Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 10:06 am GMT

PDB ID	:	6HCM
EMDB ID	:	EMD-0195
Title	:	Structure of the rabbit collided di-ribosome (stalled monosome)
Authors	:	Juszkiewicz, S.; Chandrasekaran, V.; Lin, Z.; Kraatz, S.; Ramakrishnan, V.; Hegde, R.S.
Deposited on	:	2018-08-15
Resolution	:	6.80 Å(reported)

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

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

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

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

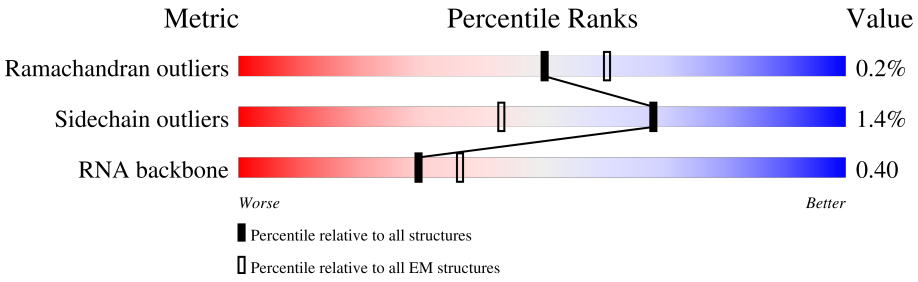
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A1	1869	65% 26% 7%
2	B1	295	25% 72% 26%
3	C1	264	39% 79% 19%
4	D1	293	25% 75% 25%
5	E1	243	30% 92% 6%
6	F1	263	33% 99%
7	G1	204	34% 90% 9%
8	H1	249	32% 94% 5%

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Mol	Chain	Length	Quality of chain
9	I1	194	31% 95% 5%
10	J1	208	41% 97%
11	K1	194	20% 93% 5%
12	L1	165	16% 57% 42%
13	M1	158	47% 89% 9%
14	N1	132	27% 86% 11%
15	O1	151	40% 97%
16	P1	168	45% 79% 19%
17	Q1	145	19% 81% 17%
18	R1	146	43% 96%
19	S1	135	39% 98%
20	T1	152	34% 94% 5%
21	U1	145	28% 97%
22	V1	119	29% 82% 16%
23	W1	83	41% 99%
24	X1	130	40% 99%
25	Y1	143	29% 97%
26	Z1	130	15% 95% 5%
27	a1	125	22% 60% 40%
28	b1	115	34% 88% 12%
29	c1	84	64% 98%
30	d1	69	29% 90% 10%
31	e1	56	38% 98%
32	f1	133	13% 40% 59%
33	g1	156	12% 43% 56%

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Mol	Chain	Length	Quality of chain
34	h1	317	50% 98%
35	j1	439	38% 94% 5%
36	k1	599	43% 95%
37	52	3634	6% 65% 31%
38	72	120	68% 31%
39	82	156	65% 29%
40	A3	257	52% 90% 5%
41	B3	403	32% 97%
42	C3	425	36% 83% 15%
43	E3	291	23% 73% 26%
44	F3	247	32% 90% 9%
45	H3	192	27% 96%
46	L3	211	30% 98%
47	M3	218	11% 63% 37%
48	N3	204	40% 97%
49	O3	203	28% 97%
50	P3	184	26% 83% 17%
51	Q3	188	38% 98%
52	R3	196	33% 86% 6% 8%
53	S3	176	36% 99%
54	T3	160	31% 98%
55	U3	128	18% 74% 23%
56	V3	140	45% 92% 6%
57	W3	157	30% 66% 32%
58	X3	156	29% 76% 24%

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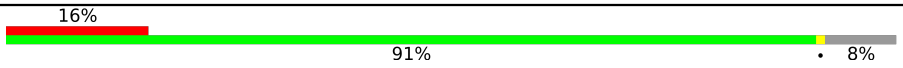
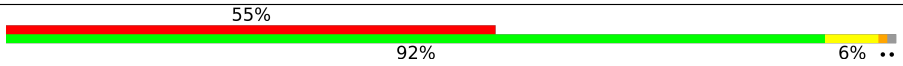
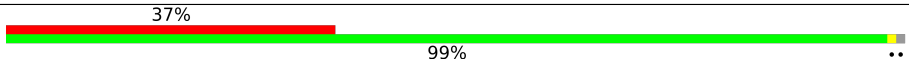
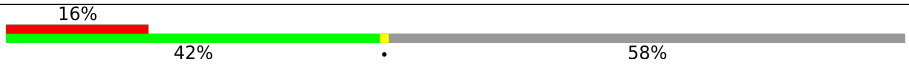
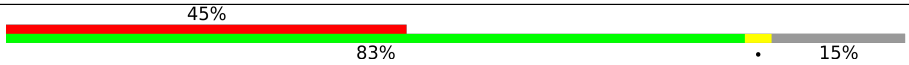
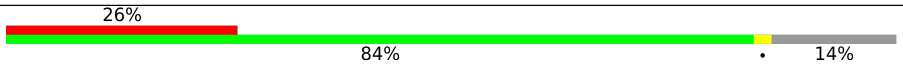
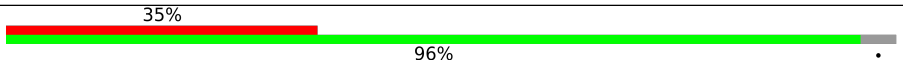
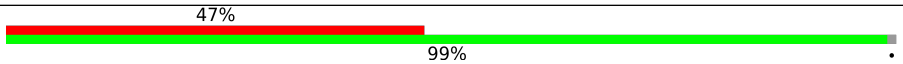
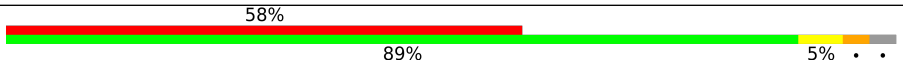
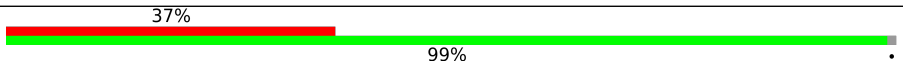
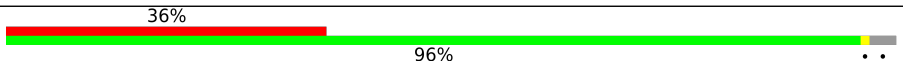
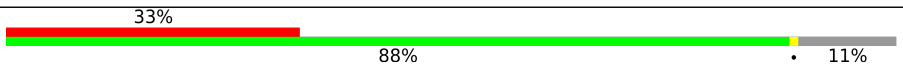
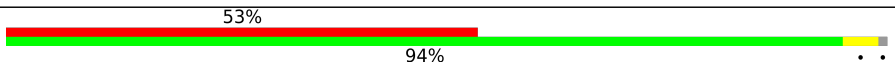
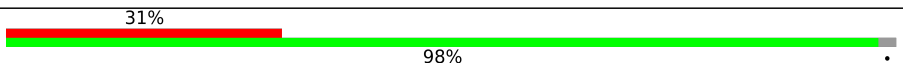
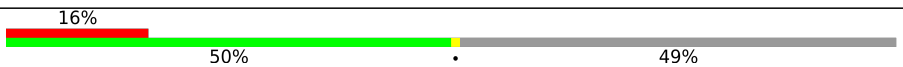
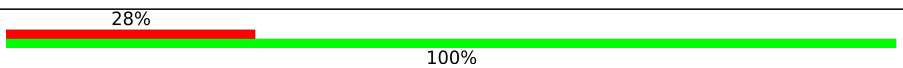
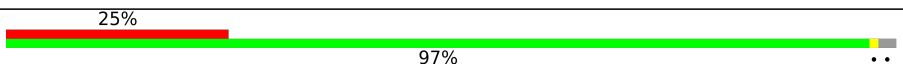
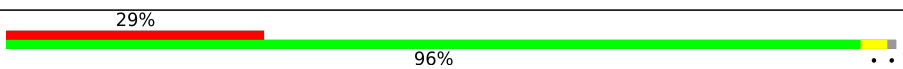
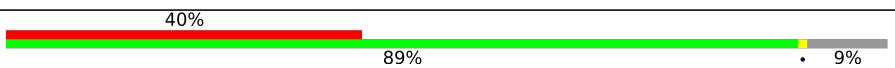
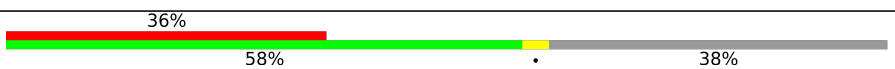
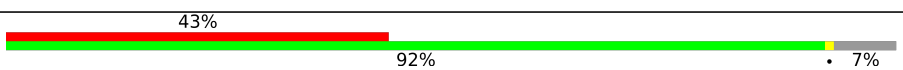
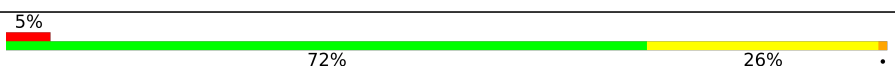
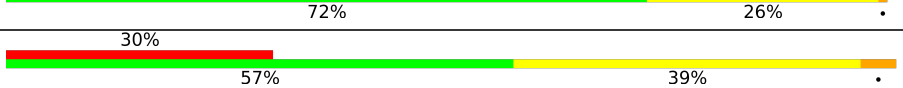
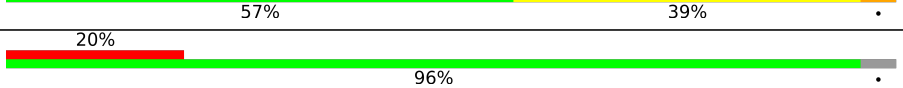
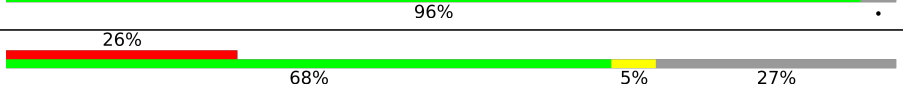
Mol	Chain	Length	Quality of chain
59	Y3	145	
60	Z3	136	
61	a3	148	
62	b3	245	
63	c3	115	
64	d3	125	
65	e3	134	
66	f3	110	
67	g3	117	
68	h3	123	
69	i3	105	
70	j3	97	
71	k3	70	
72	l3	51	
73	m3	102	
74	n3	25	
75	o3	106	
76	p3	92	
77	r3	137	
78	s3	318	
79	t3	165	
80	23	76	
81	w3	23	
82	J3	178	
83	G3	319	

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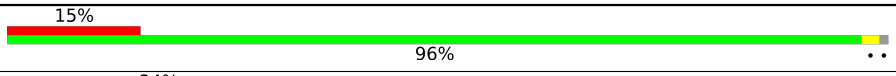
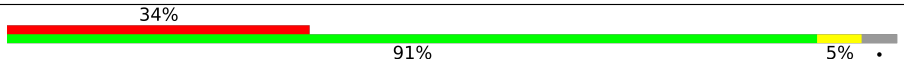
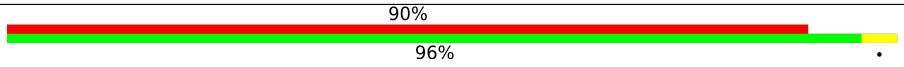
Mol	Chain	Length	Quality of chain
84	D3	297	
85	I3	214	
86	1	22	
87	u3	217	

2 Entry composition (i)

There are 91 unique types of molecules in this entry. The entry contains 226754 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A1	1732	36969	16502	6637	12099	1731	0	0

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B1	217	1710	1086	300	316	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C1	213	1729	1098	309	308	14	0	0

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D1	221	1716	1111	295	301	9	0	0

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E1	228	1768	1126	318	316	8	0	0

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F1	262	2076	1324	386	358	8	0	0

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 18 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R1	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V1	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W1	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X1	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y1	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z1	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a1	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b1	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 30 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d1	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 31 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f1	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 33 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g1	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h1	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a protein called eRF1(AAQ).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j1	419	Total	C	N	O	S	0	0
			3309	2106	562	629	12		

- Molecule 36 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k1	577	Total	C	N	O	S	0	0
			4555	2914	780	830	31		

- Molecule 37 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	52	3634	Total	C	N	O	P	0	0
			77819	34651	14241	25293	3634		

- Molecule 38 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	72	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 39 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	82	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 40 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A3	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 41 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B3	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 42 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	C3	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	E3	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 44 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	F3	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	61	ARG	GLY	conflict	UNP G1TUB1
F3	93	ARG	GLY	conflict	UNP G1TUB1
F3	131	MET	VAL	conflict	UNP G1TUB1
F3	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 45 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	H3	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 46 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L3	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 47 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M3	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 48 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N3	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 49 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O3	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 50 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	P3	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 51 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Q3	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 52 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	R3	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 53 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S3	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 54 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T3	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 55 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U3	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 56 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	V3	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 57 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	W3	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 58 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	X3	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 59 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Y3	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 60 is a protein called eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Z3	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 61 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	a3	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 62 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	b3	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 63 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c3	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 64 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	d3	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 65 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	e3	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 66 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	f3	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 67 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	g3	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 68 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	h3	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 69 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	i3	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j3	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 71 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k3	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 72 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	l3	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 73 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	m3	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 74 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	n3	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 75 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o3	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 76 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	p3	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 77 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	r3	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 78 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	s3	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 79 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	t3	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 80 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	23	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 81 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	w3	23	Total	C	N	O	P	0	0
			493	222	94	154	23		

- Molecule 82 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	J3	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 83 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	G3	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

- Molecule 84 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	D3	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 85 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	I3	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 86 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	1	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 87 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	u3	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

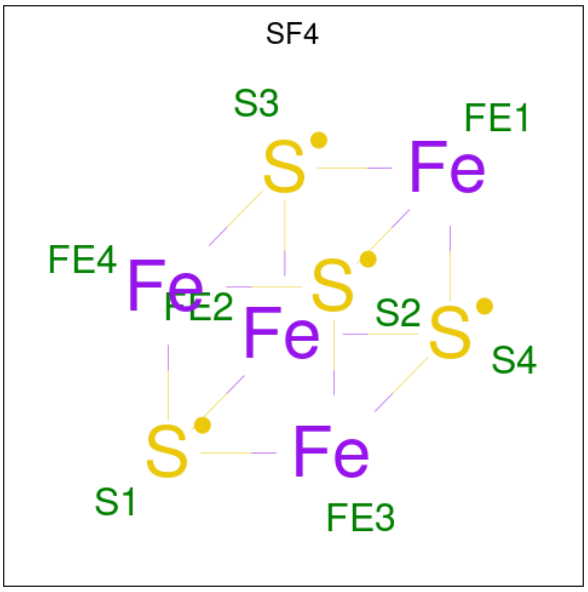
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
88	A1	77	Total Mg 77 77	0
88	G1	1	Total Mg 1 1	0
88	M1	1	Total Mg 1 1	0
88	52	204	Total Mg 204 204	0
88	72	7	Total Mg 7 7	0
88	82	5	Total Mg 5 5	0
88	P3	1	Total Mg 1 1	0
88	V3	1	Total Mg 1 1	0
88	a3	1	Total Mg 1 1	0
88	g3	1	Total Mg 1 1	0
88	w3	1	Total Mg 1 1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
89	b1	1	Total Zn 1 1	0
89	e1	1	Total Zn 1 1	0
89	g1	1	Total Zn 1 1	0
89	g3	1	Total Zn 1 1	0
89	j3	1	Total Zn 1 1	0
89	m3	1	Total Zn 1 1	0
89	o3	1	Total Zn 1 1	0
89	p3	1	Total Zn 1 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
90	k1	1	Total	Fe	S	0
			16	8	8	
90	k1	1	Total	Fe	S	0
			16	8	8	

- Molecule 91 is water.

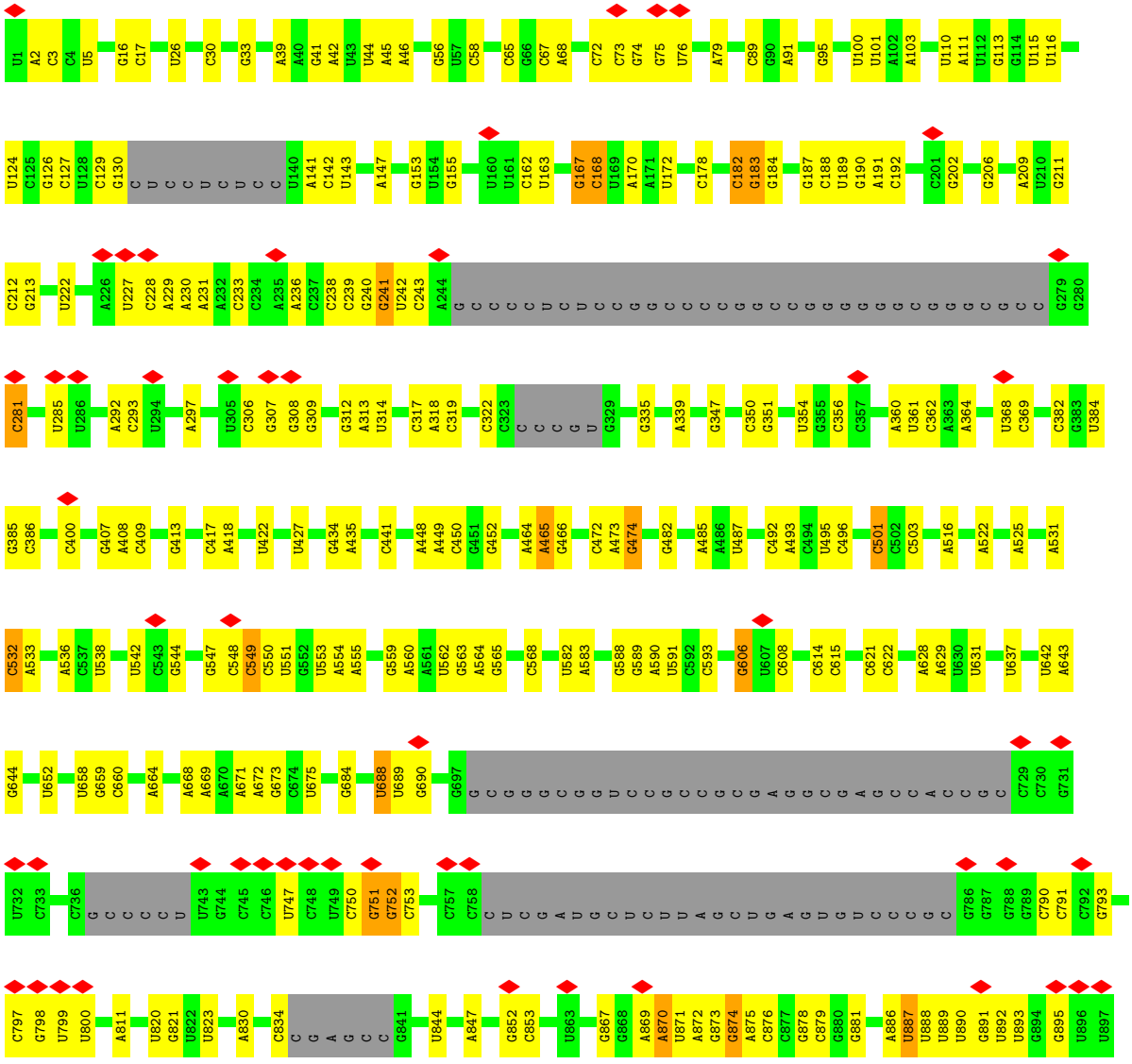
Mol	Chain	Residues	Atoms		AltConf
91	52	3	Total	O	0
			3	3	
91	1	1	Total	O	0
			1	1	

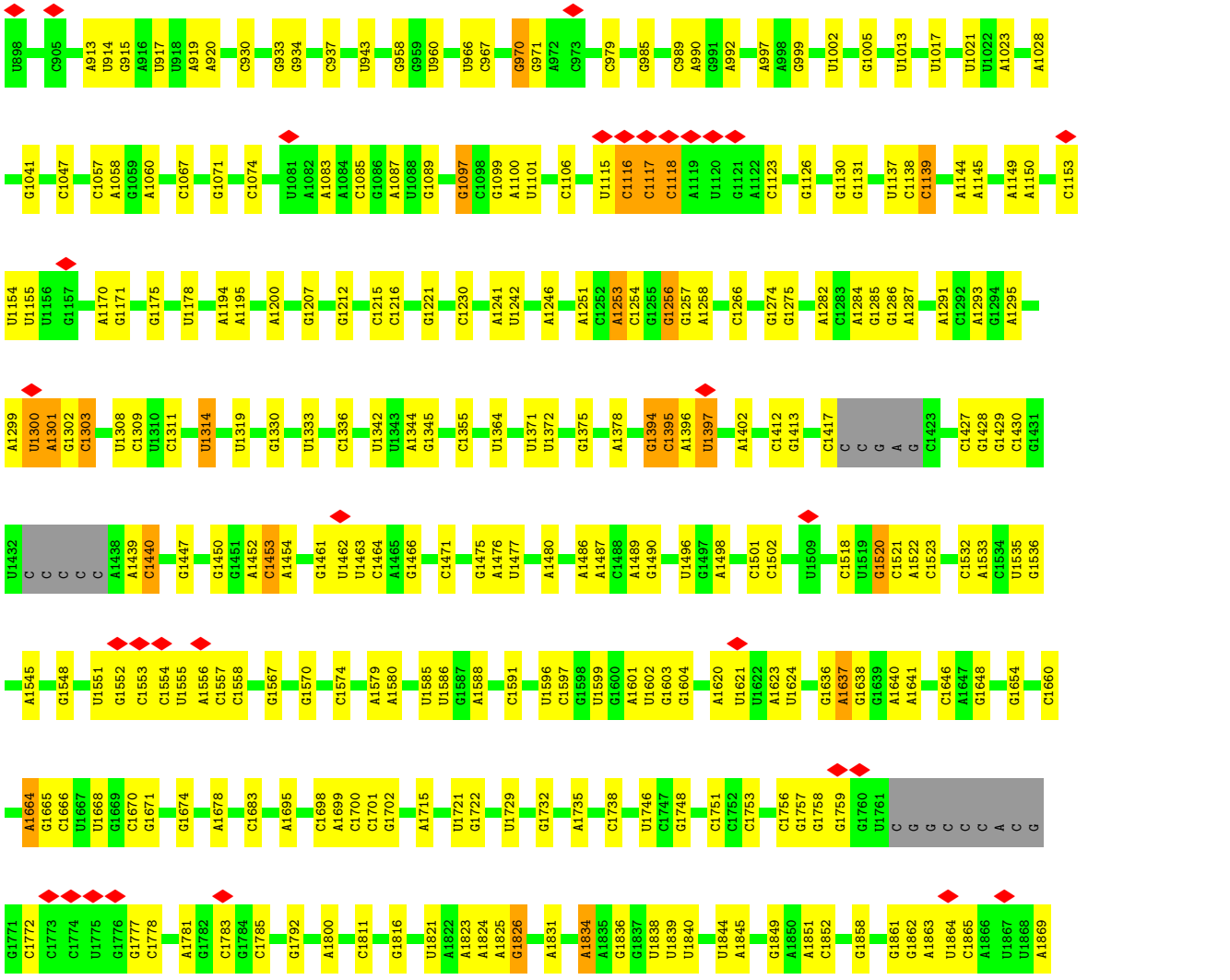
3 Residue-property plots (i)

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

- Molecule 1: 18S ribosomal RNA

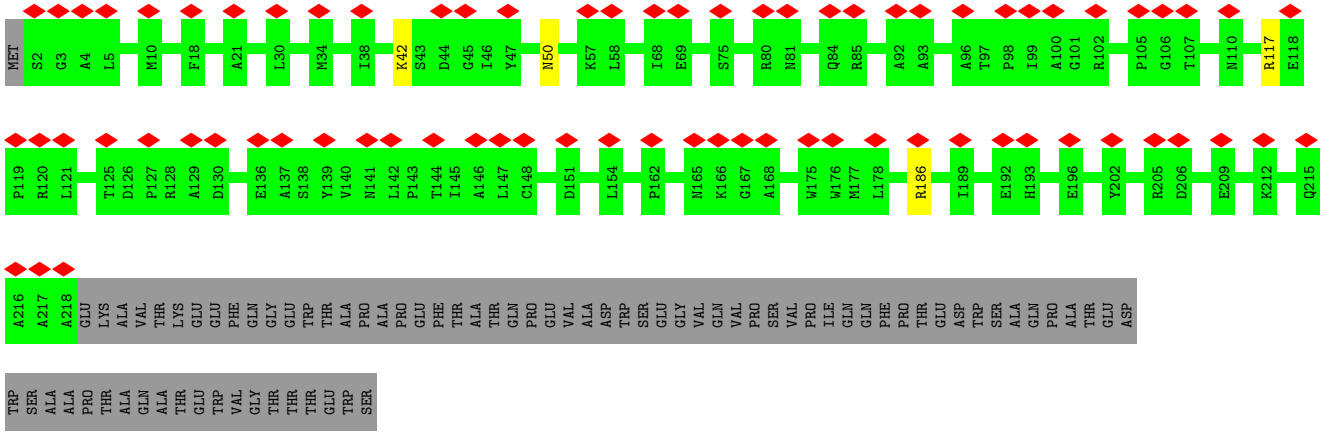
Chain A1:





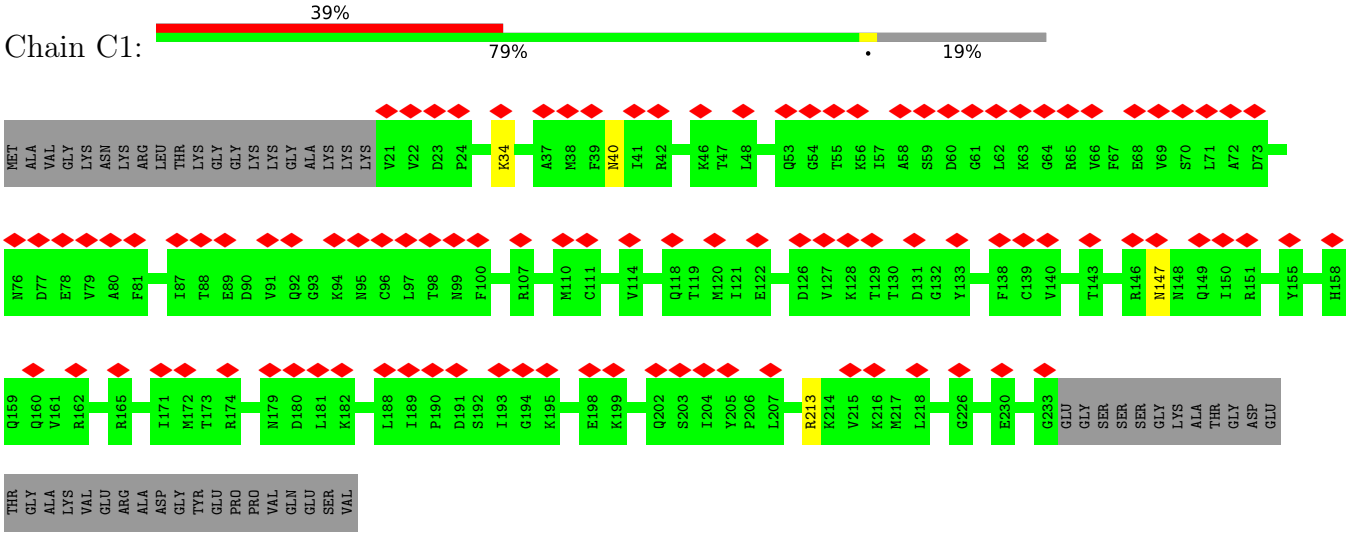
- Molecule 2: uS2

Chain B1:



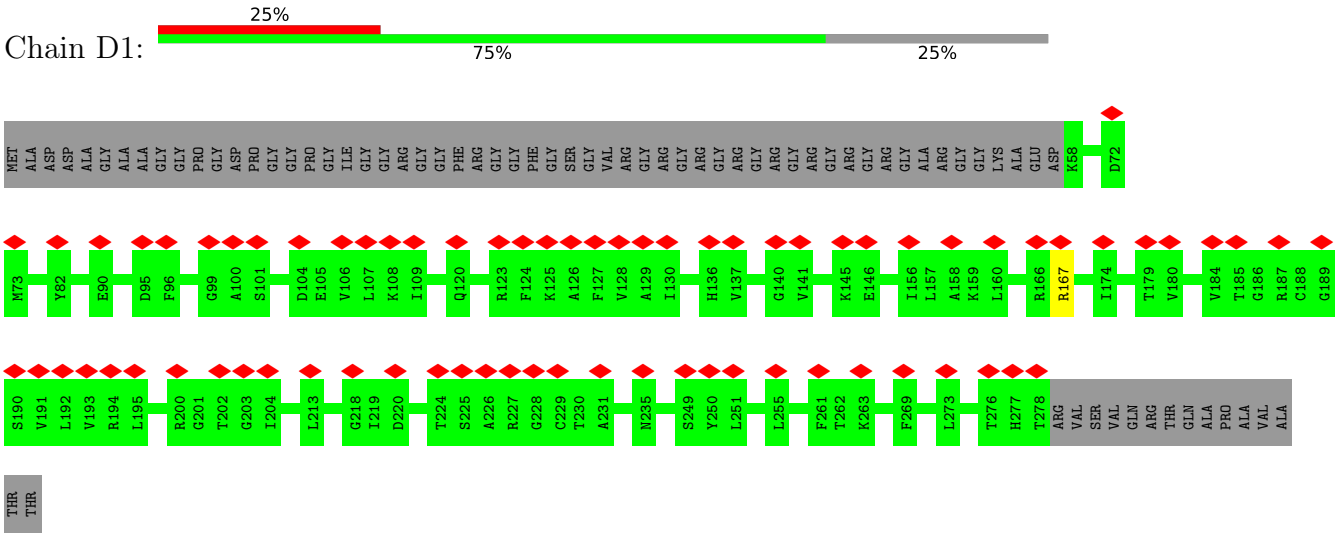
- Molecule 3: 40S ribosomal protein S3a

Chain C1:



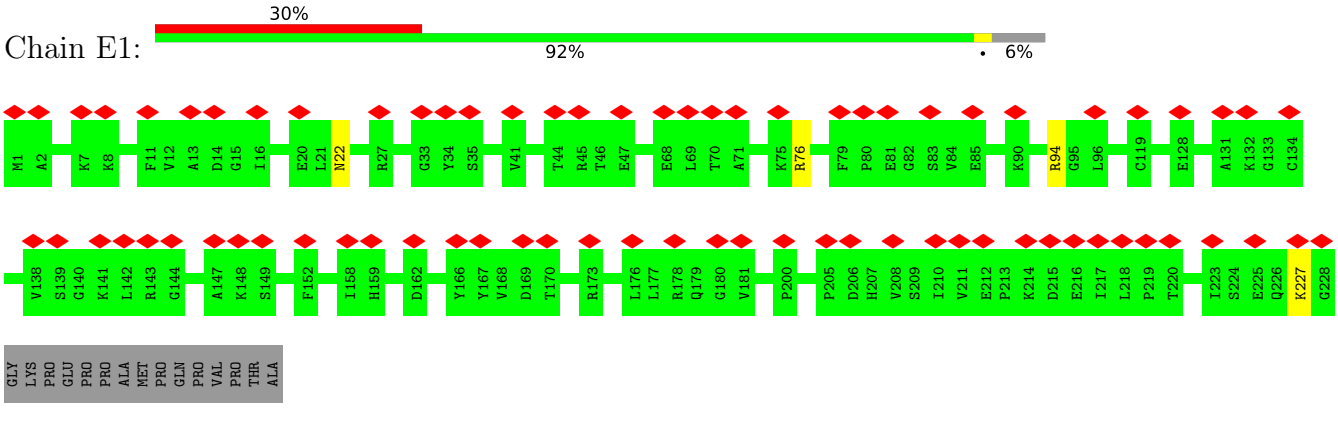
• Molecule 4: uS5

Chain D1:



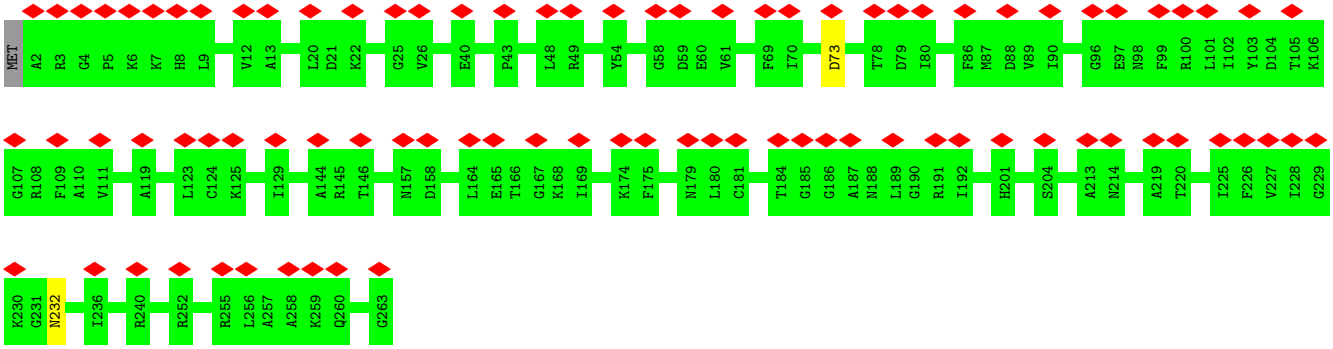
• Molecule 5: uS3

Chain E1:



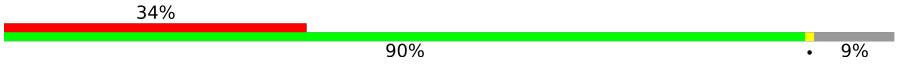
• Molecule 6: eS4

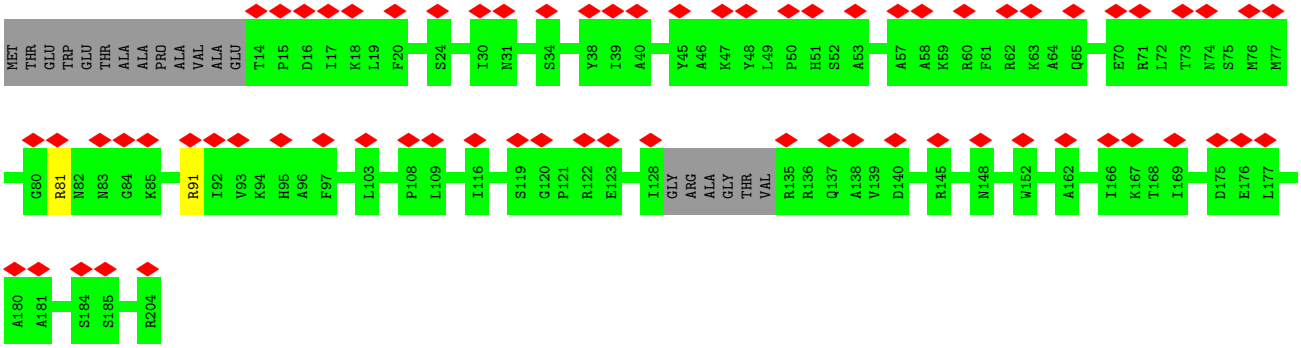
Chain F1:



• Molecule 7: Ribosomal protein S5

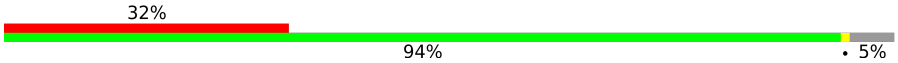
Chain G1:

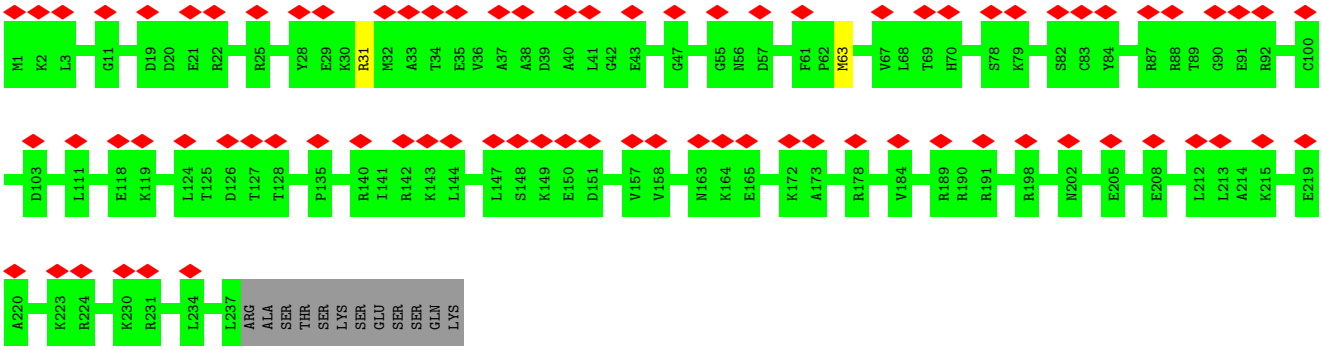




• Molecule 8: 40S ribosomal protein S6

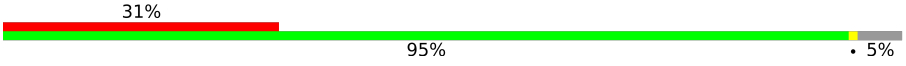
Chain H1:

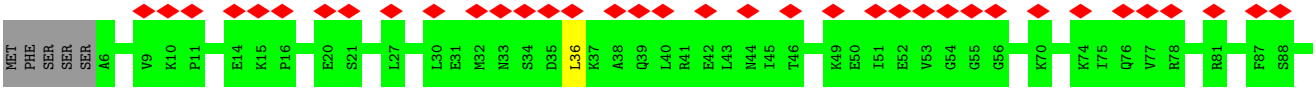


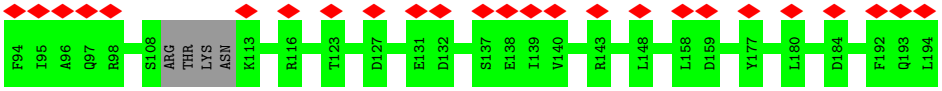


• Molecule 9: 40S ribosomal protein S7

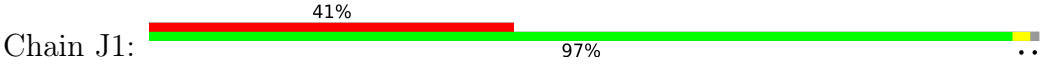
Chain I1:

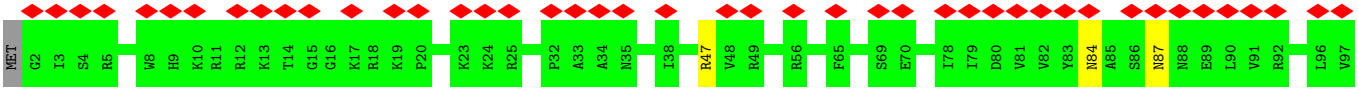


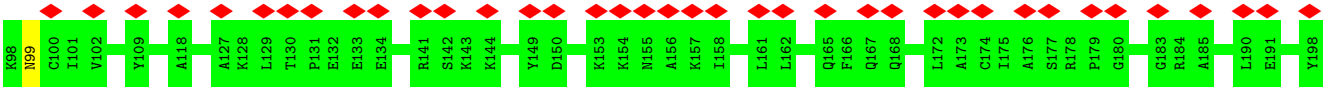


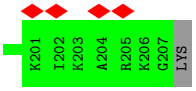


• Molecule 10: eS8

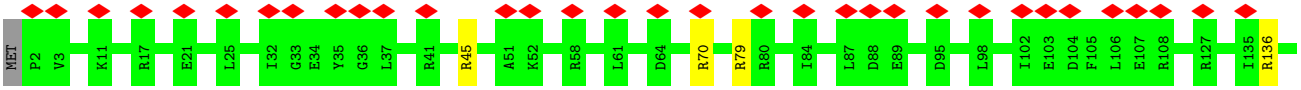


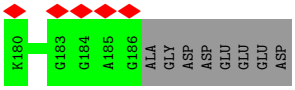




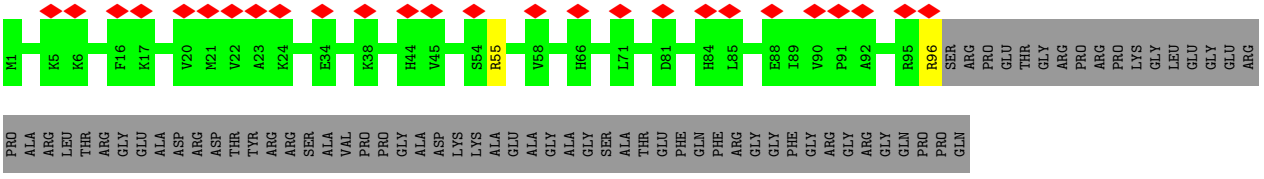


• Molecule 11: Ribosomal protein S9 (Predicted)

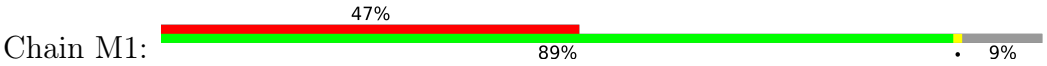


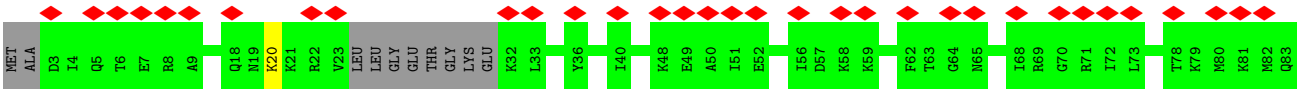


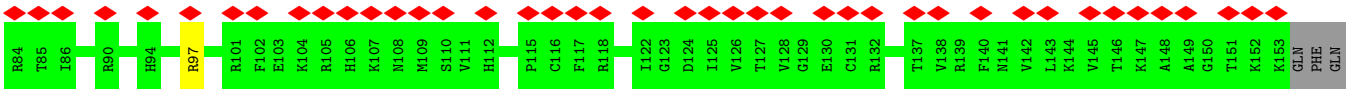
• Molecule 12: eS10



• Molecule 13: Ribosomal protein S11

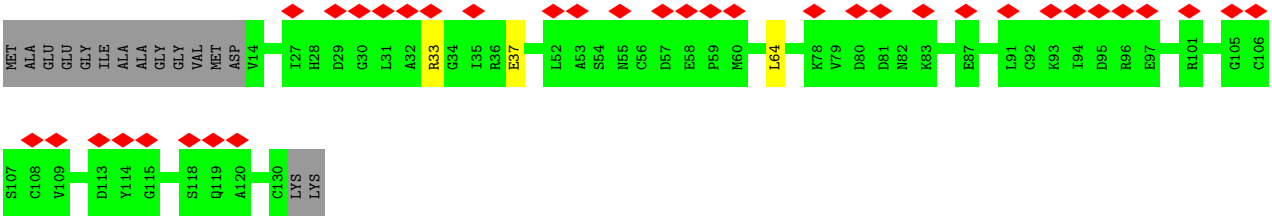






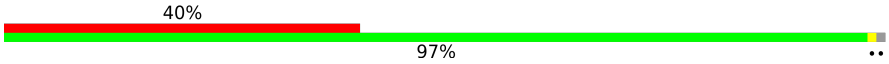
• Molecule 14: 40S ribosomal protein S12

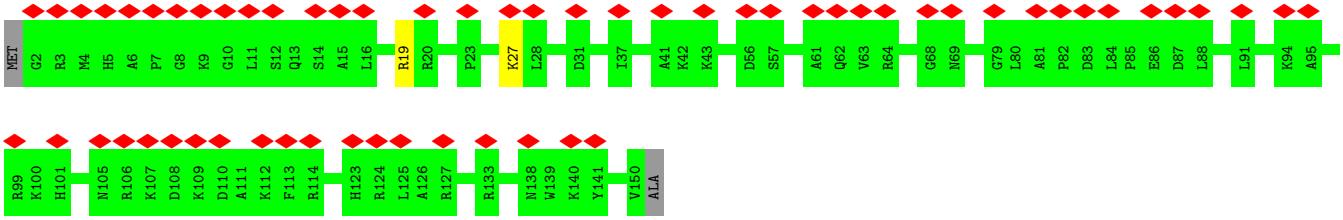
Chain N1:



• Molecule 15: uS15

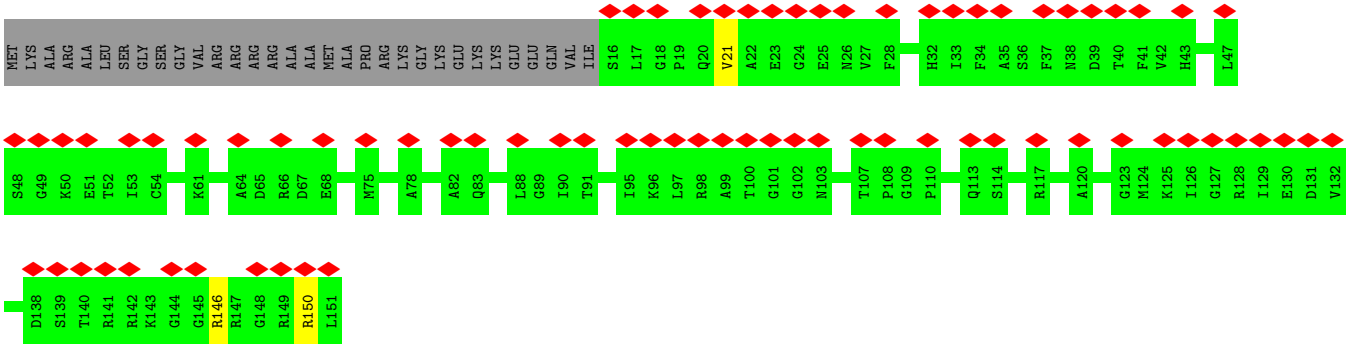
Chain O1:





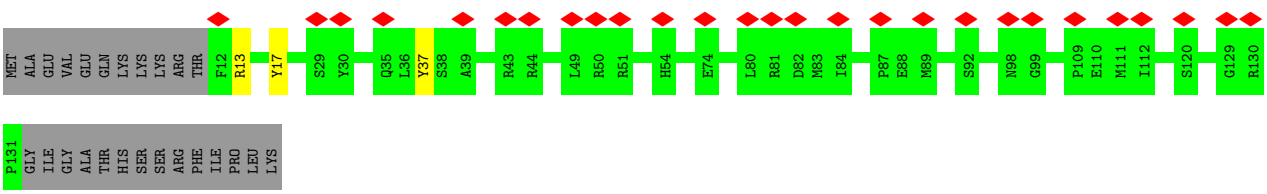
• Molecule 16: uS11

Chain P1:



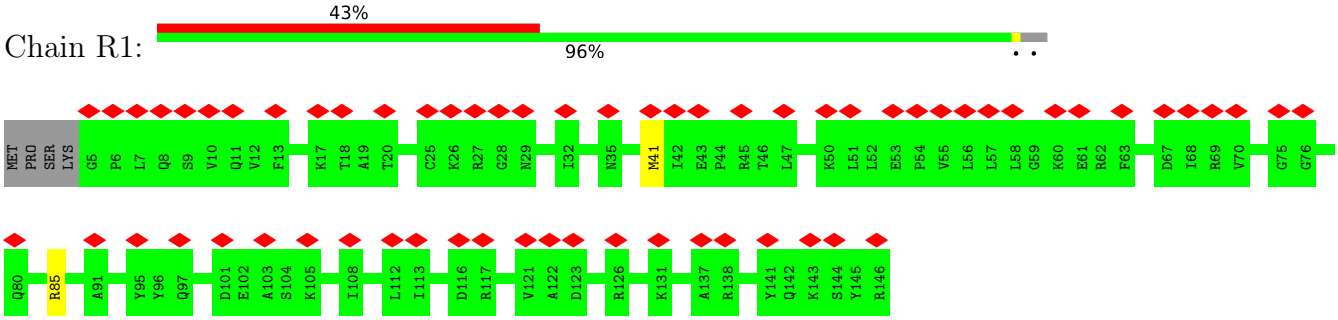
• Molecule 17: uS19

Chain Q1:



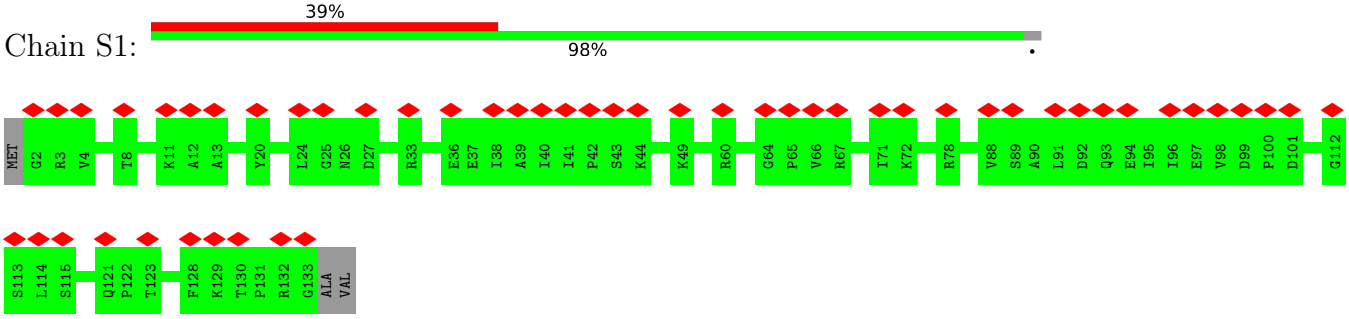
• Molecule 18: Ribosomal protein S16

Chain R1:



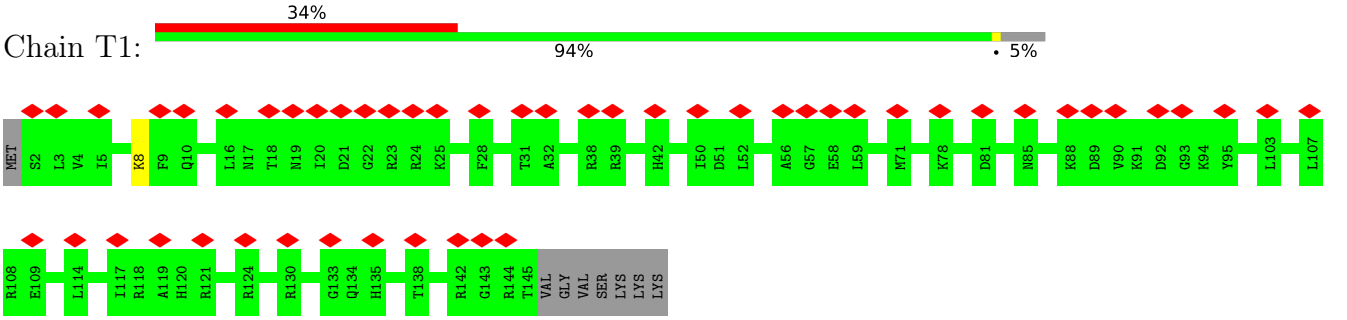
• Molecule 19: eS17

Chain S1:



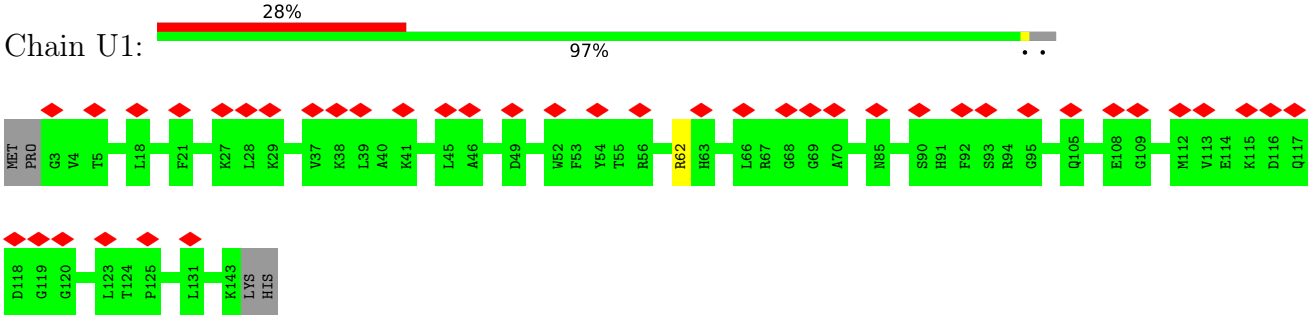
• Molecule 20: uS13

Chain T1:



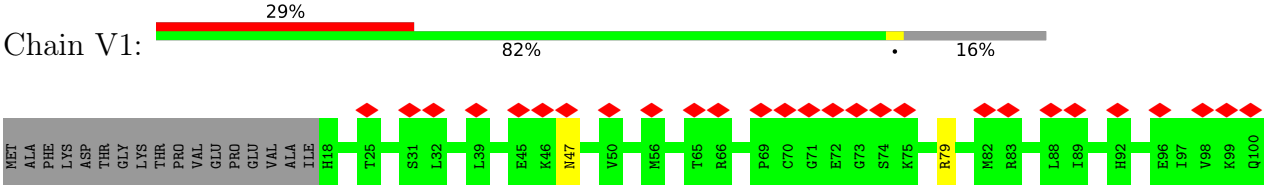
• Molecule 21: eS19

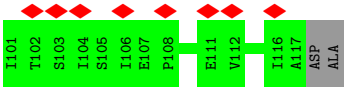
Chain U1:



• Molecule 22: uS10

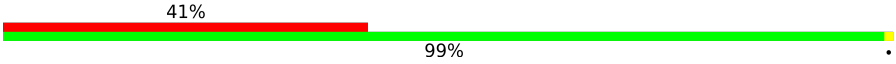
Chain V1:

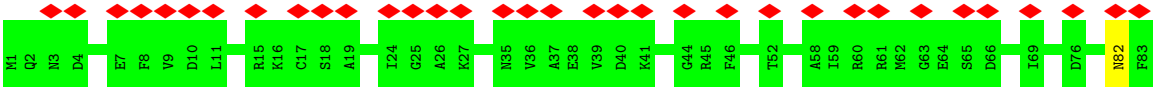




• Molecule 23: eS21

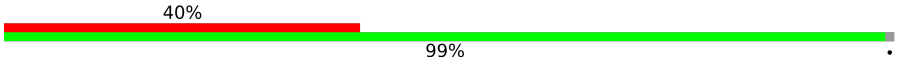
Chain W1:

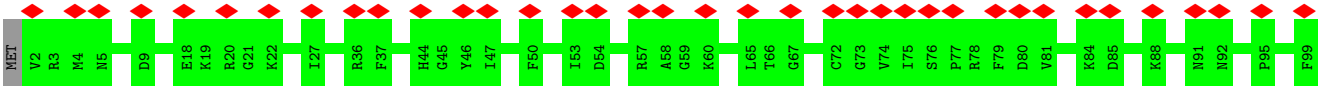


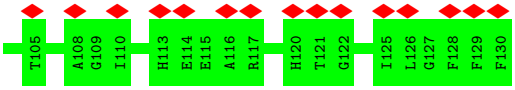


• Molecule 24: Ribosomal protein S15a

Chain X1:

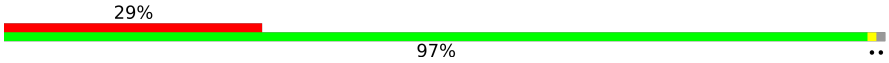


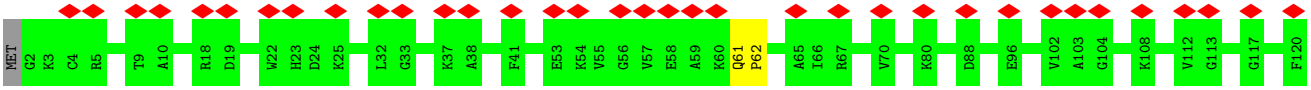


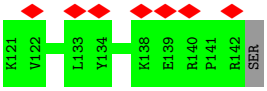


• Molecule 25: uS12

Chain Y1:

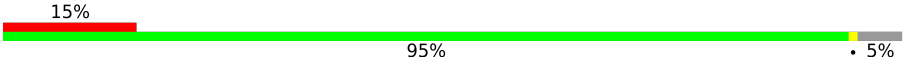


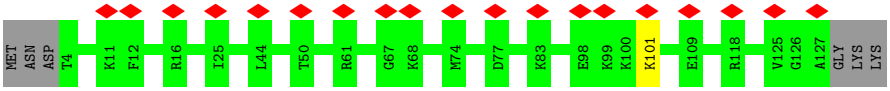




• Molecule 26: eS24

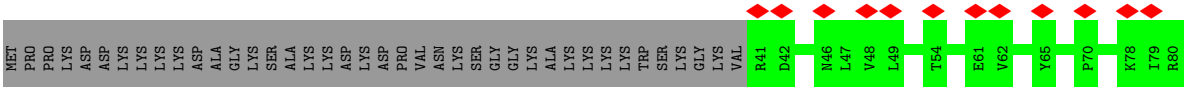
Chain Z1:

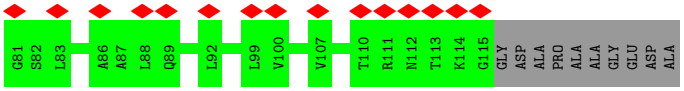




• Molecule 27: eS25

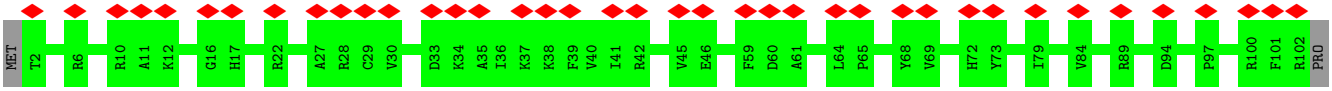
Chain a1:





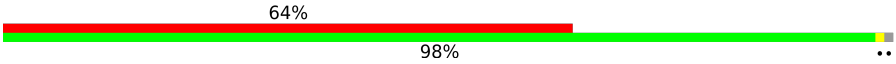
• Molecule 28: eS26

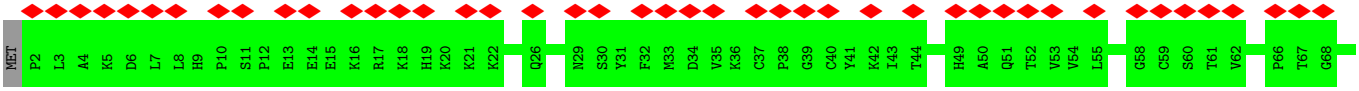
Chain b1:

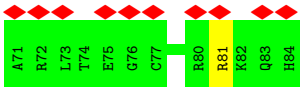


• Molecule 29: 40S ribosomal protein S27

Chain c1:

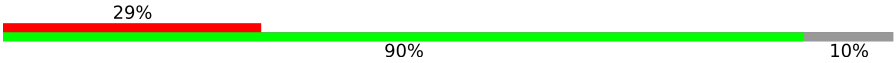


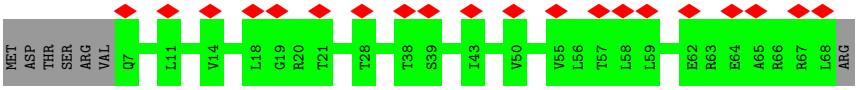




• Molecule 30: Ribosomal protein S28

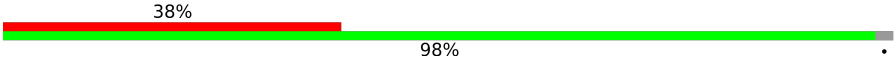
Chain d1:

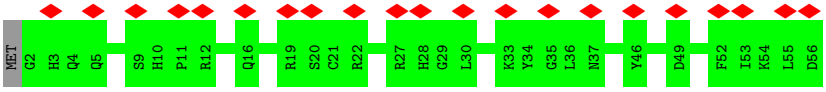




• Molecule 31: uS14

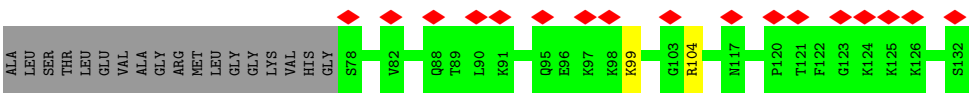
Chain e1:





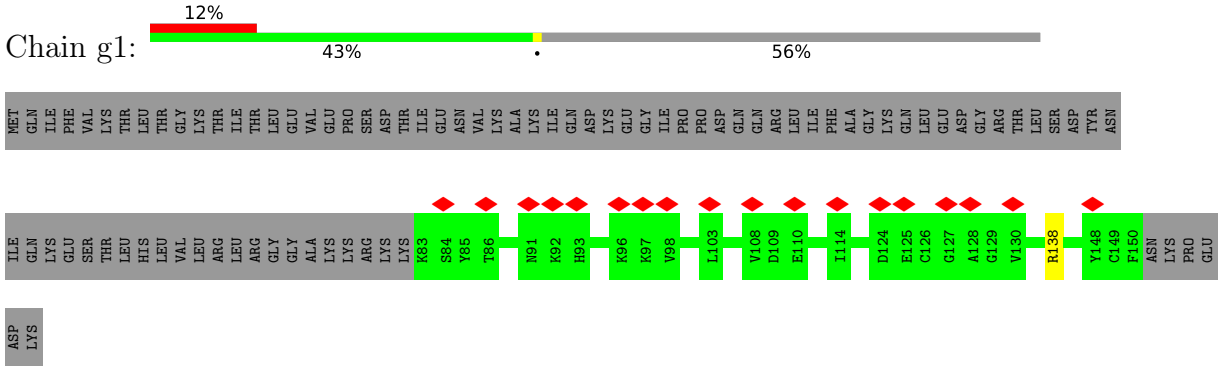
• Molecule 32: 40S ribosomal protein S30

Chain f1:



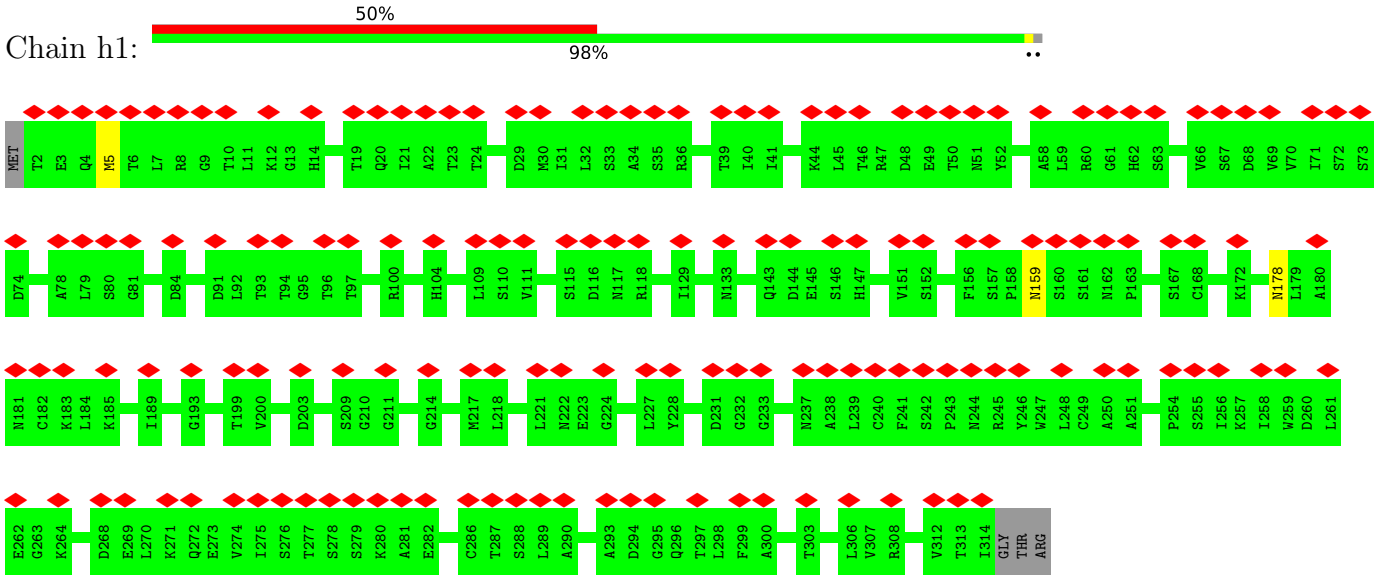
• Molecule 33: Ribosomal protein S27a

Chain g1:



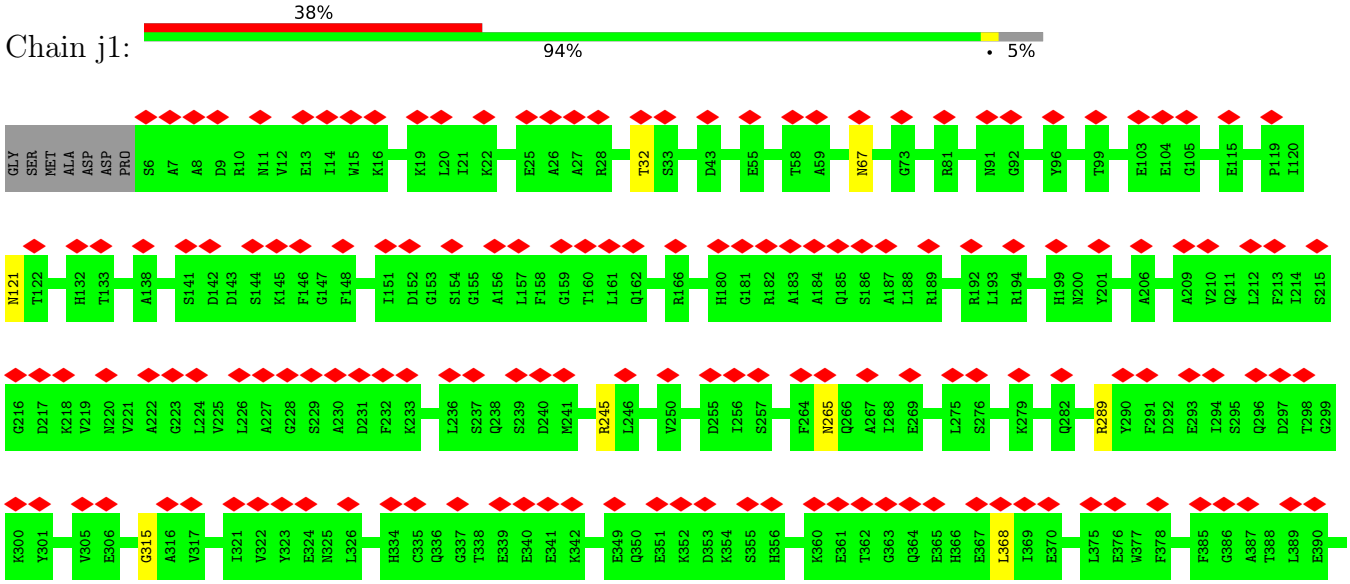
• Molecule 34: RACK1

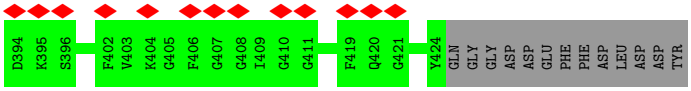
Chain h1:



• Molecule 35: eRF1(AAQ)

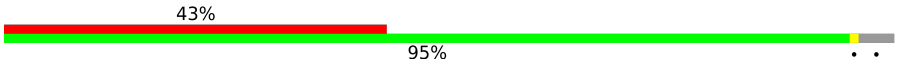
Chain j1:

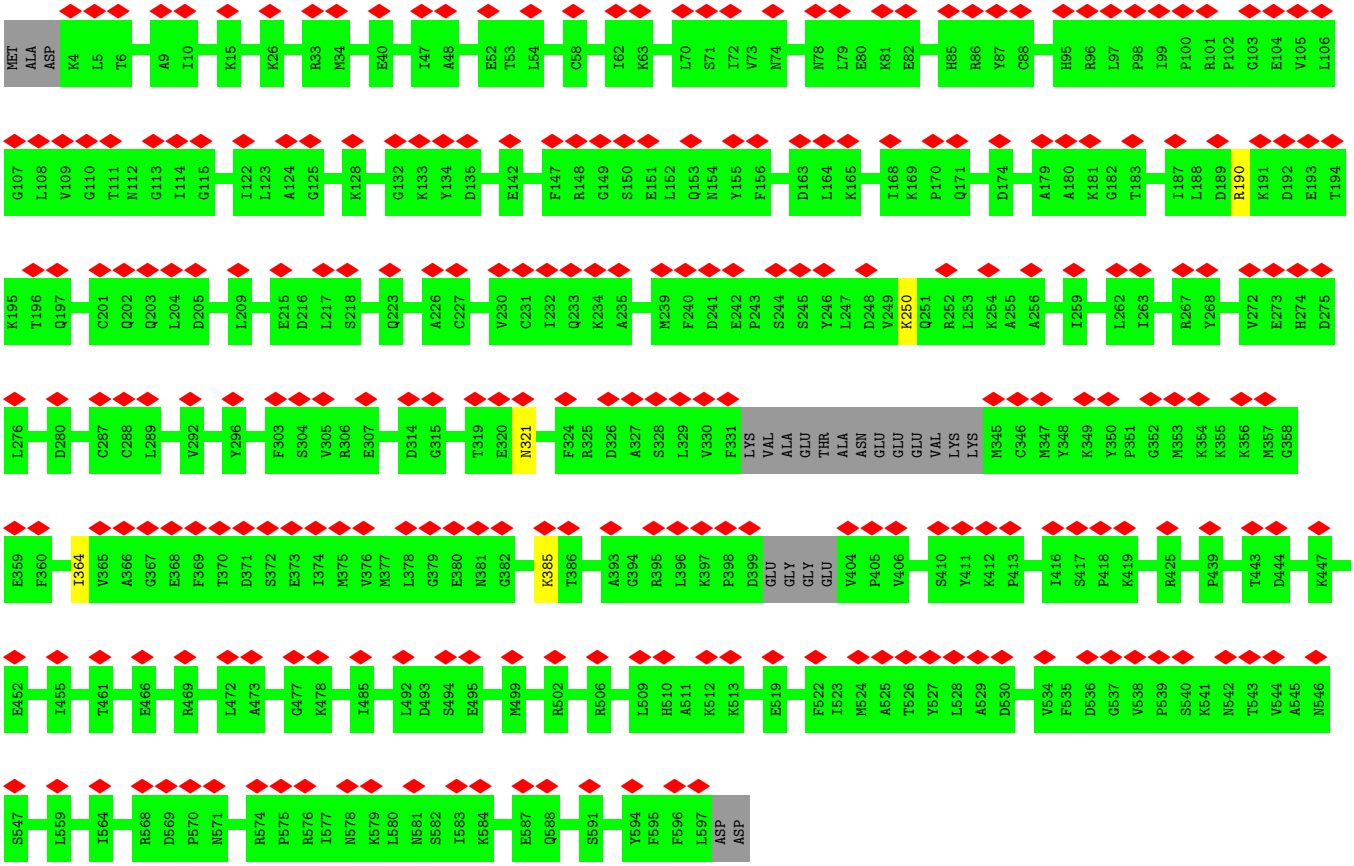




• Molecule 36: ATP binding cassette subfamily E member 1

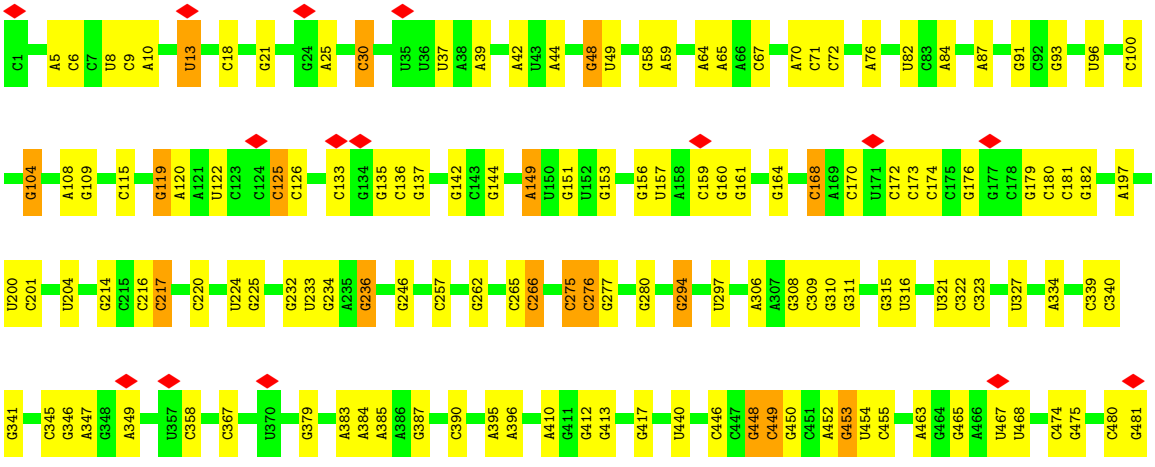
Chain k1:

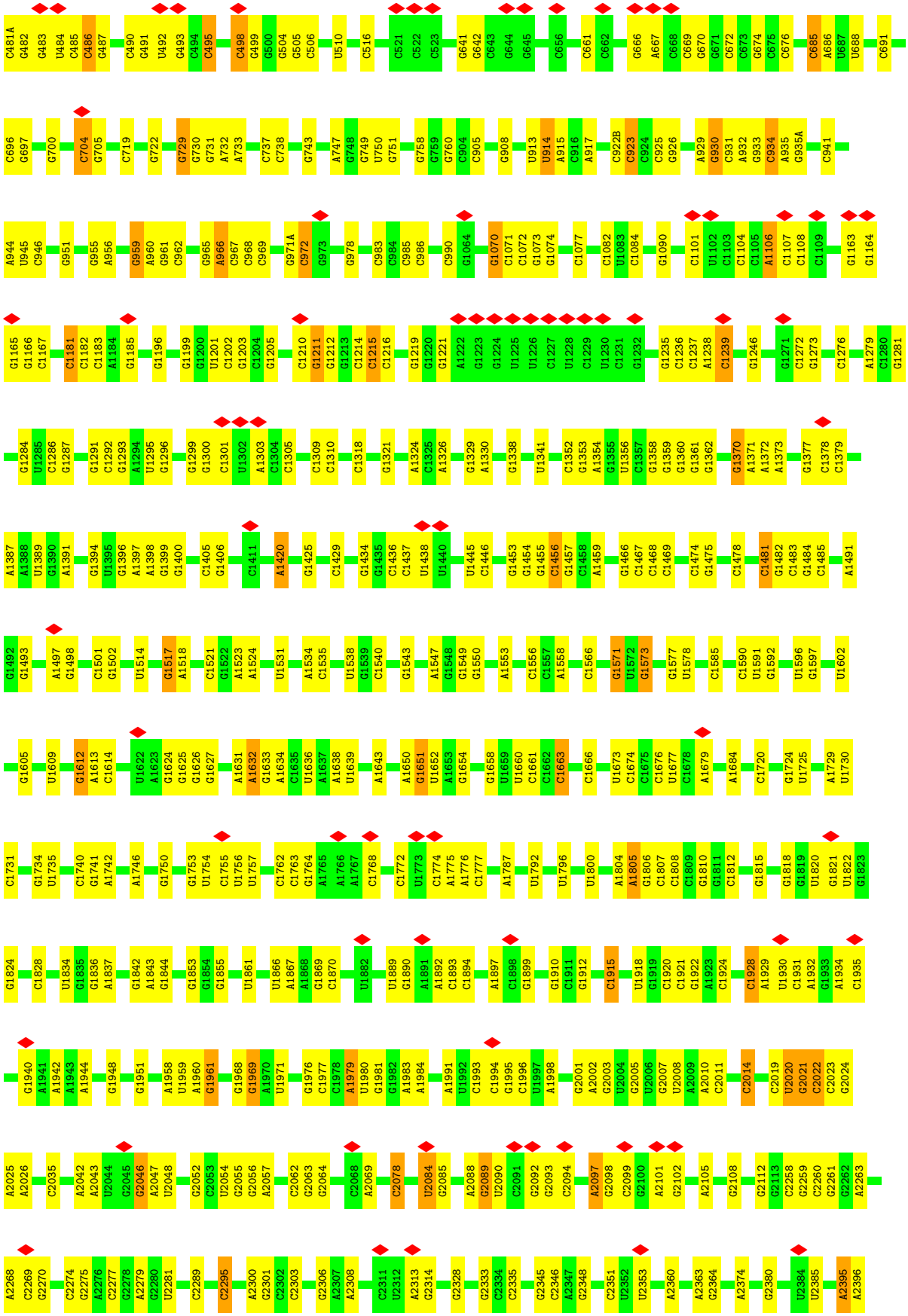




• Molecule 37: 28S ribosomal RNA

Chain 52:




C481A G482 G483 U484 C485 C486 G487 C490 G491 U492 G493 C494 C495 C498 G499 G500 G504 G505 C506 U510 C516 C521 C522 C523 G641 G642 G643 G644 G645 C656 C661 C662 G666 A667 C668 C669 G670 G671 C672 C673 G674 C675 C676 C685 A686 U687 U688 C691
C696 G697 G700 C704 G705 C719 G722 G729 G730 G731 A732 A733 C737 C738 G743 A747 G748 G749 U750 G751 G758 G759 G760 C904 C905 G908 U913 U914 A915 C916 A917 C922B C923 C924 C925 G926 A929 G930 C931 A932 G933 C934 A935 G935A C941
A944 U945 C946 G951 G955 A956 G959 A960 G961 C962 G965 A966 C967 C968 C969 G971A C972 G973 G978 C983 C984 C985 C986 C990 G1064 G1070 C1071 C1072 G1073 G1074 C1077 C1082 U1083 C1084 G1090 C1101 U1102 C1103 C1104 C1105 A1106 C1107 C1108 C1109 G1163 G1164
G1165 G1166 C1167 C1181 C1182 C1183 A1184 G1185 G1196 G1199 G1200 U1201 C1202 G1203 C1204 G1205 C1210 G1211 G1212 G1213 C1214 C1215 C1216 G1219 G1220 G1221 A1222 G1223 G1224 U1225 U1226 C1227 U1228 C1229 U1230 C1231 G1232 G1235 C1236 C1237 A1238 C1239 G1246 G1271 C1272 G1273 C1276 A1279 C1280 G1281
G1284 U1285 C1286 G1287 G1291 C1292 G1293 A1294 U1295 G1296 G1299 G1300 C1301 U1302 A1303 C1304 C1305 C1309 C1310 C1318 G1321 A1324 C1325 A1326 G1329 A1330 G1338 U1341 C1352 G1353 A1354 G1355 U1356 C1357 G1358 G1359 G1360 G1361 G1362 G1370 A1371 A1372 A1373 G1377 C1378 C1379
A1387 A1388 U1389 G1390 A1391 G1394 U1395 G1396 A1397 A1398 G1399 G1400 C1405 G1406 C1411 A1420 G1425 C1429 G1434 G1435 C1436 C1437 U1438 U1440 U1445 C1446 G1453 G1454 G1455 C1456 G1457 C1458 A1459 G1466 C1467 C1468 C1469 C1474 G1475 C1478 C1481 G1482 C1483 G1484 C1485 A1491
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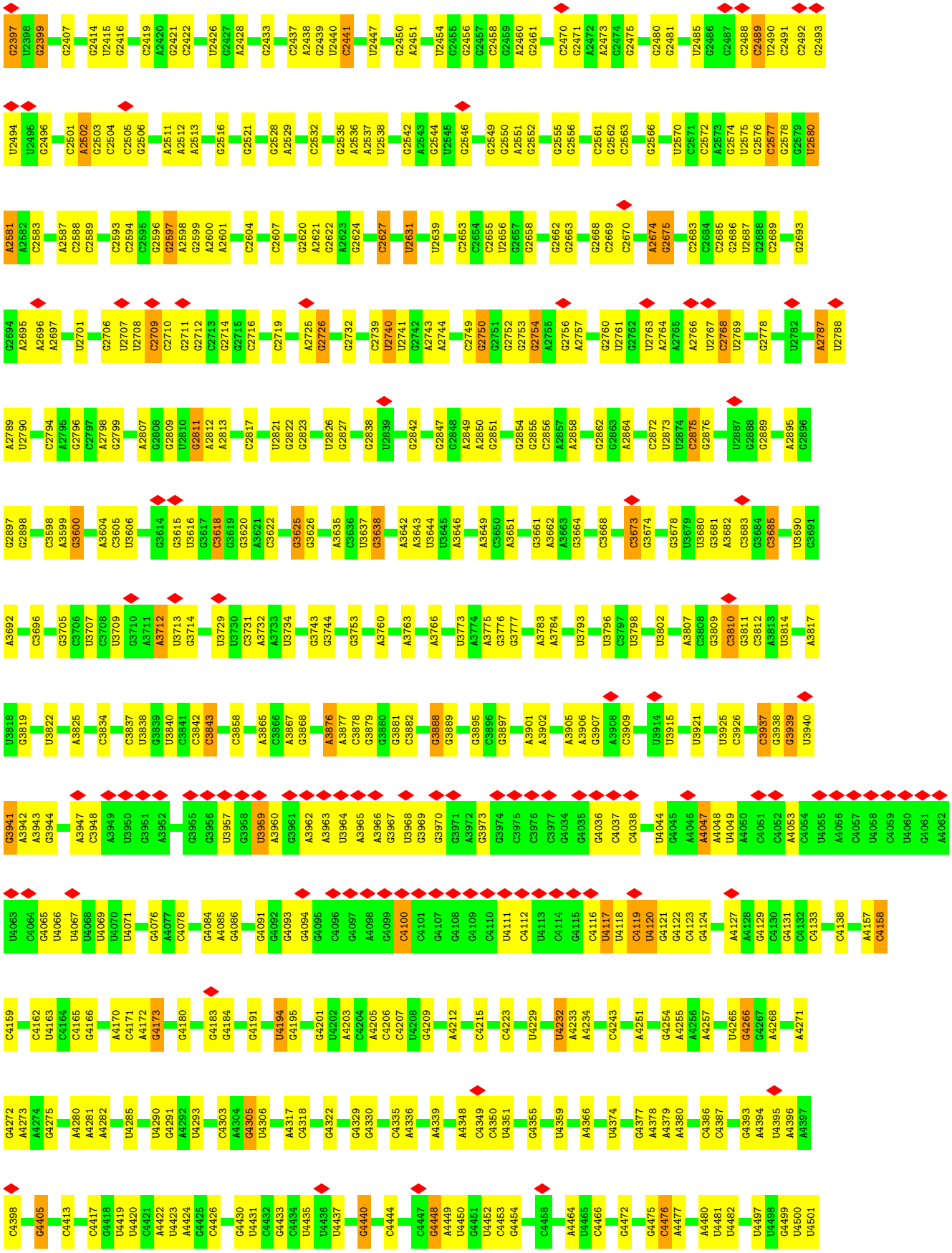
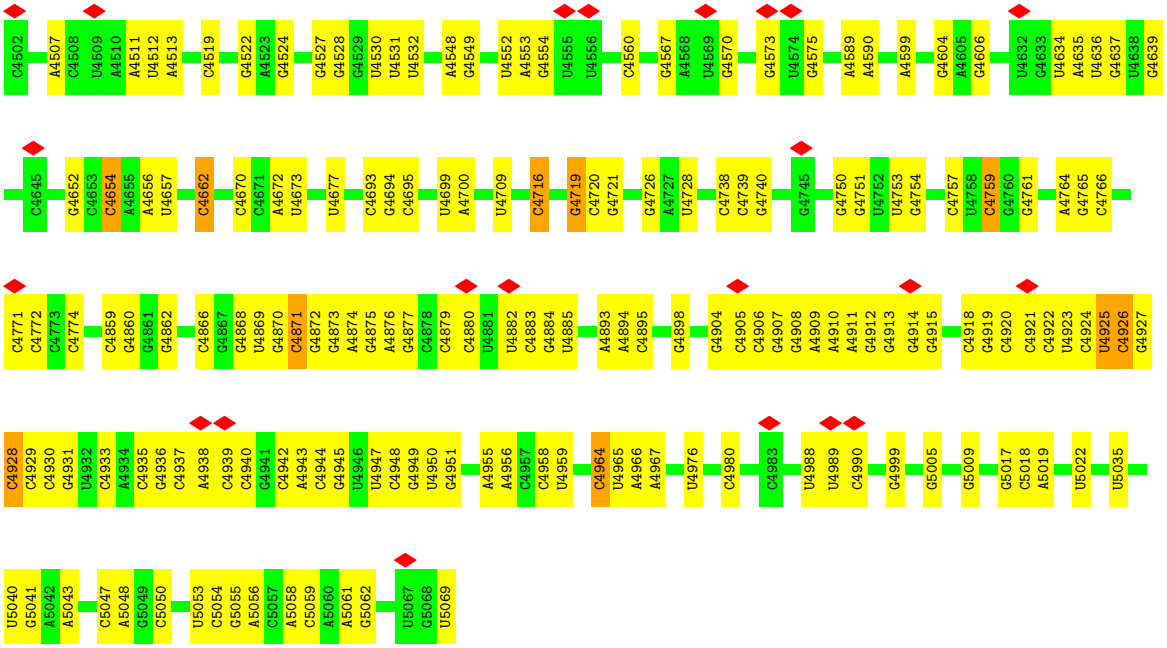
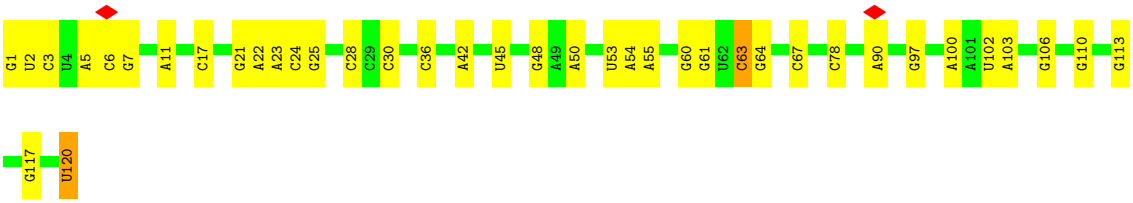
G1605 U1609 G1612 A1613 C1614 U1622 A1623 G1624 G1625 G1626 G1627 A1631 A1632 G1633 A1634 C1635 U1636 A1637 A1638 U1639 A1643 A1650 G1651 U1652 A1653 G1654 C1658 U1659 U1660 C1661 C1662 C1663 C1666 U1673 C1674 C1675 C1676 U1677 C1678 A1679 A1684 C1720 G1724 U1725 A1729 U1730
C1731 G1734 U1735 C1740 G1741 A1742 A1746 G1750 G1753 U1754 C1755 U1756 U1757 C1762 C1763 G1764 A1765 A1766 A1767 C1768 C1772 U1773 C1774 A1775 A1776 C1777 A1787 U1792 U1796 U1800 A1804 A1805 G1806 C1807 C1808 C1809 G1810 G1811 C1812 G1815 G1818 G1819 U1820 G1821 U1822 G1823
G1824 C1828 U1834 G1835 G1836 A1837 G1842 A1843 A1844 G1853 G1854 G1855 U1861 U1866 A1867 A1868 G1869 C1870 U1882 U1889 G1890 A1891 A1892 C1893 C1894 A1897 C1898 G1899 G1910 C1911 G1912 C1915 U1918 G1919 C1920 C1921 G1922 A1923 C1924 C1928 A1929 U1930 C1931 A1932 G1933 A1934 C1935
G1940 A1941 A1942 A1943 A1944 G1948 G1951 A1958 U1959 A1960 G1961 G1968 G1969 A1970 U1971 G1976 C1977 C1978 A1979 U1980 G1981 G1982 A1983 A1984 A1991 U1992 C1993 C1994 G1995 C1996 U1997 A1998 G2001 A2002 G2003 U2004 G2005 U2006 G2007 U2008 A2009 A2010 C2011 C2014 C2019 U2020 G2021 C2022 C2023 G2024
A2025 A2026 C2035 A2042 A2043 U2044 G2045 G2046 A2047 U2048 G2052 C2053 U2054 G2055 G2056 A2057 C2062 G2063 G2064 C2068 A2069 C2078 U2084 G2085 A2088 G2089 U2090 C2091 G2092 G2093 C2094 A2097 G2098 C2099 G2100 A2101 G2102 A2105 G2108 G2112 G2113 C2258 G2259 C2260 G2261 G2262 A2263
A2268 C2269 G2270 C2274 G2275 A2276 C2277 G2278 A2279 G2280 U2281 C2289 C2295 A2300 G2301 C2302 C2303 G2306 A2307 A2308 C2311 U2312 A2313 C2314 G2328 G2333 C2334 C2335 G2345 C2346 A2347 C2348 C2351 U2352 U2353 A2360 A2363 C2364 A2374 G2380 U2384 U2385 A2396





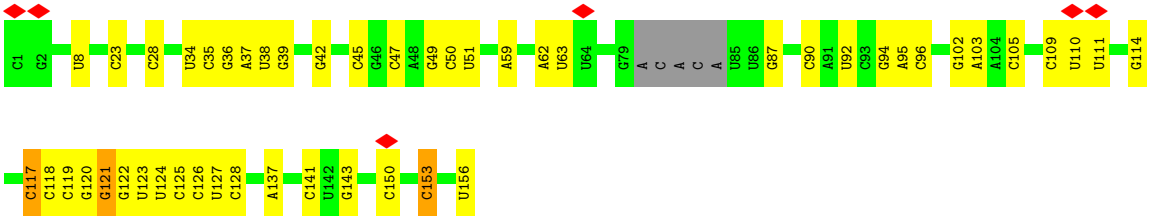
• Molecule 38: 5S ribosomal RNA

Chain 72:



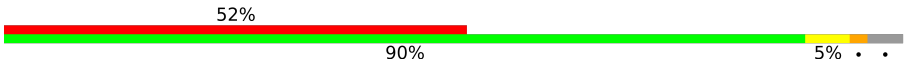
• Molecule 39: 5.8S ribosomal RNA

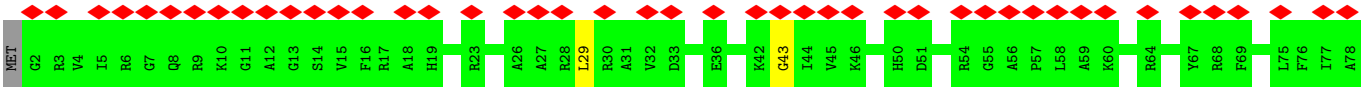
Chain 82:

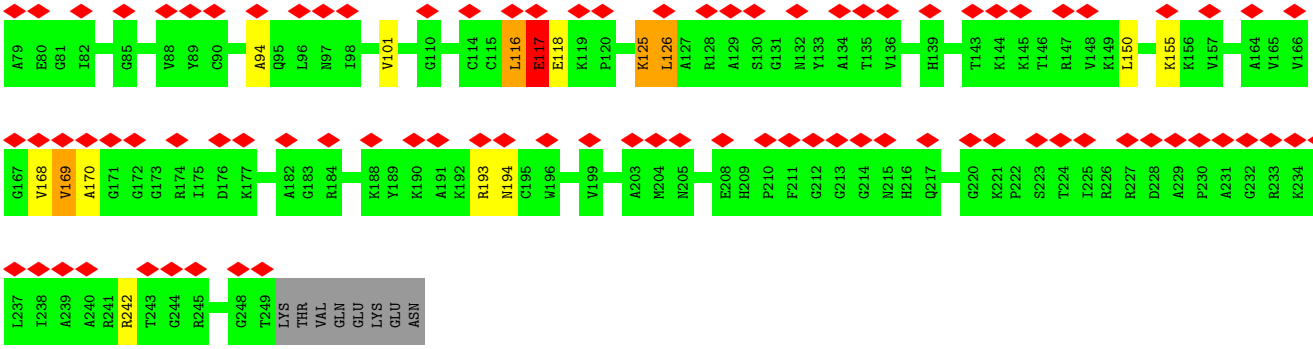


• Molecule 40: Ribosomal protein L8

Chain A3:

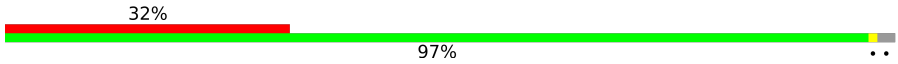


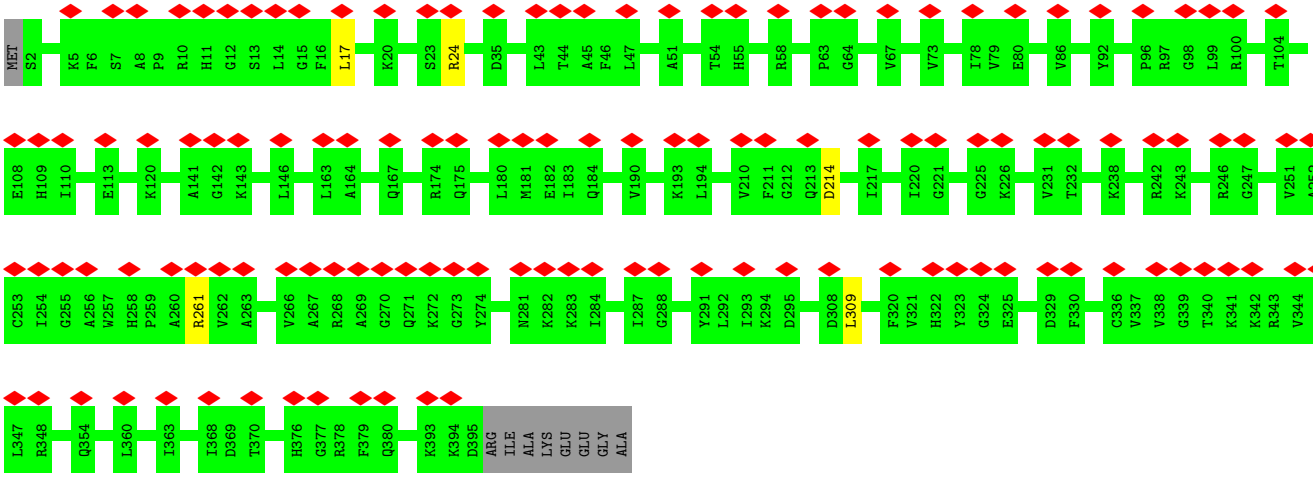




• Molecule 41: uL3

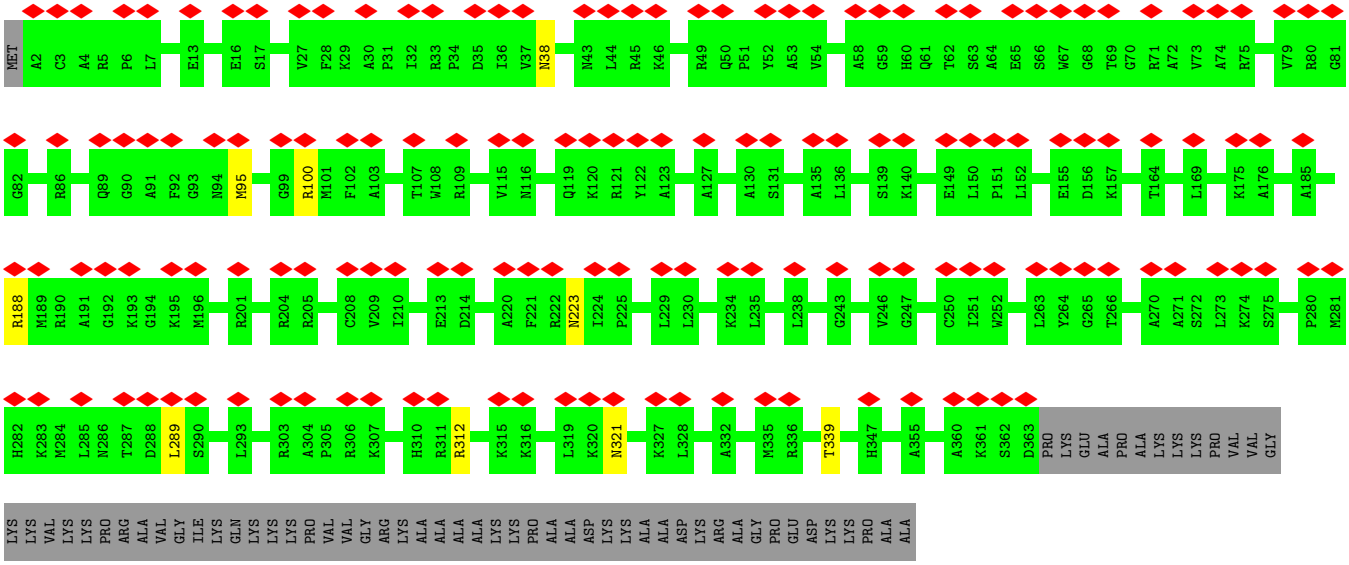
Chain B3:





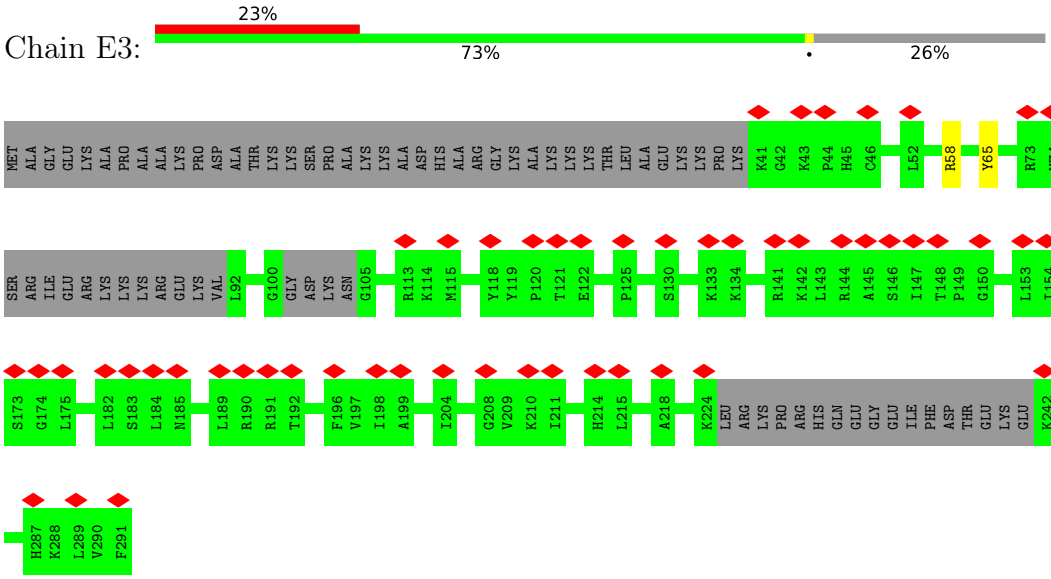
• Molecule 42: uL4

Chain C3:



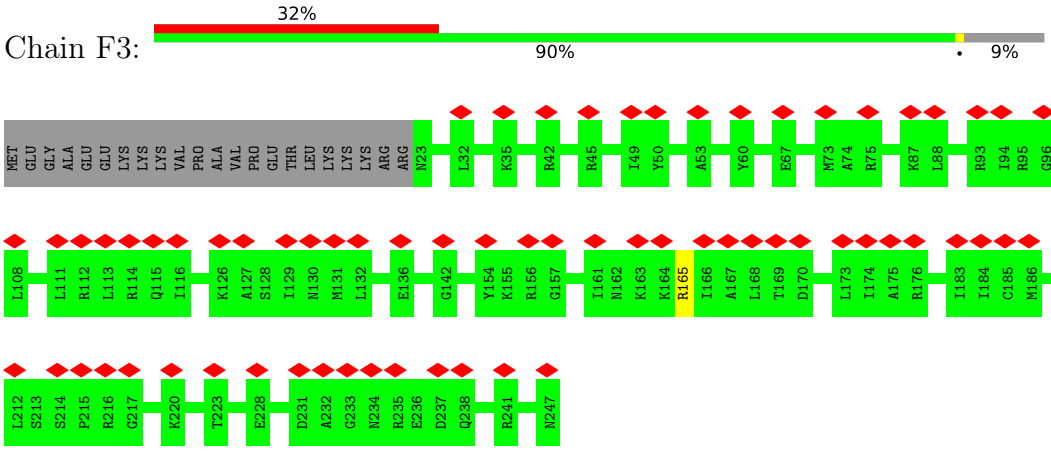
• Molecule 43: 60S ribosomal protein L6

Chain E3:



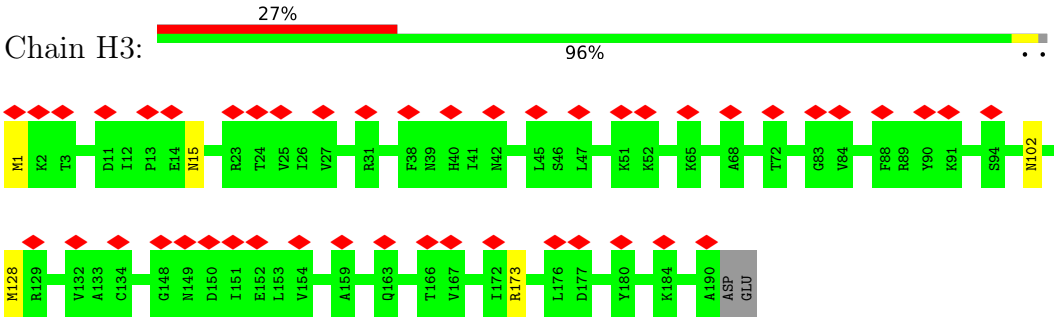
• Molecule 44: uL30

Chain F3:



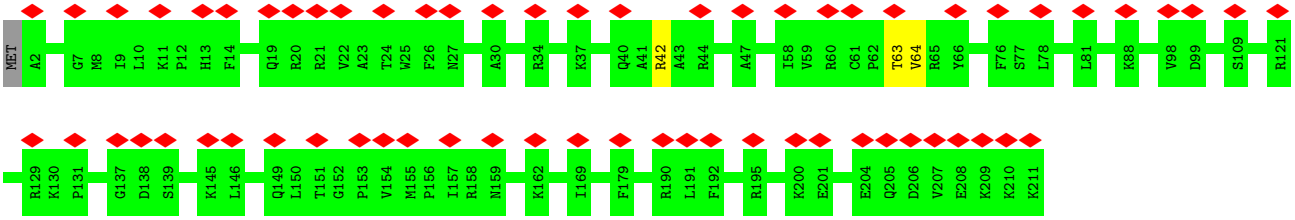
• Molecule 45: uL6

Chain H3:

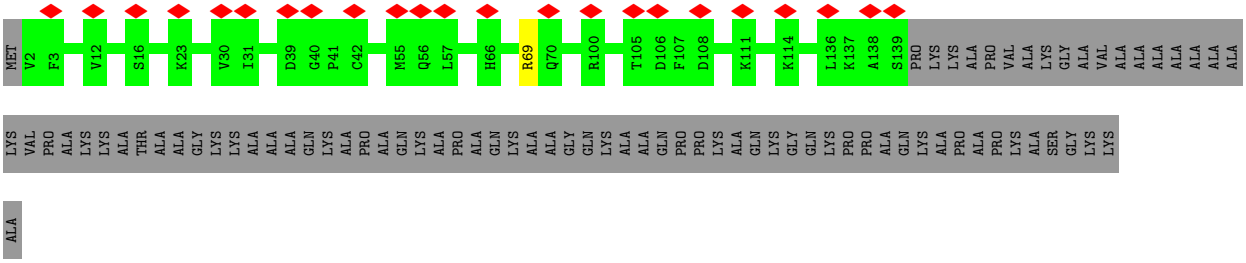


• Molecule 46: eL13

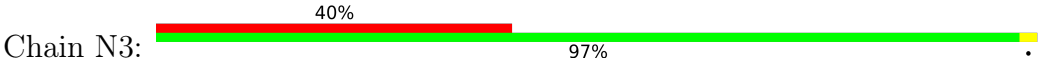
Chain L3:

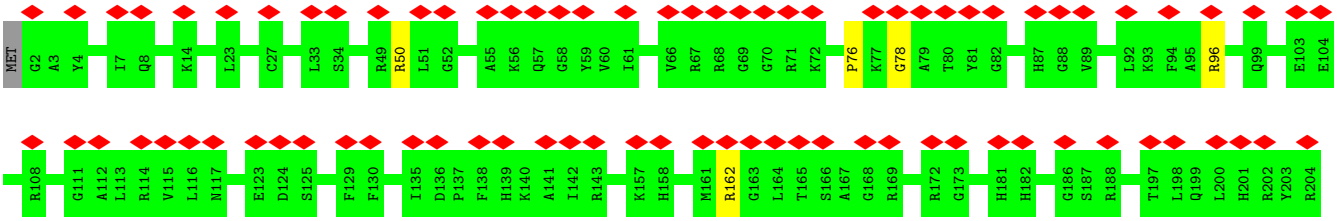


• Molecule 47: Ribosomal protein L14

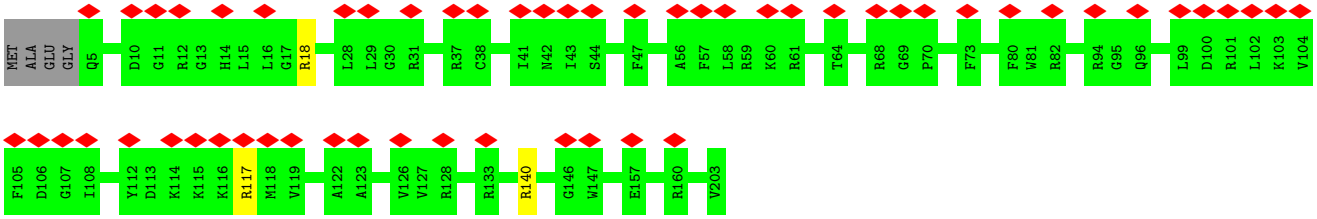


• Molecule 48: Ribosomal protein L15

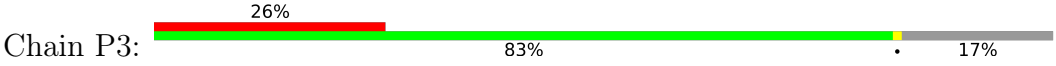


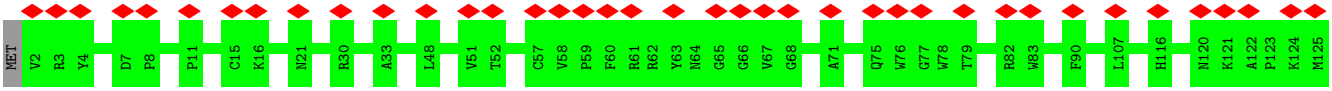


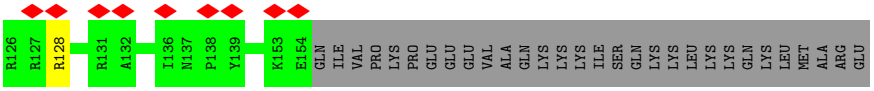
• Molecule 49: uL13



• Molecule 50: uL22

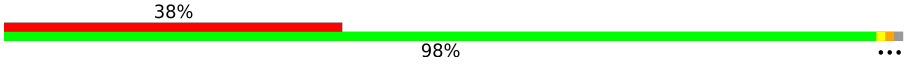


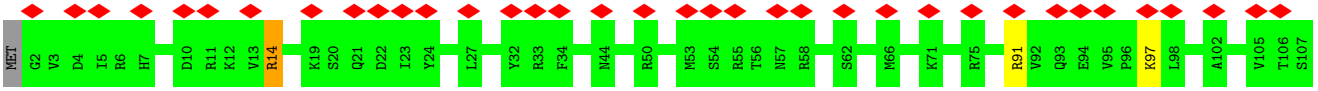


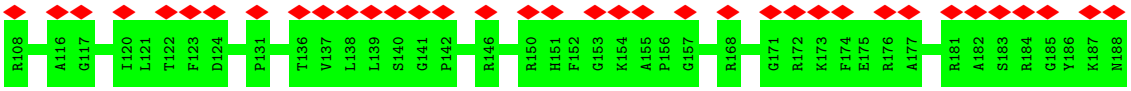


• Molecule 51: eL18

Chain Q3:

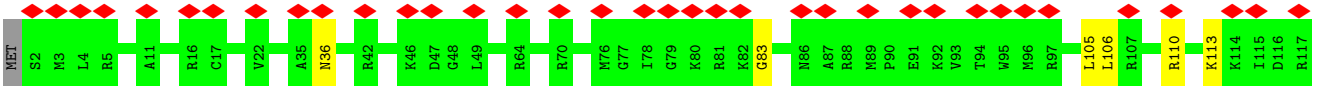


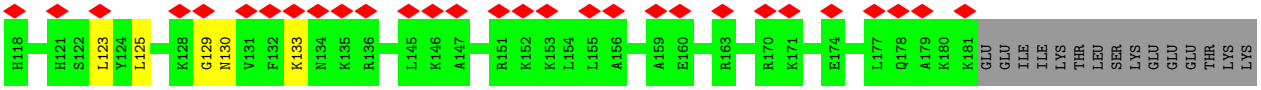




• Molecule 52: eL19

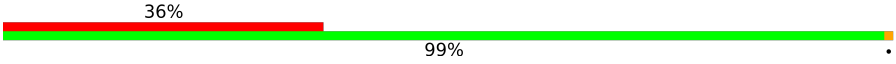
Chain R3:

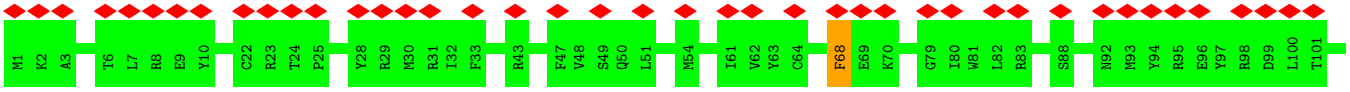


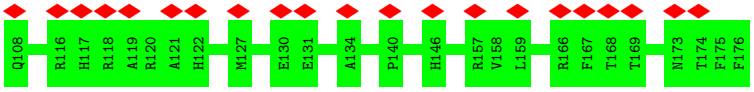


• Molecule 53: eL20

Chain S3:

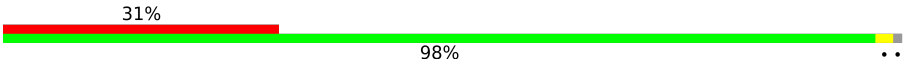


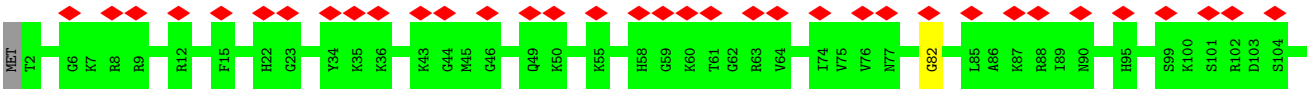


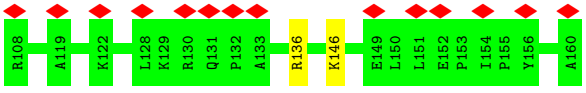


• Molecule 54: eL21

Chain T3:

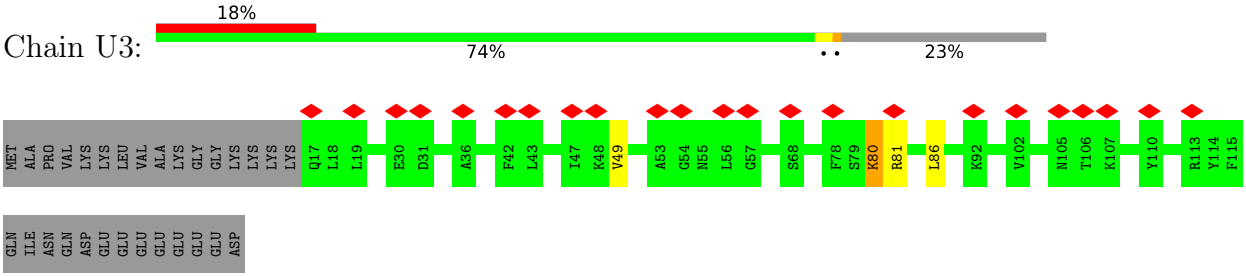






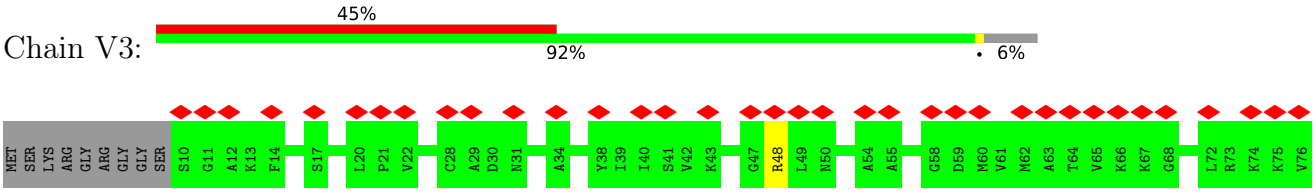
• Molecule 55: eL22

Chain U3:



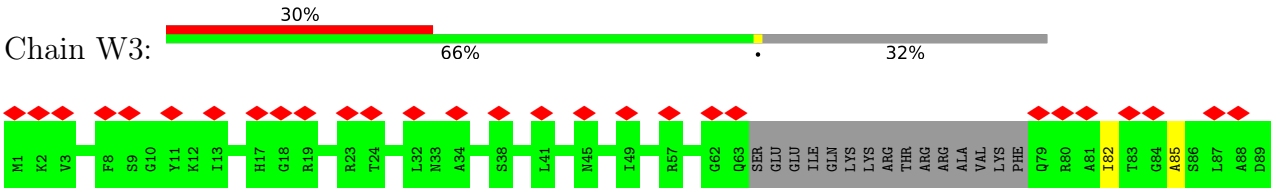
• Molecule 56: Ribosomal protein L23

Chain V3:



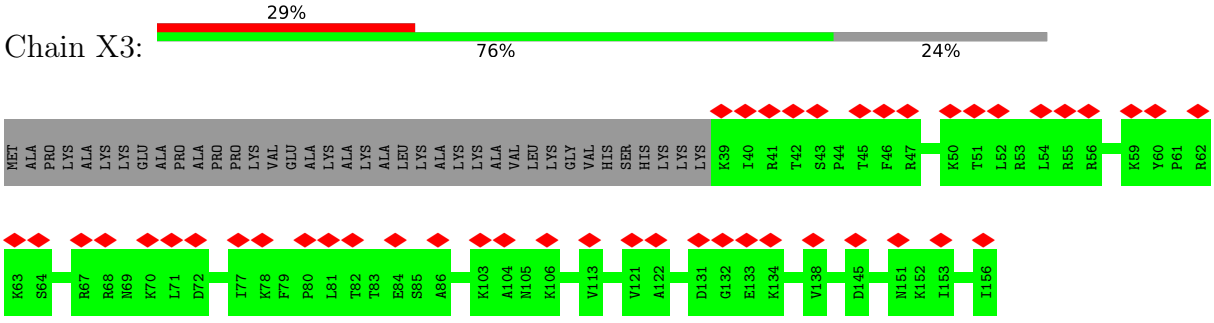
• Molecule 57: eL24

Chain W3:



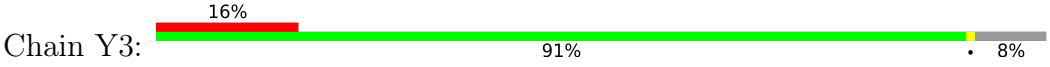
• Molecule 58: uL23

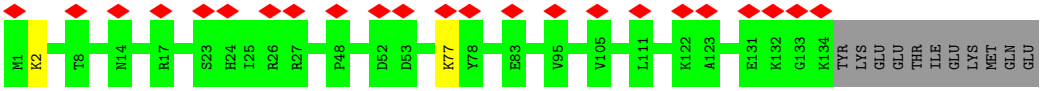
Chain X3:



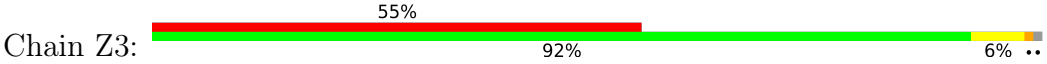
• Molecule 59: Ribosomal protein L26

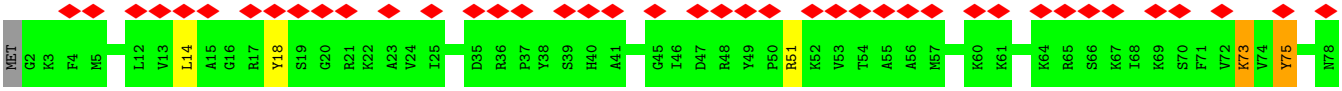
Chain Y3:

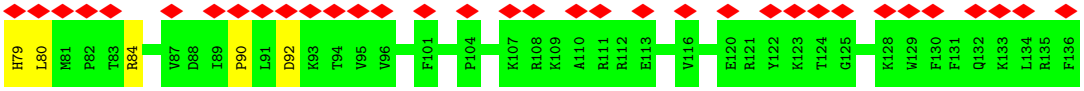




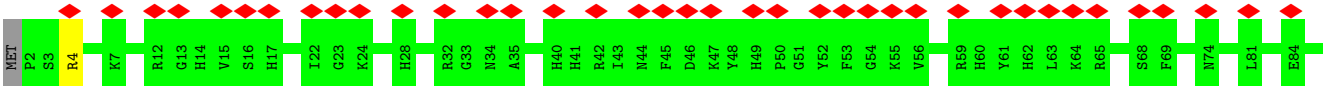
• Molecule 60: eL27

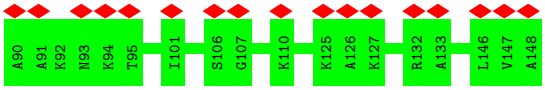




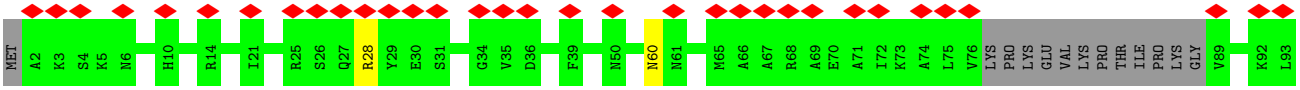


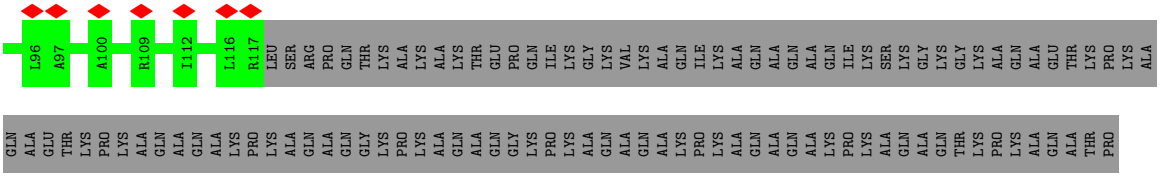
• Molecule 61: uL15



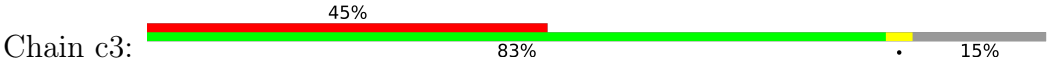


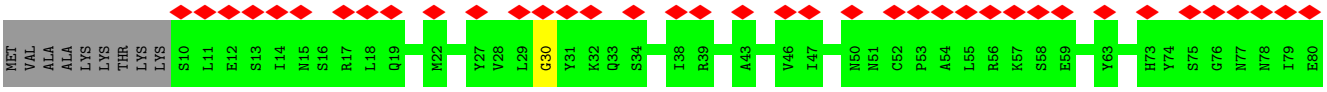
• Molecule 62: eL29

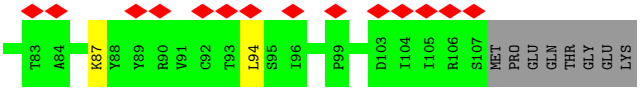




• Molecule 63: eL30

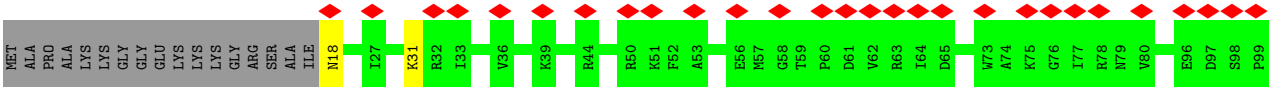


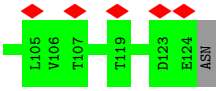




• Molecule 64: eL31

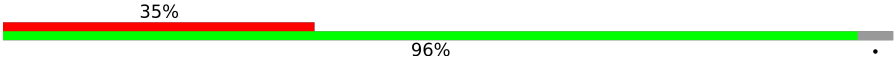
Chain d3:

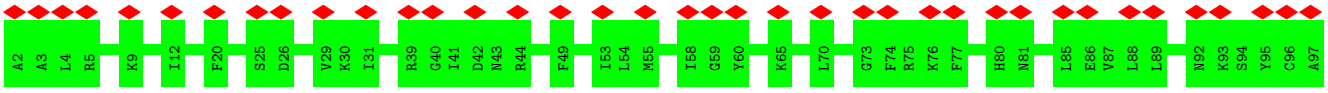


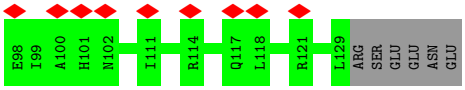


• Molecule 65: eL32

Chain e3:

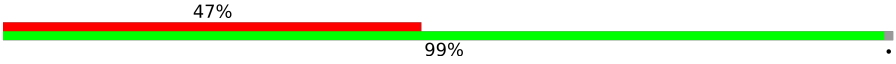


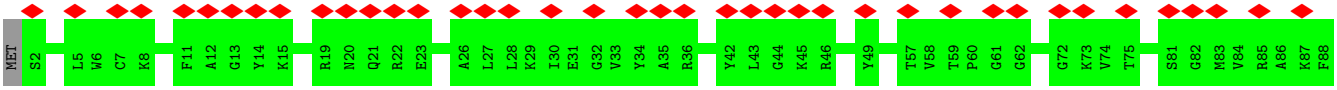


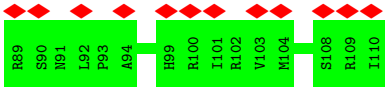


• Molecule 66: eL33

Chain f3:

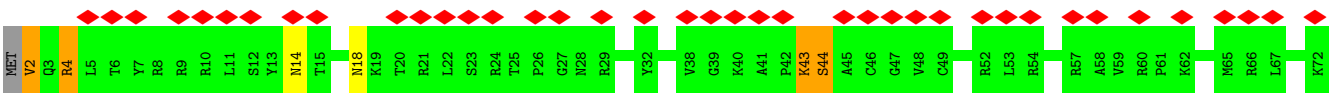


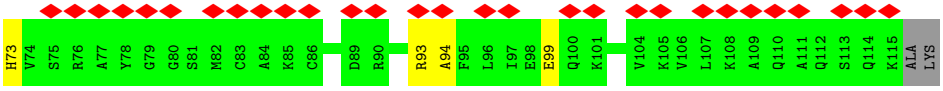




• Molecule 67: eL34

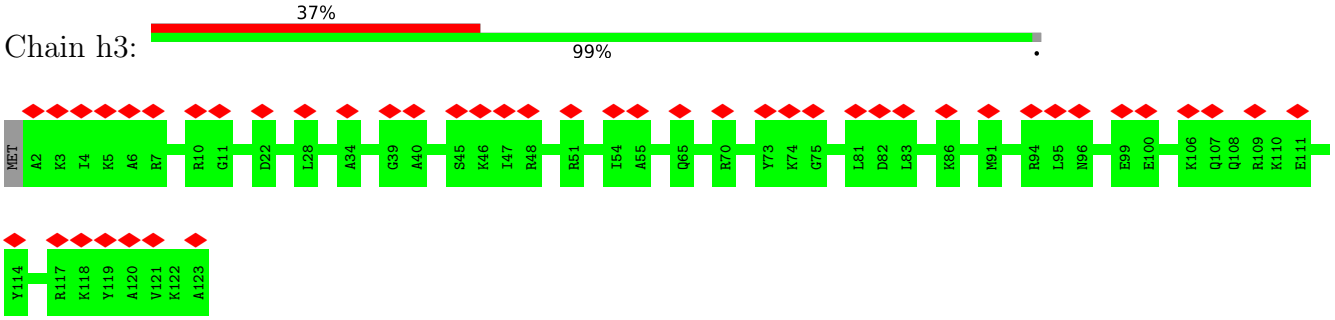
Chain g3:





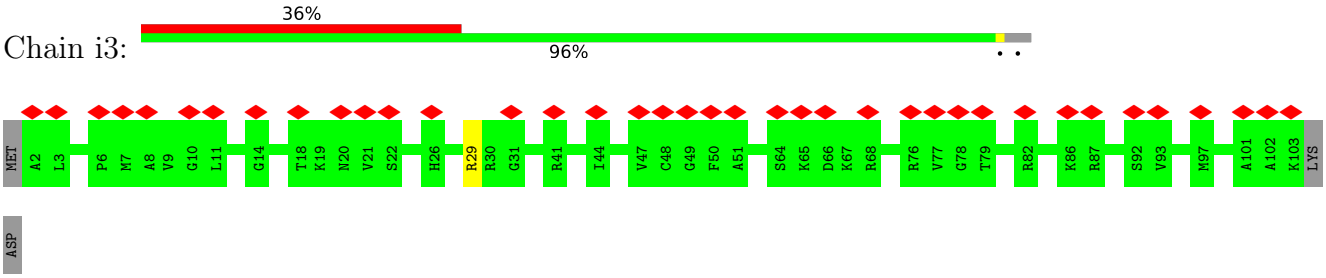
• Molecule 68: uL29

Chain h3:



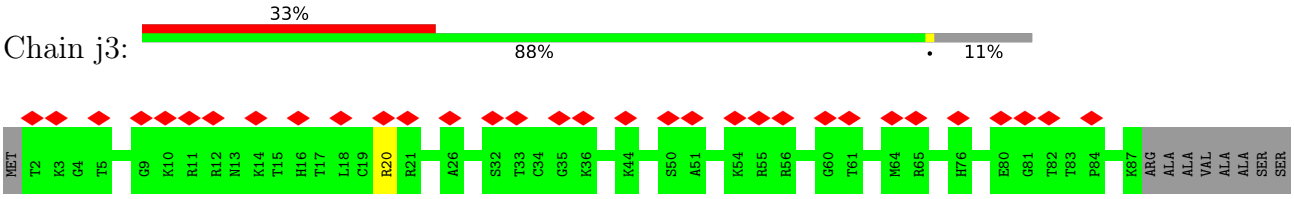
• Molecule 69: 60S ribosomal protein L36

Chain i3:



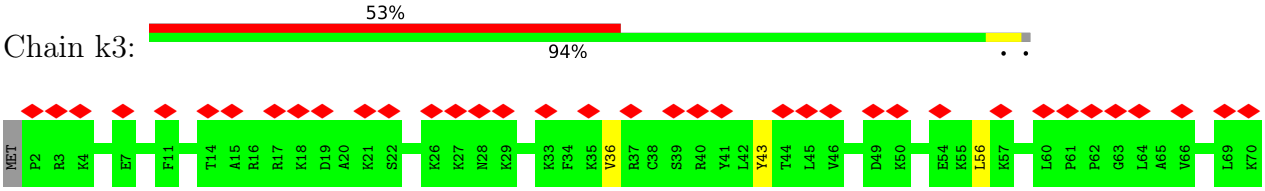
• Molecule 70: Ribosomal protein L37

Chain j3:



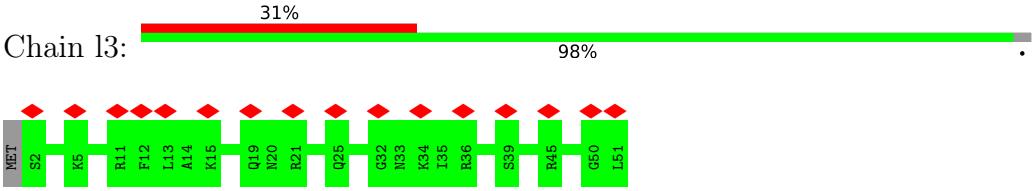
• Molecule 71: eL38

Chain k3:



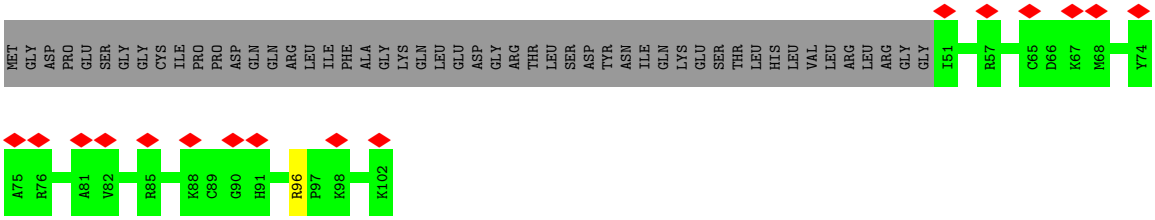
• Molecule 72: eL39

Chain l3:



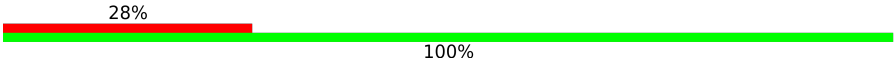
• Molecule 73: eL40

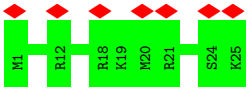
Chain m3:



• Molecule 74: eL41

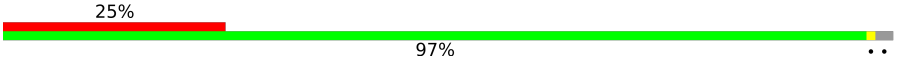
Chain n3:

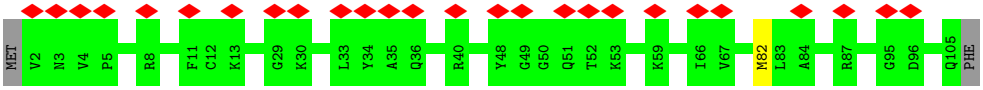




• Molecule 75: eL42

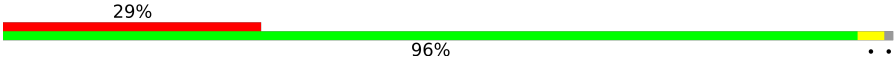
Chain o3:

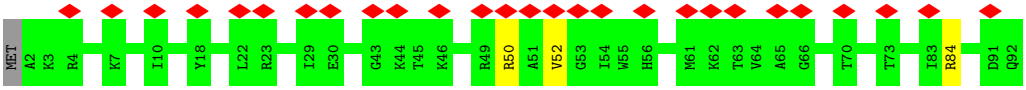




• Molecule 76: eL43

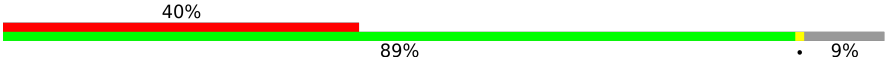
Chain p3:

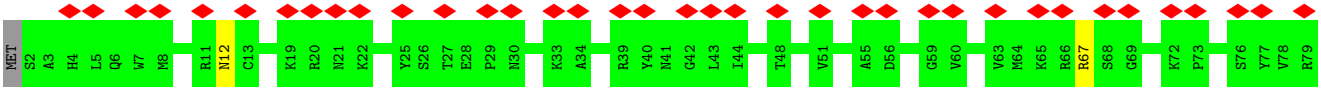


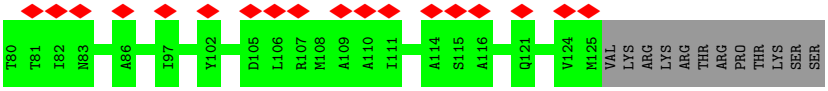


• Molecule 77: eL28

Chain r3:

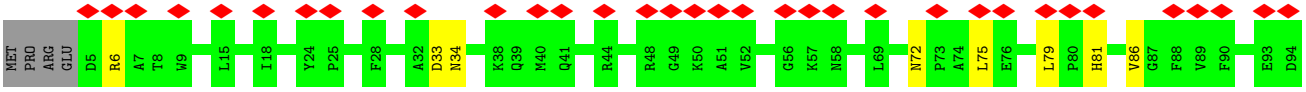


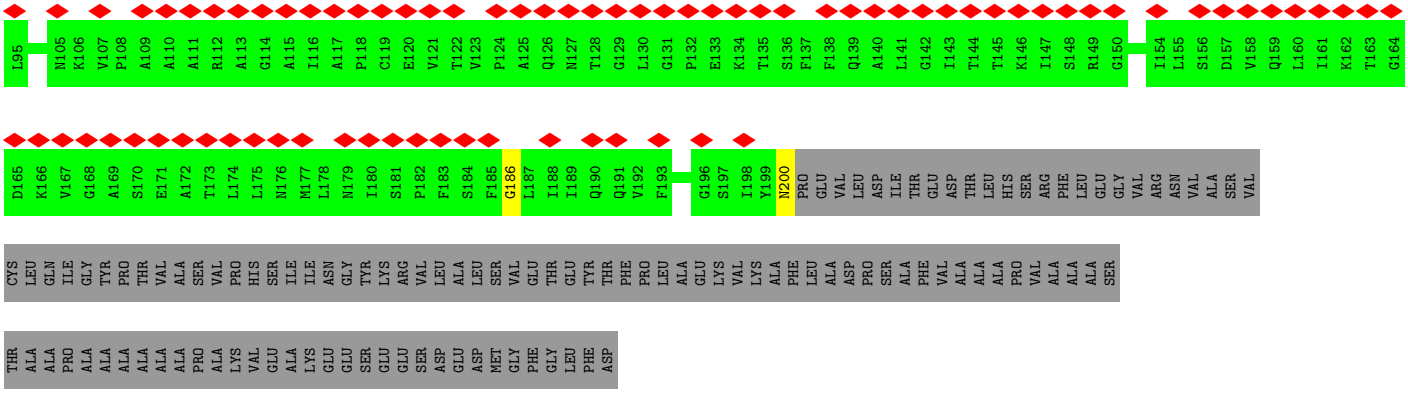




• Molecule 78: uL10

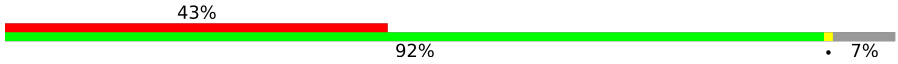
Chain s3:

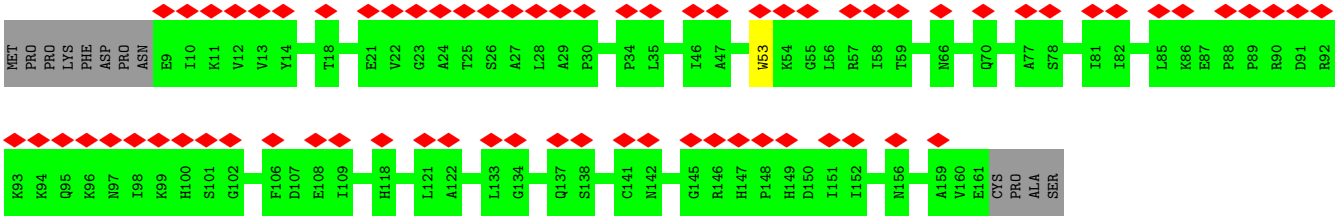




• Molecule 79: Ribosomal protein L12

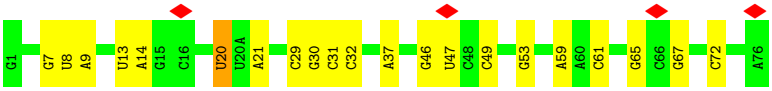
Chain t3:





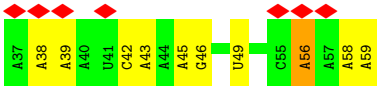
• Molecule 80: P-site tRNA

Chain 23:



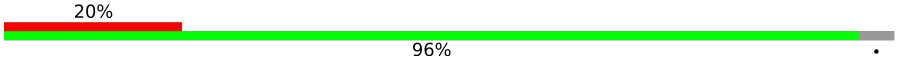
• Molecule 81: mRNA

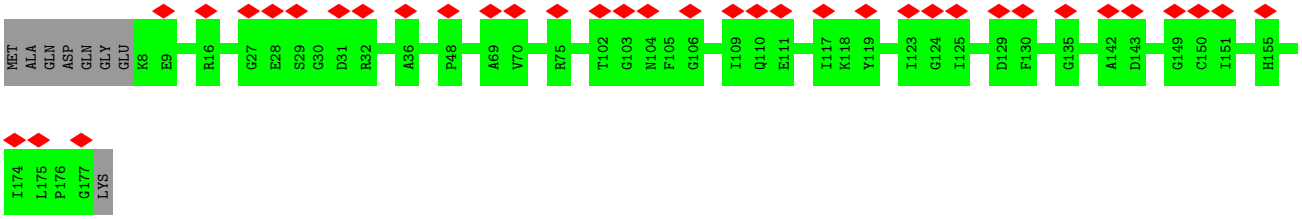
Chain w3:



• Molecule 82: Ribosomal protein L11

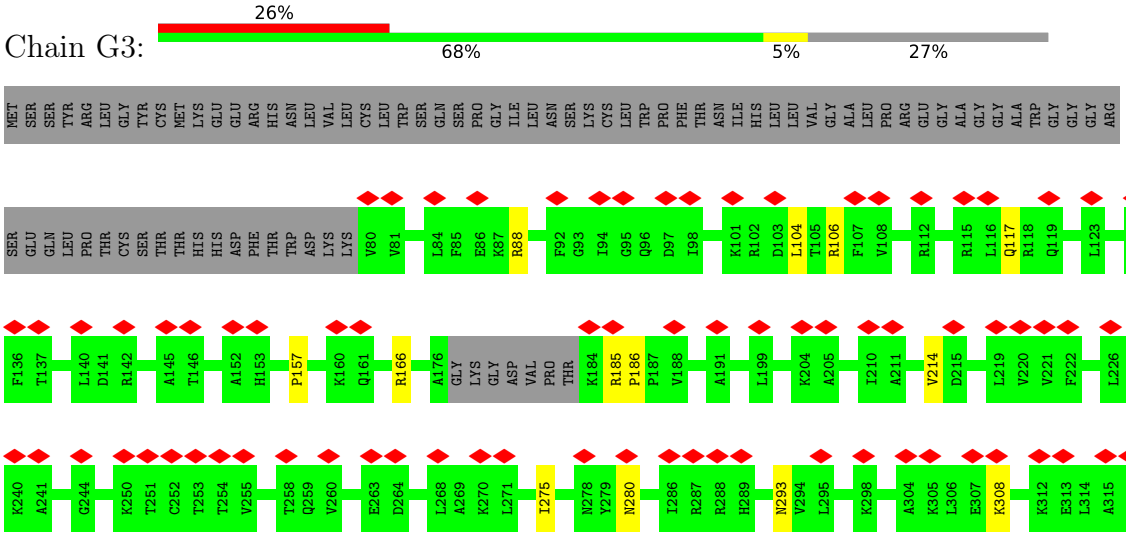
Chain J3:





• Molecule 83: eL8

Chain G3:

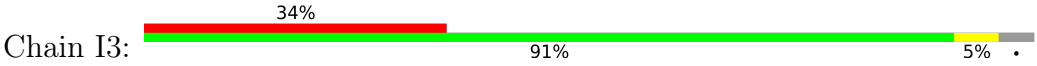


• Molecule 84: 60S ribosomal protein L5

Chain D3:

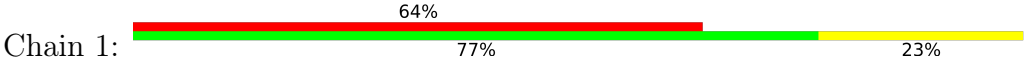
• Molecule 85: 60S ribosomal protein L10

Chain I3:



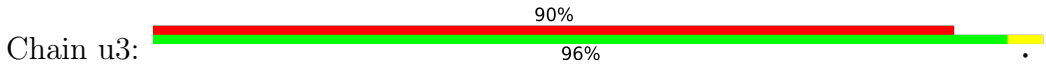
• Molecule 86: nascent chain

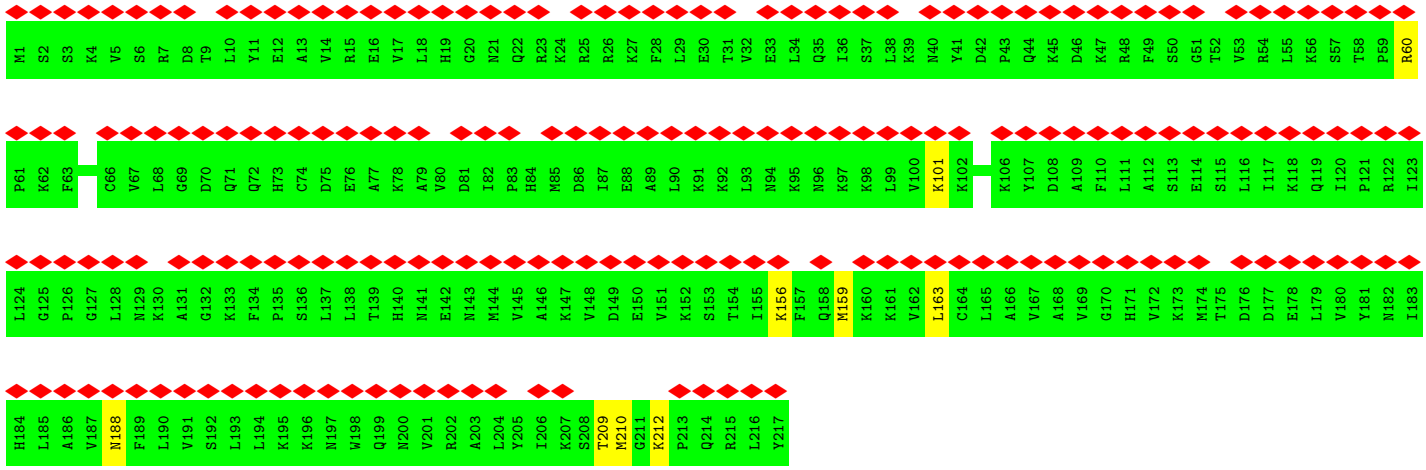
Chain 1:



• Molecule 87: Ribosomal protein

Chain u3:


90%
96%


M1 S2 S3 K4 V5 S6 R7 D8 T9 L10 Y11 E12 A13 V14 R15 E16 V17 L18 H19 G20 N21 Q22 R23 K24 R25 R26 K27 F28 L29 E30 T31 V32 E33 L34 Q35 I36 S37 L38 K39 N40 Y41 D42 P43 Q44 K45 D46 K47 R48 F49 S50 G51 T52 V53 R54 L55 K56 S57 T58 P59 R60
P61 K62 F63 C66 V67 L68 G69 D70 Q71 Q72 H73 C74 D75 E76 A77 K78 A79 V80 D81 I82 P83 H84 M85 D86 I87 E88 A89 L90 K91 K92 L93 N94 K95 N96 K97 K98 L99 V100 K101 K102 K106 Y107 D108 A109 F110 L111 A112 S113 E114 S115 L116 I117 K118 Q119 I120 P121 R122 I123
L124 G125 P126 G127 L128 N129 K130 A131 G132 K133 F134 P135 S136 L137 L138 T139 H140 N141 E142 N143 M144 V145 A146 K147 V148 D149 E150 V151 K152 S153 T154 I155 K156 F157 Q158 M159 K160 K161 V162 L163 C164 L165 A166 V167 A168 V169 G170 H171 V172 K173 M174 T175 D176 D177 E178 L179 V180 Y181 N182 I183
H184 L185 A186 V187 N188 F189 L190 V191 S192 L193 L194 K195 K196 N197 W198 Q199 N200 V201 R202 A203 L204 Y205 I206 K207 S208 T209 M210 G211 K212 P213 Q214 R215 L216 Y217

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14634	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.79	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.373	Depositor
Minimum map value	-0.246	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	1070.0, 1070.0, 1070.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.14, 2.14, 2.14	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A1	1.76	9/41324 (0.0%)	1.12	171/64370 (0.3%)
2	B1	0.39	0/1747	0.57	0/2374
3	C1	0.38	0/1756	0.58	1/2350 (0.0%)
4	D1	0.44	0/1753	0.58	0/2369
5	E1	0.38	0/1796	0.59	0/2417
6	F1	0.39	0/2118	0.57	1/2849 (0.0%)
7	G1	0.38	0/1492	0.56	0/2005
8	H1	0.36	0/1946	0.62	0/2590
9	I1	0.34	0/1510	0.60	1/2022 (0.0%)
10	J1	0.42	0/1715	0.57	0/2287
11	K1	0.38	0/1550	0.60	0/2069
12	L1	0.37	0/834	0.59	0/1125
13	M1	0.46	0/1195	0.57	0/1597
14	N1	0.32	0/918	0.65	1/1233 (0.1%)
15	O1	0.38	0/1226	0.55	0/1649
16	P1	0.39	0/1029	0.57	0/1380
17	Q1	0.42	0/1017	0.60	0/1358
18	R1	0.41	0/1146	0.59	0/1534
19	S1	0.35	0/1082	0.55	0/1452
20	T1	0.39	0/1208	0.59	0/1618
21	U1	0.39	0/1115	0.57	0/1493
22	V1	0.33	0/805	0.54	0/1081
23	W1	0.40	0/643	0.59	0/860
24	X1	0.42	0/1051	0.58	0/1406
25	Y1	0.43	0/1116	0.59	0/1490
26	Z1	0.36	0/1028	0.53	0/1366
27	a1	0.37	0/604	0.67	0/810
28	b1	0.42	0/828	0.54	0/1109
29	c1	0.36	0/665	0.57	0/891
30	d1	0.38	0/490	0.55	0/656
31	e1	0.44	0/470	0.57	0/623
32	f1	0.35	0/447	0.51	0/587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	g1	0.28	0/567	0.57	0/753
34	h1	0.34	0/2493	0.58	0/3394
35	j1	0.35	0/3363	0.57	1/4523 (0.0%)
36	k1	0.36	0/4640	0.57	0/6264
37	52	2.86	73/87026 (0.1%)	1.46	554/135683 (0.4%)
38	72	5.70	7/2858 (0.2%)	1.28	21/4455 (0.5%)
39	82	1.02	0/3581	1.12	15/5577 (0.3%)
40	A3	0.56	2/1936 (0.1%)	0.85	7/2596 (0.3%)
41	B3	0.51	0/3240	0.63	3/4339 (0.1%)
42	C3	0.53	0/2937	0.63	1/3946 (0.0%)
43	E3	2.24	3/1762 (0.2%)	0.69	3/2362 (0.1%)
44	F3	0.57	0/1911	0.61	0/2549
45	H3	0.47	0/1535	0.60	0/2063
46	L3	0.50	0/1733	0.62	0/2316
47	M3	0.52	0/1158	0.59	0/1547
48	N3	0.58	0/1746	0.64	0/2338
49	O3	0.54	0/1662	0.65	1/2222 (0.0%)
50	P3	0.55	0/1268	0.58	0/1700
51	Q3	1.98	2/1539 (0.1%)	0.95	4/2054 (0.2%)
52	R3	0.46	0/1524	0.71	1/2013 (0.0%)
53	S3	1.00	1/1501 (0.1%)	0.82	5/2012 (0.2%)
54	T3	0.53	0/1326	0.56	0/1770
55	U3	1.95	3/823 (0.4%)	1.36	7/1104 (0.6%)
56	V3	0.49	0/993	0.60	0/1332
57	W3	0.43	0/873	0.60	0/1158
58	X3	0.45	0/984	0.55	0/1323
59	Y3	0.51	0/1132	0.60	0/1504
60	Z3	0.61	0/1130	1.00	4/1507 (0.3%)
61	a3	0.52	0/1191	0.59	0/1590
62	b3	1.83	2/861 (0.2%)	0.84	4/1138 (0.4%)
63	c3	0.46	0/771	0.84	3/1034 (0.3%)
64	d3	0.51	0/903	0.62	0/1216
65	e3	0.52	0/1071	0.60	0/1429
66	f3	0.59	0/895	0.63	0/1198
67	g3	5.33	4/916 (0.4%)	1.34	7/1220 (0.6%)
68	h3	0.47	0/1021	0.59	0/1348
69	i3	0.43	0/841	0.59	0/1112
70	j3	0.54	0/720	0.61	0/952
71	k3	0.42	0/575	0.80	1/761 (0.1%)
72	l3	0.47	0/459	0.58	0/608
73	m3	0.46	0/435	0.55	0/575
74	n3	0.40	0/240	0.66	0/305
75	o3	0.46	0/864	0.58	0/1140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	p3	0.55	0/718	0.74	0/953
77	r3	0.53	0/1010	0.63	0/1354
78	s3	0.50	1/1530 (0.1%)	0.89	5/2064 (0.2%)
79	t3	0.31	0/1174	0.64	0/1582
80	23	0.61	0/1805	1.13	10/2809 (0.4%)
81	w3	0.62	0/553	1.24	2/859 (0.2%)
82	J3	0.41	0/1385	0.58	0/1852
83	G3	1.53	2/1910 (0.1%)	0.98	6/2569 (0.2%)
84	D3	0.48	0/2437	0.61	0/3264
85	I3	1.09	2/1702 (0.1%)	0.76	4/2272 (0.2%)
86	1	0.45	0/109	0.65	0/151
87	u3	0.29	0/1769	0.64	1/2371 (0.0%)
All	All	2.04	111/242730 (0.0%)	1.12	845/355150 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B1	0	1
14	N1	0	1
16	P1	0	1
17	Q1	0	2
25	Y1	0	1
35	j1	0	1
36	k1	0	1
40	A3	0	5
42	C3	0	1
47	M3	0	1
48	N3	0	2
52	R3	0	5
53	S3	0	1
55	U3	0	1
57	W3	0	1
60	Z3	0	3
63	c3	0	1
67	g3	0	8
71	k3	0	1
76	p3	0	2
78	s3	0	4
79	t3	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
83	G3	0	3
85	I3	0	1
87	u3	0	2
All	All	0	51

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	52	732	A	N3-C4	183.92	2.45	1.34
37	52	1805	A	N3-C4	177.18	2.41	1.34
37	52	732	A	C6-N1	163.94	2.50	1.35
1	A1	970	G	C6-N1	162.04	2.52	1.39
37	52	2631	U	C2-N3	160.43	2.50	1.37
37	52	1805	A	C6-N1	156.98	2.45	1.35
38	72	63	C	N3-C4	154.10	2.41	1.33
1	A1	970	G	N1-C2	147.62	2.55	1.37
67	g3	2	VAL	CA-CB	147.00	4.63	1.54
38	72	63	C	C2-N3	141.12	2.48	1.35
37	52	2399	G	N3-C4	140.98	2.34	1.35
37	52	119	G	N3-C4	140.74	2.33	1.35
38	72	63	C	N1-C6	137.26	2.19	1.37
37	52	1805	A	C5-C4	131.30	2.30	1.38
1	A1	970	G	N3-C4	130.52	2.26	1.35
37	52	2631	U	N1-C2	129.23	2.54	1.38
37	52	2084	U	C2-N3	128.24	2.27	1.37
37	52	732	A	C5-C4	128.21	2.28	1.38
37	52	2631	U	N3-C4	126.02	2.51	1.38
37	52	119	G	C2-N3	125.41	2.33	1.32
37	52	2399	G	C2-N3	125.05	2.32	1.32
37	52	732	A	N1-C2	123.46	2.45	1.34
37	52	1805	A	N1-C2	119.63	2.42	1.34
37	52	732	A	C2-N3	119.41	2.41	1.33
37	52	1805	A	C5-C6	119.35	2.48	1.41
37	52	1239	C	N3-C4	118.41	2.16	1.33
37	52	2631	U	N1-C6	118.05	2.44	1.38
1	A1	970	G	C5-C4	117.54	2.20	1.38
37	52	2631	U	C4-C5	115.95	2.48	1.43
1	A1	970	G	C2-N3	115.88	2.25	1.32
37	52	1805	A	C2-N3	114.84	2.37	1.33
37	52	119	G	C6-N1	114.36	2.19	1.39
37	52	2399	G	C6-N1	111.68	2.17	1.39
37	52	732	A	C5-C6	109.11	2.39	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	52	2631	U	C5-C6	108.83	2.32	1.34
37	52	1239	C	C2-N3	104.50	2.19	1.35
38	72	63	C	C4-C5	101.87	2.24	1.43
37	52	2084	U	N3-C4	100.61	2.29	1.38
37	52	2084	U	N1-C2	99.49	2.28	1.38
37	52	119	G	N1-C2	98.51	2.16	1.37
37	52	2399	G	N1-C2	97.19	2.15	1.37
37	52	2084	U	N1-C6	95.14	2.23	1.38
37	52	2399	G	C5-C4	94.78	2.04	1.38
38	72	63	C	C5-C6	94.72	2.10	1.34
37	52	119	G	C5-C4	94.06	2.04	1.38
37	52	1239	C	N1-C6	93.41	1.93	1.37
1	A1	970	G	C5-C6	91.53	2.33	1.42
43	E3	65	TYR	CZ-OH	90.98	2.92	1.37
37	52	2084	U	C4-C5	90.28	2.24	1.43
38	72	63	C	N1-C2	89.65	2.29	1.40
37	52	2084	U	C5-C6	85.61	2.11	1.34
37	52	3712	A	N1-C2	82.18	2.08	1.34
37	52	3712	A	C2-N3	81.71	2.07	1.33
51	Q3	14	ARG	CD-NE	74.43	2.73	1.46
37	52	3712	A	N3-C4	72.92	1.78	1.34
37	52	2399	G	C5-C6	72.46	2.14	1.42
37	52	119	G	C5-C6	72.38	2.14	1.42
37	52	2395	A	N3-C4	68.04	1.75	1.34
37	52	3712	A	C6-N1	65.58	1.81	1.35
37	52	1239	C	C4-C5	65.57	1.95	1.43
37	52	2395	A	C6-N1	62.98	1.79	1.35
83	G3	185	ARG	CD-NE	62.81	2.53	1.46
67	g3	4	ARG	CD-NE	62.75	2.53	1.46
37	52	1239	C	C5-C6	61.88	1.83	1.34
37	52	1239	C	N1-C2	60.55	2.00	1.40
62	b3	28	ARG	CA-CB	51.93	2.68	1.53
37	52	2395	A	C5-C4	51.01	1.74	1.38
55	U3	49	VAL	CA-CB	49.09	2.57	1.54
37	52	2395	A	N1-C2	47.58	1.77	1.34
37	52	2395	A	C2-N3	44.34	1.73	1.33
37	52	2395	A	C5-C6	43.11	1.79	1.41
85	I3	203	ARG	C-N	35.18	1.96	1.33
53	S3	68	PHE	CA-C	31.86	2.35	1.52
85	I3	204	GLY	N-CA	20.27	1.76	1.46
55	U3	49	VAL	CB-CG1	16.48	1.87	1.52
55	U3	49	VAL	CB-CG2	14.17	1.82	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	s3	186	GLY	C-N	14.08	1.66	1.34
83	G3	185	ARG	NE-CZ	11.39	1.47	1.33
67	g3	4	ARG	NE-CZ	10.93	1.47	1.33
37	52	1805	A	C8-N7	9.37	1.38	1.31
1	A1	970	G	C8-N7	9.09	1.36	1.30
43	E3	65	TYR	CE1-CZ	9.00	1.50	1.38
37	52	3712	A	C5-C4	-8.59	1.32	1.38
43	E3	65	TYR	CE2-CZ	8.12	1.49	1.38
37	52	3712	A	C5-C6	-7.77	1.34	1.41
37	52	1969	G	C8-N7	-7.63	1.26	1.30
37	52	3712	A	N9-C4	7.29	1.42	1.37
67	g3	4	ARG	CG-CD	7.29	1.70	1.51
51	Q3	14	ARG	NE-CZ	7.00	1.42	1.33
37	52	2598	A	N7-C5	-6.99	1.35	1.39
37	52	732	A	C8-N7	6.90	1.36	1.31
37	52	119	G	C8-N7	6.89	1.35	1.30
37	52	1805	A	N9-C8	6.84	1.43	1.37
37	52	2675	G	N7-C5	-6.83	1.35	1.39
62	b3	28	ARG	CB-CG	6.64	1.70	1.52
37	52	2597	G	N9-C8	-6.59	1.33	1.37
38	72	5	A	N9-C4	-6.48	1.33	1.37
40	A3	117	GLU	CB-CG	-6.34	1.40	1.52
37	52	2598	A	N9-C4	6.09	1.41	1.37
1	A1	970	G	N9-C8	6.06	1.42	1.37
37	52	1969	G	N7-C5	-6.04	1.35	1.39
37	52	347	A	N9-C4	-5.69	1.34	1.37
1	A1	970	G	N9-C4	-5.33	1.33	1.38
37	52	2399	G	N7-C5	-5.31	1.36	1.39
37	52	3681	G	N3-C4	-5.29	1.31	1.35
37	52	2675	G	N9-C8	-5.22	1.34	1.37
37	52	1805	A	N9-C4	-5.21	1.34	1.37
40	A3	169	VAL	CB-CG2	-5.15	1.42	1.52
37	52	1324	A	N7-C5	-5.08	1.36	1.39
37	52	1577	G	C8-N7	-5.04	1.27	1.30
37	52	2597	G	O3'-P	5.00	1.67	1.61

All (845) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	3712	A	N1-C2-N3	-240.06	9.27	129.30
37	52	3712	A	C2-N3-C4	88.06	154.63	110.60
37	52	3712	A	C6-N1-C2	69.44	160.27	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	3712	A	C4-C5-C6	-48.11	92.94	117.00
1	A1	970	G	C4-C5-N7	-38.21	95.52	110.80
37	52	732	A	N7-C8-N9	36.97	132.28	113.80
37	52	2395	A	N1-C2-N3	-36.01	111.29	129.30
37	52	2399	G	N3-C4-N9	35.70	147.42	126.00
37	52	2399	G	C4-C5-N7	-35.19	96.72	110.80
37	52	732	A	N1-C2-N3	-34.80	111.90	129.30
37	52	1805	A	C4-C5-N7	-34.61	93.39	110.70
37	52	119	G	N3-C4-N9	34.04	146.43	126.00
37	52	2399	G	C2-N3-C4	34.01	128.90	111.90
37	52	119	G	C4-C5-N7	-33.38	97.45	110.80
37	52	119	G	C2-N3-C4	33.31	128.56	111.90
37	52	1805	A	N7-C8-N9	33.28	130.44	113.80
37	52	1805	A	N1-C2-N3	-32.84	112.88	129.30
37	52	2399	G	N3-C4-C5	-32.84	112.18	128.60
37	52	732	A	C4-C5-N7	-32.65	94.38	110.70
37	52	3712	A	N3-C4-N9	32.63	153.51	127.40
37	52	2395	A	C2-N3-C4	31.58	126.39	110.60
37	52	119	G	N3-C4-C5	-31.52	112.84	128.60
1	A1	970	G	C2-N3-C4	31.24	127.52	111.90
1	A1	970	G	N7-C8-N9	30.40	128.30	113.10
37	52	732	A	C2-N3-C4	29.97	125.59	110.60
37	52	1805	A	C2-N3-C4	29.80	125.50	110.60
37	52	2399	G	N1-C2-N3	-28.61	106.73	123.90
37	52	119	G	N1-C2-N3	-28.47	106.82	123.90
1	A1	168	C	OP1-P-OP2	-28.25	77.22	119.60
1	A1	168	C	O5'-P-OP1	-28.05	77.04	110.70
37	52	3712	A	N3-C4-C5	-27.29	107.70	126.80
37	52	119	G	N7-C8-N9	27.13	126.67	113.10
37	52	1239	C	N3-C4-C5	-26.82	111.17	121.90
1	A1	970	G	N1-C2-N3	-26.76	107.84	123.90
37	52	2399	G	N7-C8-N9	26.48	126.34	113.10
67	g3	4	ARG	CD-NE-CZ	24.97	158.55	123.60
83	G3	185	ARG	CD-NE-CZ	24.43	157.80	123.60
37	52	732	A	N9-C4-C5	-24.39	96.04	105.80
51	Q3	14	ARG	CD-NE-CZ	23.72	156.81	123.60
37	52	3712	A	C5-C6-N1	-22.82	106.29	117.70
37	52	1239	C	N1-C2-N3	-22.41	103.52	119.20
37	52	1805	A	N9-C4-C5	-22.33	96.87	105.80
37	52	732	A	N3-C4-N9	21.84	144.87	127.40
37	52	3712	A	C4-C5-N7	21.66	121.53	110.70
1	A1	970	G	N9-C4-C5	-21.06	96.98	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	1805	A	C6-C5-N7	21.00	147.00	132.30
38	72	63	C	N3-C4-C5	-20.97	113.51	121.90
1	A1	970	G	N3-C4-N9	20.84	138.50	126.00
55	U3	49	VAL	CG1-CB-CG2	-20.81	77.61	110.90
38	72	63	C	C6-N1-C2	20.71	128.58	120.30
38	72	63	C	N1-C2-N3	-20.56	104.81	119.20
37	52	2395	A	N7-C8-N9	20.00	123.80	113.80
37	52	1239	C	C6-N1-C2	19.73	128.19	120.30
83	G3	185	ARG	NE-CZ-NH1	19.70	130.15	120.30
37	52	2399	G	C5-C6-N1	19.68	121.34	111.50
55	U3	49	VAL	CA-CB-CG1	19.63	140.34	110.90
1	A1	970	G	C6-C5-N7	19.14	141.88	130.40
37	52	119	G	C5-C6-N1	19.05	121.03	111.50
37	52	1805	A	N3-C4-N9	19.03	142.62	127.40
37	52	3712	A	C6-C5-N7	18.83	145.48	132.30
85	I3	203	ARG	C-N-CA	18.40	160.93	122.30
55	U3	49	VAL	CA-CB-CG2	18.34	138.41	110.90
37	52	3712	A	N9-C4-C5	-17.62	98.75	105.80
38	72	63	C	N1-C2-O2	16.64	128.88	118.90
67	g3	4	ARG	NE-CZ-NH1	16.46	128.53	120.30
37	52	1239	C	C2-N3-C4	16.43	128.11	119.90
37	52	3712	A	N1-C6-N6	16.16	128.30	118.60
62	b3	28	ARG	CA-CB-CG	15.94	148.46	113.40
78	s3	186	GLY	O-C-N	-15.86	97.33	122.70
51	Q3	14	ARG	NE-CZ-NH1	15.68	128.14	120.30
1	A1	167	G	OP1-P-O3'	15.25	138.75	105.20
37	52	2399	G	N9-C4-C5	-15.06	99.38	105.40
53	S3	68	PHE	O-C-N	-14.92	98.83	122.70
53	S3	68	PHE	CB-CA-C	14.87	140.14	110.40
37	52	2399	G	C6-C5-N7	14.70	139.22	130.40
37	52	1239	C	N1-C2-O2	14.39	127.53	118.90
1	A1	281	C	N1-C2-O2	14.23	127.44	118.90
37	52	732	A	C6-C5-N7	14.18	142.23	132.30
37	52	2395	A	C6-N1-C2	13.84	126.91	118.60
37	52	2399	G	N3-C2-N2	13.80	129.56	119.90
1	A1	168	C	O5'-P-OP2	13.74	127.19	110.70
38	72	63	C	C2-N3-C4	13.53	126.67	119.90
1	A1	167	G	OP2-P-O3'	-13.48	75.54	105.20
37	52	119	G	C6-C5-N7	13.47	138.49	130.40
1	A1	281	C	C2-N1-C1'	13.40	133.54	118.80
37	52	1805	A	C5-N7-C8	13.34	110.57	103.90
37	52	2397	G	N1-C6-O6	-13.31	111.91	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	G3	185	ARG	NE-CZ-NH2	-13.16	113.72	120.30
37	52	119	G	N9-C4-C5	-12.52	100.39	105.40
37	52	3712	A	C5-N7-C8	-12.52	97.64	103.90
37	52	4123	C	C6-N1-C2	-12.50	115.30	120.30
37	52	4123	C	C2-N1-C1'	12.41	132.45	118.80
67	g3	4	ARG	NE-CZ-NH2	-12.31	114.14	120.30
37	52	2395	A	C4-C5-N7	-12.16	104.62	110.70
51	Q3	14	ARG	CG-CD-NE	12.08	137.17	111.80
37	52	2399	G	C5-N7-C8	11.93	110.27	104.30
37	52	2395	A	N3-C4-N9	11.78	136.82	127.40
37	52	4123	C	N1-C2-O2	11.67	125.90	118.90
37	52	732	A	N3-C4-C5	-11.65	118.64	126.80
1	A1	281	C	N3-C2-O2	-11.62	113.77	121.90
37	52	732	A	C4-C5-C6	11.56	122.78	117.00
37	52	2021	G	C8-N9-C4	-11.50	101.80	106.40
37	52	2258	C	N1-C2-O2	11.45	125.77	118.90
37	52	4119	C	N1-C2-O2	11.31	125.69	118.90
37	52	2397	G	C5-C6-O6	11.30	135.38	128.60
37	52	1239	C	C4-C5-C6	11.16	122.98	117.40
37	52	4120	U	C2-N1-C1'	11.10	131.02	117.70
37	52	4123	C	N3-C2-O2	-11.10	114.13	121.90
1	A1	887	U	N1-C2-O2	11.01	130.51	122.80
55	U3	49	VAL	CB-CA-C	10.97	132.25	111.40
1	A1	887	U	C2-N1-C1'	10.97	130.86	117.70
37	52	732	A	C5-N7-C8	10.97	109.38	103.90
40	A3	126	LEU	CA-CB-CG	10.91	140.39	115.30
78	s3	186	GLY	CA-C-N	10.81	140.97	117.20
78	s3	186	GLY	C-N-CA	10.79	148.68	121.70
37	52	119	G	N1-C2-N2	10.76	125.88	116.20
1	A1	356	C	N1-C2-O2	10.73	125.34	118.90
62	b3	28	ARG	CB-CA-C	10.71	131.82	110.40
37	52	1805	A	C6-N1-C2	10.69	125.01	118.60
37	52	327	U	C2-N1-C1'	10.57	130.38	117.70
80	23	20	U	N1-C2-O2	10.56	130.19	122.80
37	52	3810	C	N1-C2-O2	10.53	125.22	118.90
37	52	2597	G	N3-C4-C5	-10.50	123.35	128.60
80	23	20	U	C2-N1-C1'	10.47	130.26	117.70
37	52	2021	G	O4'-C1'-N9	10.43	116.54	108.20
1	A1	970	G	C5-N7-C8	10.42	109.51	104.30
37	52	119	G	N3-C2-N2	10.39	127.17	119.90
37	52	2021	G	C4-N9-C1'	10.29	139.87	126.50
37	52	2021	G	N3-C4-C5	-10.24	123.48	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
67	g3	4	ARG	CG-CD-NE	10.17	133.16	111.80
80	23	20	U	N3-C2-O2	-10.12	115.12	122.20
37	52	1915	C	N1-C2-O2	10.05	124.93	118.90
37	52	2021	G	C2-N3-C4	9.90	116.85	111.90
37	52	2258	C	N3-C2-O2	-9.83	115.02	121.90
37	52	2399	G	N1-C6-O6	-9.83	114.00	119.90
37	52	3810	C	C6-N1-C2	-9.79	116.38	120.30
38	72	63	C	C4-C5-C6	9.75	122.28	117.40
37	52	2019	C	N1-C2-O2	9.72	124.73	118.90
37	52	2597	G	C4-N9-C1'	9.70	139.11	126.50
37	52	1915	C	N3-C2-O2	-9.70	115.11	121.90
37	52	4119	C	N3-C2-O2	-9.65	115.14	121.90
37	52	2397	G	C6-C5-N7	9.61	136.17	130.40
37	52	2598	A	C8-N9-C4	-9.57	101.97	105.80
37	52	2581	A	O5'-P-OP2	9.56	122.18	110.70
1	A1	970	G	N3-C2-N2	9.51	126.56	119.90
83	G3	185	ARG	CG-CD-NE	9.50	131.75	111.80
55	U3	49	VAL	N-CA-C	-9.43	85.53	111.00
1	A1	887	U	N3-C2-O2	-9.38	115.63	122.20
37	52	732	A	C6-N1-C2	9.37	124.22	118.60
1	A1	970	G	N1-C2-N2	9.35	124.61	116.20
37	52	2397	G	N9-C4-C5	9.34	109.13	105.40
37	52	1996	C	C5-C6-N1	9.33	125.67	121.00
37	52	2581	A	O5'-P-OP1	-9.33	97.30	105.70
43	E3	65	TYR	CE1-CZ-CE2	-9.32	104.89	119.80
37	52	1639	U	C2-N1-C1'	9.28	128.83	117.70
1	A1	356	C	C2-N1-C1'	9.27	129.00	118.80
37	52	3810	C	C5-C6-N1	9.25	125.63	121.00
1	A1	281	C	C6-N1-C1'	-9.25	109.70	120.80
37	52	2397	G	N3-C4-N9	-9.15	120.51	126.00
37	52	119	G	C5-N7-C8	9.13	108.86	104.30
37	52	4948	C	C2-N1-C1'	9.12	128.83	118.80
37	52	1805	A	N3-C4-C5	-9.09	120.44	126.80
37	52	119	G	C5-C6-O6	-9.08	123.15	128.60
37	52	3810	C	C2-N1-C1'	9.01	128.71	118.80
37	52	1915	C	C6-N1-C2	-8.94	116.73	120.30
37	52	2395	A	N3-C4-C5	-8.94	120.55	126.80
1	A1	281	C	C6-N1-C2	-8.91	116.73	120.30
37	52	4948	C	N1-C2-O2	8.91	124.24	118.90
1	A1	1520	G	N3-C4-N9	8.87	131.32	126.00
37	52	1239	C	N3-C2-O2	8.82	128.08	121.90
1	A1	501	C	N1-C2-O2	8.82	124.19	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	4123	C	C5-C6-N1	8.78	125.39	121.00
1	A1	356	C	N3-C2-O2	-8.77	115.76	121.90
37	52	1239	C	C5-C6-N1	8.75	125.38	121.00
37	52	119	G	C4-C5-C6	8.74	124.05	118.80
37	52	1915	C	C2-N1-C1'	8.71	128.38	118.80
37	52	2399	G	C4-C5-C6	8.68	124.01	118.80
37	52	4928	C	N1-C2-O2	8.67	124.10	118.90
37	52	2674	A	OP1-P-OP2	-8.65	106.63	119.60
37	52	2397	G	C4-C5-N7	-8.62	107.35	110.80
37	52	275	C	C6-N1-C2	-8.57	116.87	120.30
1	A1	970	G	N3-C4-C5	-8.53	124.34	128.60
85	I3	203	ARG	CA-C-O	-8.46	102.33	120.10
1	A1	1518	C	C2-N1-C1'	8.46	128.10	118.80
1	A1	1520	G	N3-C4-C5	-8.45	124.38	128.60
37	52	2395	A	N9-C4-C5	-8.43	102.43	105.80
37	52	327	U	N3-C2-O2	-8.37	116.34	122.20
67	g3	2	VAL	CA-CB-CG1	8.35	123.42	110.90
37	52	2399	G	N1-C2-N2	8.34	123.71	116.20
37	52	2258	C	C6-N1-C2	-8.30	116.98	120.30
37	52	4119	C	C2-N1-C1'	8.29	127.92	118.80
1	A1	369	C	N1-C2-O2	8.29	123.87	118.90
37	52	358	C	N1-C2-O2	8.28	123.86	118.90
1	A1	1518	C	N1-C2-O2	8.27	123.86	118.90
53	S3	68	PHE	N-CA-CB	-8.26	95.73	110.60
1	A1	1520	G	C4-N9-C1'	8.24	137.22	126.50
37	52	2019	C	C5-C6-N1	8.20	125.10	121.00
37	52	2597	G	N7-C8-N9	8.19	117.19	113.10
37	52	2597	G	C8-N9-C4	-8.16	103.14	106.40
37	52	4928	C	C2-N1-C1'	8.16	127.78	118.80
37	52	3941	G	N3-C4-C5	-8.15	124.52	128.60
37	52	4928	C	N3-C2-O2	-8.13	116.21	121.90
37	52	3810	C	N3-C2-O2	-8.12	116.22	121.90
1	A1	1518	C	N3-C2-O2	-8.08	116.24	121.90
37	52	4120	U	N1-C2-O2	8.02	128.41	122.80
37	52	4120	U	C5-C6-N1	8.01	126.70	122.70
37	52	3941	G	C4-N9-C1'	8.01	136.91	126.50
37	52	257	C	N1-C2-O2	7.99	123.70	118.90
1	A1	970	G	C8-N9-C4	7.94	109.58	106.40
37	52	4948	C	N3-C2-O2	-7.91	116.36	121.90
37	52	2019	C	C6-N1-C2	-7.86	117.16	120.30
37	52	3661	G	C4-C5-N7	7.86	113.94	110.80
37	52	3941	G	N3-C4-N9	7.86	130.71	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	Q3	14	ARG	NE-CZ-NH2	-7.84	116.38	120.30
37	52	2583	C	C6-N1-C2	-7.79	117.19	120.30
78	s3	75	LEU	CA-CB-CG	7.76	133.16	115.30
37	52	358	C	N3-C2-O2	-7.76	116.47	121.90
37	52	737	C	N1-C2-O2	7.75	123.55	118.90
1	A1	887	U	C6-N1-C1'	-7.74	110.37	121.20
43	E3	65	TYR	CD1-CE1-CZ	7.72	126.75	119.80
37	52	1239	C	C5-C4-N4	7.72	125.60	120.20
37	52	1070	G	C4-N9-C1'	7.64	136.43	126.50
55	U3	49	VAL	N-CA-CB	7.63	128.28	111.50
37	52	672	C	N1-C2-O2	7.63	123.48	118.90
1	A1	1624	U	N3-C2-O2	-7.62	116.86	122.20
1	A1	1303	C	N1-C2-O2	7.61	123.46	118.90
38	72	1	G	N3-C4-C5	-7.60	124.80	128.60
37	52	327	U	N1-C2-O2	7.59	128.12	122.80
37	52	1556	C	N1-C2-O2	7.59	123.45	118.90
37	52	2598	A	N3-C4-C5	-7.59	121.49	126.80
85	I3	203	ARG	CA-C-N	7.57	131.35	116.20
37	52	4120	U	C6-N1-C1'	-7.54	110.64	121.20
37	52	1639	U	N1-C2-O2	7.51	128.06	122.80
1	A1	1624	U	C2-N1-C1'	7.51	126.71	117.70
37	52	2597	G	N3-C4-N9	7.50	130.50	126.00
37	52	2552	G	N3-C4-N9	7.49	130.49	126.00
67	g3	2	VAL	CA-CB-CG2	7.46	122.09	110.90
37	52	2021	G	N7-C8-N9	7.45	116.83	113.10
37	52	3843	C	N1-C2-O2	7.44	123.36	118.90
38	72	63	C	C6-N1-C1'	-7.39	111.93	120.80
37	52	4123	C	C6-N1-C1'	-7.39	111.94	120.80
1	A1	501	C	C2-N1-C1'	7.39	126.93	118.80
37	52	737	C	N3-C2-O2	-7.36	116.75	121.90
37	52	2019	C	C2-N3-C4	7.34	123.57	119.90
37	52	2528	G	C4-N9-C1'	7.32	136.01	126.50
1	A1	751	G	P-O3'-C3'	7.29	128.45	119.70
1	A1	369	C	C2-N1-C1'	7.29	126.82	118.80
1	A1	501	C	N3-C2-O2	-7.29	116.80	121.90
37	52	1612	G	C4-N9-C1'	7.26	135.94	126.50
38	72	1	G	N3-C4-N9	7.26	130.35	126.00
37	52	2084	U	C2-N3-C4	-7.25	122.65	127.00
37	52	48	G	P-O3'-C3'	7.24	128.39	119.70
37	52	2598	A	C4-C5-C6	7.24	120.62	117.00
37	52	2046	G	P-O3'-C3'	7.23	128.38	119.70
43	E3	65	TYR	CZ-CE2-CD2	7.23	126.30	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	1805	A	C8-N9-C4	7.21	108.69	105.80
1	A1	751	G	OP1-P-O3'	7.21	121.06	105.20
37	52	1305	C	C6-N1-C2	-7.20	117.42	120.30
37	52	1310	C	C6-N1-C2	-7.19	117.42	120.30
37	52	2597	G	C8-N9-C1'	-7.16	117.70	127.00
37	52	2022	C	O5'-P-OP2	-7.11	99.30	105.70
37	52	1556	C	N3-C2-O2	-7.11	116.92	121.90
37	52	2395	A	C6-C5-N7	7.11	137.27	132.30
39	82	36	G	C4-N9-C1'	7.09	135.72	126.50
37	52	1239	C	N3-C4-N4	7.09	122.96	118.00
53	S3	68	PHE	CA-C-O	7.07	134.94	120.10
1	A1	1520	G	C8-N9-C1'	-7.06	117.82	127.00
37	52	3661	G	N9-C4-C5	-7.05	102.58	105.40
37	52	3941	G	C8-N9-C1'	-7.05	117.83	127.00
52	R3	125	LEU	CB-CG-CD1	-7.04	99.03	111.00
37	52	1996	C	C6-N1-C2	-7.04	117.48	120.30
37	52	2580	U	OP2-P-O3'	-7.04	89.72	105.20
37	52	4528	G	C4-N9-C1'	7.02	135.62	126.50
1	A1	241	G	N3-C4-N9	6.99	130.19	126.00
1	A1	1664	A	P-O3'-C3'	6.99	128.09	119.70
1	A1	1303	C	N3-C2-O2	-6.98	117.02	121.90
37	52	2580	U	OP1-P-O3'	6.97	120.53	105.20
37	52	2875	C	P-O3'-C3'	6.96	128.05	119.70
1	A1	1303	C	C2-N1-C1'	6.96	126.45	118.80
37	52	2078	C	C5-C6-N1	6.95	124.48	121.00
37	52	3809	G	N3-C4-N9	6.95	130.17	126.00
1	A1	183	G	N3-C4-N9	6.95	130.17	126.00
37	52	2597	G	C4-C5-C6	6.94	122.97	118.80
37	52	2084	U	C6-N1-C2	6.94	125.17	121.00
37	52	2581	A	C5'-C4'-C3'	6.93	127.09	116.00
37	52	4119	C	C6-N1-C2	-6.91	117.54	120.30
37	52	4138	C	N1-C2-O2	6.91	123.04	118.90
37	52	2504	C	C6-N1-C2	-6.90	117.54	120.30
37	52	3651	A	O5'-P-OP1	-6.89	99.50	105.70
71	k3	56	LEU	CA-CB-CG	6.88	131.13	115.30
37	52	3661	G	C5-C6-O6	-6.87	124.48	128.60
37	52	119	G	N1-C6-O6	-6.84	115.80	119.90
1	A1	356	C	C6-N1-C1'	-6.84	112.60	120.80
37	52	3637	U	N3-C2-O2	-6.83	117.42	122.20
80	23	20	U	C6-N1-C1'	-6.82	111.65	121.20
37	52	1639	U	N3-C2-O2	-6.78	117.45	122.20
1	A1	183	G	C4-N9-C1'	6.74	135.27	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	4117	U	N3-C2-O2	-6.73	117.49	122.20
1	A1	75	G	N3-C4-N9	6.72	130.03	126.00
1	A1	970	G	C4-N9-C1'	-6.71	117.78	126.50
87	u3	163	LEU	CA-CB-CG	6.71	130.72	115.30
37	52	2580	U	C4-C5-C6	6.70	123.72	119.70
37	52	2258	C	C2-N1-C1'	6.70	126.16	118.80
37	52	2397	G	C8-N9-C1'	6.70	135.70	127.00
37	52	2089	G	P-O3'-C3'	6.69	127.73	119.70
37	52	2768	C	O4'-C1'-N1	6.69	113.56	108.20
37	52	1612	G	C8-N9-C1'	-6.68	118.32	127.00
37	52	2021	G	C8-N9-C1'	-6.67	118.32	127.00
37	52	2875	C	OP2-P-O3'	6.67	119.87	105.20
37	52	1210	C	N1-C2-O2	6.66	122.89	118.90
1	A1	281	C	C5-C6-N1	6.65	124.32	121.00
1	A1	1858	G	C4-N9-C1'	6.64	135.13	126.50
37	52	48	G	OP2-P-O3'	6.64	119.81	105.20
37	52	358	C	C2-N1-C1'	6.64	126.10	118.80
37	52	327	U	C6-N1-C1'	-6.63	111.92	121.20
1	A1	751	G	N3-C4-N9	6.62	129.97	126.00
37	52	1210	C	C2-N1-C1'	6.62	126.08	118.80
1	A1	1057	C	C2-N1-C1'	6.61	126.08	118.80
49	O3	18	ARG	NE-CZ-NH2	-6.61	117.00	120.30
37	52	2631	U	C2-N3-C4	-6.60	123.04	127.00
37	52	2399	G	C5-C6-O6	-6.60	124.64	128.60
1	A1	75	G	C4-N9-C1'	6.60	135.07	126.50
1	A1	293	C	N1-C2-O2	6.59	122.86	118.90
1	A1	688	U	P-O3'-C3'	6.58	127.60	119.70
37	52	1517	G	C4-N9-C1'	6.58	135.06	126.50
37	52	4243	C	N3-C2-O2	-6.58	117.30	121.90
1	A1	212	C	C6-N1-C2	-6.56	117.68	120.30
37	52	2574	G	O5'-P-OP1	6.55	118.57	110.70
1	A1	369	C	N3-C2-O2	-6.55	117.32	121.90
60	Z3	80	LEU	CA-CB-CG	6.55	130.36	115.30
37	52	672	C	N3-C2-O2	-6.55	117.32	121.90
37	52	2750	G	C6-C5-N7	-6.54	126.47	130.40
37	52	1305	C	C2-N1-C1'	6.54	125.99	118.80
1	A1	1637	A	P-O3'-C3'	6.53	127.54	119.70
37	52	2084	U	N3-C4-C5	6.52	118.51	114.60
39	82	36	G	N3-C4-C5	-6.51	125.35	128.60
1	A1	1518	C	C6-N1-C2	-6.50	117.70	120.30
37	52	217	C	N1-C2-O2	6.50	122.80	118.90
37	52	2528	G	C8-N9-C1'	-6.50	118.55	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	2580	U	N3-C4-O4	6.50	123.95	119.40
37	52	4243	C	N1-C2-O2	6.49	122.79	118.90
37	52	3959	U	P-O3'-C3'	6.48	127.48	119.70
78	s3	79	LEU	CA-CB-CG	-6.48	100.40	115.30
37	52	1805	A	C4-N9-C1'	-6.47	114.66	126.30
37	52	2572	C	C5-C4-N4	-6.47	115.67	120.20
40	A3	117	GLU	CB-CA-C	-6.47	97.46	110.40
37	52	2489	C	N1-C2-O2	6.46	122.78	118.90
1	A1	1118	C	C2-N1-C1'	6.46	125.90	118.80
1	A1	532	C	C6-N1-C2	-6.46	117.72	120.30
37	52	4880	C	C2-N1-C1'	6.46	125.90	118.80
37	52	1651	G	C4-N9-C1'	6.46	134.89	126.50
39	82	36	G	N3-C4-N9	6.45	129.87	126.00
37	52	4926	C	C2-N1-C1'	6.42	125.86	118.80
1	A1	1314	U	C2-N1-C1'	6.41	125.40	117.70
37	52	100	C	C2-N1-C1'	6.41	125.85	118.80
37	52	4948	C	C6-N1-C1'	-6.39	113.13	120.80
37	52	2580	U	P-O3'-C3'	6.39	127.37	119.70
80	23	30	G	N3-C4-N9	6.38	129.83	126.00
37	52	2014	C	N1-C2-O2	6.37	122.72	118.90
63	c3	30	GLY	N-CA-C	6.37	129.03	113.10
37	52	1573	G	O5'-P-OP1	-6.34	100.00	105.70
37	52	2078	C	C6-N1-C2	-6.34	117.77	120.30
37	52	2552	G	N3-C4-C5	-6.33	125.43	128.60
1	A1	474	G	C4-N9-C1'	6.33	134.73	126.50
1	A1	970	G	C4-C5-C6	6.33	122.60	118.80
37	52	1070	G	C8-N9-C1'	-6.33	118.77	127.00
37	52	1961	G	C8-N9-C4	-6.33	103.87	106.40
37	52	4919	G	N3-C4-C5	-6.32	125.44	128.60
1	A1	1300	U	N3-C2-O2	-6.31	117.78	122.20
37	52	4423	U	N3-C2-O2	-6.31	117.78	122.20
1	A1	241	G	N3-C4-C5	-6.30	125.45	128.60
37	52	2084	U	C5-C6-N1	-6.28	119.56	122.70
37	52	1185	G	C8-N9-C4	-6.28	103.89	106.40
37	52	4942	C	N1-C2-O2	6.28	122.67	118.90
37	52	4926	C	N1-C2-O2	6.27	122.66	118.90
37	52	1612	G	N3-C4-N9	6.27	129.76	126.00
1	A1	1636	G	C4-N9-C1'	6.26	134.64	126.50
63	c3	94	LEU	CA-CB-CG	6.26	129.71	115.30
37	52	2019	C	N3-C2-O2	-6.26	117.52	121.90
37	52	986	C	N1-C2-O2	6.26	122.66	118.90
37	52	4560	C	N3-C2-O2	-6.26	117.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	751	G	C4-N9-C1'	6.25	134.63	126.50
37	52	4919	G	N3-C4-N9	6.25	129.75	126.00
37	52	4759	C	C2-N1-C1'	6.25	125.67	118.80
62	b3	28	ARG	N-CA-C	-6.24	94.14	111.00
37	52	1979	A	P-O3'-C3'	6.24	127.19	119.70
37	52	1632	A	C2-N3-C4	6.24	113.72	110.60
38	72	63	C	N3-C2-O2	6.24	126.26	121.90
37	52	4869	U	C2-N1-C1'	6.22	125.17	117.70
1	A1	1130	G	N3-C4-C5	-6.22	125.49	128.60
37	52	1639	U	C6-N1-C1'	-6.22	112.50	121.20
1	A1	870	A	P-O3'-C3'	6.21	127.16	119.70
14	N1	64	LEU	CA-CB-CG	6.21	129.58	115.30
37	52	2528	G	N3-C4-N9	6.20	129.72	126.00
37	52	449	C	P-O3'-C3'	6.20	127.14	119.70
37	52	294	G	C4-N9-C1'	6.20	134.56	126.50
37	52	1968	G	C8-N9-C4	-6.19	103.92	106.40
37	52	4303	C	C2-N1-C1'	6.19	125.61	118.80
37	52	1961	G	N3-C4-C5	-6.19	125.51	128.60
37	52	1961	G	C4-N9-C1'	6.17	134.52	126.50
37	52	3888	G	P-O3'-C3'	6.17	127.10	119.70
37	52	2597	G	C6-C5-N7	-6.16	126.70	130.40
37	52	4528	G	C8-N9-C1'	-6.15	119.01	127.00
37	52	1456	C	C6-N1-C2	-6.14	117.84	120.30
62	b3	28	ARG	N-CA-CB	6.14	121.64	110.60
37	52	4413	C	N1-C2-O2	6.13	122.58	118.90
37	52	2594	C	C6-N1-C2	-6.13	117.85	120.30
37	52	2811	G	C8-N9-C4	-6.12	103.95	106.40
37	52	4413	C	N3-C2-O2	-6.11	117.62	121.90
39	82	36	G	C8-N9-C1'	-6.09	119.08	127.00
85	I3	204	GLY	N-CA-C	6.09	128.31	113.10
39	82	153	C	N1-C2-O2	6.08	122.55	118.90
1	A1	1364	U	C2-N1-C1'	6.08	125.00	117.70
37	52	4413	C	C2-N1-C1'	6.07	125.48	118.80
38	72	1	G	C4-N9-C1'	6.05	134.36	126.50
37	52	2397	G	C4-N9-C1'	-6.04	118.64	126.50
37	52	2550	G	N7-C8-N9	6.04	116.12	113.10
37	52	1805	A	O4'-C1'-N9	-6.04	103.37	108.20
37	52	104	G	C4-N9-C1'	6.04	134.35	126.50
37	52	180	C	N1-C2-O2	6.04	122.52	118.90
1	A1	183	G	C8-N9-C1'	-6.04	119.15	127.00
1	A1	1130	G	N3-C4-N9	6.04	129.62	126.00
38	72	63	C	N3-C4-N4	6.04	122.22	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	1556	C	C2-N1-C1'	6.02	125.42	118.80
37	52	2598	A	C2-N3-C4	6.02	113.61	110.60
37	52	4759	C	N3-C2-O2	-6.02	117.69	121.90
37	52	3809	G	N3-C4-C5	-6.02	125.59	128.60
1	A1	1394	G	P-O3'-C3'	6.02	126.92	119.70
1	A1	1453	C	C2-N1-C1'	6.01	125.42	118.80
1	A1	1397	U	N3-C2-O2	-6.01	117.99	122.20
37	52	704	C	C2-N1-C1'	6.00	125.40	118.80
37	52	4919	G	C4-N9-C1'	5.99	134.29	126.50
37	52	4454	G	C4-N9-C1'	5.99	134.28	126.50
37	52	275	C	N3-C2-O2	-5.98	117.71	121.90
37	52	1612	G	C6-C5-N7	-5.98	126.81	130.40
37	52	966	A	N7-C8-N9	5.98	116.79	113.80
1	A1	1314	U	N3-C2-O2	-5.98	118.02	122.20
37	52	2754	G	C5'-C4'-O4'	5.98	116.27	109.10
1	A1	465	A	P-O3'-C3'	5.97	126.87	119.70
37	52	1215	C	N1-C2-O2	5.96	122.48	118.90
37	52	4423	U	C2-N1-C1'	5.96	124.86	117.70
1	A1	183	G	N3-C4-C5	-5.96	125.62	128.60
37	52	4120	U	N3-C2-O2	-5.96	118.03	122.20
37	52	4266	G	C4-N9-C1'	5.96	134.24	126.50
1	A1	75	G	C8-N9-C1'	-5.95	119.26	127.00
37	52	3712	A	C8-N9-C1'	-5.94	117.00	127.70
37	52	1469	C	C6-N1-C2	-5.94	117.92	120.30
37	52	2740	U	N3-C2-O2	-5.94	118.04	122.20
37	52	2750	G	C4-N9-C1'	5.93	134.21	126.50
37	52	3941	G	C2-N3-C4	5.93	114.87	111.90
80	23	29	C	O4'-C1'-N1	5.93	112.94	108.20
37	52	2583	C	C5-C6-N1	5.91	123.96	121.00
1	A1	1333	U	N3-C2-O2	-5.91	118.06	122.20
37	52	1070	G	N7-C8-N9	5.91	116.06	113.10
1	A1	823	U	C2-N1-C1'	5.91	124.79	117.70
37	52	1485	C	N1-C2-O2	5.91	122.44	118.90
37	52	2594	C	N3-C2-O2	-5.90	117.77	121.90
37	52	3948	C	N1-C2-O2	5.90	122.44	118.90
37	52	3842	C	N1-C2-O2	5.89	122.44	118.90
38	72	63	C	C5-C6-N1	5.88	123.94	121.00
37	52	972	C	N1-C2-O2	5.88	122.43	118.90
37	52	30	C	C6-N1-C2	-5.87	117.95	120.30
37	52	1185	G	N3-C4-C5	-5.87	125.66	128.60
37	52	4173	G	C6-C5-N7	-5.87	126.88	130.40
40	A3	43	GLY	N-CA-C	5.87	127.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	2578	G	C4-C5-N7	5.87	113.15	110.80
37	52	959	G	P-O3'-C3'	5.87	126.74	119.70
37	52	1181	C	N1-C2-O2	5.87	122.42	118.90
37	52	2726	G	C4-N9-C1'	5.86	134.11	126.50
37	52	2577	C	C6-N1-C2	-5.85	117.96	120.30
37	52	257	C	N3-C2-O2	-5.85	117.81	121.90
37	52	2258	C	C5-C6-N1	5.85	123.92	121.00
37	52	2597	G	P-O3'-C3'	5.84	126.71	119.70
37	52	2303	C	C6-N1-C2	-5.83	117.97	120.30
37	52	2407	G	C4-N9-C1'	5.83	134.08	126.50
37	52	37	U	C2-N1-C1'	5.83	124.70	117.70
37	52	4243	C	C2-N1-C1'	5.83	125.21	118.80
37	52	257	C	C2-N1-C1'	5.83	125.21	118.80
37	52	3712	A	C4-N9-C1'	5.83	136.79	126.30
1	A1	853	C	C2-N1-C1'	5.82	125.20	118.80
37	52	495	C	N1-C2-O2	5.82	122.39	118.90
37	52	1961	G	N7-C8-N9	5.82	116.01	113.10
1	A1	501	C	C6-N1-C2	-5.81	117.98	120.30
37	52	1915	C	C5-C6-N1	5.81	123.90	121.00
37	52	4232	U	P-O3'-C3'	5.81	126.67	119.70
1	A1	823	U	N3-C2-O2	-5.80	118.14	122.20
1	A1	1475	G	C4-N9-C1'	5.80	134.05	126.50
37	52	327	U	C5-C6-N1	5.80	125.60	122.70
40	A3	126	LEU	CB-CA-C	-5.80	99.17	110.20
37	52	1720	C	C6-N1-C2	-5.80	117.98	120.30
37	52	4759	C	N1-C2-O2	5.80	122.38	118.90
37	52	276	C	C6-N1-C2	-5.80	117.98	120.30
37	52	115	C	N1-C2-O2	5.79	122.38	118.90
37	52	2749	C	C6-N1-C2	-5.79	117.98	120.30
37	52	3842	C	C2-N1-C1'	5.79	125.17	118.80
1	A1	538	U	N1-C2-O2	5.79	126.85	122.80
37	52	4138	C	N3-C2-O2	-5.79	117.85	121.90
37	52	4942	C	N3-C2-O2	-5.78	117.85	121.90
37	52	4928	C	C6-N1-C2	-5.78	117.99	120.30
1	A1	1624	U	N1-C2-O2	5.77	126.84	122.80
1	A1	182	C	P-O3'-C3'	5.77	126.63	119.70
1	A1	1300	U	N1-C2-O2	5.77	126.84	122.80
1	A1	241	G	C2-N3-C4	5.76	114.78	111.90
1	A1	751	G	N3-C4-C5	-5.76	125.72	128.60
37	52	1762	C	C6-N1-C2	-5.76	118.00	120.30
80	23	72	C	N1-C2-O2	5.75	122.35	118.90
1	A1	874	G	P-O3'-C3'	5.75	126.60	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	1738	C	C6-N1-C2	-5.74	118.00	120.30
37	52	1467	C	C6-N1-C2	-5.74	118.00	120.30
37	52	1571	G	C2-N3-C4	5.74	114.77	111.90
37	52	2470	C	N1-C2-O2	5.74	122.34	118.90
37	52	104	G	C8-N9-C1'	-5.74	119.54	127.00
37	52	914	U	C5-C6-N1	5.74	125.57	122.70
37	52	327	U	C6-N1-C2	-5.73	117.56	121.00
37	52	3649	A	C4-N9-C1'	5.73	136.62	126.30
1	A1	659	G	C4-N9-C1'	5.73	133.95	126.50
1	A1	75	G	N3-C4-C5	-5.73	125.74	128.60
37	52	1912	G	C4-N9-C1'	5.73	133.95	126.50
63	c3	30	GLY	C-N-CA	5.73	136.02	121.70
1	A1	1772	C	C6-N1-C2	-5.73	118.01	120.30
1	A1	1811	C	C6-N1-C2	-5.73	118.01	120.30
1	A1	1551	U	C2-N1-C1'	5.72	124.56	117.70
37	52	1182	C	N1-C2-O2	5.72	122.33	118.90
37	52	1550	G	C4-N9-C1'	5.72	133.94	126.50
1	A1	1397	U	N1-C2-O2	5.72	126.80	122.80
37	52	4662	C	C6-N1-C2	-5.72	118.01	120.30
37	52	1651	G	C6-C5-N7	-5.71	126.97	130.40
1	A1	752	G	O5'-P-OP1	-5.69	100.58	105.70
37	52	275	C	P-O3'-C3'	5.69	126.53	119.70
37	52	1517	G	N3-C4-C5	-5.69	125.75	128.60
37	52	1969	G	C5-C6-O6	5.69	132.01	128.60
37	52	2014	C	C2-N1-C1'	5.69	125.06	118.80
1	A1	751	G	C8-N9-C1'	-5.68	119.61	127.00
1	A1	958	G	C4-N9-C1'	5.67	133.87	126.50
38	72	113	G	C4-N9-C1'	5.67	133.87	126.50
37	52	4964	C	C6-N1-C2	-5.66	118.03	120.30
37	52	498	C	P-O3'-C3'	5.66	126.49	119.70
37	52	4194	U	N3-C2-O2	-5.66	118.24	122.20
80	23	30	G	C4-N9-C1'	5.66	133.85	126.50
37	52	4948	C	C6-N1-C2	-5.65	118.04	120.30
37	52	311	G	C4-N9-C1'	5.65	133.84	126.50
1	A1	1834	A	C4-N9-C1'	5.64	136.45	126.30
1	A1	1253	A	P-O3'-C3'	5.63	126.45	119.70
37	52	3843	C	C2-N1-C1'	5.62	124.99	118.80
1	A1	1624	U	C6-N1-C2	-5.62	117.63	121.00
37	52	672	C	C2-N1-C1'	5.62	124.98	118.80
41	B3	309	LEU	CA-CB-CG	5.62	128.22	115.30
37	52	1632	A	N3-C4-N9	5.62	131.89	127.40
37	52	2594	C	C2-N1-C1'	5.62	124.98	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	729	G	N3-C4-C5	-5.62	125.79	128.60
1	A1	1117	C	N1-C2-O2	5.61	122.27	118.90
37	52	1969	G	N1-C2-N2	-5.61	111.15	116.20
37	52	1286	C	N1-C2-O2	5.61	122.27	118.90
39	82	47	C	C6-N1-C2	-5.61	118.06	120.30
37	52	934	C	C6-N1-C2	-5.60	118.06	120.30
37	52	1928	C	N3-C2-O2	-5.60	117.98	121.90
37	52	4925	U	P-O3'-C3'	5.60	126.42	119.70
37	52	1663	C	C6-N1-C2	-5.60	118.06	120.30
37	52	685	C	O5'-P-OP2	-5.59	100.66	105.70
37	52	204	U	N3-C2-O2	-5.59	118.29	122.20
37	52	4476	C	C2-N1-C1'	5.59	124.95	118.80
37	52	339	C	C6-N1-C2	-5.58	118.07	120.30
37	52	115	C	C2-N1-C1'	5.58	124.94	118.80
1	A1	427	U	C2-N1-C1'	5.58	124.39	117.70
37	52	1639	U	C5-C6-N1	5.58	125.49	122.70
1	A1	532	C	N1-C2-O2	5.57	122.24	118.90
37	52	4871	C	C2-N1-C1'	5.57	124.93	118.80
37	52	37	U	N1-C2-O2	5.57	126.70	122.80
37	52	2020	U	C5-C6-N1	5.57	125.48	122.70
1	A1	30	C	C6-N1-C2	-5.56	118.08	120.30
37	52	37	U	N3-C2-O2	-5.56	118.31	122.20
1	A1	1440	C	N1-C2-O2	5.56	122.23	118.90
37	52	3937	C	C6-N1-C2	-5.55	118.08	120.30
37	52	4528	G	N3-C4-N9	5.55	129.33	126.00
37	52	4869	U	N3-C2-O2	-5.55	118.31	122.20
37	52	3625	G	P-O3'-C3'	5.55	126.36	119.70
37	52	4866	C	C6-N1-C2	-5.55	118.08	120.30
37	52	4117	U	C2-N1-C1'	5.55	124.36	117.70
37	52	4223	C	C6-N1-C2	-5.55	118.08	120.30
1	A1	1518	C	C6-N1-C1'	-5.54	114.15	120.80
37	52	3843	C	N3-C2-O2	-5.54	118.02	121.90
37	52	4560	C	N1-C2-O2	5.54	122.22	118.90
37	52	704	C	N1-C2-O2	5.54	122.22	118.90
37	52	1310	C	C5-C6-N1	5.53	123.77	121.00
37	52	4047	A	OP1-P-O3'	5.53	117.36	105.20
1	A1	1826	G	C4-N9-C1'	5.53	133.69	126.50
37	52	930	G	P-O3'-C3'	5.53	126.33	119.70
37	52	4939	C	N1-C2-O2	5.53	122.22	118.90
37	52	217	C	N3-C2-O2	-5.53	118.03	121.90
37	52	1420	A	C2-N3-C4	5.52	113.36	110.60
1	A1	1660	C	C2-N1-C1'	5.52	124.87	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	1853	G	C4-N9-C1'	5.52	133.67	126.50
37	52	4716	C	C6-N1-C2	-5.52	118.09	120.30
37	52	4999	G	C4-N9-C1'	5.51	133.66	126.50
37	52	3638	G	C6-C5-N7	-5.50	127.10	130.40
37	52	4448	G	P-O3'-C3'	5.50	126.30	119.70
37	52	2753	G	P-O3'-C3'	5.50	126.30	119.70
37	52	2631	U	N3-C4-C5	5.50	117.90	114.60
37	52	2675	G	C8-N9-C1'	-5.50	119.86	127.00
37	52	294	G	N3-C4-N9	5.49	129.30	126.00
37	52	1968	G	N7-C8-N9	5.49	115.85	113.10
39	82	141	C	C6-N1-C2	-5.49	118.10	120.30
37	52	3876	A	P-O3'-C3'	5.49	126.28	119.70
37	52	2489	C	C6-N1-C2	-5.48	118.11	120.30
37	52	311	G	C6-C5-N7	-5.48	127.11	130.40
37	52	4405	G	C4-N9-C1'	5.48	133.62	126.50
1	A1	1301	A	C2-N3-C4	5.47	113.34	110.60
37	52	4928	C	C6-N1-C1'	-5.47	114.23	120.80
37	52	732	A	O4'-C1'-N9	5.47	112.57	108.20
37	52	2014	C	N3-C2-O2	-5.47	118.07	121.90
39	82	28	C	C6-N1-C2	-5.47	118.11	120.30
1	A1	1309	C	N1-C2-O2	5.46	122.17	118.90
37	52	2550	G	C6-C5-N7	-5.46	127.12	130.40
1	A1	549	C	C6-N1-C2	-5.46	118.12	120.30
37	52	2594	C	N1-C2-O2	5.46	122.17	118.90
1	A1	1785	C	N1-C2-O2	5.45	122.17	118.90
37	52	4528	G	N3-C4-C5	-5.45	125.87	128.60
37	52	2014	C	C6-N1-C2	-5.45	118.12	120.30
37	52	2021	G	N9-C4-C5	5.45	107.58	105.40
38	72	63	C	C5-C4-N4	5.45	124.01	120.20
37	52	1420	A	N3-C4-N9	5.44	131.75	127.40
37	52	3600	G	C4-N9-C1'	5.44	133.57	126.50
1	A1	606	G	C4-N9-C1'	5.44	133.57	126.50
37	52	448	G	C4-N9-C1'	5.43	133.56	126.50
39	82	153	C	N3-C2-O2	-5.43	118.10	121.90
37	52	2441	C	C6-N1-C2	-5.43	118.13	120.30
37	52	934	C	N3-C2-O2	-5.43	118.10	121.90
37	52	1084	C	C5-C6-N1	5.43	123.71	121.00
37	52	3709	U	C2-N1-C1'	5.42	124.21	117.70
1	A1	1664	A	OP1-P-O3'	5.42	117.12	105.20
37	52	1674	C	C6-N1-C2	-5.42	118.13	120.30
37	52	1666	C	C6-N1-C2	-5.41	118.14	120.30
37	52	115	C	N3-C2-O2	-5.41	118.11	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	1239	C	C6-N1-C1'	-5.41	114.31	120.80
37	52	1305	C	N3-C2-O2	-5.40	118.12	121.90
37	52	4527	G	C4-N9-C1'	5.39	133.51	126.50
37	52	2008	U	C2-N1-C1'	5.39	124.17	117.70
39	82	117	C	N1-C2-O2	5.39	122.14	118.90
37	52	4100	C	C6-N1-C2	-5.39	118.14	120.30
1	A1	853	C	N3-C2-O2	-5.39	118.13	121.90
37	52	257	C	C6-N1-C2	-5.39	118.14	120.30
37	52	1517	G	C8-N9-C1'	-5.38	120.00	127.00
37	52	1651	G	C8-N9-C1'	-5.38	120.00	127.00
37	52	2035	C	C6-N1-C2	-5.38	118.15	120.30
37	52	2580	U	C5'-C4'-O4'	-5.38	102.65	109.10
81	w3	56	A	C2-N3-C4	5.37	113.28	110.60
37	52	3943	A	C2-N3-C4	5.37	113.28	110.60
80	23	20	U	C5-C6-N1	5.37	125.38	122.70
60	Z3	73	LYS	CB-CA-C	5.36	121.13	110.40
1	A1	474	G	C8-N9-C1'	-5.36	120.03	127.00
37	52	236	G	N3-C2-N2	-5.36	116.15	119.90
1	A1	1364	U	N1-C2-O2	5.36	126.55	122.80
37	52	3618	C	C6-N1-C2	-5.35	118.16	120.30
37	52	3809	G	C4-N9-C1'	5.35	133.45	126.50
35	j1	368	LEU	CA-CB-CG	5.34	127.58	115.30
37	52	1969	G	N3-C2-N2	5.34	123.64	119.90
37	52	1370	G	P-O3'-C3'	5.33	126.10	119.70
37	52	4654	C	C6-N1-C2	-5.33	118.17	120.30
37	52	2787	A	C4-N9-C1'	5.33	135.89	126.30
1	A1	652	U	N3-C2-O2	-5.33	118.47	122.20
39	82	42	G	C6-C5-N7	-5.32	127.21	130.40
1	A1	1453	C	N1-C2-O2	5.32	122.09	118.90
37	52	125	C	P-O3'-C3'	5.32	126.08	119.70
53	S3	68	PHE	CB-CG-CD1	5.32	124.53	120.80
1	A1	1256	G	C4-N9-C1'	5.32	133.41	126.50
37	52	4243	C	C6-N1-C2	-5.32	118.17	120.30
37	52	2577	C	C5-C6-N1	5.32	123.66	121.00
83	G3	275	ILE	CG1-CB-CG2	-5.32	99.70	111.40
37	52	1286	C	C2-N1-C1'	5.31	124.65	118.80
1	A1	1520	G	C6-C5-N7	-5.31	127.22	130.40
37	52	2851	G	C6-C5-N7	-5.30	127.22	130.40
37	52	4926	C	N3-C2-O2	-5.30	118.19	121.90
37	52	1084	C	C6-N1-C2	-5.30	118.18	120.30
1	A1	1395	C	O4'-C1'-N1	5.30	112.44	108.20
37	52	4305	G	C4-N9-C1'	5.30	133.39	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I1	36	LEU	CA-CB-CG	5.30	127.48	115.30
37	52	1485	C	C2-N1-C1'	5.29	124.62	118.80
37	52	4173	G	C5-C6-O6	-5.28	125.43	128.60
1	A1	1751	C	C5-C6-N1	5.28	123.64	121.00
39	82	117	C	N3-C2-O2	-5.28	118.20	121.90
37	52	966	A	C5-N7-C8	-5.28	101.26	103.90
37	52	2489	C	N3-C2-O2	-5.28	118.21	121.90
60	Z3	14	LEU	CA-CB-CG	5.28	127.44	115.30
81	w3	56	A	C4-N9-C1'	5.28	135.80	126.30
1	A1	532	C	N3-C2-O2	-5.26	118.22	121.90
37	52	2581	A	C8-N9-C4	-5.26	103.70	105.80
37	52	2750	G	C4-C5-N7	5.26	112.91	110.80
1	A1	1314	U	N1-C2-O2	5.26	126.48	122.80
37	52	176	G	N3-C4-N9	-5.26	122.84	126.00
37	52	204	U	N1-C2-O2	5.26	126.48	122.80
37	52	13	U	N3-C2-O2	-5.26	118.52	122.20
37	52	294	G	N3-C4-C5	-5.26	125.97	128.60
37	52	1556	C	C6-N1-C2	-5.26	118.20	120.30
37	52	1636	U	C2-N1-C1'	5.26	124.01	117.70
37	52	2598	A	N3-C4-N9	5.26	131.60	127.40
1	A1	142	C	N1-C2-O2	5.25	122.05	118.90
1	A1	1116	C	N1-C2-O2	5.25	122.05	118.90
37	52	149	A	C4-N9-C1'	5.25	135.76	126.30
39	82	121	G	C4-N9-C1'	5.25	133.33	126.50
1	A1	967	C	C6-N1-C2	-5.25	118.20	120.30
37	52	1070	G	C6-C5-N7	-5.25	127.25	130.40
1	A1	1118	C	N1-C2-O2	5.24	122.05	118.90
37	52	3600	G	N3-C4-N9	5.24	129.15	126.00
37	52	1571	G	O4'-C1'-N9	5.24	112.39	108.20
37	52	986	C	N3-C2-O2	-5.24	118.23	121.90
37	52	1481	C	C2-N1-C1'	5.24	124.56	118.80
37	52	923	C	O5'-P-OP1	5.24	116.98	110.70
37	52	4119	C	C6-N1-C1'	-5.24	114.52	120.80
38	72	5	A	N3-C4-C5	5.23	130.46	126.80
41	B3	214	ASP	CB-CG-OD1	5.23	123.01	118.30
37	52	1467	C	C5-C6-N1	5.23	123.61	121.00
1	A1	1139	C	N1-C2-O2	5.22	122.03	118.90
37	52	1632	A	C4-N9-C1'	5.22	135.70	126.30
37	52	4440	G	C4-N9-C1'	5.22	133.29	126.50
37	52	4303	C	N3-C2-O2	-5.22	118.25	121.90
1	A1	1858	G	C6-C5-N7	-5.21	127.27	130.40
37	52	1774	C	C6-N1-C2	-5.21	118.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	A3	29	LEU	CA-CB-CG	5.21	127.29	115.30
37	52	2750	G	N7-C8-N9	5.21	115.71	113.10
37	52	2019	C	C2-N1-C1'	5.21	124.53	118.80
37	52	2753	G	O3'-P-O5'	5.21	113.89	104.00
37	52	1211	G	P-O3'-C3'	5.20	125.94	119.70
80	23	30	G	C8-N9-C1'	-5.20	120.25	127.00
1	A1	937	C	C6-N1-C2	-5.19	118.22	120.30
1	A1	1057	C	N3-C2-O2	-5.19	118.27	121.90
1	A1	1620	A	C4-N9-C1'	5.19	135.65	126.30
37	52	30	C	C5-C6-N1	5.19	123.60	121.00
37	52	4165	C	C6-N1-C2	-5.19	118.22	120.30
37	52	4173	G	N1-C6-O6	5.19	123.02	119.90
1	A1	1858	G	C8-N9-C1'	-5.19	120.25	127.00
1	A1	958	G	O4'-C1'-N9	5.19	112.35	108.20
37	52	3809	G	C8-N9-C1'	-5.19	120.26	127.00
1	A1	1364	U	N3-C2-O2	-5.18	118.57	122.20
37	52	1485	C	N3-C2-O2	-5.18	118.27	121.90
37	52	2021	G	N9-C1'-C2'	5.18	120.74	114.00
1	A1	853	C	N1-C2-O2	5.18	122.01	118.90
37	52	257	C	C5-C6-N1	5.18	123.59	121.00
37	52	2502	A	P-O3'-C3'	5.18	125.92	119.70
1	A1	688	U	OP2-P-O3'	5.18	116.59	105.20
37	52	1912	G	C8-N9-C1'	-5.17	120.28	127.00
37	52	4880	C	N1-C2-O2	5.17	122.00	118.90
1	A1	870	A	OP2-P-O3'	5.17	116.57	105.20
1	A1	369	C	C6-N1-C2	-5.17	118.23	120.30
3	C1	34	LYS	C-N-CA	5.17	134.61	121.70
37	52	168	C	N1-C2-O2	5.17	122.00	118.90
37	52	4948	C	O4'-C1'-N1	5.17	112.33	108.20
37	52	2097	A	C4-N9-C1'	5.16	135.59	126.30
1	A1	1300	U	C2-N1-C1'	5.16	123.89	117.70
37	52	3939	G	P-O3'-C3'	5.16	125.89	119.70
1	A1	1074	C	C6-N1-C2	-5.16	118.24	120.30
37	52	2726	G	C8-N9-C1'	-5.16	120.30	127.00
1	A1	538	U	N3-C2-O2	-5.16	118.59	122.20
38	72	120	U	C5-C6-N1	5.16	125.28	122.70
1	A1	915	G	O4'-C1'-N9	5.15	112.32	108.20
1	A1	887	U	C5-C6-N1	5.15	125.28	122.70
37	52	1474	C	C6-N1-C2	-5.15	118.24	120.30
37	52	495	C	C6-N1-C2	-5.15	118.24	120.30
37	52	2787	A	N3-C4-N9	5.15	131.52	127.40
37	52	1805	A	C4-C5-C6	5.15	119.57	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	1106	A	P-O3'-C3'	5.14	125.87	119.70
37	52	4201	G	C4-N9-C1'	5.14	133.19	126.50
37	52	4871	C	N1-C2-O2	5.14	121.99	118.90
1	A1	1333	U	N1-C2-O2	5.14	126.40	122.80
83	G3	104	LEU	CA-CB-CG	5.14	127.13	115.30
37	52	2441	C	C5-C6-N1	5.14	123.57	121.00
1	A1	791	C	C6-N1-C2	-5.14	118.24	120.30
37	52	2528	G	N3-C4-C5	-5.14	126.03	128.60
37	52	2838	G	C4-N9-C1'	5.14	133.18	126.50
37	52	2295	C	C6-N1-C2	-5.14	118.25	120.30
38	72	36	C	C6-N1-C2	-5.14	118.25	120.30
60	Z3	51	ARG	CD-NE-CZ	5.14	130.79	123.60
1	A1	1636	G	C6-C5-N7	-5.13	127.32	130.40
1	A1	1130	G	C2-N3-C4	5.13	114.46	111.90
37	52	453	G	N3-C4-N9	5.13	129.08	126.00
37	52	1202	C	C6-N1-C2	-5.12	118.25	120.30
37	52	4527	G	N3-C4-N9	5.12	129.07	126.00
41	B3	17	LEU	CA-CB-CG	5.12	127.09	115.30
37	52	4454	G	C8-N9-C1'	-5.12	120.34	127.00
37	52	4879	C	C6-N1-C2	-5.12	118.25	120.30
1	A1	1097	G	C4-N9-C1'	5.12	133.16	126.50
37	52	1517	G	N3-C4-N9	5.12	129.07	126.00
37	52	2740	U	C2-N1-C1'	5.12	123.84	117.70
37	52	3842	C	N3-C2-O2	-5.12	118.32	121.90
37	52	4423	U	N1-C2-O2	5.12	126.38	122.80
40	A3	125	LYS	C-N-CA	5.11	134.48	121.70
37	52	4232	U	OP2-P-O3'	5.11	116.44	105.20
37	52	1890	G	C4-C5-N7	5.11	112.84	110.80
38	72	1	G	C2-N3-C4	5.10	114.45	111.90
37	52	1899	G	C4-N9-C1'	5.10	133.13	126.50
37	52	3685	C	C6-N1-C2	-5.10	118.26	120.30
37	52	3938	G	C8-N9-C4	5.10	108.44	106.40
38	72	67	C	C6-N1-C2	-5.09	118.26	120.30
37	52	385	A	OP1-P-O3'	5.09	116.40	105.20
37	52	1070	G	N3-C4-N9	5.09	129.05	126.00
37	52	1286	C	C6-N1-C2	-5.08	118.27	120.30
37	52	2596	G	N1-C2-N2	-5.08	111.62	116.20
37	52	4158	C	O5'-P-OP1	-5.08	101.13	105.70
37	52	486	C	C5-C6-N1	5.08	123.54	121.00
37	52	3673	C	N1-C2-O2	5.08	121.94	118.90
37	52	13	U	N1-C2-O2	5.07	126.35	122.80
37	52	2504	C	C5-C6-N1	5.07	123.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	82	38	U	N3-C2-O2	-5.07	118.65	122.20
37	52	4719	G	OP1-P-O3'	5.07	116.35	105.20
1	A1	465	A	OP2-P-O3'	5.07	116.35	105.20
37	52	2419	C	C6-N1-C2	-5.07	118.27	120.30
37	52	2709	C	C6-N1-C2	-5.07	118.27	120.30
1	A1	1834	A	N7-C8-N9	5.06	116.33	113.80
37	52	4774	C	N1-C2-O2	5.06	121.94	118.90
37	52	4527	G	N3-C4-C5	-5.06	126.07	128.60
37	52	1853	G	C8-N9-C1'	-5.06	120.42	127.00
37	52	1305	C	N1-C2-O2	5.06	121.94	118.90
37	52	266	C	O5'-P-OP2	-5.05	101.15	105.70
37	52	1286	C	N3-C2-O2	-5.05	118.36	121.90
37	52	498	C	OP2-P-O3'	5.05	116.32	105.20
55	U3	80	LYS	CD-CE-NZ	5.05	123.32	111.70
37	52	729	G	N3-C4-N9	5.05	129.03	126.00
37	52	2550	G	C5-N7-C8	-5.05	101.78	104.30
37	52	236	G	N1-C2-N3	5.05	126.93	123.90
37	52	294	G	C8-N9-C1'	-5.05	120.44	127.00
37	52	3661	G	O4'-C1'-N9	-5.05	104.16	108.20
37	52	4078	C	C6-N1-C2	-5.05	118.28	120.30
37	52	4272	G	N3-C4-C5	-5.05	126.08	128.60
37	52	1577	G	C8-N9-C1'	-5.04	120.45	127.00
67	g3	43	LYS	C-N-CA	5.04	134.30	121.70
42	C3	289	LEU	CA-CB-CG	5.03	126.87	115.30
1	A1	1751	C	C6-N1-C2	-5.03	118.29	120.30
6	F1	73	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A1	1118	C	C6-N1-C2	-5.03	118.29	120.30
37	52	2740	U	N1-C2-O2	5.03	126.32	122.80
37	52	3810	C	C2-N3-C4	5.03	122.41	119.90
37	52	1894	C	C6-N1-C2	-5.03	118.29	120.30
39	82	42	G	C4-C5-N7	5.03	112.81	110.80
37	52	4919	G	C8-N9-C1'	-5.02	120.47	127.00
1	A1	1057	C	C6-N1-C2	-5.02	118.29	120.30
37	52	3876	A	OP2-P-O3'	5.01	116.23	105.20
1	A1	1858	G	N7-C8-N9	5.01	115.61	113.10
37	52	2627	C	C6-N1-C2	-5.01	118.30	120.30
40	A3	117	GLU	N-CA-C	5.01	124.53	111.00
38	72	113	G	C8-N9-C1'	-5.01	120.49	127.00
37	52	2008	U	N3-C2-O2	-5.01	118.69	122.20
37	52	3888	G	C8-N9-C4	-5.01	104.40	106.40
37	52	4266	G	C8-N9-C1'	-5.01	120.49	127.00
1	A1	659	G	C8-N9-C1'	-5.00	120.49	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	52	1929	A	C2-N3-C4	5.00	113.10	110.60
37	52	4929	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	A3	116	LEU	Peptide
40	A3	117	GLU	Peptide
40	A3	168	VAL	Peptide
40	A3	170	ALA	Peptide
40	A3	94	ALA	Peptide
2	B1	42	LYS	Peptide
42	C3	339	THR	Peptide
83	G3	157	PRO	Peptide
83	G3	186	PRO	Peptide
83	G3	214	VAL	Peptide
85	I3	204	GLY	Peptide
47	M3	69	ARG	Peptide
14	N1	37	GLU	Peptide
48	N3	76	PRO	Peptide
48	N3	78	GLY	Peptide
16	P1	21	VAL	Peptide
17	Q1	17	TYR	Peptide
17	Q1	37	TYR	Peptide
52	R3	106	LEU	Peptide
52	R3	113	LYS	Peptide
52	R3	123	LEU	Peptide
52	R3	129	GLY	Peptide
52	R3	83	GLY	Peptide
53	S3	68	PHE	Peptide
55	U3	86	LEU	Peptide
57	W3	85	ALA	Peptide
25	Y1	61	GLN	Peptide
60	Z3	18	TYR	Peptide
60	Z3	79	HIS	Peptide
60	Z3	92	ASP	Peptide
63	c3	87	LYS	Peptide
67	g3	2	VAL	Peptide
67	g3	4	ARG	Sidechain
67	g3	43	LYS	Mainchain
67	g3	44	SER	Peptide

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Mol	Chain	Res	Type	Group
67	g3	73	HIS	Peptide
67	g3	93	ARG	Peptide
67	g3	94	ALA	Peptide
67	g3	99	GLU	Peptide
35	j1	315	GLY	Peptide
36	k1	364	ILE	Peptide
71	k3	43	TYR	Peptide
76	p3	50	ARG	Peptide
76	p3	52	VAL	Peptide
78	s3	33	ASP	Peptide
78	s3	72	ASN	Peptide
78	s3	81	HIS	Peptide
78	s3	86	VAL	Peptide
79	t3	53	TRP	Peptide
87	u3	209	THR	Peptide
87	u3	60	ARG	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B1	215/295 (73%)	199 (93%)	16 (7%)	0	100	100
3	C1	211/264 (80%)	191 (90%)	20 (10%)	0	100	100
4	D1	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
5	E1	226/243 (93%)	211 (93%)	15 (7%)	0	100	100
6	F1	260/263 (99%)	227 (87%)	33 (13%)	0	100	100
7	G1	181/204 (89%)	167 (92%)	14 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H1	235/249 (94%)	218 (93%)	17 (7%)	0	100	100
9	I1	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
10	J1	204/208 (98%)	184 (90%)	20 (10%)	0	100	100
11	K1	183/194 (94%)	173 (94%)	10 (6%)	0	100	100
12	L1	94/165 (57%)	83 (88%)	11 (12%)	0	100	100
13	M1	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
14	N1	115/132 (87%)	101 (88%)	14 (12%)	0	100	100
15	O1	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
16	P1	134/168 (80%)	123 (92%)	11 (8%)	0	100	100
17	Q1	118/145 (81%)	106 (90%)	12 (10%)	0	100	100
18	R1	140/146 (96%)	126 (90%)	14 (10%)	0	100	100
19	S1	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
20	T1	142/152 (93%)	128 (90%)	14 (10%)	0	100	100
21	U1	139/145 (96%)	128 (92%)	11 (8%)	0	100	100
22	V1	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
23	W1	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
24	X1	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
25	Y1	139/143 (97%)	124 (89%)	14 (10%)	1 (1%)	22	63
26	Z1	122/130 (94%)	109 (89%)	13 (11%)	0	100	100
27	a1	73/125 (58%)	65 (89%)	8 (11%)	0	100	100
28	b1	99/115 (86%)	92 (93%)	7 (7%)	0	100	100
29	c1	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
30	d1	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
31	e1	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
32	f1	53/133 (40%)	49 (92%)	4 (8%)	0	100	100
33	g1	66/156 (42%)	58 (88%)	8 (12%)	0	100	100
34	h1	311/317 (98%)	268 (86%)	43 (14%)	0	100	100
35	j1	417/439 (95%)	388 (93%)	29 (7%)	0	100	100
36	k1	571/599 (95%)	517 (90%)	54 (10%)	0	100	100
40	A3	246/257 (96%)	185 (75%)	54 (22%)	7 (3%)	5	30
41	B3	392/403 (97%)	355 (91%)	37 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	C3	360/425 (85%)	325 (90%)	35 (10%)	0	100	100
43	E3	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
44	F3	223/247 (90%)	205 (92%)	18 (8%)	0	100	100
45	H3	188/192 (98%)	174 (93%)	13 (7%)	1 (0%)	29	69
46	L3	208/211 (99%)	194 (93%)	12 (6%)	2 (1%)	15	54
47	M3	136/218 (62%)	121 (89%)	15 (11%)	0	100	100
48	N3	201/204 (98%)	181 (90%)	20 (10%)	0	100	100
49	O3	197/203 (97%)	185 (94%)	12 (6%)	0	100	100
50	P3	151/184 (82%)	143 (95%)	8 (5%)	0	100	100
51	Q3	185/188 (98%)	167 (90%)	18 (10%)	0	100	100
52	R3	178/196 (91%)	161 (90%)	17 (10%)	0	100	100
53	S3	174/176 (99%)	154 (88%)	20 (12%)	0	100	100
54	T3	157/160 (98%)	144 (92%)	12 (8%)	1 (1%)	25	66
55	U3	97/128 (76%)	79 (81%)	18 (19%)	0	100	100
56	V3	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
57	W3	102/157 (65%)	92 (90%)	10 (10%)	0	100	100
58	X3	116/156 (74%)	109 (94%)	7 (6%)	0	100	100
59	Y3	132/145 (91%)	120 (91%)	12 (9%)	0	100	100
60	Z3	133/136 (98%)	105 (79%)	25 (19%)	3 (2%)	6	34
61	a3	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
62	b3	100/245 (41%)	94 (94%)	6 (6%)	0	100	100
63	c3	96/115 (84%)	81 (84%)	15 (16%)	0	100	100
64	d3	105/125 (84%)	90 (86%)	15 (14%)	0	100	100
65	e3	126/134 (94%)	115 (91%)	11 (9%)	0	100	100
66	f3	107/110 (97%)	96 (90%)	11 (10%)	0	100	100
67	g3	112/117 (96%)	98 (88%)	13 (12%)	1 (1%)	17	57
68	h3	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
69	i3	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
70	j3	84/97 (87%)	75 (89%)	9 (11%)	0	100	100
71	k3	67/70 (96%)	59 (88%)	8 (12%)	0	100	100
72	l3	48/51 (94%)	41 (85%)	7 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
73	m3	50/102 (49%)	48 (96%)	2 (4%)	0	100 100
74	n3	23/25 (92%)	23 (100%)	0	0	100 100
75	o3	102/106 (96%)	96 (94%)	6 (6%)	0	100 100
76	p3	89/92 (97%)	77 (86%)	12 (14%)	0	100 100
77	r3	122/137 (89%)	110 (90%)	12 (10%)	0	100 100
78	s3	194/318 (61%)	156 (80%)	37 (19%)	1 (0%)	29 69
79	t3	151/165 (92%)	127 (84%)	24 (16%)	0	100 100
82	J3	168/178 (94%)	158 (94%)	10 (6%)	0	100 100
83	G3	229/319 (72%)	195 (85%)	34 (15%)	0	100 100
84	D3	291/297 (98%)	253 (87%)	38 (13%)	0	100 100
85	I3	201/214 (94%)	167 (83%)	33 (16%)	1 (0%)	29 69
86	1	20/22 (91%)	11 (55%)	4 (20%)	5 (25%)	0 1
87	u3	215/217 (99%)	183 (85%)	30 (14%)	2 (1%)	17 57
All	All	12742/14651 (87%)	11466 (90%)	1251 (10%)	25 (0%)	50 81

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	A3	116	LEU
40	A3	118	GLU
40	A3	126	LEU
46	L3	64	VAL
60	Z3	73	LYS
86	1	15	ALA
87	u3	101	LYS
40	A3	169	VAL
78	s3	34	ASN
86	1	7	ALA
87	u3	210	MET
46	L3	63	THR
60	Z3	75	TYR
67	g3	44	SER
86	1	13	ALA
86	1	14	ALA
40	A3	117	GLU
86	1	8	ALA
40	A3	125	LYS

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Mol	Chain	Res	Type
45	H3	108	ASN
40	A3	150	LEU
25	Y1	62	PRO
85	I3	205	PRO
54	T3	82	GLY
60	Z3	90	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B1	180/245 (74%)	177 (98%)	3 (2%)	60 78
3	C1	194/231 (84%)	191 (98%)	3 (2%)	65 80
4	D1	187/225 (83%)	186 (100%)	1 (0%)	88 93
5	E1	190/202 (94%)	186 (98%)	4 (2%)	53 72
6	F1	224/225 (100%)	223 (100%)	1 (0%)	91 94
7	G1	158/170 (93%)	156 (99%)	2 (1%)	69 82
8	H1	207/218 (95%)	205 (99%)	2 (1%)	76 86
9	I1	165/174 (95%)	165 (100%)	0	100 100
10	J1	178/180 (99%)	174 (98%)	4 (2%)	52 71
11	K1	161/168 (96%)	157 (98%)	4 (2%)	47 68
12	L1	87/136 (64%)	85 (98%)	2 (2%)	50 70
13	M1	130/142 (92%)	128 (98%)	2 (2%)	65 80
14	N1	99/108 (92%)	98 (99%)	1 (1%)	76 86
15	O1	130/131 (99%)	128 (98%)	2 (2%)	65 80
16	P1	106/130 (82%)	104 (98%)	2 (2%)	57 75
17	Q1	109/130 (84%)	108 (99%)	1 (1%)	78 87
18	R1	117/121 (97%)	115 (98%)	2 (2%)	60 78
19	S1	119/121 (98%)	119 (100%)	0	100 100
20	T1	125/132 (95%)	124 (99%)	1 (1%)	81 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	U1	111/115 (96%)	110 (99%)	1 (1%)	78 87
22	V1	92/107 (86%)	90 (98%)	2 (2%)	52 71
23	W1	67/67 (100%)	66 (98%)	1 (2%)	65 80
24	X1	112/113 (99%)	112 (100%)	0	100 100
25	Y1	113/115 (98%)	113 (100%)	0	100 100
26	Z1	107/112 (96%)	106 (99%)	1 (1%)	78 87
27	a1	66/103 (64%)	66 (100%)	0	100 100
28	b1	88/98 (90%)	88 (100%)	0	100 100
29	c1	75/76 (99%)	74 (99%)	1 (1%)	69 82
30	d1	55/62 (89%)	55 (100%)	0	100 100
31	e1	48/49 (98%)	48 (100%)	0	100 100
32	f1	46/106 (43%)	44 (96%)	2 (4%)	29 53
33	g1	61/140 (44%)	60 (98%)	1 (2%)	62 79
34	h1	272/275 (99%)	269 (99%)	3 (1%)	73 84
35	j1	361/377 (96%)	355 (98%)	6 (2%)	60 78
36	k1	509/526 (97%)	505 (99%)	4 (1%)	81 89
40	A3	190/199 (96%)	185 (97%)	5 (3%)	46 66
41	B3	342/348 (98%)	340 (99%)	2 (1%)	86 92
42	C3	302/347 (87%)	295 (98%)	7 (2%)	50 70
43	E3	190/251 (76%)	188 (99%)	2 (1%)	73 84
44	F3	196/215 (91%)	194 (99%)	2 (1%)	76 86
45	H3	169/171 (99%)	164 (97%)	5 (3%)	41 63
46	L3	175/176 (99%)	174 (99%)	1 (1%)	86 92
47	M3	117/161 (73%)	117 (100%)	0	100 100
48	N3	171/172 (99%)	168 (98%)	3 (2%)	59 77
49	O3	171/173 (99%)	169 (99%)	2 (1%)	71 83
50	P3	134/163 (82%)	133 (99%)	1 (1%)	84 90
51	Q3	164/165 (99%)	161 (98%)	3 (2%)	59 77
52	R3	159/175 (91%)	154 (97%)	5 (3%)	40 62
53	S3	157/157 (100%)	157 (100%)	0	100 100
54	T3	139/140 (99%)	137 (99%)	2 (1%)	67 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	U3	89/114 (78%)	87 (98%)	2 (2%)	52	71
56	V3	101/107 (94%)	99 (98%)	2 (2%)	55	74
57	W3	86/126 (68%)	85 (99%)	1 (1%)	71	83
58	X3	106/134 (79%)	106 (100%)	0	100	100
59	Y3	124/135 (92%)	122 (98%)	2 (2%)	62	79
60	Z3	117/118 (99%)	115 (98%)	2 (2%)	60	78
61	a3	119/120 (99%)	118 (99%)	1 (1%)	81	89
62	b3	84/184 (46%)	83 (99%)	1 (1%)	71	83
63	c3	84/98 (86%)	84 (100%)	0	100	100
64	d3	98/110 (89%)	96 (98%)	2 (2%)	55	74
65	e3	114/120 (95%)	114 (100%)	0	100	100
66	f3	88/89 (99%)	88 (100%)	0	100	100
67	g3	98/100 (98%)	96 (98%)	2 (2%)	55	74
68	h3	109/110 (99%)	109 (100%)	0	100	100
69	i3	86/89 (97%)	85 (99%)	1 (1%)	71	83
70	j3	73/80 (91%)	72 (99%)	1 (1%)	67	80
71	k3	64/65 (98%)	63 (98%)	1 (2%)	62	79
72	l3	47/48 (98%)	47 (100%)	0	100	100
73	m3	48/90 (53%)	47 (98%)	1 (2%)	53	72
74	n3	24/24 (100%)	24 (100%)	0	100	100
75	o3	92/94 (98%)	91 (99%)	1 (1%)	73	84
76	p3	74/75 (99%)	73 (99%)	1 (1%)	67	80
77	r3	108/121 (89%)	106 (98%)	2 (2%)	57	75
78	s3	164/258 (64%)	162 (99%)	2 (1%)	71	83
79	t3	126/137 (92%)	126 (100%)	0	100	100
82	J3	143/149 (96%)	143 (100%)	0	100	100
83	G3	200/272 (74%)	191 (96%)	9 (4%)	27	52
84	D3	247/250 (99%)	240 (97%)	7 (3%)	43	65
85	I3	175/181 (97%)	167 (95%)	8 (5%)	27	52
87	u3	195/196 (100%)	191 (98%)	4 (2%)	53	72
All	All	11108/12437 (89%)	10956 (99%)	152 (1%)	68	80

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B1	50	ASN
2	B1	117	ARG
2	B1	186	ARG
3	C1	40	ASN
3	C1	147	ASN
3	C1	213	ARG
4	D1	167	ARG
5	E1	22	ASN
5	E1	76	ARG
5	E1	94	ARG
5	E1	227	LYS
6	F1	232	ASN
7	G1	81	ARG
7	G1	91	ARG
8	H1	31	ARG
8	H1	63	MET
10	J1	47	ARG
10	J1	84	ASN
10	J1	87	ASN
10	J1	99	ASN
11	K1	45	ARG
11	K1	70	ARG
11	K1	79	ARG
11	K1	136	ARG
12	L1	55	ARG
12	L1	96	ARG
13	M1	20	LYS
13	M1	97	ARG
14	N1	33	ARG
15	O1	19	ARG
15	O1	27	LYS
16	P1	146	ARG
16	P1	150	ARG
17	Q1	13	ARG
18	R1	41	MET
18	R1	85	ARG
20	T1	8	LYS
21	U1	62	ARG
22	V1	47	ASN
22	V1	79	ARG
23	W1	82	ASN
26	Z1	101	LYS

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Mol	Chain	Res	Type
29	c1	81	ARG
32	f1	99	LYS
32	f1	104	ARG
33	g1	138	ARG
34	h1	5	MET
34	h1	159	ASN
34	h1	178	ASN
35	j1	32	THR
35	j1	67	ASN
35	j1	121	ASN
35	j1	245	ARG
35	j1	265	ASN
35	j1	289	ARG
36	k1	190	ARG
36	k1	250	LYS
36	k1	321	ASN
36	k1	385	LYS
40	A3	101	VAL
40	A3	155	LYS
40	A3	193	ARG
40	A3	194	ASN
40	A3	242	ARG
41	B3	24	ARG
41	B3	261	ARG
42	C3	38	ASN
42	C3	95	MET
42	C3	100	ARG
42	C3	188	ARG
42	C3	223	ASN
42	C3	312	ARG
42	C3	321	ASN
43	E3	58	ARG
43	E3	164	ARG
44	F3	165	ARG
44	F3	205	ASN
45	H3	1	MET
45	H3	15	ASN
45	H3	102	ASN
45	H3	128	MET
45	H3	173	ARG
46	L3	42	ARG
48	N3	50	ARG

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Mol	Chain	Res	Type
48	N3	96	ARG
48	N3	162	ARG
49	O3	117	ARG
49	O3	140	ARG
50	P3	128	ARG
51	Q3	14	ARG
51	Q3	91	ARG
51	Q3	97	LYS
52	R3	36	ASN
52	R3	105	LEU
52	R3	110	ARG
52	R3	130	ASN
52	R3	133	LYS
54	T3	136	ARG
54	T3	146	LYS
55	U3	80	LYS
55	U3	81	ARG
56	V3	48	ARG
56	V3	85	ARG
57	W3	82	ILE
59	Y3	2	LYS
59	Y3	77	LYS
60	Z3	75	TYR
60	Z3	84	ARG
61	a3	4	ARG
62	b3	60	ASN
64	d3	18	ASN
64	d3	31	LYS
67	g3	14	ASN
67	g3	18	ASN
69	i3	29	ARG
70	j3	20	ARG
71	k3	36	VAL
73	m3	96	ARG
75	o3	82	MET
76	p3	84	ARG
77	r3	12	ASN
77	r3	67	ARG
78	s3	6	ARG
78	s3	200	ASN
83	G3	88	ARG
83	G3	106	ARG

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Mol	Chain	Res	Type
83	G3	117	GLN
83	G3	134	ASN
83	G3	166	ARG
83	G3	228	ARG
83	G3	280	ASN
83	G3	293	ASN
83	G3	308	LYS
84	D3	23	ARG
84	D3	33	ARG
84	D3	50	ARG
84	D3	143	THR
84	D3	220	LYS
84	D3	242	LYS
84	D3	293	ARG
85	I3	3	ARG
85	I3	10	ARG
85	I3	39	LYS
85	I3	100	ASN
85	I3	102	MET
85	I3	162	ARG
85	I3	164	LYS
85	I3	175	LYS
87	u3	156	LYS
87	u3	159	MET
87	u3	188	ASN
87	u3	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
2	B1	141	ASN
3	C1	40	ASN
3	C1	147	ASN
4	D1	113	GLN
5	E1	22	ASN
6	F1	138	HIS
6	F1	142	HIS
6	F1	209	HIS
6	F1	232	ASN
7	G1	82	ASN
7	G1	114	ASN
8	H1	81	HIS

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Mol	Chain	Res	Type
8	H1	186	GLN
8	H1	202	ASN
9	I1	33	ASN
9	I1	186	ASN
10	J1	84	ASN
10	J1	87	ASN
10	J1	99	ASN
12	L1	7	ASN
13	M1	19	ASN
13	M1	106	HIS
14	N1	28	HIS
14	N1	82	ASN
15	O1	5	HIS
15	O1	105	ASN
16	P1	94	HIS
17	Q1	104	GLN
18	R1	97	GLN
20	T1	120	HIS
20	T1	135	HIS
22	V1	47	ASN
23	W1	33	GLN
24	X1	113	HIS
26	Z1	15	ASN
30	d1	26	GLN
30	d1	29	GLN
33	g1	111	ASN
33	g1	135	HIS
34	h1	133	ASN
34	h1	159	ASN
34	h1	178	ASN
35	j1	11	ASN
35	j1	121	ASN
35	j1	380	ASN
36	k1	171	GLN
36	k1	251	GLN
36	k1	321	ASN
36	k1	381	ASN
36	k1	440	GLN
36	k1	520	HIS
40	A3	194	ASN
41	B3	179	HIS
41	B3	245	HIS

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Mol	Chain	Res	Type
42	C3	38	ASN
42	C3	245	HIS
42	C3	321	ASN
44	F3	38	GLN
44	F3	79	ASN
44	F3	205	ASN
45	H3	8	GLN
45	H3	15	ASN
45	H3	102	ASN
48	N3	199	GLN
49	O3	5	GLN
50	P3	25	HIS
50	P3	80	GLN
50	P3	120	ASN
52	R3	36	ASN
52	R3	130	ASN
52	R3	143	HIS
52	R3	178	GLN
53	S3	156	HIS
53	S3	163	HIS
54	T3	95	HIS
58	X3	93	ASN
58	X3	105	ASN
58	X3	111	GLN
64	d3	18	ASN
66	f3	65	ASN
66	f3	99	HIS
67	g3	14	ASN
67	g3	114	GLN
70	j3	76	HIS
77	r3	12	ASN
82	J3	104	ASN
83	G3	134	ASN
83	G3	280	ASN
83	G3	293	ASN
84	D3	195	HIS
84	D3	202	GLN
84	D3	222	GLN
84	D3	275	GLN
85	I3	95	HIS
85	I3	100	ASN
87	u3	40	ASN

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Mol	Chain	Res	Type
87	u3	188	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1709/1869 (91%)	474 (27%)	23 (1%)
37	52	3591/3634 (98%)	1136 (31%)	45 (1%)
38	72	119/120 (99%)	34 (28%)	0
39	82	149/156 (95%)	43 (28%)	0
80	23	74/76 (97%)	18 (24%)	0
81	w3	22/23 (95%)	10 (45%)	0
All	All	5664/5878 (96%)	1715 (30%)	68 (1%)

All (1715) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	2	A
1	A1	3	C
1	A1	5	U
1	A1	16	G
1	A1	17	C
1	A1	26	U
1	A1	33	G
1	A1	39	A
1	A1	41	G
1	A1	42	A
1	A1	44	U
1	A1	45	A
1	A1	46	A
1	A1	56	G
1	A1	58	C
1	A1	65	C
1	A1	67	C
1	A1	68	A
1	A1	72	C
1	A1	73	C
1	A1	74	G
1	A1	76	U
1	A1	79	A
1	A1	89	C
1	A1	91	A

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Mol	Chain	Res	Type
1	A1	95	G
1	A1	100	U
1	A1	101	U
1	A1	103	A
1	A1	111	A
1	A1	113	G
1	A1	115	U
1	A1	116	U
1	A1	124	U
1	A1	126	G
1	A1	127	C
1	A1	129	C
1	A1	130	G
1	A1	141	A
1	A1	143	U
1	A1	147	A
1	A1	153	G
1	A1	155	G
1	A1	162	C
1	A1	163	U
1	A1	167	G
1	A1	168	C
1	A1	170	A
1	A1	172	U
1	A1	178	C
1	A1	182	C
1	A1	183	G
1	A1	184	G
1	A1	187	G
1	A1	188	C
1	A1	189	U
1	A1	190	G
1	A1	191	A
1	A1	192	C
1	A1	202	G
1	A1	206	G
1	A1	209	A
1	A1	211	G
1	A1	213	G
1	A1	222	U
1	A1	227	U
1	A1	228	C

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Mol	Chain	Res	Type
1	A1	229	A
1	A1	230	A
1	A1	231	A
1	A1	233	C
1	A1	236	A
1	A1	238	C
1	A1	239	C
1	A1	240	G
1	A1	241	G
1	A1	242	U
1	A1	243	C
1	A1	281	C
1	A1	285	U
1	A1	292	A
1	A1	297	A
1	A1	306	C
1	A1	307	G
1	A1	308	G
1	A1	309	G
1	A1	312	G
1	A1	313	A
1	A1	314	U
1	A1	317	C
1	A1	318	A
1	A1	319	C
1	A1	322	C
1	A1	335	G
1	A1	339	A
1	A1	347	G
1	A1	350	C
1	A1	351	G
1	A1	354	U
1	A1	360	A
1	A1	361	U
1	A1	362	C
1	A1	364	A
1	A1	368	U
1	A1	382	C
1	A1	384	U
1	A1	385	G
1	A1	386	C
1	A1	400	C

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Mol	Chain	Res	Type
1	A1	407	G
1	A1	408	A
1	A1	409	C
1	A1	413	G
1	A1	417	C
1	A1	418	A
1	A1	422	U
1	A1	435	A
1	A1	441	C
1	A1	448	A
1	A1	449	A
1	A1	450	C
1	A1	452	G
1	A1	464	A
1	A1	465	A
1	A1	466	G
1	A1	472	C
1	A1	473	A
1	A1	474	G
1	A1	482	G
1	A1	485	A
1	A1	487	U
1	A1	492	C
1	A1	493	A
1	A1	495	U
1	A1	496	C
1	A1	501	C
1	A1	503	C
1	A1	516	A
1	A1	522	A
1	A1	525	A
1	A1	531	A
1	A1	532	C
1	A1	533	A
1	A1	536	A
1	A1	542	U
1	A1	544	G
1	A1	547	G
1	A1	548	C
1	A1	549	C
1	A1	550	C
1	A1	551	U

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Mol	Chain	Res	Type
1	A1	554	A
1	A1	555	A
1	A1	559	G
1	A1	560	A
1	A1	562	U
1	A1	563	G
1	A1	564	A
1	A1	565	G
1	A1	568	C
1	A1	582	U
1	A1	583	A
1	A1	588	G
1	A1	589	G
1	A1	590	A
1	A1	591	U
1	A1	593	C
1	A1	606	G
1	A1	608	C
1	A1	614	C
1	A1	615	C
1	A1	621	C
1	A1	622	C
1	A1	628	A
1	A1	629	A
1	A1	631	U
1	A1	637	U
1	A1	642	U
1	A1	643	A
1	A1	644	G
1	A1	658	U
1	A1	660	C
1	A1	664	A
1	A1	668	A
1	A1	669	A
1	A1	671	A
1	A1	672	A
1	A1	673	G
1	A1	675	U
1	A1	684	G
1	A1	688	U
1	A1	689	U
1	A1	690	G

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Mol	Chain	Res	Type
1	A1	747	U
1	A1	750	C
1	A1	752	G
1	A1	753	C
1	A1	790	C
1	A1	793	G
1	A1	797	C
1	A1	798	G
1	A1	799	U
1	A1	800	U
1	A1	811	A
1	A1	820	U
1	A1	821	G
1	A1	830	A
1	A1	834	C
1	A1	844	U
1	A1	847	A
1	A1	852	G
1	A1	867	G
1	A1	869	A
1	A1	870	A
1	A1	871	U
1	A1	872	A
1	A1	873	G
1	A1	874	G
1	A1	875	A
1	A1	876	C
1	A1	878	G
1	A1	879	C
1	A1	881	G
1	A1	886	A
1	A1	887	U
1	A1	888	U
1	A1	889	U
1	A1	890	U
1	A1	891	G
1	A1	892	U
1	A1	893	U
1	A1	895	G
1	A1	913	A
1	A1	914	U
1	A1	917	U

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Mol	Chain	Res	Type
1	A1	919	A
1	A1	920	A
1	A1	930	C
1	A1	933	G
1	A1	934	G
1	A1	943	U
1	A1	960	U
1	A1	966	U
1	A1	970	G
1	A1	971	G
1	A1	979	C
1	A1	985	G
1	A1	989	C
1	A1	990	A
1	A1	992	A
1	A1	997	A
1	A1	999	G
1	A1	1002	U
1	A1	1005	G
1	A1	1013	U
1	A1	1017	U
1	A1	1021	U
1	A1	1023	A
1	A1	1028	A
1	A1	1041	G
1	A1	1047	C
1	A1	1058	A
1	A1	1060	A
1	A1	1067	C
1	A1	1071	G
1	A1	1083	A
1	A1	1085	C
1	A1	1087	A
1	A1	1089	G
1	A1	1097	G
1	A1	1099	G
1	A1	1100	A
1	A1	1101	U
1	A1	1106	C
1	A1	1115	U
1	A1	1116	C
1	A1	1117	C

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Mol	Chain	Res	Type
1	A1	1118	C
1	A1	1123	C
1	A1	1126	G
1	A1	1131	G
1	A1	1138	C
1	A1	1139	C
1	A1	1144	A
1	A1	1145	A
1	A1	1149	A
1	A1	1150	A
1	A1	1153	C
1	A1	1154	U
1	A1	1155	U
1	A1	1170	A
1	A1	1171	G
1	A1	1175	G
1	A1	1178	U
1	A1	1194	A
1	A1	1195	A
1	A1	1200	A
1	A1	1207	G
1	A1	1212	G
1	A1	1215	C
1	A1	1216	C
1	A1	1221	G
1	A1	1230	C
1	A1	1241	A
1	A1	1242	U
1	A1	1246	A
1	A1	1251	A
1	A1	1253	A
1	A1	1254	C
1	A1	1256	G
1	A1	1257	G
1	A1	1258	A
1	A1	1266	C
1	A1	1274	G
1	A1	1275	G
1	A1	1282	A
1	A1	1284	A
1	A1	1285	G
1	A1	1286	G

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Mol	Chain	Res	Type
1	A1	1287	A
1	A1	1291	A
1	A1	1293	A
1	A1	1295	A
1	A1	1299	A
1	A1	1300	U
1	A1	1301	A
1	A1	1302	G
1	A1	1303	C
1	A1	1308	U
1	A1	1311	C
1	A1	1314	U
1	A1	1319	U
1	A1	1330	G
1	A1	1336	C
1	A1	1342	U
1	A1	1344	A
1	A1	1345	G
1	A1	1355	C
1	A1	1371	U
1	A1	1372	U
1	A1	1375	G
1	A1	1378	A
1	A1	1395	C
1	A1	1396	A
1	A1	1397	U
1	A1	1402	A
1	A1	1412	C
1	A1	1413	G
1	A1	1417	C
1	A1	1427	C
1	A1	1428	G
1	A1	1429	G
1	A1	1430	C
1	A1	1439	A
1	A1	1440	C
1	A1	1447	G
1	A1	1450	G
1	A1	1452	A
1	A1	1453	C
1	A1	1454	A
1	A1	1461	G

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Mol	Chain	Res	Type
1	A1	1462	U
1	A1	1463	U
1	A1	1464	C
1	A1	1466	G
1	A1	1471	C
1	A1	1476	A
1	A1	1477	U
1	A1	1480	A
1	A1	1486	A
1	A1	1487	A
1	A1	1489	A
1	A1	1490	G
1	A1	1496	U
1	A1	1498	A
1	A1	1501	C
1	A1	1502	C
1	A1	1521	C
1	A1	1522	A
1	A1	1523	C
1	A1	1532	C
1	A1	1533	A
1	A1	1535	U
1	A1	1536	G
1	A1	1545	A
1	A1	1548	G
1	A1	1552	G
1	A1	1553	C
1	A1	1554	C
1	A1	1555	U
1	A1	1556	A
1	A1	1557	C
1	A1	1558	C
1	A1	1567	G
1	A1	1570	G
1	A1	1574	C
1	A1	1579	A
1	A1	1580	A
1	A1	1585	U
1	A1	1586	U
1	A1	1588	A
1	A1	1591	C
1	A1	1596	U

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Mol	Chain	Res	Type
1	A1	1597	C
1	A1	1599	U
1	A1	1601	A
1	A1	1602	U
1	A1	1603	G
1	A1	1604	G
1	A1	1621	U
1	A1	1623	A
1	A1	1637	A
1	A1	1638	G
1	A1	1640	A
1	A1	1641	A
1	A1	1646	C
1	A1	1648	G
1	A1	1654	G
1	A1	1665	G
1	A1	1666	C
1	A1	1668	U
1	A1	1670	C
1	A1	1671	G
1	A1	1674	G
1	A1	1678	A
1	A1	1683	C
1	A1	1695	A
1	A1	1698	C
1	A1	1699	A
1	A1	1700	C
1	A1	1701	C
1	A1	1702	G
1	A1	1715	A
1	A1	1721	U
1	A1	1722	G
1	A1	1729	U
1	A1	1732	G
1	A1	1735	A
1	A1	1746	U
1	A1	1748	G
1	A1	1753	C
1	A1	1756	C
1	A1	1757	G
1	A1	1758	G
1	A1	1759	G

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Mol	Chain	Res	Type
1	A1	1777	G
1	A1	1778	C
1	A1	1781	A
1	A1	1783	C
1	A1	1792	G
1	A1	1800	A
1	A1	1816	G
1	A1	1821	U
1	A1	1823	A
1	A1	1824	A
1	A1	1825	A
1	A1	1826	G
1	A1	1831	A
1	A1	1834	A
1	A1	1836	G
1	A1	1838	U
1	A1	1839	U
1	A1	1840	U
1	A1	1844	U
1	A1	1845	A
1	A1	1849	G
1	A1	1851	A
1	A1	1852	C
1	A1	1861	G
1	A1	1862	G
1	A1	1863	A
1	A1	1864	U
1	A1	1865	C
1	A1	1869	A
37	52	5	A
37	52	6	C
37	52	8	U
37	52	9	C
37	52	10	A
37	52	13	U
37	52	18	C
37	52	21	G
37	52	25	A
37	52	30	C
37	52	39	A
37	52	42	A
37	52	44	A

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Mol	Chain	Res	Type
37	52	48	G
37	52	49	U
37	52	58	G
37	52	59	A
37	52	64	A
37	52	65	A
37	52	67	C
37	52	70	A
37	52	71	C
37	52	72	C
37	52	76	A
37	52	82	U
37	52	84	A
37	52	87	A
37	52	91	G
37	52	93	G
37	52	96	U
37	52	104	G
37	52	108	A
37	52	109	G
37	52	119	G
37	52	120	A
37	52	122	U
37	52	126	C
37	52	133	C
37	52	135	G
37	52	136	C
37	52	137	G
37	52	142	G
37	52	144	G
37	52	149	A
37	52	151	G
37	52	153	G
37	52	156	G
37	52	157	U
37	52	159	C
37	52	160	G
37	52	161	G
37	52	164	G
37	52	168	C
37	52	170	C
37	52	172	C

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Mol	Chain	Res	Type
37	52	173	C
37	52	174	C
37	52	179	G
37	52	181	C
37	52	182	G
37	52	197	A
37	52	200	U
37	52	201	C
37	52	214	G
37	52	216	C
37	52	217	C
37	52	220	C
37	52	224	U
37	52	225	G
37	52	232	G
37	52	233	U
37	52	234	G
37	52	236	G
37	52	246	G
37	52	262	G
37	52	265	C
37	52	266	C
37	52	276	C
37	52	277	G
37	52	280	G
37	52	294	G
37	52	297	U
37	52	306	A
37	52	308	G
37	52	309	C
37	52	310	G
37	52	315	G
37	52	316	U
37	52	321	U
37	52	322	C
37	52	323	C
37	52	334	A
37	52	340	C
37	52	341	G
37	52	345	C
37	52	346	G
37	52	349	A

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Mol	Chain	Res	Type
37	52	367	C
37	52	379	G
37	52	383	A
37	52	384	A
37	52	387	G
37	52	390	C
37	52	395	A
37	52	396	A
37	52	410	A
37	52	412	G
37	52	413	G
37	52	417	G
37	52	440	U
37	52	446	C
37	52	448	G
37	52	449	C
37	52	450	G
37	52	452	A
37	52	453	G
37	52	454	U
37	52	455	C
37	52	463	A
37	52	465	G
37	52	467	U
37	52	468	U
37	52	474	C
37	52	475	G
37	52	481	G
37	52	481(A)	C
37	52	482	G
37	52	483	G
37	52	484	U
37	52	485	C
37	52	486	C
37	52	487	G
37	52	490	C
37	52	491	G
37	52	492	U
37	52	493	G
37	52	495	C
37	52	498	C
37	52	499	G

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Mol	Chain	Res	Type
37	52	505	G
37	52	506	C
37	52	510	U
37	52	516	C
37	52	641	G
37	52	642	G
37	52	661	C
37	52	666	G
37	52	667	A
37	52	669	C
37	52	670	G
37	52	674	G
37	52	676	C
37	52	685	C
37	52	686	A
37	52	688	U
37	52	691	C
37	52	696	C
37	52	697	G
37	52	700	G
37	52	704	C
37	52	705	G
37	52	719	C
37	52	722	G
37	52	729	G
37	52	730	G
37	52	731	G
37	52	733	A
37	52	738	C
37	52	743	G
37	52	747	A
37	52	749	G
37	52	750	U
37	52	751	G
37	52	758	G
37	52	760	G
37	52	905	C
37	52	908	G
37	52	913	U
37	52	914	U
37	52	915	A
37	52	917	A

Continued on next page...

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Mol	Chain	Res	Type
37	52	922(B)	C
37	52	923	C
37	52	925	C
37	52	926	G
37	52	929	A
37	52	930	G
37	52	931	C
37	52	932	A
37	52	933	G
37	52	934	C
37	52	935	A
37	52	935(A)	G
37	52	941	C
37	52	944	A
37	52	945	U
37	52	946	C
37	52	951	G
37	52	955	G
37	52	956	A
37	52	959	G
37	52	960	A
37	52	961	G
37	52	962	C
37	52	965	G
37	52	966	A
37	52	967	C
37	52	968	C
37	52	969	C
37	52	972	C
37	52	978	G
37	52	983	C
37	52	985	C
37	52	990	C
37	52	1070	G
37	52	1071	C
37	52	1072	C
37	52	1073	G
37	52	1074	G
37	52	1077	C
37	52	1082	C
37	52	1090	G
37	52	1101	C

Continued on next page...

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Mol	Chain	Res	Type
37	52	1104	C
37	52	1107	C
37	52	1108	C
37	52	1163	G
37	52	1164	G
37	52	1165	G
37	52	1166	G
37	52	1167	C
37	52	1181	C
37	52	1183	C
37	52	1196	G
37	52	1199	G
37	52	1201	U
37	52	1203	G
37	52	1205	G
37	52	1211	G
37	52	1212	G
37	52	1214	C
37	52	1215	C
37	52	1216	C
37	52	1219	G
37	52	1221	G
37	52	1235	G
37	52	1236	C
37	52	1237	C
37	52	1238	A
37	52	1239	C
37	52	1246	G
37	52	1272	C
37	52	1273	G
37	52	1276	C
37	52	1279	A
37	52	1281	G
37	52	1284	G
37	52	1287	G
37	52	1292	C
37	52	1293	G
37	52	1295	U
37	52	1296	G
37	52	1299	G
37	52	1300	G
37	52	1301	C

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Mol	Chain	Res	Type
37	52	1303	A
37	52	1309	C
37	52	1318	C
37	52	1321	G
37	52	1326	A
37	52	1330	A
37	52	1338	G
37	52	1341	U
37	52	1352	C
37	52	1353	G
37	52	1354	A
37	52	1356	U
37	52	1358	G
37	52	1359	G
37	52	1360	G
37	52	1361	G
37	52	1362	G
37	52	1371	A
37	52	1372	A
37	52	1373	A
37	52	1377	G
37	52	1378	C
37	52	1379	C
37	52	1387	A
37	52	1389	U
37	52	1391	A
37	52	1394	G
37	52	1396	G
37	52	1397	A
37	52	1398	A
37	52	1399	G
37	52	1400	G
37	52	1405	C
37	52	1406	G
37	52	1420	A
37	52	1425	G
37	52	1429	C
37	52	1434	G
37	52	1436	C
37	52	1437	C
37	52	1438	U
37	52	1445	U

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Mol	Chain	Res	Type
37	52	1446	C
37	52	1453	G
37	52	1454	G
37	52	1456	C
37	52	1457	G
37	52	1459	A
37	52	1466	G
37	52	1468	C
37	52	1475	G
37	52	1478	C
37	52	1481	C
37	52	1482	G
37	52	1483	C
37	52	1484	G
37	52	1491	A
37	52	1493	G
37	52	1497	A
37	52	1498	G
37	52	1501	C
37	52	1502	G
37	52	1514	U
37	52	1517	G
37	52	1518	A
37	52	1521	C
37	52	1523	A
37	52	1524	A
37	52	1531	U
37	52	1534	A
37	52	1535	C
37	52	1538	U
37	52	1540	C
37	52	1543	G
37	52	1547	A
37	52	1549	G
37	52	1553	A
37	52	1558	A
37	52	1566	C
37	52	1571	G
37	52	1573	G
37	52	1578	U
37	52	1585	C
37	52	1590	C

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Mol	Chain	Res	Type
37	52	1591	U
37	52	1592	G
37	52	1596	U
37	52	1597	G
37	52	1602	U
37	52	1605	G
37	52	1609	U
37	52	1612	G
37	52	1613	A
37	52	1614	C
37	52	1624	G
37	52	1625	G
37	52	1626	G
37	52	1627	G
37	52	1631	A
37	52	1632	A
37	52	1633	G
37	52	1634	A
37	52	1638	A
37	52	1643	A
37	52	1650	A
37	52	1651	G
37	52	1652	U
37	52	1654	G
37	52	1658	G
37	52	1660	U
37	52	1661	C
37	52	1663	C
37	52	1673	U
37	52	1676	C
37	52	1677	U
37	52	1679	A
37	52	1684	A
37	52	1724	G
37	52	1725	U
37	52	1729	A
37	52	1730	U
37	52	1731	C
37	52	1734	G
37	52	1735	U
37	52	1740	C
37	52	1741	G

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Mol	Chain	Res	Type
37	52	1742	A
37	52	1746	A
37	52	1750	G
37	52	1753	G
37	52	1754	U
37	52	1755	C
37	52	1756	U
37	52	1757	U
37	52	1763	C
37	52	1764	G
37	52	1768	C
37	52	1772	C
37	52	1775	A
37	52	1776	A
37	52	1777	C
37	52	1787	A
37	52	1792	U
37	52	1796	U
37	52	1800	U
37	52	1804	A
37	52	1805	A
37	52	1806	G
37	52	1807	C
37	52	1808	C
37	52	1810	G
37	52	1812	C
37	52	1815	G
37	52	1818	G
37	52	1820	U
37	52	1821	G
37	52	1822	U
37	52	1824	G
37	52	1828	C
37	52	1834	U
37	52	1836	G
37	52	1837	A
37	52	1842	G
37	52	1843	A
37	52	1844	G
37	52	1855	G
37	52	1861	U
37	52	1866	U

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Mol	Chain	Res	Type
37	52	1867	A
37	52	1869	G
37	52	1870	C
37	52	1889	U
37	52	1892	A
37	52	1893	C
37	52	1897	A
37	52	1910	G
37	52	1915	C
37	52	1918	U
37	52	1920	C
37	52	1921	C
37	52	1922	G
37	52	1924	C
37	52	1928	C
37	52	1930	U
37	52	1931	C
37	52	1932	A
37	52	1934	A
37	52	1935	C
37	52	1940	G
37	52	1942	A
37	52	1944	A
37	52	1948	G
37	52	1951	G
37	52	1958	A
37	52	1959	U
37	52	1960	A
37	52	1961	G
37	52	1969	G
37	52	1971	U
37	52	1976	G
37	52	1977	C
37	52	1979	A
37	52	1980	U
37	52	1981	G
37	52	1983	A
37	52	1984	A
37	52	1991	A
37	52	1993	C
37	52	1994	C
37	52	1995	G

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Mol	Chain	Res	Type
37	52	1998	A
37	52	2001	G
37	52	2002	A
37	52	2003	G
37	52	2005	G
37	52	2007	G
37	52	2010	A
37	52	2011	C
37	52	2014	C
37	52	2020	U
37	52	2021	G
37	52	2022	C
37	52	2023	C
37	52	2024	G
37	52	2025	A
37	52	2026	A
37	52	2042	A
37	52	2043	A
37	52	2046	G
37	52	2047	A
37	52	2048	U
37	52	2052	G
37	52	2054	U
37	52	2055	G
37	52	2056	G
37	52	2057	A
37	52	2062	C
37	52	2063	G
37	52	2064	G
37	52	2069	A
37	52	2078	C
37	52	2084	U
37	52	2085	G
37	52	2088	A
37	52	2089	G
37	52	2090	U
37	52	2092	G
37	52	2093	G
37	52	2094	C
37	52	2097	A
37	52	2098	G
37	52	2099	C

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Mol	Chain	Res	Type
37	52	2101	A
37	52	2102	G
37	52	2105	A
37	52	2108	G
37	52	2112	G
37	52	2259	G
37	52	2260	C
37	52	2261	G
37	52	2263	A
37	52	2268	A
37	52	2269	C
37	52	2270	G
37	52	2274	C
37	52	2275	G
37	52	2277	C
37	52	2279	A
37	52	2281	U
37	52	2289	C
37	52	2295	C
37	52	2300	A
37	52	2301	G
37	52	2306	G
37	52	2308	A
37	52	2313	A
37	52	2314	G
37	52	2328	G
37	52	2333	G
37	52	2335	C
37	52	2345	G
37	52	2346	C
37	52	2348	G
37	52	2351	C
37	52	2353	U
37	52	2360	A
37	52	2363	A
37	52	2364	G
37	52	2374	A
37	52	2380	G
37	52	2385	U
37	52	2395	A
37	52	2396	A
37	52	2397	G

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Mol	Chain	Res	Type
37	52	2399	G
37	52	2414	G
37	52	2415	U
37	52	2416	G
37	52	2421	G
37	52	2422	C
37	52	2426	U
37	52	2428	A
37	52	2433	G
37	52	2437	C
37	52	2438	A
37	52	2439	G
37	52	2440	U
37	52	2441	C
37	52	2447	U
37	52	2450	G
37	52	2451	A
37	52	2454	U
37	52	2456	G
37	52	2458	C
37	52	2460	A
37	52	2461	G
37	52	2471	G
37	52	2473	A
37	52	2475	G
37	52	2480	G
37	52	2481	G
37	52	2485	U
37	52	2488	C
37	52	2489	C
37	52	2490	U
37	52	2491	C
37	52	2492	C
37	52	2493	G
37	52	2494	U
37	52	2496	G
37	52	2501	C
37	52	2503	G
37	52	2505	C
37	52	2506	G
37	52	2511	A
37	52	2512	A

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Mol	Chain	Res	Type
37	52	2513	A
37	52	2516	G
37	52	2521	G
37	52	2529	A
37	52	2532	C
37	52	2535	G
37	52	2536	A
37	52	2537	A
37	52	2538	U
37	52	2542	G
37	52	2544	G
37	52	2546	G
37	52	2549	G
37	52	2551	A
37	52	2555	G
37	52	2556	G
37	52	2561	C
37	52	2562	G
37	52	2563	C
37	52	2566	G
37	52	2570	U
37	52	2575	U
37	52	2576	G
37	52	2577	C
37	52	2580	U
37	52	2581	A
37	52	2587	A
37	52	2588	C
37	52	2589	C
37	52	2593	C
37	52	2597	G
37	52	2599	G
37	52	2600	A
37	52	2601	A
37	52	2604	C
37	52	2607	C
37	52	2620	G
37	52	2621	A
37	52	2622	G
37	52	2624	G
37	52	2627	C
37	52	2631	U

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Mol	Chain	Res	Type
37	52	2639	U
37	52	2653	C
37	52	2655	C
37	52	2656	U
37	52	2658	G
37	52	2662	G
37	52	2663	G
37	52	2668	G
37	52	2669	C
37	52	2670	C
37	52	2674	A
37	52	2675	G
37	52	2683	C
37	52	2685	C
37	52	2686	G
37	52	2687	U
37	52	2689	C
37	52	2693	G
37	52	2695	A
37	52	2696	A
37	52	2697	A
37	52	2701	U
37	52	2706	G
37	52	2707	U
37	52	2708	U
37	52	2709	C
37	52	2710	C
37	52	2711	G
37	52	2712	G
37	52	2714	G
37	52	2716	C
37	52	2719	C
37	52	2725	A
37	52	2726	G
37	52	2732	G
37	52	2739	C
37	52	2740	U
37	52	2741	U
37	52	2743	A
37	52	2744	A
37	52	2750	G
37	52	2752	G

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Mol	Chain	Res	Type
37	52	2754	G
37	52	2756	G
37	52	2757	A
37	52	2760	G
37	52	2761	U
37	52	2763	U
37	52	2764	A
37	52	2766	A
37	52	2767	U
37	52	2768	C
37	52	2769	U
37	52	2778	G
37	52	2787	A
37	52	2788	U
37	52	2789	A
37	52	2790	U
37	52	2794	C
37	52	2796	G
37	52	2798	A
37	52	2799	G
37	52	2807	A
37	52	2809	G
37	52	2811	G
37	52	2812	A
37	52	2813	A
37	52	2817	C
37	52	2821	U
37	52	2822	G
37	52	2823	G
37	52	2826	U
37	52	2827	G
37	52	2842	G
37	52	2847	G
37	52	2849	A
37	52	2850	A
37	52	2854	G
37	52	2855	G
37	52	2856	C
37	52	2858	A
37	52	2862	G
37	52	2864	A
37	52	2872	C

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Mol	Chain	Res	Type
37	52	2873	U
37	52	2875	C
37	52	2876	G
37	52	2889	G
37	52	2895	A
37	52	2897	G
37	52	2898	G
37	52	3598	C
37	52	3599	A
37	52	3600	G
37	52	3604	A
37	52	3605	C
37	52	3606	U
37	52	3615	G
37	52	3616	U
37	52	3618	C
37	52	3620	G
37	52	3622	C
37	52	3625	G
37	52	3626	G
37	52	3635	A
37	52	3638	G
37	52	3642	A
37	52	3643	A
37	52	3644	U
37	52	3646	A
37	52	3662	A
37	52	3664	G
37	52	3668	C
37	52	3673	C
37	52	3674	G
37	52	3678	G
37	52	3680	U
37	52	3682	A
37	52	3683	C
37	52	3685	C
37	52	3690	U
37	52	3692	A
37	52	3696	C
37	52	3705	G
37	52	3707	U
37	52	3712	A

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Mol	Chain	Res	Type
37	52	3713	U
37	52	3714	G
37	52	3729	U
37	52	3731	C
37	52	3732	A
37	52	3734	U
37	52	3743	G
37	52	3744	G
37	52	3753	G
37	52	3760	A
37	52	3763	A
37	52	3766	A
37	52	3773	U
37	52	3775	A
37	52	3776	G
37	52	3777	G
37	52	3783	A
37	52	3784	A
37	52	3793	U
37	52	3796	U
37	52	3798	U
37	52	3802	U
37	52	3807	A
37	52	3810	C
37	52	3811	G
37	52	3812	C
37	52	3814	U
37	52	3817	A
37	52	3819	G
37	52	3822	U
37	52	3825	A
37	52	3834	C
37	52	3837	C
37	52	3838	U
37	52	3840	U
37	52	3843	C
37	52	3858	C
37	52	3865	A
37	52	3867	A
37	52	3868	G
37	52	3876	A
37	52	3877	A

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Mol	Chain	Res	Type
37	52	3878	C
37	52	3879	G
37	52	3881	G
37	52	3882	C
37	52	3889	G
37	52	3895	G
37	52	3897	G
37	52	3901	A
37	52	3902	A
37	52	3905	A
37	52	3906	A
37	52	3907	G
37	52	3909	C
37	52	3915	U
37	52	3921	U
37	52	3925	U
37	52	3926	C
37	52	3937	C
37	52	3940	U
37	52	3941	G
37	52	3942	A
37	52	3944	G
37	52	3947	A
37	52	3957	U
37	52	3959	U
37	52	3960	A
37	52	3962	A
37	52	3963	A
37	52	3964	U
37	52	3965	A
37	52	3966	A
37	52	3967	G
37	52	3969	G
37	52	3970	G
37	52	3973	G
37	52	4037	C
37	52	4038	C
37	52	4044	U
37	52	4047	A
37	52	4048	A
37	52	4049	U
37	52	4053	A

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Mol	Chain	Res	Type
37	52	4065	G
37	52	4066	U
37	52	4067	U
37	52	4069	U
37	52	4071	U
37	52	4076	G
37	52	4084	G
37	52	4085	A
37	52	4086	G
37	52	4091	G
37	52	4093	G
37	52	4094	G
37	52	4100	C
37	52	4111	U
37	52	4112	C
37	52	4116	C
37	52	4117	U
37	52	4118	U
37	52	4119	C
37	52	4120	U
37	52	4121	G
37	52	4122	G
37	52	4124	G
37	52	4127	A
37	52	4129	G
37	52	4131	G
37	52	4133	C
37	52	4157	A
37	52	4158	C
37	52	4159	C
37	52	4162	C
37	52	4163	U
37	52	4166	G
37	52	4170	A
37	52	4171	C
37	52	4172	A
37	52	4173	G
37	52	4180	G
37	52	4183	G
37	52	4184	G
37	52	4191	G
37	52	4194	U

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Mol	Chain	Res	Type
37	52	4195	G
37	52	4203	A
37	52	4205	A
37	52	4206	C
37	52	4207	C
37	52	4209	G
37	52	4212	A
37	52	4215	C
37	52	4229	U
37	52	4233	A
37	52	4234	A
37	52	4251	A
37	52	4254	G
37	52	4255	A
37	52	4257	A
37	52	4265	U
37	52	4266	G
37	52	4268	A
37	52	4271	A
37	52	4273	A
37	52	4275	G
37	52	4280	A
37	52	4281	A
37	52	4282	A
37	52	4285	U
37	52	4290	U
37	52	4291	G
37	52	4293	U
37	52	4305	G
37	52	4306	U
37	52	4317	A
37	52	4318	C
37	52	4322	G
37	52	4329	G
37	52	4330	G
37	52	4335	C
37	52	4336	A
37	52	4339	A
37	52	4348	A
37	52	4349	C
37	52	4350	C
37	52	4351	U

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Mol	Chain	Res	Type
37	52	4355	G
37	52	4359	U
37	52	4366	A
37	52	4374	U
37	52	4377	G
37	52	4378	A
37	52	4379	A
37	52	4380	A
37	52	4386	C
37	52	4387	C
37	52	4393	G
37	52	4394	A
37	52	4395	U
37	52	4396	A
37	52	4398	C
37	52	4405	G
37	52	4417	C
37	52	4419	U
37	52	4420	U
37	52	4422	A
37	52	4424	A
37	52	4426	C
37	52	4430	G
37	52	4431	U
37	52	4433	G
37	52	4435	U
37	52	4437	U
37	52	4440	G
37	52	4444	C
37	52	4448	G
37	52	4449	A
37	52	4450	U
37	52	4452	U
37	52	4453	C
37	52	4464	A
37	52	4466	C
37	52	4472	G
37	52	4475	G
37	52	4476	C
37	52	4477	A
37	52	4480	A
37	52	4481	U

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Mol	Chain	Res	Type
37	52	4482	U
37	52	4497	U
37	52	4499	G
37	52	4500	U
37	52	4501	U
37	52	4507	A
37	52	4511	A
37	52	4512	U
37	52	4513	A
37	52	4519	C
37	52	4522	G
37	52	4524	G
37	52	4530	U
37	52	4531	U
37	52	4532	U
37	52	4548	A
37	52	4549	G
37	52	4552	U
37	52	4553	A
37	52	4554	G
37	52	4567	G
37	52	4570	G
37	52	4573	G
37	52	4575	G
37	52	4589	A
37	52	4590	A
37	52	4599	A
37	52	4604	G
37	52	4606	G
37	52	4634	U
37	52	4635	A
37	52	4636	U
37	52	4637	G
37	52	4639	G
37	52	4652	G
37	52	4654	C
37	52	4656	A
37	52	4657	U
37	52	4662	C
37	52	4670	C
37	52	4672	A
37	52	4673	U

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Mol	Chain	Res	Type
37	52	4677	U
37	52	4693	C
37	52	4694	G
37	52	4695	C
37	52	4700	A
37	52	4709	U
37	52	4716	C
37	52	4719	G
37	52	4720	C
37	52	4721	G
37	52	4726	G
37	52	4728	U
37	52	4738	C
37	52	4739	C
37	52	4740	G
37	52	4750	G
37	52	4751	G
37	52	4753	U
37	52	4754	G
37	52	4757	C
37	52	4759	C
37	52	4761	G
37	52	4764	A
37	52	4765	G
37	52	4766	C
37	52	4771	C
37	52	4772	C
37	52	4860	G
37	52	4862	G
37	52	4868	G
37	52	4870	G
37	52	4871	C
37	52	4872	G
37	52	4873	G
37	52	4874	A
37	52	4875	G
37	52	4876	A
37	52	4877	G
37	52	4882	U
37	52	4883	C
37	52	4885	U
37	52	4893	A

Continued on next page...

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Mol	Chain	Res	Type
37	52	4894	A
37	52	4895	C
37	52	4898	G
37	52	4904	G
37	52	4905	C
37	52	4906	C
37	52	4907	G
37	52	4908	G
37	52	4909	A
37	52	4910	A
37	52	4911	A
37	52	4912	G
37	52	4913	G
37	52	4914	G
37	52	4915	G
37	52	4918	C
37	52	4920	C
37	52	4921	C
37	52	4922	C
37	52	4923	U
37	52	4924	C
37	52	4926	C
37	52	4927	G
37	52	4928	C
37	52	4930	C
37	52	4931	G
37	52	4933	C
37	52	4935	C
37	52	4937	C
37	52	4938	A
37	52	4940	C
37	52	4943	A
37	52	4944	C
37	52	4945	G
37	52	4947	U
37	52	4949	G
37	52	4950	U
37	52	4951	G
37	52	4955	A
37	52	4956	A
37	52	4958	C
37	52	4959	U

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Mol	Chain	Res	Type
37	52	4964	C
37	52	4965	U
37	52	4966	A
37	52	4967	A
37	52	4976	U
37	52	4980	C
37	52	4988	U
37	52	4989	U
37	52	4990	C
37	52	5005	G
37	52	5009	G
37	52	5017	G
37	52	5018	C
37	52	5019	A
37	52	5022	U
37	52	5035	U
37	52	5040	U
37	52	5041	G
37	52	5043	A
37	52	5047	C
37	52	5048	A
37	52	5050	C
37	52	5053	U
37	52	5054	C
37	52	5055	G
37	52	5056	A
37	52	5058	A
37	52	5059	C
37	52	5061	A
37	52	5062	G
37	52	5069	U
38	72	2	U
38	72	3	C
38	72	6	C
38	72	7	G
38	72	11	A
38	72	17	C
38	72	21	G
38	72	22	A
38	72	23	A
38	72	24	C
38	72	25	G

Continued on next page...

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Mol	Chain	Res	Type
38	72	28	C
38	72	30	C
38	72	42	A
38	72	45	U
38	72	48	G
38	72	50	A
38	72	53	U
38	72	54	A
38	72	55	A
38	72	60	G
38	72	61	G
38	72	63	C
38	72	64	G
38	72	78	C
38	72	90	A
38	72	97	G
38	72	100	A
38	72	102	U
38	72	103	A
38	72	106	G
38	72	110	G
38	72	117	G
38	72	120	U
39	82	8	U
39	82	23	C
39	82	34	U
39	82	35	C
39	82	37	A
39	82	39	G
39	82	45	C
39	82	49	G
39	82	50	C
39	82	51	U
39	82	59	A
39	82	62	A
39	82	63	U
39	82	87	G
39	82	90	C
39	82	92	U
39	82	94	G
39	82	95	A
39	82	96	C

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Mol	Chain	Res	Type
39	82	102	G
39	82	103	A
39	82	105	C
39	82	109	C
39	82	110	U
39	82	111	U
39	82	114	G
39	82	117	C
39	82	118	C
39	82	119	C
39	82	120	G
39	82	121	G
39	82	122	G
39	82	123	U
39	82	124	U
39	82	125	C
39	82	126	C
39	82	127	U
39	82	128	C
39	82	137	A
39	82	143	G
39	82	150	C
39	82	153	C
39	82	156	U
80	23	7	G
80	23	8	U
80	23	9	A
80	23	13	U
80	23	14	A
80	23	20	U
80	23	21	A
80	23	31	C
80	23	32	C
80	23	37	A
80	23	46	G
80	23	47	U
80	23	49	C
80	23	53	G
80	23	59	A
80	23	61	C
80	23	65	G
80	23	67	G

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Mol	Chain	Res	Type
81	w3	38	A
81	w3	39	A
81	w3	42	C
81	w3	43	A
81	w3	45	A
81	w3	46	G
81	w3	49	U
81	w3	56	A
81	w3	58	A
81	w3	59	A

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	110	U
1	A1	182	C
1	A1	228	C
1	A1	241	G
1	A1	434	G
1	A1	465	A
1	A1	532	C
1	A1	553	U
1	A1	642	U
1	A1	688	U
1	A1	751	G
1	A1	870	A
1	A1	874	G
1	A1	1137	U
1	A1	1253	A
1	A1	1394	G
1	A1	1395	C
1	A1	1396	A
1	A1	1489	A
1	A1	1520	G
1	A1	1637	A
1	A1	1664	A
1	A1	1824	A
37	52	48	G
37	52	125	C
37	52	265	C
37	52	275	C
37	52	449	C

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Mol	Chain	Res	Type
37	52	480	C
37	52	498	C
37	52	504	G
37	52	930	G
37	52	959	G
37	52	966	A
37	52	971(A)	G
37	52	1106	A
37	52	1211	G
37	52	1238	A
37	52	1291	G
37	52	1329	G
37	52	1370	G
37	52	1445	U
37	52	1455	G
37	52	1979	A
37	52	1994	C
37	52	2046	G
37	52	2089	G
37	52	2502	A
37	52	2536	A
37	52	2875	C
37	52	3625	G
37	52	3876	A
37	52	3888	G
37	52	3939	G
37	52	3940	U
37	52	3959	U
37	52	3965	A
37	52	3968	U
37	52	4036	G
37	52	4157	A
37	52	4232	U
37	52	4448	G
37	52	4699	U
37	52	4719	G
37	52	4859	C
37	52	4884	G
37	52	4925	U
37	52	4936	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 310 ligands modelled in this entry, 308 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
90	SF4	k1	601	-	0,12,12	-	-	-		
90	SF4	k1	600	-	0,12,12	-	-	-		

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
90	SF4	k1	601	-	-	-	0/6/5/5
90	SF4	k1	600	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	52	37
1	A1	12
80	23	1
85	I3	1
78	s3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	52	2113:G	O3'	2258:C	P	42.99
1	52	1252:C	O3'	1271:G	P	36.84
1	52	1406(C):G	O3'	1411:C	P	19.26
1	52	1109:C	O3'	1161:G	P	17.69
1	52	3977:C	O3'	4034:G	P	16.37
1	52	1696:C	O3'	1720:C	P	16.22
1	52	4101:C	O3'	4107:G	P	15.99
1	52	990:C	O3'	1064:G	P	15.06
1	52	5022:U	O3'	5028:G	P	14.93
1	52	4777:C	O3'	4859:C	P	14.91
1	52	523:C	O3'	638:G	P	14.66
1	52	1364:U	O3'	1368:A	P	14.61
1	52	2901:G	O3'	3597:G	P	13.74
1	52	4138:C	O3'	4146:G	P	13.54
1	52	760:G	O3'	904:C	P	12.47
1	52	4729:A	O3'	4735:G	P	9.89
1	52	182:G	O3'	189:G	P	9.08
1	52	500:G	O3'	504:G	P	7.93
1	A1	745:C	O3'	746:C	P	7.34
1	52	512:U	O3'	515:C	P	7.27
1	52	3938:G	O3'	3939:G	P	6.79
1	52	3937:C	O3'	3938:G	P	6.76
1	52	4740:G	O3'	4743:G	P	6.72
1	A1	787:G	O3'	788:G	P	6.10
1	52	3948:C	O3'	3949:A	P	5.77
1	52	4899:G	O3'	4902:C	P	5.75

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	52	1222:A	O3'	1223:G	P	5.52
1	23	16:C	O3'	18:G	P	5.52
1	52	3942:A	O3'	3943:A	P	5.07
1	52	1219:G	O3'	1220:G	P	4.89
1	A1	225:G	O3'	226:A	P	4.57
1	52	1221:G	O3'	1222:A	P	4.51
1	52	3947:A	O3'	3948:C	P	4.39
1	52	170:C	O3'	171:U	P	4.17
1	52	5020:G	O3'	5021:C	P	4.08
1	A1	748:C	O3'	749:U	P	4.02
1	A1	322:C	O3'	323:C	P	3.93
1	A1	747:U	O3'	748:C	P	3.87
1	A1	286:U	O3'	287:U	P	3.86
1	A1	304:C	O3'	305:U	P	3.66
1	A1	903:A	O3'	904:A	P	3.65
1	52	1239:C	O3'	1244:G	P	3.53
1	52	1088:C	O3'	1089:G	P	3.45
1	A1	309:G	O3'	310:C	P	3.43
1	A1	902:G	O3'	903:A	P	3.29
1	52	1438:U	O3'	1440:U	P	3.24
1	52	751:G	O3'	752:G	P	3.23
1	A1	1295:A	O3'	1296:U	P	3.20
1	52	267:G	O3'	268:G	P	3.20
1	52	4076:G	O3'	4077:A	P	3.11
1	I3	203:ARG	C	204:GLY	N	1.96
1	s3	186:GLY	C	187:LEU	N	1.66

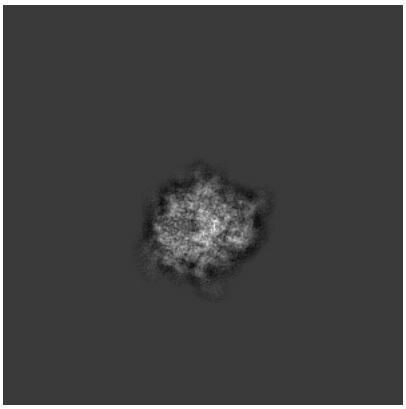
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0195. These allow visual inspection of the internal detail of the map and identification of artifacts.

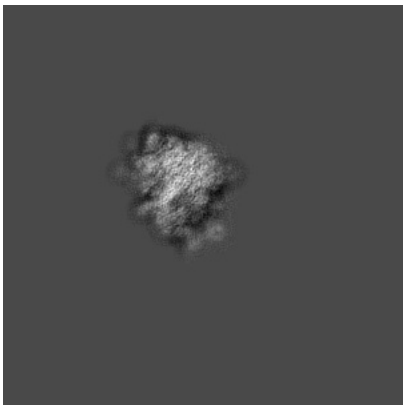
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

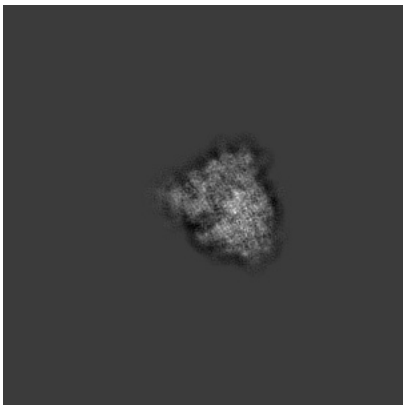
6.1.1 Primary map



X

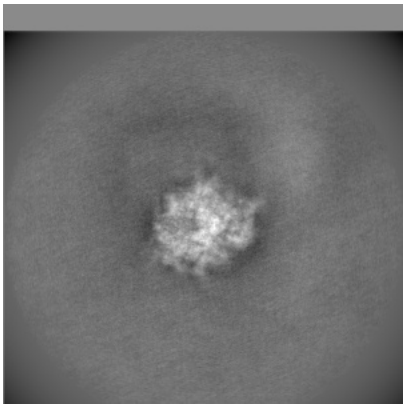


Y

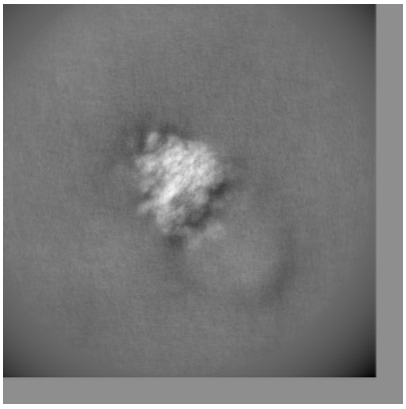


Z

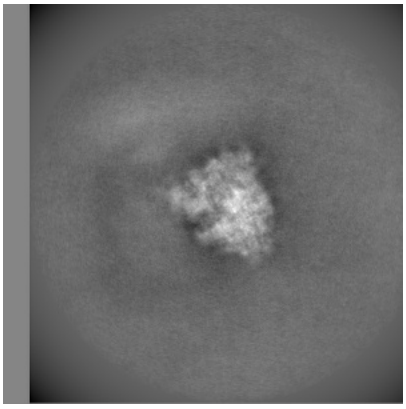
6.1.2 Raw map



X



Y

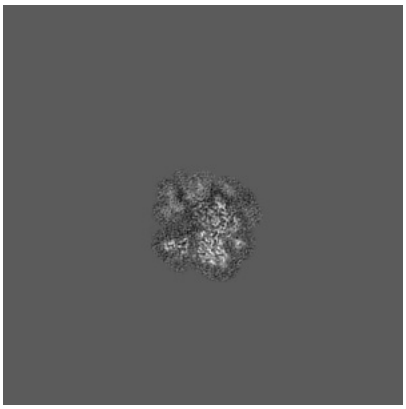


Z

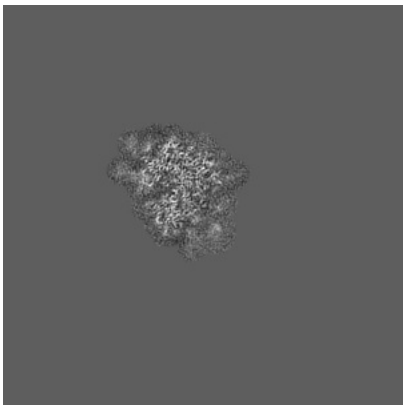
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

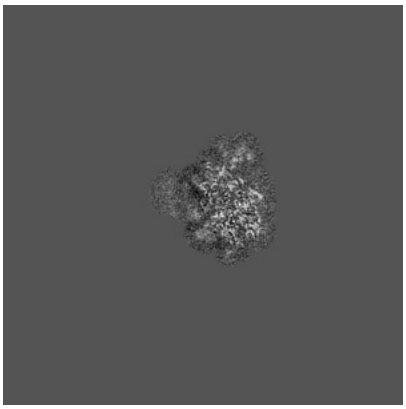
6.2.1 Primary map



X Index: 250

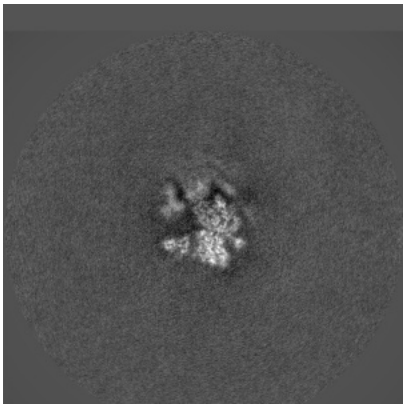


Y Index: 250

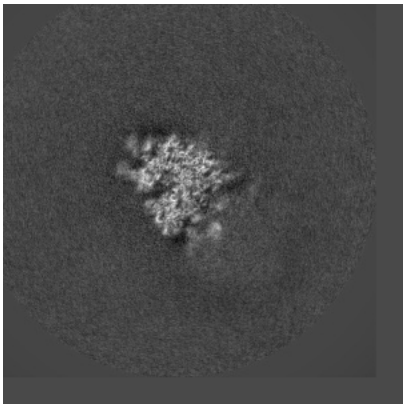


Z Index: 250

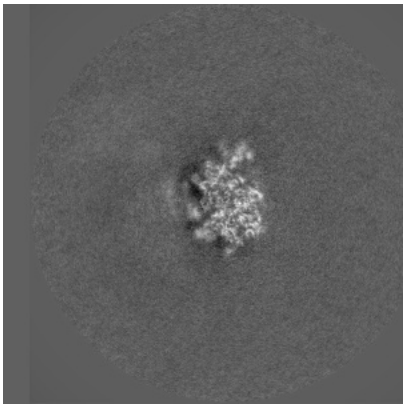
6.2.2 Raw map



X Index: 250



Y Index: 250

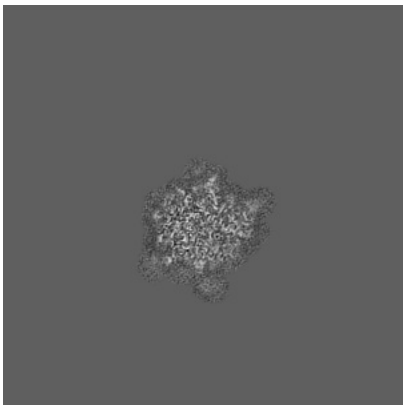


Z Index: 250

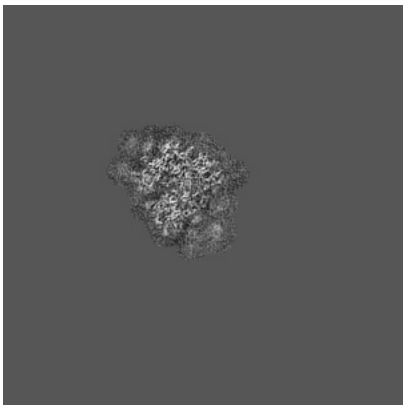
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

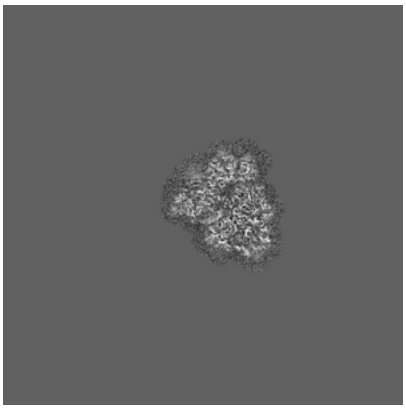
6.3.1 Primary map



X Index: 293

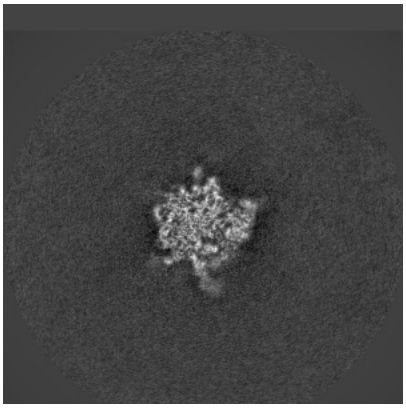


Y Index: 251

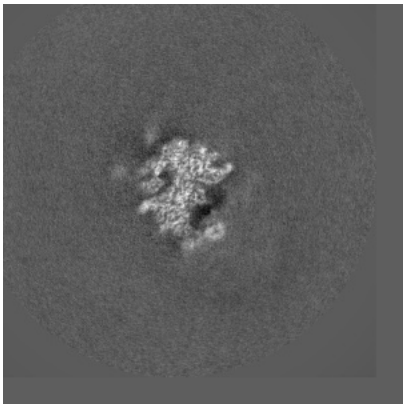


Z Index: 208

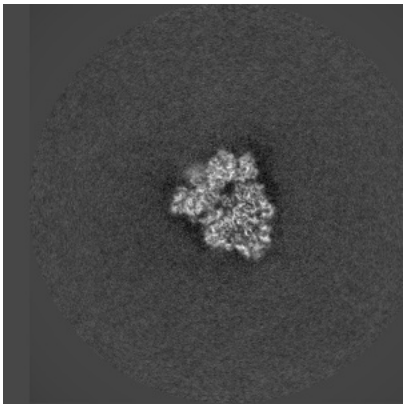
6.3.2 Raw map



X Index: 290



Y Index: 264



Z Index: 207

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

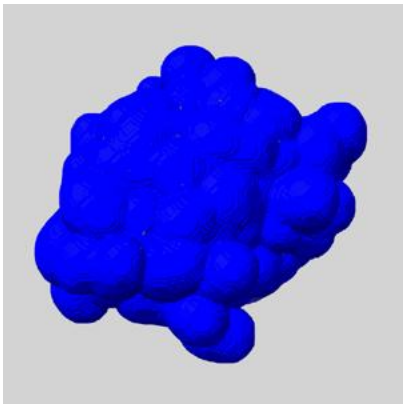
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

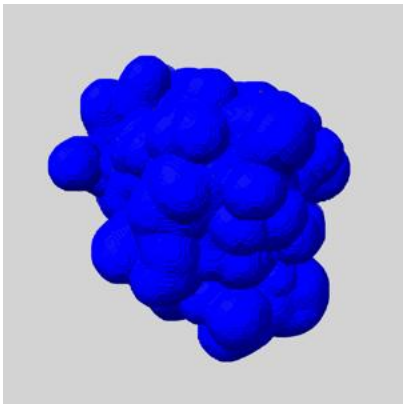
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

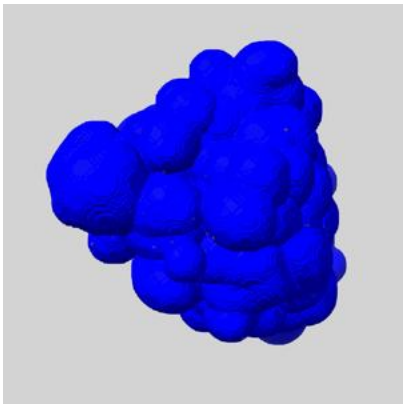
6.5.1 emd_0195_msk_1.map (i)



X



Y

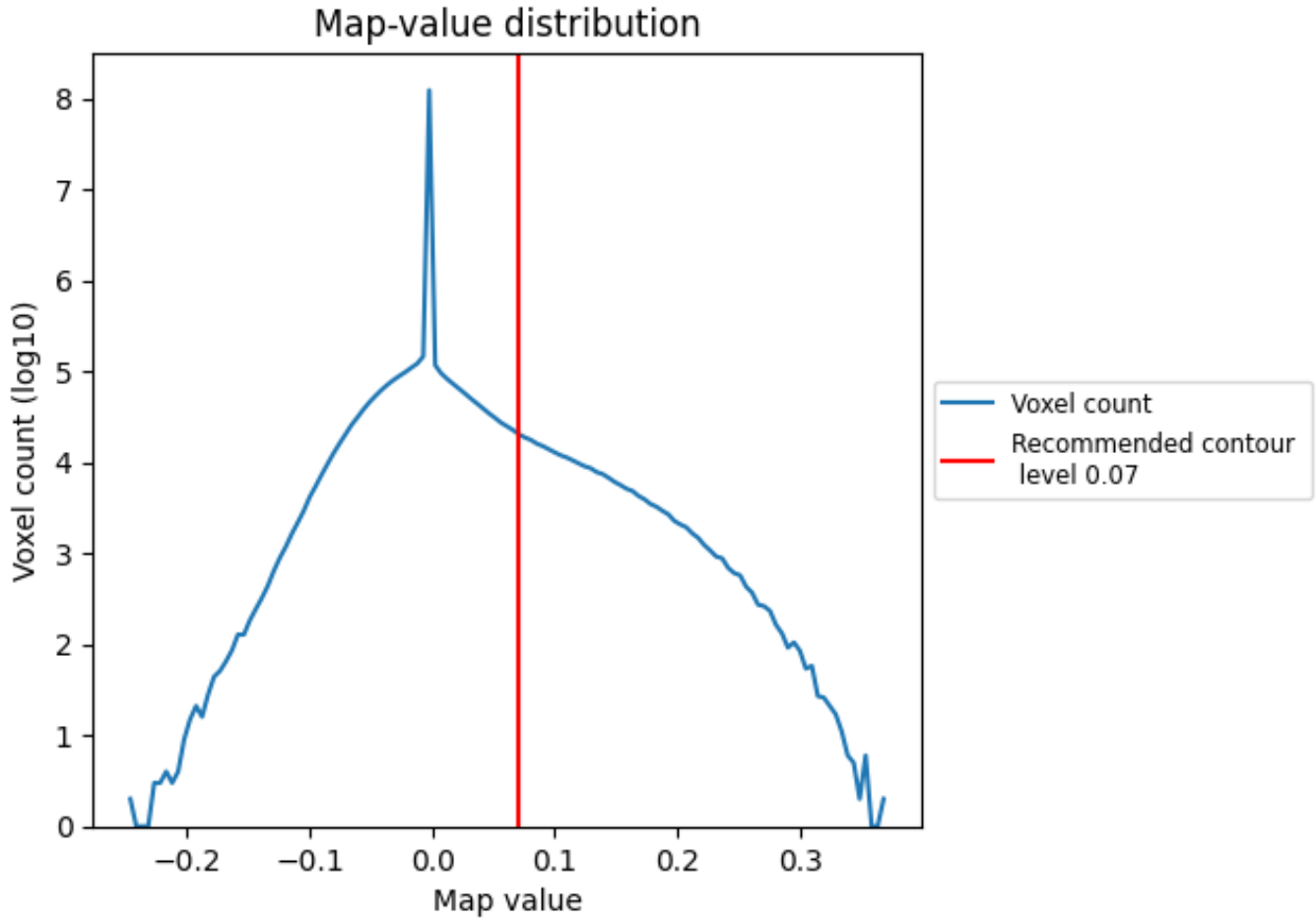


Z

7 Map analysis

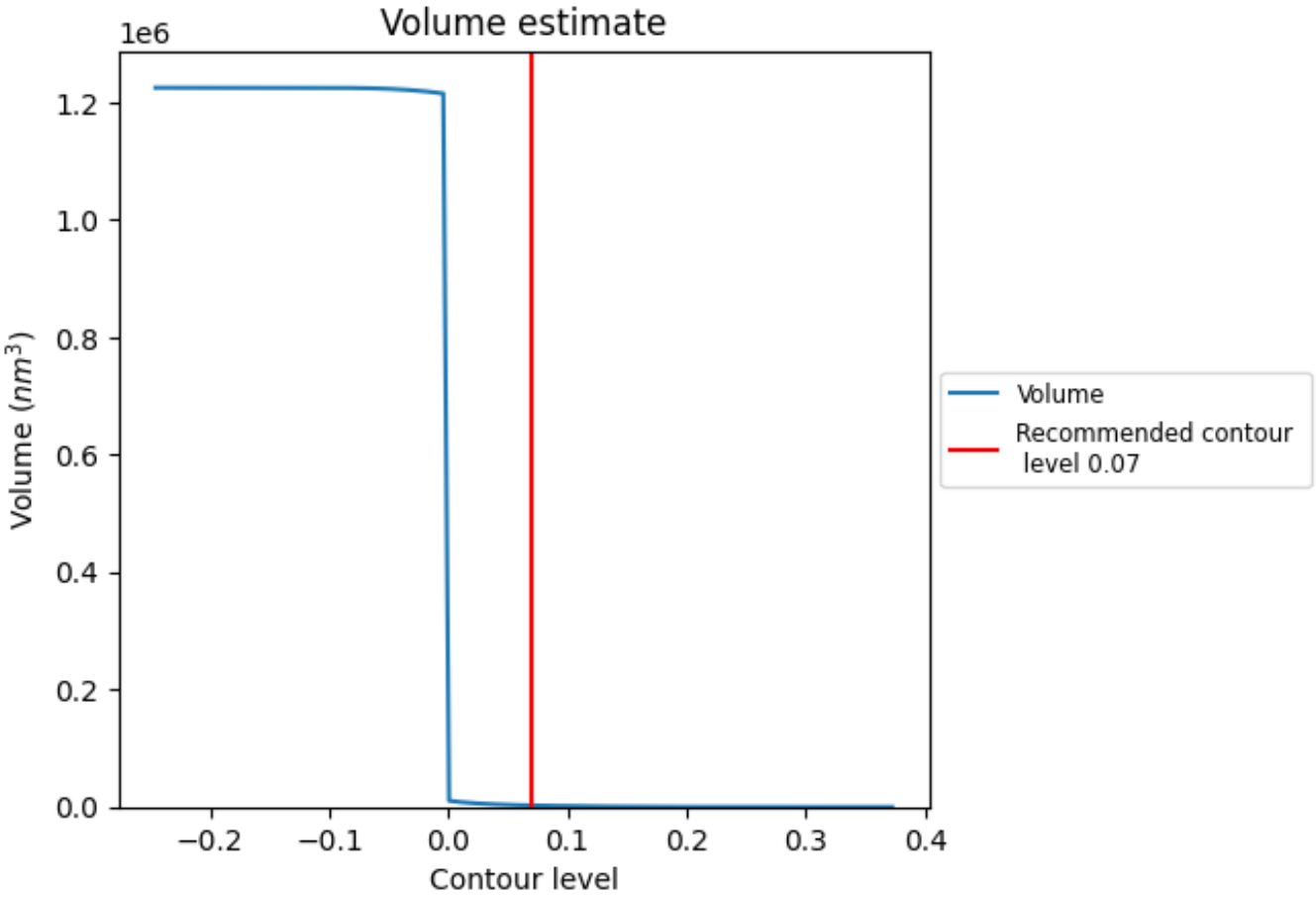
This section contains the results of statistical analysis of the map.

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.

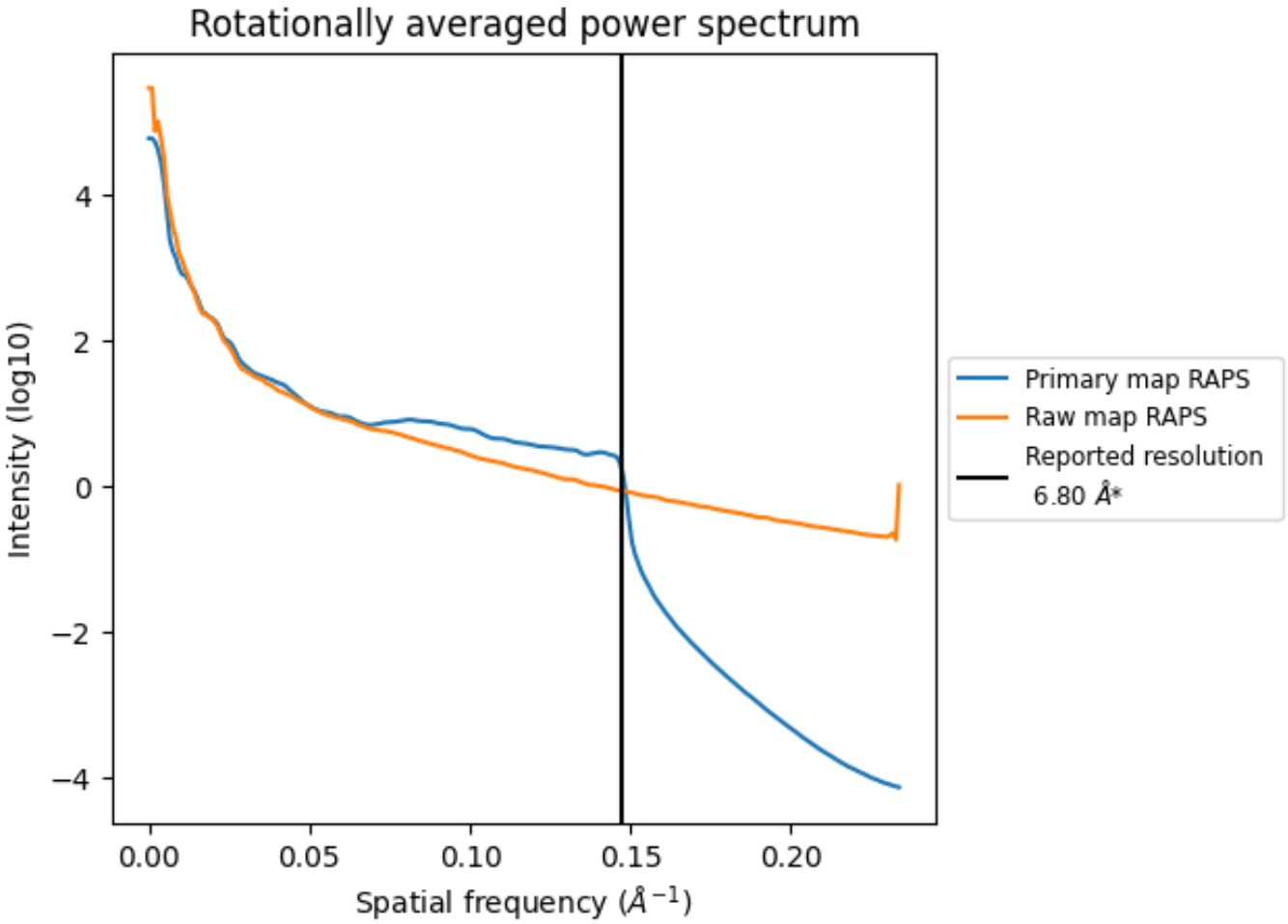
7.2 Volume estimate



The volume at the recommended contour level is 2563 nm^3; this corresponds to an approximate mass of 2315 kDa.

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

7.3 Rotationally averaged power spectrum (i)

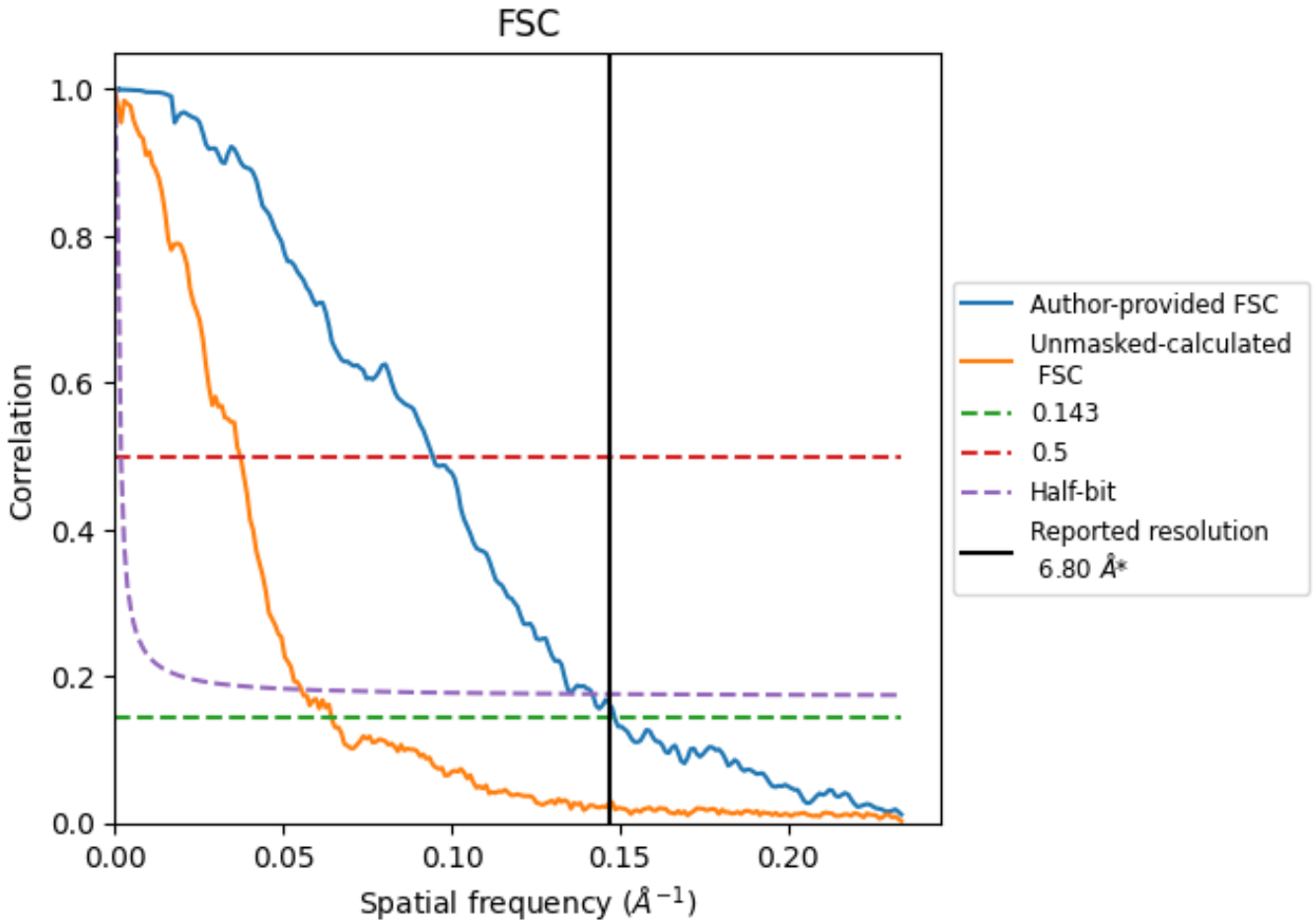


*Reported resolution corresponds to spatial frequency of 0.147 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.147 Å^{-1}

8.2 Resolution estimates (i)

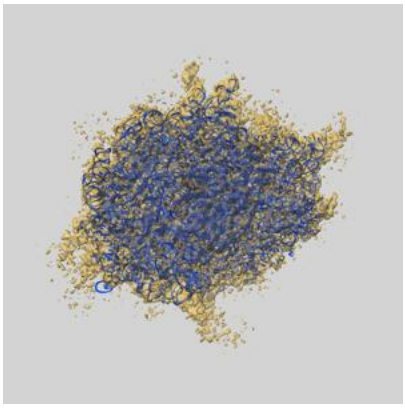
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.80	-	-
Author-provided FSC curve	6.73	10.59	7.05
Unmasked-calculated*	15.53	26.81	18.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 15.53 differs from the reported value 6.8 by more than 10 %

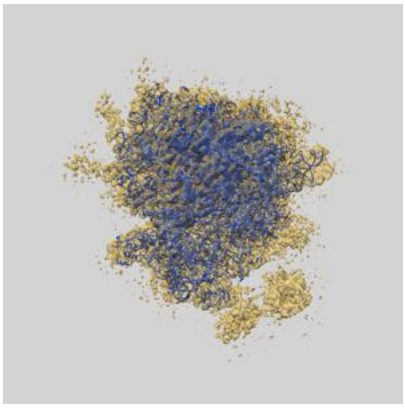
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0195 and PDB model 6HCM. Per-residue inclusion information can be found in section 3 on page 22.

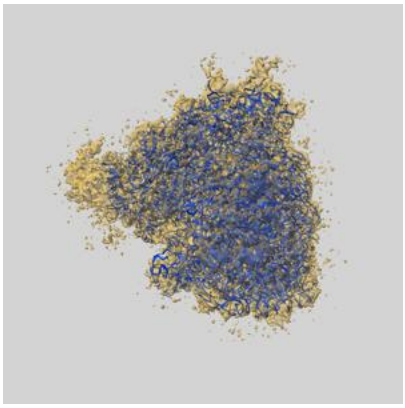
9.1 Map-model overlay



X



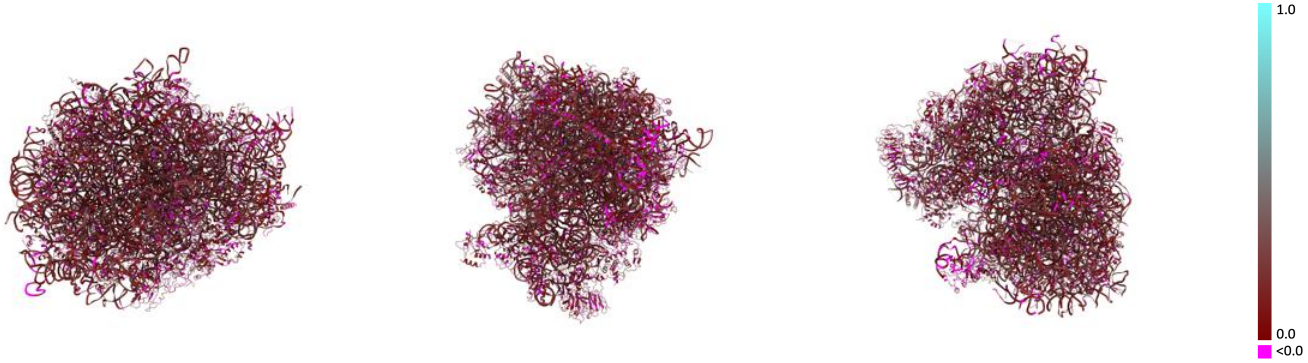
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

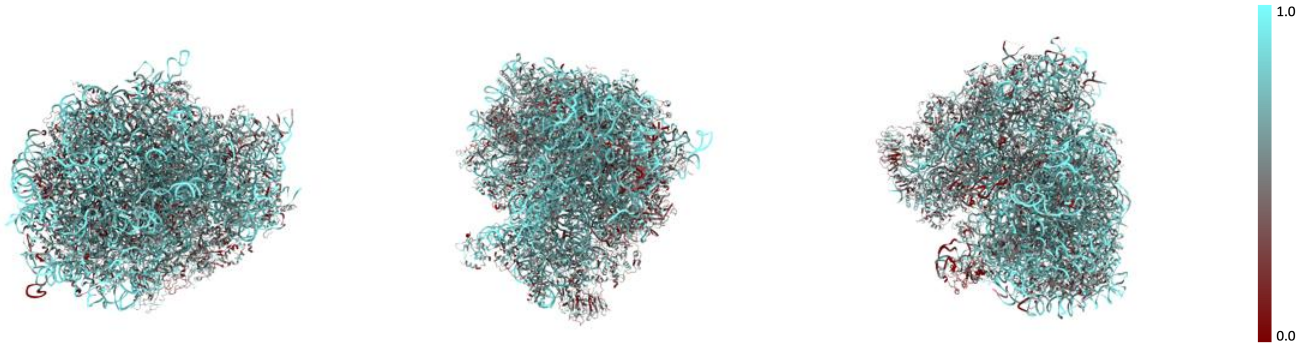
9.2 Q-score mapped to coordinate model



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.

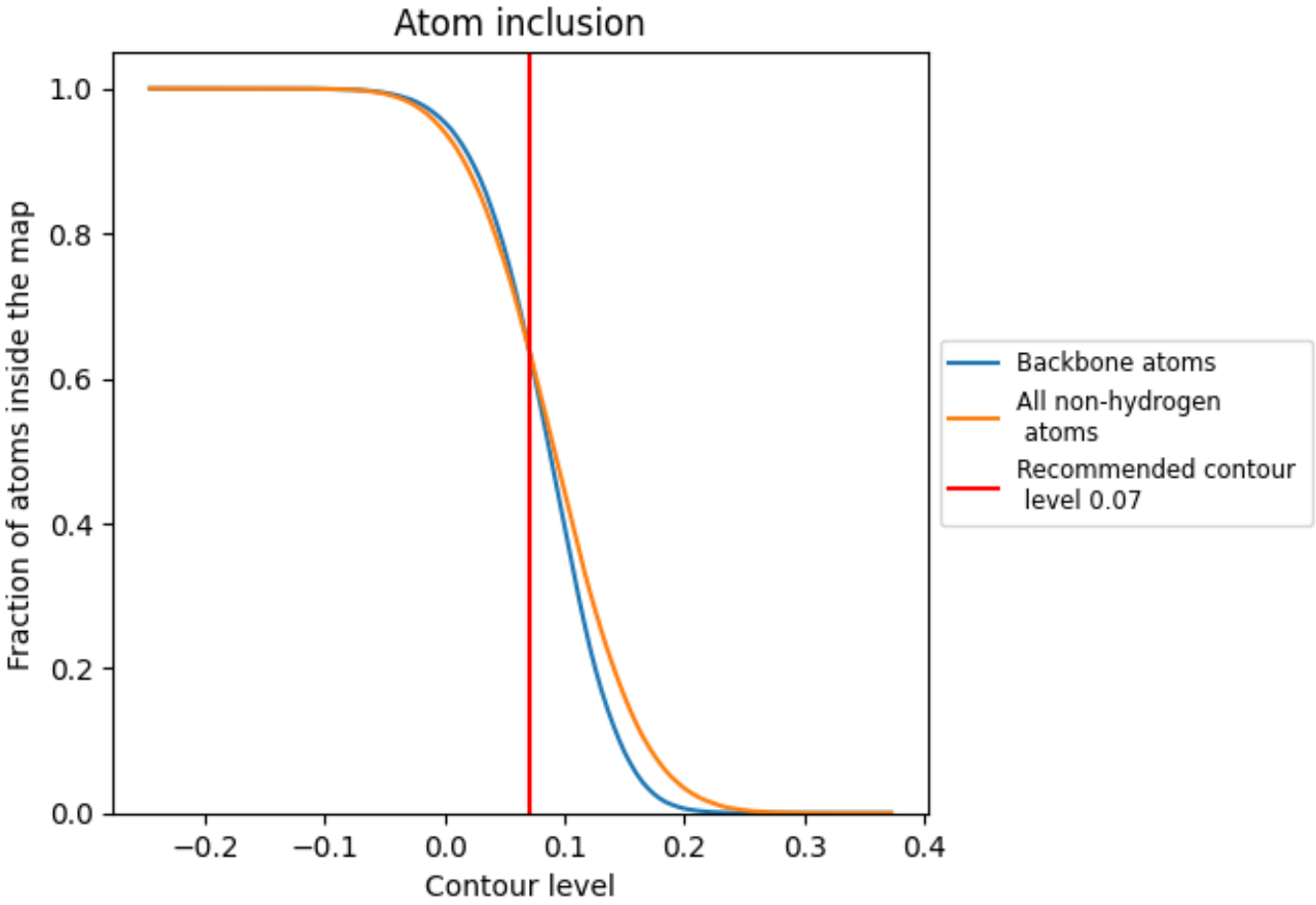
9.3 Atom inclusion mapped to coordinate model



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 64% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6430	0.1560
1	0.3818	0.2540
23	0.8379	0.1860
52	0.7755	0.1840
72	0.8573	0.1930
82	0.7815	0.1910
A1	0.8008	0.1860
A3	0.3995	0.1180
B1	0.5045	0.1410
B3	0.5100	0.1250
C1	0.3843	0.1360
C3	0.4490	0.1210
D1	0.5042	0.1390
D3	0.6498	0.1380
E1	0.5009	0.1310
E3	0.5313	0.1480
F1	0.5086	0.1320
F3	0.4768	0.1160
G1	0.4836	0.1100
G3	0.4953	0.1370
H1	0.5175	0.1190
H3	0.5210	0.1440
I1	0.4928	0.1200
I3	0.5112	0.1390
J1	0.4677	0.1170
J3	0.5988	0.1310
K1	0.5904	0.1370
L1	0.5418	0.1290
L3	0.5190	0.1400
M1	0.3742	0.1340
M3	0.6005	0.1400
N1	0.5391	0.1050
N3	0.4741	0.1140
O1	0.4683	0.1380
O3	0.5238	0.1390

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Chain	Atom inclusion	Q-score
P1	0.3759	0.1270
P3	0.4855	0.1130
Q1	0.5751	0.1100
Q3	0.4545	0.1380
R1	0.4505	0.1160
R3	0.4976	0.0900
S1	0.4374	0.1370
S3	0.5057	0.1360
T1	0.5153	0.1230
T3	0.5051	0.1470
U1	0.5333	0.1170
U3	0.5841	0.1070
V1	0.4884	0.1300
V3	0.4029	0.1360
W1	0.4373	0.1090
W3	0.4681	0.0970
X1	0.4535	0.1250
X3	0.4766	0.1340
Y1	0.5107	0.1410
Y3	0.6076	0.1250
Z1	0.6340	0.1340
Z3	0.3849	0.0220
a1	0.4425	0.1270
a3	0.4969	0.1220
b1	0.4463	0.1270
b3	0.4626	0.1180
c1	0.3521	0.1230
c3	0.3696	0.0290
d1	0.5064	0.1370
d3	0.5228	0.1210
e1	0.5271	0.1260
e3	0.4710	0.1410
f1	0.5423	0.1390
f3	0.4335	0.1350
g1	0.6580	0.1120
g3	0.3674	0.0690
h1	0.4136	0.1270
h3	0.5117	0.1120
i3	0.4887	0.1140
j1	0.4506	0.1310
j3	0.5067	0.1090
k1	0.4340	0.1300

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Chain	Atom inclusion	Q-score
k3	0.4075	0.0340
l3	0.5176	0.1500
m3	0.5433	0.1360
n3	0.4908	0.1060
o3	0.5751	0.1300
p3	0.5181	0.1170
r3	0.4462	0.1340
s3	0.3872	0.0720
t3	0.4490	0.1160
u3	0.1266	0.0230
w3	0.5850	0.1600