Full wwPDB EM Validation Report ⓘ

Feb 27, 2024 – 03:44 PM EST

PDB ID	:	6UZ7
EMDB ID	:	EMD-20952
Title	:	K.lactis 80S ribosome with p/PE tRNA and eIF5B
Authors	:	Fernandez, I.S.; Huang, B.Y.
Deposited on	:	2019-11-14
Resolution	:	3.60 Å(reported)
Based on initial model	:	3U5B

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

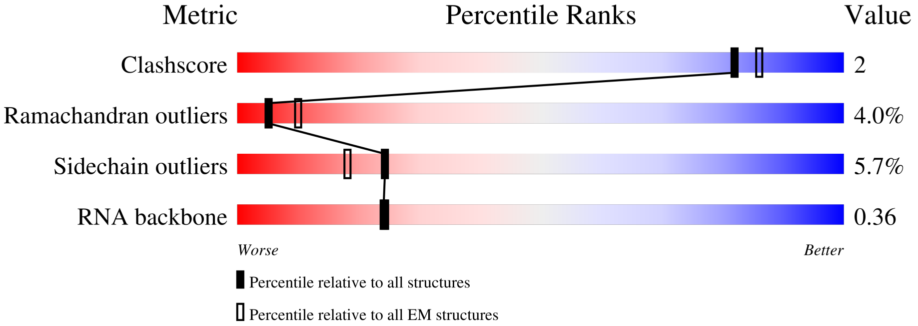
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

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

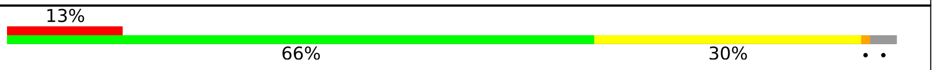
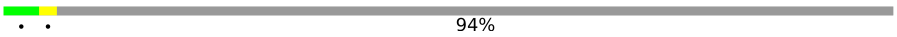
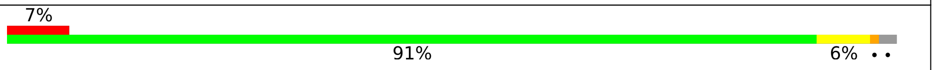
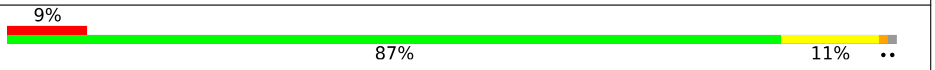
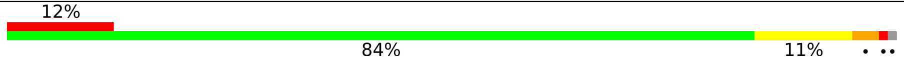
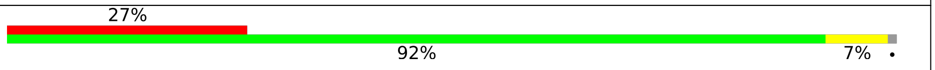
The reported resolution of this entry is 3.60 Å.

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



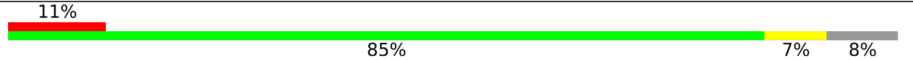
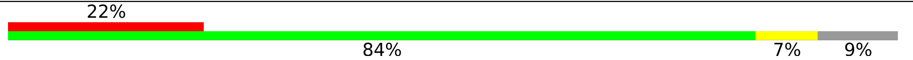
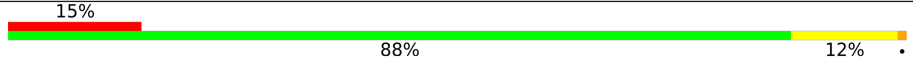
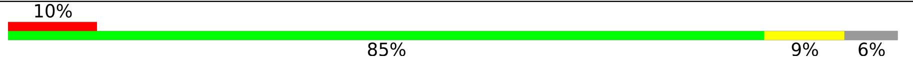
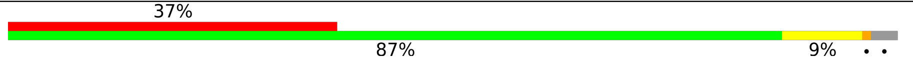
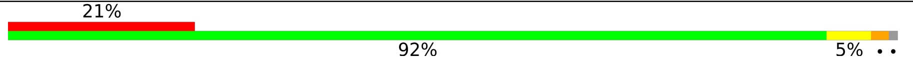
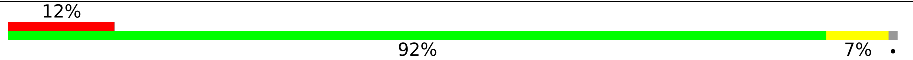
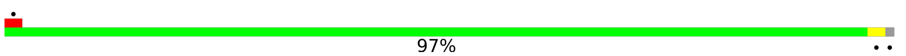
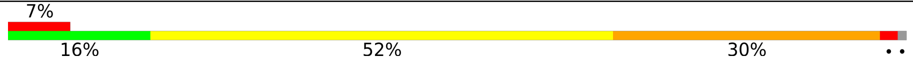
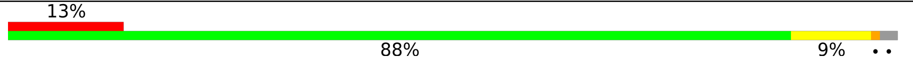
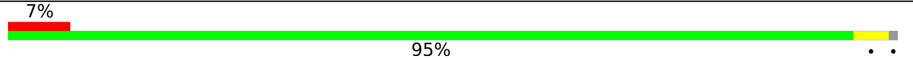
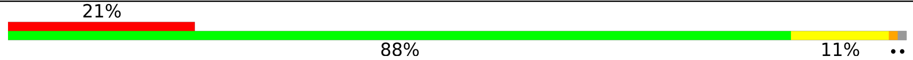
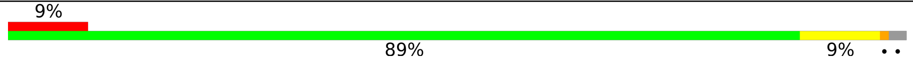
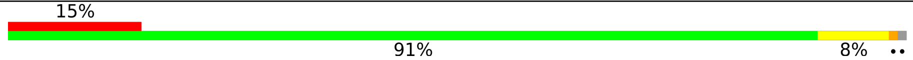
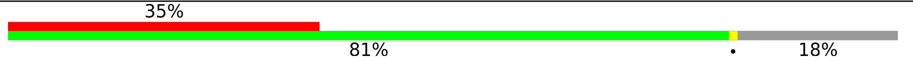
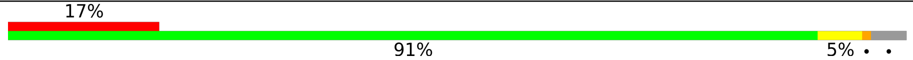
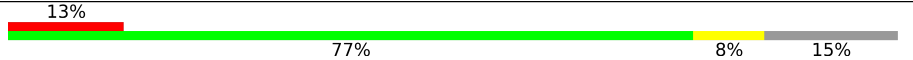
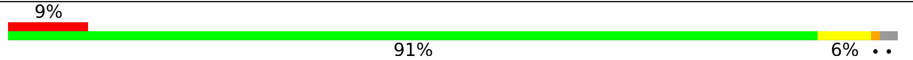
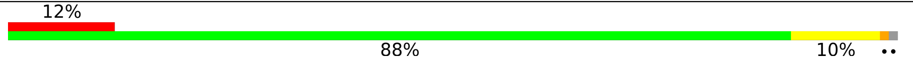
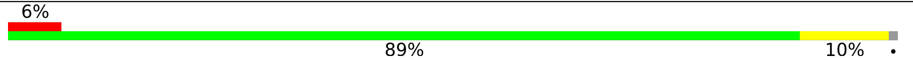
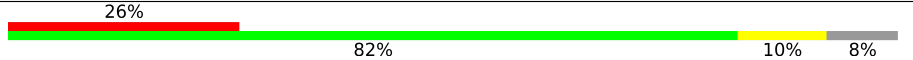
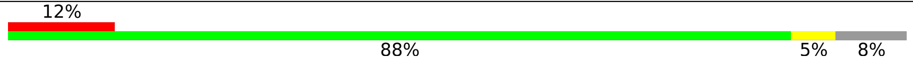
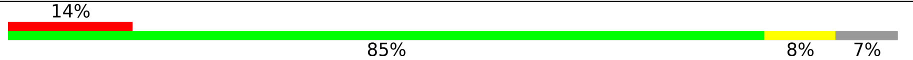
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	5	3364	
2	7	121	
3	8	2825	
4	AA	254	
5	AB	387	
6	AC	363	
7	AD	297	

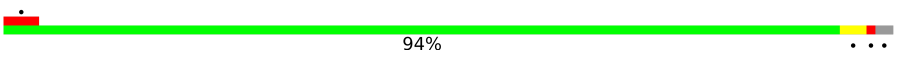
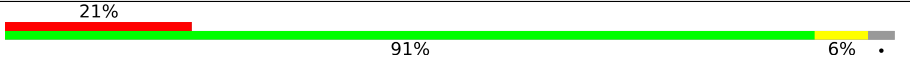
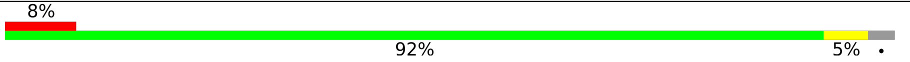
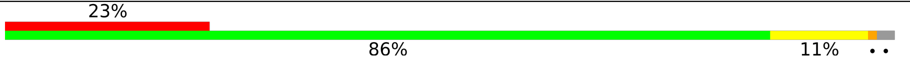
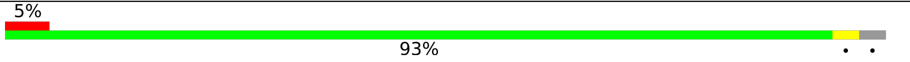
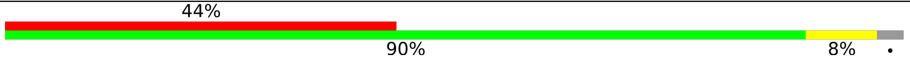
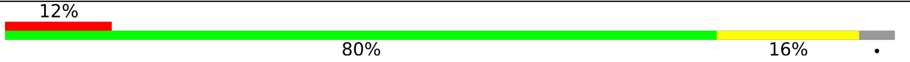
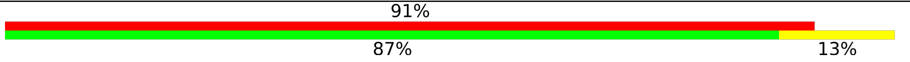
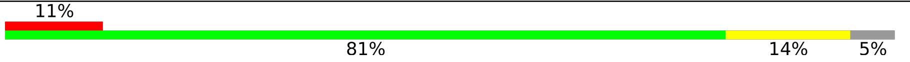
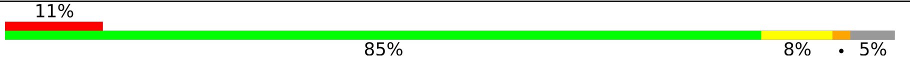
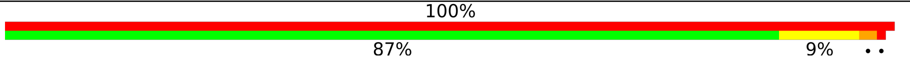
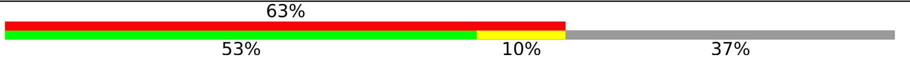
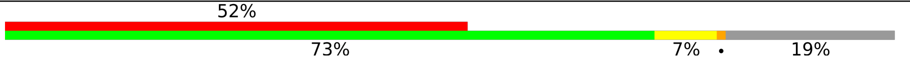
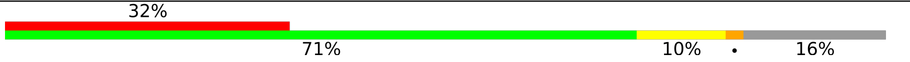
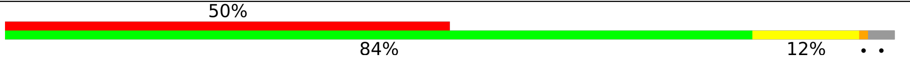
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	AE	175	
9	AF	241	
10	AG	255	
11	AH	191	
12	AI	220	
13	AJ	174	
14	AL	199	
15	AM	138	
16	AN	204	
17	AO	199	
18	AP	184	
19	AQ	186	
20	AR	189	
21	AS	172	
22	AT	160	
23	AU	122	
24	AV	137	
25	AW	155	
26	AX	142	
27	AY	127	
28	AZ	136	
29	Ba	149	
30	Bb	62	
31	Bc	105	
32	Bd	114	

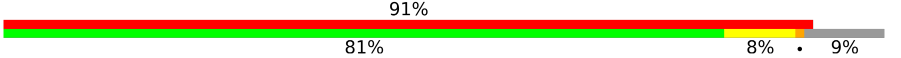
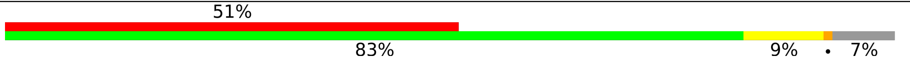
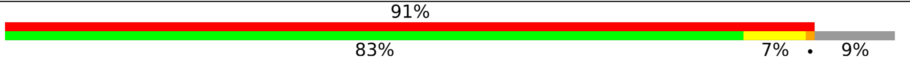
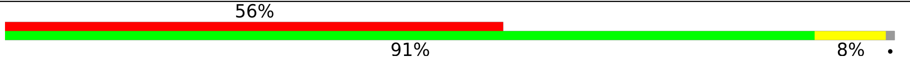
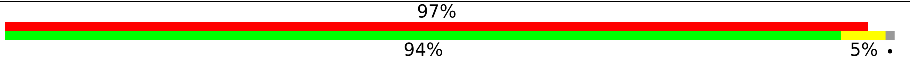
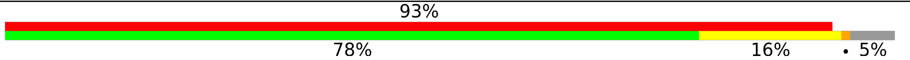
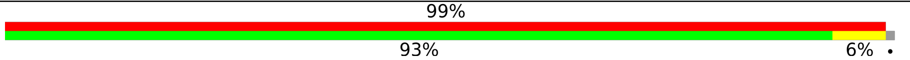
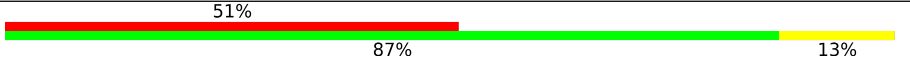
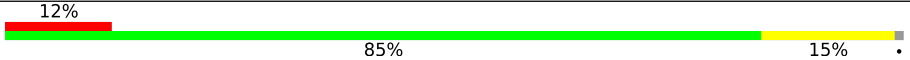
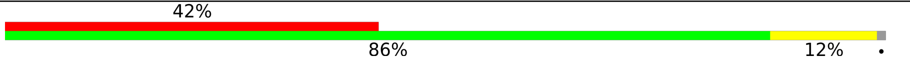
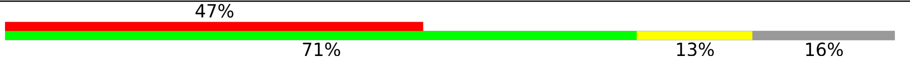
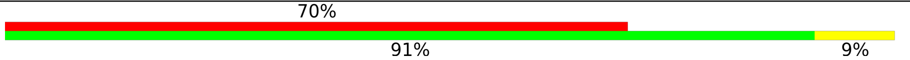
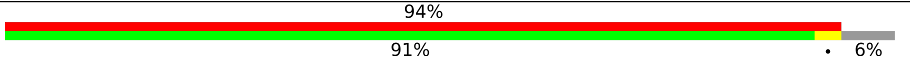
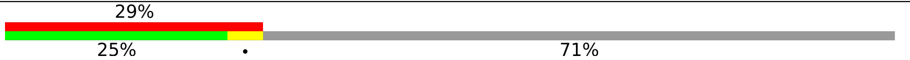
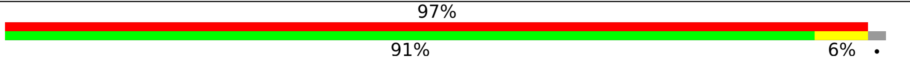
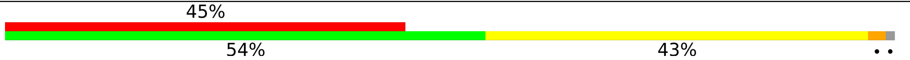
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	Be	130	
34	Bf	107	
35	Bg	125	
36	Bh	120	
37	Bi	100	
38	Bj	88	
39	Bk	78	
40	Bl	51	
41	Bm	128	
42	Bn	23	
43	Bo	106	
44	Bp	92	
45	Bq	217	
46	Br	311	
47	AK	147	
48	A	254	
49	B	255	
50	C	259	
51	D	237	
52	E	261	
53	F	227	
54	G	236	
55	H	190	
56	I	201	
57	J	188	

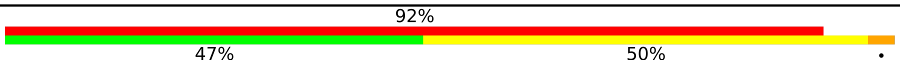
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	K	106	
59	L	156	
60	M	134	
61	N	151	
62	O	137	
63	P	142	
64	Q	143	
65	R	136	
66	S	146	
67	T	144	
68	U	117	
69	V	87	
70	W	130	
71	X	145	
72	Y	135	
73	Z	108	
74	a	119	
75	b	82	
76	c	67	
77	d	56	
78	e	63	
79	f	150	
80	g	326	
81	2	1798	
82	1	967	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
83	3	76	

2 Entry composition ⓘ

There are 85 unique types of molecules in this entry. The entry contains 211187 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3269	69874	31213	12576	22816	3269	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1923	A	C	conflict	GB 1241923359
5	2021	U	C	conflict	GB 1241923359
5	2051	U	C	conflict	GB 1241923359

- Molecule 2 is a RNA chain called RNA (121-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	7	121	2579	1152	461	845	121	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	157	3326	1488	573	1108	157	0	0

- Molecule 4 is a protein called KLLA0D16027p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AA	249	1892	1176	385	330	1	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AB	384	3064	1946	580	533	5	0	0

- Molecule 6 is a protein called KLLA0B07139p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	360	Total 2743	C 1725	N 522	O 493	S 3	0	0

- Molecule 7 is a protein called KLLA0D06941p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AD	295	Total 2384	C 1510	N 417	O 456	S 1	0	0

- Molecule 8 is a protein called KLLA0B04686p.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AE	164	Total 1321	C 847	N 247	O 227	0	0

- Molecule 9 is a protein called KLLA0D03410p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AF	222	Total 1774	C 1138	N 319	O 316	S 1	0	0

- Molecule 10 is a protein called KLLA0E00573p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AG	233	Total 1817	C 1160	N 324	O 330	S 3	0	0

- Molecule 11 is a protein called KLLA0F04499p.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AH	191	Total 1528	C 965	N 277	O 284	S 2	0	0

- Molecule 12 is a protein called KLLA0D05643p.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AI	207	Total 1690	C 1074	N 319	O 292	S 5	0	0

- Molecule 13 is a protein called KLLA0F08261p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	AJ	168	1349	845	255	245	4	0	0

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	AL	197	1581	988	317	276	0	0

- Molecule 15 is a protein called KLLA0B13409p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	AM	136	1045	666	196	183	0	0

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	AN	202	1709	1069	359	280	1	0	0

- Molecule 17 is a protein called KLLA0F04675p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AO	198	1571	1013	290	267	1	0	0

- Molecule 18 is a protein called KLLA0A06336p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	AP	180	1432	885	287	260	0	0

- Molecule 19 is a protein called KLLA0A07227p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	AQ	184	1444	911	290	243	0	0

- Molecule 20 is a protein called KLLA0E12453p.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AR	188	Total 1522	C 933	N 328	O 259	S 2	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AS	169	Total 1422	C 916	N 265	O 238	S 3	0	0

- Molecule 22 is a protein called KLLA0E23651p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AT	158	Total 1262	C 797	N 240	O 220	S 5	0	0

- Molecule 23 is a protein called KLLA0D05181p.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	AU	100	Total 807	C 524	N 131	O 152	0	0

- Molecule 24 is a protein called KLLA0E06997p.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AV	132	Total 976	C 612	N 182	O 174	S 8	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	AW	62	Total 515	C 330	N 103	O 82	0	0

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AX	121	Total 964	C 620	N 169	O 174	S 1	0	0

- Molecule 27 is a protein called KLLA0B05742p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	AY	125	992	622	189	181	0	0

- Molecule 28 is a protein called KLLA0E03455p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	AZ	134	1089	708	199	182	0	0

- Molecule 29 is a protein called RPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Ba	147	1156	740	225	189	2	0	0

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	Bb	57	458	287	99	72	0	0

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Bc	97	740	477	125	137	1	0	0

- Molecule 32 is a protein called KLLA0B02937p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Bd	106	869	553	167	147	2	0	0

- Molecule 33 is a protein called KLLA0E06843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Be	122	980	618	198	162	2	0	0

- Molecule 34 is a protein called KLLA0D07405p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Bf	105	837	531	161	144	1	0	0

- Molecule 35 is a protein called KLLA0C08371p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Bg	121	951	591	192	167	1	0	0

- Molecule 36 is a protein called KLLA0F05247p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	Bh	116	961	608	187	166	0	0

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	Bi	98	766	479	155	131	1	0	0

- Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Bj	85	675	410	148	111	6	0	0

- Molecule 39 is a protein called KLLA0C18216p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
39	Bk	76	619	398	114	107	0	0

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Bl	49	428	266	96	64	2	0	0

- Molecule 41 is a protein called Ubiquitin fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Bm	51	410	254	85	66	5	0	0

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Bn	23	218	133	60	24	1	0	0

- Molecule 43 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Bo	101	814	509	163	136	6	0	0

- Molecule 44 is a protein called KLLA0E05941p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Bp	87	660	404	133	117	6	0	0

- Molecule 45 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Bq	217	1716	1097	297	313	9	0	0

- Molecule 46 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Br	195	1508	968	258	278	4	0	0

- Molecule 47 is a protein called GDPCP.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	AK	147	735	441	147	147	0	0

- Molecule 48 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	A	206	1616	1035	285	294	2	0	0

- Molecule 49 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	B	214	1722	1089	313	317	3	0	0

- Molecule 50 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	C	217	1629	1041	287	297	4	0	0

- Molecule 51 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	D	223	1744	1108	313	318	5	0	0

- Molecule 52 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	E	260	2078	1322	393	359	4	0	0

- Molecule 53 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	F	206	1609	1008	298	300	3	0	0

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	G	226	1812	1134	348	326	4	0	0

- Molecule 55 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	H	184	1483	950	270	263	0	0

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	I	188	1493	926	301	265	1	0	0

- Molecule 57 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	J	182	1471	929	287	254	1	0	0

- Molecule 58 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	K	96	809	533	129	146	1	0	0

- Molecule 59 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	L	145	1168	745	222	198	3	0	0

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
60	M	122	922	575	167	180	0	0

- Molecule 61 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	N	150	1187	756	223	206	2	0	0

- Molecule 62 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	O	127	Total 942	C 578	N 188	O 173	S 3	0	0

- Molecule 63 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	P	119	Total 950	C 611	N 170	O 164	S 5	0	0

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	Q	141	Total 1105	C 709	N 204	O 192	0	0

- Molecule 65 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	R	123	Total 983	C 614	N 181	O 185	S 3	0	0

- Molecule 66 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	S	138	Total 1138	C 707	N 231	O 198	S 2	0	0

- Molecule 67 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	T	143	Total 1110	C 693	N 210	O 207	0	0

- Molecule 68 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	U	106	Total 845	C 540	N 152	O 152	S 1	0	0

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	V	87	687	424	126	135	2	0	0

- Molecule 70 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	W	129	1021	651	187	180	3	0	0

- Molecule 71 is a protein called RPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	X	143	1110	704	214	189	3	0	0

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
72	Y	134	1061	665	207	189	0	0

- Molecule 73 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	Z	70	558	355	104	98	1	0	0

- Molecule 74 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	a	100	798	491	170	131	6	0	0

- Molecule 75 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	b	82	617	384	113	114	6	0	0

- Molecule 76 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	c	63	494	305	98	90	1	0	0

- Molecule 77 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	d	53	446	280	89	76	1	0	0

- Molecule 78 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	e	55	443	276	90	76	1	0	0

- Molecule 79 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	f	44	337	213	65	55	4	0	0

- Molecule 80 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	g	318	2466	1561	430	470	5	0	0

- Molecule 81 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
81	2	1780	37797	16892	6658	12467	1780	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	676	G	U	conflict	GB 49642208
2	678	U	G	conflict	GB 49642208

- Molecule 82 is a protein called KLLA0F23265p.

Mol	Chain	Residues	Atoms	AltConf	Trace
82	1	600	Total C N O S 4702 2981 808 890 23	0	0

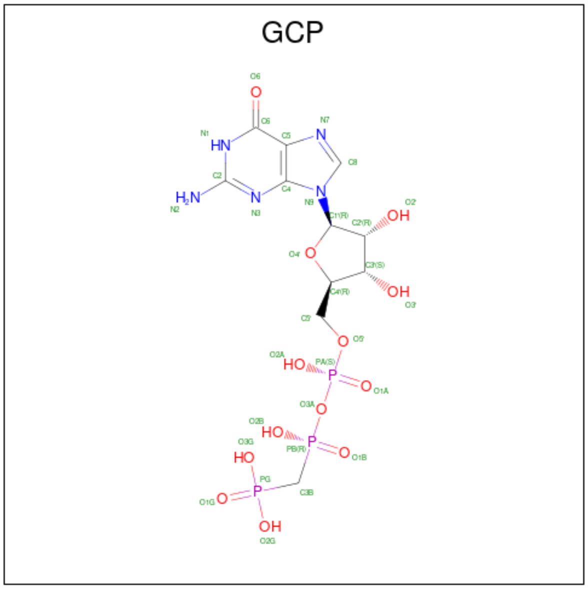
- Molecule 83 is a RNA chain called RNA (76-MER).

Mol	Chain	Residues	Atoms	AltConf	Trace
83	3	76	Total C N O P 1623 725 295 528 75	0	0

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
84	Bj	1	Total Zn 1 1	0
84	Bm	1	Total Zn 1 1	0
84	Bo	1	Total Zn 1 1	0
84	a	1	Total Zn 1 1	0
84	b	1	Total Zn 1 1	0
84	f	1	Total Zn 1 1	0

- Molecule 85 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



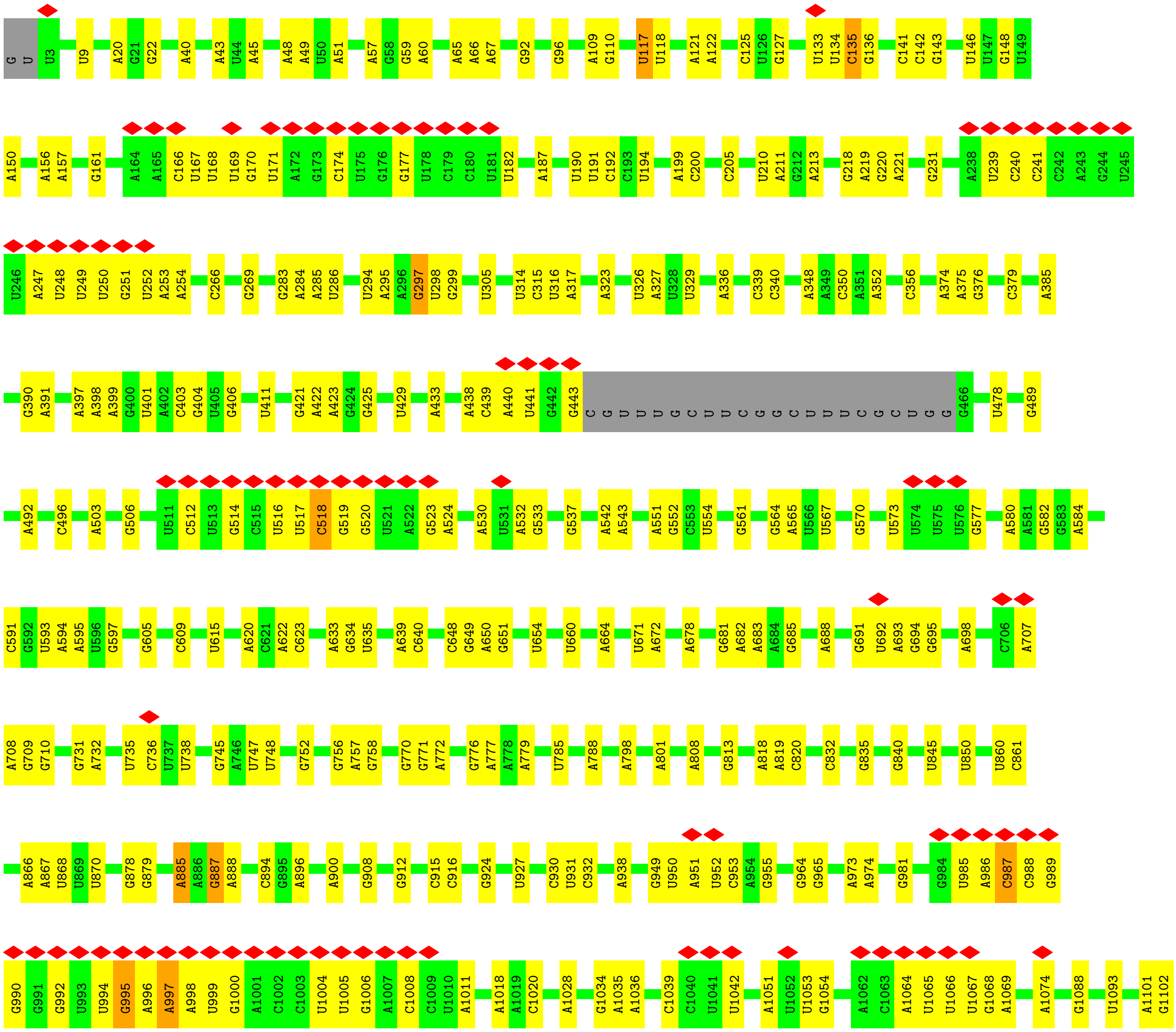
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
85	1	1	32	11	5	13	3	0

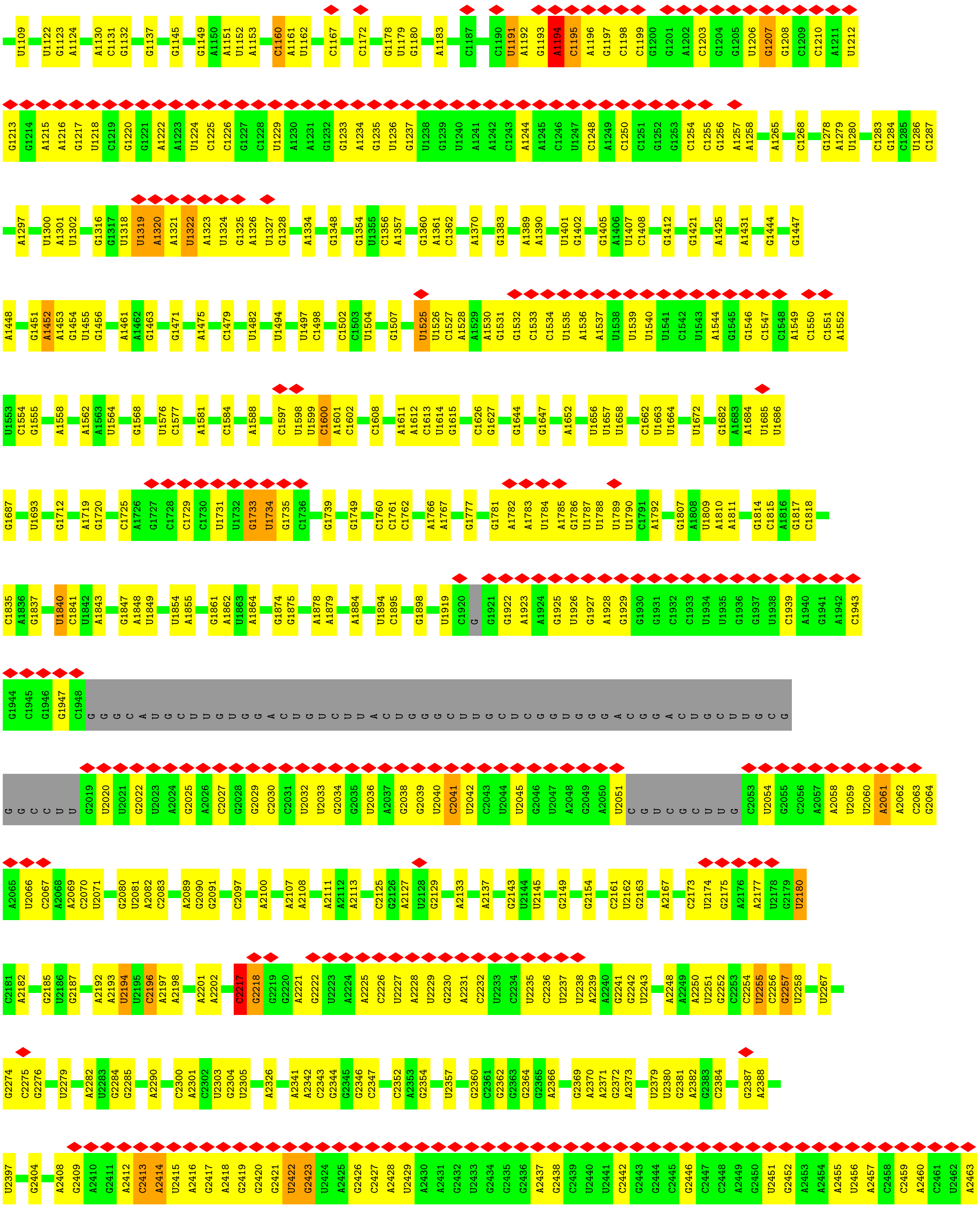
3 Residue-property plots ⓘ

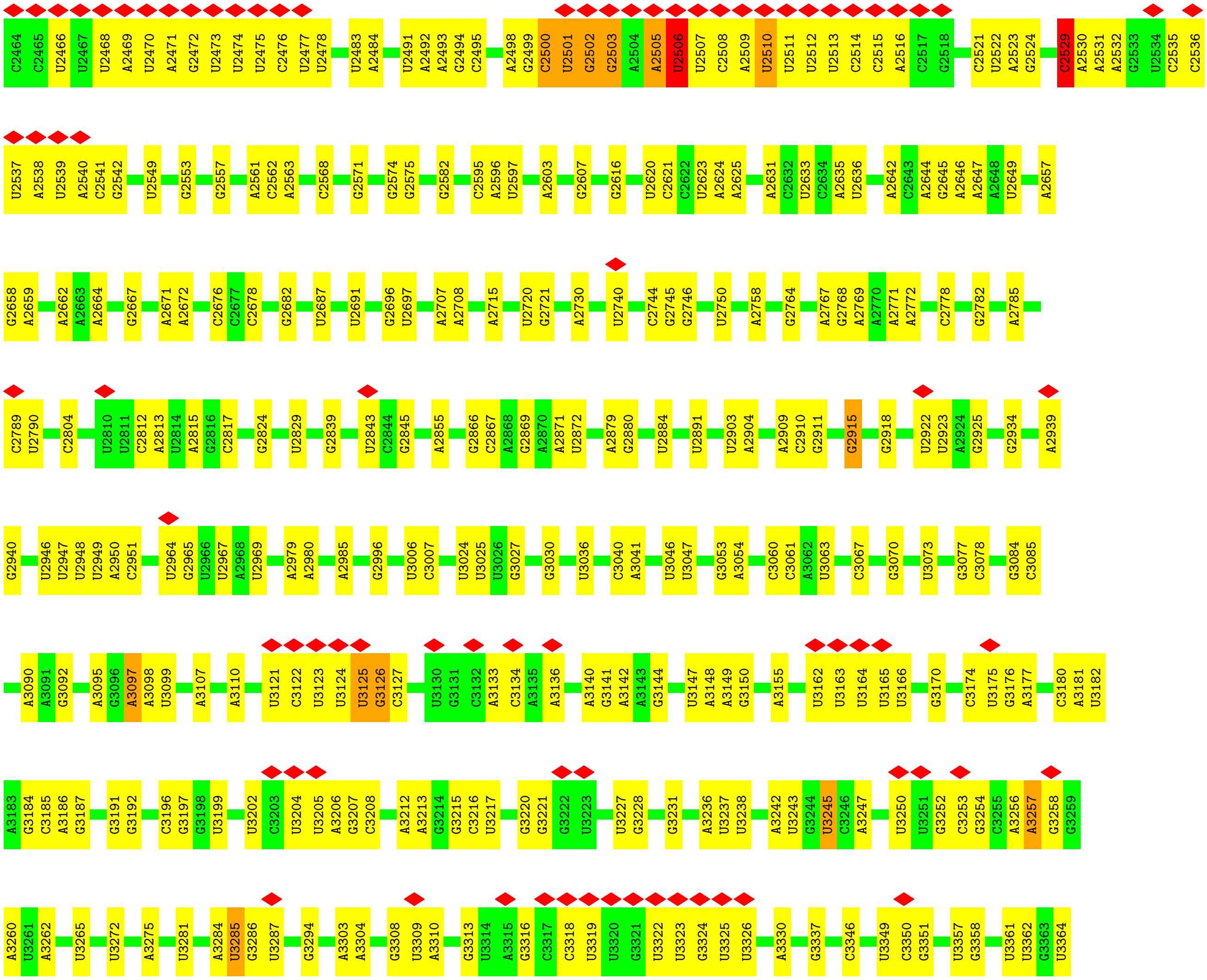
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 25S ribosomal RNA

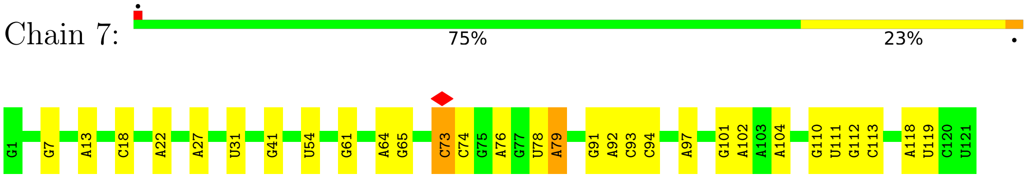
Chain 5:



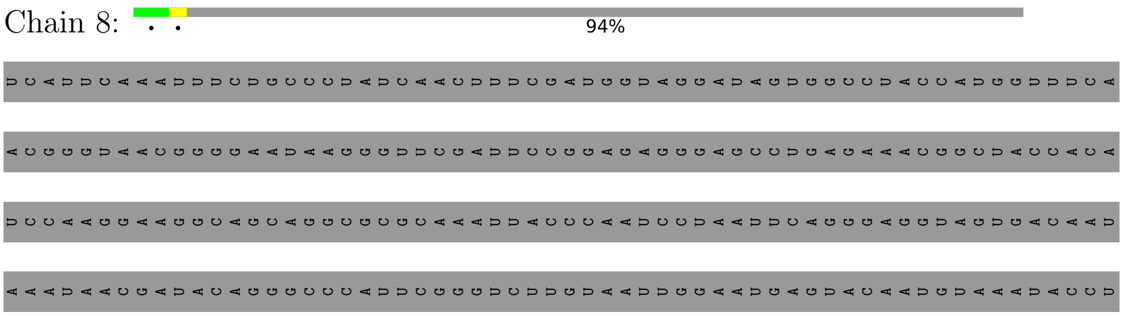

U1109 U1122 G1123 A1124 A1130 C1131 G1132 G1137 G1145 G1149 A1150 A1151 U1152 A1153 C1160 A1161 U1162 C1167 C1172 G1178 U1179 G1180 A1183 C1187 C1190 U1191 A1192 G1193 A1194 C1195 A1196 G1197 C1198 C1199 G1200 G1201 A1202 C1203 G1204 G1205 U1206 G1207 G1208 C1209 C1210 A1211 U1212
G1213 G1214 A1215 A1216 G1217 U1218 C1219 G1220 G1221 A1222 A1223 U1224 C1225 C1226 G1227 C1228 U1229 A1230 A1231 G1232 G1233 A1234 G1235 U1236 G1237 U1238 G1239 U1240 A1241 A1242 C1243 A1244 A1245 C1246 U1247 C1248 A1249 C1250 C1251 G1252 G1253 C1254 C1255 G1256 A1257 A1258 A1265 C1268 G1278 A1279 U1280 C1283 G1284 C1285 U1286 C1287
A1297 U1300 A1301 U1302 G1316 G1317 U1318 U1319 A1320 A1321 U1322 A1323 U1324 G1325 A1326 U1327 G1328 A1334 G1348 G1354 U1355 C1356 A1357 G1360 A1361 C1362 A1370 G1383 A1389 A1390 U1401 G1402 G1405 A1406 U1407 C1408 G1412 G1421 A1425 A1431 G1444 G1447
A1448 G1451 A1452 A1453 G1454 U1455 G1456 A1461 A1462 G1463 G1471 A1475 C1479 U1482 U1494 U1497 C1498 C1502 C1503 U1504 G1507 U1525 U1526 C1527 A1528 A1529 A1530 G1531 G1532 C1533 C1534 U1535 A1536 A1537 U1538 U1539 U1540 U1541 C1542 U1543 A1544 G1545 G1546 C1547 C1548 A1549 C1550 C1551 A1552
U1553 C1554 G1555 A1558 A1562 A1563 U1564 G1568 U1576 C1577 A1581 C1584 A1588 C1597 U1598 U1599 C1600 A1601 C1602 C1608 A1611 A1612 C1613 U1614 G1615 C1626 G1627 G1644 G1647 A1652 U1656 U1657 U1658 C1662 U1663 U1664 U1672 G1682 A1683 A1684 U1685 U1686
G1687 U1693 G1712 A1719 G1720 C1725 A1726 G1727 C1728 C1729 C1730 U1731 U1732 G1733 U1734 G1735 C1736 G1739 G1749 C1760 C1761 C1762 A1766 A1767 G1777 G1781 A1782 A1783 U1784 A1785 G1786 U1787 U1788 U1789 U1790 C1791 A1792 G1807 A1808 U1809 A1810 A1811 G1814 C1815 A1816 G1817 C1818
C1835 A1836 G1837 U1840 C1841 U1842 A1843 G1847 A1848 U1849 U1854 A1855 G1861 A1862 U1863 A1864 G1874 G1875 A1878 A1879 A1884 U1894 C1895 G1898 U1919 C1920 G G1921 G1922 A1923 A1924 G1925 U1926 G1927 A1928 G1929 G1930 G1931 C1932 C1933 U1934 U1935 G1936 G1937 U1938 C1939 A1940 G1941 A1942 C1943
G1944 C1945 G1946 G1947 C1948 G G G C A U G C U U G U G G A C U G U C U U A C U G G G C U U G C U C G G U G G G A C G G A C U G C U U G C G
G G C C U U G2019 U2020 G2021 G2022 U2023 A2024 G2025 A2026 C2027 G2028 G2029 C2030 C2031 U2032 U2033 G2034 G2035 U2036 A2037 G2038 G2039 U2040 C2041 U2042 C2043 U2044 U2045 G2046 U2047 A2048 G2049 A2050 U2051 C G U C G C U U G C2053 U2054 G2055 C2056 A2057 A2058 U2059 U2060 A2061 A2062 C2063 G2064
A2065 U2066 C2067 A2068 A2069 C2070 U2071 G2080 U2081 A2082 C2083 A2089 G2090 G2091 C2097 A2100 A2107 A2108 A2111 A2112 A2113 C2125 G2126 A2127 U2128 G2129 A2133 A2137 G2143 U2144 U2145 G2149 G2154 C2161 U2162 G2163 A2167 C2173 U2174 G2175 A2176 A2177 U2178 G2179 U2180
C2181 A2182 G2185 U2186 G2187 A2192 A2193 U2194 U2195 C2196 A2197 A2198 A2201 A2202 C2217 G2218 G2219 G2220 A2221 G2222 U2223 A2224 A2225 C2226 U2227 A2228 U2229 G2230 A2231 C2232 U2233 C2234 U2235 C2236 U2237 U2238 A2239 A2240 G2241 G2242 U2243 A2248 A2249 A2250 U2251 G2252 C2253 C2254 U2255 C2256 G2257 U2258 U2267
G2274 C2275 G2276 U2279 A2282 U2283 G2284 G2285 A2290 C2300 A2301 C2302 U2303 G2304 U2305 A2326 A2341 A2342 C2343 G2344 G2345 G2346 C2347 C2352 A2353 G2354 U2357 G2360 C2361 G2362 G2363 G2364 G2365 A2366 G2369 A2370 A2371 G2372 A2373 U2379 U2380 G2381 A2382 G2383 C2384 G2387 A2388
U2397 G2404 A2408 G2409 A2410 G2411 A2412 C2413 A2414 U2415 A2416 G2417 A2418 G2419 G2420 G2421 U2422 G2423 U2424 A2425 G2426 C2427 A2428 U2429 A2430 A2431 G2432 U2433 G2434 G2435 G2436 A2437 G2438 C2439 U2440 U2441 C2442 G2443 G2444 C2445 G2446 C2447 C2448 A2449 G2450 U2451 G2452 A2453 A2454 A2455 U2456 A2457 C2458 C2459 A2460 C2461 U2462 A2463

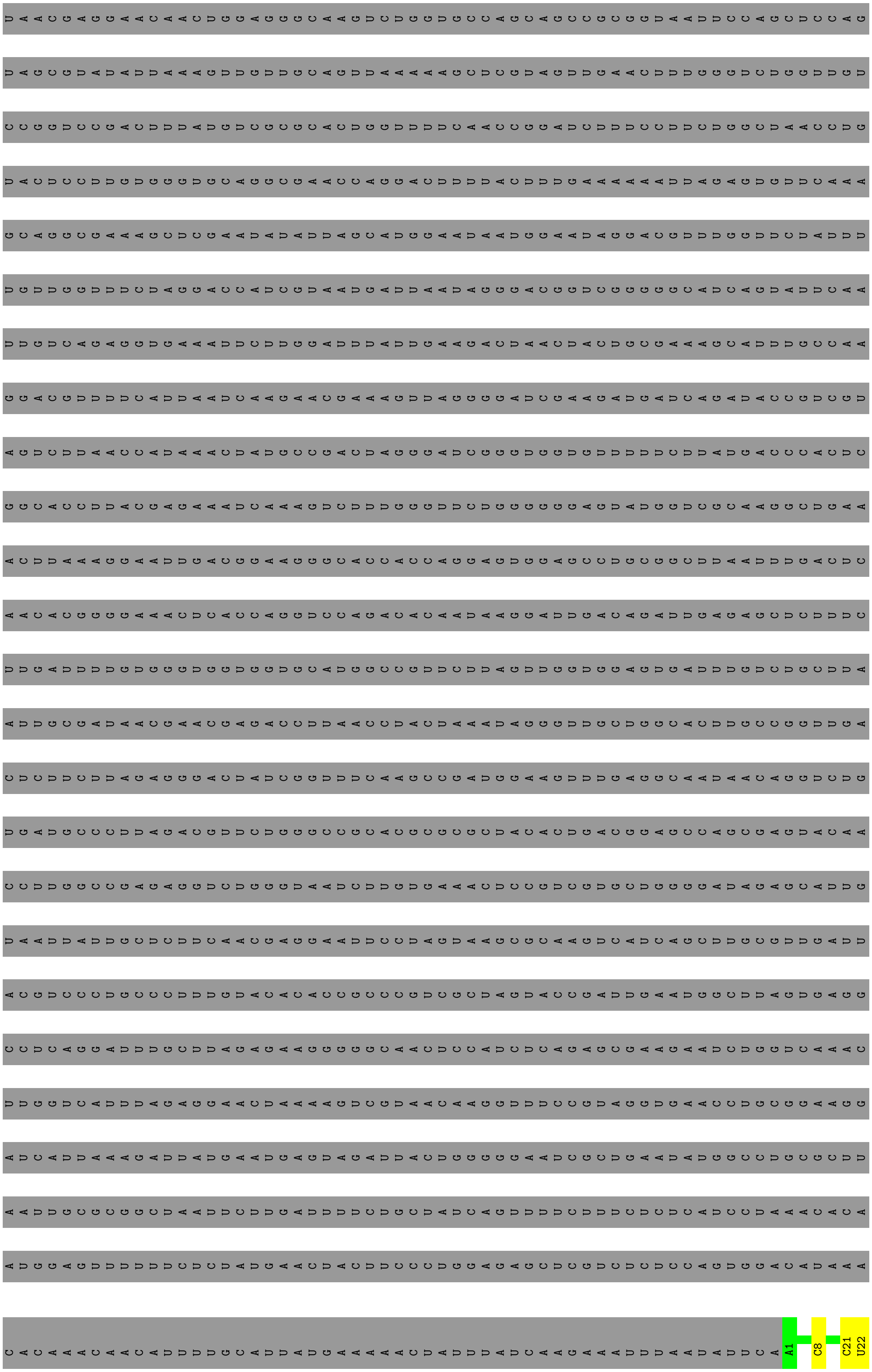


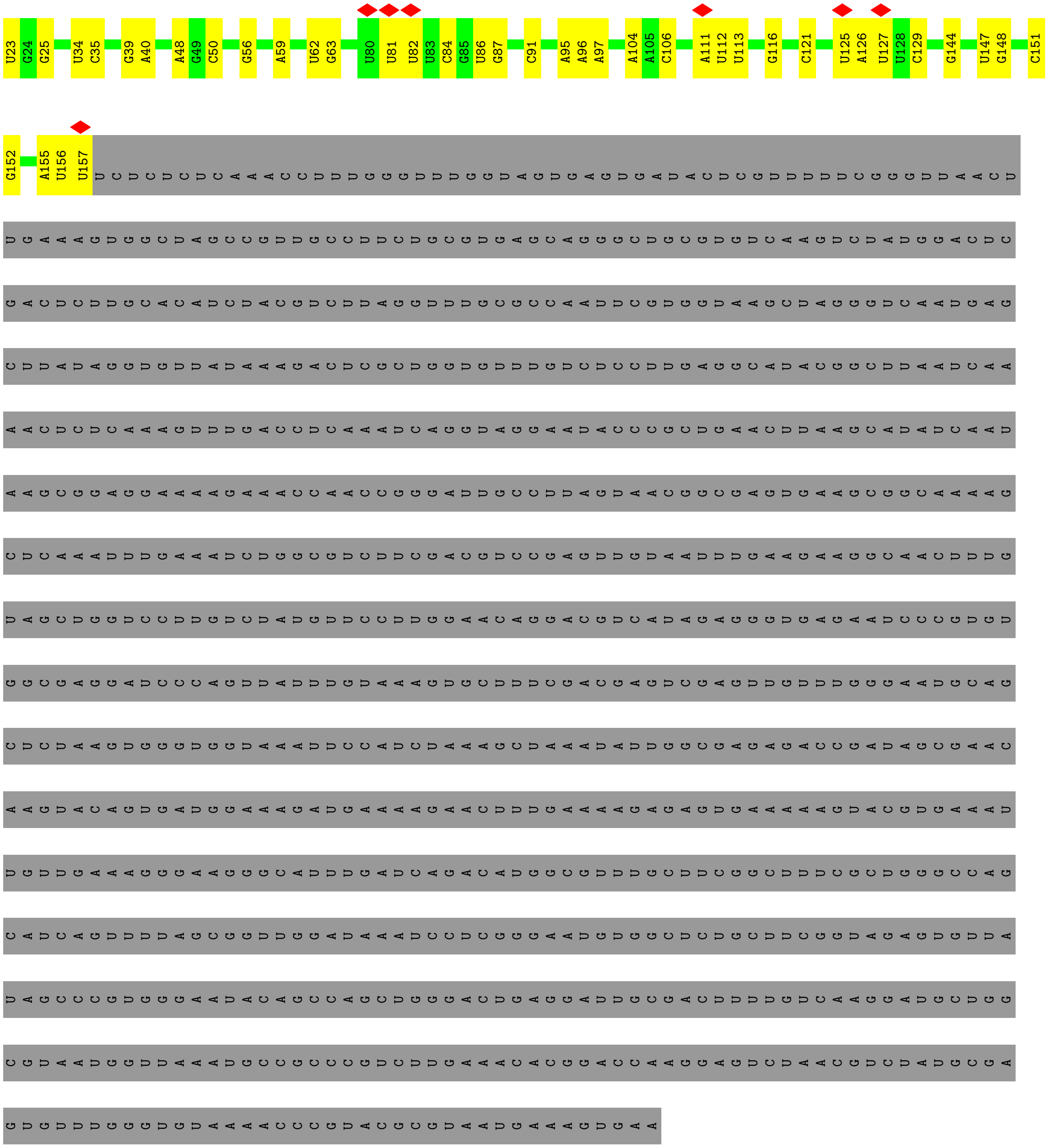
- Molecule 2: RNA (121-MER)



- Molecule 3: 5.8S ribosomal RNA

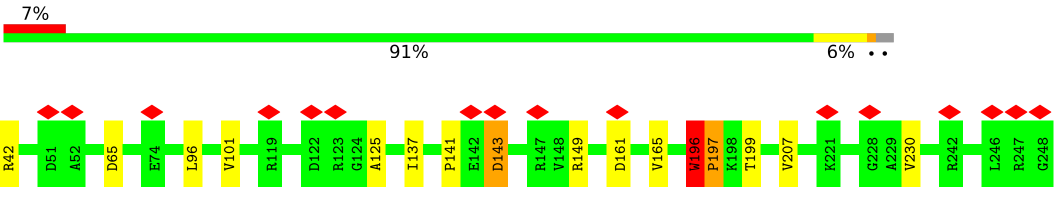



U A A C G A G G A A C A A C U G G A G G G C A A G U C U G G U G C C A G C A G C C G C G G U A A U U C C A G C U C C A G
U A G C G U A U A U U A A A G U U G U U G C A G U U A A A A A G C U C G U A G U U G A A C U U U G G G U C U G G U U G U
C C G G U C C G A C U U U A U G U C G C G C A C U G G U U U U C A A C C G G A U C U U U C C U U C U G G C U A A C C U G
U A C U C C U U G U G G G U G C A G G C G A A C C A G G A C U U U A C U U U G A A A A A A U U A G A G U G U U C A A A
G C A G G C G A A A G C U C G A A U A U A U U A G C A U G G A A U A A U G G A A U A G G A C G U U 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 A U C G U A A U G A U U A A U A G G G A C G G U C G G G G G C A U C A G U A U U C A A
U U G U C A G A G G U G A A A U U C U U G G A U U U A U U G A A G A C U A A C U A C U G C G A A A G C A U U U G C C A A
G G A C G U U U U C A U U A A U C A A G A A C G A A A G U U A G G G G A U C G A A G A U G A U C A G A U A C C G U C G U
A G U C U U A A C C A U A A A C U A U G C C G A C U A G G G A U C G G G U G G U G U U U U U C U U A U G A C C C A C U C
G G C A C C U U A C G A G A A A U C A A A G U C U U U G G G U U C U G G G G G G A G U A U G G U C G C A A G G C U G A A
A C U U A A A G G A A U U G A C G G A A G G G C A C C A C C A G G A G U G G A G C C U G C G G C U U A A U U U G A C U C
A A C A C G G G G A A A C U C A C C A G G U C C A G A C A C A A U A A G G A U U G A C A G A U U G A G A G C U C U U U C
U U G A U U U U G U G G G U G G U G G U G C A U G G C C G U U C U U A G U U G G U G G A G U G A U U U G U C U G C U U A
A U U G C G A U A A C G A A C G A G A C C U U A A C C U A C U A A A U A G G G U U G C U G G C A C U U G C C G G U U G A
C U C U U C U U A G A G G G A C U A U C G G U U U C A A G C C G A U G G A A G U U U G A G G C A A U A A C A G G U C U G
U G A U G C C C U U A G A C G U U C U G G G C C G C A C G C G C G C U A C A C U G A C G G A G C C A G C G A G U A C A A
C C U U G G C C G A G A G G U C U G G G U A A U C U U G U G A A A C U C C G U C G U G C U G G G G A U A G A G C A U U G
U A A U U A U U G C U C U U C A A C G A G G A A U U C C U A G U A A G C G C A A G U C A U C A G C U U G C G U U G A U U
A C G U C C C U G C C C U U U G U A C A C A C C G C C C G U C G C U A G U A C C G A U U G A A U G G C U U A G U G A G G
C C U C A G G A U U U G C U U A G A G A A G G G G G C A A C U C C A U C U C A G A G C G A A G A A U C U G G U C A A A C
U U G G U C A U U U A G A G G A A C U A A A A G U C G U A A C A A G G U U U C C G U A G G U G A A C C U G C G G A A G G
A U C A U U A A A G A U U A U G A A U G A G U A G A U U A C U G G G G G A A U C G C U G A A U A U G G C C U G C G C U U
A A U U G C C G G C U A A U U C U U G A U U U U C U G C U A U C A G U U U U C U U U C U C U C A U C C U A A A C A C A
A U G G A G U U U U U U C U C U A U G A A C U A C U U C C C U G G A G A G C U C G U C U C U C C A G U G G A C A U A A A
C A C A A A C A A C A U U U U G C A U U A U G A A A A A C U A U U U A U C A A G A A A U U U A A U A U U C A
A1
C8
C21
U22



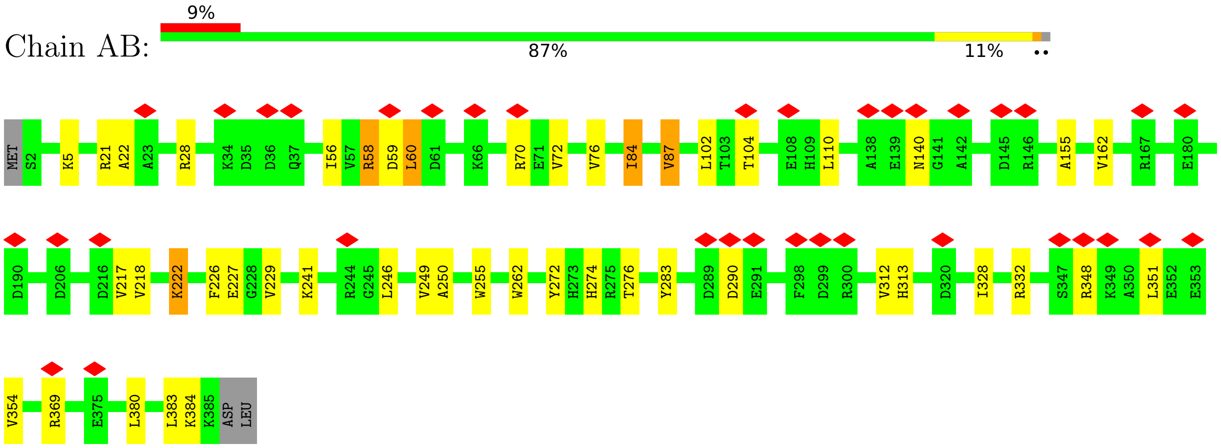
- Molecule 4: KLLA0D16027p

Chain AA:



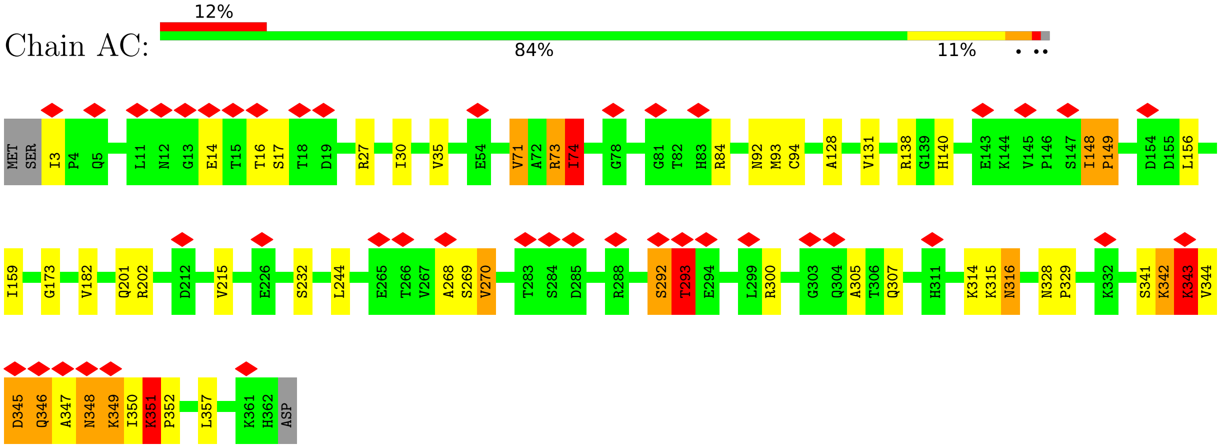
- Molecule 5: 60S ribosomal protein L3

Chain AB:



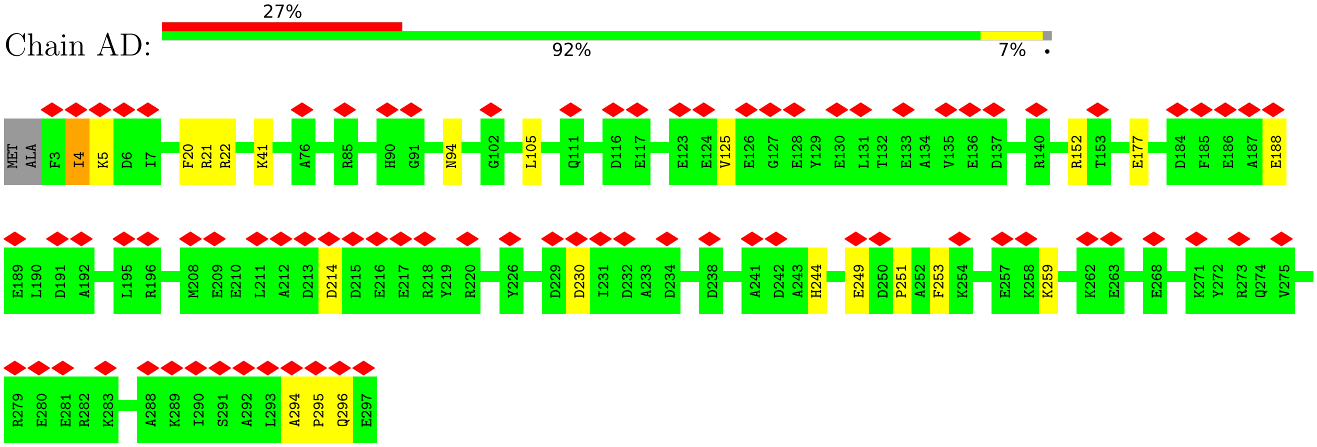
- Molecule 6: KLLA0B07139p

Chain AC:



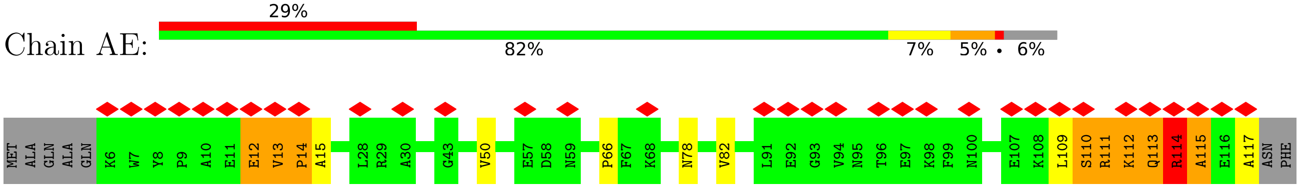
- Molecule 7: KLLA0D06941p

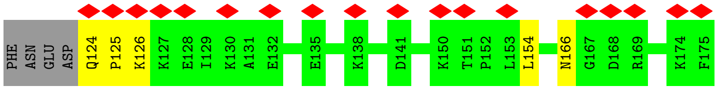
Chain AD:



- Molecule 8: KLLA0B04686p

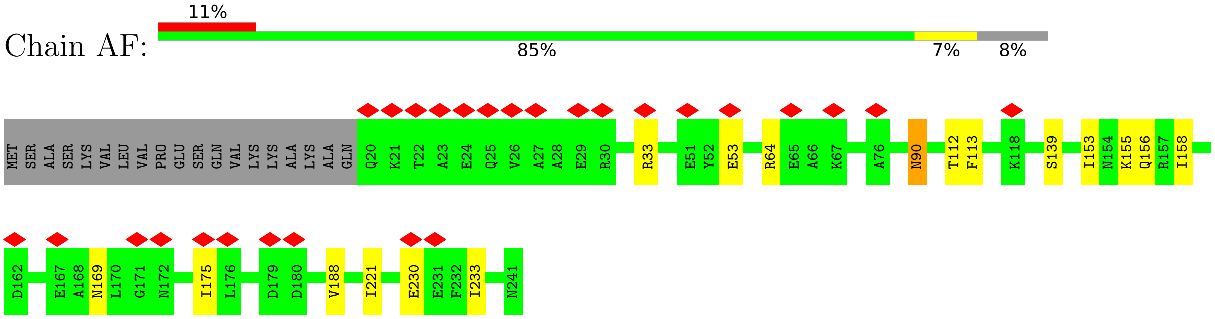
Chain AE:





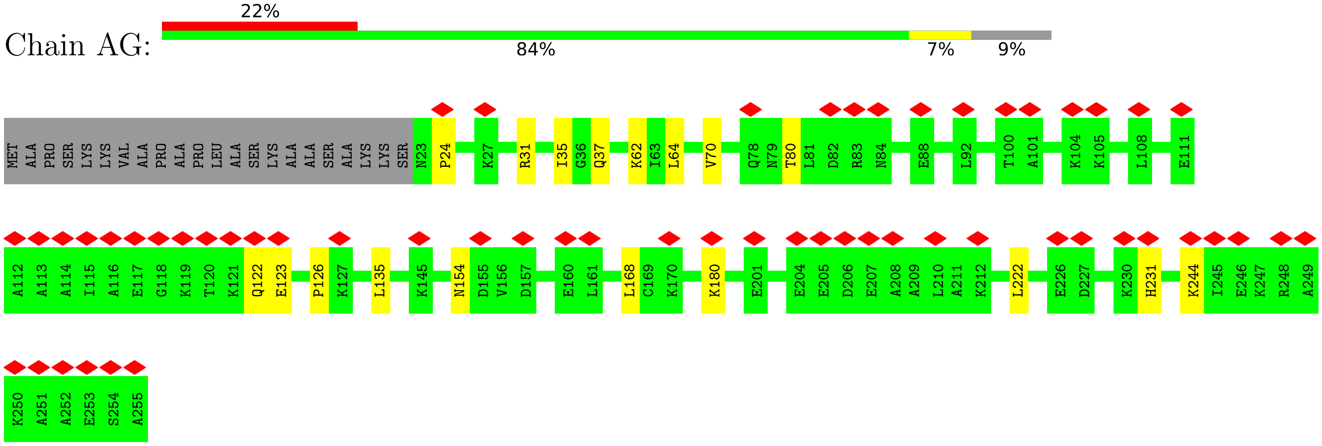
- Molecule 9: KLLA0D03410p

Chain AF:



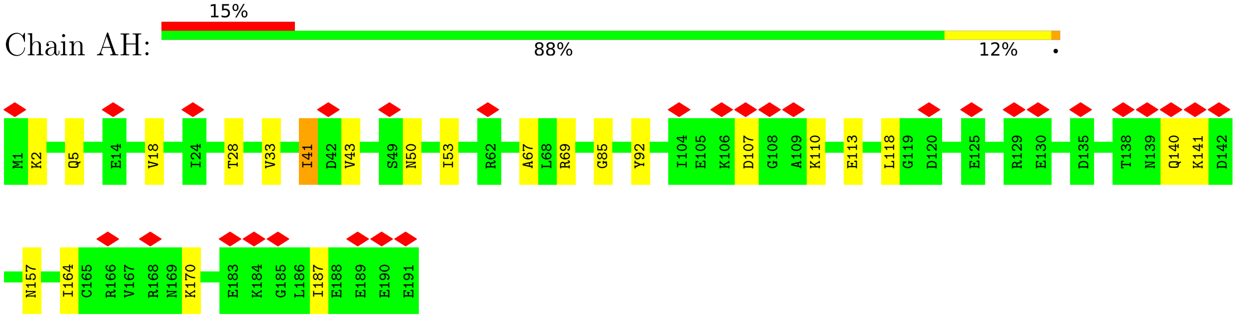
- Molecule 10: KLLA0E00573p

Chain AG:



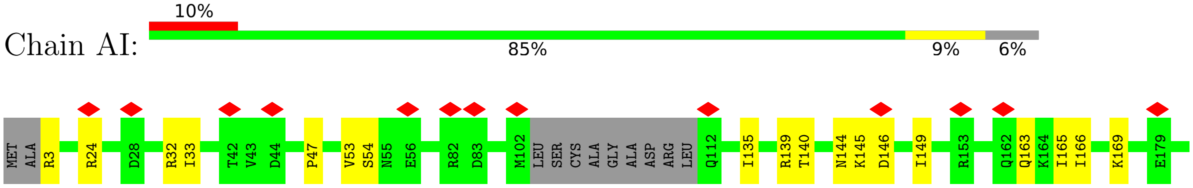
- Molecule 11: KLLA0F04499p

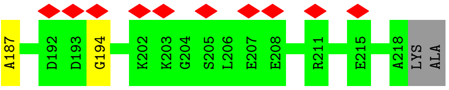
Chain AH:



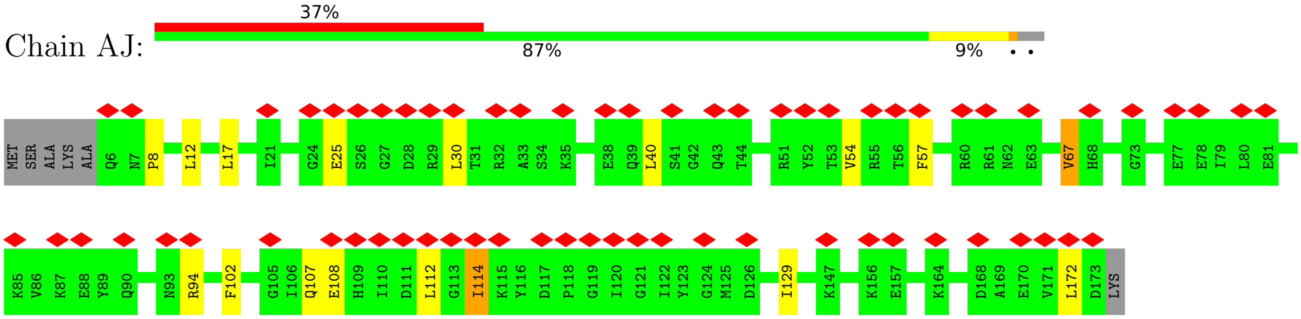
- Molecule 12: KLLA0D05643p

Chain AI:

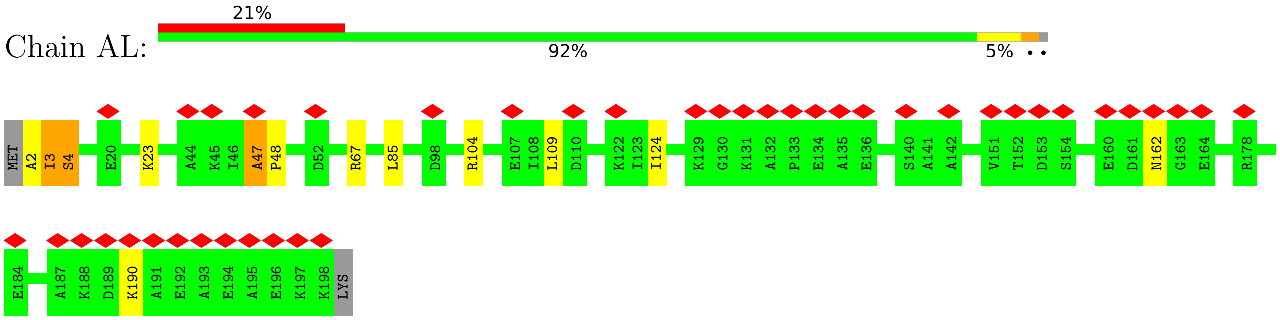




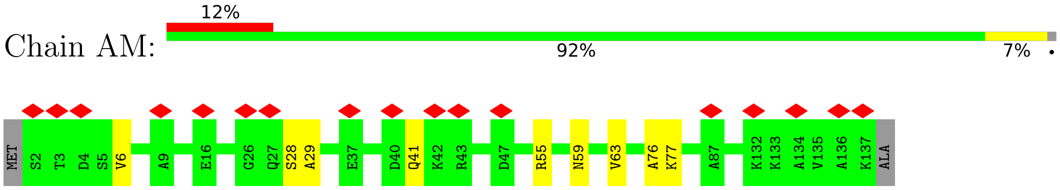
- Molecule 13: KLLA0F08261p



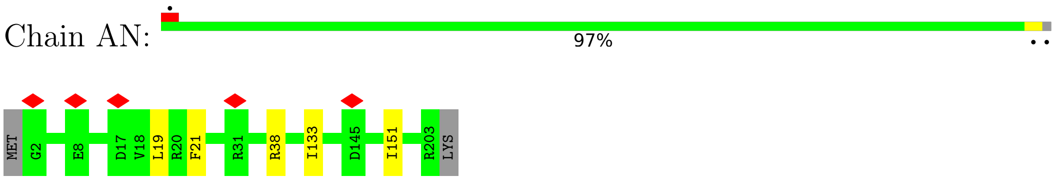
- Molecule 14: 60S ribosomal protein L13



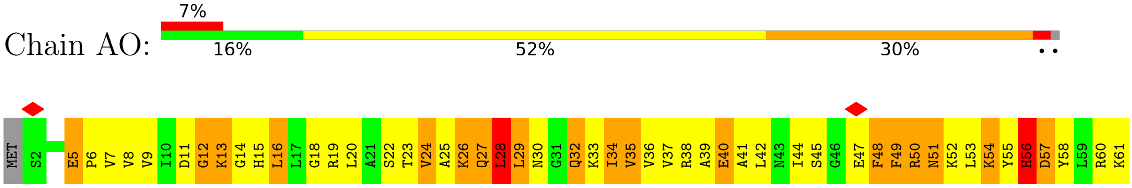
- Molecule 15: KLLA0B13409p

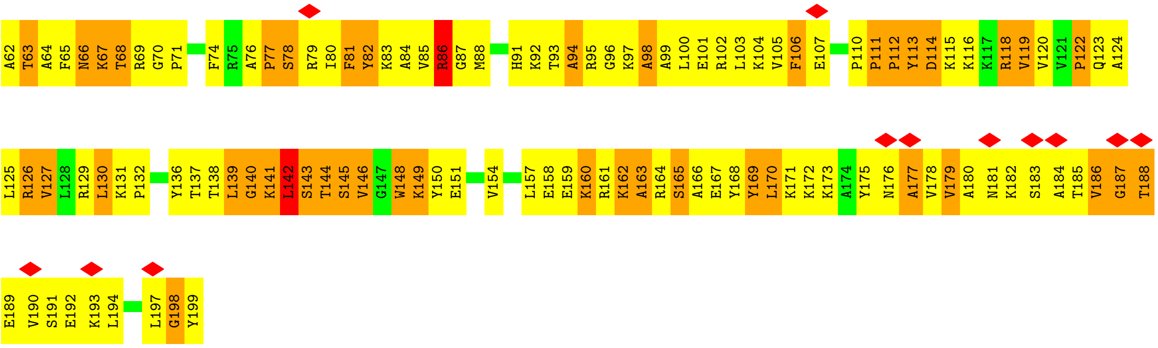


- Molecule 16: Ribosomal protein L15



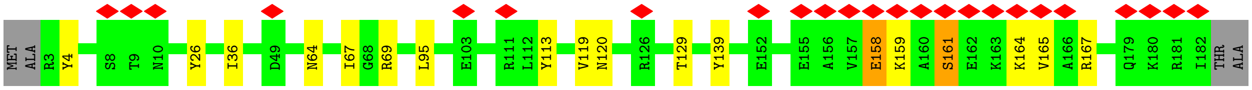
- Molecule 17: KLLA0F04675p





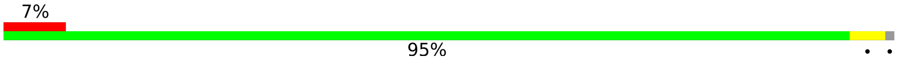
- Molecule 18: KLLA0A06336p

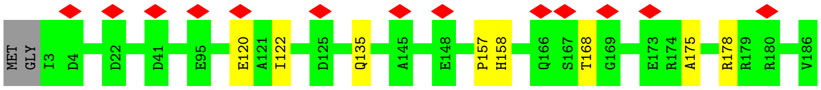
Chain AP:



- Molecule 19: KLLA0A07227p

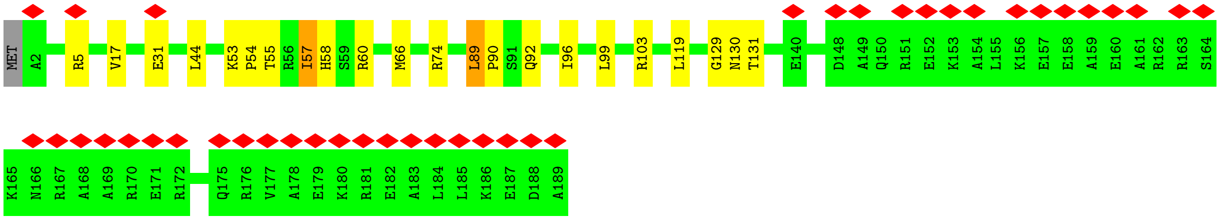
Chain AQ:





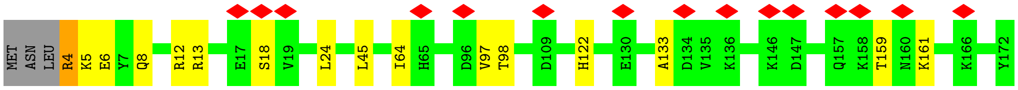
- Molecule 20: KLLA0E12453p

Chain AR:



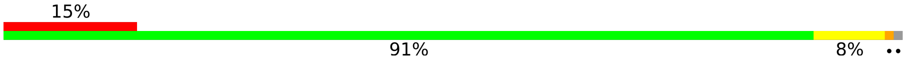
- Molecule 21: 60S ribosomal protein L20

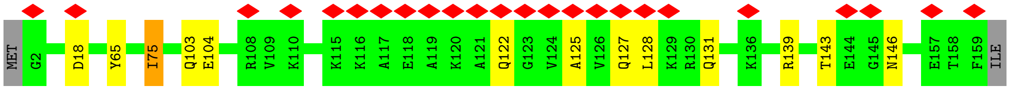
Chain AS:



- Molecule 22: KLLA0E23651p

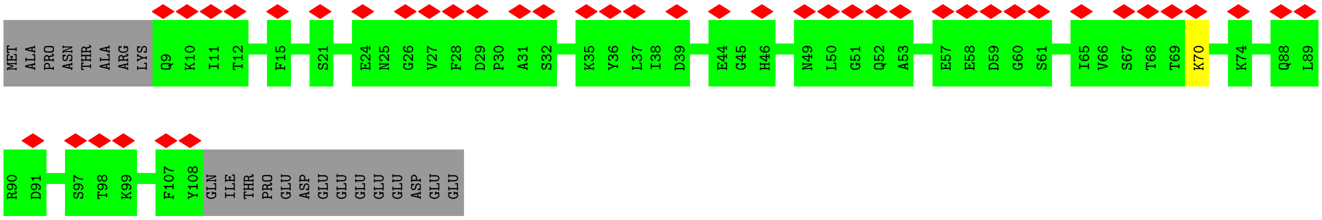
Chain AT:





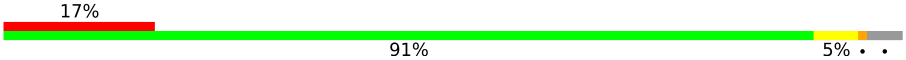
- Molecule 23: KLLA0D05181p

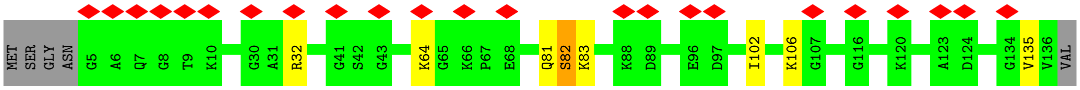
Chain AU:



- Molecule 24: KLLA0E06997p

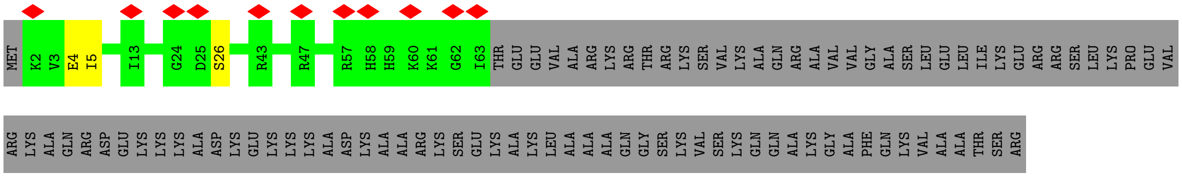
Chain AV:





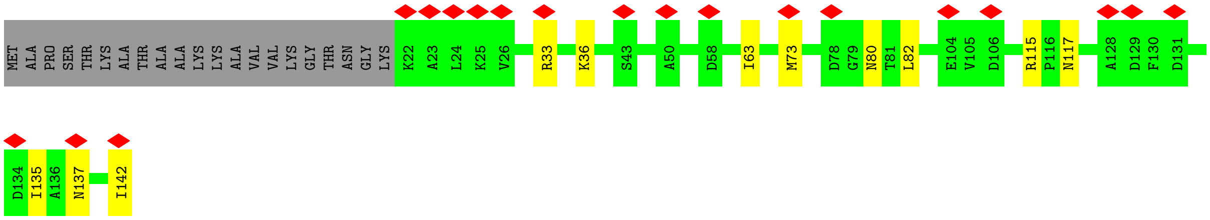
- Molecule 25: 60S ribosomal protein L24

Chain AW:



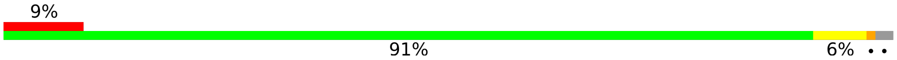
- Molecule 26: 60S ribosomal protein L25

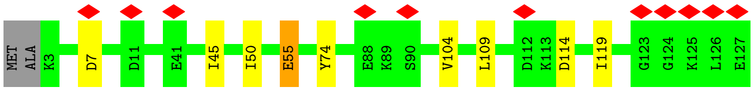
Chain AX:



- Molecule 27: KLLA0B05742p

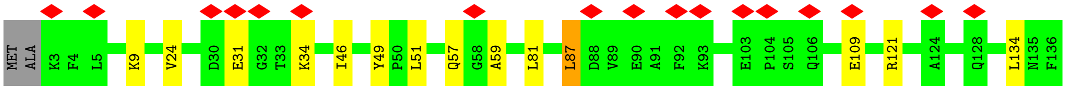
Chain AY:





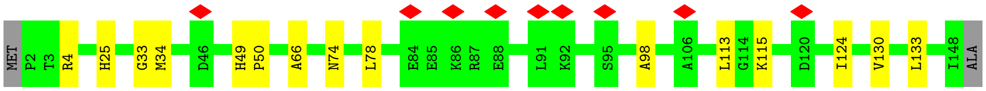
- Molecule 28: KLLA0E03455p

Chain AZ:



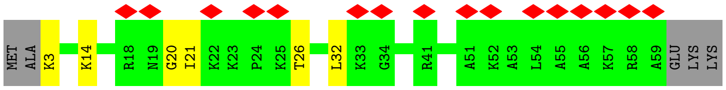
- Molecule 29: RPL28

Chain Ba:



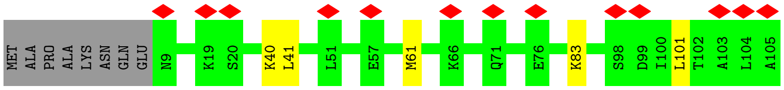
- Molecule 30: 60S ribosomal protein L29

Chain Bb:



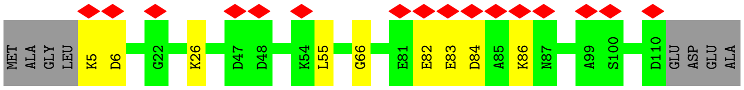
- Molecule 31: 60S ribosomal protein L30

Chain Bc:



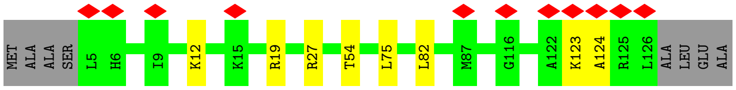
- Molecule 32: KLLA0B02937p

Chain Bd:



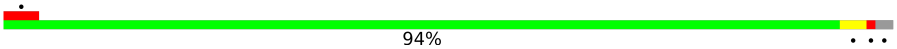
- Molecule 33: KLLA0E06843p

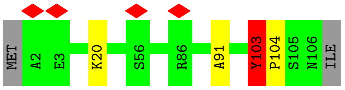
Chain Be:



- Molecule 34: KLLA0D07405p

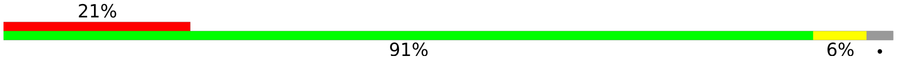
Chain Bf:

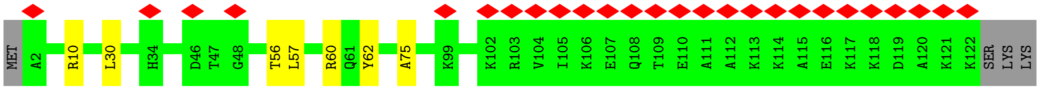




- Molecule 35: KLLA0C08371p

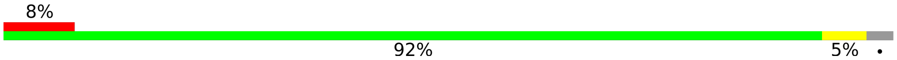
Chain Bg:

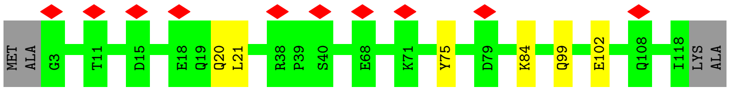




- Molecule 36: KLLA0F05247p

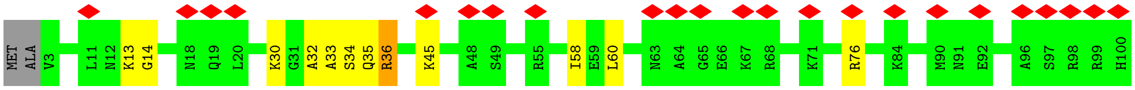
Chain Bh:





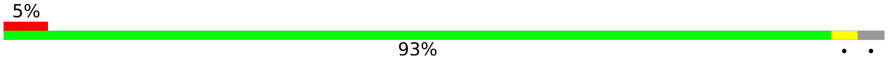
- Molecule 37: 60S ribosomal protein L36

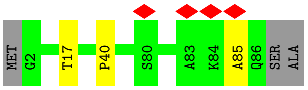
Chain Bi:



- Molecule 38: Ribosomal protein L37

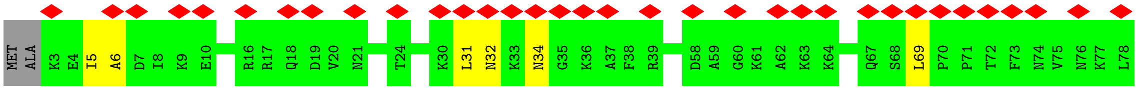
Chain Bj:





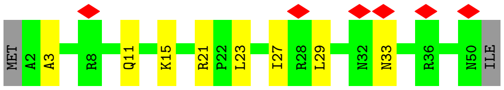
- Molecule 39: KLLA0C18216p

Chain Bk:

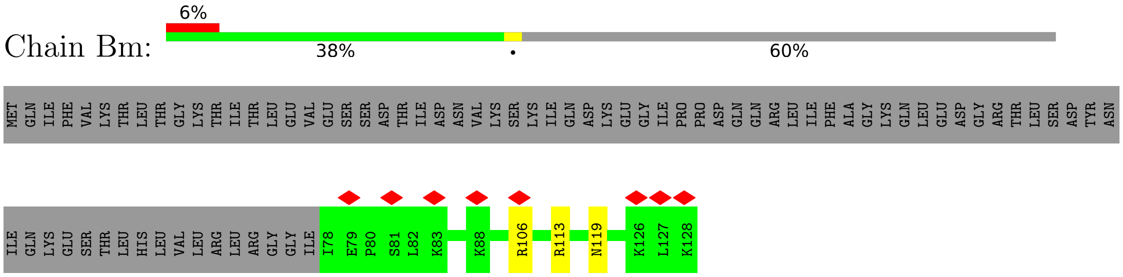


- Molecule 40: 60S ribosomal protein L39

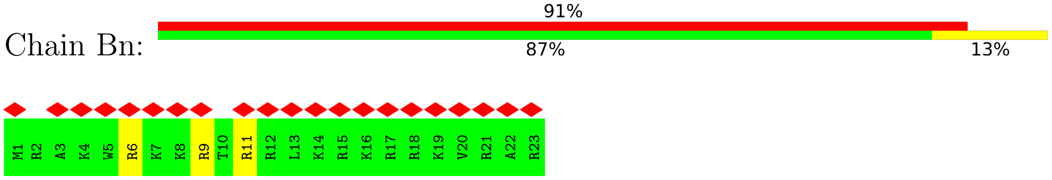
Chain Bl:



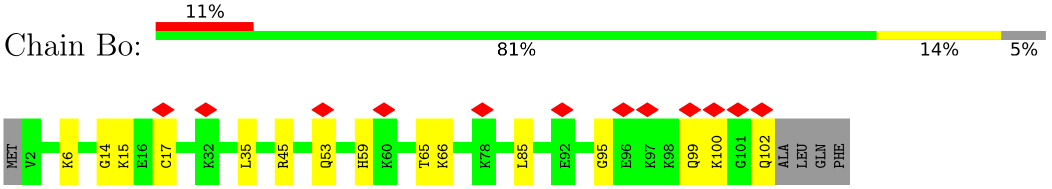
- Molecule 41: Ubiquitin fusion protein



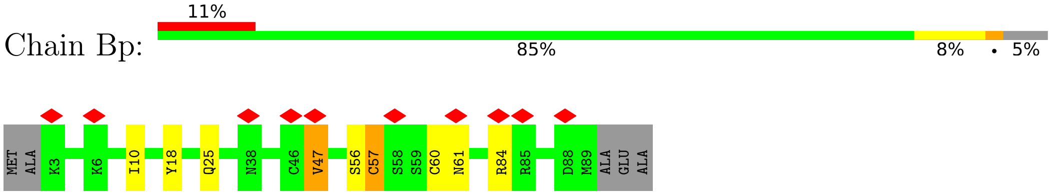
- Molecule 42: 60S ribosomal protein L41



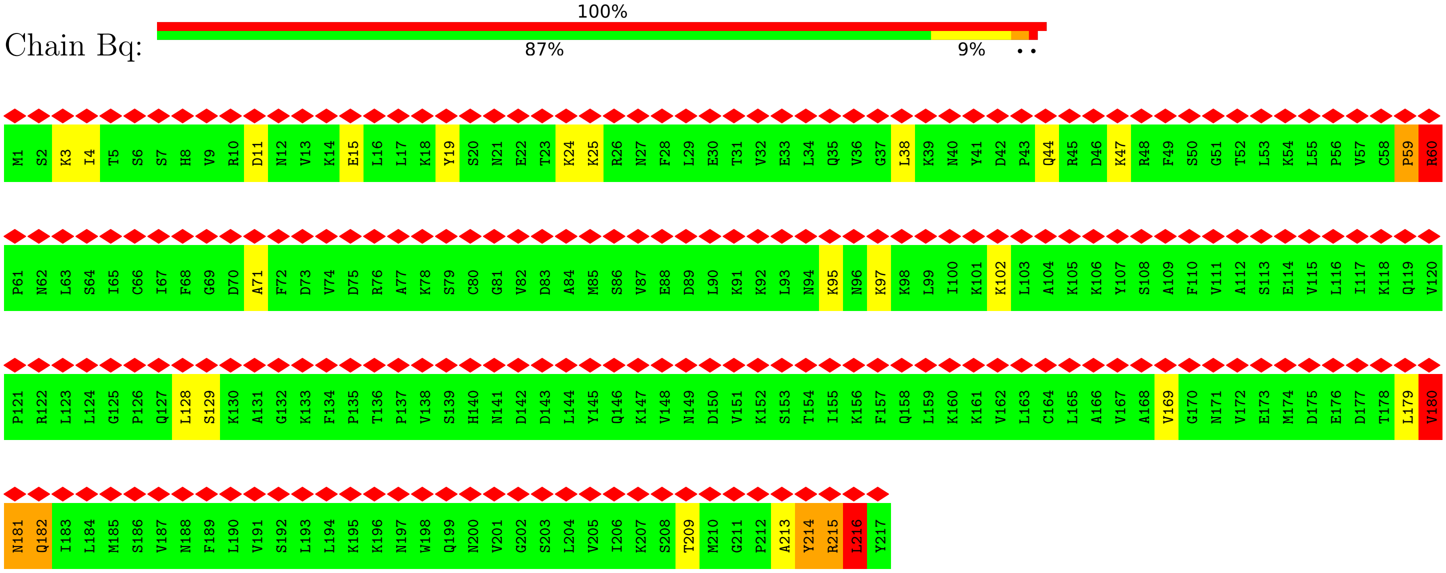
- Molecule 43: 60S ribosomal protein L44



- Molecule 44: KLLA0E05941p

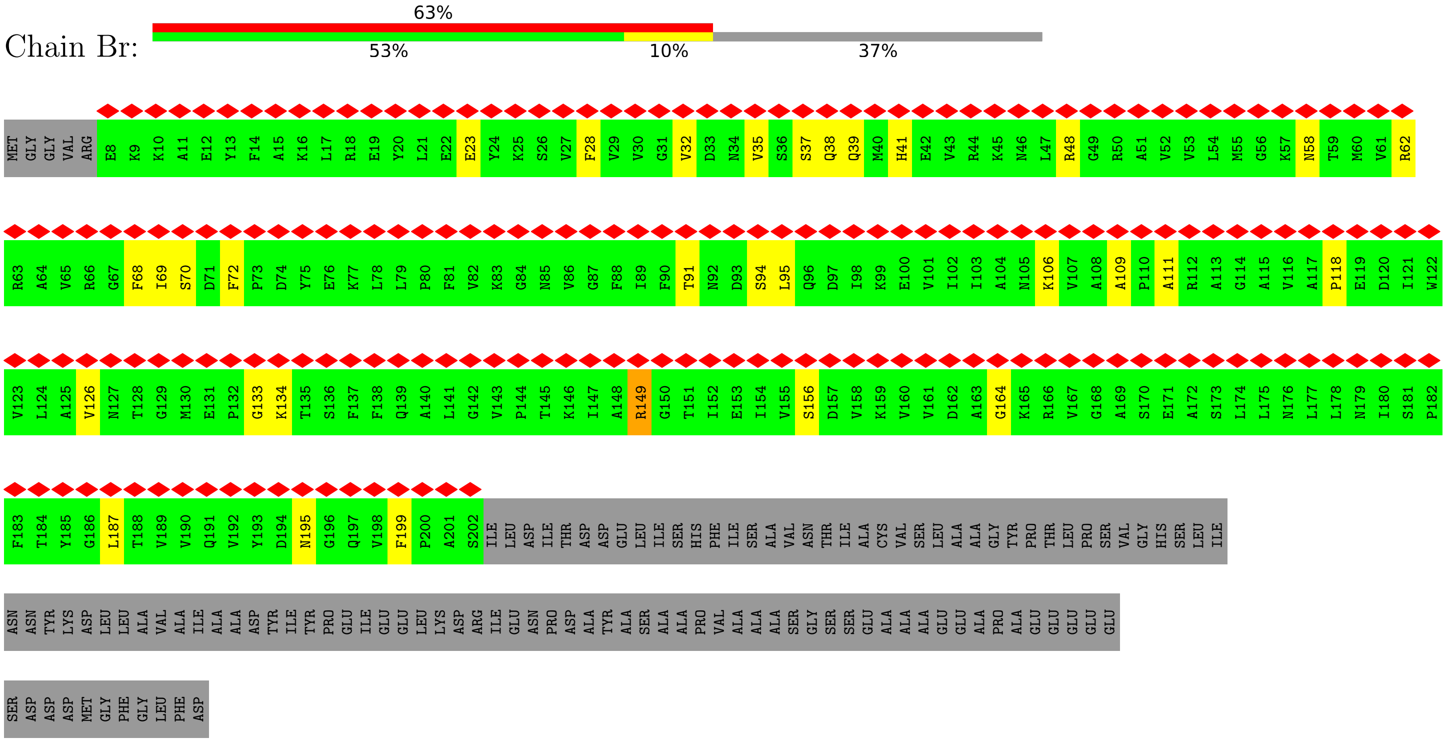


- Molecule 45: Ribosomal protein



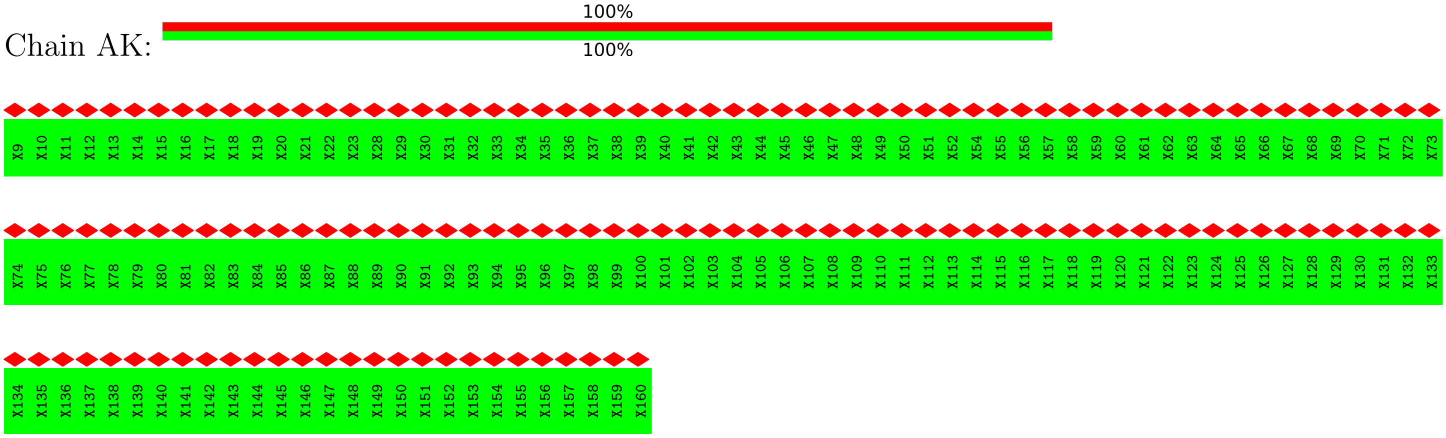
- Molecule 46: 60S acidic ribosomal protein P0

Chain Br:



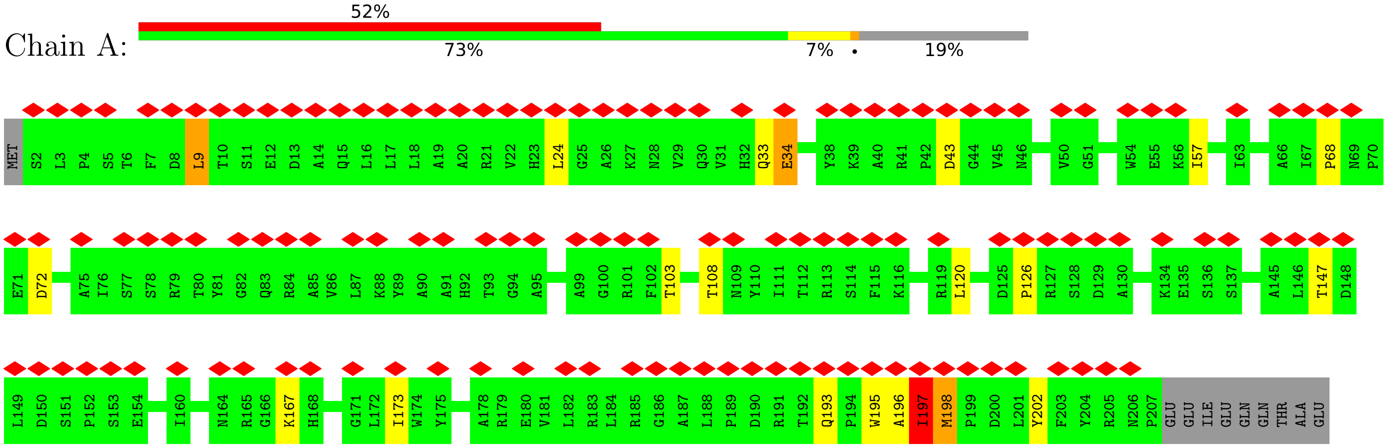
- Molecule 47: GDPCP

Chain AK:



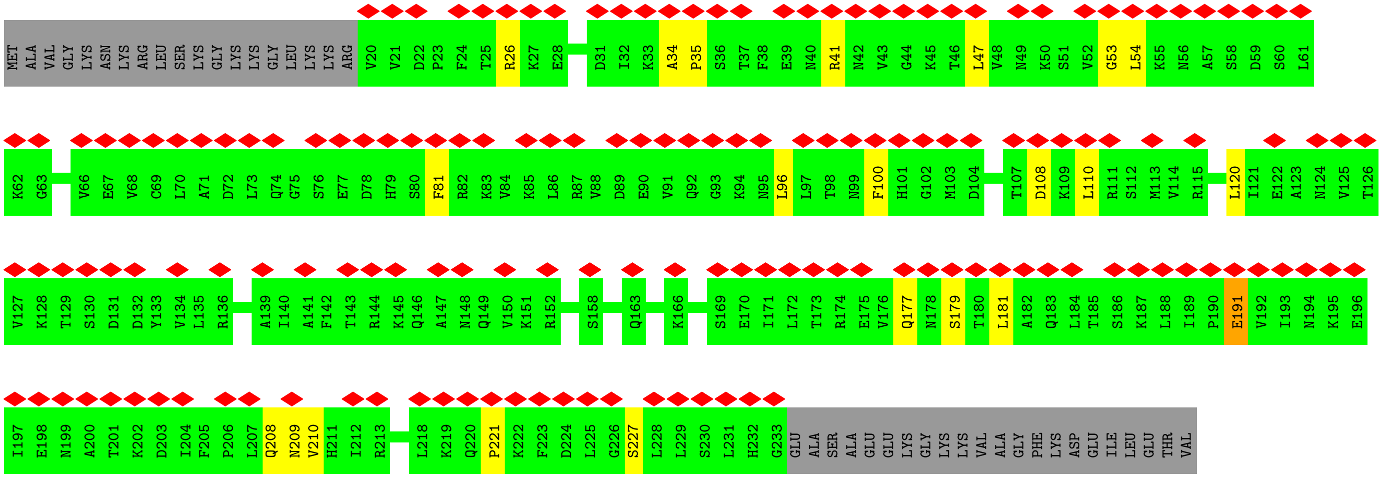
- Molecule 48: 40S ribosomal protein S0

Chain A:



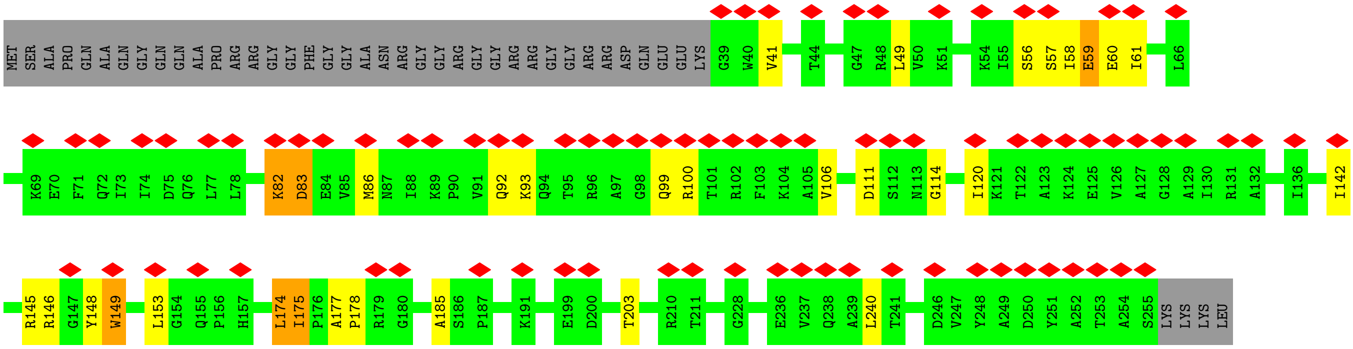
- Molecule 49: 40S ribosomal protein S1

Chain B:

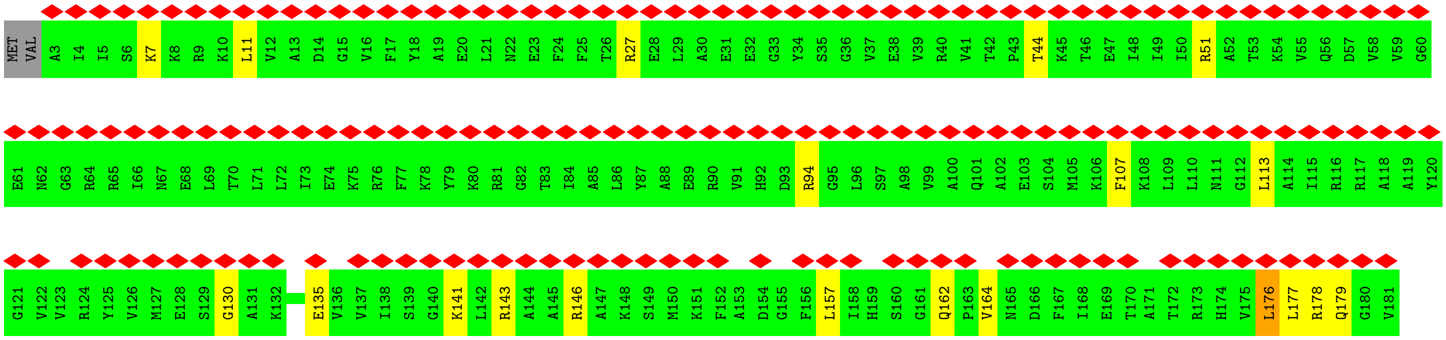
- Molecule 50: KLLA0F09812p

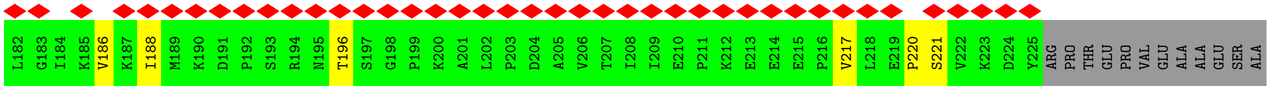
Chain C:

- Molecule 51: KLLA0D08305p

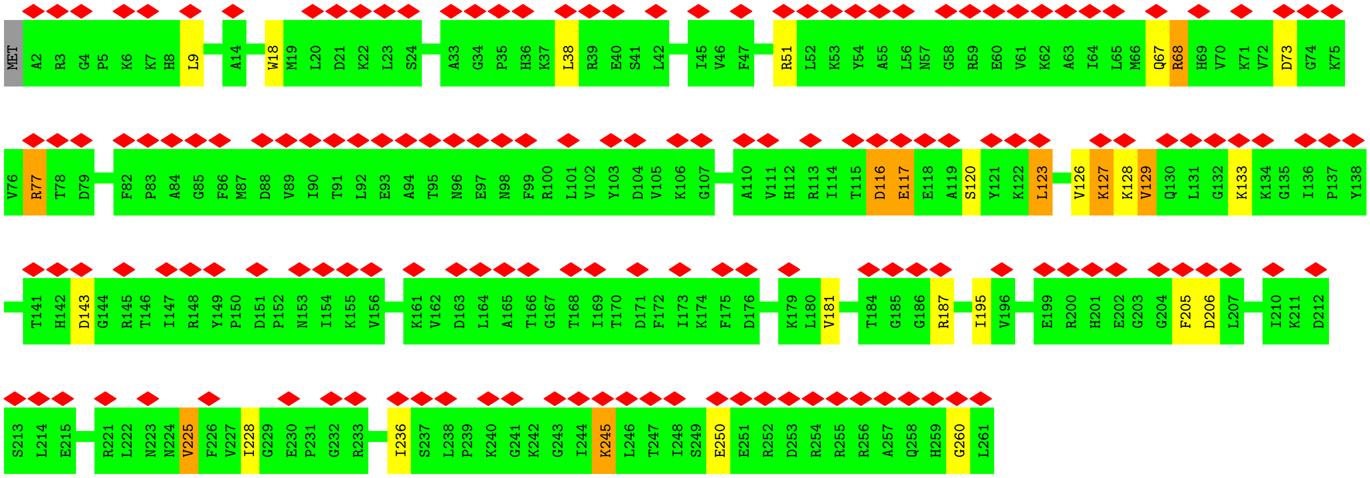
Chain D:



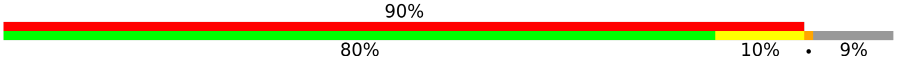
- Molecule 52: 40S ribosomal protein S4

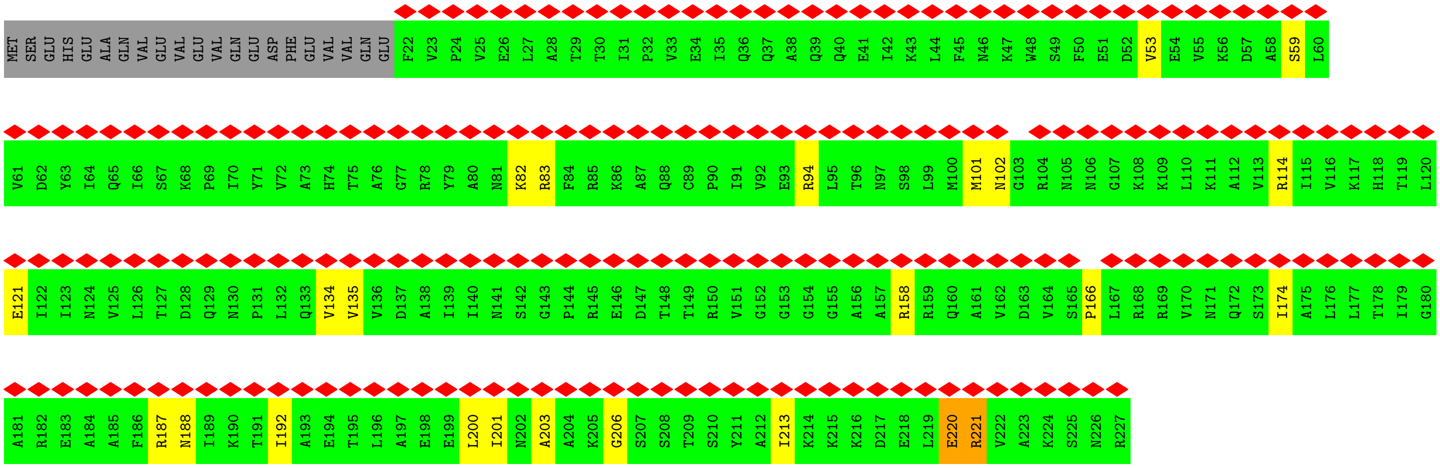
Chain E:



- Molecule 53: KLLA0D10659p

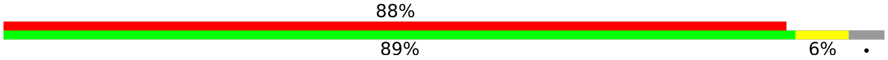
Chain F:

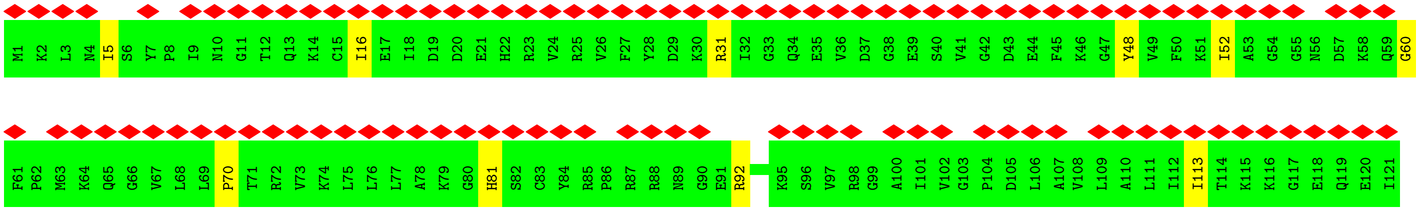


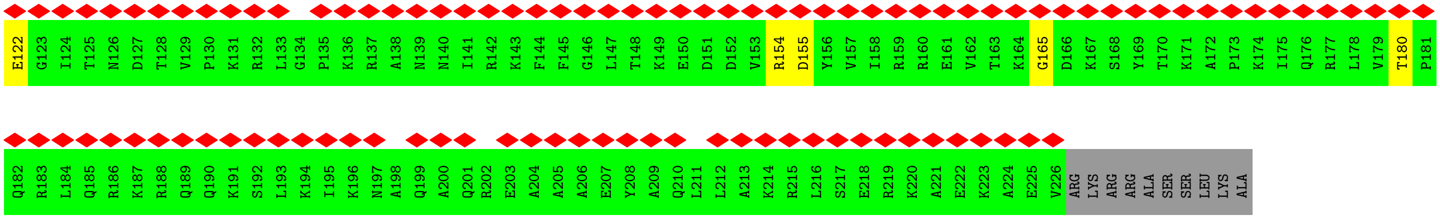


- Molecule 54: 40S ribosomal protein S6

Chain G:

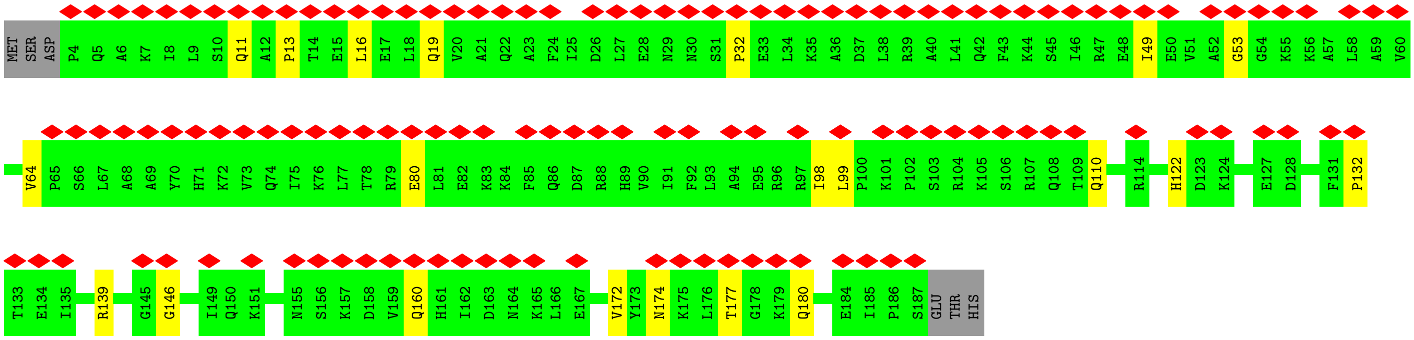






- Molecule 55: 40S ribosomal protein S7

Chain H:

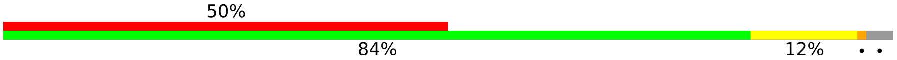


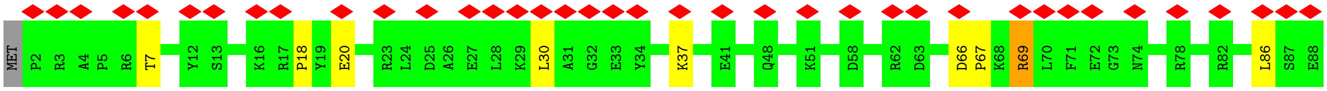
- Molecule 56: 40S ribosomal protein S8

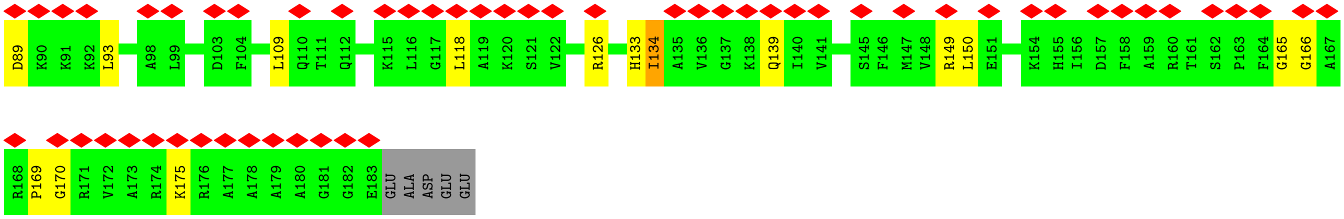
Chain I:

- Molecule 57: KLLA0E23673p

Chain J:

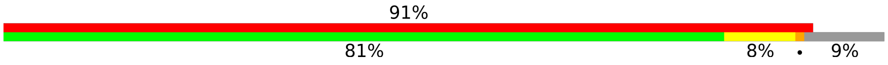


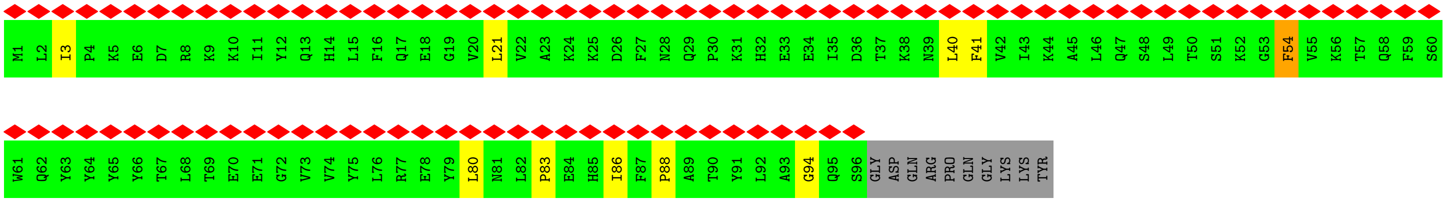




- Molecule 58: KLLA0B08173p

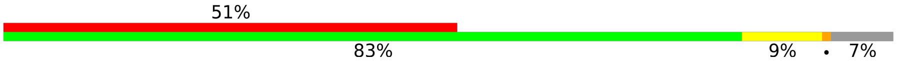
Chain K:

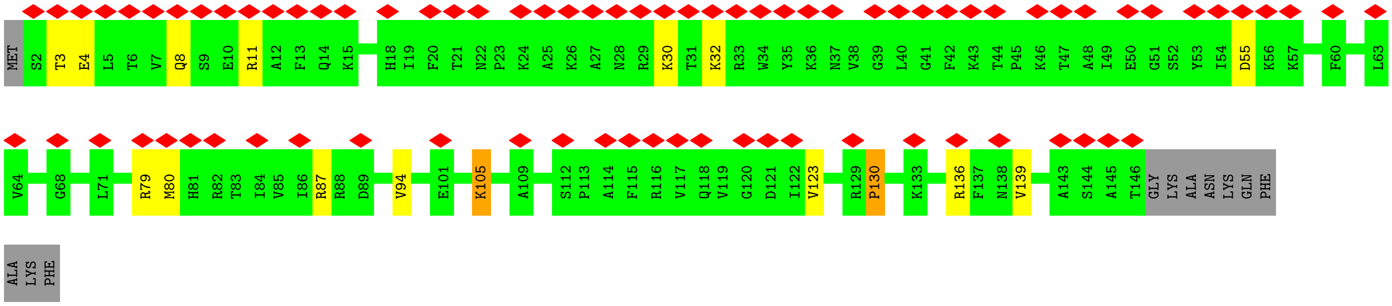




- Molecule 59: KLLA0A10483p

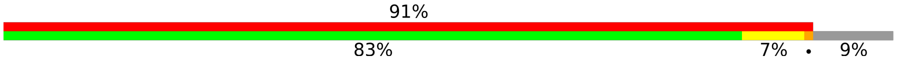
Chain L:

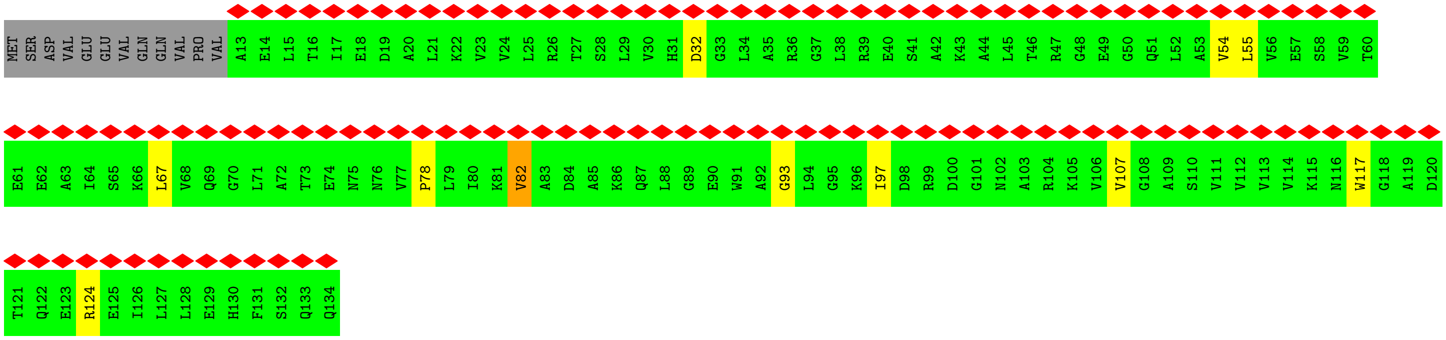




- Molecule 60: 40S ribosomal protein S12

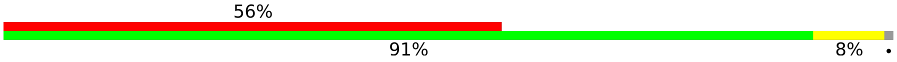
Chain M:

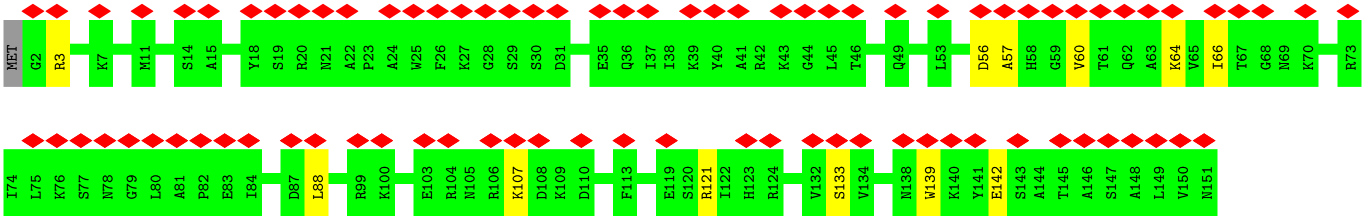




- Molecule 61: KLLA0F18040p

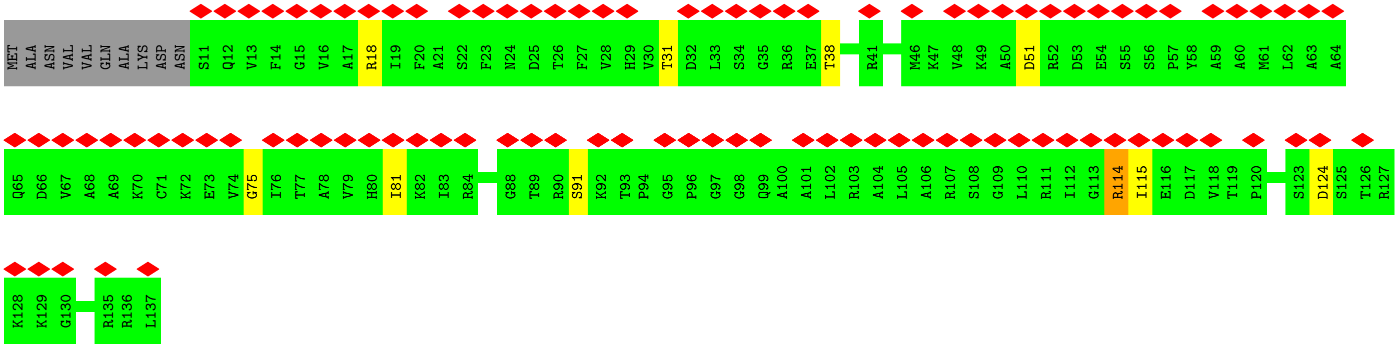
Chain N:





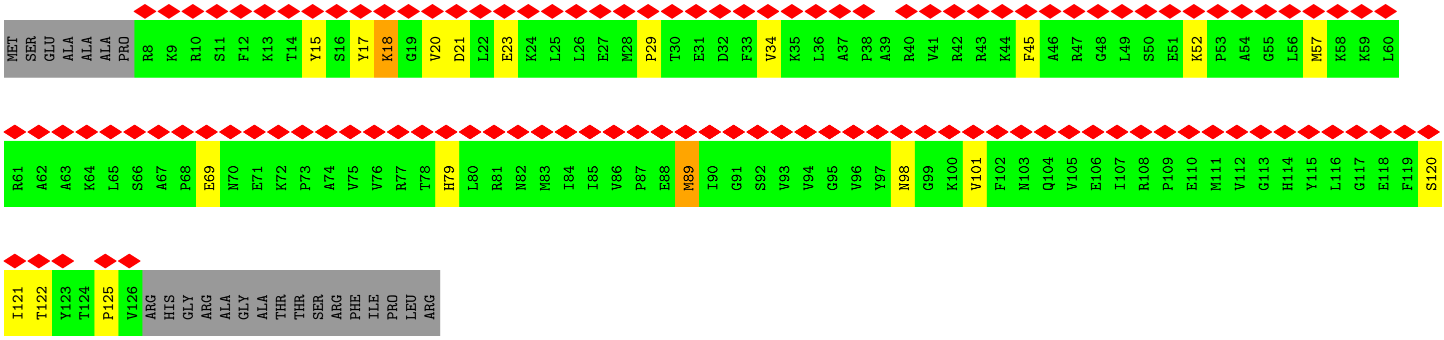
- Molecule 62: 40S ribosomal protein S14

Chain O:



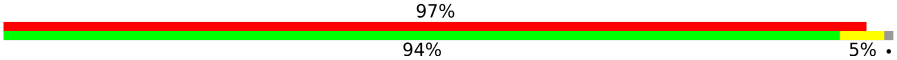
- Molecule 63: KLLA0F07843p

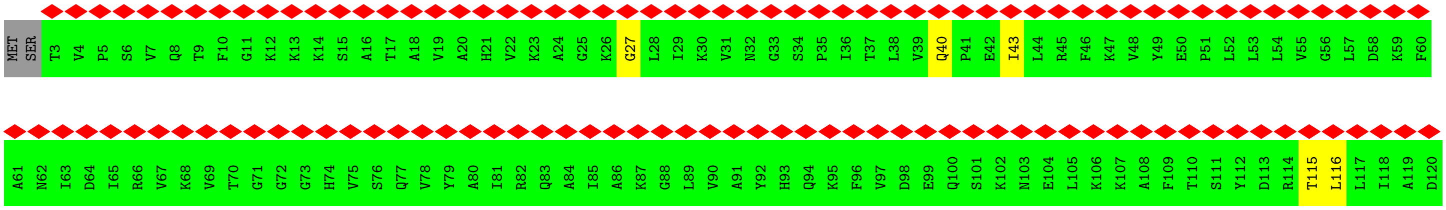
Chain P:

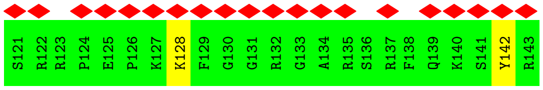


- Molecule 64: 40S ribosomal protein S16

Chain Q:

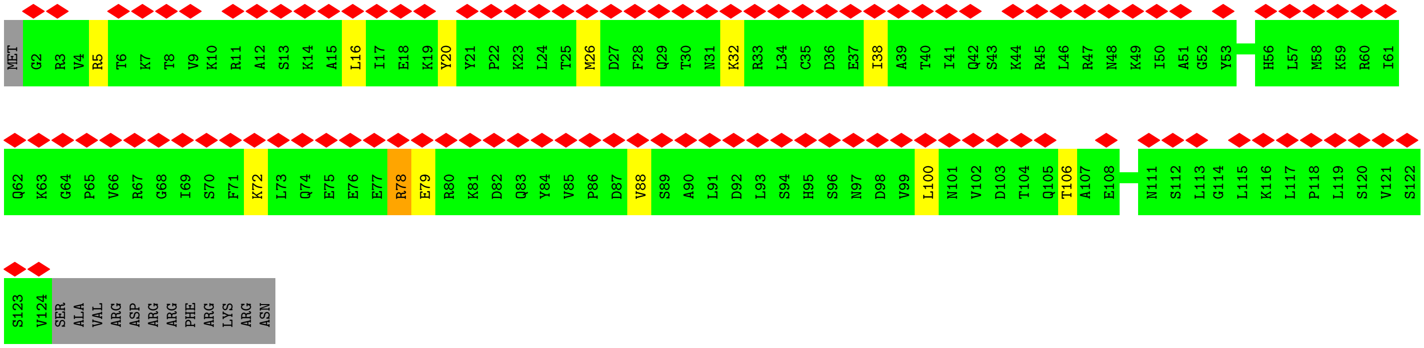






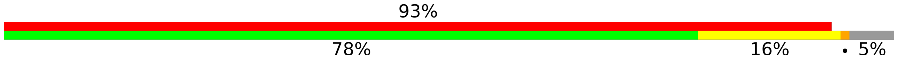
- Molecule 65: KLLA0B01474p

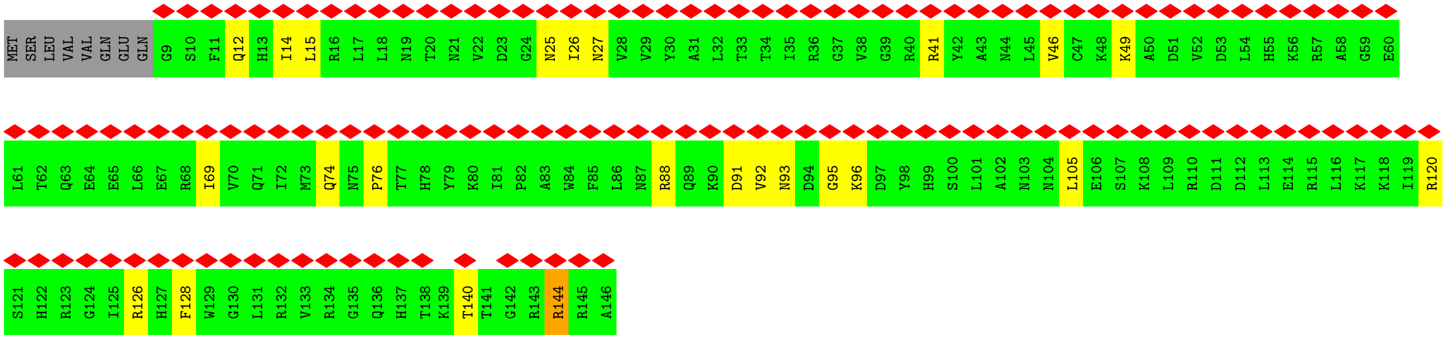
Chain R:



- Molecule 66: KLLA0B01562p

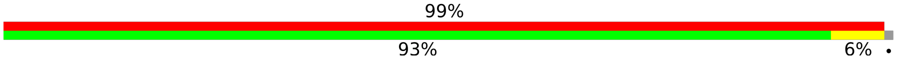
Chain S:

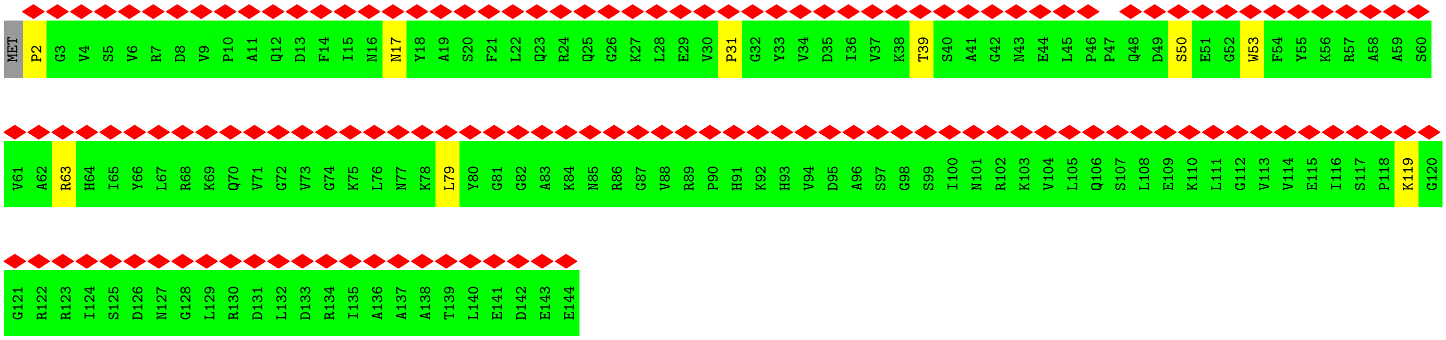




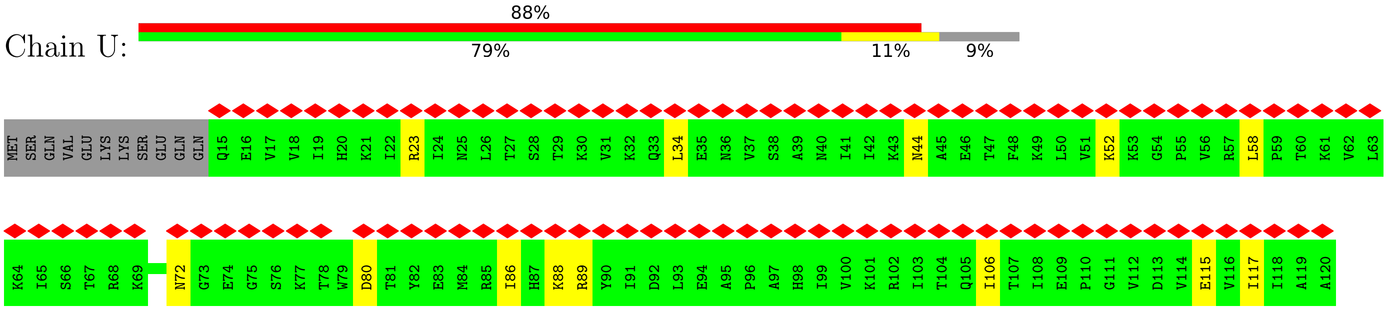
- Molecule 67: KLLA0A07194p

Chain T:

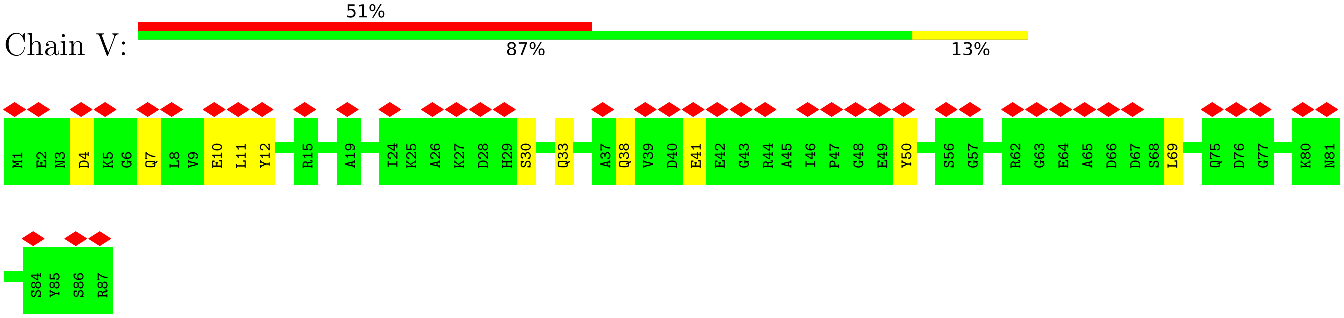




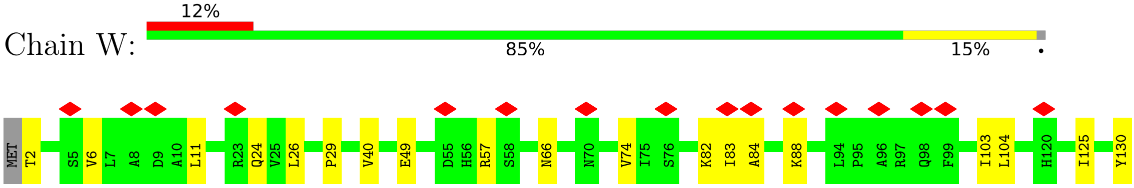
- Molecule 68: KLLA0F25542p



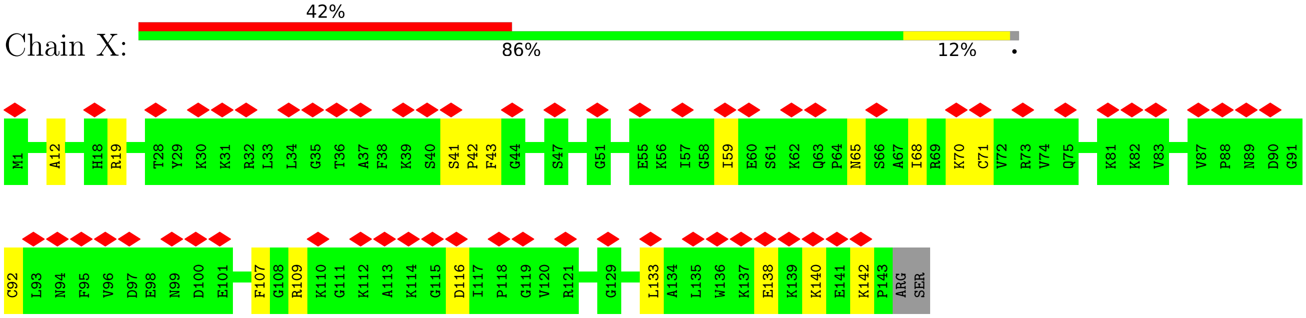
- Molecule 69: 40S ribosomal protein S21



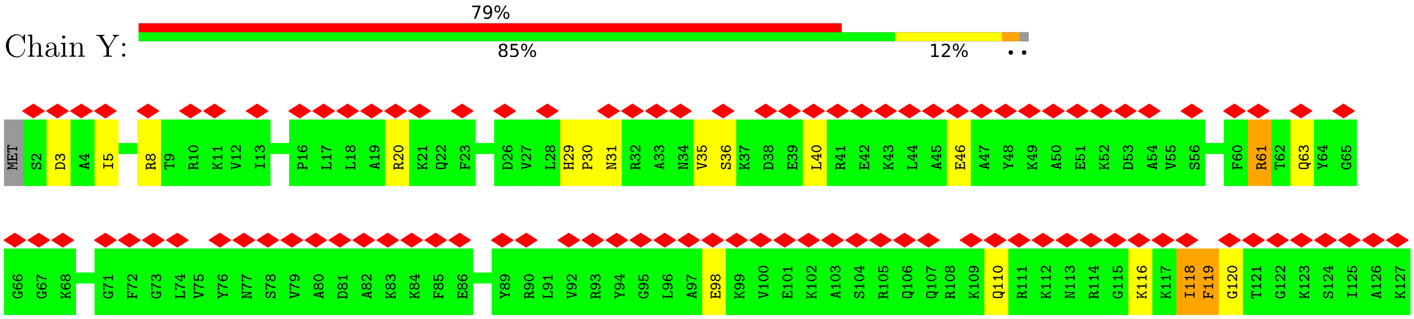
- Molecule 70: 40S ribosomal protein S22

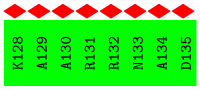


- Molecule 71: RPS23



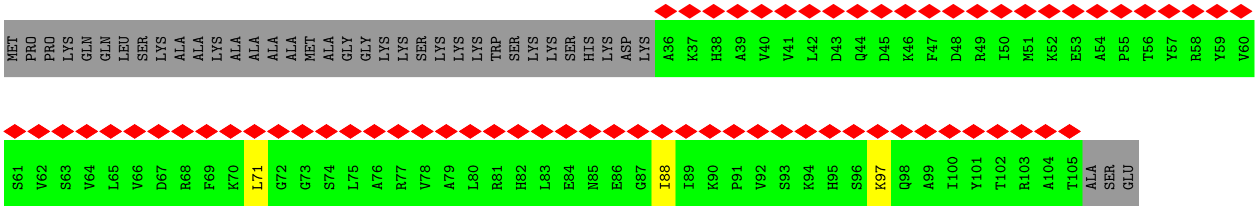
- Molecule 72: 40S ribosomal protein S24





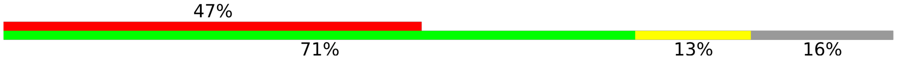
- Molecule 73: 40S ribosomal protein S25

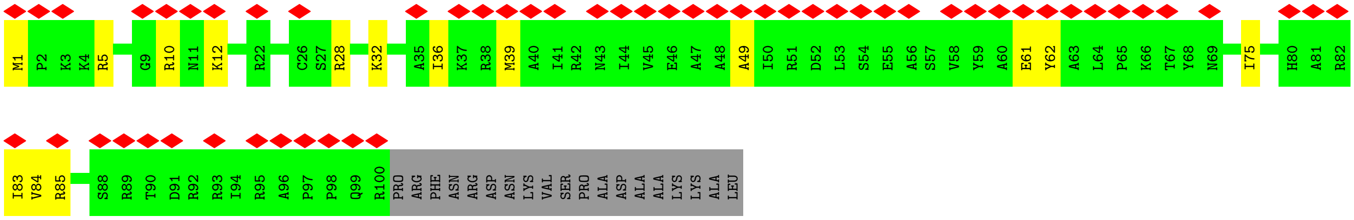
Chain Z:



- Molecule 74: 40S ribosomal protein S26

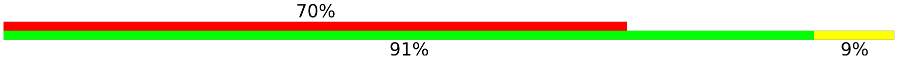
Chain a:

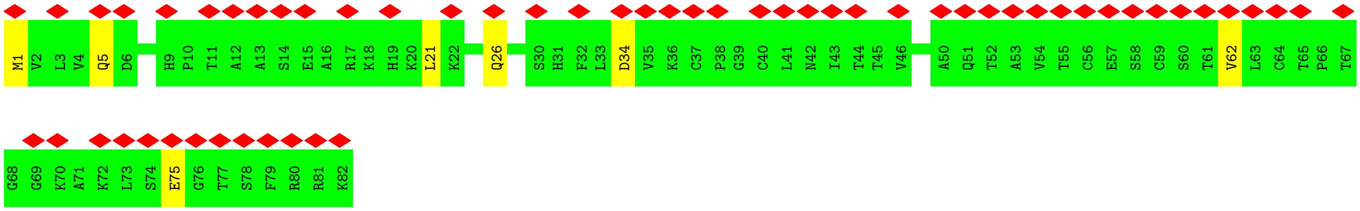




- Molecule 75: 40S ribosomal protein S27

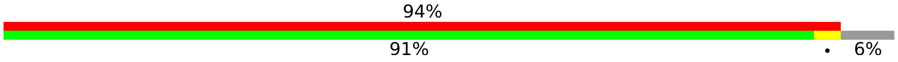
Chain b:



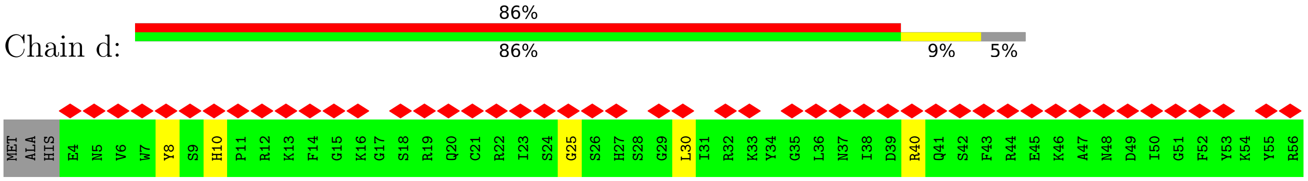


- Molecule 76: 40S ribosomal protein S28

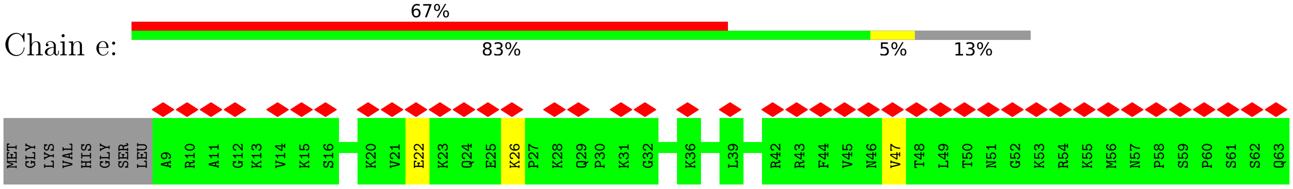
Chain c:



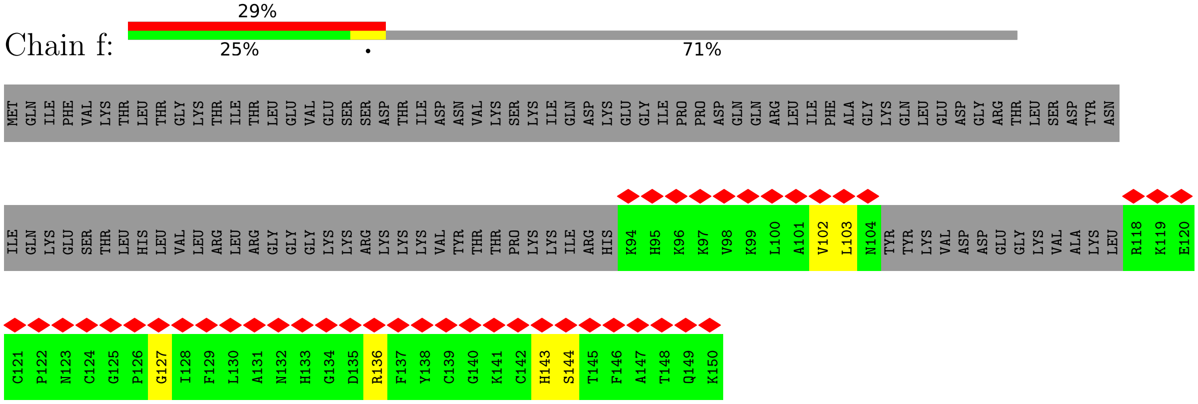
- Molecule 77: 40S ribosomal protein S29



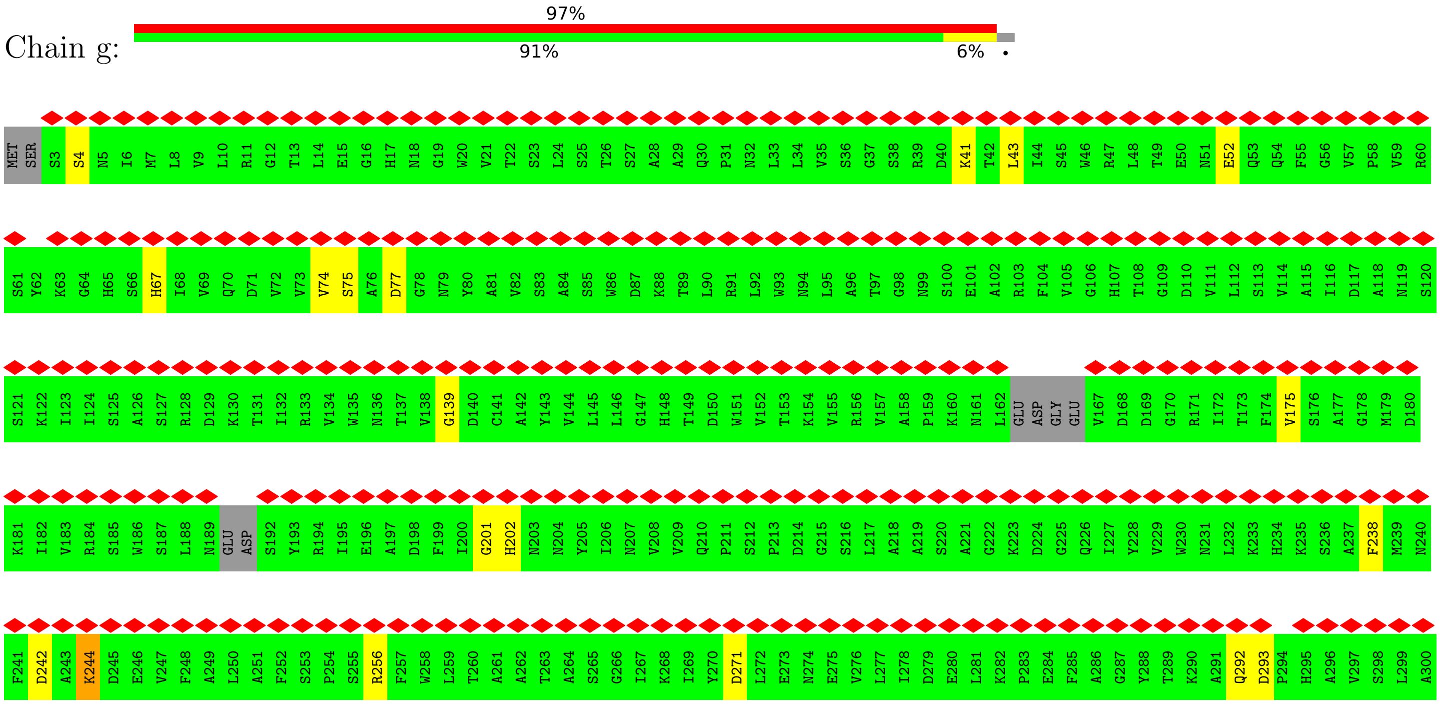
- Molecule 78: 40S ribosomal protein S30

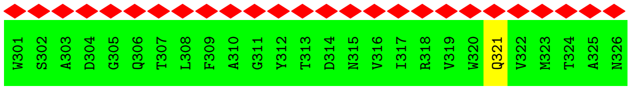


- Molecule 79: Ubiquitin-40S ribosomal protein S27a



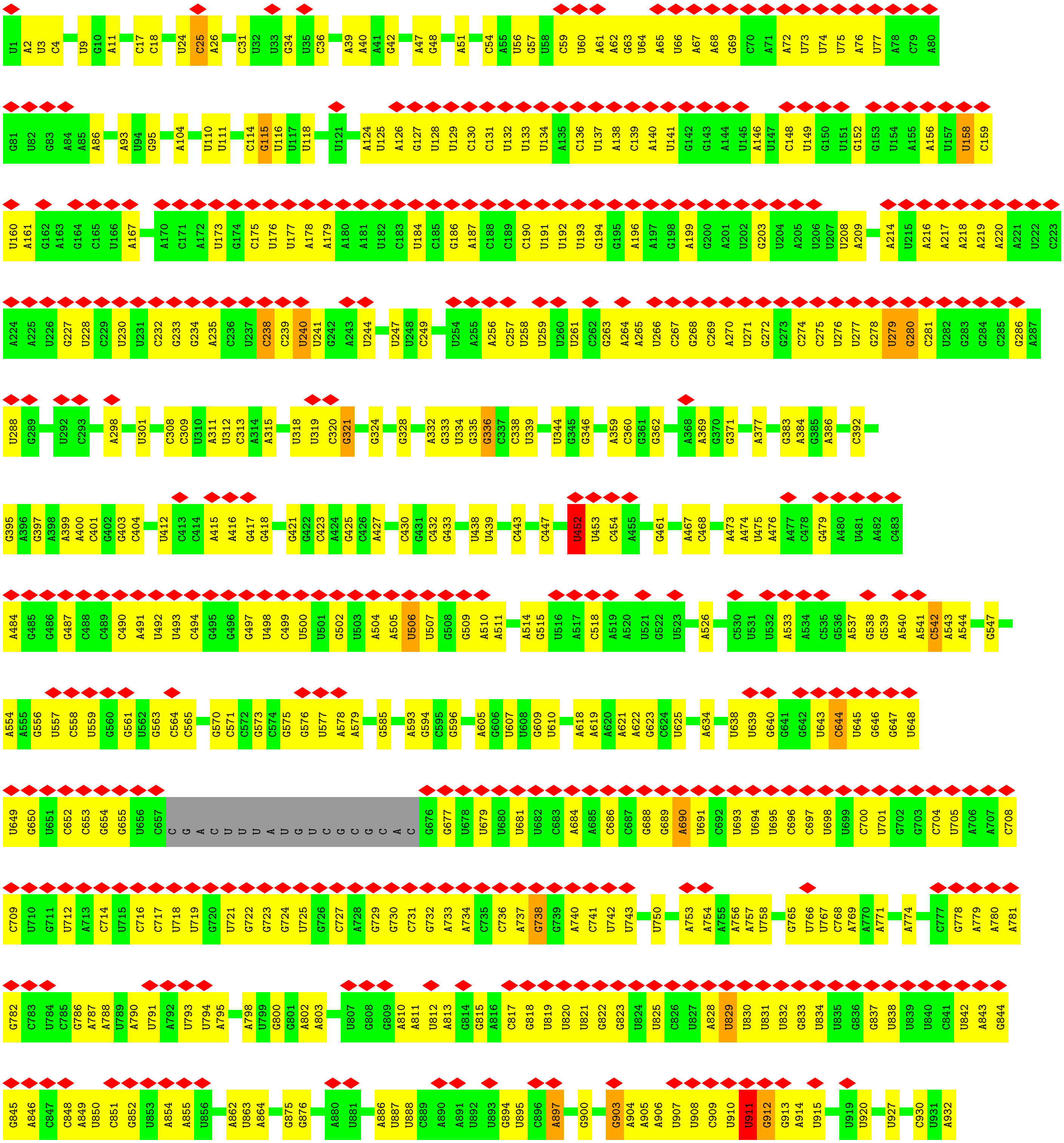
- Molecule 80: KLLA0E12277p





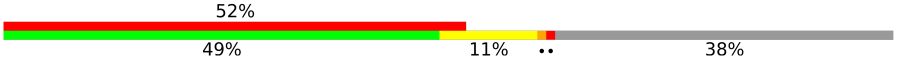
- Molecule 81: 18S ribosomal RNA

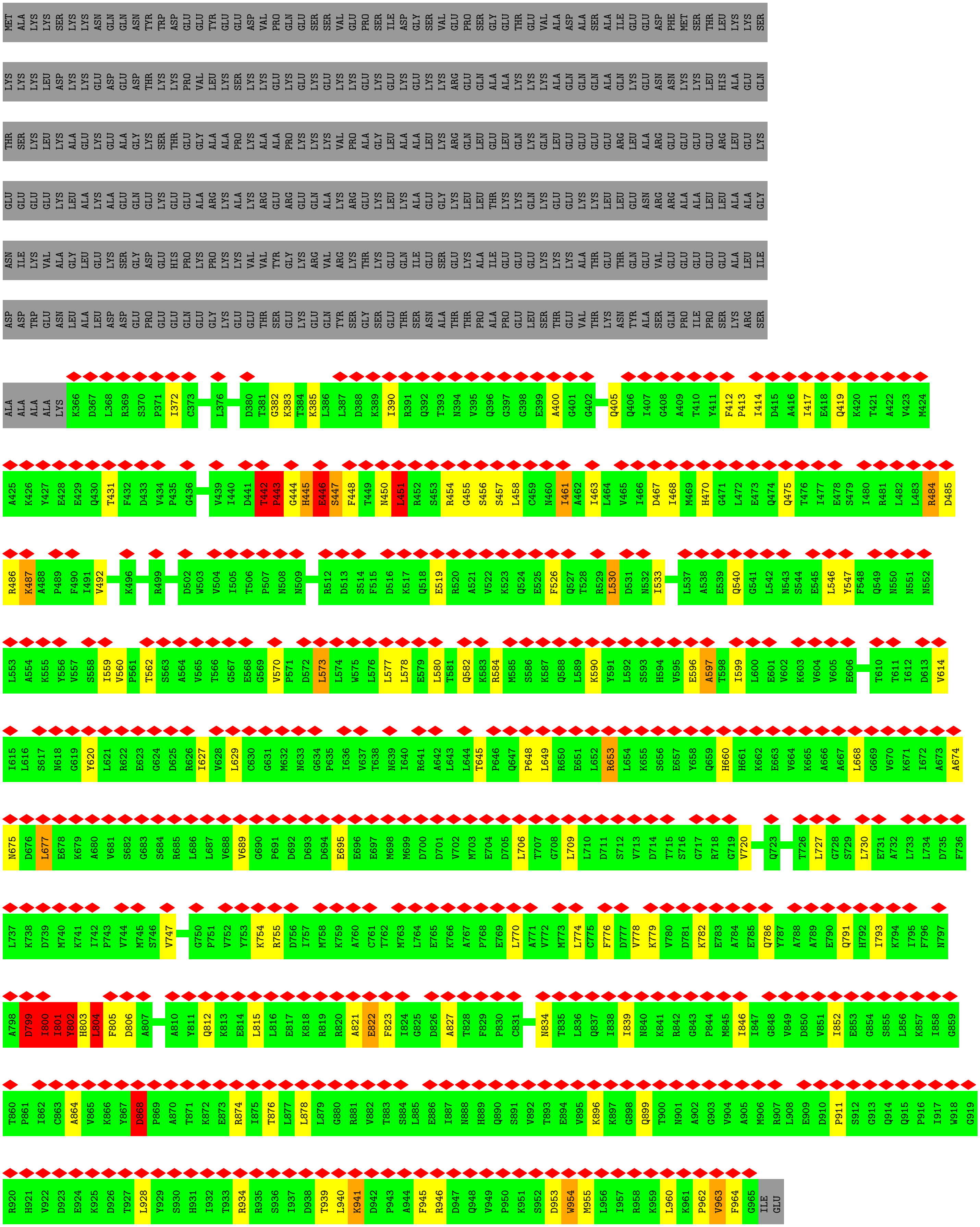
Chain 2:



- Molecule 82: KLLA0F23265p

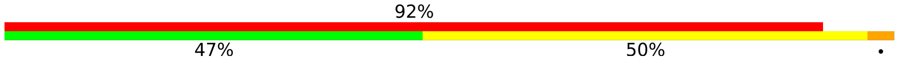
Chain 1:

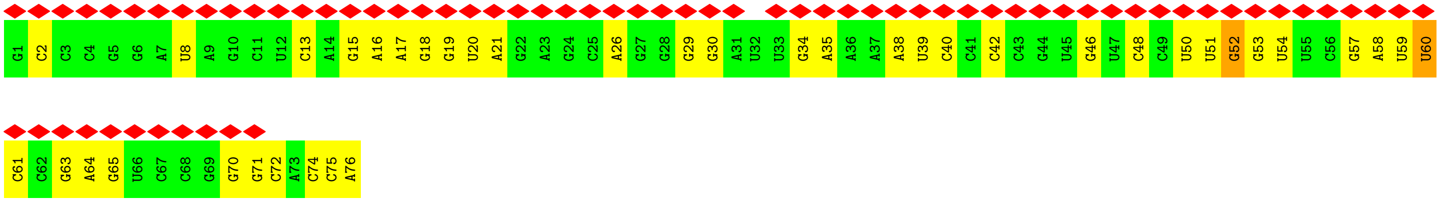



MET ALA LYS LYS SER LYS LYS ASN GLN GLN ASN TYR TRP ASP GLU GLU TYR GLU GLU ASP VAL PRO GLN GLU SER SER VAL GLU PRO SER ILE ASP GLY SER VAL GLU PRO SER GLY GLU THR GLU VAL ALA ASP ALA SER ALA ILE GLU GLU ASP PHE MET SER THR LEU LYS LYS SER
LYS LYS LYS LEU ASP LYS LYS GLU ASP GLU ASP THR LYS LYS PRO VAL LEU LYS SER LYS LYS GLU LYS GLU LYS GLU LYS LYS GLU LYS GLU LYS GLU LYS LYS ARG GLU GLN ALA ALA LYS LYS LYS ALA GLN GLN GLN ALA GLN LYS GLU ASN ASN LYS LYS LEU HIS ALA GLU GLN
THR SER LYS LEU LYS ALA GLU LYS GLU ALA GLY LYS SER THR GLU GLY ALA ALA PRO LYS ALA ALA PRO LYS LYS LYS VAL PRO ALA GLY LEU ALA ALA LEU LYS ARG GLN LEU GLU LEU GLN LYS GLN LEU GLU GLU GLU GLU ARG LEU ALA ARG GLU GLU GLU GLU ARG LEU GLU LYS
GLU GLU GLU GLU LYS LEU ALA LYS ALA GLU GLN GLU LYS GLU GLU ALA ARG LYS ALA LYS ARG GLU ARG GLU GLN ALA LYS ARG GLU LYS LEU LYS ALA GLU GLY LYS LEU LEU THR LYS LYS GLN LYS GLU GLU LYS LYS LEU LEU GLU ASN ARG ARG ALA ALA LEU LEU ALA ALA GLY
ASN ILE LYS VAL ALA GLY LEU GLU LYS SER GLY ASP GLU HIS PRO LYS PRO LYS LYS VAL VAL TYR GLY LYS ARG VAL ARG LYS THR LYS GLU GLN ILE GLU SER GLU LYS ALA ILE GLU GLU GLU LYS LYS LYS ALA THR GLU THR GLN GLU VAL GLU GLU GLU GLU GLU ALA LEU ILE
ASP ASP TRP GLU ASN LEU ALA LEU ASP ASP GLU PRO GLU GLU GLN GLU GLY LYS GLU GLU THR SER GLU LYS GLU GLN TYR SER GLY SER GLU THR SER ASN ALA THR THR PRO ALA PRO GLU LEU SER THR GLU VAL THR LYS ASN TYR ALA SER GLN PRO ILE PRO SER LYS ARG SER
ALA ALA ALA ALA LYS K366 D367 L368 R369 S370 P371 I372 C373 L376 D380 T381 G382 K383 T384 K385 L386 L387 D388 K389 I390 R391 Q392 T393 N394 V395 Q396 G397 G398 E399 A400 G401 G402 Q405 Q406 I407 G408 A409 T410 Y411 F412 P413 I414 D415 A416 I417 E418 Q419 K420 T421 A422 V423 M424
A425 K426 Y427 E428 E429 Q430 T431 F432 D433 V434 P435 G436 V439 I440 D441 T442 P443 G444 H445 E446 S447 F448 T449 N450 L451 R452 S453 R454 G455 S456 S457 L458 C459 N460 I461 A462 I463 L464 V465 I466 D467 I468 M469 H470 G471 L472 E473 Q474 Q475 T476 I477 E478 S479 I480 R481 L482 L483 R484 D485
R486 K487 A488 P489 F490 I491 V492 K496 R499 D502 W503 V504 I505 T506 P507 N508 N509 R512 D513 S514 F515 D516 K517 Q518 E519 R520 A521 V522 K523 Q524 E525 F526 Q527 T528 R529 L530 D531 N532 I533 L537 A538 E539 Q540 G541 L542 N543 S544 E545 L546 Y547 F548 Q549 N550 N551 N552
L553 A554 K555 Y556 V557 S558 I559 V560 P561 T562 S563 A564 V565 T566 G567 E568 G569 V570 P571 D572 L573 L574 W575 L576 L577 L578 E579 L580 T581 Q582 K583 R584 M585 S586 K587 Q588 L589 K590 Y591 L592 S593 H594 V595 E596 A597 T598 I599 L600 E601 V602 K603 V604 V605 E606 T610 T611 I612 D613 V614
I615 L616 S617 N618 G619 Y620 L621 R622 E623 G624 D625 R626 I627 V628 L629 C630 G631 M632 N633 G634 P635 I636 V637 T638 N639 I640 R641 A642 L643 L644 T645 P646 Q647 P648 L649 R650 E651 L652 R653 L654 K655 S656 E657 Y658 Q659 H660 H661 K662 E663 V664 K665 A666 A667 L668 G669 V670 K671 I672 A673 A674
N675 D676 L677 E678 K679 A680 V681 S682 G683 S684 R685 L686 L687 V688 V689 G690 P691 D692 D693 D694 E695 E696 E697 M698 M699 D700 D701 V702 M703 E704 D705 L706 T707 G708 L709 L710 D711 S712 V713 D714 T715 S716 G717 R718 G719 V720 Q723 T726 L727 G728 S729 L730 E731 A732 L733 L734 D735 F736
L737 K738 D739 M740 K741 I742 P743 V744 M745 S746 V747 G750 P751 V752 Y753 K754 R755 D756 I757 M758 K759 A760 C761 T762 M763 L764 E765 K766 A767 P768 E769 L770 A771 V772 M773 L774 C775 F776 D777 V778 K779 V780 D781 K782 E783 A784 E785 Q786 Y787 A788 A789 E790 Q791 H792 I793 K794 I795 F796 N797
A798 D799 I800 I801 Y802 H803 L804 F805 D806 A807 A810 Y811 Q812 K813 E814 L815 L816 E817 K818 R819 R820 A821 E822 F823 I824 G825 D826 A827 T828 F829 P830 C831 N834 T835 L836 Q837 I838 I839 N840 K841 R842 G843 P844 M845 I846 I847 G848 V849 D850 V851 I852 E853 G854 S855 L856 K857 I858 G859
T860 P861 I862 C863 A864 V865 K866 Y867 D868 P869 A870 T871 K872 E873 R874 I875 T876 L877 L878 L879 G880 R881 V882 T883 S884 L885 E886 I887 N888 H889 Q890 S891 V892 T893 E894 V895 K896 K897 G898 Q899 T900 N901 A902 G903 V904 A905 M906 R907 L908 E909 D910 P911 S912 G913 Q914 Q915 F916 I917 W918 G919
R920 H921 V922 D923 E924 K925 D926 T927 L928 Y929 S930 H931 I932 T933 R934 R935 S936 I937 D938 T939 L940 K941 D942 P943 A944 F945 R946 D947 Q948 V949 P950 K951 S952 D953 W954 M955 I956 I957 R958 K959 L960 K961 P962 V963 F964 G965 ILE GLU

- Molecule 83: RNA (76-MER)

Chain 3:





4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	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	0.588	Depositor
Minimum map value	-0.380	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	5	0.20	0/78206	0.67	9/121916 (0.0%)
2	7	0.19	0/2883	0.65	0/4491
3	8	0.20	0/3714	0.66	0/5781
4	AA	0.36	0/1926	0.58	0/2588
5	AB	0.36	0/3136	0.56	0/4225
6	AC	0.44	1/2792 (0.0%)	0.60	0/3777
7	AD	0.37	0/2436	0.56	0/3292
8	AE	0.41	0/1343	0.58	0/1804
9	AF	0.39	0/1810	0.53	0/2440
10	AG	0.37	0/1846	0.52	0/2486
11	AH	0.36	0/1547	0.54	0/2083
12	AI	0.37	0/1725	0.55	0/2310
13	AJ	0.38	0/1370	0.60	0/1835
14	AL	0.38	0/1607	0.62	0/2156
15	AM	0.38	0/1060	0.57	0/1430
16	AN	0.38	0/1746	0.61	0/2339
17	AO	0.23	0/1602	0.39	0/2151
18	AP	0.38	0/1455	0.60	0/1952
19	AQ	0.37	0/1469	0.61	0/1970
20	AR	0.40	0/1539	0.62	0/2047
21	AS	0.37	0/1458	0.56	0/1964
22	AT	0.37	0/1286	0.55	0/1722
23	AU	0.38	0/824	0.47	0/1113
24	AV	0.37	0/991	0.57	0/1331
25	AW	0.39	0/528	0.57	0/703
26	AX	0.36	0/979	0.55	0/1320
27	AY	0.37	0/1003	0.59	0/1339
28	AZ	0.39	0/1114	0.55	0/1493
29	Ba	0.37	0/1186	0.57	0/1590
30	Bb	0.37	0/468	0.53	0/621
31	Bc	0.38	0/748	0.50	0/1005
32	Bd	0.36	0/885	0.54	0/1186

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Be	0.37	0/998	0.56	0/1332
34	Bf	0.37	0/855	0.56	0/1150
35	Bg	0.37	0/961	0.59	0/1281
36	Bh	0.38	0/970	0.58	0/1291
37	Bi	0.41	0/773	0.62	0/1029
38	Bj	0.40	0/690	0.61	0/913
39	Bk	0.43	0/626	0.70	0/835
40	Bl	0.41	0/435	0.64	0/577
41	Bm	0.38	0/416	0.59	0/552
42	Bn	0.41	0/219	0.83	0/281
43	Bo	0.38	0/825	0.65	0/1086
44	Bp	0.42	0/667	0.70	0/891
45	Bq	0.45	1/1742 (0.1%)	0.59	1/2342 (0.0%)
46	Br	0.41	0/1535	0.62	0/2077
48	A	0.39	0/1656	0.57	0/2264
49	B	0.38	0/1747	0.56	0/2353
50	C	0.39	0/1659	0.60	0/2252
51	D	0.38	0/1769	0.57	0/2378
52	E	0.39	0/2122	0.62	1/2861 (0.0%)
53	F	0.39	0/1628	0.60	0/2198
54	G	0.37	0/1835	0.60	0/2451
55	H	0.37	0/1507	0.56	0/2028
56	I	0.40	0/1519	0.63	0/2033
57	J	0.40	0/1495	0.64	0/2001
58	K	0.40	0/831	0.50	0/1123
59	L	0.39	0/1194	0.63	0/1611
60	M	0.38	0/929	0.57	0/1255
61	N	0.38	0/1210	0.58	0/1628
62	O	0.38	0/953	0.61	0/1279
63	P	0.43	0/969	0.62	0/1302
64	Q	0.39	0/1125	0.58	0/1510
65	R	0.38	0/994	0.61	0/1335
66	S	0.42	0/1157	0.63	0/1554
67	T	0.38	0/1129	0.56	0/1520
68	U	0.36	0/857	0.54	0/1158
69	V	0.36	0/696	0.57	0/938
70	W	0.37	0/1039	0.58	0/1399
71	X	0.39	0/1128	0.62	0/1504
72	Y	0.40	0/1075	0.59	0/1433
73	Z	0.38	0/567	0.58	0/762
74	a	0.40	0/810	0.69	0/1084
75	b	0.35	0/627	0.55	0/847
76	c	0.37	0/496	0.63	0/666

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
77	d	0.39	0/457	0.55	0/607
78	e	0.37	0/450	0.53	0/599
79	f	0.39	0/344	0.54	0/458
80	g	0.37	0/2521	0.55	0/3431
81	2	0.21	0/42269	0.68	4/65862 (0.0%)
82	1	0.39	0/4776	0.67	0/6459
83	3	0.21	0/1815	0.67	0/2829
All	All	0.30	2/225749 (0.0%)	0.64	15/331069 (0.0%)

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	5	2	0
4	AA	0	1
6	AC	0	7
8	AE	0	8
29	Ba	0	1
34	Bf	0	1
37	Bi	0	4
39	Bk	0	1
45	Bq	0	6
65	R	0	1
72	Y	0	2
74	a	0	1
82	1	0	6
All	All	2	39

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Bq	60	ARG	C-N	8.47	1.50	1.34
6	AC	74	ILE	C-N	8.46	1.50	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1191	U	N1-C1'-C2'	10.70	127.90	114.00
1	5	2506	U	C5'-C4'-O4'	7.34	117.90	109.10
1	5	2506	U	C5'-C4'-C3'	7.24	127.58	116.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	2	1534	G	C2'-C3'-O3'	6.24	123.69	113.70
1	5	3257	A	C2'-C3'-O3'	5.95	123.22	113.70
1	5	2217	C	C4'-C3'-O3'	5.53	124.06	113.00
1	5	297	G	C2'-C3'-O3'	5.40	122.33	113.70
81	2	452	U	N1-C1'-C2'	5.32	120.91	114.00
45	Bq	11	ASP	CB-CG-OD2	5.21	122.99	118.30
52	E	116	ASP	C-N-CA	5.21	134.72	121.70
81	2	911	U	N1-C1'-C2'	5.17	120.73	114.00
81	2	903	G	C2'-C3'-O3'	5.17	121.97	113.70
1	5	1194	A	C2'-C3'-O3'	5.15	121.94	113.70
1	5	2529	C	N1-C1'-C2'	5.08	120.60	114.00
1	5	2041	C	C2'-C3'-O3'	5.01	121.72	113.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	5	1191	U	C1'
1	5	2506	U	C4'

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	1	442	THR	Peptide
82	1	443	PRO	Peptide
82	1	446	GLU	Peptide
82	1	799	ASP	Peptide
82	1	801	ILE	Peptide
82	1	802	TYR	Peptide
4	AA	196	TRP	Peptide
6	AC	343	LYS	Peptide
6	AC	345	ASP	Peptide
6	AC	346	GLN	Peptide
6	AC	347	ALA	Peptide
6	AC	349	LYS	Peptide
6	AC	351	LYS	Peptide
6	AC	73	ARG	Peptide
8	AE	110	SER	Peptide
8	AE	111	ARG	Peptide
8	AE	113	GLN	Peptide
8	AE	114	ARG	Peptide
8	AE	12	GLU	Peptide
8	AE	13	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	AE	14	PRO	Peptide
8	AE	15	ALA	Peptide
29	Ba	49	HIS	Peptide
34	Bf	103	TYR	Peptide
37	Bi	32	ALA	Peptide
37	Bi	33	ALA	Peptide
37	Bi	34	SER	Peptide
37	Bi	35	GLN	Peptide
39	Bk	5	ILE	Peptide
45	Bq	179	LEU	Peptide
45	Bq	180	VAL	Peptide
45	Bq	214	TYR	Peptide
45	Bq	215	ARG	Peptide
45	Bq	216	LEU	Peptide
45	Bq	59	PRO	Peptide
65	R	78	ARG	Peptide
72	Y	120	GLY	Peptide
72	Y	29	HIS	Peptide
74	a	49	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	69874	0	35111	118	0
2	7	2579	0	1304	3	0
3	8	3326	0	1680	0	0
4	AA	1892	0	1954	6	0
5	AB	3064	0	3140	13	0
6	AC	2743	0	2865	23	0
7	AD	2384	0	2337	1	0
8	AE	1321	0	1412	33	0
9	AF	1774	0	1832	4	0
10	AG	1817	0	1927	3	0
11	AH	1528	0	1596	7	0
12	AI	1690	0	1729	3	0
13	AJ	1349	0	1382	3	0
14	AL	1581	0	1661	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	AM	1045	0	1126	1	0
16	AN	1709	0	1763	1	0
17	AO	1571	0	1669	318	0
18	AP	1432	0	1465	4	0
19	AQ	1444	0	1541	2	0
20	AR	1522	0	1622	14	0
21	AS	1422	0	1466	8	0
22	AT	1262	0	1309	1	0
23	AU	807	0	821	0	0
24	AV	976	0	1021	2	0
25	AW	515	0	532	1	0
26	AX	964	0	1031	0	0
27	AY	992	0	1070	1	0
28	AZ	1089	0	1150	3	0
29	Ba	1156	0	1206	0	0
30	Bb	458	0	486	0	0
31	Bc	740	0	792	0	0
32	Bd	869	0	920	0	0
33	Be	980	0	1048	0	0
34	Bf	837	0	861	0	0
35	Bg	951	0	1036	0	0
36	Bh	961	0	1062	0	0
37	Bi	766	0	840	0	0
38	Bj	675	0	678	0	0
39	Bk	619	0	675	0	0
40	Bl	428	0	464	0	0
41	Bm	410	0	447	0	0
42	Bn	218	0	266	0	0
43	Bo	814	0	875	0	0
44	Bp	660	0	690	0	0
45	Bq	1716	0	1819	0	0
46	Br	1508	0	1542	0	0
47	AK	735	0	178	0	0
48	A	1616	0	1636	6	0
49	B	1722	0	1795	2	0
50	C	1629	0	1710	11	0
51	D	1744	0	1826	3	0
52	E	2078	0	2157	7	0
53	F	1609	0	1679	6	0
54	G	1812	0	1911	3	0
55	H	1483	0	1579	2	0
56	I	1493	0	1515	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	J	1471	0	1554	3	0
58	K	809	0	810	1	0
59	L	1168	0	1227	3	0
60	M	922	0	953	2	0
61	N	1187	0	1251	2	0
62	O	942	0	979	2	0
63	P	950	0	1001	7	0
64	Q	1105	0	1170	1	0
65	R	983	0	1033	3	0
66	S	1138	0	1161	4	0
67	T	1110	0	1124	1	0
68	U	845	0	913	4	0
69	V	687	0	682	0	0
70	W	1021	0	1056	6	0
71	X	1110	0	1192	4	0
72	Y	1061	0	1111	9	0
73	Z	558	0	585	0	0
74	a	798	0	854	0	0
75	b	617	0	643	0	0
76	c	494	0	534	0	0
77	d	446	0	436	0	0
78	e	443	0	481	0	0
79	f	337	0	333	0	0
80	g	2466	0	2406	0	0
81	2	37797	0	19016	89	0
82	1	4702	0	4822	59	0
83	3	1623	0	823	12	0
84	Bj	1	0	0	0	0
84	Bm	1	0	0	0	0
84	Bo	1	0	0	0	0
84	a	1	0	0	0	0
84	b	1	0	0	0	0
84	f	1	0	0	0	0
85	1	32	0	14	0	0
All	All	211187	0	157373	792	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (792) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AE:113:GLN:HA	8:AE:117:ALA:CB	1.12	1.54
81:2:214:A:C6	81:2:241:U:C4	1.95	1.54
1:5:2502:G:N2	1:5:2516:A:C4	1.77	1.51
8:AE:113:GLN:CA	8:AE:117:ALA:HB3	1.33	1.51
81:2:214:A:C2	81:2:241:U:O4	1.63	1.50
81:2:214:A:C6	81:2:241:U:C5	2.11	1.37
81:2:214:A:C5	81:2:241:U:C4	2.15	1.33
81:2:214:A:C5	81:2:241:U:N3	1.98	1.32
8:AE:13:VAL:HG22	8:AE:14:PRO:CD	1.63	1.28
1:5:3073:U:C4	1:5:3097:A:N7	2.00	1.27
17:AO:131:LYS:HG3	17:AO:132:PRO:CD	1.68	1.24
1:5:2187:G:C6	1:5:2197:A:N1	1.95	1.23
17:AO:185:THR:O	17:AO:186:VAL:O	1.54	1.23
17:AO:107:GLU:N	17:AO:107:GLU:OE2	1.72	1.20
81:2:214:A:C4	81:2:241:U:N3	2.09	1.20
8:AE:13:VAL:CG2	8:AE:14:PRO:HD3	1.72	1.19
17:AO:186:VAL:O	17:AO:188:THR:N	1.74	1.19
17:AO:144:THR:OG1	17:AO:151:GLU:OE2	1.61	1.18
17:AO:113:TYR:O	17:AO:115:LYS:N	1.74	1.17
17:AO:157:LEU:O	17:AO:159:GLU:N	1.74	1.17
81:2:214:A:N1	81:2:241:U:O4	1.76	1.17
81:2:214:A:N6	81:2:241:U:C5	2.11	1.17
17:AO:111:PRO:O	17:AO:113:TYR:N	1.76	1.17
1:5:2880:G:C2	1:5:3098:A:C8	2.33	1.16
1:5:2880:G:N1	1:5:3098:A:N7	1.93	1.16
17:AO:111:PRO:HB2	17:AO:112:PRO:CD	1.74	1.14
17:AO:169:TYR:O	17:AO:171:LYS:N	1.82	1.13
17:AO:28:LEU:H	17:AO:28:LEU:HD23	1.06	1.12
81:2:321:G:C6	81:2:336:G:O6	2.03	1.12
17:AO:34:ILE:HG22	17:AO:35:VAL:H	1.06	1.12
82:1:400:ALA:HB2	82:1:799:ASP:O	1.48	1.11
1:5:2187:G:C5	1:5:2197:A:N1	2.16	1.11
81:2:214:A:N7	81:2:241:U:C2	2.20	1.10
17:AO:182:LYS:O	17:AO:184:ALA:N	1.83	1.10
81:2:214:A:N1	81:2:241:U:C4	2.15	1.09
17:AO:91:HIS:CD2	17:AO:91:HIS:O	2.06	1.09
17:AO:182:LYS:C	17:AO:184:ALA:H	1.53	1.09
20:AR:53:LYS:HG2	20:AR:54:PRO:HD2	1.11	1.08
17:AO:111:PRO:HB2	17:AO:112:PRO:HD3	1.11	1.07
17:AO:12:GLY:O	17:AO:13:LYS:O	1.72	1.05
1:5:2502:G:C2	1:5:2516:A:C4	2.46	1.03
17:AO:131:LYS:HG3	17:AO:132:PRO:HD2	1.09	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:214:A:C8	81:2:241:U:C2	2.47	1.02
1:5:3073:U:O4	1:5:3097:A:C8	2.12	1.02
81:2:214:A:C2	81:2:241:U:C4	2.47	1.02
17:AO:129:ARG:O	17:AO:130:LEU:O	1.79	1.00
20:AR:53:LYS:HG2	20:AR:54:PRO:CD	1.91	1.00
8:AE:113:GLN:CA	8:AE:117:ALA:CB	2.09	0.99
1:5:2880:G:C6	1:5:3098:A:N7	2.28	0.99
17:AO:189:GLU:O	17:AO:191:SER:N	1.96	0.99
82:1:383:LYS:HD2	82:1:442:THR:HG23	1.43	0.98
81:2:214:A:C5	81:2:241:U:C2	2.52	0.98
17:AO:67:LYS:O	17:AO:69:ARG:N	1.97	0.98
1:5:2502:G:N2	1:5:2516:A:N3	2.11	0.97
17:AO:157:LEU:C	17:AO:159:GLU:H	1.60	0.97
81:2:214:A:C4	81:2:241:U:C4	2.49	0.96
17:AO:185:THR:HG23	17:AO:186:VAL:H	1.30	0.96
17:AO:178:VAL:O	17:AO:180:ALA:N	1.99	0.96
81:2:321:G:N1	81:2:336:G:C6	2.33	0.96
1:5:3073:U:O4	1:5:3097:A:N7	1.99	0.96
8:AE:113:GLN:HA	8:AE:117:ALA:HB1	1.47	0.96
83:3:51:U:N3	83:3:64:A:N1	2.13	0.95
1:5:2880:G:N1	1:5:3098:A:C8	2.33	0.95
1:5:2502:G:N2	1:5:2516:A:N9	1.99	0.95
17:AO:187:GLY:O	17:AO:189:GLU:N	1.99	0.94
1:5:564:G:O2’	8:AE:14:PRO:O	1.86	0.94
72:Y:119:PHE:HE1	81:2:86:A:C5’	1.82	0.93
17:AO:34:ILE:HG22	17:AO:35:VAL:N	1.83	0.92
1:5:2502:G:C2	1:5:2516:A:C5	2.59	0.91
17:AO:119:VAL:HG23	17:AO:120:VAL:N	1.86	0.90
17:AO:32:GLN:HG3	17:AO:33:LYS:H	1.36	0.89
82:1:400:ALA:CB	82:1:799:ASP:O	2.20	0.89
20:AR:53:LYS:CG	20:AR:54:PRO:HD2	2.02	0.89
8:AE:113:GLN:HA	8:AE:117:ALA:CA	2.04	0.88
17:AO:86:ARG:HE	17:AO:91:HIS:CE1	1.91	0.88
1:5:2187:G:C4	1:5:2197:A:N1	2.37	0.88
17:AO:38:ARG:C	17:AO:40:GLU:OE2	2.12	0.87
17:AO:28:LEU:HD23	17:AO:28:LEU:N	1.78	0.87
17:AO:32:GLN:O	17:AO:102:ARG:HD3	1.75	0.86
17:AO:34:ILE:CG2	17:AO:35:VAL:H	1.88	0.86
21:AS:159:THR:HG23	21:AS:161:LYS:O	1.76	0.85
17:AO:119:VAL:CG2	17:AO:120:VAL:N	2.40	0.85
17:AO:143:SER:O	17:AO:146:VAL:HG22	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:2502:G:H22	1:5:2516:A:C1’	1.90	0.85
17:AO:124:ALA:O	17:AO:125:LEU:HD22	1.78	0.84
17:AO:111:PRO:CB	17:AO:112:PRO:CD	2.56	0.84
17:AO:28:LEU:O	17:AO:30:ASN:N	2.09	0.83
17:AO:112:PRO:O	17:AO:113:TYR:CD2	2.31	0.83
17:AO:28:LEU:C	17:AO:30:ASN:H	1.81	0.83
17:AO:178:VAL:C	17:AO:180:ALA:H	1.81	0.83
81:2:214:A:C8	81:2:241:U:O2	2.31	0.83
17:AO:77:PRO:O	17:AO:80:ILE:N	2.11	0.82
17:AO:142:LEU:C	17:AO:142:LEU:HD12	2.00	0.82
17:AO:91:HIS:O	17:AO:91:HIS:HD2	1.62	0.82
17:AO:192:GLU:C	17:AO:194:LEU:H	1.81	0.82
82:1:799:ASP:N	82:1:799:ASP:OD1	2.11	0.82
17:AO:40:GLU:OE2	17:AO:40:GLU:N	2.12	0.81
17:AO:57:ASP:HA	17:AO:60:ARG:HG2	1.60	0.81
81:2:321:G:N1	81:2:336:G:O6	2.09	0.81
17:AO:131:LYS:CG	17:AO:132:PRO:HD2	2.03	0.81
17:AO:182:LYS:C	17:AO:184:ALA:N	2.25	0.81
17:AO:112:PRO:O	17:AO:113:TYR:CG	2.33	0.80
1:5:2187:G:C6	1:5:2197:A:C6	2.69	0.80
17:AO:171:LYS:NZ	17:AO:171:LYS:HB3	1.97	0.80
17:AO:124:ALA:C	17:AO:125:LEU:HD22	2.01	0.80
72:Y:119:PHE:HE1	81:2:86:A:H5”	1.45	0.79
1:5:2194:U:H6	1:5:2194:U:C5’	1.95	0.79
1:5:2257:G:C2	1:5:2258:U:N3	2.51	0.79
83:3:50:U:O2	83:3:65:G:N2	2.16	0.79
81:2:1114:U:H2’	81:2:1114:U:O2	1.82	0.78
6:AC:74:ILE:HD11	6:AC:94:CYS:SG	2.24	0.78
1:5:2880:G:N2	1:5:3098:A:C8	2.52	0.78
17:AO:175:TYR:O	17:AO:179:VAL:HG23	1.84	0.77
60:M:54:VAL:HG13	60:M:82:VAL:HG21	1.65	0.77
1:5:2501:U:H5”	1:5:2501:U:H6	1.49	0.77
17:AO:169:TYR:O	17:AO:172:LYS:N	2.15	0.77
17:AO:48:PHE:HA	17:AO:137:THR:OG1	1.84	0.77
82:1:801:ILE:HA	82:1:804:LEU:HD23	1.67	0.77
81:2:214:A:N6	81:2:241:U:C6	2.52	0.77
17:AO:85:VAL:C	17:AO:87:GLY:H	1.88	0.76
81:2:1358:C:H2’	81:2:1359:A:H8	1.50	0.75
17:AO:107:GLU:H	17:AO:107:GLU:CD	1.90	0.75
81:2:115:G:N2	81:2:333:G:N2	2.35	0.75
17:AO:186:VAL:C	17:AO:188:THR:H	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:Y:119:PHE:HE1	81:2:86:A:H5’	1.50	0.75
83:3:50:U:C2	83:3:65:G:N2	2.55	0.75
17:AO:140:GLY:O	17:AO:142:LEU:N	2.19	0.74
17:AO:32:GLN:HG3	17:AO:33:LYS:N	2.01	0.74
17:AO:159:GLU:O	17:AO:161:ARG:N	2.20	0.74
17:AO:32:GLN:CG	17:AO:33:LYS:H	2.00	0.74
17:AO:148:TRP:CZ3	17:AO:151:GLU:HB2	2.23	0.74
81:2:214:A:N3	81:2:241:U:O4	2.21	0.73
1:5:1162:U:O2	17:AO:49:PHE:CE1	2.41	0.73
17:AO:74:PHE:CD1	17:AO:79:ARG:HD2	2.23	0.73
81:2:644:C:O2	81:2:690:A:C2	2.41	0.73
72:Y:119:PHE:CE1	81:2:86:A:C5’	2.71	0.73
17:AO:164:ARG:O	17:AO:167:GLU:N	2.21	0.73
17:AO:119:VAL:HG23	17:AO:120:VAL:H	1.51	0.73
17:AO:86:ARG:NE	17:AO:91:HIS:CE1	2.57	0.73
17:AO:118:ARG:H	17:AO:118:ARG:HD3	1.54	0.72
17:AO:192:GLU:O	17:AO:194:LEU:N	2.21	0.72
72:Y:119:PHE:CE1	81:2:86:A:H5’	2.23	0.72
17:AO:157:LEU:C	17:AO:159:GLU:N	2.31	0.72
17:AO:103:LEU:HG	17:AO:104:LYS:N	2.05	0.72
17:AO:144:THR:HG22	17:AO:145:SER:N	2.05	0.71
1:5:2880:G:C6	1:5:3098:A:C5	2.78	0.71
17:AO:139:LEU:O	17:AO:140:GLY:C	2.29	0.71
6:AC:350:ILE:N	6:AC:350:ILE:HD12	2.05	0.71
82:1:596:GLU:HA	82:1:597:ALA:CB	2.21	0.71
17:AO:126:ARG:HB3	17:AO:126:ARG:HH11	1.55	0.70
17:AO:122:PRO:HA	17:AO:125:LEU:HD23	1.74	0.70
17:AO:131:LYS:CG	17:AO:132:PRO:CD	2.61	0.70
17:AO:49:PHE:O	17:AO:50:ARG:C	2.29	0.70
8:AE:113:GLN:C	8:AE:117:ALA:HB3	2.12	0.69
17:AO:173:LYS:O	17:AO:177:ALA:N	2.17	0.69
20:AR:92:GLN:O	20:AR:96:ILE:HD12	1.92	0.69
17:AO:35:VAL:HG21	17:AO:113:TYR:CZ	2.27	0.69
17:AO:82:TYR:HD1	17:AO:82:TYR:O	1.75	0.69
1:5:2502:G:N1	1:5:2516:A:C5	2.59	0.69
20:AR:89:LEU:HD12	20:AR:89:LEU:C	2.13	0.69
54:G:5:ILE:HD12	54:G:16:ILE:HD13	1.73	0.69
17:AO:140:GLY:O	17:AO:141:LYS:C	2.29	0.69
17:AO:192:GLU:C	17:AO:194:LEU:N	2.44	0.69
17:AO:33:LYS:O	17:AO:34:ILE:HG12	1.92	0.69
17:AO:178:VAL:C	17:AO:180:ALA:N	2.41	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AO:187:GLY:C	17:AO:189:GLU:H	1.96	0.69
17:AO:80:ILE:HG22	17:AO:81:PHE:N	2.07	0.69
52:E:67:GLN:HA	52:E:68:ARG:HB2	1.73	0.69
1:5:3073:U:N3	1:5:3097:A:C5	2.61	0.68
17:AO:176:ASN:C	17:AO:178:VAL:H	1.95	0.68
72:Y:35:VAL:HG21	72:Y:40:LEU:HD11	1.75	0.68
17:AO:126:ARG:HD2	17:AO:136:TYR:CG	2.27	0.68
8:AE:13:VAL:HG22	8:AE:14:PRO:HD3	0.79	0.68
8:AE:13:VAL:CG2	8:AE:14:PRO:CD	2.51	0.68
1:5:591:C:OP2	8:AE:111:ARG:NH1	2.25	0.68
17:AO:85:VAL:O	17:AO:87:GLY:N	2.27	0.68
17:AO:86:ARG:O	17:AO:86:ARG:HG2	1.94	0.68
17:AO:103:LEU:O	17:AO:104:LYS:HG3	1.92	0.68
17:AO:129:ARG:O	17:AO:130:LEU:C	2.31	0.68
6:AC:156:LEU:HD12	6:AC:159:ILE:HD12	1.76	0.68
17:AO:161:ARG:O	17:AO:162:LYS:C	2.32	0.68
1:5:3073:U:N3	1:5:3097:A:N7	2.42	0.67
17:AO:178:VAL:O	17:AO:181:ASN:N	2.28	0.67
81:2:321:G:C2	81:2:336:G:C6	2.82	0.67
17:AO:79:ARG:O	17:AO:82:TYR:HB3	1.93	0.67
17:AO:24:VAL:O	17:AO:28:LEU:HD21	1.94	0.67
17:AO:81:PHE:O	17:AO:81:PHE:CD1	2.48	0.67
17:AO:185:THR:O	17:AO:186:VAL:C	2.32	0.67
1:5:2257:G:N2	1:5:2258:U:O2	2.27	0.67
17:AO:148:TRP:HZ3	17:AO:151:GLU:CB	2.08	0.67
17:AO:35:VAL:HG22	17:AO:35:VAL:O	1.94	0.67
82:1:445:HIS:NE2	82:1:802:TYR:OH	2.27	0.66
17:AO:138:THR:O	17:AO:139:LEU:O	2.13	0.66
83:3:52:G:N1	83:3:63:G:N2	2.42	0.66
6:AC:342:LYS:O	6:AC:344:VAL:N	2.29	0.66
8:AE:113:GLN:HE21	8:AE:114:ARG:HB2	1.61	0.66
1:5:3073:U:C2	1:5:3097:A:N6	2.64	0.66
6:AC:349:LYS:HB3	6:AC:351:LYS:HB2	1.78	0.66
17:AO:93:THR:O	17:AO:94:ALA:C	2.32	0.66
17:AO:169:TYR:O	17:AO:170:LEU:C	2.34	0.66
81:2:1359:A:N3	81:2:1359:A:H2’	2.10	0.66
82:1:774:LEU:HG	82:1:804:LEU:HD12	1.77	0.66
17:AO:82:TYR:O	17:AO:82:TYR:CD1	2.48	0.65
17:AO:106:PHE:N	17:AO:106:PHE:CD1	2.65	0.65
17:AO:126:ARG:O	17:AO:127:VAL:HB	1.95	0.65
17:AO:113:TYR:O	17:AO:114:ASP:C	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AO:185:THR:HG23	17:AO:186:VAL:N	2.09	0.65
17:AO:159:GLU:C	17:AO:161:ARG:N	2.47	0.65
48:A:57:ILE:HD11	48:A:173:ILE:HD11	1.79	0.65
17:AO:47:GLU:O	17:AO:48:PHE:C	2.34	0.64
17:AO:91:HIS:O	17:AO:91:HIS:CG	2.46	0.64
8:AE:114:ARG:HG3	8:AE:115:ALA:HA	1.79	0.64
17:AO:93:THR:O	17:AO:96:GLY:N	2.31	0.64
1:5:1160:C:N3	1:5:1286:U:O2	2.31	0.64
17:AO:118:ARG:HD3	17:AO:118:ARG:N	2.11	0.64
1:5:2257:G:C2	1:5:2258:U:C2	2.86	0.64
17:AO:93:THR:O	17:AO:95:ARG:N	2.31	0.64
82:1:599:ILE:HD13	82:1:614:VAL:HG12	1.80	0.64
1:5:1319:U:H4’	1:5:1320:A:H5’	1.80	0.63
17:AO:67:LYS:O	17:AO:70:GLY:N	2.32	0.63
17:AO:83:LYS:C	17:AO:85:VAL:H	2.01	0.63
21:AS:6:GLU:O	21:AS:6:GLU:HG3	1.98	0.63
17:AO:126:ARG:HB3	17:AO:126:ARG:NH1	2.13	0.63
17:AO:148:TRP:HZ3	17:AO:151:GLU:HB2	1.62	0.63
17:AO:164:ARG:O	17:AO:166:ALA:N	2.32	0.63
63:P:122:THR:HG21	81:2:1452:G:H4’	1.79	0.63
17:AO:197:LEU:O	17:AO:199:TYR:N	2.32	0.63
1:5:2880:G:N2	1:5:3098:A:H8	1.94	0.63
17:AO:26:LYS:HD3	17:AO:26:LYS:C	2.18	0.63
2:7:97:A:H4’	9:AF:221:ILE:HD11	1.80	0.63
17:AO:159:GLU:C	17:AO:161:ARG:H	2.01	0.62
17:AO:15:HIS:CE1	17:AO:125:LEU:HD11	2.34	0.62
17:AO:103:LEU:HG	17:AO:104:LYS:H	1.62	0.62
17:AO:27:GLN:O	17:AO:30:ASN:N	2.32	0.62
1:5:2194:U:H6	1:5:2194:U:H5”	1.65	0.62
17:AO:142:LEU:O	17:AO:143:SER:C	2.38	0.62
13:AJ:30:LEU:HD21	13:AJ:67:VAL:HG13	1.80	0.62
17:AO:53:LEU:C	17:AO:55:TYR:H	2.01	0.62
8:AE:13:VAL:HG13	8:AE:14:PRO:HD2	1.80	0.62
17:AO:13:LYS:C	17:AO:15:HIS:H	2.03	0.62
17:AO:55:TYR:O	17:AO:57:ASP:N	2.33	0.62
81:2:321:G:O6	81:2:336:G:O6	2.18	0.62
1:5:2502:G:O6	1:5:2515:C:N3	2.32	0.61
17:AO:197:LEU:C	17:AO:199:TYR:N	2.52	0.61
1:5:2502:G:N2	1:5:2516:A:C1’	2.57	0.61
17:AO:81:PHE:O	17:AO:81:PHE:CG	2.53	0.61
17:AO:47:GLU:O	17:AO:49:PHE:N	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AO:85:VAL:C	17:AO:87:GLY:N	2.54	0.61
50:C:174:LEU:HA	50:C:175:ILE:HB	1.82	0.61
17:AO:5:GLU:CA	17:AO:5:GLU:OE1	2.48	0.61
1:5:518:C:H2'	1:5:518:C:O2	2.00	0.61
17:AO:80:ILE:C	17:AO:82:TYR:H	2.03	0.61
17:AO:20:LEU:HD23	17:AO:81:PHE:CE2	2.35	0.61
17:AO:97:LYS:O	17:AO:99:ALA:N	2.34	0.61
17:AO:144:THR:O	17:AO:146:VAL:N	2.34	0.61
17:AO:77:PRO:O	17:AO:78:SER:C	2.38	0.61
1:5:1321:A:O5'	1:5:1321:A:H8	1.84	0.60
6:AC:350:ILE:HD12	6:AC:350:ILE:H	1.65	0.60
17:AO:97:LYS:HB3	17:AO:101:GLU:OE1	2.01	0.60
17:AO:28:LEU:N	17:AO:28:LEU:CD2	2.52	0.60
17:AO:50:ARG:O	17:AO:51:ASN:C	2.40	0.60
17:AO:74:PHE:CD1	17:AO:79:ARG:CD	2.84	0.60
1:5:2257:G:N1	1:5:2258:U:N3	2.50	0.60
82:1:596:GLU:HA	82:1:597:ALA:HB3	1.82	0.60
17:AO:176:ASN:C	17:AO:178:VAL:N	2.55	0.60
1:5:2257:G:C6	1:5:2258:U:O4	2.55	0.59
17:AO:26:LYS:HD3	17:AO:26:LYS:O	2.02	0.59
17:AO:143:SER:O	17:AO:144:THR:C	2.40	0.59
81:2:1114:U:O2	81:2:1115:A:C8	2.54	0.59
17:AO:32:GLN:NE2	17:AO:32:GLN:HA	2.17	0.59
20:AR:57:ILE:HG22	20:AR:57:ILE:O	2.02	0.59
8:AE:109:LEU:O	8:AE:111:ARG:HA	2.02	0.59
17:AO:138:THR:O	17:AO:139:LEU:C	2.39	0.59
17:AO:148:TRP:CZ3	17:AO:151:GLU:CB	2.83	0.59
81:2:115:G:H21	81:2:333:G:N2	2.00	0.59
1:5:927:U:H6	1:5:927:U:O5'	1.86	0.59
17:AO:29:LEU:HD12	17:AO:95:ARG:CZ	2.32	0.59
17:AO:162:LYS:O	17:AO:163:ALA:C	2.41	0.59
1:5:1162:U:O2	17:AO:49:PHE:CZ	2.55	0.59
1:5:2217:C:H4'	1:5:2218:G:OP2	2.03	0.59
17:AO:162:LYS:O	17:AO:164:ARG:N	2.36	0.59
8:AE:114:ARG:N	8:AE:117:ALA:N	2.51	0.58
17:AO:16:LEU:HD12	17:AO:19:ARG:HD2	1.85	0.58
17:AO:139:LEU:O	17:AO:142:LEU:N	2.33	0.58
11:AH:41:ILE:HD11	11:AH:67:ALA:HB1	1.84	0.58
50:C:82:LYS:HA	50:C:83:ASP:HB2	1.86	0.58
17:AO:171:LYS:HB3	17:AO:171:LYS:HZ2	1.69	0.58
81:2:645:U:H1'	81:2:689:G:N2	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1600:C:H2’	1:5:1600:C:O2	2.03	0.58
6:AC:343:LYS:HB3	6:AC:344:VAL:HA	1.85	0.58
17:AO:67:LYS:O	17:AO:68:THR:C	2.42	0.58
52:E:116:ASP:HB2	52:E:117:GLU:HB2	1.86	0.58
82:1:417:ILE:HG21	82:1:578:LEU:HD11	1.85	0.58
82:1:446:GLU:HG2	82:1:447:SER:HA	1.85	0.58
1:5:2529:C:H2’	1:5:2529:C:O2	2.04	0.58
17:AO:126:ARG:CD	17:AO:136:TYR:CD2	2.87	0.58
17:AO:86:ARG:O	17:AO:86:ARG:CG	2.52	0.57
6:AC:3:ILE:HG22	6:AC:3:ILE:O	2.03	0.57
17:AO:53:LEU:C	17:AO:55:TYR:N	2.58	0.57
17:AO:38:ARG:CA	17:AO:40:GLU:OE2	2.52	0.57
17:AO:106:PHE:CD2	17:AO:110:PRO:HG3	2.39	0.57
17:AO:112:PRO:C	17:AO:113:TYR:CD2	2.77	0.57
17:AO:181:ASN:O	17:AO:184:ALA:CB	2.52	0.57
1:5:2503:G:H3’	1:5:2503:G:H8	1.69	0.57
17:AO:85:VAL:O	17:AO:88:MET:N	2.33	0.57
14:AL:47:ALA:HB3	14:AL:48:PRO:HD3	1.85	0.57
1:5:2422:U:H4’	1:5:2423:G:OP1	2.05	0.57
1:5:3073:U:C2	1:5:3097:A:C6	2.93	0.57
82:1:804:LEU:HG	82:1:804:LEU:O	2.05	0.56
17:AO:154:VAL:CG1	17:AO:154:VAL:O	2.53	0.56
17:AO:77:PRO:O	17:AO:79:ARG:N	2.38	0.56
17:AO:113:TYR:O	17:AO:116:LYS:N	2.39	0.56
17:AO:141:LYS:HA	17:AO:151:GLU:OE1	2.05	0.56
82:1:442:THR:HG22	82:1:444:GLY:H	1.70	0.56
81:2:240:U:H2’	81:2:240:U:O2	2.04	0.56
82:1:801:ILE:HD13	82:1:801:ILE:O	2.06	0.56
81:2:214:A:C6	81:2:241:U:C6	2.84	0.56
81:2:1114:U:O2	81:2:1114:U:C2’	2.54	0.56
1:5:2502:G:H3’	1:5:2503:G:H5”	1.88	0.56
17:AO:29:LEU:HD12	17:AO:95:ARG:NH2	2.21	0.55
17:AO:39:ALA:C	17:AO:41:ALA:H	2.08	0.55
6:AC:351:LYS:HD2	6:AC:351:LYS:O	2.07	0.55
17:AO:171:LYS:HB3	17:AO:171:LYS:HZ3	1.69	0.55
17:AO:187:GLY:C	17:AO:189:GLU:N	2.53	0.55
82:1:802:TYR:N	82:1:802:TYR:CD2	2.73	0.55
72:Y:118:ILE:HD13	72:Y:118:ILE:O	2.06	0.55
81:2:1454:C:O2	81:2:1454:C:O4’	2.24	0.55
17:AO:197:LEU:C	17:AO:199:TYR:H	2.09	0.55
28:AZ:24:VAL:HG11	28:AZ:87:LEU:HD23	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C:106:VAL:HG22	50:C:120:ILE:HD12	1.89	0.55
82:1:960:LEU:HD23	82:1:963:VAL:HG11	1.89	0.55
83:3:51:U:N3	83:3:64:A:C2	2.68	0.55
17:AO:32:GLN:HA	17:AO:32:GLN:HE21	1.72	0.55
2:7:73:C:O2	2:7:73:C:O4'	2.25	0.54
17:AO:122:PRO:CA	17:AO:125:LEU:HD23	2.37	0.54
17:AO:125:LEU:O	17:AO:127:VAL:N	2.40	0.54
17:AO:9:VAL:HG22	17:AO:35:VAL:HG11	1.90	0.54
17:AO:83:LYS:O	17:AO:85:VAL:N	2.41	0.54
21:AS:159:THR:CG2	21:AS:161:LYS:O	2.53	0.54
81:2:25:C:O2	81:2:25:C:O4'	2.24	0.54
1:5:1407:U:C4	6:AC:71:VAL:O	2.61	0.54
1:5:2503:G:H3'	1:5:2503:G:C8	2.42	0.54
6:AC:348:ASN:OD1	6:AC:348:ASN:N	2.41	0.54
17:AO:48:PHE:CD1	17:AO:49:PHE:N	2.76	0.54
1:5:2500:C:H3'	1:5:2501:U:H5"	1.90	0.54
17:AO:27:GLN:O	17:AO:28:LEU:C	2.46	0.54
13:AJ:102:PHE:CE2	13:AJ:129:ILE:HD13	2.42	0.54
17:AO:185:THR:C	17:AO:186:VAL:O	2.37	0.54
1:5:2502:G:N1	1:5:2516:A:N7	2.56	0.53
17:AO:33:LYS:O	17:AO:34:ILE:CG1	2.55	0.53
1:5:2196:C:H3'	1:5:2196:C:H6	1.73	0.53
17:AO:119:VAL:HG23	17:AO:120:VAL:O	2.08	0.53
17:AO:120:VAL:HG23	17:AO:122:PRO:HD3	1.89	0.53
82:1:954:TRP:HA	82:1:955:MET:HB2	1.90	0.53
17:AO:96:GLY:O	17:AO:99:ALA:HB3	2.09	0.53
17:AO:35:VAL:HA	17:AO:104:LYS:O	2.09	0.53
17:AO:38:ARG:HA	17:AO:40:GLU:OE2	2.08	0.53
70:W:2:THR:N	81:2:1033:C:HO2'	2.06	0.53
81:2:214:A:C8	81:2:241:U:N3	2.70	0.53
82:1:446:GLU:CB	82:1:475:GLN:NE2	2.72	0.53
17:AO:148:TRP:CZ3	17:AO:151:GLU:CA	2.92	0.53
81:2:158:U:H2'	81:2:158:U:O2	2.07	0.53
17:AO:131:LYS:HG3	17:AO:132:PRO:N	2.19	0.53
27:AY:45:ILE:HD11	27:AY:119:ILE:HG23	1.91	0.53
17:AO:28:LEU:C	17:AO:30:ASN:N	2.49	0.53
8:AE:114:ARG:NH1	8:AE:114:ARG:HG2	2.23	0.53
17:AO:103:LEU:CG	17:AO:104:LYS:H	2.22	0.53
17:AO:66:ASN:O	17:AO:67:LYS:C	2.48	0.53
82:1:463:ILE:HD11	82:1:577:LEU:HD21	1.91	0.53
1:5:885:A:C8	4:AA:199:THR:HG21	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AO:13:LYS:O	17:AO:15:HIS:N	2.42	0.52
17:AO:48:PHE:HD1	17:AO:49:PHE:N	2.07	0.52
56:I:10:LYS:HE2	81:2:338:C:OP1	2.09	0.52
81:2:214:A:N9	81:2:241:U:N3	2.56	0.52
8:AE:113:GLN:HE21	8:AE:114:ARG:HD3	1.73	0.52
81:2:1015:C:O4'	81:2:1015:C:O2	2.26	0.52
17:AO:29:LEU:O	17:AO:30:ASN:OD1	2.26	0.52
81:2:646:G:C5	81:2:688:G:C2	2.98	0.52
17:AO:154:VAL:O	17:AO:154:VAL:HG12	2.09	0.52
83:3:52:G:H1	83:3:63:G:N2	2.07	0.52
17:AO:7:VAL:CG1	17:AO:8:VAL:N	2.72	0.52
17:AO:57:ASP:OD1	17:AO:61:LYS:NZ	2.43	0.52
17:AO:82:TYR:CD1	17:AO:82:TYR:C	2.83	0.52
11:AH:28:THR:HG22	11:AH:33:VAL:HG12	1.92	0.52
17:AO:181:ASN:O	17:AO:184:ALA:HB2	2.10	0.52
67:T:2:PRO:HB2	81:2:1359:A:O2'	2.09	0.52
21:AS:6:GLU:HG3	21:AS:64:ILE:HB	1.92	0.52
1:5:1407:U:C5	6:AC:71:VAL:O	2.63	0.52
1:5:2510:U:O2	1:5:2510:U:C2'	2.58	0.52
17:AO:9:VAL:HG22	17:AO:35:VAL:CG1	2.40	0.52
17:AO:103:LEU:CG	17:AO:104:LYS:N	2.72	0.52
17:AO:167:GLU:O	17:AO:168:TYR:C	2.47	0.52
1:5:2413:C:O2	1:5:2413:C:C2'	2.57	0.51
17:AO:50:ARG:O	17:AO:53:LEU:N	2.26	0.51
1:5:1840:U:O2'	20:AR:58:HIS:HD2	1.93	0.51
17:AO:111:PRO:O	17:AO:114:ASP:OD1	2.28	0.51
8:AE:113:GLN:HA	8:AE:117:ALA:HB3	0.52	0.51
48:A:24:LEU:HD21	65:R:106:THR:HG21	1.92	0.51
51:D:176:LEU:HB2	51:D:177:LEU:HA	1.92	0.51
81:2:214:A:C5	81:2:241:U:C5	2.75	0.51
17:AO:38:ARG:O	17:AO:40:GLU:OE2	2.27	0.51
17:AO:141:LYS:O	17:AO:144:THR:HB	2.10	0.51
81:2:1765:G:O2'	81:2:1766:G:OP2	2.27	0.51
82:1:446:GLU:HB2	82:1:475:GLN:NE2	2.26	0.51
82:1:461:ILE:HD12	82:1:580:LEU:HD11	1.93	0.51
82:1:864:ALA:HB2	82:1:928:LEU:HD22	1.93	0.51
1:5:117:U:O2	1:5:117:U:C2'	2.58	0.51
17:AO:18:GLY:O	17:AO:22:SER:HB2	2.10	0.51
17:AO:80:ILE:C	17:AO:82:TYR:N	2.63	0.51
70:W:82:LYS:O	70:W:84:ALA:N	2.43	0.51
17:AO:51:ASN:O	17:AO:53:LEU:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:338:C:H2’	81:2:338:C:O2	2.11	0.51
83:3:51:U:O2	83:3:64:A:H2	1.94	0.51
1:5:135:C:C2’	1:5:135:C:O2	2.59	0.51
1:5:2180:U:O2	1:5:2180:U:O4’	2.29	0.51
6:AC:35:VAL:HG21	6:AC:244:LEU:HD21	1.93	0.51
6:AC:350:ILE:H	6:AC:350:ILE:CD1	2.22	0.51
68:U:34:LEU:HD11	68:U:89:ARG:HG3	1.93	0.51
17:AO:142:LEU:HG	17:AO:143:SER:N	2.25	0.51
21:AS:8:GLN:HB2	21:AS:64:ILE:HD11	1.91	0.51
82:1:774:LEU:HB3	82:1:804:LEU:CD1	2.41	0.51
82:1:776:PHE:HE2	82:1:801:ILE:HB	1.75	0.51
1:5:518:C:O2	1:5:518:C:C2’	2.58	0.50
1:5:776:G:H5’	6:AC:74:ILE:N	2.25	0.50
57:J:7:THR:HG21	81:2:758:U:H5”	1.92	0.50
71:X:41:SER:O	71:X:43:PHE:N	2.44	0.50
1:5:3245:U:O2	1:5:3245:U:O4’	2.30	0.50
17:AO:197:LEU:O	17:AO:199:TYR:O	2.28	0.50
20:AR:53:LYS:CG	20:AR:54:PRO:CD	2.76	0.50
70:W:11:LEU:HD12	70:W:74:VAL:CG2	2.41	0.50
71:X:59:ILE:HD12	71:X:71:CYS:SG	2.52	0.50
81:2:214:A:N3	81:2:241:U:C4	2.74	0.50
81:2:1714:C:H4’	81:2:1715:G:OP1	2.11	0.50
1:5:2529:C:O2	1:5:2529:C:C2’	2.59	0.50
1:5:3073:U:C4	1:5:3097:A:C5	2.89	0.50
8:AE:114:ARG:CG	8:AE:114:ARG:HH11	2.24	0.50
17:AO:139:LEU:O	17:AO:142:LEU:HB3	2.11	0.50
68:U:23:ARG:HB2	68:U:117:ILE:HD12	1.94	0.50
82:1:774:LEU:CG	82:1:804:LEU:HD12	2.41	0.50
17:AO:32:GLN:HE21	17:AO:32:GLN:CA	2.24	0.50
6:AC:350:ILE:N	6:AC:350:ILE:CD1	2.73	0.50
17:AO:5:GLU:OE1	17:AO:5:GLU:HA	2.10	0.50
17:AO:24:VAL:O	17:AO:28:LEU:CD2	2.59	0.50
17:AO:168:TYR:O	17:AO:169:TYR:O	2.29	0.50
70:W:40:VAL:HG11	70:W:103:ILE:HD12	1.93	0.50
17:AO:57:ASP:CA	17:AO:60:ARG:HG2	2.38	0.50
83:3:50:U:O2	83:3:65:G:C2	2.64	0.50
1:5:887:G:C6	4:AA:207:VAL:HG21	2.47	0.50
17:AO:57:ASP:O	17:AO:61:LYS:HG3	2.11	0.50
57:J:7:THR:HG21	81:2:758:U:C5’	2.41	0.50
28:AZ:46:ILE:HD11	28:AZ:49:TYR:CE1	2.47	0.50
1:5:987:C:O2	1:5:987:C:C2’	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
17:AO:164:ARG:C	17:AO:166:ALA:N	2.65	0.49
1:5:2384:C:H5'	4:AA:207:VAL:HG22	1.94	0.49
48:A:33:GLN:N	48:A:34:GLU:HB2	2.27	0.49
81:2:829:U:O2	81:2:829:U:C2'	2.59	0.49
82:1:443:PRO:O	82:1:451:LEU:CD1	2.60	0.49
17:AO:25:ALA:O	17:AO:26:LYS:C	2.51	0.49
17:AO:83:LYS:C	17:AO:85:VAL:N	2.64	0.49
17:AO:119:VAL:CG2	17:AO:120:VAL:O	2.60	0.49
17:AO:36:VAL:HG21	17:AO:81:PHE:CE1	2.47	0.49
17:AO:140:GLY:O	17:AO:143:SER:N	2.46	0.49
55:H:122:HIS:CE1	55:H:177:THR:HG22	2.47	0.49
5:AB:229:VAL:HG11	5:AB:249:VAL:HG23	1.93	0.49
53:F:135:VAL:HG22	53:F:200:LEU:HD13	1.94	0.49
82:1:454:ARG:N	82:1:455:GLY:HA2	2.27	0.49
17:AO:23:THR:O	17:AO:25:ALA:N	2.45	0.49
17:AO:36:VAL:HG12	17:AO:37:VAL:N	2.28	0.49
21:AS:4:ARG:HA	21:AS:4:ARG:HD3	1.58	0.49
62:O:81:ILE:HB	62:O:115:ILE:HG22	1.95	0.49
1:5:2804:C:O2	1:5:2804:C:O4'	2.30	0.49
6:AC:351:LYS:HE3	9:AF:64:ARG:HB3	1.94	0.49
17:AO:97:LYS:O	17:AO:100:LEU:N	2.46	0.49
20:AR:92:GLN:O	20:AR:92:GLN:HG3	2.13	0.49
82:1:445:HIS:CE1	82:1:802:TYR:HH	2.31	0.49
8:AE:114:ARG:HA	8:AE:117:ALA:N	2.28	0.48
17:AO:51:ASN:O	17:AO:54:LYS:N	2.45	0.48
82:1:445:HIS:C	82:1:445:HIS:CD2	2.85	0.48
8:AE:13:VAL:HG13	8:AE:14:PRO:CD	2.42	0.48
17:AO:176:ASN:O	17:AO:178:VAL:N	2.46	0.48
82:1:443:PRO:O	82:1:451:LEU:HD12	2.14	0.48
83:3:52:G:H5"	83:3:52:G:H8	1.77	0.48
51:D:176:LEU:CB	51:D:177:LEU:HA	2.43	0.48
81:2:1456:G:H2'	81:2:1456:G:N3	2.27	0.48
1:5:2194:U:C5'	1:5:2194:U:C6	2.86	0.48
17:AO:6:PRO:O	17:AO:7:VAL:HG23	2.13	0.48
72:Y:119:PHE:CE1	81:2:86:A:H5"	2.35	0.48
59:L:130:PRO:O	81:2:335:G:H5'	2.14	0.48
17:AO:25:ALA:O	17:AO:28:LEU:HG	2.12	0.48
50:C:174:LEU:HA	50:C:175:ILE:CB	2.44	0.48
17:AO:142:LEU:CG	17:AO:143:SER:N	2.77	0.48
17:AO:76:ALA:HA	17:AO:148:TRP:CD1	2.49	0.48
18:AP:158:GLU:HA	18:AP:159:LYS:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:C:58:ILE:O	50:C:60:GLU:N	2.46	0.48
81:2:1558:U:O2	81:2:1558:U:O4'	2.30	0.48
12:AI:53:VAL:HG21	12:AI:166:ILE:HD12	1.96	0.48
17:AO:23:THR:O	17:AO:24:VAL:C	2.52	0.48
17:AO:66:ASN:O	17:AO:67:LYS:O	2.31	0.48
53:F:114:ARG:HD2	64:Q:43:ILE:HD12	1.96	0.48
82:1:823:PHE:CG	82:1:823:PHE:O	2.67	0.48
6:AC:292:SER:O	6:AC:293:THR:HG23	2.13	0.48
17:AO:106:PHE:N	17:AO:106:PHE:HD1	2.11	0.48
82:1:945:PHE:HA	82:1:946:ARG:C	2.35	0.48
1:5:2257:G:N2	1:5:2258:U:C2	2.83	0.47
1:5:3073:U:N1	1:5:3097:A:N6	2.62	0.47
8:AE:113:GLN:HG2	8:AE:114:ARG:HB2	1.96	0.47
17:AO:39:ALA:O	17:AO:41:ALA:N	2.43	0.47
81:2:452:U:O2	81:2:452:U:H2'	2.12	0.47
17:AO:97:LYS:C	17:AO:99:ALA:N	2.65	0.47
59:L:3:THR:HB	59:L:4:GLU:HA	1.96	0.47
70:W:11:LEU:HD12	70:W:74:VAL:HG22	1.96	0.47
1:5:2503:G:C8	1:5:2503:G:C3'	2.98	0.47
81:2:1292:U:O2	81:2:1292:U:O4'	2.31	0.47
17:AO:11:ASP:O	17:AO:12:GLY:O	2.31	0.47
17:AO:49:PHE:O	17:AO:50:ARG:O	2.32	0.47
50:C:177:ALA:HB1	50:C:178:PRO:HD2	1.97	0.47
1:5:2413:C:O2	1:5:2413:C:O2'	2.31	0.47
82:1:839:ILE:HD12	82:1:846:ILE:HG22	1.96	0.47
1:5:2194:U:H5"	1:5:2194:U:C6	2.48	0.47
17:AO:62:ALA:HA	17:AO:71:PRO:HD2	1.96	0.47
17:AO:65:PHE:O	17:AO:66:ASN:HB2	2.14	0.47
17:AO:82:TYR:HD1	17:AO:82:TYR:C	2.17	0.47
50:C:58:ILE:HG23	50:C:61:ILE:HD12	1.96	0.47
82:1:727:LEU:HD12	82:1:730:LEU:HD23	1.96	0.47
82:1:803:HIS:O	82:1:806:ASP:N	2.48	0.47
1:5:3036:U:OP1	20:AR:58:HIS:HA	2.15	0.47
17:AO:112:PRO:C	17:AO:113:TYR:CG	2.88	0.47
82:1:468:ILE:HA	82:1:533:ILE:HD11	1.96	0.47
17:AO:53:LEU:O	17:AO:55:TYR:N	2.48	0.47
81:2:911:U:H2'	81:2:911:U:O2	2.15	0.47
11:AH:18:VAL:HG21	11:AH:53:ILE:HD11	1.97	0.47
17:AO:80:ILE:O	17:AO:82:TYR:N	2.48	0.47
82:1:940:LEU:HD13	82:1:941:LYS:N	2.30	0.46
1:5:1841:C:H5'	20:AR:58:HIS:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:U:44:ASN:HD21	68:U:106:ILE:HD11	1.81	0.46
82:1:400:ALA:HB1	82:1:800:ILE:HG12	1.97	0.46
82:1:443:PRO:O	82:1:451:LEU:HG	2.16	0.46
57:J:133:HIS:HB2	57:J:134:ILE:HD12	1.96	0.46
82:1:730:LEU:HD21	82:1:747:VAL:CG1	2.45	0.46
1:5:2506:U:OP2	49:B:227:SER:N	2.49	0.46
1:5:2915:G:N3	5:AB:250:ALA:HB1	2.31	0.46
8:AE:114:ARG:HB2	8:AE:117:ALA:O	2.15	0.46
8:AE:114:ARG:HG2	8:AE:114:ARG:HH11	1.80	0.46
17:AO:12:GLY:C	17:AO:13:LYS:O	2.48	0.46
17:AO:32:GLN:NE2	17:AO:32:GLN:CA	2.78	0.46
17:AO:35:VAL:HG21	17:AO:113:TYR:CE1	2.50	0.46
17:AO:162:LYS:O	17:AO:165:SER:N	2.49	0.46
81:2:829:U:O2	81:2:829:U:H2'	2.15	0.46
81:2:506:U:O2	81:2:506:U:O4'	2.33	0.46
81:2:1716:A:H2'	81:2:1717:A:C8	2.49	0.46
1:5:1161:A:H3'	1:5:1161:A:N3	2.30	0.46
1:5:1207:G:N2	1:5:1215:A:OP1	2.49	0.46
1:5:2510:U:O2	1:5:2510:U:H2'	2.15	0.46
1:5:3125:U:H3'	1:5:3126:G:C5'	2.46	0.46
5:AB:217:VAL:HG11	5:AB:328:ILE:HG23	1.98	0.46
8:AE:13:VAL:CB	8:AE:14:PRO:CD	2.94	0.46
13:AJ:54:VAL:HG11	13:AJ:57:PHE:CD2	2.50	0.46
17:AO:40:GLU:O	17:AO:40:GLU:HG2	2.14	0.46
52:E:128:LYS:HA	52:E:129:VAL:HB	1.98	0.46
81:2:214:A:N1	81:2:241:U:C5	2.65	0.46
82:1:484:ARG:HA	82:1:485:ASP:C	2.36	0.46
1:5:1194:A:O2'	1:5:1195:C:OP2	2.28	0.46
50:C:82:LYS:HA	50:C:83:ASP:CB	2.45	0.46
70:W:6:VAL:HG13	70:W:29:PRO:HB2	1.98	0.46
14:AL:3:ILE:HG23	14:AL:4:SER:OG	2.15	0.46
17:AO:181:ASN:O	17:AO:184:ALA:HB3	2.15	0.46
56:I:26:LYS:O	56:I:29:LEU:HD12	2.15	0.46
17:AO:29:LEU:N	17:AO:29:LEU:HD22	2.31	0.46
17:AO:149:LYS:O	17:AO:150:TYR:CG	2.69	0.46
82:1:492:VAL:CG1	82:1:559:ILE:HD13	2.45	0.46
1:5:3073:U:C4	1:5:3097:A:C8	2.76	0.45
15:AM:55:ARG:NH2	15:AM:76:ALA:O	2.50	0.45
17:AO:149:LYS:C	17:AO:150:TYR:CG	2.90	0.45
17:AO:164:ARG:O	17:AO:165:SER:C	2.53	0.45
1:5:1452:A:H2'	1:5:1452:A:N3	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AO:48:PHE:O	17:AO:49:PHE:C	2.54	0.45
81:2:333:G:H2’	81:2:334:U:H6	1.81	0.45
1:5:1321:A:C5	1:5:1322:U:H1’	2.51	0.45
11:AH:164:ILE:HG22	11:AH:164:ILE:O	2.15	0.45
17:AO:36:VAL:HB	17:AO:105:VAL:HG13	1.98	0.45
17:AO:126:ARG:CD	17:AO:136:TYR:CG	2.99	0.45
17:AO:148:TRP:CZ3	17:AO:151:GLU:HA	2.51	0.45
53:F:203:ALA:HA	53:F:213:ILE:HD11	1.97	0.45
81:2:333:G:H2’	81:2:334:U:C6	2.51	0.45
1:5:2502:G:H2’	1:5:2503:G:C5	2.51	0.45
5:AB:87:VAL:HG21	5:AB:110:LEU:HD23	1.99	0.45
5:AB:218:VAL:HG13	5:AB:276:THR:HG22	1.99	0.45
53:F:220:GLU:HB3	53:F:221:ARG:HB2	1.97	0.45
83:3:60:U:H2’	83:3:60:U:O2	2.17	0.45
4:AA:137:ILE:HD11	4:AA:149:ARG:HB2	1.97	0.45
17:AO:107:GLU:HG2	17:AO:107:GLU:O	2.17	0.45
17:AO:159:GLU:O	17:AO:160:LYS:C	2.52	0.45
83:3:50:U:C2	83:3:65:G:C2	3.04	0.45
1:5:995:G:N2	1:5:997:A:OP2	2.49	0.45
1:5:2194:U:C6	1:5:2194:U:C4’	2.99	0.45
2:7:78:U:H2’	2:7:79:A:H5’	1.98	0.45
17:AO:136:TYR:CD1	17:AO:136:TYR:N	2.84	0.45
17:AO:179:VAL:HG12	17:AO:179:VAL:O	2.16	0.45
81:2:452:U:O2	81:2:452:U:C2’	2.64	0.45
82:1:390:ILE:HG22	82:1:570:VAL:HG13	1.99	0.45
1:5:2414:A:H2’	1:5:2414:A:N3	2.32	0.45
17:AO:9:VAL:HA	17:AO:35:VAL:HG13	1.98	0.45
59:L:123:VAL:HG13	59:L:139:VAL:HG13	1.98	0.45
1:5:327:A:OP1	14:AL:23:LYS:NZ	2.49	0.45
81:2:646:G:C5	81:2:688:G:N1	2.85	0.45
10:AG:70:VAL:HG12	16:AN:21:PHE:CZ	2.51	0.45
17:AO:32:GLN:HE21	17:AO:33:LYS:N	2.14	0.45
81:2:279:U:O2’	81:2:280:G:OP2	2.29	0.45
1:5:2255:U:OP1	1:5:2255:U:C6	2.69	0.44
17:AO:146:VAL:O	17:AO:146:VAL:HG23	2.16	0.44
62:O:31:THR:HG22	62:O:38:THR:HG22	1.99	0.44
82:1:405:GLN:HB3	82:1:448:PHE:CE1	2.53	0.44
12:AI:146:ASP:HA	12:AI:149:ILE:HG22	1.99	0.44
17:AO:13:LYS:C	17:AO:15:HIS:N	2.70	0.44
17:AO:105:VAL:C	17:AO:106:PHE:CD1	2.90	0.44
19:AQ:120:GLU:HB3	19:AQ:122:ILE:HD13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:R:20:TYR:CE2	65:R:38:ILE:HD13	2.52	0.44
82:1:562:THR:HG21	82:1:573:LEU:HD23	1.98	0.44
82:1:827:ALA:HB2	82:1:939:THR:HG21	2.00	0.44
17:AO:63:THR:HG22	17:AO:64:ALA:N	2.31	0.44
17:AO:161:ARG:O	17:AO:164:ARG:N	2.42	0.44
66:S:46:VAL:HG11	66:S:69:ILE:HG23	2.00	0.44
68:U:58:LEU:HD12	68:U:88:LYS:HG2	2.00	0.44
1:5:2196:C:C3'	1:5:2196:C:C6	3.01	0.44
81:2:336:G:H4'	81:2:336:G:OP2	2.18	0.44
81:2:1712:A:H2'	81:2:1713:G:O4'	2.18	0.44
1:5:1162:U:C2	17:AO:49:PHE:CE1	3.05	0.44
1:5:1733:G:H3'	1:5:1734:U:H5"	1.99	0.44
8:AE:114:ARG:NH1	8:AE:114:ARG:CG	2.81	0.44
17:AO:113:TYR:O	17:AO:115:LYS:CA	2.61	0.44
17:AO:29:LEU:H	17:AO:29:LEU:CD2	2.30	0.44
81:2:1598:A:H2'	81:2:1598:A:N3	2.32	0.44
1:5:1161:A:N3	1:5:1161:A:C2'	2.80	0.43
17:AO:39:ALA:HA	17:AO:42:LEU:HD13	1.99	0.43
55:H:49:ILE:HG21	55:H:172:VAL:HG22	2.00	0.43
56:I:101:ILE:HD12	56:I:101:ILE:N	2.33	0.43
81:2:1396:U:H3'	81:2:1397:C:C5'	2.48	0.43
5:AB:84:ILE:HG23	5:AB:162:VAL:HG13	2.00	0.43
71:X:65:ASN:ND2	71:X:116:ASP:OD2	2.50	0.43
72:Y:119:PHE:C	72:Y:119:PHE:CD1	2.92	0.43
82:1:821:ALA:HB1	82:1:822:GLU:HA	2.00	0.43
1:5:1194:A:C4	1:5:1195:C:C5	3.06	0.43
17:AO:142:LEU:HD12	17:AO:142:LEU:O	2.18	0.43
5:AB:218:VAL:HG22	5:AB:276:THR:HG22	2.01	0.43
6:AC:351:LYS:HB3	6:AC:351:LYS:HE2	1.50	0.43
17:AO:29:LEU:N	17:AO:29:LEU:CD2	2.82	0.43
17:AO:141:LYS:N	17:AO:151:GLU:OE1	2.52	0.43
53:F:134:VAL:HG11	53:F:201:ILE:HD12	2.00	0.43
1:5:2501:U:H5"	1:5:2501:U:C6	2.40	0.43
1:5:2502:G:N2	1:5:2516:A:H1'	2.31	0.43
52:E:126:VAL:HA	52:E:127:LYS:CB	2.48	0.43
17:AO:97:LYS:O	17:AO:98:ALA:C	2.55	0.43
17:AO:178:VAL:O	17:AO:179:VAL:C	2.55	0.43
21:AS:97:VAL:HG13	21:AS:98:THR:HG23	2.01	0.43
1:5:1161:A:N3	1:5:1161:A:H2'	2.34	0.43
7:AD:294:ALA:HB3	7:AD:295:PRO:HD3	2.01	0.43
17:AO:33:LYS:C	17:AO:34:ILE:CG1	2.88	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:A:126:PRO:CG	48:A:147:THR:HG22	2.48	0.43
58:K:3:ILE:HG23	58:K:41:PHE:CD2	2.54	0.43
10:AG:80:THR:HG21	10:AG:180:LYS:HE3	2.00	0.43
17:AO:36:VAL:HG21	17:AO:81:PHE:CZ	2.54	0.43
8:AE:112:LYS:O	8:AE:117:ALA:HB1	2.19	0.42
8:AE:124:GLN:N	8:AE:125:PRO:CD	2.82	0.42
17:AO:32:GLN:CG	17:AO:33:LYS:N	2.64	0.42
17:AO:27:GLN:HB2	17:AO:28:LEU:HD23	2.00	0.42
53:F:94:ARG:HB3	53:F:174:ILE:HD13	2.02	0.42
1:5:2502:G:N1	1:5:2516:A:C8	2.87	0.42
5:AB:58:ARG:HD3	5:AB:354:VAL:HG13	2.01	0.42
17:AO:32:GLN:O	17:AO:102:ARG:CD	2.57	0.42
24:AV:135:VAL:HG11	25:AW:26:SER:HB3	2.02	0.42
63:P:21:ASP:O	66:S:93:ASN:ND2	2.52	0.42
82:1:674:ALA:HB3	82:1:677:LEU:HD21	2.01	0.42
1:5:591:C:P	8:AE:111:ARG:NH1	2.93	0.42
17:AO:169:TYR:C	17:AO:171:LYS:N	2.63	0.42
48:A:197:ILE:HG23	48:A:198:MET:N	2.34	0.42
81:2:1513:A:O2'	81:2:1516:C:N4	2.52	0.42
1:5:1525:U:O2	1:5:1525:U:C2'	2.68	0.42
1:5:2061:A:N3	1:5:2061:A:H2'	2.34	0.42
9:AF:153:ILE:HG23	9:AF:169:ASN:HD21	1.84	0.42
20:AR:58:HIS:ND1	20:AR:58:HIS:C	2.73	0.42
81:2:646:G:O6	81:2:688:G:C6	2.72	0.42
82:1:596:GLU:HA	82:1:597:ALA:HB2	1.99	0.42
83:3:60:U:O2	83:3:60:U:C2'	2.66	0.42
5:AB:60:LEU:HD12	5:AB:72:VAL:HG21	2.01	0.42
8:AE:114:ARG:CA	8:AE:117:ALA:N	2.83	0.42
17:AO:51:ASN:C	17:AO:53:LEU:N	2.73	0.42
17:AO:144:THR:CB	17:AO:151:GLU:OE2	2.63	0.42
17:AO:185:THR:CG2	17:AO:186:VAL:H	2.10	0.42
28:AZ:46:ILE:HD11	28:AZ:49:TYR:CD1	2.54	0.42
81:2:1712:A:C2	81:2:1713:G:C5	3.07	0.42
17:AO:11:ASP:C	17:AO:11:ASP:OD1	2.58	0.42
17:AO:15:HIS:CD2	17:AO:124:ALA:O	2.73	0.42
17:AO:139:LEU:HD12	17:AO:139:LEU:HA	1.80	0.42
20:AR:99:LEU:HD11	20:AR:103:ARG:NH1	2.33	0.42
48:A:196:ALA:HA	48:A:197:ILE:HG22	2.00	0.42
50:C:148:TYR:HA	50:C:149:TRP:CB	2.49	0.42
56:I:154:GLU:O	56:I:156:ALA:N	2.53	0.42
63:P:18:LYS:O	66:S:95:GLY:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1322:U:C3'	1:5:1322:U:C6	3.02	0.42
12:AI:54:SER:HB2	12:AI:135:ILE:HD11	2.00	0.42
17:AO:113:TYR:C	17:AO:114:ASP:OD1	2.58	0.42
17:AO:141:LYS:CA	17:AO:151:GLU:OE1	2.67	0.42
18:AP:64:ASN:HA	18:AP:67:ILE:HD12	2.01	0.42
52:E:67:GLN:CA	52:E:68:ARG:HB2	2.46	0.42
1:5:2255:U:O2	1:5:2255:U:O2'	2.22	0.42
4:AA:101:VAL:HG22	4:AA:165:VAL:HG22	2.02	0.42
5:AB:222:LYS:O	5:AB:272:TYR:N	2.51	0.42
56:I:82:VAL:HG12	56:I:197:LEU:HD21	2.02	0.42
61:N:60:VAL:HG13	61:N:66:ILE:HD12	2.02	0.42
82:1:834:ASN:CG	82:1:852:ILE:HD11	2.40	0.42
1:5:2505:A:N3	1:5:2505:A:H2'	2.34	0.42
5:AB:283:TYR:CD1	5:AB:354:VAL:HG11	2.55	0.42
1:5:2257:G:C6	1:5:2258:U:C4	3.07	0.41
11:AH:85:GLY:HA3	11:AH:187:ILE:HD12	2.01	0.41
14:AL:2:ALA:O	14:AL:3:ILE:HG22	2.20	0.41
17:AO:149:LYS:O	17:AO:150:TYR:CD1	2.73	0.41
54:G:48:TYR:CD1	54:G:113:ILE:HD11	2.55	0.41
54:G:48:TYR:HB3	54:G:113:ILE:HD11	2.01	0.41
1:5:2529:C:O2'	10:AG:31:ARG:NH1	2.53	0.41
5:AB:383:LEU:HA	5:AB:384:LYS:HA	1.90	0.41
17:AO:48:PHE:C	17:AO:48:PHE:CD1	2.93	0.41
24:AV:81:GLN:O	24:AV:82:SER:CB	2.68	0.41
51:D:186:VAL:HG12	51:D:188:ILE:CD1	2.50	0.41
82:1:963:VAL:HG12	82:1:964:PHE:CD1	2.55	0.41
17:AO:44:ILE:HG22	17:AO:45:SER:O	2.20	0.41
17:AO:56:HIS:O	17:AO:57:ASP:HB2	2.20	0.41
17:AO:126:ARG:HD2	17:AO:136:TYR:CD2	2.55	0.41
17:AO:140:GLY:C	17:AO:142:LEU:N	2.73	0.41
18:AP:129:THR:HG23	18:AP:139:TYR:HB2	2.02	0.41
22:AT:65:TYR:CD1	22:AT:75:ILE:HG23	2.54	0.41
1:5:1322:U:C6	1:5:1322:U:H3'	2.55	0.41
11:AH:41:ILE:HD12	11:AH:43:VAL:HG13	2.01	0.41
18:AP:36:ILE:CD1	18:AP:95:LEU:HD11	2.50	0.41
71:X:68:ILE:HD12	71:X:68:ILE:N	2.36	0.41
82:1:800:ILE:HG13	82:1:803:HIS:CD2	2.56	0.41
82:1:803:HIS:O	82:1:805:PHE:N	2.54	0.41
82:1:954:TRP:HA	82:1:955:MET:CB	2.50	0.41
6:AC:148:ILE:HB	6:AC:149:PRO:CD	2.51	0.41
17:AO:20:LEU:HD23	17:AO:81:PHE:HE2	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AQ:157:PRO:HA	19:AQ:158:HIS:HA	1.86	0.41
20:AR:89:LEU:HD12	20:AR:90:PRO:N	2.35	0.41
52:E:123:LEU:HD13	52:E:236:ILE:HD11	2.01	0.41
52:E:181:VAL:CG2	52:E:225:VAL:HG22	2.51	0.41
65:R:78:ARG:CB	65:R:79:GLU:HA	2.50	0.41
81:2:238:C:H3'	81:2:238:C:C6	2.56	0.41
21:AS:6:GLU:O	21:AS:6:GLU:CG	2.66	0.41
81:2:542:C:O2	81:2:542:C:O4'	2.39	0.41
4:AA:196:TRP:HB3	4:AA:197:PRO:CD	2.50	0.41
17:AO:92:LYS:O	17:AO:93:THR:HG23	2.21	0.41
49:B:34:ALA:HB3	49:B:41:ARG:HA	2.03	0.41
63:P:89:MET:SD	63:P:89:MET:N	2.94	0.41
82:1:560:VAL:HG11	82:1:573:LEU:HD22	2.03	0.41
5:AB:312:VAL:HG12	5:AB:313:HIS:CD2	2.56	0.41
8:AE:114:ARG:HG3	8:AE:115:ALA:CA	2.48	0.41
17:AO:169:TYR:O	17:AO:171:LYS:CA	2.65	0.41
61:N:56:ASP:OD1	61:N:57:ALA:N	2.54	0.41
1:5:3285:U:O2	1:5:3285:U:O4'	2.35	0.41
17:AO:39:ALA:C	17:AO:41:ALA:N	2.73	0.41
17:AO:55:TYR:O	17:AO:58:TYR:N	2.52	0.41
17:AO:114:ASP:OD1	17:AO:114:ASP:N	2.53	0.41
63:P:18:LYS:HA	66:S:91:ASP:C	2.40	0.41
63:P:98:ASN:HB3	63:P:122:THR:HG22	2.02	0.41
81:2:238:C:C6	81:2:238:C:C3'	3.03	0.41
81:2:737:A:O2'	81:2:738:G:O5'	2.37	0.41
82:1:526:PHE:CE2	82:1:530:LEU:HD12	2.56	0.41
82:1:953:ASP:HB3	82:1:954:TRP:CG	2.56	0.41
6:AC:30:ILE:HD11	6:AC:128:ALA:HB2	2.03	0.41
6:AC:315:LYS:O	6:AC:316:ASN:CB	2.69	0.41
17:AO:11:ASP:HB2	17:AO:118:ARG:HG3	2.03	0.41
17:AO:63:THR:CG2	17:AO:64:ALA:N	2.84	0.41
17:AO:139:LEU:HB3	17:AO:140:GLY:H	1.65	0.41
81:2:897:A:N6	81:2:911:U:H1'	2.36	0.41
82:1:868:ASP:OD1	82:1:868:ASP:N	2.54	0.41
1:5:2501:U:H2'	1:5:2502:G:H4'	2.03	0.40
17:AO:185:THR:CG2	17:AO:186:VAL:N	2.78	0.40
63:P:34:VAL:HG21	63:P:45:PHE:CG	2.56	0.40
17:AO:23:THR:C	17:AO:25:ALA:N	2.74	0.40
50:C:177:ALA:HB1	50:C:178:PRO:CD	2.50	0.40
1:5:2502:G:C2	1:5:2516:A:C6	3.08	0.40
17:AO:126:ARG:NE	17:AO:136:TYR:CE2	2.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:646:G:C6	81:2:688:G:C6	3.09	0.40
81:2:911:U:H4’	81:2:912:G:O3’	2.20	0.40
1:5:2254:C:H6	1:5:2254:C:O5’	2.03	0.40
6:AC:74:ILE:O	6:AC:74:ILE:CG2	2.70	0.40
9:AF:153:ILE:HB	9:AF:158:ILE:HD12	2.03	0.40
11:AH:41:ILE:HD11	11:AH:67:ALA:CB	2.49	0.40
17:AO:80:ILE:O	17:AO:83:LYS:N	2.52	0.40
17:AO:197:LEU:O	17:AO:198:GLY:C	2.60	0.40
50:C:185:ALA:HB2	50:C:203:THR:HG21	2.03	0.40
60:M:107:VAL:HG21	81:2:1226:A:OP1	2.21	0.40
81:2:214:A:N7	81:2:241:U:N1	2.64	0.40
17:AO:148:TRP:CE3	17:AO:151:GLU:HB2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
4	AA	247/254 (97%)	216 (87%)	24 (10%)	7 (3%)	5	34
5	AB	382/387 (99%)	321 (84%)	51 (13%)	10 (3%)	5	35
6	AC	358/363 (99%)	279 (78%)	54 (15%)	25 (7%)	1	14
7	AD	293/297 (99%)	266 (91%)	15 (5%)	12 (4%)	3	26
8	AE	159/175 (91%)	138 (87%)	16 (10%)	5 (3%)	4	32
9	AF	220/241 (91%)	196 (89%)	17 (8%)	7 (3%)	4	31
10	AG	231/255 (91%)	213 (92%)	14 (6%)	4 (2%)	9	45
11	AH	189/191 (99%)	162 (86%)	24 (13%)	3 (2%)	9	46
12	AI	203/220 (92%)	181 (89%)	16 (8%)	6 (3%)	4	33
13	AJ	166/174 (95%)	147 (89%)	12 (7%)	7 (4%)	3	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	AL	195/199 (98%)	172 (88%)	19 (10%)	4 (2%)	7	40
15	AM	134/138 (97%)	116 (87%)	14 (10%)	4 (3%)	4	33
16	AN	200/204 (98%)	189 (94%)	11 (6%)	0	100	100
17	AO	196/199 (98%)	94 (48%)	38 (19%)	64 (33%)	0	0
18	AP	178/184 (97%)	156 (88%)	17 (10%)	5 (3%)	5	34
19	AQ	182/186 (98%)	163 (90%)	18 (10%)	1 (0%)	29	68
20	AR	186/189 (98%)	171 (92%)	12 (6%)	3 (2%)	9	46
21	AS	167/172 (97%)	152 (91%)	10 (6%)	5 (3%)	4	33
22	AT	156/160 (98%)	138 (88%)	16 (10%)	2 (1%)	12	50
23	AU	98/122 (80%)	89 (91%)	9 (9%)	0	100	100
24	AV	130/137 (95%)	118 (91%)	10 (8%)	2 (2%)	10	47
25	AW	60/155 (39%)	57 (95%)	3 (5%)	0	100	100
26	AX	119/142 (84%)	110 (92%)	9 (8%)	0	100	100
27	AY	123/127 (97%)	107 (87%)	14 (11%)	2 (2%)	9	46
28	AZ	132/136 (97%)	111 (84%)	17 (13%)	4 (3%)	4	33
29	Ba	145/149 (97%)	120 (83%)	19 (13%)	6 (4%)	3	26
30	Bb	55/62 (89%)	47 (86%)	6 (11%)	2 (4%)	3	29
31	Bc	95/105 (90%)	88 (93%)	7 (7%)	0	100	100
32	Bd	104/114 (91%)	94 (90%)	6 (6%)	4 (4%)	3	27
33	Be	120/130 (92%)	111 (92%)	6 (5%)	3 (2%)	5	36
34	Bf	103/107 (96%)	94 (91%)	6 (6%)	3 (3%)	4	33
35	Bg	119/125 (95%)	105 (88%)	9 (8%)	5 (4%)	3	25
36	Bh	114/120 (95%)	106 (93%)	5 (4%)	3 (3%)	5	35
37	Bi	96/100 (96%)	81 (84%)	10 (10%)	5 (5%)	2	20
38	Bj	83/88 (94%)	75 (90%)	6 (7%)	2 (2%)	6	37
39	Bk	74/78 (95%)	61 (82%)	11 (15%)	2 (3%)	5	35
40	Bl	47/51 (92%)	41 (87%)	4 (8%)	2 (4%)	2	24
41	Bm	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
42	Bn	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
43	Bo	99/106 (93%)	76 (77%)	15 (15%)	8 (8%)	1	11
44	Bp	85/92 (92%)	71 (84%)	8 (9%)	6 (7%)	1	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	Bq	215/217 (99%)	171 (80%)	29 (14%)	15 (7%)	1	14
46	Br	193/311 (62%)	140 (72%)	33 (17%)	20 (10%)	0	7
48	A	204/254 (80%)	174 (85%)	21 (10%)	9 (4%)	2	23
49	B	212/255 (83%)	181 (85%)	22 (10%)	9 (4%)	3	25
50	C	215/259 (83%)	178 (83%)	29 (14%)	8 (4%)	3	28
51	D	221/237 (93%)	193 (87%)	19 (9%)	9 (4%)	3	26
52	E	258/261 (99%)	225 (87%)	22 (8%)	11 (4%)	2	24
53	F	204/227 (90%)	166 (81%)	29 (14%)	9 (4%)	2	23
54	G	224/236 (95%)	196 (88%)	22 (10%)	6 (3%)	5	35
55	H	182/190 (96%)	155 (85%)	18 (10%)	9 (5%)	2	21
56	I	184/201 (92%)	158 (86%)	19 (10%)	7 (4%)	3	27
57	J	180/188 (96%)	146 (81%)	25 (14%)	9 (5%)	2	21
58	K	94/106 (89%)	81 (86%)	9 (10%)	4 (4%)	2	24
59	L	143/156 (92%)	127 (89%)	12 (8%)	4 (3%)	5	34
60	M	120/134 (90%)	99 (82%)	15 (12%)	6 (5%)	2	21
61	N	148/151 (98%)	137 (93%)	10 (7%)	1 (1%)	22	61
62	O	125/137 (91%)	106 (85%)	13 (10%)	6 (5%)	2	22
63	P	117/142 (82%)	90 (77%)	18 (15%)	9 (8%)	1	12
64	Q	139/143 (97%)	121 (87%)	14 (10%)	4 (3%)	4	33
65	R	121/136 (89%)	96 (79%)	22 (18%)	3 (2%)	5	36
66	S	136/146 (93%)	112 (82%)	17 (12%)	7 (5%)	2	20
67	T	141/144 (98%)	123 (87%)	14 (10%)	4 (3%)	5	34
68	U	104/117 (89%)	89 (86%)	13 (12%)	2 (2%)	8	42
69	V	85/87 (98%)	70 (82%)	11 (13%)	4 (5%)	2	22
70	W	127/130 (98%)	106 (84%)	19 (15%)	2 (2%)	9	46
71	X	141/145 (97%)	116 (82%)	21 (15%)	4 (3%)	5	34
72	Y	132/135 (98%)	112 (85%)	15 (11%)	5 (4%)	3	27
73	Z	68/108 (63%)	60 (88%)	6 (9%)	2 (3%)	4	33
74	a	98/119 (82%)	78 (80%)	12 (12%)	8 (8%)	1	10
75	b	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	3	27
76	c	61/67 (91%)	58 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
77	d	51/56 (91%)	42 (82%)	8 (16%)	1 (2%)	7	41
78	e	53/63 (84%)	50 (94%)	2 (4%)	1 (2%)	8	42
79	f	40/150 (27%)	28 (70%)	8 (20%)	4 (10%)	0	8
80	g	312/326 (96%)	250 (80%)	52 (17%)	10 (3%)	4	31
82	1	598/967 (62%)	465 (78%)	103 (17%)	30 (5%)	2	21
All	All	11839/13368 (89%)	10064 (85%)	1297 (11%)	478 (4%)	5	26

All (478) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AA	34	TYR
4	AA	196	TRP
4	AA	197	PRO
5	AB	5	LYS
5	AB	351	LEU
6	AC	74	ILE
6	AC	148	ILE
6	AC	149	PRO
6	AC	182	VAL
6	AC	270	VAL
6	AC	300	ARG
6	AC	316	ASN
6	AC	342	LYS
6	AC	352	PRO
7	AD	4	ILE
10	AG	126	PRO
13	AJ	25	GLU
13	AJ	114	ILE
14	AL	3	ILE
14	AL	4	SER
14	AL	47	ALA
17	AO	13	LYS
17	AO	16	LEU
17	AO	29	LEU
17	AO	35	VAL
17	AO	48	PHE
17	AO	50	ARG
17	AO	56	HIS
17	AO	57	ASP
17	AO	67	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	AO	68	THR
17	AO	78	SER
17	AO	86	ARG
17	AO	94	ALA
17	AO	112	PRO
17	AO	114	ASP
17	AO	122	PRO
17	AO	123	GLN
17	AO	126	ARG
17	AO	127	VAL
17	AO	130	LEU
17	AO	139	LEU
17	AO	141	LYS
17	AO	146	VAL
17	AO	158	GLU
17	AO	160	LYS
17	AO	162	LYS
17	AO	169	TYR
17	AO	170	LEU
17	AO	179	VAL
17	AO	183	SER
17	AO	186	VAL
17	AO	187	GLY
17	AO	188	THR
17	AO	190	VAL
17	AO	193	LYS
21	AS	18	SER
27	AY	55	GLU
28	AZ	51	LEU
28	AZ	59	ALA
29	Ba	50	PRO
29	Ba	78	LEU
34	Bf	104	PRO
37	Bi	30	LYS
39	Bk	6	ALA
39	Bk	32	ASN
40	Bl	33	ASN
43	Bo	66	LYS
45	Bq	24	LYS
45	Bq	59	PRO
45	Bq	181	ASN
46	Br	41	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	Br	70	SER
48	A	197	ILE
49	B	35	PRO
49	B	191	GLU
50	C	59	GLU
51	D	176	LEU
52	E	117	GLU
53	F	192	ILE
53	F	221	ARG
54	G	122	GLU
54	G	154	ARG
55	H	64	VAL
56	I	22	ARG
56	I	35	ASN
56	I	148	ALA
56	I	155	HIS
58	K	88	PRO
59	L	105	LYS
62	O	91	SER
63	P	20	VAL
63	P	29	PRO
64	Q	40	GLN
66	S	92	VAL
69	V	10	GLU
70	W	83	ILE
71	X	12	ALA
71	X	42	PRO
71	X	138	GLU
72	Y	30	PRO
74	a	10	ARG
74	a	75	ILE
79	f	143	HIS
80	g	52	GLU
82	1	442	THR
82	1	461	ILE
82	1	597	ALA
82	1	653	ARG
82	1	868	ASP
82	1	876	THR
82	1	911	PRO
82	1	941	LYS
4	AA	33	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AB	226	PHE
6	AC	16	THR
6	AC	268	ALA
6	AC	292	SER
6	AC	293	THR
6	AC	305	ALA
6	AC	341	SER
6	AC	343	LYS
7	AD	5	LYS
7	AD	20	PHE
7	AD	21	ARG
7	AD	188	GLU
7	AD	296	GLN
8	AE	114	ARG
9	AF	90	ASN
9	AF	139	SER
9	AF	156	GLN
12	AI	145	LYS
12	AI	187	ALA
15	AM	6	VAL
17	AO	12	GLY
17	AO	34	ILE
17	AO	40	GLU
17	AO	49	PHE
17	AO	51	ASN
17	AO	66	ASN
17	AO	81	PHE
17	AO	84	ALA
17	AO	98	ALA
17	AO	113	TYR
17	AO	140	GLY
17	AO	144	THR
17	AO	145	SER
17	AO	148	TRP
17	AO	163	ALA
17	AO	165	SER
17	AO	177	ALA
17	AO	198	GLY
18	AP	165	VAL
21	AS	133	ALA
24	AV	82	SER
24	AV	106	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	AY	109	LEU
28	AZ	87	LEU
29	Ba	124	ILE
33	Be	124	ALA
35	Bg	60	ARG
35	Bg	75	ALA
37	Bi	14	GLY
37	Bi	36	ARG
38	Bj	85	ALA
43	Bo	6	LYS
44	Bp	56	SER
44	Bp	60	CYS
44	Bp	61	ASN
46	Br	69	ILE
46	Br	95	LEU
46	Br	126	VAL
49	B	177	GLN
50	C	57	SER
51	D	217	VAL
52	E	68	ARG
52	E	120	SER
52	E	127	LYS
52	E	195	ILE
53	F	59	SER
53	F	206	GLY
55	H	53	GLY
56	I	62	THR
56	I	153	ILE
59	L	55	ASP
60	M	78	PRO
62	O	18	ARG
63	P	101	VAL
63	P	121	ILE
66	S	26	ILE
67	T	39	THR
69	V	30	SER
73	Z	71	LEU
74	a	84	VAL
74	a	85	ARG
75	b	21	LEU
80	g	77	ASP
80	g	201	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
82	1	382	GLY
82	1	431	THR
82	1	445	HIS
82	1	457	SER
82	1	487	LYS
82	1	793	ILE
82	1	800	ILE
82	1	801	ILE
5	AB	140	ASN
6	AC	84	ARG
6	AC	140	HIS
6	AC	173	GLY
6	AC	232	SER
6	AC	269	SER
7	AD	214	ASP
7	AD	253	PHE
8	AE	66	PRO
8	AE	112	LYS
8	AE	115	ALA
9	AF	230	GLU
12	AI	24	ARG
13	AJ	8	PRO
14	AL	190	LYS
15	AM	28	SER
15	AM	29	ALA
15	AM	41	GLN
17	AO	24	VAL
17	AO	27	GLN
17	AO	54	LYS
17	AO	77	PRO
17	AO	111	PRO
17	AO	143	SER
18	AP	161	SER
19	AQ	175	ALA
20	AR	131	THR
28	AZ	9	LYS
32	Bd	83	GLU
32	Bd	84	ASP
35	Bg	10	ARG
35	Bg	56	THR
35	Bg	57	LEU
40	Bl	3	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	Bo	14	GLY
43	Bo	65	THR
45	Bq	71	ALA
45	Bq	129	SER
45	Bq	209	THR
46	Br	23	GLU
46	Br	38	GLN
46	Br	58	ASN
46	Br	111	ALA
48	A	72	ASP
49	B	181	LEU
49	B	209	ASN
50	C	111	ASP
50	C	153	LEU
50	C	175	ILE
51	D	220	PRO
52	E	205	PHE
54	G	70	PRO
54	G	165	GLY
55	H	98	ILE
57	J	18	PRO
57	J	67	PRO
57	J	118	LEU
58	K	54	PHE
58	K	83	PRO
59	L	30	LYS
60	M	82	VAL
62	O	51	ASP
62	O	114	ARG
63	P	125	PRO
64	Q	116	LEU
65	R	26	MET
65	R	72	LYS
65	R	100	LEU
66	S	140	THR
67	T	119	LYS
69	V	4	ASP
70	W	57	ARG
72	Y	61	ARG
74	a	61	GLU
79	f	144	SER
80	g	244	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	g	256	ARG
82	1	443	PRO
82	1	451	LEU
82	1	695	GLU
82	1	720	VAL
4	AA	143	ASP
6	AC	131	VAL
6	AC	345	ASP
7	AD	249	GLU
8	AE	110	SER
11	AH	50	ASN
12	AI	47	PRO
12	AI	144	ASN
13	AJ	108	GLU
17	AO	28	LEU
17	AO	52	LYS
17	AO	142	LEU
18	AP	4	TYR
18	AP	158	GLU
20	AR	130	ASN
21	AS	13	ARG
21	AS	24	LEU
22	AT	125	ALA
29	Ba	66	ALA
29	Ba	98	ALA
32	Bd	82	GLU
34	Bf	91	ALA
37	Bi	13	LYS
43	Bo	53	GLN
44	Bp	47	VAL
45	Bq	25	LYS
45	Bq	128	LEU
45	Bq	182	GLN
45	Bq	213	ALA
46	Br	68	PHE
46	Br	106	LYS
46	Br	149	ARG
46	Br	156	SER
48	A	9	LEU
48	A	167	LYS
48	A	193	GLN
48	A	202	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	D	196	THR
52	E	77	ARG
53	F	82	LYS
53	F	83	ARG
53	F	166	PRO
54	G	155	ASP
55	H	32	PRO
55	H	110	GLN
56	I	120	SER
57	J	69	ARG
57	J	169	PRO
60	M	117	TRP
62	O	75	GLY
62	O	124	ASP
63	P	52	LYS
66	S	12	GLN
67	T	50	SER
67	T	53	TRP
72	Y	63	GLN
75	b	75	GLU
80	g	4	SER
80	g	41	LYS
80	g	75	SER
80	g	139	GLY
82	1	467	ASP
82	1	519	GLU
82	1	590	LYS
82	1	804	LEU
82	1	963	VAL
4	AA	125	ALA
5	AB	22	ALA
5	AB	28	ARG
5	AB	155	ALA
5	AB	348	ARG
6	AC	14	GLU
7	AD	259	LYS
9	AF	113	PHE
10	AG	24	PRO
10	AG	122	GLN
11	AH	110	LYS
13	AJ	94	ARG
17	AO	14	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	AO	63	THR
21	AS	12	ARG
22	AT	122	GLN
29	Ba	33	GLY
33	Be	12	LYS
33	Be	123	LYS
36	Bh	75	TYR
36	Bh	99	GLN
43	Bo	15	LYS
43	Bo	17	CYS
44	Bp	57	CYS
45	Bq	216	LEU
46	Br	28	PHE
48	A	103	THR
48	A	195	TRP
49	B	179	SER
50	C	41	VAL
50	C	56	SER
51	D	44	THR
51	D	143	ARG
51	D	164	VAL
52	E	245	LYS
55	H	13	PRO
55	H	160	GLN
60	M	32	ASP
64	Q	27	GLY
66	S	14	ILE
66	S	76	PRO
66	S	144	ARG
69	V	7	GLN
71	X	70	LYS
72	Y	36	SER
74	a	62	TYR
75	b	62	VAL
79	f	127	GLY
80	g	293	ASP
82	1	413	PRO
4	AA	141	PRO
5	AB	227	GLU
7	AD	125	VAL
11	AH	2	LYS
13	AJ	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AJ	172	LEU
30	Bb	20	GLY
30	Bb	21	ILE
34	Bf	103	TYR
36	Bh	84	LYS
37	Bi	45	LYS
44	Bp	18	TYR
46	Br	94	SER
48	A	68	PRO
49	B	53	GLY
49	B	210	VAL
51	D	221	SER
52	E	260	GLY
53	F	102	ASN
55	H	146	GLY
57	J	134	ILE
61	N	133	SER
63	P	23	GLU
63	P	69	GLU
63	P	120	SER
64	Q	115	THR
68	U	72	ASN
73	Z	88	ILE
78	e	47	VAL
79	f	102	VAL
82	1	372	ILE
10	AG	35	ILE
12	AI	194	GLY
57	J	165	GLY
57	J	166	GLY
60	M	93	GLY
60	M	97	ILE
74	a	36	ILE
43	Bo	95	GLY
45	Bq	4	ILE
45	Bq	60	ARG
46	Br	32	VAL
46	Br	118	PRO
51	D	130	GLY
54	G	60	GLY
55	H	132	PRO
5	AB	87	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	AC	328	ASN
7	AD	251	PRO
20	AR	129	GLY
45	Bq	180	VAL
46	Br	109	ALA
46	Br	133	GLY
52	E	129	VAL
53	F	53	VAL
68	U	86	ILE
9	AF	175	ILE
9	AF	188	VAL
18	AP	119	VAL
32	Bd	66	GLY
45	Bq	169	VAL
46	Br	164	GLY
50	C	114	GLY
52	E	228	ILE
57	J	170	GLY
58	K	94	GLY
59	L	130	PRO
74	a	83	ILE
82	1	414	ILE
49	B	221	PRO
72	Y	5	ILE
77	d	25	GLY
38	Bj	40	PRO
82	1	648	PRO
82	1	962	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AA	190/195 (97%)	183 (96%)	7 (4%)	34	66
5	AB	323/326 (99%)	303 (94%)	20 (6%)	18	53
6	AC	291/294 (99%)	271 (93%)	20 (7%)	15	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AD	243/244 (100%)	234 (96%)	9 (4%)	34	66
8	AE	141/150 (94%)	133 (94%)	8 (6%)	20	55
9	AF	188/204 (92%)	182 (97%)	6 (3%)	39	70
10	AG	192/209 (92%)	182 (95%)	10 (5%)	23	58
11	AH	173/173 (100%)	162 (94%)	11 (6%)	17	52
12	AI	177/187 (95%)	169 (96%)	8 (4%)	27	62
13	AJ	144/148 (97%)	138 (96%)	6 (4%)	30	63
14	AL	162/164 (99%)	156 (96%)	6 (4%)	34	66
15	AM	109/110 (99%)	106 (97%)	3 (3%)	43	72
16	AN	175/177 (99%)	171 (98%)	4 (2%)	50	76
17	AO	163/164 (99%)	151 (93%)	12 (7%)	13	46
18	AP	148/150 (99%)	141 (95%)	7 (5%)	26	61
19	AQ	150/151 (99%)	147 (98%)	3 (2%)	55	79
20	AR	152/153 (99%)	141 (93%)	11 (7%)	14	47
21	AS	154/157 (98%)	150 (97%)	4 (3%)	46	74
22	AT	135/137 (98%)	125 (93%)	10 (7%)	13	46
23	AU	90/110 (82%)	89 (99%)	1 (1%)	73	88
24	AV	101/105 (96%)	97 (96%)	4 (4%)	31	65
25	AW	54/127 (42%)	52 (96%)	2 (4%)	34	66
26	AX	106/120 (88%)	95 (90%)	11 (10%)	7	33
27	AY	111/112 (99%)	105 (95%)	6 (5%)	22	57
28	AZ	115/116 (99%)	108 (94%)	7 (6%)	18	53
29	Ba	117/118 (99%)	109 (93%)	8 (7%)	16	50
30	Bb	45/49 (92%)	41 (91%)	4 (9%)	9	40
31	Bc	79/85 (93%)	74 (94%)	5 (6%)	18	53
32	Bd	95/100 (95%)	90 (95%)	5 (5%)	22	58
33	Be	106/110 (96%)	101 (95%)	5 (5%)	26	61
34	Bf	90/92 (98%)	88 (98%)	2 (2%)	52	77
35	Bg	102/106 (96%)	100 (98%)	2 (2%)	55	79
36	Bh	104/106 (98%)	101 (97%)	3 (3%)	42	72
37	Bi	79/80 (99%)	75 (95%)	4 (5%)	24	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Bj	69/71 (97%)	68 (99%)	1 (1%)	67	85
39	Bk	68/69 (99%)	65 (96%)	3 (4%)	28	63
40	Bl	44/46 (96%)	38 (86%)	6 (14%)	3	22
41	Bm	46/116 (40%)	43 (94%)	3 (6%)	17	51
42	Bn	21/21 (100%)	18 (86%)	3 (14%)	3	21
43	Bo	86/90 (96%)	79 (92%)	7 (8%)	11	43
44	Bp	69/71 (97%)	64 (93%)	5 (7%)	14	47
45	Bq	198/198 (100%)	182 (92%)	16 (8%)	11	43
46	Br	162/251 (64%)	150 (93%)	12 (7%)	13	46
48	A	174/211 (82%)	167 (96%)	7 (4%)	31	65
49	B	196/228 (86%)	185 (94%)	11 (6%)	21	56
50	C	176/203 (87%)	161 (92%)	15 (8%)	10	41
51	D	185/196 (94%)	171 (92%)	14 (8%)	13	45
52	E	223/224 (100%)	209 (94%)	14 (6%)	18	53
53	F	174/194 (90%)	168 (97%)	6 (3%)	37	69
54	G	192/200 (96%)	187 (97%)	5 (3%)	46	74
55	H	164/170 (96%)	156 (95%)	8 (5%)	25	59
56	I	148/159 (93%)	134 (90%)	14 (10%)	8	37
57	J	153/158 (97%)	139 (91%)	14 (9%)	9	39
58	K	88/96 (92%)	83 (94%)	5 (6%)	20	55
59	L	129/137 (94%)	120 (93%)	9 (7%)	15	48
60	M	97/109 (89%)	94 (97%)	3 (3%)	40	71
61	N	127/128 (99%)	120 (94%)	7 (6%)	21	57
62	O	96/104 (92%)	95 (99%)	1 (1%)	76	88
63	P	103/119 (87%)	97 (94%)	6 (6%)	20	55
64	Q	117/119 (98%)	115 (98%)	2 (2%)	60	82
65	R	112/124 (90%)	108 (96%)	4 (4%)	35	67
66	S	121/129 (94%)	108 (89%)	13 (11%)	6	32
67	T	117/118 (99%)	113 (97%)	4 (3%)	37	69
68	U	96/107 (90%)	93 (97%)	3 (3%)	40	71
69	V	73/73 (100%)	66 (90%)	7 (10%)	8	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	W	110/111 (99%)	102 (93%)	8 (7%)	14	46
71	X	118/120 (98%)	111 (94%)	7 (6%)	19	55
72	Y	108/109 (99%)	97 (90%)	11 (10%)	7	34
73	Z	60/88 (68%)	59 (98%)	1 (2%)	60	82
74	a	85/100 (85%)	79 (93%)	6 (7%)	14	48
75	b	72/72 (100%)	68 (94%)	4 (6%)	21	56
76	c	55/59 (93%)	53 (96%)	2 (4%)	35	67
77	d	46/48 (96%)	42 (91%)	4 (9%)	10	41
78	e	49/55 (89%)	47 (96%)	2 (4%)	30	64
79	f	35/133 (26%)	33 (94%)	2 (6%)	20	55
80	g	265/272 (97%)	254 (96%)	11 (4%)	30	63
82	1	522/836 (62%)	465 (89%)	57 (11%)	6	32
All	All	10153/11271 (90%)	9576 (94%)	577 (6%)	24	55

All (577) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AA	21	ARG
4	AA	42	ARG
4	AA	65	ASP
4	AA	96	LEU
4	AA	143	ASP
4	AA	161	ASP
4	AA	230	VAL
5	AB	21	ARG
5	AB	56	ILE
5	AB	58	ARG
5	AB	59	ASP
5	AB	60	LEU
5	AB	70	ARG
5	AB	76	VAL
5	AB	84	ILE
5	AB	102	LEU
5	AB	104	THR
5	AB	222	LYS
5	AB	241	LYS
5	AB	246	LEU
5	AB	255	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AB	262	TRP
5	AB	274	HIS
5	AB	290	ASP
5	AB	332	ARG
5	AB	369	ARG
5	AB	380	LEU
6	AC	17	SER
6	AC	27	ARG
6	AC	71	VAL
6	AC	73	ARG
6	AC	74	ILE
6	AC	92	ASN
6	AC	93	MET
6	AC	138	ARG
6	AC	201	GLN
6	AC	202	ARG
6	AC	215	VAL
6	AC	270	VAL
6	AC	293	THR
6	AC	307	GLN
6	AC	314	LYS
6	AC	329	PRO
6	AC	346	GLN
6	AC	348	ASN
6	AC	351	LYS
6	AC	357	LEU
7	AD	4	ILE
7	AD	22	ARG
7	AD	41	LYS
7	AD	94	ASN
7	AD	105	LEU
7	AD	152	ARG
7	AD	177	GLU
7	AD	230	ASP
7	AD	244	HIS
8	AE	12	GLU
8	AE	50	VAL
8	AE	78	ASN
8	AE	82	VAL
8	AE	114	ARG
8	AE	126	LYS
8	AE	154	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	AE	166	ASN
9	AF	33	ARG
9	AF	53	GLU
9	AF	90	ASN
9	AF	112	THR
9	AF	155	LYS
9	AF	233	ILE
10	AG	37	GLN
10	AG	62	LYS
10	AG	64	LEU
10	AG	123	GLU
10	AG	135	LEU
10	AG	154	ASN
10	AG	168	LEU
10	AG	222	LEU
10	AG	231	HIS
10	AG	244	LYS
11	AH	5	GLN
11	AH	41	ILE
11	AH	69	ARG
11	AH	92	TYR
11	AH	107	ASP
11	AH	113	GLU
11	AH	118	LEU
11	AH	140	GLN
11	AH	141	LYS
11	AH	157	ASN
11	AH	170	LYS
12	AI	3	ARG
12	AI	32	ARG
12	AI	33	ILE
12	AI	139	ARG
12	AI	140	THR
12	AI	163	GLN
12	AI	165	ILE
12	AI	169	LYS
13	AJ	17	LEU
13	AJ	40	LEU
13	AJ	67	VAL
13	AJ	107	GLN
13	AJ	112	LEU
13	AJ	114	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	AL	67	ARG
14	AL	85	LEU
14	AL	104	ARG
14	AL	109	LEU
14	AL	124	ILE
14	AL	162	ASN
15	AM	59	ASN
15	AM	63	VAL
15	AM	77	LYS
16	AN	19	LEU
16	AN	38	ARG
16	AN	133	ILE
16	AN	151	ILE
17	AO	5	GLU
17	AO	26	LYS
17	AO	28	LEU
17	AO	32	GLN
17	AO	56	HIS
17	AO	82	TYR
17	AO	86	ARG
17	AO	106	PHE
17	AO	118	ARG
17	AO	119	VAL
17	AO	142	LEU
17	AO	149	LYS
18	AP	26	TYR
18	AP	69	ARG
18	AP	113	TYR
18	AP	120	ASN
18	AP	161	SER
18	AP	164	LYS
18	AP	167	ARG
19	AQ	135	GLN
19	AQ	168	THR
19	AQ	178	ARG
20	AR	5	ARG
20	AR	17	VAL
20	AR	31	GLU
20	AR	44	LEU
20	AR	55	THR
20	AR	57	ILE
20	AR	60	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	AR	66	MET
20	AR	74	ARG
20	AR	89	LEU
20	AR	119	LEU
21	AS	4	ARG
21	AS	5	LYS
21	AS	45	LEU
21	AS	122	HIS
22	AT	18	ASP
22	AT	75	ILE
22	AT	103	GLN
22	AT	104	GLU
22	AT	127	GLN
22	AT	128	LEU
22	AT	131	GLN
22	AT	139	ARG
22	AT	143	THR
22	AT	146	ASN
23	AU	70	LYS
24	AV	32	ARG
24	AV	64	LYS
24	AV	83	LYS
24	AV	102	ILE
25	AW	4	GLU
25	AW	5	ILE
26	AX	33	ARG
26	AX	36	LYS
26	AX	63	ILE
26	AX	73	MET
26	AX	80	ASN
26	AX	82	LEU
26	AX	115	ARG
26	AX	117	ASN
26	AX	135	ILE
26	AX	137	ASN
26	AX	142	ILE
27	AY	7	ASP
27	AY	50	ILE
27	AY	55	GLU
27	AY	74	TYR
27	AY	104	VAL
27	AY	114	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	AZ	31	GLU
28	AZ	34	LYS
28	AZ	57	GLN
28	AZ	81	LEU
28	AZ	109	GLU
28	AZ	121	ARG
28	AZ	134	LEU
29	Ba	4	ARG
29	Ba	25	HIS
29	Ba	34	MET
29	Ba	74	ASN
29	Ba	113	LEU
29	Ba	115	LYS
29	Ba	130	VAL
29	Ba	133	LEU
30	Bb	3	LYS
30	Bb	14	LYS
30	Bb	26	THR
30	Bb	32	LEU
31	Bc	40	LYS
31	Bc	41	LEU
31	Bc	61	MET
31	Bc	83	LYS
31	Bc	101	LEU
32	Bd	5	LYS
32	Bd	6	ASP
32	Bd	26	LYS
32	Bd	55	LEU
32	Bd	86	LYS
33	Be	19	ARG
33	Be	27	ARG
33	Be	54	THR
33	Be	75	LEU
33	Be	82	LEU
34	Bf	20	LYS
34	Bf	103	TYR
35	Bg	30	LEU
35	Bg	62	TYR
36	Bh	20	GLN
36	Bh	21	LEU
36	Bh	102	GLU
37	Bi	36	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	Bi	58	ILE
37	Bi	60	LEU
37	Bi	76	ARG
38	Bj	17	THR
39	Bk	31	LEU
39	Bk	34	ASN
39	Bk	69	LEU
40	Bl	11	GLN
40	Bl	15	LYS
40	Bl	21	ARG
40	Bl	23	LEU
40	Bl	27	ILE
40	Bl	29	LEU
41	Bm	106	ARG
41	Bm	113	ARG
41	Bm	119	ASN
42	Bn	6	ARG
42	Bn	9	ARG
42	Bn	11	ARG
43	Bo	35	LEU
43	Bo	45	ARG
43	Bo	59	HIS
43	Bo	85	LEU
43	Bo	99	GLN
43	Bo	100	LYS
43	Bo	102	GLN
44	Bp	10	ILE
44	Bp	25	GLN
44	Bp	47	VAL
44	Bp	57	CYS
44	Bp	84	ARG
45	Bq	3	LYS
45	Bq	15	GLU
45	Bq	19	TYR
45	Bq	38	LEU
45	Bq	44	GLN
45	Bq	47	LYS
45	Bq	60	ARG
45	Bq	95	LYS
45	Bq	97	LYS
45	Bq	102	LYS
45	Bq	180	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	Bq	181	ASN
45	Bq	182	GLN
45	Bq	214	TYR
45	Bq	215	ARG
45	Bq	216	LEU
46	Br	35	VAL
46	Br	37	SER
46	Br	39	GLN
46	Br	48	ARG
46	Br	62	ARG
46	Br	72	PHE
46	Br	91	THR
46	Br	134	LYS
46	Br	149	ARG
46	Br	187	LEU
46	Br	195	ASN
46	Br	199	PHE
48	A	9	LEU
48	A	34	GLU
48	A	43	ASP
48	A	108	THR
48	A	120	LEU
48	A	197	ILE
48	A	198	MET
49	B	26	ARG
49	B	47	LEU
49	B	54	LEU
49	B	81	PHE
49	B	96	LEU
49	B	100	PHE
49	B	108	ASP
49	B	110	LEU
49	B	120	LEU
49	B	191	GLU
49	B	208	GLN
50	C	49	LEU
50	C	59	GLU
50	C	82	LYS
50	C	83	ASP
50	C	86	MET
50	C	92	GLN
50	C	93	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	C	99	GLN
50	C	100	ARG
50	C	142	ILE
50	C	145	ARG
50	C	146	ARG
50	C	149	TRP
50	C	174	LEU
50	C	240	LEU
51	D	7	LYS
51	D	11	LEU
51	D	27	ARG
51	D	51	ARG
51	D	94	ARG
51	D	107	PHE
51	D	113	LEU
51	D	135	GLU
51	D	141	LYS
51	D	146	ARG
51	D	157	LEU
51	D	162	GLN
51	D	178	ARG
51	D	179	GLN
52	E	9	LEU
52	E	18	TRP
52	E	38	LEU
52	E	51	ARG
52	E	73	ASP
52	E	77	ARG
52	E	123	LEU
52	E	133	LYS
52	E	143	ASP
52	E	187	ARG
52	E	206	ASP
52	E	225	VAL
52	E	245	LYS
52	E	250	GLU
53	F	101	MET
53	F	121	GLU
53	F	158	ARG
53	F	187	ARG
53	F	188	ASN
53	F	220	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	G	31	ARG
54	G	52	ILE
54	G	81	HIS
54	G	92	ARG
54	G	180	THR
55	H	11	GLN
55	H	16	LEU
55	H	19	GLN
55	H	80	GLU
55	H	99	LEU
55	H	139	ARG
55	H	174	ASN
55	H	180	GLN
56	I	8	ARG
56	I	9	HIS
56	I	29	LEU
56	I	35	ASN
56	I	67	TRP
56	I	72	VAL
56	I	74	ARG
56	I	75	LYS
56	I	89	GLU
56	I	107	THR
56	I	138	LYS
56	I	144	TRP
56	I	152	LYS
56	I	192	PHE
57	J	20	GLU
57	J	30	LEU
57	J	37	LYS
57	J	66	ASP
57	J	69	ARG
57	J	86	LEU
57	J	89	ASP
57	J	93	LEU
57	J	109	LEU
57	J	126	ARG
57	J	139	GLN
57	J	149	ARG
57	J	150	LEU
57	J	175	LYS
58	K	21	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	K	40	LEU
58	K	54	PHE
58	K	80	LEU
58	K	86	ILE
59	L	8	GLN
59	L	11	ARG
59	L	32	LYS
59	L	79	ARG
59	L	80	MET
59	L	87	ARG
59	L	94	VAL
59	L	105	LYS
59	L	136	ARG
60	M	55	LEU
60	M	67	LEU
60	M	124	ARG
61	N	3	ARG
61	N	64	LYS
61	N	88	LEU
61	N	107	LYS
61	N	121	ARG
61	N	139	TRP
61	N	142	GLU
62	O	114	ARG
63	P	15	TYR
63	P	17	TYR
63	P	18	LYS
63	P	57	MET
63	P	79	HIS
63	P	89	MET
64	Q	128	LYS
64	Q	142	TYR
65	R	5	ARG
65	R	16	LEU
65	R	32	LYS
65	R	88	VAL
66	S	15	LEU
66	S	25	ASN
66	S	27	ASN
66	S	41	ARG
66	S	49	LYS
66	S	74	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	S	88	ARG
66	S	96	LYS
66	S	105	LEU
66	S	120	ARG
66	S	126	ARG
66	S	128	PHE
66	S	144	ARG
67	T	17	ASN
67	T	31	PRO
67	T	63	ARG
67	T	79	LEU
68	U	52	LYS
68	U	80	ASP
68	U	115	GLU
69	V	11	LEU
69	V	12	TYR
69	V	33	GLN
69	V	38	GLN
69	V	41	GLU
69	V	50	TYR
69	V	69	LEU
70	W	24	GLN
70	W	26	LEU
70	W	49	GLU
70	W	66	ASN
70	W	88	LYS
70	W	104	LEU
70	W	125	ILE
70	W	130	TYR
71	X	19	ARG
71	X	92	CYS
71	X	107	PHE
71	X	109	ARG
71	X	133	LEU
71	X	140	LYS
71	X	142	LYS
72	Y	3	ASP
72	Y	8	ARG
72	Y	20	ARG
72	Y	31	ASN
72	Y	46	GLU
72	Y	61	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
72	Y	98	GLU
72	Y	110	GLN
72	Y	116	LYS
72	Y	118	ILE
72	Y	119	PHE
73	Z	97	LYS
74	a	1	MET
74	a	5	ARG
74	a	12	LYS
74	a	28	ARG
74	a	32	LYS
74	a	39	MET
75	b	1	MET
75	b	5	GLN
75	b	26	GLN
75	b	34	ASP
76	c	16	LEU
76	c	56	LEU
77	d	8	TYR
77	d	10	HIS
77	d	30	LEU
77	d	40	ARG
78	e	22	GLU
78	e	26	LYS
79	f	103	LEU
79	f	136	ARG
80	g	43	LEU
80	g	67	HIS
80	g	74	VAL
80	g	175	VAL
80	g	202	HIS
80	g	238	PHE
80	g	242	ASP
80	g	244	LYS
80	g	271	ASP
80	g	292	GLN
80	g	321	GLN
82	1	385	LYS
82	1	412	PHE
82	1	419	GLN
82	1	442	THR
82	1	446	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
82	1	447	SER
82	1	450	ASN
82	1	451	LEU
82	1	456	SER
82	1	458	LEU
82	1	470	HIS
82	1	484	ARG
82	1	486	ARG
82	1	487	LYS
82	1	530	LEU
82	1	540	GLN
82	1	546	LEU
82	1	547	TYR
82	1	573	LEU
82	1	582	GLN
82	1	584	ARG
82	1	620	TYR
82	1	627	ILE
82	1	629	LEU
82	1	645	THR
82	1	649	LEU
82	1	653	ARG
82	1	660	HIS
82	1	668	LEU
82	1	675	ASN
82	1	677	LEU
82	1	689	VAL
82	1	706	LEU
82	1	709	LEU
82	1	754	LYS
82	1	755	ARG
82	1	770	LEU
82	1	778	VAL
82	1	779	LYS
82	1	782	LYS
82	1	786	GLN
82	1	791	GLN
82	1	799	ASP
82	1	800	ILE
82	1	801	ILE
82	1	802	TYR
82	1	804	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
82	1	812	GLN
82	1	815	LEU
82	1	822	GLU
82	1	868	ASP
82	1	874	ARG
82	1	878	LEU
82	1	896	LYS
82	1	899	GLN
82	1	934	ARG
82	1	954	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
4	AA	83	HIS
4	AA	86	GLN
4	AA	97	ASN
4	AA	233	GLN
5	AB	182	GLN
6	AC	92	ASN
6	AC	296	GLN
6	AC	346	GLN
7	AD	90	HIS
8	AE	78	ASN
8	AE	113	GLN
8	AE	166	ASN
9	AF	90	ASN
9	AF	169	ASN
11	AH	50	ASN
11	AH	140	GLN
11	AH	169	ASN
12	AI	12	GLN
12	AI	14	ASN
14	AL	137	GLN
14	AL	162	ASN
15	AM	59	ASN
17	AO	32	GLN
17	AO	51	ASN
17	AO	91	HIS
19	AQ	58	ASN
19	AQ	73	GLN
20	AR	58	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	AT	131	GLN
22	AT	146	ASN
24	AV	98	ASN
34	Bf	106	ASN
40	Bl	4	GLN
40	Bl	11	GLN
41	Bm	119	ASN
43	Bo	47	GLN
43	Bo	82	GLN
43	Bo	102	GLN
45	Bq	27	ASN
45	Bq	35	GLN
45	Bq	44	GLN
45	Bq	182	GLN
45	Bq	188	ASN
46	Br	39	GLN
48	A	109	ASN
48	A	193	GLN
49	B	95	ASN
49	B	178	ASN
50	C	152	ASN
50	C	225	ASN
52	E	224	ASN
53	F	40	GLN
53	F	105	ASN
54	G	4	ASN
54	G	140	ASN
54	G	182	GLN
54	G	197	ASN
55	H	19	GLN
55	H	170	GLN
56	I	160	GLN
58	K	17	GLN
58	K	47	GLN
59	L	14	GLN
62	O	29	HIS
67	T	17	ASN
69	V	33	GLN
69	V	38	GLN
70	W	66	ASN
71	X	22	ASN
72	Y	31	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	f	132	ASN
80	g	32	ASN
80	g	226	GLN
80	g	321	GLN
80	g	326	ASN
82	1	475	GLN
82	1	540	GLN
82	1	786	GLN
82	1	803	HIS
82	1	812	GLN
82	1	899	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3261/3364 (96%)	978 (29%)	153 (4%)
2	7	120/121 (99%)	27 (22%)	2 (1%)
3	8	156/2825 (5%)	41 (26%)	5 (3%)
81	2	1778/1798 (98%)	770 (43%)	94 (5%)
83	3	75/76 (98%)	35 (46%)	6 (8%)
All	All	5390/8184 (65%)	1851 (34%)	260 (4%)

All (1851) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	9	U
1	5	20	A
1	5	22	G
1	5	40	A
1	5	43	A
1	5	45	A
1	5	48	A
1	5	49	A
1	5	51	A
1	5	57	A
1	5	59	G
1	5	60	A
1	5	65	A
1	5	66	A
1	5	67	A
1	5	92	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	96	G
1	5	109	A
1	5	110	G
1	5	117	U
1	5	118	U
1	5	121	A
1	5	122	A
1	5	125	C
1	5	127	G
1	5	133	U
1	5	134	U
1	5	135	C
1	5	136	G
1	5	141	C
1	5	142	C
1	5	143	G
1	5	146	U
1	5	148	G
1	5	150	A
1	5	156	A
1	5	157	A
1	5	161	G
1	5	167	U
1	5	168	U
1	5	169	U
1	5	170	G
1	5	171	U
1	5	174	C
1	5	177	G
1	5	182	U
1	5	187	A
1	5	190	U
1	5	191	U
1	5	192	C
1	5	194	U
1	5	199	A
1	5	200	C
1	5	205	C
1	5	210	U
1	5	211	A
1	5	213	A
1	5	218	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	219	A
1	5	220	G
1	5	221	A
1	5	231	G
1	5	239	U
1	5	240	C
1	5	241	C
1	5	247	A
1	5	248	U
1	5	249	U
1	5	250	U
1	5	251	G
1	5	252	U
1	5	253	A
1	5	254	A
1	5	266	C
1	5	269	G
1	5	284	A
1	5	285	A
1	5	286	U
1	5	294	U
1	5	295	A
1	5	297	G
1	5	298	U
1	5	299	G
1	5	305	U
1	5	314	U
1	5	315	C
1	5	316	U
1	5	317	A
1	5	323	A
1	5	326	U
1	5	329	U
1	5	336	A
1	5	339	C
1	5	340	C
1	5	348	A
1	5	350	C
1	5	352	A
1	5	356	C
1	5	374	A
1	5	375	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	376	G
1	5	379	C
1	5	385	A
1	5	390	G
1	5	391	A
1	5	398	A
1	5	399	A
1	5	401	U
1	5	403	C
1	5	404	G
1	5	411	U
1	5	421	G
1	5	422	A
1	5	423	A
1	5	425	G
1	5	429	U
1	5	433	A
1	5	438	A
1	5	439	C
1	5	440	A
1	5	441	U
1	5	443	G
1	5	478	U
1	5	492	A
1	5	496	C
1	5	503	A
1	5	506	G
1	5	512	C
1	5	514	G
1	5	516	U
1	5	518	C
1	5	519	G
1	5	520	G
1	5	523	G
1	5	524	A
1	5	530	A
1	5	532	A
1	5	533	G
1	5	537	G
1	5	542	A
1	5	543	A
1	5	551	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	552	G
1	5	554	U
1	5	565	A
1	5	570	G
1	5	573	U
1	5	577	G
1	5	582	G
1	5	584	A
1	5	594	A
1	5	595	A
1	5	597	G
1	5	605	G
1	5	609	C
1	5	615	U
1	5	620	A
1	5	622	A
1	5	623	C
1	5	633	A
1	5	634	G
1	5	635	U
1	5	639	A
1	5	640	C
1	5	648	C
1	5	649	G
1	5	650	A
1	5	651	G
1	5	654	U
1	5	660	U
1	5	664	A
1	5	671	U
1	5	672	A
1	5	678	A
1	5	681	G
1	5	682	A
1	5	683	A
1	5	685	G
1	5	688	A
1	5	691	G
1	5	692	U
1	5	693	A
1	5	694	G
1	5	695	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	698	A
1	5	708	A
1	5	709	G
1	5	710	G
1	5	732	A
1	5	736	C
1	5	738	U
1	5	745	G
1	5	747	U
1	5	748	U
1	5	752	G
1	5	756	G
1	5	757	A
1	5	758	G
1	5	770	G
1	5	771	G
1	5	772	A
1	5	777	A
1	5	779	A
1	5	785	U
1	5	788	A
1	5	798	A
1	5	801	A
1	5	808	A
1	5	813	G
1	5	818	A
1	5	819	A
1	5	820	C
1	5	832	C
1	5	835	G
1	5	840	G
1	5	845	U
1	5	850	U
1	5	860	U
1	5	861	C
1	5	866	A
1	5	867	A
1	5	868	U
1	5	870	U
1	5	878	G
1	5	879	G
1	5	885	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	887	G
1	5	888	A
1	5	894	C
1	5	896	A
1	5	900	A
1	5	908	G
1	5	912	G
1	5	915	C
1	5	916	C
1	5	924	G
1	5	930	C
1	5	931	U
1	5	938	A
1	5	949	G
1	5	950	U
1	5	952	U
1	5	953	C
1	5	955	G
1	5	964	G
1	5	965	G
1	5	973	A
1	5	974	A
1	5	981	G
1	5	985	U
1	5	986	A
1	5	987	C
1	5	988	C
1	5	989	G
1	5	990	G
1	5	992	G
1	5	994	U
1	5	995	G
1	5	996	A
1	5	997	A
1	5	999	U
1	5	1000	G
1	5	1004	U
1	5	1005	U
1	5	1006	G
1	5	1008	C
1	5	1011	A
1	5	1018	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1020	C
1	5	1028	A
1	5	1034	G
1	5	1035	A
1	5	1036	A
1	5	1039	C
1	5	1042	U
1	5	1051	A
1	5	1053	U
1	5	1054	G
1	5	1064	A
1	5	1065	U
1	5	1066	U
1	5	1067	U
1	5	1068	G
1	5	1069	A
1	5	1074	A
1	5	1088	G
1	5	1093	U
1	5	1101	A
1	5	1102	G
1	5	1109	U
1	5	1122	U
1	5	1123	G
1	5	1124	A
1	5	1130	A
1	5	1132	G
1	5	1137	G
1	5	1145	G
1	5	1149	G
1	5	1151	A
1	5	1152	U
1	5	1153	A
1	5	1160	C
1	5	1167	C
1	5	1172	C
1	5	1178	G
1	5	1180	G
1	5	1183	A
1	5	1191	U
1	5	1192	A
1	5	1193	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1194	A
1	5	1195	C
1	5	1196	A
1	5	1197	G
1	5	1198	C
1	5	1199	C
1	5	1203	C
1	5	1206	U
1	5	1207	G
1	5	1208	G
1	5	1210	C
1	5	1212	U
1	5	1213	G
1	5	1216	A
1	5	1217	G
1	5	1218	U
1	5	1220	G
1	5	1222	A
1	5	1224	U
1	5	1225	C
1	5	1226	C
1	5	1229	U
1	5	1233	G
1	5	1234	A
1	5	1235	G
1	5	1236	U
1	5	1237	G
1	5	1244	A
1	5	1248	C
1	5	1250	C
1	5	1254	C
1	5	1255	C
1	5	1256	G
1	5	1257	A
1	5	1258	A
1	5	1265	A
1	5	1268	C
1	5	1278	G
1	5	1279	A
1	5	1280	U
1	5	1283	C
1	5	1284	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1287	C
1	5	1297	A
1	5	1301	A
1	5	1302	U
1	5	1316	G
1	5	1318	U
1	5	1319	U
1	5	1320	A
1	5	1322	U
1	5	1323	A
1	5	1324	U
1	5	1325	G
1	5	1327	U
1	5	1328	G
1	5	1334	A
1	5	1348	G
1	5	1354	G
1	5	1356	C
1	5	1357	A
1	5	1360	G
1	5	1361	A
1	5	1362	C
1	5	1370	A
1	5	1383	G
1	5	1389	A
1	5	1390	A
1	5	1401	U
1	5	1402	G
1	5	1405	G
1	5	1408	C
1	5	1412	G
1	5	1421	G
1	5	1425	A
1	5	1431	A
1	5	1444	G
1	5	1447	G
1	5	1448	A
1	5	1451	G
1	5	1452	A
1	5	1453	A
1	5	1454	G
1	5	1455	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1456	G
1	5	1461	A
1	5	1463	G
1	5	1471	G
1	5	1475	A
1	5	1479	C
1	5	1482	U
1	5	1494	U
1	5	1497	U
1	5	1498	C
1	5	1502	C
1	5	1504	U
1	5	1507	G
1	5	1525	U
1	5	1526	U
1	5	1527	C
1	5	1528	A
1	5	1530	A
1	5	1531	G
1	5	1532	G
1	5	1533	C
1	5	1534	C
1	5	1535	U
1	5	1536	A
1	5	1537	A
1	5	1539	U
1	5	1540	U
1	5	1544	A
1	5	1546	G
1	5	1547	C
1	5	1549	A
1	5	1550	C
1	5	1551	C
1	5	1552	A
1	5	1554	C
1	5	1555	G
1	5	1558	A
1	5	1562	A
1	5	1564	U
1	5	1568	G
1	5	1576	U
1	5	1577	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1581	A
1	5	1584	C
1	5	1588	A
1	5	1597	C
1	5	1598	U
1	5	1599	U
1	5	1600	C
1	5	1601	A
1	5	1602	C
1	5	1608	C
1	5	1612	A
1	5	1613	C
1	5	1614	U
1	5	1615	G
1	5	1626	C
1	5	1627	G
1	5	1644	G
1	5	1647	G
1	5	1652	A
1	5	1656	U
1	5	1657	U
1	5	1658	U
1	5	1662	C
1	5	1663	U
1	5	1672	U
1	5	1682	G
1	5	1684	A
1	5	1685	U
1	5	1686	U
1	5	1687	G
1	5	1693	U
1	5	1712	G
1	5	1719	A
1	5	1720	G
1	5	1725	C
1	5	1729	C
1	5	1731	U
1	5	1733	G
1	5	1734	U
1	5	1735	G
1	5	1739	G
1	5	1749	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1760	C
1	5	1761	C
1	5	1766	A
1	5	1767	A
1	5	1777	G
1	5	1781	G
1	5	1782	A
1	5	1783	A
1	5	1784	U
1	5	1785	A
1	5	1786	G
1	5	1787	U
1	5	1788	U
1	5	1789	U
1	5	1790	U
1	5	1792	A
1	5	1807	G
1	5	1809	U
1	5	1810	A
1	5	1811	A
1	5	1814	G
1	5	1815	C
1	5	1817	G
1	5	1818	C
1	5	1835	C
1	5	1837	G
1	5	1840	U
1	5	1843	A
1	5	1847	G
1	5	1848	A
1	5	1849	U
1	5	1854	U
1	5	1855	A
1	5	1861	G
1	5	1862	A
1	5	1864	A
1	5	1874	G
1	5	1875	G
1	5	1878	A
1	5	1879	A
1	5	1884	A
1	5	1895	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1898	G
1	5	1919	U
1	5	1922	G
1	5	1923	A
1	5	1925	G
1	5	1926	U
1	5	1927	G
1	5	1928	A
1	5	1929	G
1	5	1939	C
1	5	1943	C
1	5	1947	G
1	5	2020	U
1	5	2022	G
1	5	2025	G
1	5	2027	C
1	5	2029	G
1	5	2030	C
1	5	2033	U
1	5	2034	G
1	5	2036	U
1	5	2038	G
1	5	2039	G
1	5	2041	C
1	5	2042	U
1	5	2045	U
1	5	2051	U
1	5	2054	U
1	5	2058	A
1	5	2059	U
1	5	2060	U
1	5	2061	A
1	5	2062	A
1	5	2063	C
1	5	2064	G
1	5	2066	U
1	5	2067	C
1	5	2069	A
1	5	2070	C
1	5	2071	U
1	5	2080	G
1	5	2081	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2082	A
1	5	2083	C
1	5	2089	A
1	5	2090	G
1	5	2091	G
1	5	2097	C
1	5	2100	A
1	5	2107	A
1	5	2108	A
1	5	2111	A
1	5	2125	C
1	5	2127	A
1	5	2129	G
1	5	2133	A
1	5	2137	A
1	5	2143	G
1	5	2145	U
1	5	2149	G
1	5	2154	G
1	5	2161	C
1	5	2162	U
1	5	2163	G
1	5	2167	A
1	5	2174	U
1	5	2175	G
1	5	2177	A
1	5	2180	U
1	5	2182	A
1	5	2185	G
1	5	2192	A
1	5	2193	A
1	5	2194	U
1	5	2196	C
1	5	2198	A
1	5	2201	A
1	5	2202	A
1	5	2217	C
1	5	2218	G
1	5	2221	A
1	5	2222	G
1	5	2225	A
1	5	2226	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2227	U
1	5	2228	A
1	5	2229	U
1	5	2230	G
1	5	2231	A
1	5	2232	C
1	5	2235	U
1	5	2236	C
1	5	2237	U
1	5	2238	U
1	5	2239	A
1	5	2241	G
1	5	2242	G
1	5	2243	U
1	5	2248	A
1	5	2250	A
1	5	2251	U
1	5	2252	G
1	5	2255	U
1	5	2256	C
1	5	2257	G
1	5	2267	U
1	5	2275	C
1	5	2276	G
1	5	2279	U
1	5	2282	A
1	5	2284	G
1	5	2285	G
1	5	2290	A
1	5	2300	C
1	5	2301	A
1	5	2303	U
1	5	2304	G
1	5	2305	U
1	5	2326	A
1	5	2342	A
1	5	2343	C
1	5	2344	G
1	5	2346	G
1	5	2347	C
1	5	2352	C
1	5	2354	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2357	U
1	5	2360	G
1	5	2362	G
1	5	2364	G
1	5	2366	A
1	5	2369	G
1	5	2370	A
1	5	2371	A
1	5	2372	G
1	5	2373	A
1	5	2379	U
1	5	2380	U
1	5	2381	G
1	5	2382	A
1	5	2387	G
1	5	2388	A
1	5	2397	U
1	5	2404	G
1	5	2408	A
1	5	2409	G
1	5	2412	A
1	5	2413	C
1	5	2414	A
1	5	2415	U
1	5	2416	A
1	5	2417	G
1	5	2418	A
1	5	2419	G
1	5	2420	G
1	5	2421	G
1	5	2422	U
1	5	2423	G
1	5	2426	G
1	5	2427	C
1	5	2428	A
1	5	2429	U
1	5	2438	G
1	5	2442	C
1	5	2446	G
1	5	2451	U
1	5	2452	G
1	5	2456	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2457	A
1	5	2459	C
1	5	2460	A
1	5	2463	A
1	5	2466	U
1	5	2468	U
1	5	2469	A
1	5	2470	U
1	5	2471	A
1	5	2472	G
1	5	2473	U
1	5	2474	U
1	5	2475	U
1	5	2476	C
1	5	2477	U
1	5	2478	U
1	5	2483	U
1	5	2484	A
1	5	2491	U
1	5	2492	A
1	5	2493	A
1	5	2494	G
1	5	2495	C
1	5	2498	A
1	5	2499	G
1	5	2500	C
1	5	2501	U
1	5	2502	G
1	5	2503	G
1	5	2505	A
1	5	2506	U
1	5	2507	U
1	5	2508	C
1	5	2509	A
1	5	2510	U
1	5	2511	U
1	5	2512	U
1	5	2513	U
1	5	2514	C
1	5	2521	C
1	5	2522	U
1	5	2523	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2524	G
1	5	2529	C
1	5	2530	A
1	5	2531	A
1	5	2532	A
1	5	2535	C
1	5	2536	C
1	5	2537	U
1	5	2540	A
1	5	2541	C
1	5	2542	G
1	5	2549	U
1	5	2553	G
1	5	2557	G
1	5	2562	C
1	5	2563	A
1	5	2568	C
1	5	2571	G
1	5	2574	G
1	5	2575	G
1	5	2582	G
1	5	2595	C
1	5	2596	A
1	5	2597	U
1	5	2607	G
1	5	2616	G
1	5	2620	U
1	5	2621	C
1	5	2623	U
1	5	2624	A
1	5	2625	A
1	5	2631	A
1	5	2633	U
1	5	2635	A
1	5	2636	U
1	5	2642	A
1	5	2645	G
1	5	2646	A
1	5	2647	A
1	5	2649	U
1	5	2657	A
1	5	2658	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2659	A
1	5	2662	A
1	5	2664	A
1	5	2667	G
1	5	2671	A
1	5	2672	A
1	5	2676	C
1	5	2678	C
1	5	2682	G
1	5	2687	U
1	5	2691	U
1	5	2696	G
1	5	2697	U
1	5	2707	A
1	5	2708	A
1	5	2715	A
1	5	2720	U
1	5	2721	G
1	5	2730	A
1	5	2740	U
1	5	2744	C
1	5	2745	G
1	5	2746	G
1	5	2750	U
1	5	2758	A
1	5	2764	G
1	5	2767	A
1	5	2768	G
1	5	2769	A
1	5	2771	A
1	5	2772	A
1	5	2778	C
1	5	2782	G
1	5	2785	A
1	5	2789	C
1	5	2790	U
1	5	2812	C
1	5	2813	A
1	5	2815	A
1	5	2817	C
1	5	2824	G
1	5	2829	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2839	G
1	5	2843	U
1	5	2845	G
1	5	2855	A
1	5	2866	G
1	5	2867	C
1	5	2869	G
1	5	2871	A
1	5	2872	U
1	5	2879	A
1	5	2884	U
1	5	2891	U
1	5	2903	U
1	5	2904	A
1	5	2910	C
1	5	2911	G
1	5	2915	G
1	5	2922	U
1	5	2923	U
1	5	2925	G
1	5	2934	G
1	5	2940	G
1	5	2946	U
1	5	2947	U
1	5	2948	U
1	5	2949	U
1	5	2950	A
1	5	2951	C
1	5	2964	U
1	5	2965	G
1	5	2967	U
1	5	2969	U
1	5	2979	A
1	5	2980	A
1	5	2985	A
1	5	2996	G
1	5	3006	U
1	5	3007	C
1	5	3024	U
1	5	3025	U
1	5	3027	G
1	5	3030	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	3040	C
1	5	3041	A
1	5	3046	U
1	5	3047	U
1	5	3053	G
1	5	3054	A
1	5	3060	C
1	5	3063	U
1	5	3067	C
1	5	3070	G
1	5	3077	G
1	5	3078	C
1	5	3084	G
1	5	3085	C
1	5	3090	A
1	5	3092	G
1	5	3095	A
1	5	3097	A
1	5	3099	U
1	5	3107	A
1	5	3110	A
1	5	3121	U
1	5	3123	U
1	5	3124	U
1	5	3125	U
1	5	3126	G
1	5	3127	C
1	5	3133	A
1	5	3134	C
1	5	3136	A
1	5	3140	A
1	5	3141	G
1	5	3142	A
1	5	3144	G
1	5	3147	U
1	5	3148	A
1	5	3149	A
1	5	3150	G
1	5	3155	A
1	5	3162	U
1	5	3163	U
1	5	3164	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	3165	U
1	5	3166	U
1	5	3170	G
1	5	3174	C
1	5	3175	U
1	5	3176	G
1	5	3177	A
1	5	3180	C
1	5	3181	A
1	5	3182	U
1	5	3184	G
1	5	3185	C
1	5	3186	A
1	5	3187	G
1	5	3191	G
1	5	3192	G
1	5	3197	G
1	5	3199	U
1	5	3202	U
1	5	3204	U
1	5	3205	U
1	5	3206	A
1	5	3207	G
1	5	3208	C
1	5	3212	A
1	5	3213	A
1	5	3215	G
1	5	3216	C
1	5	3217	U
1	5	3220	G
1	5	3221	G
1	5	3227	U
1	5	3228	G
1	5	3231	G
1	5	3236	A
1	5	3237	U
1	5	3238	U
1	5	3243	U
1	5	3245	U
1	5	3247	A
1	5	3250	U
1	5	3252	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	3253	C
1	5	3254	G
1	5	3256	A
1	5	3258	G
1	5	3260	A
1	5	3262	A
1	5	3265	U
1	5	3272	U
1	5	3275	A
1	5	3281	U
1	5	3284	A
1	5	3285	U
1	5	3286	G
1	5	3287	U
1	5	3294	G
1	5	3303	A
1	5	3304	A
1	5	3309	U
1	5	3310	A
1	5	3313	G
1	5	3316	G
1	5	3318	C
1	5	3319	U
1	5	3322	U
1	5	3323	U
1	5	3324	G
1	5	3325	U
1	5	3326	U
1	5	3330	A
1	5	3337	G
1	5	3346	C
1	5	3350	C
1	5	3351	G
1	5	3357	U
1	5	3358	G
1	5	3361	U
1	5	3362	U
1	5	3364	U
2	7	7	G
2	7	13	A
2	7	18	C
2	7	22	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	7	27	A
2	7	31	U
2	7	41	G
2	7	54	U
2	7	61	G
2	7	64	A
2	7	65	G
2	7	73	C
2	7	74	C
2	7	76	A
2	7	79	A
2	7	91	G
2	7	92	A
2	7	93	C
2	7	94	C
2	7	101	G
2	7	102	A
2	7	104	A
2	7	110	G
2	7	112	G
2	7	113	C
2	7	118	A
2	7	119	U
3	8	8	C
3	8	21	C
3	8	23	U
3	8	25	G
3	8	34	U
3	8	35	C
3	8	39	G
3	8	40	A
3	8	48	A
3	8	50	C
3	8	56	G
3	8	59	A
3	8	62	U
3	8	63	G
3	8	81	U
3	8	82	U
3	8	84	C
3	8	86	U
3	8	87	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	8	91	C
3	8	95	A
3	8	96	A
3	8	97	A
3	8	104	A
3	8	106	C
3	8	111	A
3	8	112	U
3	8	113	U
3	8	116	G
3	8	121	C
3	8	126	A
3	8	127	U
3	8	129	C
3	8	144	G
3	8	147	U
3	8	148	G
3	8	151	C
3	8	152	G
3	8	155	A
3	8	156	U
3	8	157	U
81	2	2	A
81	2	3	U
81	2	4	C
81	2	9	U
81	2	11	A
81	2	17	C
81	2	18	C
81	2	24	U
81	2	25	C
81	2	26	A
81	2	31	C
81	2	34	G
81	2	36	C
81	2	39	A
81	2	40	A
81	2	42	G
81	2	47	A
81	2	48	G
81	2	51	A
81	2	54	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	56	U
81	2	57	G
81	2	59	C
81	2	60	U
81	2	61	A
81	2	62	A
81	2	63	G
81	2	64	U
81	2	65	A
81	2	66	U
81	2	67	A
81	2	68	A
81	2	69	G
81	2	72	A
81	2	73	U
81	2	74	U
81	2	75	U
81	2	76	A
81	2	77	U
81	2	93	A
81	2	95	G
81	2	104	A
81	2	110	U
81	2	111	U
81	2	114	C
81	2	115	G
81	2	116	U
81	2	118	U
81	2	124	A
81	2	125	U
81	2	126	A
81	2	127	G
81	2	128	U
81	2	129	U
81	2	131	C
81	2	132	U
81	2	133	U
81	2	134	U
81	2	136	C
81	2	137	U
81	2	138	A
81	2	139	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	140	A
81	2	141	U
81	2	146	A
81	2	148	C
81	2	149	U
81	2	152	G
81	2	156	A
81	2	158	U
81	2	159	C
81	2	160	U
81	2	161	A
81	2	167	A
81	2	173	U
81	2	175	C
81	2	176	U
81	2	177	U
81	2	178	A
81	2	179	A
81	2	184	U
81	2	186	G
81	2	187	A
81	2	190	C
81	2	191	U
81	2	192	U
81	2	193	U
81	2	194	G
81	2	196	A
81	2	199	A
81	2	203	G
81	2	208	U
81	2	209	A
81	2	216	A
81	2	217	A
81	2	218	A
81	2	219	A
81	2	220	A
81	2	227	G
81	2	228	U
81	2	230	U
81	2	232	C
81	2	233	G
81	2	234	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	235	A
81	2	238	C
81	2	239	C
81	2	240	U
81	2	244	U
81	2	247	U
81	2	249	C
81	2	256	A
81	2	257	C
81	2	258	U
81	2	259	U
81	2	261	U
81	2	263	G
81	2	264	A
81	2	265	A
81	2	266	U
81	2	267	C
81	2	268	G
81	2	269	C
81	2	270	A
81	2	271	U
81	2	272	G
81	2	274	C
81	2	275	C
81	2	276	U
81	2	277	U
81	2	278	G
81	2	279	U
81	2	280	G
81	2	281	C
81	2	286	G
81	2	288	U
81	2	298	A
81	2	301	U
81	2	308	C
81	2	309	C
81	2	311	A
81	2	312	U
81	2	313	C
81	2	315	A
81	2	318	U
81	2	319	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	320	C
81	2	321	G
81	2	324	G
81	2	328	G
81	2	332	A
81	2	336	G
81	2	339	U
81	2	344	U
81	2	346	G
81	2	359	A
81	2	360	C
81	2	362	G
81	2	369	A
81	2	371	G
81	2	377	A
81	2	383	G
81	2	384	A
81	2	386	A
81	2	392	C
81	2	395	G
81	2	397	G
81	2	399	A
81	2	400	A
81	2	401	C
81	2	403	G
81	2	404	C
81	2	412	U
81	2	415	A
81	2	416	A
81	2	417	G
81	2	418	G
81	2	421	G
81	2	423	C
81	2	425	G
81	2	427	A
81	2	430	C
81	2	432	C
81	2	433	G
81	2	438	U
81	2	439	U
81	2	443	C
81	2	447	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	452	U
81	2	453	U
81	2	454	C
81	2	461	G
81	2	467	A
81	2	468	C
81	2	473	A
81	2	474	A
81	2	475	U
81	2	476	A
81	2	479	G
81	2	484	A
81	2	487	G
81	2	490	C
81	2	491	A
81	2	492	U
81	2	493	U
81	2	494	C
81	2	497	G
81	2	498	U
81	2	499	C
81	2	500	U
81	2	502	G
81	2	504	A
81	2	505	A
81	2	506	U
81	2	507	U
81	2	509	G
81	2	510	A
81	2	511	A
81	2	514	A
81	2	515	G
81	2	518	C
81	2	526	A
81	2	533	A
81	2	538	G
81	2	539	G
81	2	540	A
81	2	541	A
81	2	542	C
81	2	543	A
81	2	544	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	547	G
81	2	554	A
81	2	556	G
81	2	557	U
81	2	558	C
81	2	559	U
81	2	561	G
81	2	563	G
81	2	565	C
81	2	570	G
81	2	571	C
81	2	573	G
81	2	575	G
81	2	576	G
81	2	577	U
81	2	578	A
81	2	579	A
81	2	585	G
81	2	593	A
81	2	594	G
81	2	596	G
81	2	607	U
81	2	609	G
81	2	610	U
81	2	618	A
81	2	619	A
81	2	622	A
81	2	623	G
81	2	625	U
81	2	634	A
81	2	638	U
81	2	639	U
81	2	640	G
81	2	643	U
81	2	644	C
81	2	647	G
81	2	648	U
81	2	649	U
81	2	650	G
81	2	652	C
81	2	653	C
81	2	654	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	655	G
81	2	677	G
81	2	679	U
81	2	681	U
81	2	684	A
81	2	686	C
81	2	690	A
81	2	691	U
81	2	693	U
81	2	695	U
81	2	696	C
81	2	697	C
81	2	698	U
81	2	701	U
81	2	704	C
81	2	705	U
81	2	708	C
81	2	709	C
81	2	712	U
81	2	714	C
81	2	716	C
81	2	717	C
81	2	718	U
81	2	719	U
81	2	721	U
81	2	722	G
81	2	723	G
81	2	724	G
81	2	725	U
81	2	727	C
81	2	729	G
81	2	730	G
81	2	731	C
81	2	732	G
81	2	733	A
81	2	734	A
81	2	736	C
81	2	738	G
81	2	740	A
81	2	741	C
81	2	742	U
81	2	743	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	750	U
81	2	753	A
81	2	754	A
81	2	756	A
81	2	757	A
81	2	765	G
81	2	766	U
81	2	767	U
81	2	768	C
81	2	769	A
81	2	771	A
81	2	774	A
81	2	778	G
81	2	779	A
81	2	780	A
81	2	781	A
81	2	782	G
81	2	786	G
81	2	787	A
81	2	788	A
81	2	790	A
81	2	791	U
81	2	793	U
81	2	794	U
81	2	795	A
81	2	798	A
81	2	800	G
81	2	802	A
81	2	803	A
81	2	810	A
81	2	811	A
81	2	812	U
81	2	813	A
81	2	815	G
81	2	817	C
81	2	819	U
81	2	820	U
81	2	821	U
81	2	822	G
81	2	823	G
81	2	825	U
81	2	828	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	829	U
81	2	830	U
81	2	831	U
81	2	832	U
81	2	833	G
81	2	834	U
81	2	837	G
81	2	838	U
81	2	842	U
81	2	843	A
81	2	844	G
81	2	845	G
81	2	846	A
81	2	848	C
81	2	849	A
81	2	850	U
81	2	851	C
81	2	852	G
81	2	854	A
81	2	855	A
81	2	862	A
81	2	863	U
81	2	864	A
81	2	875	G
81	2	876	G
81	2	886	A
81	2	887	U
81	2	888	U
81	2	894	G
81	2	895	U
81	2	897	A
81	2	900	G
81	2	903	G
81	2	904	A
81	2	905	A
81	2	906	A
81	2	907	U
81	2	908	U
81	2	909	C
81	2	910	U
81	2	912	G
81	2	913	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	914	A
81	2	915	U
81	2	920	U
81	2	927	U
81	2	930	C
81	2	932	A
81	2	934	U
81	2	941	G
81	2	942	C
81	2	944	U
81	2	948	C
81	2	950	A
81	2	951	A
81	2	958	U
81	2	959	U
81	2	963	U
81	2	965	A
81	2	969	A
81	2	981	U
81	2	983	G
81	2	984	G
81	2	991	A
81	2	992	A
81	2	994	A
81	2	996	G
81	2	1003	U
81	2	1004	A
81	2	1005	C
81	2	1006	C
81	2	1011	U
81	2	1015	C
81	2	1016	U
81	2	1019	A
81	2	1020	C
81	2	1025	A
81	2	1026	A
81	2	1027	C
81	2	1029	A
81	2	1030	U
81	2	1031	G
81	2	1038	A
81	2	1039	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	1041	G
81	2	1044	C
81	2	1048	U
81	2	1049	G
81	2	1050	G
81	2	1051	U
81	2	1052	G
81	2	1054	U
81	2	1057	U
81	2	1058	C
81	2	1060	U
81	2	1066	C
81	2	1075	A
81	2	1079	U
81	2	1080	A
81	2	1081	C
81	2	1082	G
81	2	1087	A
81	2	1091	A
81	2	1096	U
81	2	1097	U
81	2	1099	G
81	2	1108	G
81	2	1110	G
81	2	1112	A
81	2	1113	G
81	2	1114	U
81	2	1123	A
81	2	1125	G
81	2	1130	A
81	2	1134	U
81	2	1137	A
81	2	1138	A
81	2	1139	G
81	2	1142	A
81	2	1149	G
81	2	1150	A
81	2	1154	G
81	2	1157	C
81	2	1158	C
81	2	1161	C
81	2	1163	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	1164	G
81	2	1166	G
81	2	1169	G
81	2	1172	C
81	2	1173	C
81	2	1175	G
81	2	1184	U
81	2	1185	U
81	2	1186	U
81	2	1189	C
81	2	1190	U
81	2	1191	C
81	2	1193	A
81	2	1195	A
81	2	1196	C
81	2	1198	G
81	2	1199	G
81	2	1201	A
81	2	1202	A
81	2	1203	A
81	2	1206	C
81	2	1208	C
81	2	1209	C
81	2	1210	A
81	2	1212	G
81	2	1215	C
81	2	1216	A
81	2	1217	G
81	2	1218	A
81	2	1222	A
81	2	1223	A
81	2	1225	A
81	2	1227	G
81	2	1228	G
81	2	1229	A
81	2	1232	G
81	2	1234	C
81	2	1236	G
81	2	1237	A
81	2	1240	G
81	2	1241	A
81	2	1242	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	1243	A
81	2	1244	G
81	2	1245	C
81	2	1247	C
81	2	1250	U
81	2	1254	G
81	2	1255	A
81	2	1258	U
81	2	1259	U
81	2	1260	G
81	2	1261	U
81	2	1268	U
81	2	1269	G
81	2	1271	U
81	2	1272	G
81	2	1277	G
81	2	1282	U
81	2	1284	U
81	2	1286	A
81	2	1289	U
81	2	1292	U
81	2	1293	G
81	2	1306	U
81	2	1311	A
81	2	1313	U
81	2	1314	U
81	2	1320	A
81	2	1321	A
81	2	1322	C
81	2	1323	G
81	2	1330	A
81	2	1336	A
81	2	1339	U
81	2	1340	A
81	2	1342	U
81	2	1344	A
81	2	1345	A
81	2	1347	A
81	2	1348	G
81	2	1349	G
81	2	1351	U
81	2	1352	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	1353	G
81	2	1355	U
81	2	1356	G
81	2	1359	A
81	2	1360	C
81	2	1361	U
81	2	1362	U
81	2	1363	G
81	2	1364	C
81	2	1365	C
81	2	1366	G
81	2	1367	G
81	2	1369	U
81	2	1370	G
81	2	1373	U
81	2	1374	C
81	2	1375	U
81	2	1378	U
81	2	1384	G
81	2	1388	U
81	2	1389	A
81	2	1390	U
81	2	1395	U
81	2	1396	U
81	2	1397	C
81	2	1398	A
81	2	1400	G
81	2	1402	C
81	2	1403	G
81	2	1406	G
81	2	1410	G
81	2	1411	U
81	2	1412	U
81	2	1413	U
81	2	1419	A
81	2	1425	A
81	2	1426	G
81	2	1430	U
81	2	1432	U
81	2	1433	G
81	2	1434	A
81	2	1438	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	1441	U
81	2	1443	G
81	2	1444	A
81	2	1447	U
81	2	1448	U
81	2	1449	C
81	2	1451	G
81	2	1453	G
81	2	1454	C
81	2	1455	C
81	2	1456	G
81	2	1457	C
81	2	1458	A
81	2	1459	C
81	2	1463	C
81	2	1469	A
81	2	1471	U
81	2	1474	C
81	2	1476	G
81	2	1481	A
81	2	1484	G
81	2	1485	A
81	2	1487	U
81	2	1488	A
81	2	1489	C
81	2	1490	A
81	2	1491	A
81	2	1492	C
81	2	1494	U
81	2	1495	U
81	2	1502	G
81	2	1503	A
81	2	1504	G
81	2	1506	U
81	2	1507	C
81	2	1508	U
81	2	1509	G
81	2	1512	U
81	2	1514	A
81	2	1515	U
81	2	1516	C
81	2	1519	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	1521	G
81	2	1522	A
81	2	1528	C
81	2	1532	G
81	2	1533	U
81	2	1534	G
81	2	1535	C
81	2	1536	U
81	2	1538	G
81	2	1540	G
81	2	1543	A
81	2	1546	G
81	2	1551	G
81	2	1553	A
81	2	1555	U
81	2	1556	U
81	2	1557	A
81	2	1566	C
81	2	1567	A
81	2	1569	C
81	2	1580	U
81	2	1581	A
81	2	1583	U
81	2	1588	G
81	2	1590	A
81	2	1595	A
81	2	1598	A
81	2	1599	G
81	2	1600	C
81	2	1604	C
81	2	1606	U
81	2	1608	G
81	2	1611	U
81	2	1612	A
81	2	1614	G
81	2	1615	U
81	2	1616	C
81	2	1619	U
81	2	1620	G
81	2	1621	C
81	2	1622	C
81	2	1626	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	1629	A
81	2	1633	A
81	2	1636	G
81	2	1637	C
81	2	1638	C
81	2	1640	G
81	2	1643	G
81	2	1647	G
81	2	1649	A
81	2	1655	U
81	2	1656	G
81	2	1660	G
81	2	1668	G
81	2	1672	C
81	2	1674	U
81	2	1679	A
81	2	1682	U
81	2	1685	U
81	2	1686	U
81	2	1687	A
81	2	1688	G
81	2	1689	A
81	2	1692	A
81	2	1693	G
81	2	1694	G
81	2	1695	G
81	2	1696	G
81	2	1697	G
81	2	1698	C
81	2	1699	A
81	2	1700	A
81	2	1701	C
81	2	1702	U
81	2	1703	C
81	2	1705	A
81	2	1706	U
81	2	1707	C
81	2	1708	U
81	2	1709	C
81	2	1710	A
81	2	1711	G
81	2	1712	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	1713	G
81	2	1714	C
81	2	1715	G
81	2	1716	A
81	2	1721	U
81	2	1729	A
81	2	1736	U
81	2	1738	A
81	2	1746	G
81	2	1748	A
81	2	1751	A
81	2	1752	A
81	2	1753	A
81	2	1754	A
81	2	1758	G
81	2	1760	A
81	2	1763	A
81	2	1764	A
81	2	1766	G
81	2	1767	U
81	2	1768	U
81	2	1776	G
81	2	1778	G
81	2	1780	A
81	2	1781	C
81	2	1784	G
81	2	1786	G
81	2	1789	A
81	2	1790	G
81	2	1791	G
81	2	1792	A
81	2	1793	U
81	2	1794	C
81	2	1795	A
81	2	1796	U
81	2	1798	A
83	3	2	C
83	3	8	U
83	3	13	C
83	3	15	G
83	3	16	A
83	3	17	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
83	3	18	G
83	3	19	G
83	3	20	U
83	3	21	A
83	3	26	A
83	3	29	G
83	3	30	G
83	3	34	G
83	3	35	A
83	3	38	A
83	3	39	U
83	3	40	C
83	3	42	C
83	3	46	G
83	3	48	C
83	3	52	G
83	3	53	G
83	3	54	U
83	3	57	G
83	3	58	A
83	3	59	U
83	3	60	U
83	3	61	C
83	3	70	G
83	3	71	G
83	3	72	C
83	3	74	C
83	3	75	C
83	3	76	A

All (260) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	65	A
1	5	121	A
1	5	148	G
1	5	166	C
1	5	240	C
1	5	248	U
1	5	249	U
1	5	283	G
1	5	297	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	298	U
1	5	397	A
1	5	401	U
1	5	406	G
1	5	489	G
1	5	517	U
1	5	518	C
1	5	561	G
1	5	567	U
1	5	580	A
1	5	593	U
1	5	634	G
1	5	691	G
1	5	692	U
1	5	707	A
1	5	731	G
1	5	735	U
1	5	756	G
1	5	867	A
1	5	887	G
1	5	932	C
1	5	949	G
1	5	951	A
1	5	964	G
1	5	985	U
1	5	987	C
1	5	998	A
1	5	1035	A
1	5	1066	U
1	5	1068	G
1	5	1123	G
1	5	1131	C
1	5	1152	U
1	5	1167	C
1	5	1179	U
1	5	1191	U
1	5	1193	G
1	5	1194	A
1	5	1212	U
1	5	1234	A
1	5	1255	C
1	5	1278	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	1300	U
1	5	1319	U
1	5	1323	A
1	5	1326	A
1	5	1451	G
1	5	1453	A
1	5	1526	U
1	5	1531	G
1	5	1539	U
1	5	1551	C
1	5	1576	U
1	5	1600	C
1	5	1611	A
1	5	1612	A
1	5	1626	C
1	5	1664	U
1	5	1685	U
1	5	1720	G
1	5	1762	C
1	5	1785	A
1	5	1790	U
1	5	1809	U
1	5	1810	A
1	5	1815	C
1	5	1894	U
1	5	2032	U
1	5	2040	U
1	5	2041	C
1	5	2059	U
1	5	2061	A
1	5	2081	U
1	5	2107	A
1	5	2113	A
1	5	2173	C
1	5	2217	C
1	5	2225	A
1	5	2228	A
1	5	2230	G
1	5	2231	A
1	5	2237	U
1	5	2250	A
1	5	2251	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	2274	G
1	5	2341	A
1	5	2343	C
1	5	2416	A
1	5	2422	U
1	5	2437	A
1	5	2455	A
1	5	2456	U
1	5	2468	U
1	5	2469	A
1	5	2472	G
1	5	2474	U
1	5	2477	U
1	5	2483	U
1	5	2506	U
1	5	2507	U
1	5	2511	U
1	5	2512	U
1	5	2522	U
1	5	2529	C
1	5	2530	A
1	5	2538	A
1	5	2539	U
1	5	2540	A
1	5	2553	G
1	5	2561	A
1	5	2595	C
1	5	2603	A
1	5	2644	A
1	5	2645	G
1	5	2672	A
1	5	2696	G
1	5	2745	G
1	5	2879	A
1	5	2909	A
1	5	2918	G
1	5	2922	U
1	5	2939	A
1	5	2946	U
1	5	2947	U
1	5	3024	U
1	5	3046	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	3061	C
1	5	3084	G
1	5	3122	C
1	5	3162	U
1	5	3174	C
1	5	3176	G
1	5	3184	G
1	5	3186	A
1	5	3196	C
1	5	3237	U
1	5	3242	A
1	5	3252	G
1	5	3257	A
1	5	3285	U
1	5	3308	G
1	5	3309	U
1	5	3325	U
1	5	3349	U
2	7	13	A
2	7	111	U
3	8	22	U
3	8	39	G
3	8	112	U
3	8	125	U
3	8	126	A
81	2	3	U
81	2	61	A
81	2	65	A
81	2	66	U
81	2	72	A
81	2	73	U
81	2	130	C
81	2	131	C
81	2	177	U
81	2	216	A
81	2	217	A
81	2	258	U
81	2	263	G
81	2	271	U
81	2	277	U
81	2	278	G
81	2	279	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	452	U
81	2	497	G
81	2	537	A
81	2	542	C
81	2	556	G
81	2	564	C
81	2	570	G
81	2	605	A
81	2	621	A
81	2	694	U
81	2	695	U
81	2	697	C
81	2	700	C
81	2	708	C
81	2	721	U
81	2	740	A
81	2	742	U
81	2	765	G
81	2	794	U
81	2	810	A
81	2	818	G
81	2	828	A
81	2	854	A
81	2	903	G
81	2	909	C
81	2	911	U
81	2	912	G
81	2	943	A
81	2	958	U
81	2	1056	U
81	2	1060	U
81	2	1080	A
81	2	1107	G
81	2	1157	C
81	2	1185	U
81	2	1189	C
81	2	1192	A
81	2	1195	A
81	2	1216	A
81	2	1228	G
81	2	1241	A
81	2	1243	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
81	2	1343	A
81	2	1369	U
81	2	1374	C
81	2	1389	A
81	2	1397	C
81	2	1410	G
81	2	1412	U
81	2	1429	C
81	2	1444	A
81	2	1447	U
81	2	1455	C
81	2	1456	G
81	2	1491	A
81	2	1514	A
81	2	1520	U
81	2	1532	G
81	2	1534	G
81	2	1535	C
81	2	1554	A
81	2	1580	U
81	2	1598	A
81	2	1613	C
81	2	1628	U
81	2	1643	G
81	2	1655	U
81	2	1678	G
81	2	1686	U
81	2	1713	G
81	2	1714	C
81	2	1752	A
81	2	1753	A
81	2	1765	G
81	2	1767	U
81	2	1791	G
81	2	1792	A
83	3	16	A
83	3	19	G
83	3	34	G
83	3	58	A
83	3	71	G
83	3	74	C

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 7 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
85	GCP	1	1001	-	27,34,34	1.60	6 (22%)	34,54,54	1.93	9 (26%)

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
85	GCP	1	1001	-	-	6/15/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	1	1001	GCP	C5-C6	4.48	1.49	1.41
85	1	1001	GCP	PB-O3A	3.01	1.61	1.58
85	1	1001	GCP	PG-O2G	2.85	1.61	1.54
85	1	1001	GCP	PG-O3G	2.80	1.61	1.54
85	1	1001	GCP	C5-C4	2.61	1.47	1.40
85	1	1001	GCP	PB-O2B	2.14	1.61	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	1	1001	GCP	C2-N3-C4	5.14	121.23	115.36
85	1	1001	GCP	C4-C5-C6	-3.99	116.99	120.80
85	1	1001	GCP	C2-N1-C6	3.87	122.07	115.93
85	1	1001	GCP	C5-C6-N1	-3.61	118.49	123.43
85	1	1001	GCP	N3-C2-N1	-3.49	122.57	127.22
85	1	1001	GCP	PB-O3A-PA	-3.15	122.58	132.56
85	1	1001	GCP	C3'-C2'-C1'	2.89	105.33	100.98
85	1	1001	GCP	C4-C5-N7	-2.69	106.60	109.40
85	1	1001	GCP	O3G-PG-C3B	2.05	111.37	106.40

There are no chirality outliers.

All (6) torsion outliers are listed below:

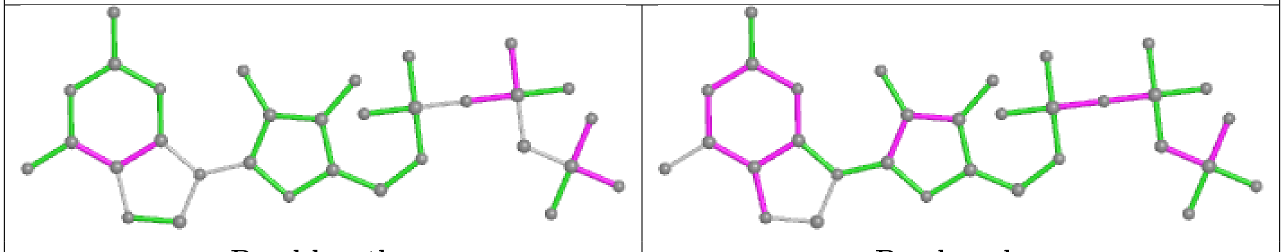
Mol	Chain	Res	Type	Atoms
85	1	1001	GCP	PB-C3B-PG-O1G
85	1	1001	GCP	PB-C3B-PG-O2G
85	1	1001	GCP	PB-C3B-PG-O3G
85	1	1001	GCP	PG-C3B-PB-O3A
85	1	1001	GCP	O4'-C4'-C5'-O5'
85	1	1001	GCP	PG-C3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

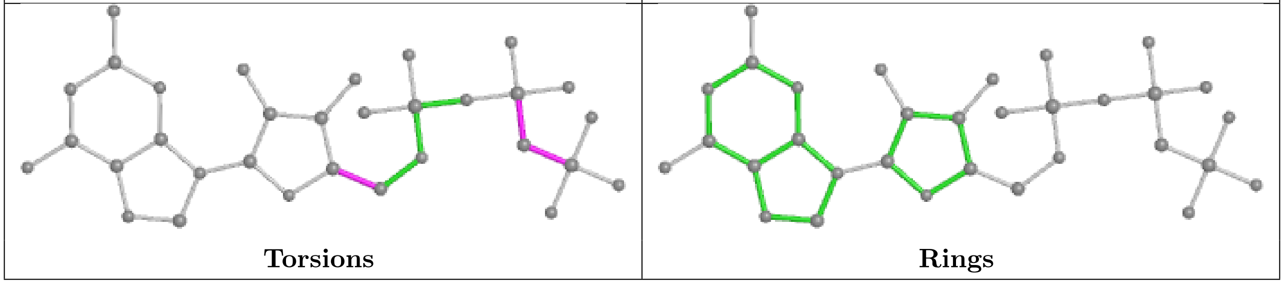
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GCP 1 1001



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
1	5	2
47	AK	2
8	AE	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AE	116:GLU	C	117:ALA	N	6.39
1	5	2049:G	O3’	2050:A	P	6.33
1	AK	52:UNK	C	54:UNK	N	5.65
1	AK	23:UNK	C	28:UNK	N	3.69
1	5	2196:C	O3’	2197:A	P	3.40

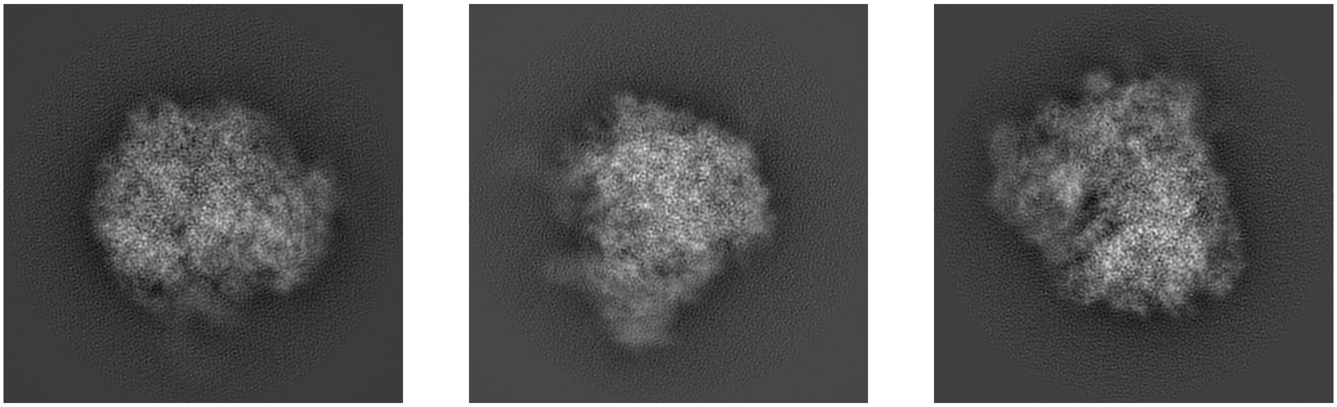
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20952. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

6.1.1 Primary map

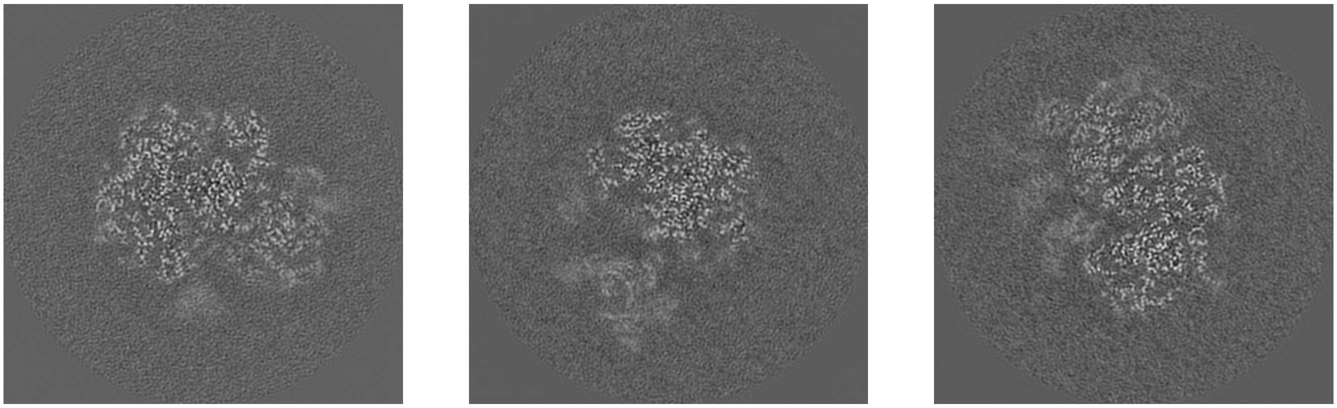


X Y Z

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

6.2 Central slices

6.2.1 Primary map

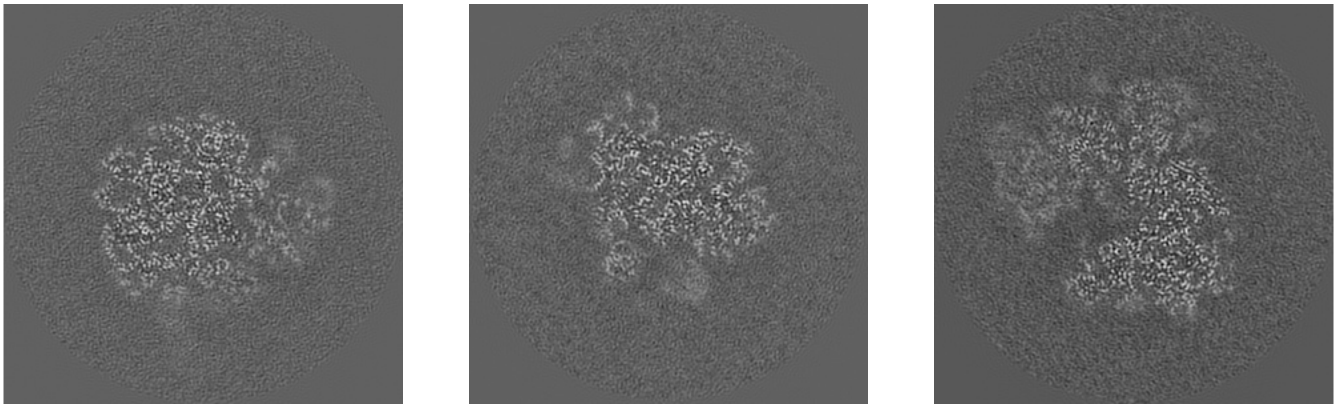


X Index: 200 Y Index: 200 Z Index: 200

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

6.3 Largest variance slices

6.3.1 Primary map

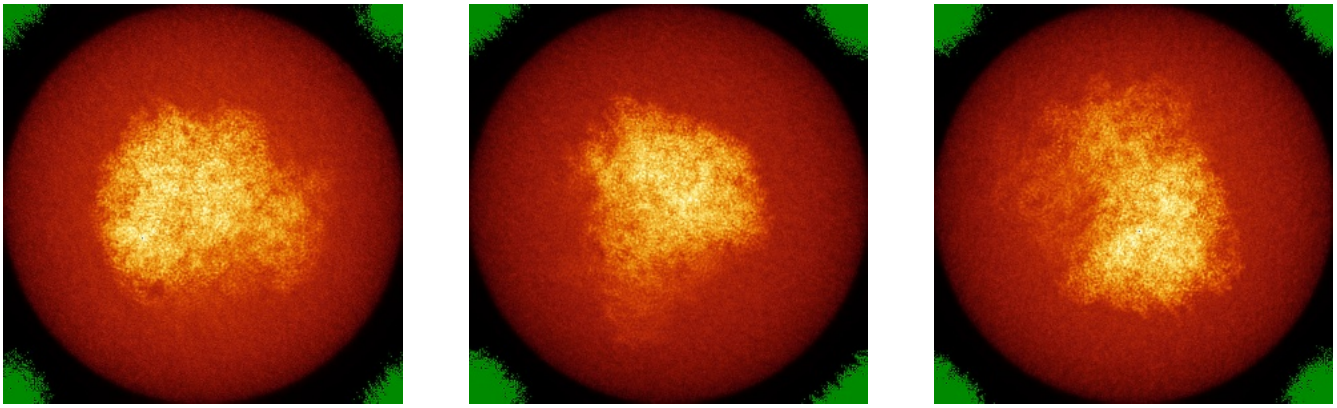


X Index: 230 Y Index: 158 Z Index: 176

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

6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

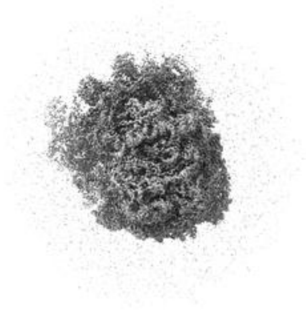
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

6.5.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

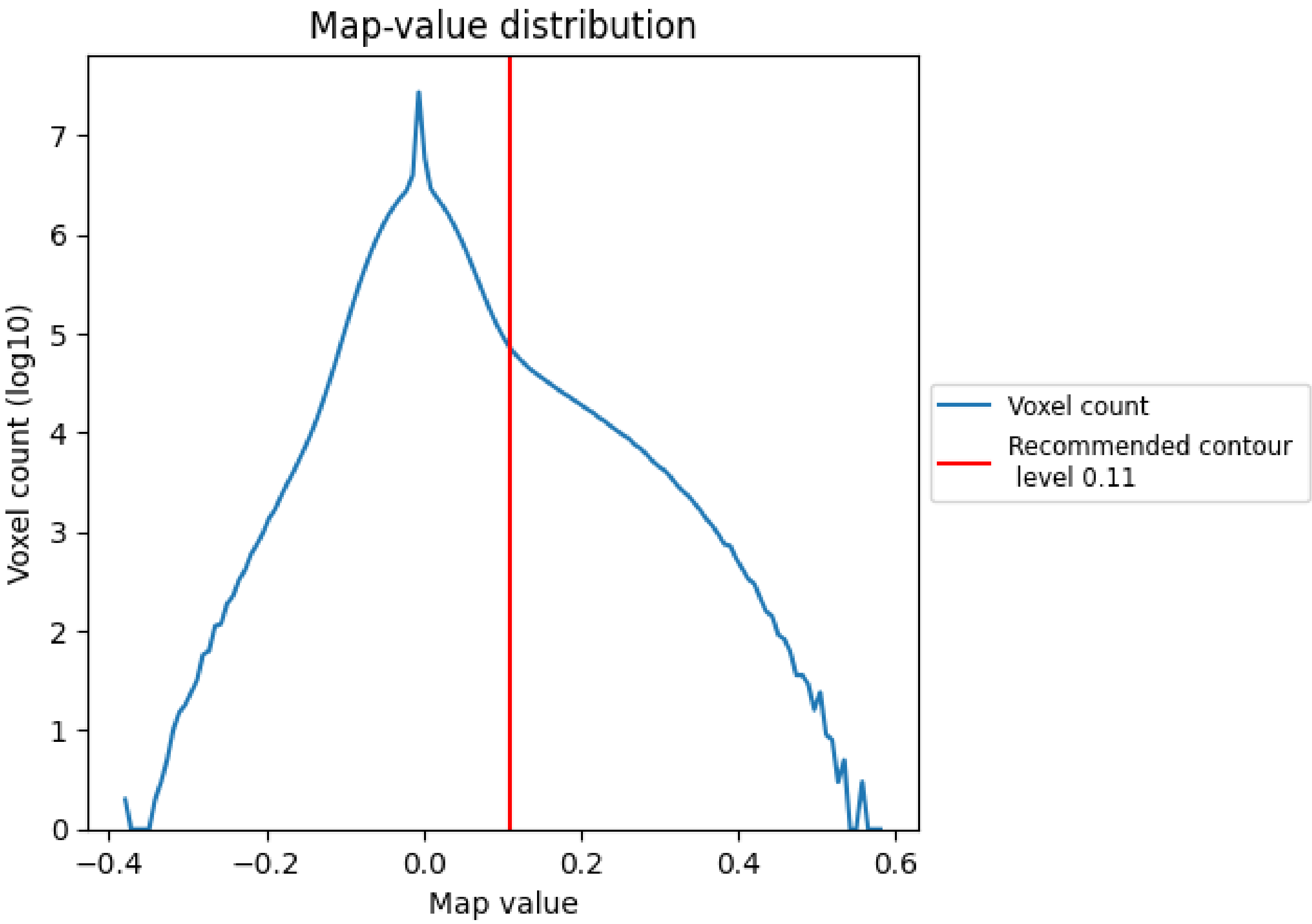
6.6 Mask visualisation

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

7 Map analysis ⓘ

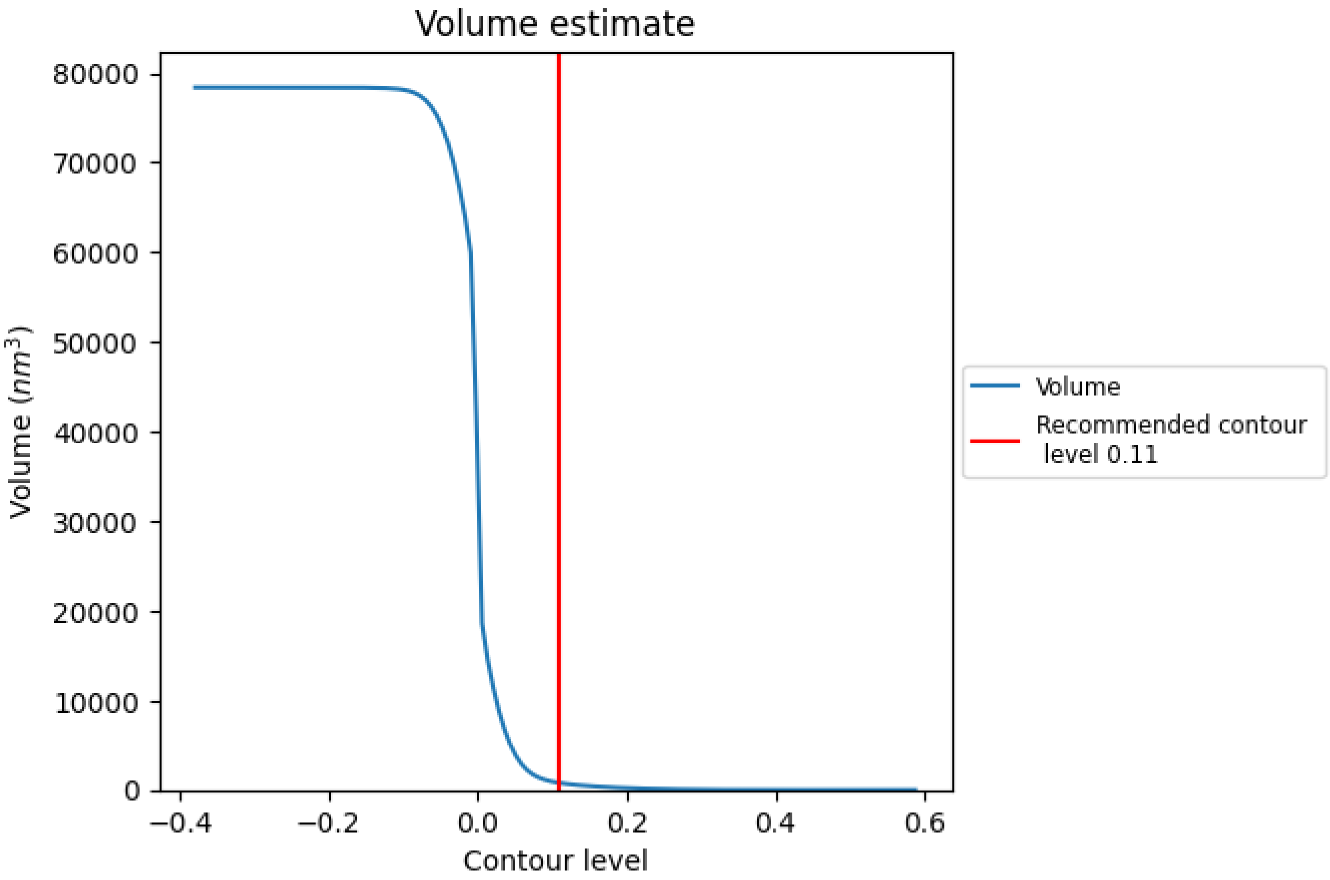
This section contains the results of statistical analysis of the map.

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.

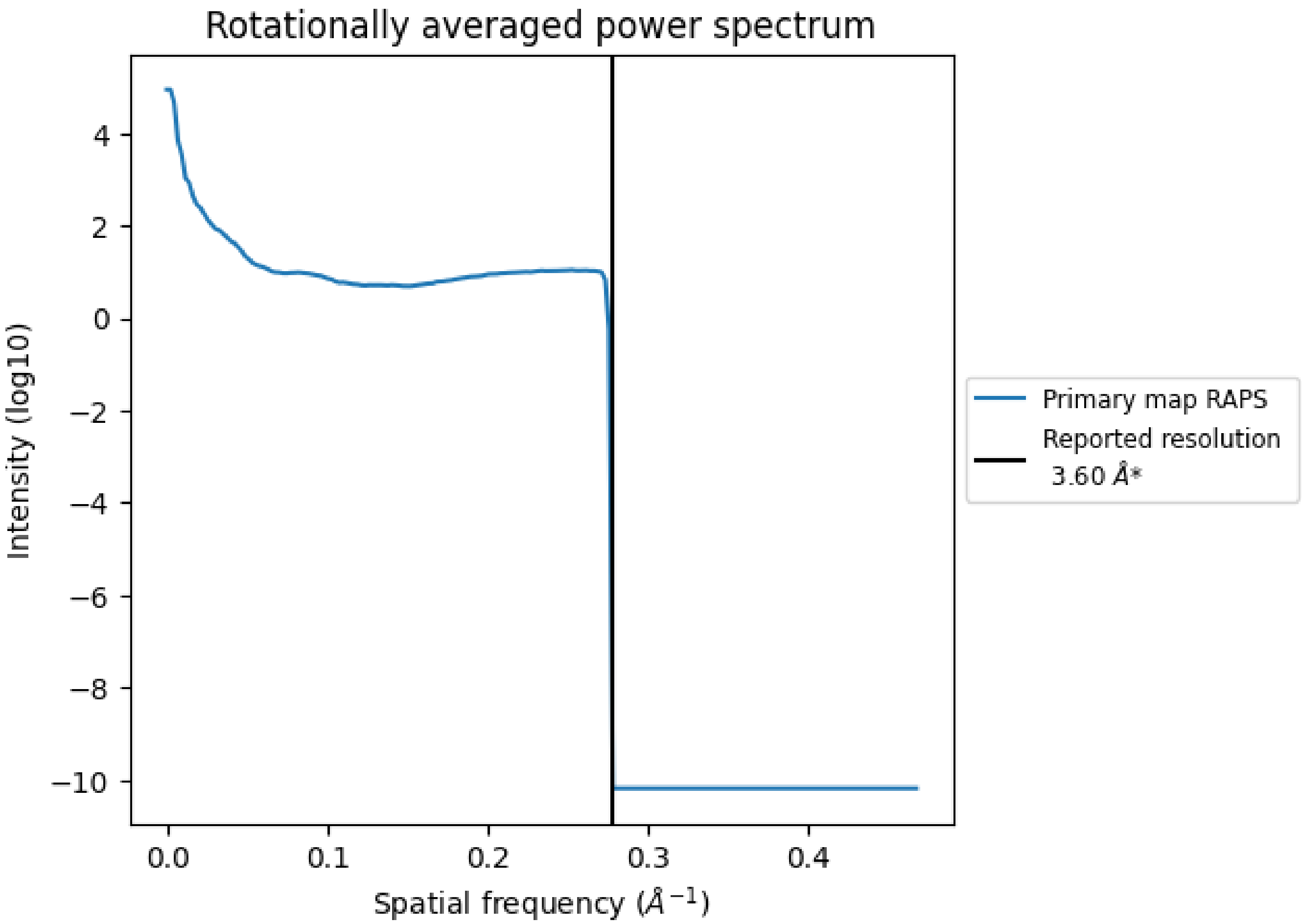
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 787 nm^3; this corresponds to an approximate mass of 711 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 0.278 Å^{-1}

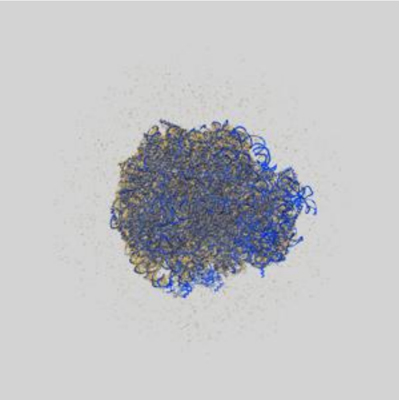
8 Fourier-Shell correlation ⓘ

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

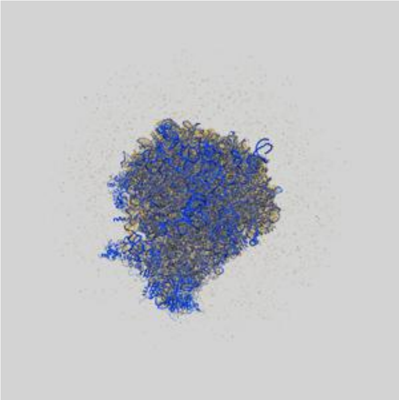
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20952 and PDB model 6UZ7. Per-residue inclusion information can be found in section 3 on page 21.

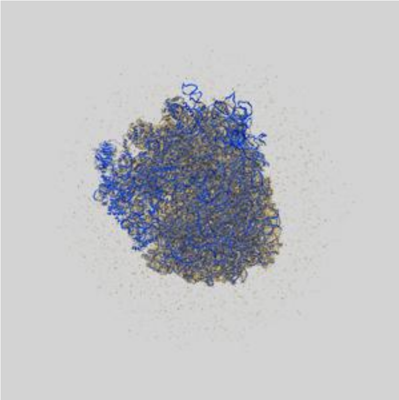
9.1 Map-model overlay



X



Y



Z

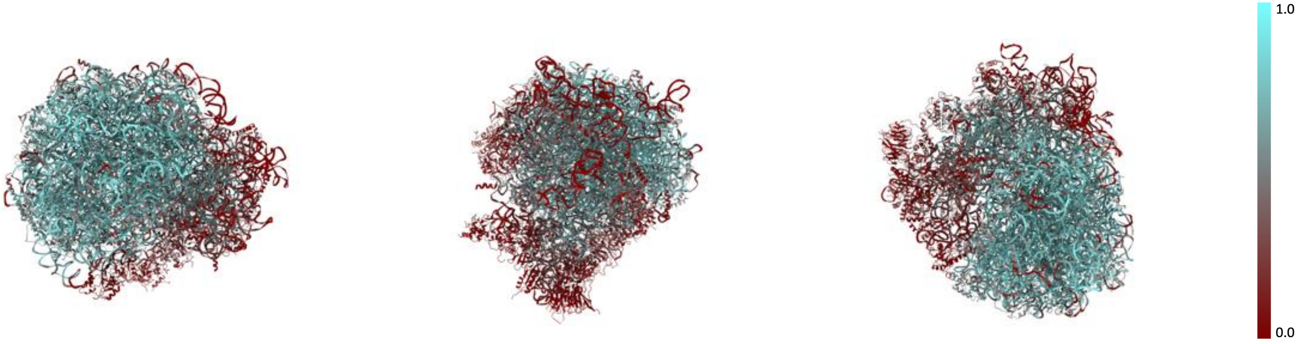
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

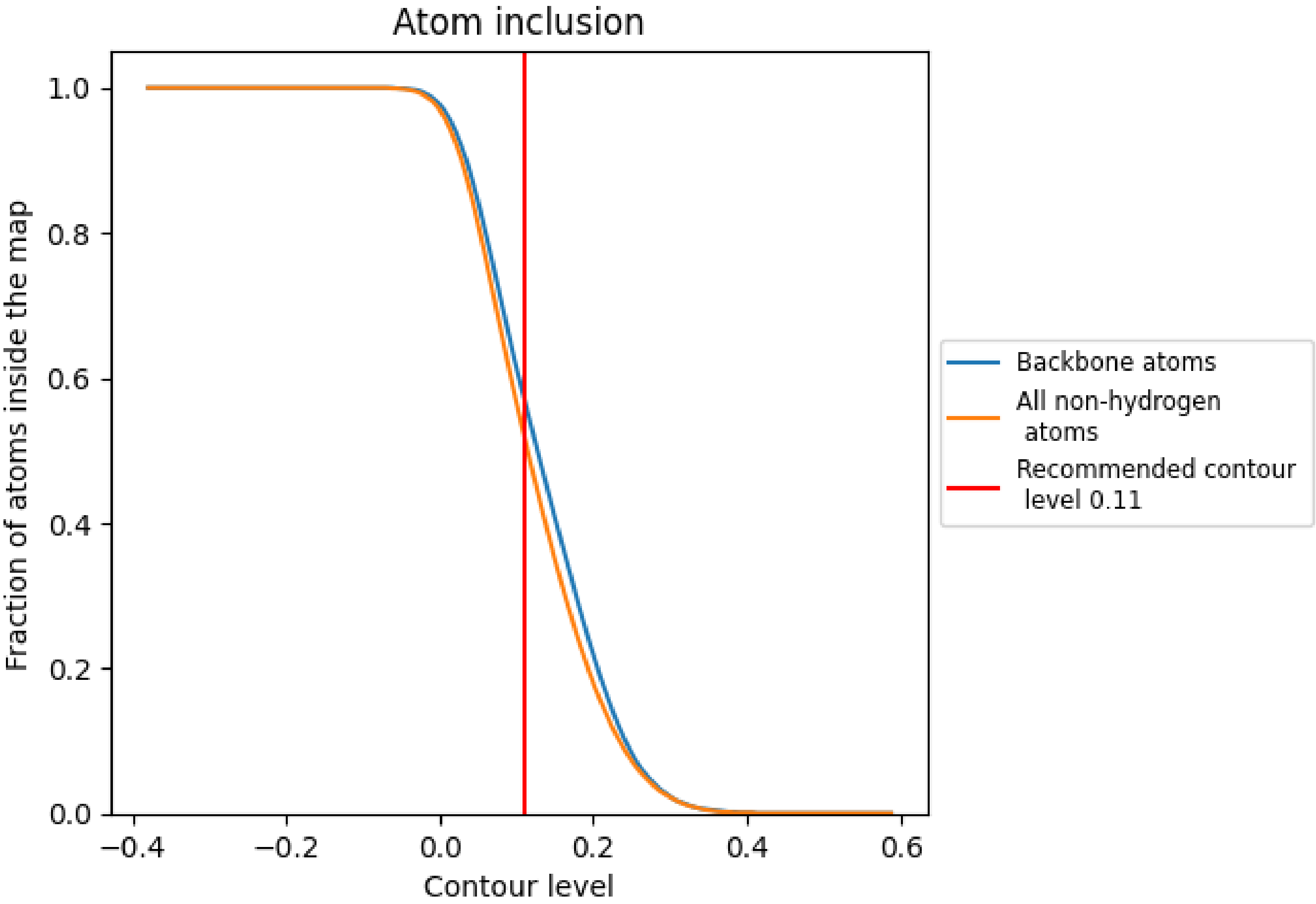
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.11).

9.4 Atom inclusion ⓘ



At the recommended contour level, 57% of all backbone atoms, 52% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5200	0.3900
1	0.2170	0.3570
2	0.4230	0.3290
3	0.2380	0.2170
5	0.7020	0.4420
7	0.7830	0.4790
8	0.7630	0.4730
A	0.3340	0.3440
AA	0.6580	0.4920
AB	0.6710	0.4920
AC	0.6330	0.4730
AD	0.5450	0.4330
AE	0.5100	0.4230
AF	0.6550	0.4730
AG	0.5510	0.4400
AH	0.5830	0.4690
AI	0.6300	0.4810
AJ	0.4720	0.4050
AK	0.0080	0.0410
AL	0.5730	0.4520
AM	0.5940	0.4720
AN	0.7240	0.5110
AO	0.6910	0.5000
AP	0.6410	0.4700
AQ	0.6470	0.4950
AR	0.5540	0.4380
AS	0.6530	0.4920
AT	0.6200	0.4710
AU	0.4240	0.4050
AV	0.6040	0.4940
AW	0.6190	0.4790
AX	0.5980	0.4580
AY	0.6180	0.4580
AZ	0.6010	0.4430
B	0.2850	0.3630

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ba	0.7030	0.5000
Bb	0.5630	0.4500
Bc	0.5810	0.4590
Bd	0.6290	0.4830
Be	0.6170	0.4760
Bf	0.7070	0.5080
Bg	0.5670	0.4440
Bh	0.6150	0.4740
Bi	0.5270	0.4310
Bj	0.7320	0.5150
Bk	0.4300	0.3690
Bl	0.6340	0.4810
Bm	0.5820	0.4800
Bn	0.1730	0.2430
Bo	0.5890	0.4680
Bp	0.6170	0.4680
Bq	0.0250	0.0860
Br	0.0150	0.1060
C	0.4500	0.4040
D	0.1030	0.2240
E	0.3540	0.3740
F	0.0390	0.1680
G	0.1440	0.2400
H	0.2770	0.3410
I	0.2180	0.2820
J	0.3910	0.3650
K	0.0530	0.1820
L	0.3920	0.3760
M	0.0050	0.0710
N	0.3870	0.3750
O	0.2760	0.3630
P	0.0710	0.1780
Q	0.0690	0.2130
R	0.1370	0.2480
S	0.0610	0.1430
T	0.0690	0.2050
U	0.0750	0.2000
V	0.4320	0.4250
W	0.5880	0.4640
X	0.4470	0.4300
Y	0.2230	0.3260
Z	0.0050	0.0990

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	🟥 0.3660	🟥 0.3450
b	🟥 0.2920	🟥 0.3310
c	🟥 0.0440	🟥 0.2110
d	🟥 0.1920	🟥 0.3010
e	🟥 0.2210	🟥 0.2980
f	🟥 0.0090	🟥 0.1220
g	🟥 0.0270	🟥 0.1600