Full wwPDB EM Validation Report (i)

Dec 11, 2022 – 08:14 am GMT

PDB ID	:	4D67
EMDB ID	:	EMD-2813
Title	:	Cryo-EM structures of ribosomal 80S complexes with termination factors and cricket paralysis virus IRES reveal the IRES in the translocated state
Authors	:	Muhs, M.; Hilal, T.; Mielke, T.; Skabkin, M.A.; Sanbonmatsu, K.Y.; Pestova, T.V.; Spahn, C.M.T.
Deposited on	:	2014-11-10
Resolution	:	9.00 Å(reported)
Based on initial model	:	4CXD

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 (i) 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 (i)) were used in the production of this report:

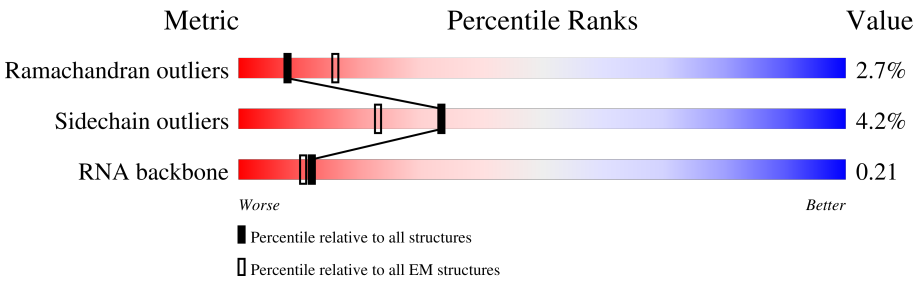
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	257	20% 93% • •
2	B	403	13% 90% 7% •
3	C	427	11% 78% 6% • 15%
4	D	297	15% 93% • •
5	E	288	15% 50% 5% 45%
6	F	248	12% 90% • 6%
7	G	266	17% 83% 5% • 12%
8	H	192	9% 95% 5%

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Mol	Chain	Length	Quality of chain
9	I	214	14% 86% 6% 8%
10	J	178	10% 85% 10%
11	L	211	20% 84% 9% 5%
12	M	215	11% 62% 35%
13	N	204	15% 98%
14	O	203	10% 94%
15	P	184	10% 78% 5% 17%
16	Q	188	19% 92% 6%
17	R	196	15% 86% 7% 7%
18	S	176	13% 91% 7%
19	T	160	19% 95%
20	U	128	13% 77% 20%
21	V	140	19% 89% 9%
22	W	157	5% 39% 59%
23	X	156	16% 75% 24%
24	Y	145	8% 83% 6% 12%
25	Z	136	18% 93% 7%
26	a	148	16% 94% 5%
27	b	159	8% 40% 57%
28	c	115	17% 88% 10%
29	d	125	7% 83% 13%
30	e	135	20% 90% 5%
31	f	110	19% 86% 10%
32	g	117	15% 87% 10%
33	h	123	14% 94% 5%

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Mol	Chain	Length	Quality of chain
34	i	105	11% 83% 8% 8%
35	j	97	6% 84% 12%
36	k	70	24% 97%
37	l	51	6% 94%
38	m	128	9% 38% 59%
39	n	25	100%
40	o	106	25% 93% 7%
41	p	92	14% 93% 5%
42	t	137	20% 86% 7% 5%
43	u	210	40% 92% 8%
44	2	5025	30% 41% 28%
45	3	194	39% 41% 19%
46	4	121	40% 56%

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 136495 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S RIBOSOMAL PROTEIN L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	247	1888	1183	388	311	6	0	1

- Molecule 2 is a protein called 60S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	396	3190	2030	601	545	14	0	1

- Molecule 3 is a protein called 60S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	364	2889	1817	578	480	14	0	1

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	290	2361	1489	431	427	14	0	0

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	158	1286	834	238	214	0	0

- Molecule 6 is a protein called 60S RIBOSOMAL PROTEIN L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	234	1949	1252	376	312	9	0	0

- Molecule 7 is a protein called 60S RIBOSOMAL PROTEIN L7A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	235	1881	1197	363	317	4	0	1

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	192	1535	965	286	278	6	0	0

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	196	1604	1022	308	262	12	0	0

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L11.

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

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	200	1617	1013	335	265	4	0	1

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	140	1139	730	219	183	7	0	1

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	204	1708	1077	360	266	5	0	0

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	196	1607	1034	316	252	5	0	1

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	153	1234	771	241	213	9	0	1

- Molecule 16 is a protein called 60S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	184	1493	933	311	244	5	0	0

- Molecule 17 is a protein called 60S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	R	183	1526	943	331	242	10	0	1

- Molecule 18 is a protein called 60S RIBOSOMAL PROTEIN L18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	173	1438	916	280	232	10	0	0

- Molecule 19 is a protein called 60S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	159	1297	823	252	216	6	0	0

- Molecule 20 is a protein called 60S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	U	102	827	529	146	150	2	0	1

- Molecule 21 is a protein called 60S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	128	963	610	181	167	5	0	0

- Molecule 22 is a protein called 60S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	64	529	337	104	85	3	0	1

- Molecule 23 is a protein called 60S RIBOSOMAL PROTEIN L23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	119	975	624	183	167	1	0	0

- Molecule 24 is a protein called 60S RIBOSOMAL PROTEIN L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	128	1065	668	217	177	3	0	1

- Molecule 25 is a protein called 60S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Z	136	1114	719	209	182	4	0	0

- Molecule 26 is a protein called 60S RIBOSOMAL PROTEIN L27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	a	147	1161	736	237	185	3	0	0

- Molecule 27 is a protein called 60S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b	69	560	344	123	90	3	0	1

- Molecule 28 is a protein called 60S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	104	802	508	142	145	7	0	1

- Molecule 29 is a protein called 60S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	109	904	570	174	158	2	0	0

- Molecule 30 is a protein called 60S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	e	128	1053	664	219	165	5	0	1

- Molecule 31 is a protein called 60S RIBOSOMAL PROTEIN L35A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	f	107	865	550	172	140	3	0	0

- Molecule 32 is a protein called 60S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	115	907	566	188	147	6	0	1

- Molecule 33 is a protein called 60S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	122	1014	641	205	167	1	0	0

- Molecule 34 is a protein called 60S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	i	97	783	488	168	122	5	0	1

- Molecule 35 is a protein called 60S RIBOSOMAL PROTEIN L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	j	85	690	423	153	109	5	0	1

- Molecule 36 is a protein called 60S RIBOSOMAL PROTEIN L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	k	69	568	366	103	98	1	0	0

- Molecule 37 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	l	50	443	281	98	63	1	0	0

- Molecule 38 is a protein called UBIQUITIN-60S RIBOSOMAL PROTEIN L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	m	52	428	266	90	66	6	0	0

- Molecule 39 is a protein called 60S RIBOSOMAL PROTEIN L41.

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

- Molecule 40 is a protein called 60S RIBOSOMAL PROTEIN L36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	o	106	870	547	176	140	7	0	0

- Molecule 41 is a protein called 60S RIBOSOMAL PROTEIN L37A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	p	91	707	445	136	119	7	0	0

- Molecule 42 is a protein called 60S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	t	130	1043	646	220	172	5	0	1

- Molecule 43 is a protein called 60S RIBOSOMAL PROTEIN L10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	u	210	1621	990	278	347	6	0	0

- Molecule 44 is a RNA chain called 28S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
44	2	3616	77488	34508	14153	25212	3615	0	0

- Molecule 45 is a RNA chain called 5.8S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
45	3	157	3334	1489	587	1102	156	0	0

- Molecule 46 is a RNA chain called 5S RRNA.

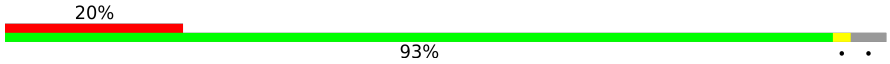
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	4	119	2538	1132	454	834	118	0	0

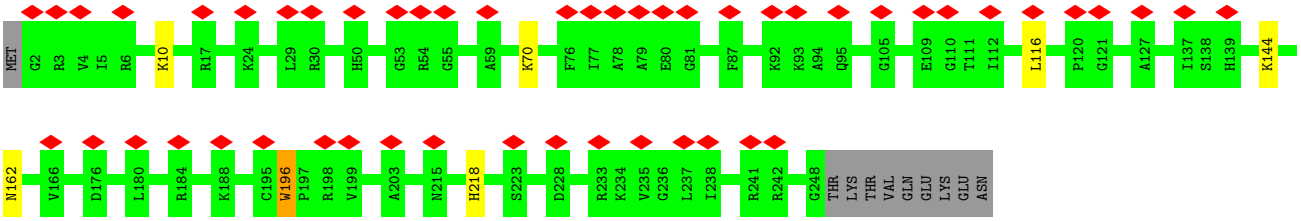
3 Residue-property plots (i)

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: 60S RIBOSOMAL PROTEIN L8

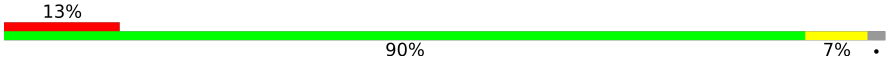
Chain A:

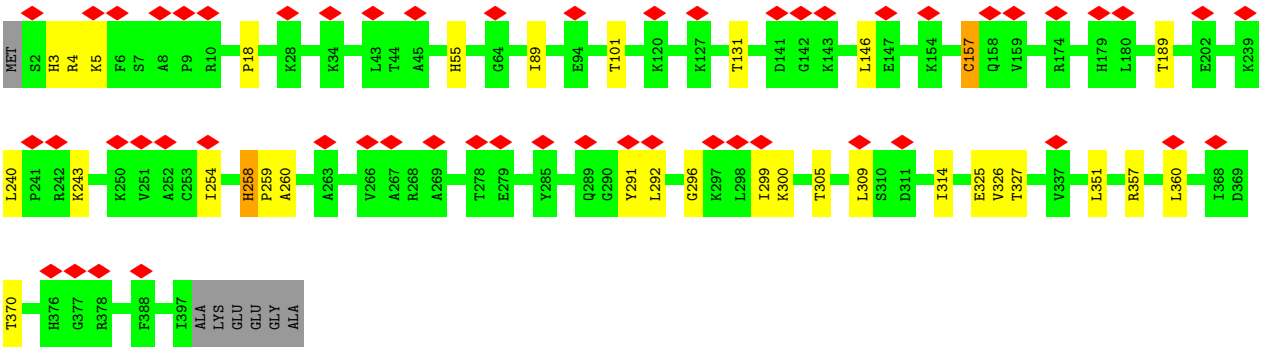




- Molecule 2: 60S RIBOSOMAL PROTEIN L3

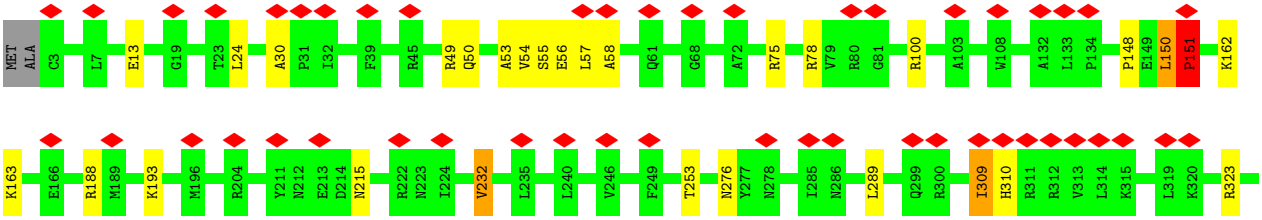
Chain B:

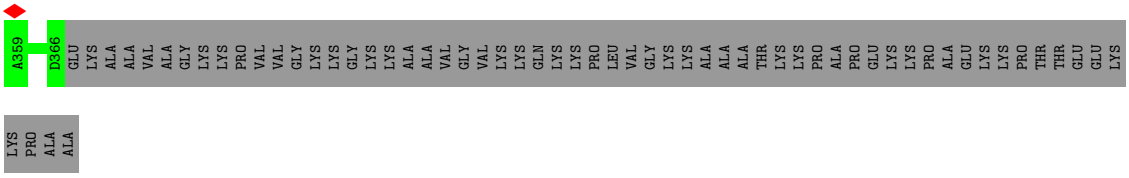




- Molecule 3: 60S RIBOSOMAL PROTEIN L4

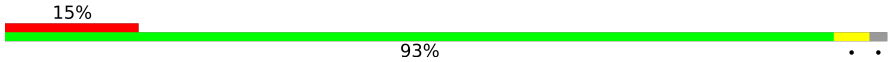
Chain C:

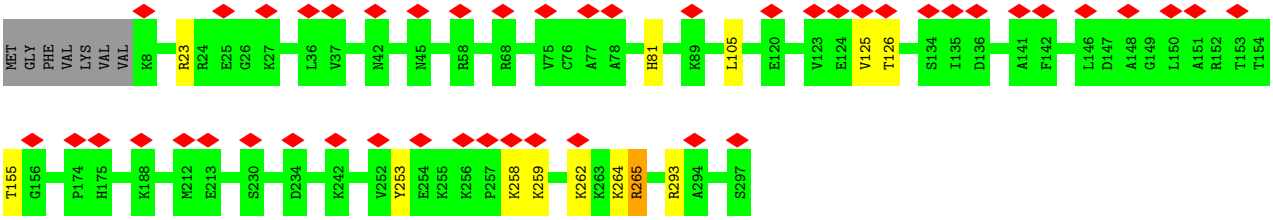




• Molecule 4: 60S RIBOSOMAL PROTEIN L5

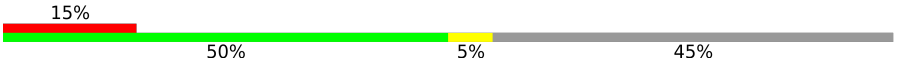
Chain D:

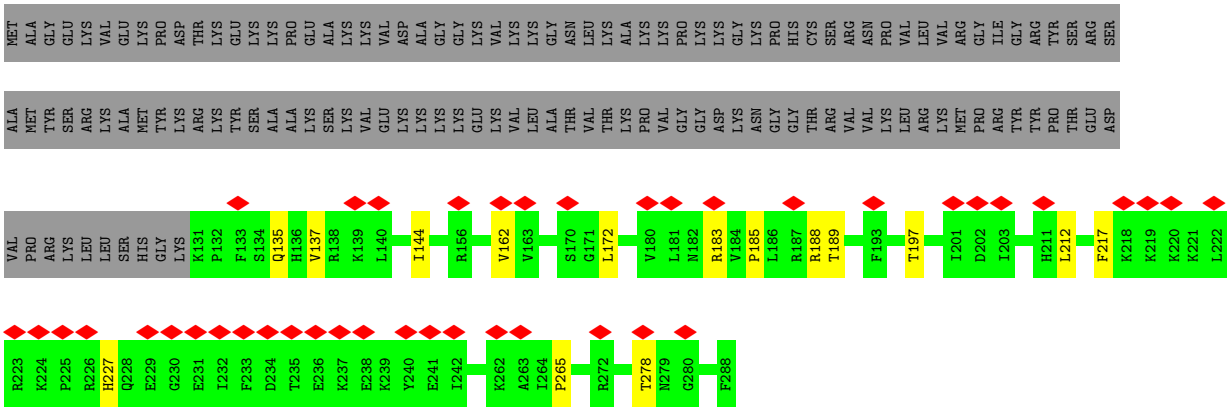




• Molecule 5: 60S RIBOSOMAL PROTEIN L6

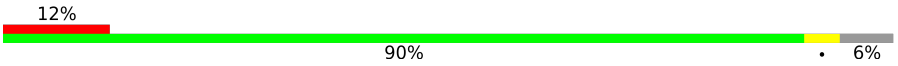
Chain E:

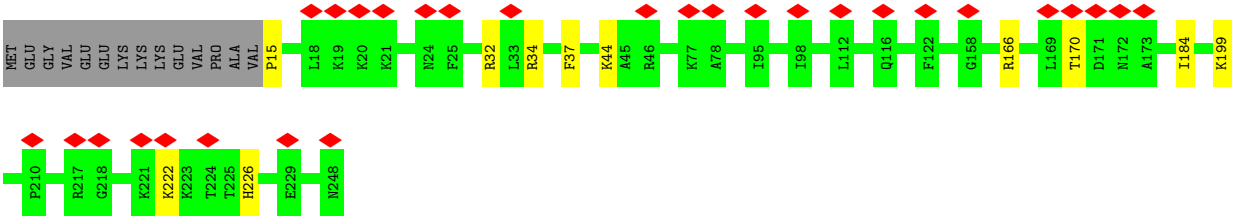




• Molecule 6: 60S RIBOSOMAL PROTEIN L7

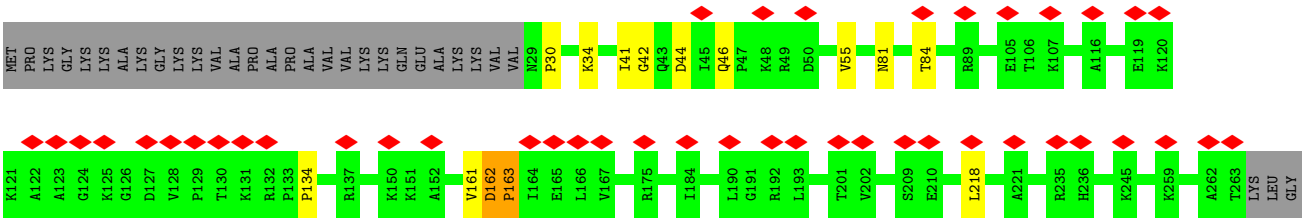
Chain F:





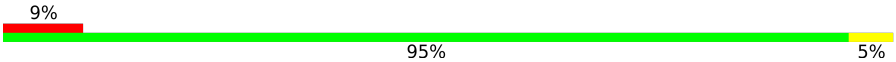
• Molecule 7: 60S RIBOSOMAL PROTEIN L7A

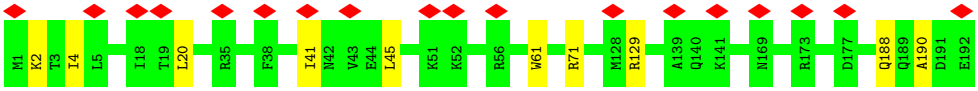
Chain G:



- Molecule 8: 60S RIBOSOMAL PROTEIN L9

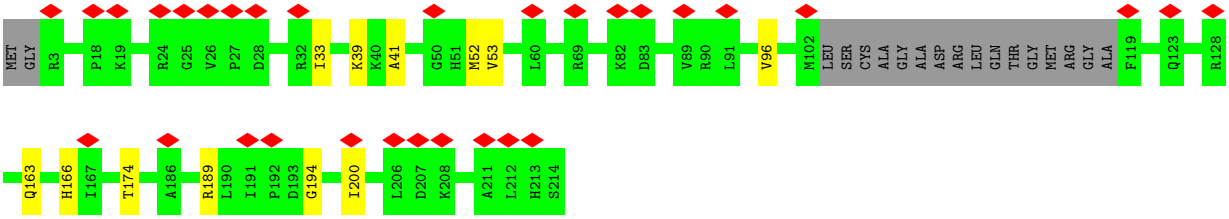
Chain H:





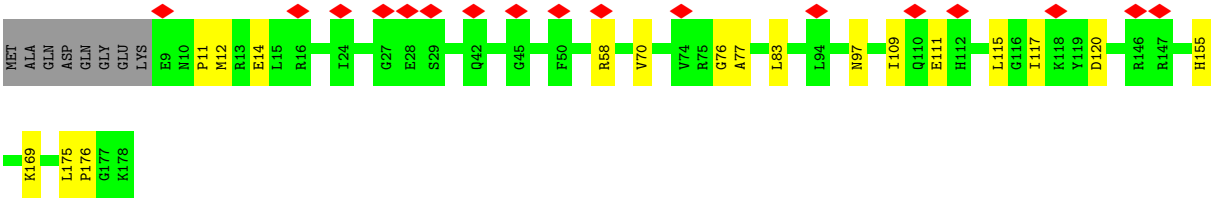
- Molecule 9: 60S RIBOSOMAL PROTEIN L10

Chain I:



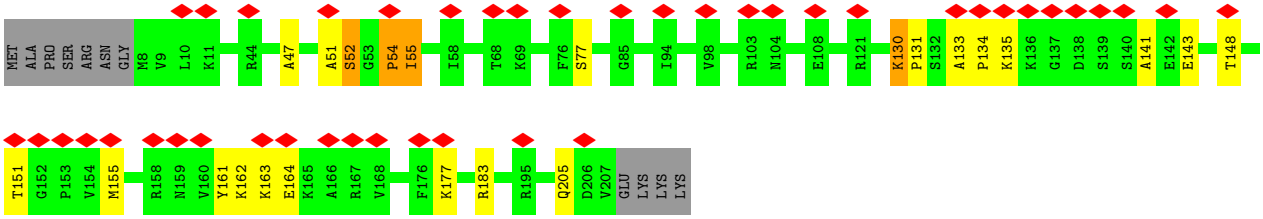
- Molecule 10: 60S RIBOSOMAL PROTEIN L11

Chain J:



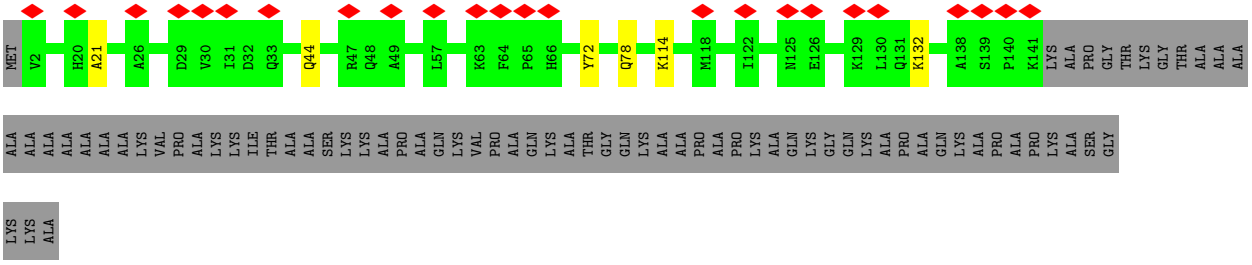
- Molecule 11: 60S RIBOSOMAL PROTEIN L13

Chain L:



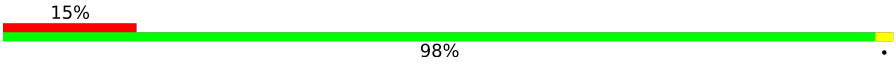
- Molecule 12: 60S RIBOSOMAL PROTEIN L14

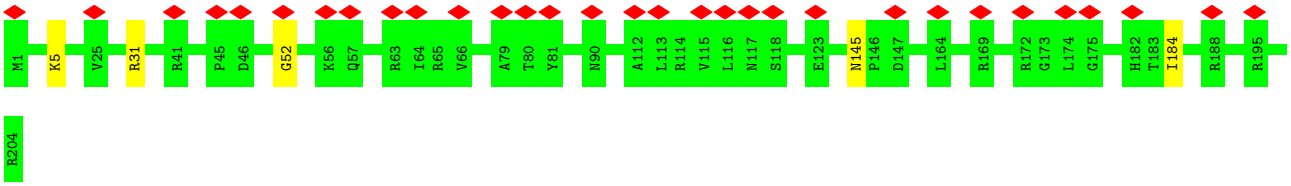
Chain M:



- Molecule 13: 60S RIBOSOMAL PROTEIN L15

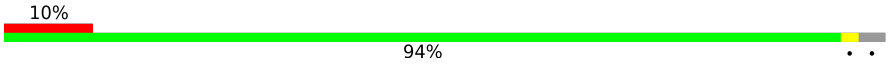
Chain N:

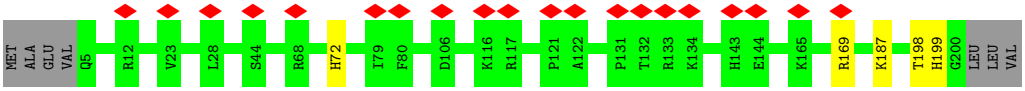




- Molecule 14: 60S RIBOSOMAL PROTEIN L13A

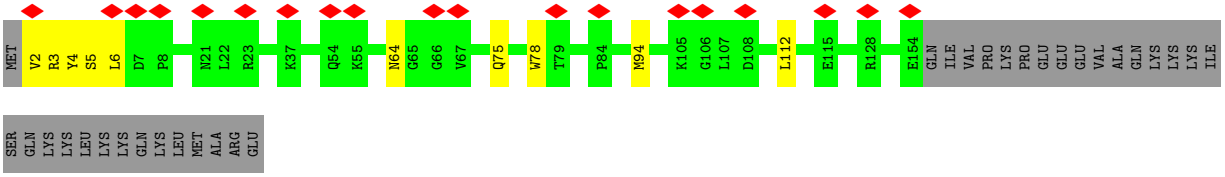
Chain O:





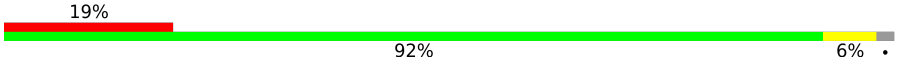
- Molecule 15: 60S RIBOSOMAL PROTEIN L17

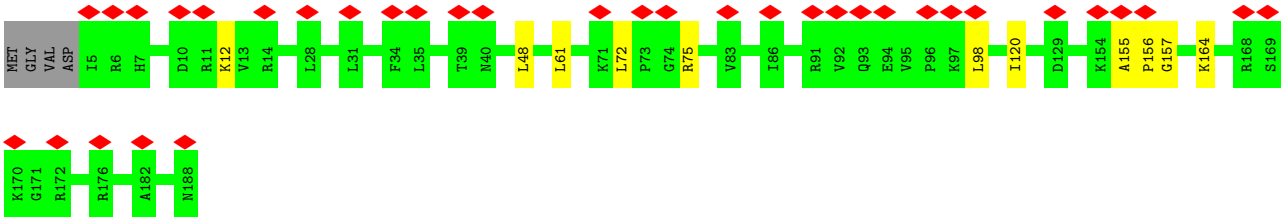
Chain P:



- Molecule 16: 60S RIBOSOMAL PROTEIN L18

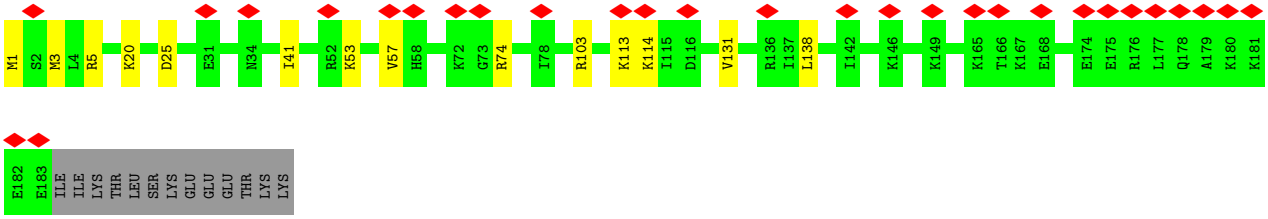
Chain Q:





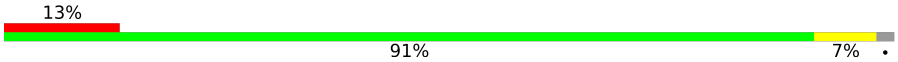
- Molecule 17: 60S RIBOSOMAL PROTEIN L19

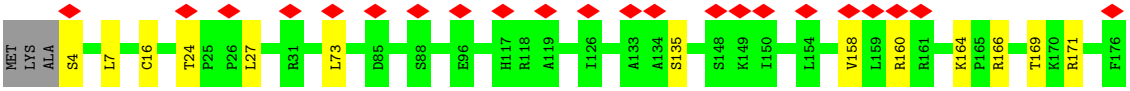
Chain R:



• Molecule 18: 60S RIBOSOMAL PROTEIN L18A

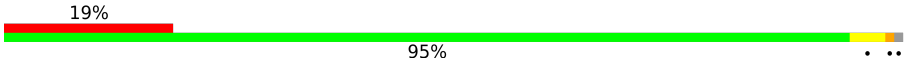
Chain S:

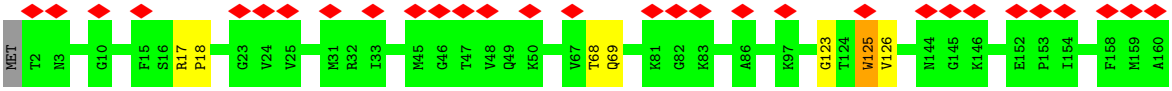




• Molecule 19: 60S RIBOSOMAL PROTEIN L21

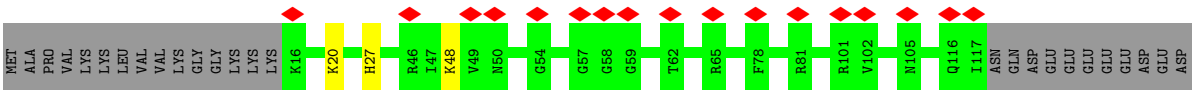
Chain T:





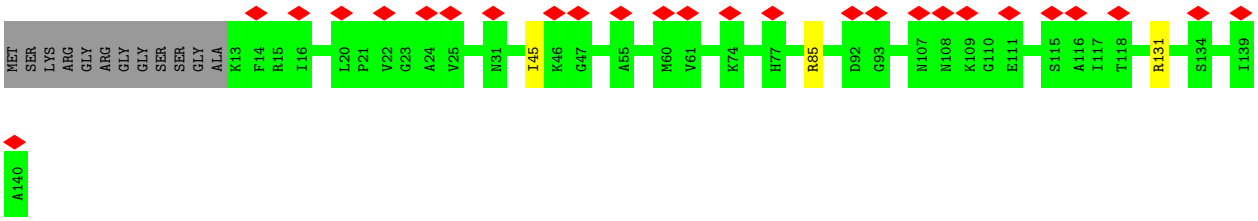
• Molecule 20: 60S RIBOSOMAL PROTEIN L22

Chain U:



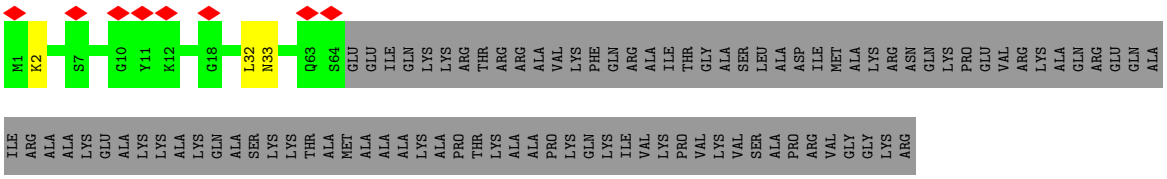
• Molecule 21: 60S RIBOSOMAL PROTEIN L23

Chain V:



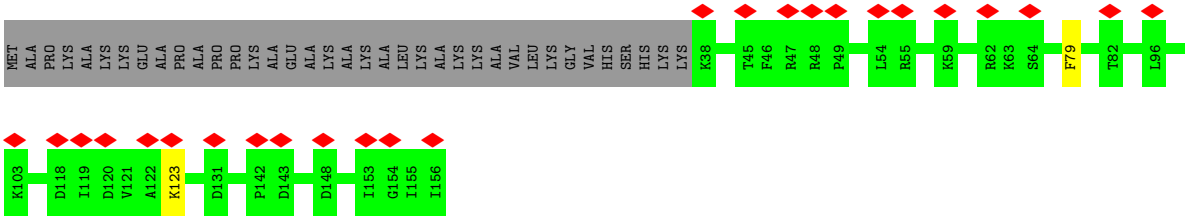
• Molecule 22: 60S RIBOSOMAL PROTEIN L24

Chain W:



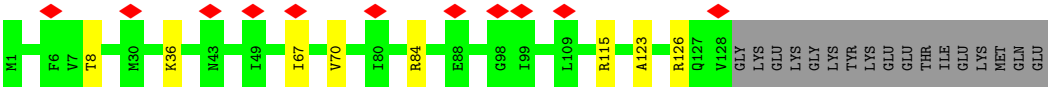
• Molecule 23: 60S RIBOSOMAL PROTEIN L23A

Chain X:



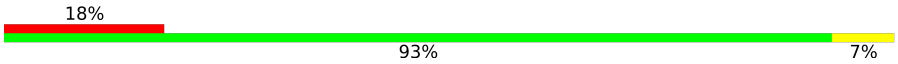
• Molecule 24: 60S RIBOSOMAL PROTEIN L26

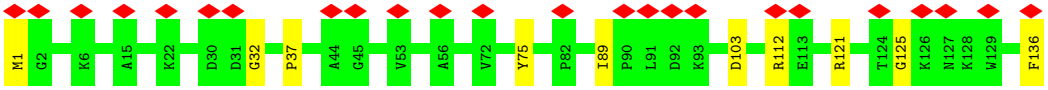
Chain Y:



• Molecule 25: 60S RIBOSOMAL PROTEIN L27

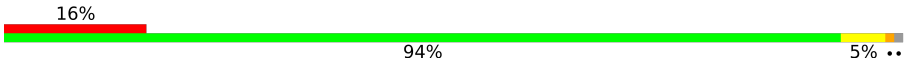
Chain Z:

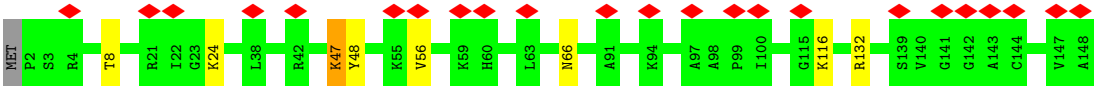




• Molecule 26: 60S RIBOSOMAL PROTEIN L27A

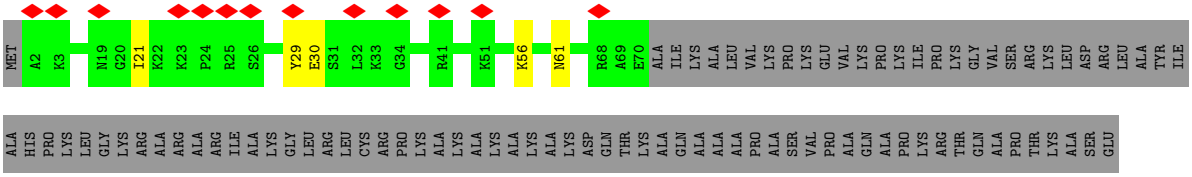
Chain a:





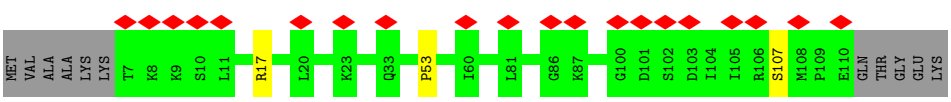
• Molecule 27: 60S RIBOSOMAL PROTEIN L29

Chain b:



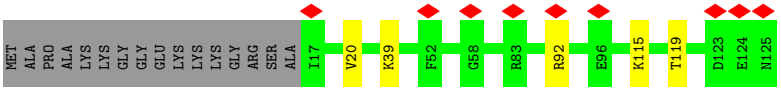
• Molecule 28: 60S RIBOSOMAL PROTEIN L30

Chain c:



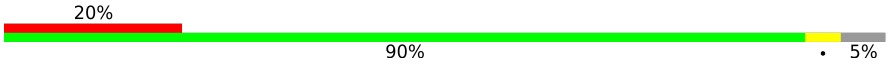
• Molecule 29: 60S RIBOSOMAL PROTEIN L31

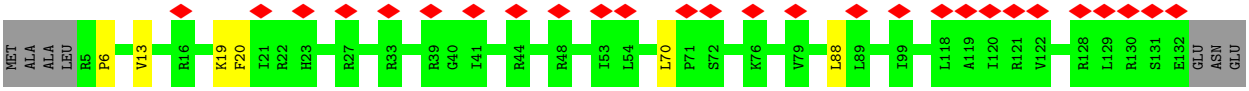
Chain d:



• Molecule 30: 60S RIBOSOMAL PROTEIN L32

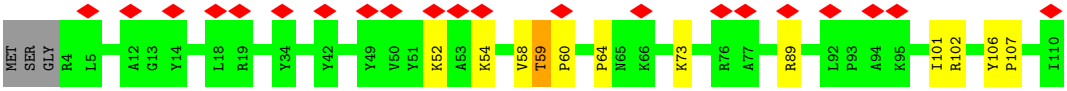
Chain e:





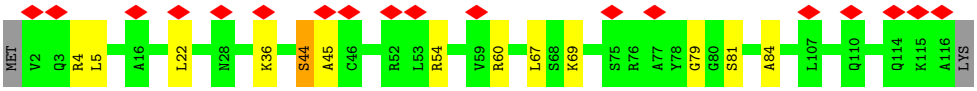
• Molecule 31: 60S RIBOSOMAL PROTEIN L35A

Chain f:



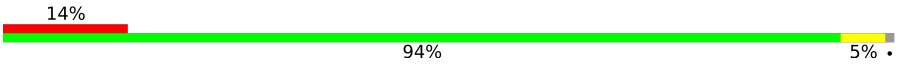
• Molecule 32: 60S RIBOSOMAL PROTEIN L34

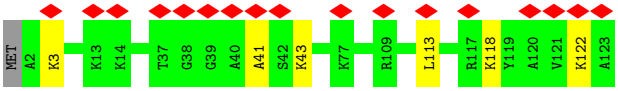
Chain g:



• Molecule 33: 60S RIBOSOMAL PROTEIN L35

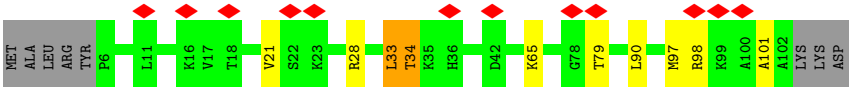
Chain h:





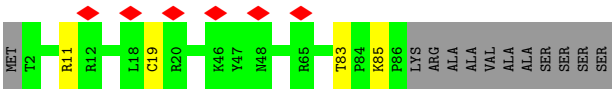
• Molecule 34: 60S RIBOSOMAL PROTEIN L36

Chain i:



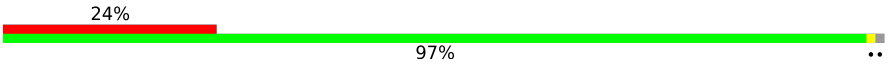
• Molecule 35: 60S RIBOSOMAL PROTEIN L37

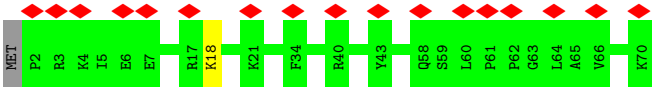
Chain j:



• Molecule 36: 60S RIBOSOMAL PROTEIN L38

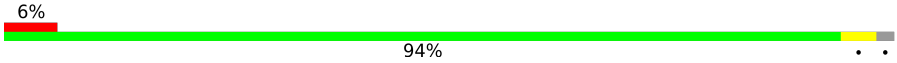
Chain k:

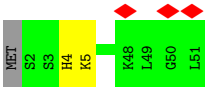




• Molecule 37: 60S RIBOSOMAL PROTEIN L39

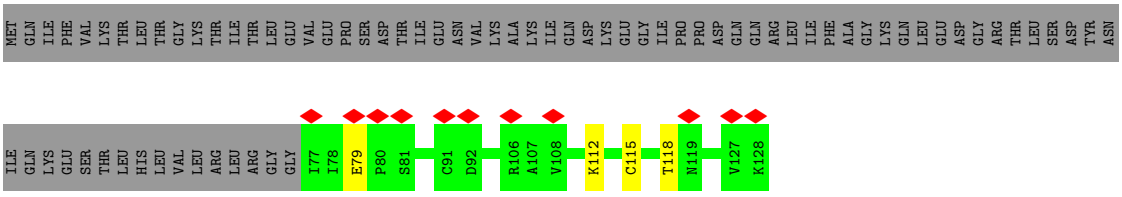
Chain l:





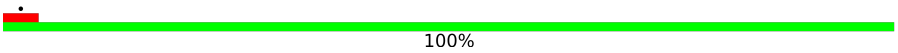
• Molecule 38: UBIQUITIN-60S RIBOSOMAL PROTEIN L40

Chain m:



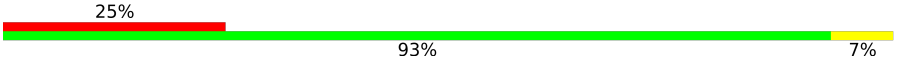
• Molecule 39: 60S RIBOSOMAL PROTEIN L41

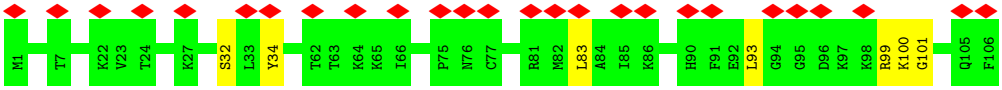
Chain n:



• Molecule 40: 60S RIBOSOMAL PROTEIN L36A

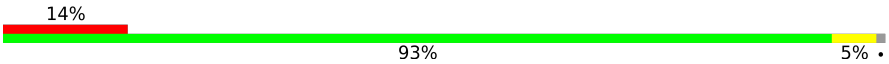
Chain o:

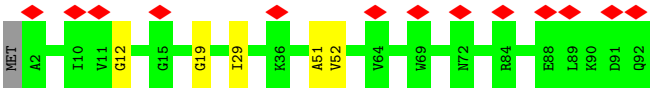




• Molecule 41: 60S RIBOSOMAL PROTEIN L37A

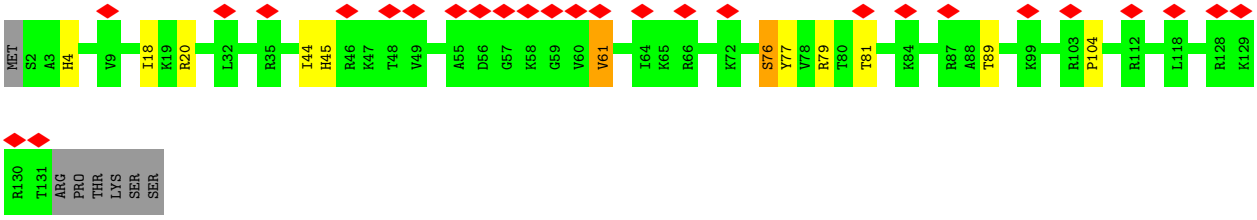
Chain p:





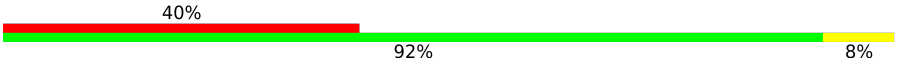
- Molecule 42: 60S RIBOSOMAL PROTEIN L28

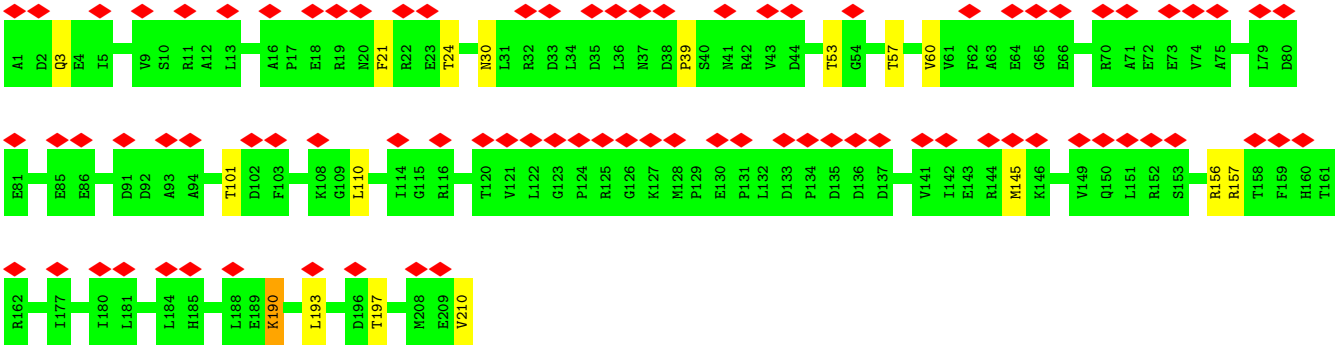
Chain t:



- Molecule 43: 60S RIBOSOMAL PROTEIN L10A

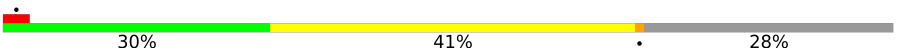
Chain u:

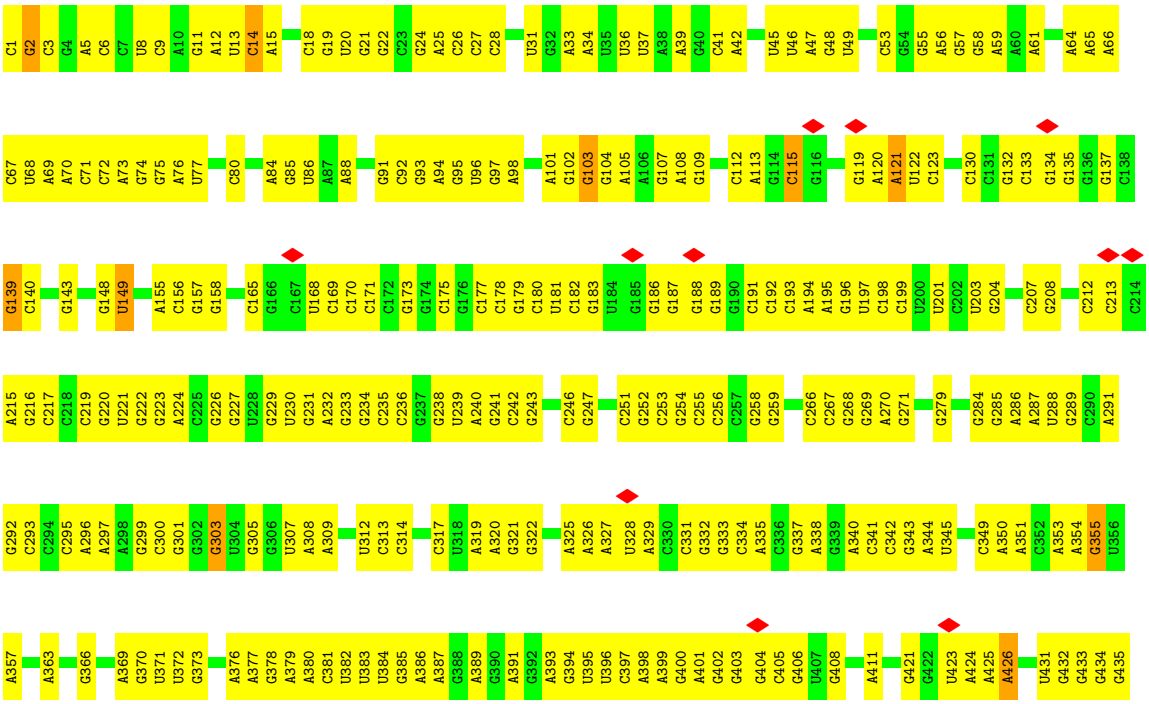


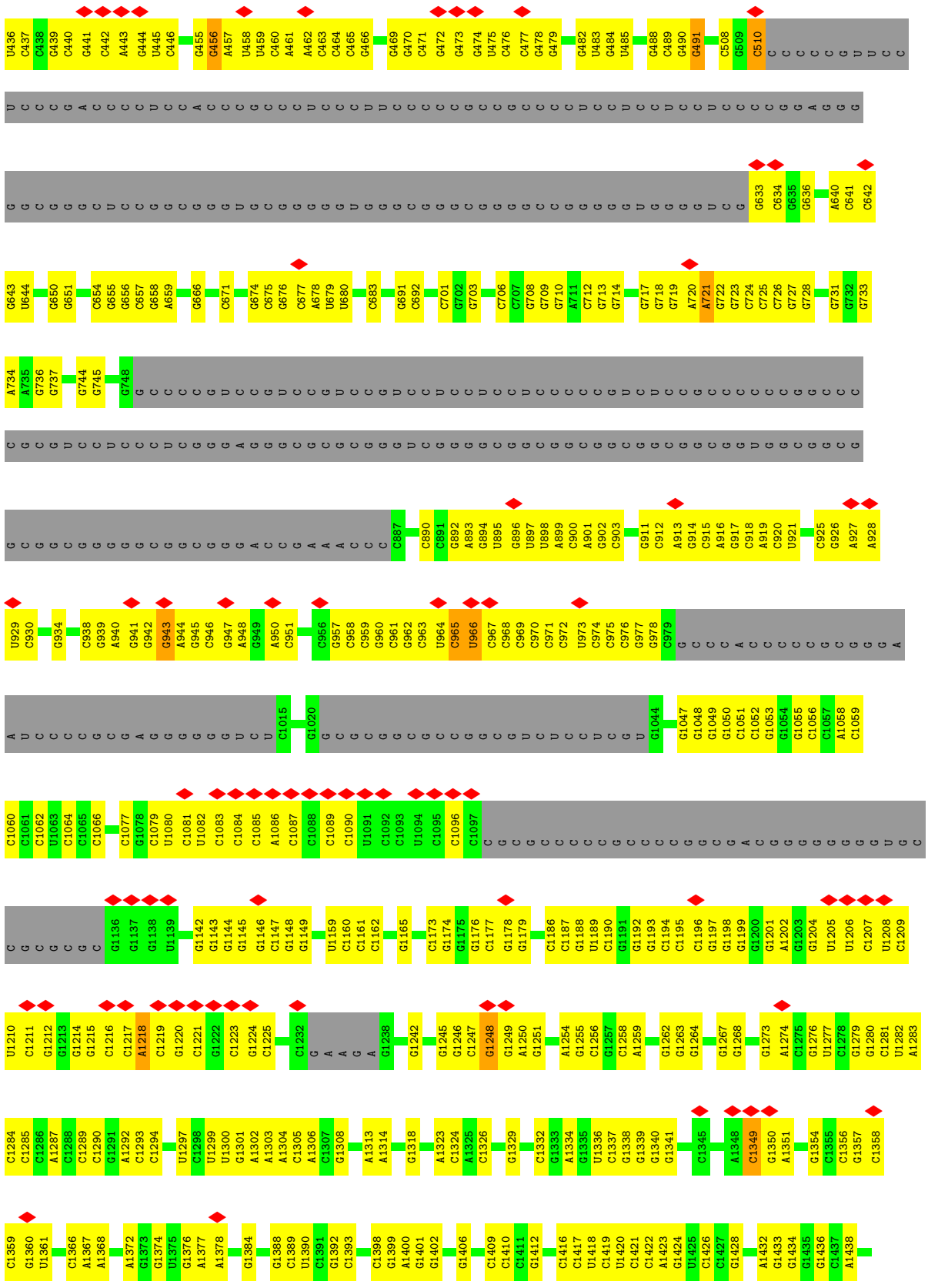


- Molecule 44: 28S RRNA

Chain 2:



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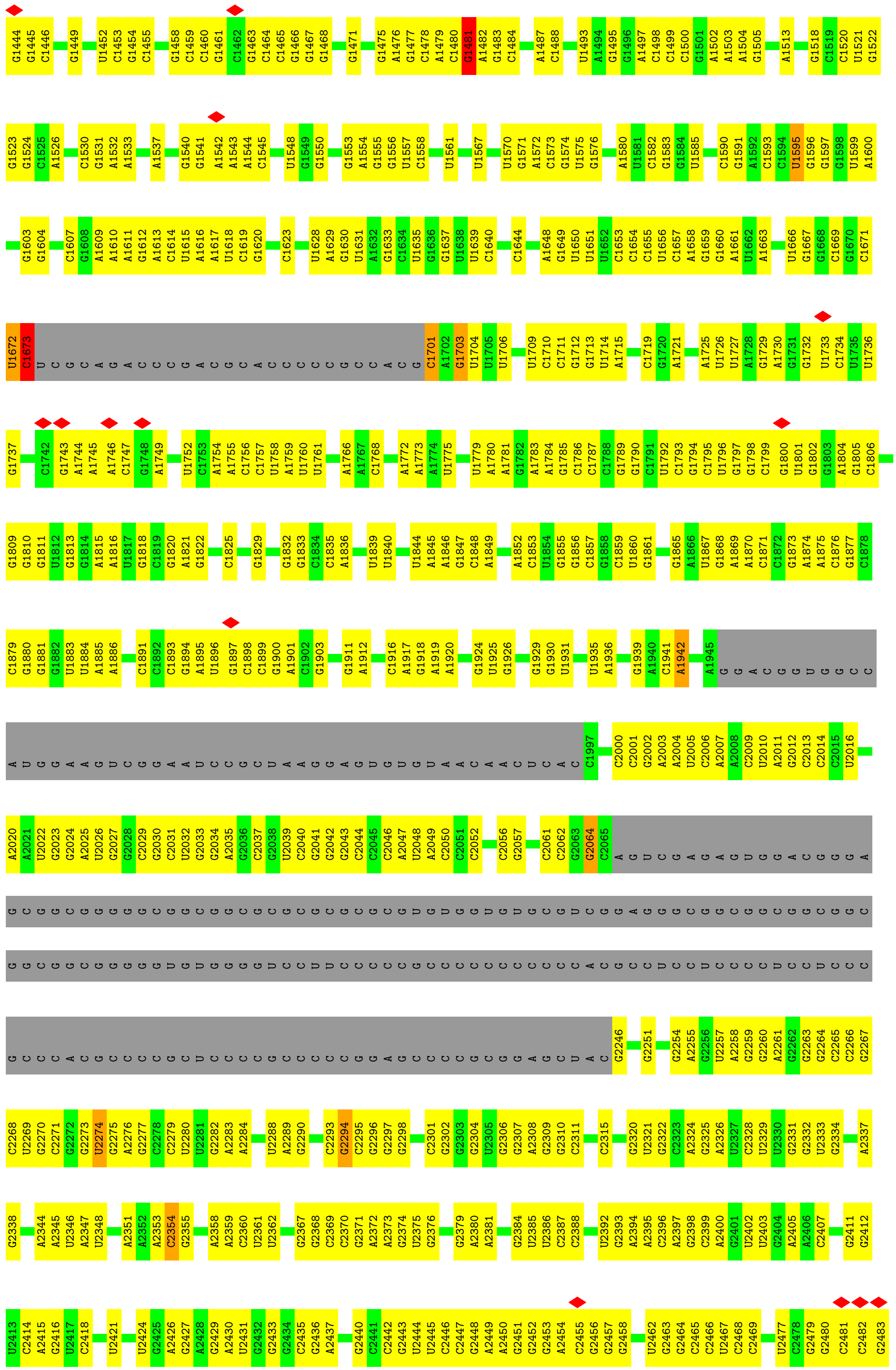
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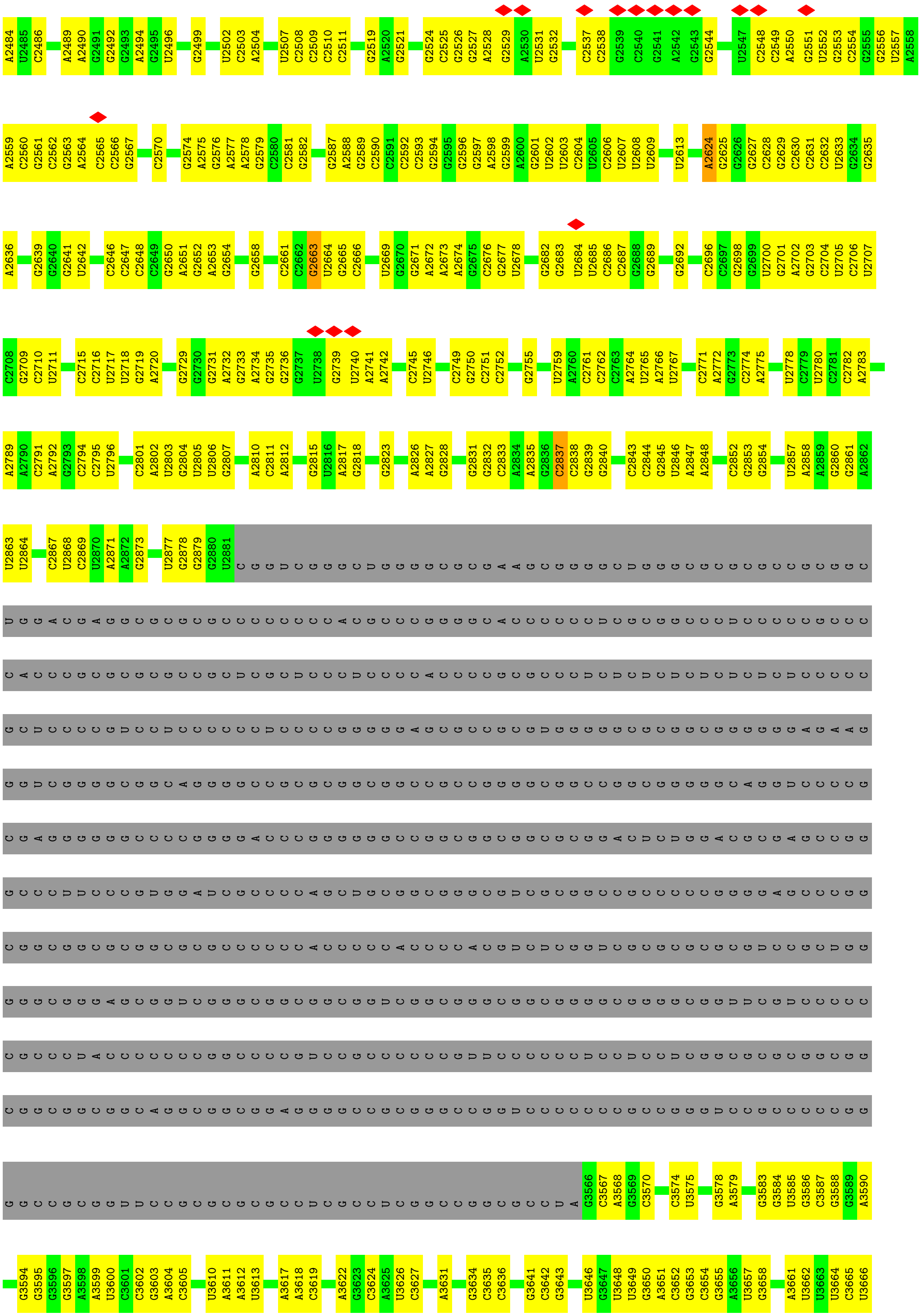
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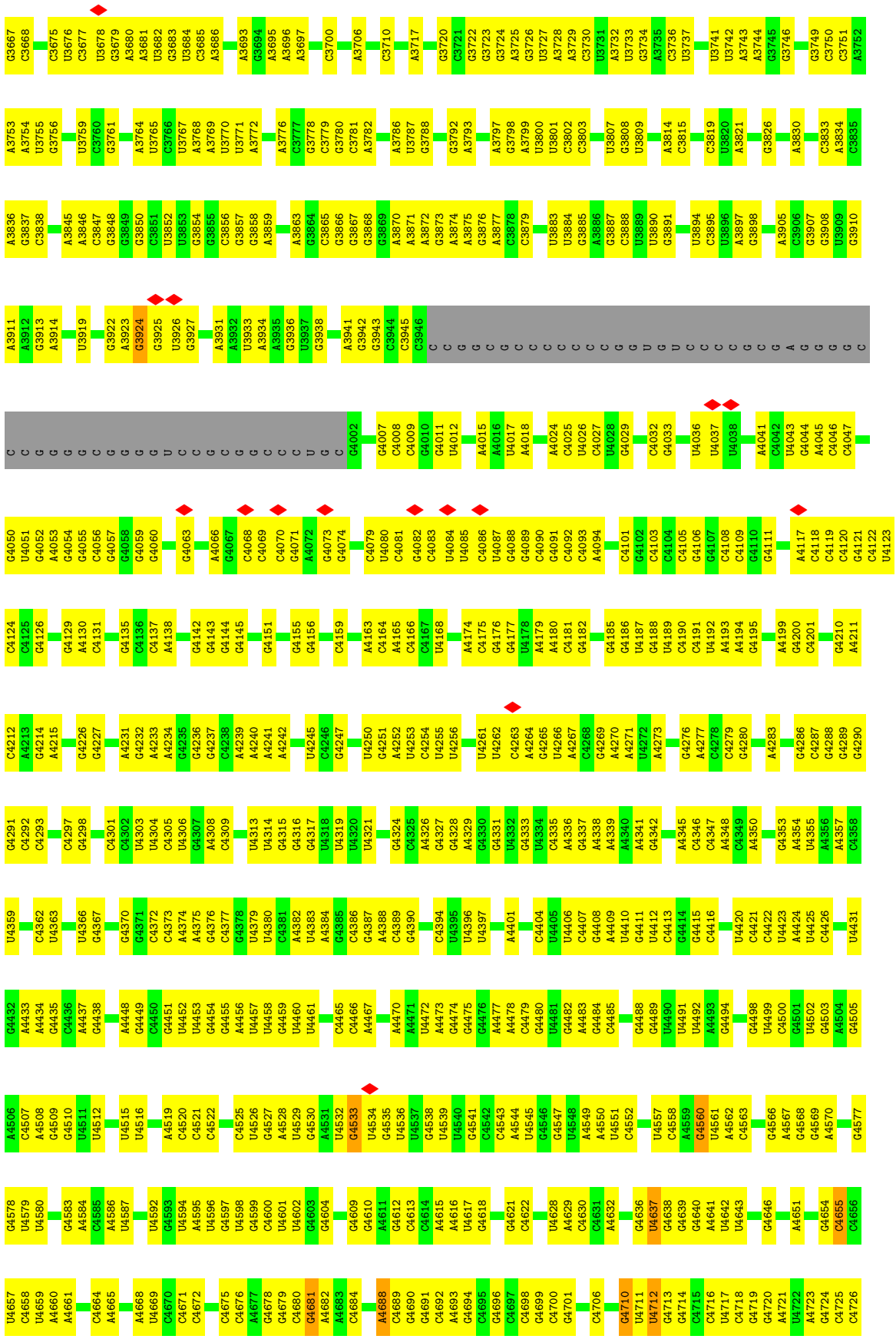

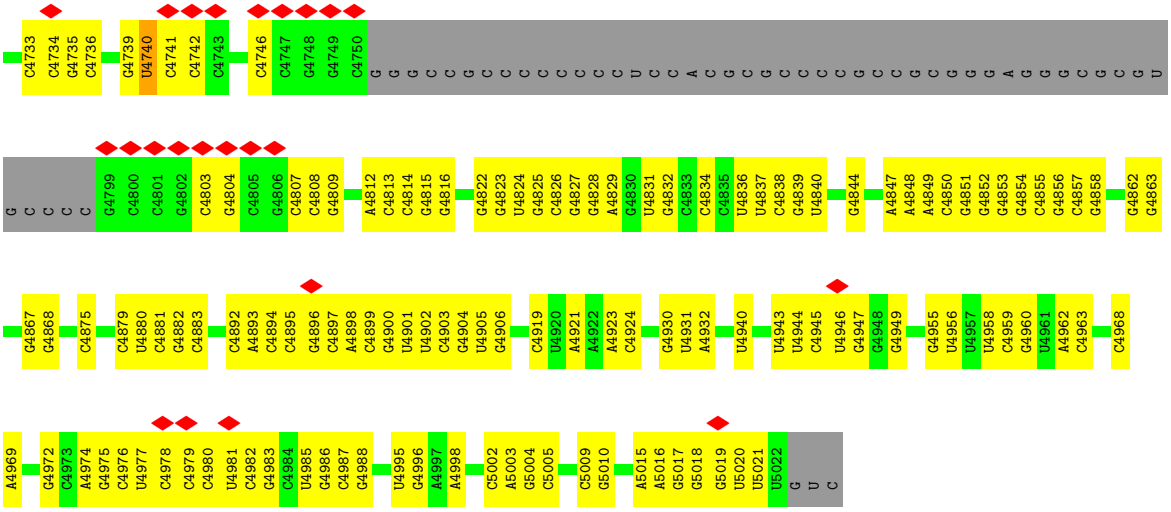

- Molecule 45: 5.8S RRNA

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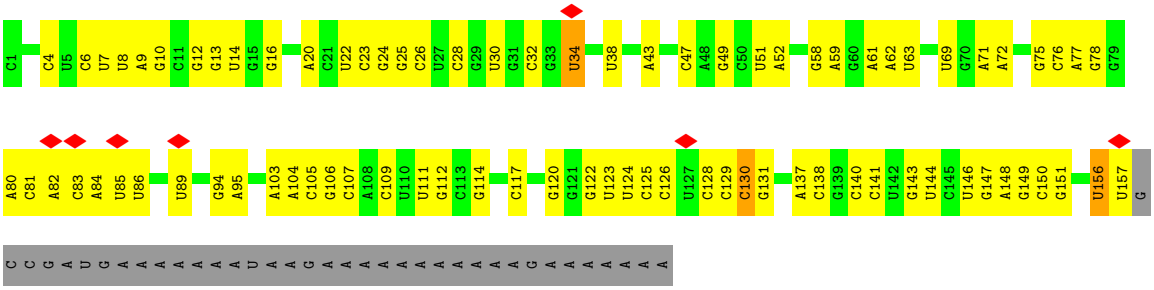
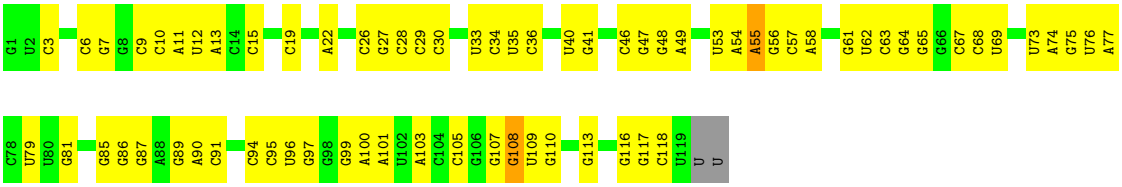


- Molecule 46: 5S RRNA

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64902	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	194805	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	12.165	Depositor
Minimum map value	-4.363	Depositor
Average map value	0.164	Depositor
Map value standard deviation	0.954	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	467.99997, 467.99997, 467.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	A	0.44	0/1926	0.67	0/2583
2	B	0.45	0/3258	0.73	2/4361 (0.0%)
3	C	0.47	0/2943	0.73	1/3953 (0.0%)
4	D	0.49	1/2406 (0.0%)	0.70	1/3221 (0.0%)
5	E	0.52	0/1311	0.73	0/1763
6	F	0.45	0/1985	0.68	0/2644
7	G	0.46	0/1914	0.72	0/2578
8	H	0.43	0/1554	0.69	0/2089
9	I	0.42	0/1642	0.67	0/2194
10	J	0.49	0/1385	0.71	0/1852
11	L	0.53	2/1647 (0.1%)	0.73	3/2205 (0.1%)
12	M	0.49	0/1162	0.70	0/1556
13	N	0.43	0/1753	0.65	0/2348
14	O	0.44	0/1639	0.69	0/2193
15	P	0.44	0/1260	0.70	0/1691
16	Q	0.45	0/1517	0.74	0/2026
17	R	0.41	0/1542	0.64	0/2037
18	S	0.45	0/1478	0.73	0/1985
19	T	0.46	0/1325	0.72	0/1770
20	U	0.47	0/841	0.71	0/1128
21	V	0.43	0/977	0.63	0/1312
22	W	0.43	0/542	0.59	0/722
23	X	0.41	0/992	0.67	0/1334
24	Y	0.47	0/1082	0.72	1/1441 (0.1%)
25	Z	0.47	0/1137	0.79	0/1517
26	a	0.45	0/1190	0.71	0/1591
27	b	0.45	0/570	0.72	0/752
28	c	0.46	0/813	0.70	0/1091
29	d	0.45	0/919	0.67	0/1238
30	e	0.45	0/1071	0.68	0/1428
31	f	0.50	0/884	0.81	0/1185
32	g	0.48	0/917	0.74	0/1222
33	h	0.38	0/1022	0.64	0/1351
34	i	0.43	0/793	0.75	0/1048

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	j	0.49	0/704	0.76	0/931
36	k	0.43	0/574	0.73	0/761
37	l	0.40	0/453	0.61	0/599
38	m	0.42	0/434	0.70	0/575
39	n	0.40	0/240	0.50	0/305
40	o	0.46	0/884	0.74	0/1166
41	p	0.40	0/717	0.61	0/953
42	t	0.48	0/1058	0.75	0/1416
43	u	0.45	0/1638	0.69	1/2222 (0.0%)
44	2	0.41	22/86672 (0.0%)	0.81	41/135198 (0.0%)
45	3	0.36	0/3723	0.79	1/5800 (0.0%)
46	4	0.38	0/2836	0.82	3/4421 (0.1%)
All	All	0.43	25/147330 (0.0%)	0.77	54/217756 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
44	2	0	34
45	3	0	2
All	All	0	36

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	1701	C	C5'-C4'	18.32	1.73	1.51
44	2	1673	C	C3'-O3'	15.33	1.63	1.42
44	2	1701	C	O5'-C5'	14.40	1.67	1.44
44	2	1673	C	O3'-P	14.19	1.78	1.61
44	2	1701	C	P-O5'	13.52	1.73	1.59
44	2	1673	C	C5'-C4'	11.33	1.65	1.51
44	2	1701	C	C4'-C3'	10.23	1.64	1.53
44	2	1701	C	O3'-P	10.17	1.73	1.61
44	2	1673	C	C4'-C3'	9.86	1.64	1.53
44	2	1673	C	P-O5'	8.84	1.68	1.59
44	2	1673	C	O5'-C5'	8.74	1.58	1.44
44	2	943	G	C5-C6	-7.74	1.34	1.42
44	2	1701	C	C3'-O3'	7.38	1.52	1.42
44	2	2663	G	C6-O6	-6.68	1.18	1.24
44	2	1673	C	C2-N3	-6.40	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	264	LYS	N-CA	5.89	1.58	1.46
44	2	1481	G	C2-N2	-5.78	1.28	1.34
44	2	1673	C	N3-C4	-5.73	1.29	1.33
11	L	131	PRO	N-CD	5.54	1.55	1.47
44	2	1701	C	C4'-O4'	5.44	1.52	1.45
11	L	134	PRO	N-CD	5.41	1.55	1.47
44	2	3924	G	C2-N2	-5.33	1.29	1.34
44	2	1701	C	N1-C2	5.17	1.45	1.40
44	2	456	G	C2-N2	-5.11	1.29	1.34
44	2	1701	C	O4'-C1'	5.01	1.48	1.41

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	1701	C	O4'-C4'-C3'	-15.18	88.82	104.00
2	B	258	HIS	C-N-CD	-13.98	89.84	120.60
44	2	1701	C	O4'-C1'-N1	12.32	118.06	108.20
44	2	1701	C	C4'-C3'-O3'	12.21	137.41	113.00
44	2	1701	C	C2'-C3'-O3'	-10.63	86.10	109.50
44	2	1673	C	C5'-C4'-O4'	-8.01	99.49	109.10
44	2	1701	C	C5'-C4'-C3'	7.95	128.72	116.00
44	2	1673	C	O3'-P-O5'	7.17	117.62	104.00
44	2	1673	C	C2-N1-C1'	-7.12	110.97	118.80
45	3	34	U	C3'-C2'-C1'	-6.96	95.93	101.50
44	2	1673	C	C5-C4-N4	6.51	124.76	120.20
44	2	139	G	C3'-C2'-C1'	-6.40	96.38	101.50
44	2	103	G	C3'-C2'-C1'	-6.35	96.42	101.50
44	2	1673	C	N3-C4-N4	-6.31	113.58	118.00
44	2	4688	A	C3'-C2'-C1'	-6.16	96.58	101.50
44	2	1673	C	C4'-C3'-C2'	-6.15	96.45	102.60
44	2	4560	G	C3'-C2'-C1'	-6.14	96.59	101.50
44	2	1673	C	C6-N1-C1'	6.13	128.15	120.80
44	2	1673	C	C4'-C3'-O3'	6.09	125.19	113.00
44	2	1673	C	C5'-C4'-C3'	6.07	125.72	116.00
44	2	683	C	C3'-C2'-C1'	-5.87	96.80	101.50
44	2	1942	A	N9-C1'-C2'	-5.83	105.58	112.00
44	2	3677	C	C3'-C2'-C1'	-5.83	96.83	101.50
44	2	1673	C	N1-C1'-C2'	5.82	121.56	114.00
44	2	3742	U	C3'-C2'-C1'	-5.79	96.87	101.50
44	2	943	G	C5-C6-O6	-5.78	125.13	128.60
4	D	265	ARG	N-CA-C	5.72	126.45	111.00
44	2	3868	G	C3'-C2'-C1'	-5.55	97.06	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	2	2837	C	C3'-C2'-C1'	-5.49	97.11	101.50
11	L	133	ALA	C-N-CD	5.48	139.91	128.40
11	L	130	LYS	C-N-CD	5.43	139.81	128.40
44	2	1703	G	O4'-C1'-C2'	-5.43	100.37	105.80
46	4	108	G	O4'-C4'-C3'	-5.37	98.63	104.00
44	2	1548	U	C3'-C2'-C1'	-5.36	97.21	101.50
44	2	4475	G	C3'-C2'-C1'	-5.34	97.23	101.50
44	2	1672	U	C3'-C2'-C1'	-5.33	97.23	101.50
44	2	4987	C	C3'-C2'-C1'	-5.33	97.23	101.50
46	4	108	G	C5'-C4'-O4'	5.33	115.50	109.10
44	2	28	C	C3'-C2'-C1'	-5.29	97.27	101.50
44	2	355	G	C3'-C2'-C1'	-5.21	97.33	101.50
44	2	1432	A	C3'-C2'-C1'	-5.18	97.36	101.50
43	u	157	ARG	N-CA-CB	-5.14	101.35	110.60
44	2	303	G	C3'-C2'-C1'	-5.14	97.39	101.50
44	2	4547	G	C3'-C2'-C1'	-5.10	97.42	101.50
44	2	14	C	OP2-P-O3'	5.09	116.40	105.20
11	L	55	ILE	N-CA-C	-5.09	97.27	111.00
44	2	1595	U	C3'-C2'-C1'	-5.08	97.43	101.50
44	2	4467	A	C3'-C2'-C1'	-5.07	97.44	101.50
2	B	325	GLU	N-CA-C	5.05	124.63	111.00
46	4	55	A	C3'-C2'-C1'	-5.05	97.46	101.50
24	Y	126	ARG	CB-CA-C	-5.05	100.31	110.40
44	2	491	G	C3'-C2'-C1'	-5.04	97.47	101.50
3	C	151	PRO	CA-N-CD	-5.02	104.47	111.50
44	2	2261	A	C3'-C2'-C1'	-5.02	97.49	101.50

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	2	1	C	Sidechain
44	2	115	C	Sidechain
44	2	121	A	Sidechain
44	2	1218	A	Sidechain
44	2	1248	G	Sidechain
44	2	1349	C	Sidechain
44	2	1481	G	Sidechain
44	2	149	U	Sidechain
44	2	1618	U	Sidechain
44	2	1673	C	Sidechain
44	2	2	G	Sidechain

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Mol	Chain	Res	Type	Group
44	2	2064	G	Sidechain
44	2	2246	G	Sidechain
44	2	2274	U	Sidechain
44	2	2294	G	Sidechain
44	2	2338	G	Sidechain
44	2	2354	C	Sidechain
44	2	2570	C	Sidechain
44	2	2581	C	Sidechain
44	2	2624	A	Sidechain
44	2	2795	C	Sidechain
44	2	426	A	Sidechain
44	2	4533	G	Sidechain
44	2	4637	U	Sidechain
44	2	4655	C	Sidechain
44	2	4681	G	Sidechain
44	2	4710	G	Sidechain
44	2	4712	U	Sidechain
44	2	4740	U	Sidechain
44	2	510	C	Sidechain
44	2	721	A	Sidechain
44	2	902	G	Sidechain
44	2	965	C	Sidechain
44	2	966	U	Sidechain
45	3	130	C	Sidechain
45	3	156	U	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/257 (95%)	236 (96%)	6 (2%)	3 (1%)	13	50
2	B	394/403 (98%)	369 (94%)	11 (3%)	14 (4%)	3	25
3	C	362/427 (85%)	338 (93%)	9 (2%)	15 (4%)	3	23
4	D	288/297 (97%)	279 (97%)	4 (1%)	5 (2%)	9	42
5	E	156/288 (54%)	141 (90%)	8 (5%)	7 (4%)	2	22
6	F	232/248 (94%)	225 (97%)	3 (1%)	4 (2%)	9	42
7	G	233/266 (88%)	217 (93%)	7 (3%)	9 (4%)	3	23
8	H	190/192 (99%)	184 (97%)	3 (2%)	3 (2%)	9	44
9	I	192/214 (90%)	187 (97%)	2 (1%)	3 (2%)	9	44
10	J	168/178 (94%)	153 (91%)	3 (2%)	12 (7%)	1	14
11	L	198/211 (94%)	178 (90%)	9 (4%)	11 (6%)	2	19
12	M	138/215 (64%)	132 (96%)	4 (3%)	2 (1%)	11	46
13	N	202/204 (99%)	193 (96%)	6 (3%)	3 (2%)	10	46
14	O	194/203 (96%)	187 (96%)	4 (2%)	3 (2%)	10	46
15	P	151/184 (82%)	141 (93%)	7 (5%)	3 (2%)	7	38
16	Q	182/188 (97%)	169 (93%)	7 (4%)	6 (3%)	4	26
17	R	181/196 (92%)	174 (96%)	4 (2%)	3 (2%)	9	42
18	S	171/176 (97%)	158 (92%)	7 (4%)	6 (4%)	3	25
19	T	157/160 (98%)	150 (96%)	4 (2%)	3 (2%)	8	38
20	U	100/128 (78%)	97 (97%)	3 (3%)	0	100	100
21	V	126/140 (90%)	119 (94%)	5 (4%)	2 (2%)	9	44
22	W	62/157 (40%)	61 (98%)	1 (2%)	0	100	100
23	X	117/156 (75%)	113 (97%)	4 (3%)	0	100	100
24	Y	126/145 (87%)	119 (94%)	4 (3%)	3 (2%)	6	33
25	Z	134/136 (98%)	125 (93%)	5 (4%)	4 (3%)	4	28
26	a	145/148 (98%)	134 (92%)	6 (4%)	5 (3%)	3	26
27	b	67/159 (42%)	60 (90%)	3 (4%)	4 (6%)	1	17
28	c	102/115 (89%)	99 (97%)	1 (1%)	2 (2%)	7	38
29	d	107/125 (86%)	103 (96%)	3 (3%)	1 (1%)	17	57
30	e	126/135 (93%)	117 (93%)	6 (5%)	3 (2%)	6	33
31	f	105/110 (96%)	96 (91%)	4 (4%)	5 (5%)	2	21
32	g	113/117 (97%)	103 (91%)	6 (5%)	4 (4%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	120/123 (98%)	112 (93%)	5 (4%)	3 (2%)	5	32
34	i	95/105 (90%)	85 (90%)	4 (4%)	6 (6%)	1	17
35	j	83/97 (86%)	75 (90%)	6 (7%)	2 (2%)	6	33
36	k	67/70 (96%)	64 (96%)	2 (3%)	1 (2%)	10	46
37	l	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	7	36
38	m	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	7	38
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	8	38
41	p	89/92 (97%)	83 (93%)	3 (3%)	3 (3%)	3	26
42	t	128/137 (93%)	112 (88%)	9 (7%)	7 (6%)	2	19
43	u	208/210 (99%)	199 (96%)	6 (3%)	3 (1%)	11	46
All	All	6479/7422 (87%)	6102 (94%)	200 (3%)	177 (3%)	8	31

All (177) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	LYS
1	A	196	TRP
2	B	4	ARG
2	B	5	LYS
2	B	157	CYS
2	B	259	PRO
2	B	260	ALA
2	B	360	LEU
3	C	50	GLN
3	C	53	ALA
3	C	54	VAL
3	C	151	PRO
3	C	309	ILE
4	D	258	LYS
5	E	137	VAL
5	E	183	ARG
5	E	185	PRO
6	F	222	LYS
7	G	41	ILE
7	G	42	GLY
7	G	162	ASP
8	H	4	ILE

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Mol	Chain	Res	Type
8	H	61	TRP
9	I	189	ARG
10	J	11	PRO
10	J	14	GLU
10	J	77	ALA
10	J	155	HIS
10	J	175	LEU
11	L	47	ALA
11	L	52	SER
11	L	54	PRO
11	L	77	SER
11	L	205	GLN
12	M	21	ALA
13	N	184	ILE
15	P	3	ARG
15	P	6	LEU
16	Q	98	LEU
16	Q	155	ALA
17	R	131	VAL
18	S	171	ARG
19	T	18	PRO
24	Y	67	ILE
25	Z	32	GLY
25	Z	103	ASP
25	Z	125	GLY
26	a	48	TYR
27	b	30	GLU
27	b	56	LYS
28	c	107	SER
30	e	19	LYS
30	e	20	PHE
31	f	60	PRO
31	f	64	PRO
31	f	106	TYR
31	f	107	PRO
32	g	84	ALA
33	h	122	LYS
34	i	28	ARG
34	i	33	LEU
34	i	34	THR
35	j	11	ARG
35	j	85	LYS

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Mol	Chain	Res	Type
36	k	18	LYS
37	l	4	HIS
42	t	44	ILE
42	t	61	VAL
42	t	76	SER
42	t	104	PRO
43	u	190	LYS
2	B	299	ILE
2	B	309	LEU
2	B	357	ARG
3	C	55	SER
3	C	58	ALA
3	C	148	PRO
3	C	276	ASN
6	F	166	ARG
6	F	170	THR
7	G	84	THR
8	H	190	ALA
9	I	41	ALA
9	I	194	GLY
10	J	97	ASN
10	J	117	ILE
11	L	51	ALA
11	L	143	GLU
11	L	162	LYS
14	O	199	HIS
16	Q	157	GLY
17	R	113	LYS
21	V	85	ARG
24	Y	84	ARG
26	a	47	LYS
26	a	66	ASN
26	a	116	LYS
32	g	44	SER
32	g	45	ALA
40	o	34	TYR
41	p	12	GLY
2	B	292	LEU
2	B	296	GLY
3	C	57	LEU
3	C	75	ARG
3	C	150	LEU

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Mol	Chain	Res	Type
4	D	265	ARG
5	E	135	GLN
5	E	265	PRO
7	G	161	VAL
7	G	163	PRO
10	J	111	GLU
11	L	141	ALA
11	L	161	TYR
11	L	177	LYS
14	O	72	HIS
14	O	198	THR
15	P	5	SER
16	Q	12	LYS
18	S	135	SER
24	Y	123	ALA
25	Z	37	PRO
27	b	29	TYR
33	h	41	ALA
34	i	101	ALA
38	m	79	GLU
41	p	51	ALA
43	u	3	GLN
1	A	70	LYS
4	D	253	TYR
5	E	227	HIS
7	G	44	ASP
10	J	120	ASP
10	J	176	PRO
12	M	44	GLN
13	N	145	ASN
16	Q	164	LYS
18	S	16	CYS
18	S	158	VAL
18	S	160	ARG
19	T	125	TRP
28	c	53	PRO
33	h	3	LYS
42	t	79	ARG
42	t	89	THR
2	B	189	THR
3	C	30	ALA
3	C	56	GLU

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Mol	Chain	Res	Type
7	G	134	PRO
16	Q	156	PRO
18	S	164	LYS
42	t	45	HIS
43	u	39	PRO
2	B	326	VAL
4	D	125	VAL
4	D	259	LYS
6	F	184	ILE
10	J	58	ARG
17	R	53	LYS
19	T	123	GLY
26	a	24	LYS
27	b	21	ILE
31	f	59	THR
34	i	21	VAL
34	i	65	LYS
7	G	30	PRO
10	J	76	GLY
32	g	79	GLY
41	p	19	GLY
2	B	18	PRO
3	C	232	VAL
5	E	144	ILE
13	N	52	GLY
29	d	20	VAL
30	e	6	PRO
40	o	101	GLY
21	V	45	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/199 (95%)	184 (97%)	5 (3%)	46	66
2	B	344/349 (99%)	326 (95%)	18 (5%)	23	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	302/348 (87%)	284 (94%)	18 (6%)	19	44
4	D	244/250 (98%)	237 (97%)	7 (3%)	42	64
5	E	143/252 (57%)	135 (94%)	8 (6%)	21	46
6	F	203/215 (94%)	196 (97%)	7 (3%)	37	60
7	G	199/223 (89%)	192 (96%)	7 (4%)	36	59
8	H	171/171 (100%)	164 (96%)	7 (4%)	30	55
9	I	170/181 (94%)	161 (95%)	9 (5%)	22	47
10	J	143/149 (96%)	137 (96%)	6 (4%)	30	54
11	L	167/177 (94%)	156 (93%)	11 (7%)	16	41
12	M	118/161 (73%)	114 (97%)	4 (3%)	37	60
13	N	172/172 (100%)	170 (99%)	2 (1%)	71	83
14	O	168/174 (97%)	166 (99%)	2 (1%)	71	83
15	P	133/163 (82%)	126 (95%)	7 (5%)	22	47
16	Q	162/165 (98%)	157 (97%)	5 (3%)	40	62
17	R	161/175 (92%)	150 (93%)	11 (7%)	16	41
18	S	155/157 (99%)	148 (96%)	7 (4%)	27	52
19	T	139/140 (99%)	134 (96%)	5 (4%)	35	59
20	U	91/115 (79%)	88 (97%)	3 (3%)	38	61
21	V	100/107 (94%)	99 (99%)	1 (1%)	76	86
22	W	55/126 (44%)	52 (94%)	3 (6%)	21	47
23	X	107/133 (80%)	105 (98%)	2 (2%)	57	75
24	Y	119/135 (88%)	115 (97%)	4 (3%)	37	60
25	Z	118/118 (100%)	112 (95%)	6 (5%)	24	48
26	a	120/121 (99%)	116 (97%)	4 (3%)	38	61
27	b	58/126 (46%)	57 (98%)	1 (2%)	60	78
28	c	88/97 (91%)	87 (99%)	1 (1%)	73	84
29	d	100/110 (91%)	96 (96%)	4 (4%)	31	55
30	e	115/121 (95%)	112 (97%)	3 (3%)	46	66
31	f	87/89 (98%)	79 (91%)	8 (9%)	9	29
32	g	98/100 (98%)	88 (90%)	10 (10%)	7	25
33	h	109/110 (99%)	106 (97%)	3 (3%)	43	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	i	82/89 (92%)	76 (93%)	6 (7%)	14	39
35	j	71/80 (89%)	69 (97%)	2 (3%)	43	65
36	k	64/65 (98%)	64 (100%)	0	100	100
37	l	47/48 (98%)	46 (98%)	1 (2%)	53	72
38	m	48/116 (41%)	45 (94%)	3 (6%)	18	43
39	n	24/24 (100%)	24 (100%)	0	100	100
40	o	94/94 (100%)	89 (95%)	5 (5%)	22	47
41	p	74/75 (99%)	72 (97%)	2 (3%)	44	65
42	t	113/121 (93%)	106 (94%)	7 (6%)	18	43
43	u	177/177 (100%)	163 (92%)	14 (8%)	12	35
All	All	5642/6318 (89%)	5403 (96%)	239 (4%)	33	54

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	116	LEU
1	A	162	ASN
1	A	196	TRP
1	A	218	HIS
2	B	3	HIS
2	B	55	HIS
2	B	89	ILE
2	B	101	THR
2	B	131	THR
2	B	146	LEU
2	B	157	CYS
2	B	240	LEU
2	B	243	LYS
2	B	254	ILE
2	B	258	HIS
2	B	291	TYR
2	B	300	LYS
2	B	305	THR
2	B	314	ILE
2	B	327	THR
2	B	351	LEU
2	B	370	THR

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Mol	Chain	Res	Type
3	C	13	GLU
3	C	24	LEU
3	C	49	ARG
3	C	78	ARG
3	C	100	ARG
3	C	150	LEU
3	C	151	PRO
3	C	162	LYS
3	C	163	LYS
3	C	188	ARG
3	C	193	LYS
3	C	215	ASN
3	C	232	VAL
3	C	253	THR
3	C	289	LEU
3	C	309	ILE
3	C	310	HIS
3	C	323	ARG
4	D	23	ARG
4	D	81	HIS
4	D	105	LEU
4	D	126	THR
4	D	155	THR
4	D	262	LYS
4	D	293	ARG
5	E	162	VAL
5	E	172	LEU
5	E	188	ARG
5	E	189	THR
5	E	197	THR
5	E	212	LEU
5	E	217	PHE
5	E	278	THR
6	F	15	PRO
6	F	32	ARG
6	F	34	ARG
6	F	37	PHE
6	F	44	LYS
6	F	199	LYS
6	F	226	HIS
7	G	34	LYS
7	G	46	GLN

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Mol	Chain	Res	Type
7	G	55	VAL
7	G	81	ASN
7	G	162	ASP
7	G	163	PRO
7	G	218	LEU
8	H	2	LYS
8	H	20	LEU
8	H	41	ILE
8	H	45	LEU
8	H	71	ARG
8	H	129	ARG
8	H	188	GLN
9	I	33	ILE
9	I	39	LYS
9	I	52	MET
9	I	53	VAL
9	I	96	VAL
9	I	163	GLN
9	I	166	HIS
9	I	174	THR
9	I	200	ILE
10	J	12	MET
10	J	70	VAL
10	J	83	LEU
10	J	109	ILE
10	J	115	LEU
10	J	169	LYS
11	L	52	SER
11	L	54	PRO
11	L	55	ILE
11	L	130	LYS
11	L	135	LYS
11	L	148	THR
11	L	151	THR
11	L	155	MET
11	L	163	LYS
11	L	164	GLU
11	L	183	ARG
12	M	72	TYR
12	M	78	GLN
12	M	114	LYS
12	M	132	LYS

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Mol	Chain	Res	Type
13	N	5	LYS
13	N	31	ARG
14	O	169	ARG
14	O	187	LYS
15	P	2	VAL
15	P	4	TYR
15	P	64	ASN
15	P	75	GLN
15	P	78	TRP
15	P	94	MET
15	P	112	LEU
16	Q	48	LEU
16	Q	61	LEU
16	Q	72	LEU
16	Q	75	ARG
16	Q	120	ILE
17	R	1	MET
17	R	3	MET
17	R	5	ARG
17	R	20	LYS
17	R	25	ASP
17	R	41	ILE
17	R	57	VAL
17	R	74	ARG
17	R	103	ARG
17	R	114	LYS
17	R	138	LEU
18	S	4	SER
18	S	7	LEU
18	S	24	THR
18	S	27	LEU
18	S	73	LEU
18	S	166	ARG
18	S	169	THR
19	T	17	ARG
19	T	68	THR
19	T	69	GLN
19	T	125	TRP
19	T	126	VAL
20	U	20	LYS
20	U	27	HIS
20	U	48	LYS

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Mol	Chain	Res	Type
21	V	131	ARG
22	W	2	LYS
22	W	32	LEU
22	W	33	ASN
23	X	79	PHE
23	X	123	LYS
24	Y	8	THR
24	Y	36	LYS
24	Y	70	VAL
24	Y	115	ARG
25	Z	1	MET
25	Z	75	TYR
25	Z	89	ILE
25	Z	112	ARG
25	Z	121	ARG
25	Z	136	PHE
26	a	8	THR
26	a	47	LYS
26	a	56	VAL
26	a	132	ARG
27	b	61	ASN
28	c	17	ARG
29	d	39	LYS
29	d	92	ARG
29	d	115	LYS
29	d	119	THR
30	e	13	VAL
30	e	70	LEU
30	e	88	LEU
31	f	52	LYS
31	f	54	LYS
31	f	58	VAL
31	f	59	THR
31	f	73	LYS
31	f	89	ARG
31	f	101	ILE
31	f	102	ARG
32	g	4	ARG
32	g	5	LEU
32	g	22	LEU
32	g	36	LYS
32	g	44	SER

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Mol	Chain	Res	Type
32	g	54	ARG
32	g	60	ARG
32	g	67	LEU
32	g	69	LYS
32	g	81	SER
33	h	43	LYS
33	h	113	LEU
33	h	118	LYS
34	i	33	LEU
34	i	34	THR
34	i	79	THR
34	i	90	LEU
34	i	97	MET
34	i	98	ARG
35	j	19	CYS
35	j	83	THR
37	l	5	LYS
38	m	112	LYS
38	m	115	CYS
38	m	118	THR
40	o	32	SER
40	o	83	LEU
40	o	93	LEU
40	o	99	ARG
40	o	100	LYS
41	p	29	ILE
41	p	52	VAL
42	t	4	HIS
42	t	18	ILE
42	t	20	ARG
42	t	61	VAL
42	t	76	SER
42	t	77	TYR
42	t	81	THR
43	u	21	PHE
43	u	24	THR
43	u	30	ASN
43	u	53	THR
43	u	57	THR
43	u	60	VAL
43	u	101	THR
43	u	110	LEU

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Mol	Chain	Res	Type
43	u	145	MET
43	u	156	ARG
43	u	190	LYS
43	u	193	LEU
43	u	197	THR
43	u	210	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (125) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	A	209	HIS
1	A	215	ASN
2	B	25	HIS
2	B	167	GLN
2	B	175	GLN
2	B	208	ASN
2	B	213	GLN
2	B	271	GLN
2	B	328	ASN
2	B	354	GLN
3	C	43	ASN
3	C	50	GLN
3	C	187	GLN
3	C	245	HIS
3	C	329	ASN
3	C	347	HIS
3	C	362	GLN
4	D	57	ASN
4	D	191	ASN
4	D	195	HIS
4	D	244	HIS
4	D	291	GLN
5	E	135	GLN
5	E	182	ASN
5	E	205	ASN
5	E	211	HIS
5	E	228	GLN
5	E	256	GLN
6	F	80	ASN
6	F	116	GLN
6	F	131	ASN

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Mol	Chain	Res	Type
6	F	151	ASN
7	G	66	GLN
7	G	108	GLN
8	H	15	ASN
8	H	162	GLN
9	I	14	ASN
9	I	51	HIS
9	I	59	GLN
9	I	144	ASN
10	J	97	ASN
10	J	112	HIS
10	J	167	GLN
10	J	168	GLN
11	L	19	GLN
11	L	27	ASN
11	L	149	GLN
12	M	20	HIS
12	M	33	GLN
12	M	131	GLN
13	N	8	GLN
13	N	15	GLN
13	N	139	HIS
13	N	158	HIS
13	N	201	HIS
14	O	180	GLN
15	P	25	HIS
15	P	54	GLN
15	P	64	ASN
15	P	120	ASN
16	Q	40	ASN
16	Q	45	GLN
16	Q	162	HIS
17	R	39	GLN
17	R	40	GLN
17	R	118	HIS
17	R	141	HIS
18	S	91	HIS
18	S	117	HIS
18	S	122	HIS
18	S	125	GLN
18	S	146	HIS
18	S	156	HIS

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Mol	Chain	Res	Type
19	T	69	GLN
19	T	127	GLN
19	T	131	GLN
19	T	139	HIS
19	T	144	ASN
20	U	17	GLN
20	U	44	GLN
20	U	116	GLN
21	V	36	ASN
21	V	84	GLN
21	V	135	ASN
22	W	48	GLN
22	W	63	GLN
23	X	93	ASN
23	X	107	HIS
23	X	111	GLN
23	X	125	ASN
24	Y	66	GLN
24	Y	72	GLN
25	Z	132	GLN
26	a	17	HIS
26	a	40	HIS
26	a	67	GLN
26	a	74	ASN
26	a	93	ASN
27	b	12	GLN
27	b	19	ASN
27	b	42	ASN
27	b	50	ASN
27	b	60	ASN
28	c	15	ASN
29	d	125	ASN
31	f	21	GLN
31	f	65	ASN
32	g	3	GLN
32	g	100	GLN
33	h	101	ASN
34	i	36	HIS
34	i	80	HIS
35	j	30	GLN
36	k	28	ASN
38	m	87	GLN

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Mol	Chain	Res	Type
38	m	90	ASN
39	n	22	GLN
40	o	45	GLN
40	o	51	GLN
40	o	102	GLN
42	t	23	GLN
43	u	3	GLN
43	u	55	GLN
43	u	194	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	2	3605/5025 (71%)	2046 (56%)	325 (9%)
45	3	156/194 (80%)	81 (51%)	6 (3%)
46	4	118/121 (97%)	68 (57%)	9 (7%)
All	All	3879/5340 (72%)	2195 (56%)	340 (8%)

All (2195) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	2	2	G
44	2	3	C
44	2	5	A
44	2	6	C
44	2	8	U
44	2	9	C
44	2	11	G
44	2	12	A
44	2	13	U
44	2	14	C
44	2	15	A
44	2	18	C
44	2	19	G
44	2	20	U
44	2	21	G
44	2	22	G
44	2	24	G
44	2	25	A
44	2	26	C
44	2	27	C

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Mol	Chain	Res	Type
44	2	31	U
44	2	33	A
44	2	34	A
44	2	36	U
44	2	37	U
44	2	39	A
44	2	41	C
44	2	42	A
44	2	45	U
44	2	46	U
44	2	47	A
44	2	48	G
44	2	49	U
44	2	53	C
44	2	55	G
44	2	56	A
44	2	57	G
44	2	58	G
44	2	59	A
44	2	61	A
44	2	64	A
44	2	65	A
44	2	66	A
44	2	67	C
44	2	68	U
44	2	69	A
44	2	70	A
44	2	71	C
44	2	72	C
44	2	73	A
44	2	74	G
44	2	75	G
44	2	76	A
44	2	77	U
44	2	80	C
44	2	84	A
44	2	85	G
44	2	86	U
44	2	88	A
44	2	91	G
44	2	92	C
44	2	93	G

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Mol	Chain	Res	Type
44	2	94	A
44	2	95	G
44	2	96	U
44	2	97	G
44	2	98	A
44	2	101	A
44	2	102	G
44	2	103	G
44	2	104	G
44	2	105	A
44	2	107	G
44	2	108	A
44	2	109	G
44	2	112	C
44	2	113	A
44	2	115	C
44	2	119	G
44	2	120	A
44	2	121	A
44	2	122	U
44	2	123	C
44	2	130	C
44	2	132	G
44	2	133	C
44	2	134	G
44	2	135	G
44	2	137	G
44	2	139	G
44	2	140	C
44	2	143	G
44	2	148	G
44	2	149	U
44	2	155	A
44	2	156	C
44	2	157	G
44	2	158	G
44	2	165	C
44	2	168	U
44	2	169	C
44	2	170	C
44	2	171	C
44	2	173	G

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Mol	Chain	Res	Type
44	2	175	C
44	2	177	C
44	2	178	C
44	2	179	G
44	2	180	C
44	2	181	U
44	2	182	C
44	2	183	G
44	2	186	G
44	2	187	G
44	2	188	G
44	2	189	G
44	2	191	C
44	2	193	C
44	2	194	A
44	2	195	A
44	2	196	G
44	2	197	U
44	2	198	C
44	2	199	C
44	2	201	U
44	2	203	U
44	2	204	G
44	2	207	C
44	2	208	G
44	2	212	C
44	2	213	C
44	2	215	A
44	2	216	G
44	2	217	C
44	2	219	C
44	2	220	G
44	2	221	U
44	2	222	G
44	2	223	G
44	2	224	A
44	2	226	G
44	2	227	G
44	2	229	G
44	2	230	U
44	2	231	G
44	2	232	A

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Mol	Chain	Res	Type
44	2	233	G
44	2	234	G
44	2	235	C
44	2	236	C
44	2	238	G
44	2	239	U
44	2	240	A
44	2	241	G
44	2	242	C
44	2	243	G
44	2	246	C
44	2	247	G
44	2	251	C
44	2	252	G
44	2	253	C
44	2	254	G
44	2	255	C
44	2	256	C
44	2	258	G
44	2	259	G
44	2	266	C
44	2	267	C
44	2	268	G
44	2	269	G
44	2	270	A
44	2	271	G
44	2	279	G
44	2	284	G
44	2	285	G
44	2	286	A
44	2	287	A
44	2	288	U
44	2	289	G
44	2	291	A
44	2	292	G
44	2	293	C
44	2	295	C
44	2	296	A
44	2	297	A
44	2	299	G
44	2	300	C
44	2	301	G

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Mol	Chain	Res	Type
44	2	303	G
44	2	305	G
44	2	307	U
44	2	308	A
44	2	309	A
44	2	312	U
44	2	313	C
44	2	314	C
44	2	317	C
44	2	319	A
44	2	320	A
44	2	321	G
44	2	322	G
44	2	325	A
44	2	326	A
44	2	327	A
44	2	328	U
44	2	329	A
44	2	331	C
44	2	332	G
44	2	333	G
44	2	334	C
44	2	335	A
44	2	337	G
44	2	338	A
44	2	340	A
44	2	341	C
44	2	342	C
44	2	343	G
44	2	344	A
44	2	345	U
44	2	349	C
44	2	350	A
44	2	351	A
44	2	353	A
44	2	354	A
44	2	355	G
44	2	357	A
44	2	363	A
44	2	366	G
44	2	369	A
44	2	370	G

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Mol	Chain	Res	Type
44	2	372	U
44	2	373	G
44	2	376	A
44	2	377	A
44	2	378	G
44	2	379	A
44	2	380	A
44	2	381	C
44	2	382	U
44	2	383	U
44	2	384	U
44	2	385	G
44	2	386	A
44	2	387	A
44	2	389	A
44	2	391	A
44	2	393	A
44	2	394	G
44	2	395	U
44	2	396	U
44	2	397	C
44	2	398	A
44	2	399	A
44	2	400	G
44	2	401	A
44	2	402	G
44	2	403	G
44	2	404	G
44	2	405	C
44	2	406	G
44	2	408	G
44	2	411	A
44	2	421	G
44	2	423	U
44	2	424	A
44	2	425	A
44	2	426	A
44	2	431	U
44	2	432	G
44	2	433	G
44	2	434	G
44	2	435	G

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Mol	Chain	Res	Type
44	2	436	U
44	2	437	C
44	2	439	G
44	2	440	C
44	2	441	G
44	2	442	C
44	2	443	A
44	2	444	G
44	2	445	U
44	2	446	C
44	2	455	G
44	2	456	G
44	2	457	A
44	2	458	U
44	2	459	U
44	2	460	C
44	2	461	A
44	2	462	A
44	2	463	C
44	2	464	C
44	2	465	C
44	2	466	G
44	2	469	G
44	2	470	G
44	2	471	C
44	2	472	G
44	2	473	G
44	2	474	G
44	2	475	U
44	2	476	C
44	2	477	C
44	2	478	G
44	2	479	G
44	2	482	G
44	2	483	U
44	2	484	G
44	2	485	U
44	2	488	G
44	2	489	C
44	2	490	G
44	2	491	G
44	2	508	C

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Mol	Chain	Res	Type
44	2	510	C
44	2	634	C
44	2	636	G
44	2	640	A
44	2	641	C
44	2	642	C
44	2	643	G
44	2	644	U
44	2	650	G
44	2	651	G
44	2	654	C
44	2	655	G
44	2	656	G
44	2	657	C
44	2	658	G
44	2	659	A
44	2	666	G
44	2	671	C
44	2	674	G
44	2	675	C
44	2	676	G
44	2	677	C
44	2	678	A
44	2	679	U
44	2	680	U
44	2	691	G
44	2	692	C
44	2	701	C
44	2	703	G
44	2	706	C
44	2	708	G
44	2	709	G
44	2	710	G
44	2	712	C
44	2	713	G
44	2	714	G
44	2	717	G
44	2	718	G
44	2	719	G
44	2	720	A
44	2	721	A
44	2	722	G

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Mol	Chain	Res	Type
44	2	723	G
44	2	724	C
44	2	725	C
44	2	726	C
44	2	727	G
44	2	728	G
44	2	731	G
44	2	733	G
44	2	734	A
44	2	736	G
44	2	737	G
44	2	744	G
44	2	745	G
44	2	890	C
44	2	892	G
44	2	893	A
44	2	894	G
44	2	895	U
44	2	896	G
44	2	897	U
44	2	898	U
44	2	899	A
44	2	900	C
44	2	901	A
44	2	903	C
44	2	911	G
44	2	912	C
44	2	913	A
44	2	914	G
44	2	915	C
44	2	916	A
44	2	917	G
44	2	918	C
44	2	919	A
44	2	920	C
44	2	921	U
44	2	925	C
44	2	926	G
44	2	927	A
44	2	928	A
44	2	929	U
44	2	930	C

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Mol	Chain	Res	Type
44	2	934	G
44	2	938	C
44	2	939	G
44	2	940	A
44	2	941	G
44	2	942	G
44	2	943	G
44	2	944	A
44	2	945	G
44	2	946	C
44	2	947	G
44	2	948	A
44	2	950	A
44	2	951	C
44	2	957	G
44	2	958	C
44	2	959	C
44	2	960	G
44	2	961	C
44	2	962	G
44	2	963	C
44	2	964	U
44	2	965	C
44	2	966	U
44	2	967	C
44	2	968	C
44	2	969	C
44	2	970	C
44	2	971	C
44	2	972	C
44	2	973	U
44	2	974	C
44	2	975	C
44	2	976	C
44	2	977	G
44	2	978	G
44	2	1047	G
44	2	1048	G
44	2	1049	G
44	2	1050	G
44	2	1051	C
44	2	1052	C

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Mol	Chain	Res	Type
44	2	1053	G
44	2	1055	G
44	2	1056	C
44	2	1058	A
44	2	1059	C
44	2	1060	C
44	2	1062	C
44	2	1064	C
44	2	1066	C
44	2	1077	C
44	2	1079	C
44	2	1080	U
44	2	1081	C
44	2	1082	U
44	2	1083	C
44	2	1084	C
44	2	1085	C
44	2	1086	A
44	2	1087	C
44	2	1089	C
44	2	1090	C
44	2	1096	C
44	2	1142	G
44	2	1143	G
44	2	1144	G
44	2	1145	G
44	2	1146	G
44	2	1147	C
44	2	1148	G
44	2	1149	G
44	2	1159	U
44	2	1160	C
44	2	1161	C
44	2	1162	C
44	2	1165	G
44	2	1173	C
44	2	1174	G
44	2	1176	G
44	2	1177	C
44	2	1178	G
44	2	1179	G
44	2	1186	C

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Mol	Chain	Res	Type
44	2	1187	C
44	2	1188	G
44	2	1189	U
44	2	1190	C
44	2	1192	G
44	2	1193	G
44	2	1194	C
44	2	1195	C
44	2	1196	C
44	2	1197	G
44	2	1198	G
44	2	1199	G
44	2	1201	G
44	2	1202	A
44	2	1204	G
44	2	1205	U
44	2	1206	U
44	2	1207	C
44	2	1208	U
44	2	1209	C
44	2	1210	U
44	2	1212	G
44	2	1214	G
44	2	1215	G
44	2	1216	C
44	2	1217	C
44	2	1218	A
44	2	1219	C
44	2	1220	G
44	2	1221	C
44	2	1223	C
44	2	1224	G
44	2	1225	C
44	2	1242	G
44	2	1245	G
44	2	1246	G
44	2	1247	C
44	2	1248	G
44	2	1249	G
44	2	1250	A
44	2	1251	G
44	2	1254	A

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Mol	Chain	Res	Type
44	2	1255	G
44	2	1256	C
44	2	1258	C
44	2	1259	A
44	2	1262	G
44	2	1263	G
44	2	1264	G
44	2	1267	G
44	2	1268	G
44	2	1273	G
44	2	1274	A
44	2	1276	G
44	2	1277	U
44	2	1279	G
44	2	1280	G
44	2	1281	C
44	2	1282	U
44	2	1283	A
44	2	1284	C
44	2	1285	C
44	2	1287	A
44	2	1289	C
44	2	1290	C
44	2	1292	A
44	2	1293	C
44	2	1294	C
44	2	1297	U
44	2	1299	U
44	2	1300	U
44	2	1301	G
44	2	1302	A
44	2	1303	A
44	2	1305	C
44	2	1306	A
44	2	1308	G
44	2	1313	A
44	2	1314	A
44	2	1318	G
44	2	1323	A
44	2	1324	C
44	2	1326	C
44	2	1329	G

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Mol	Chain	Res	Type
44	2	1332	C
44	2	1334	A
44	2	1336	U
44	2	1337	C
44	2	1338	G
44	2	1339	G
44	2	1340	G
44	2	1341	G
44	2	1349	C
44	2	1350	G
44	2	1351	A
44	2	1354	G
44	2	1356	C
44	2	1357	G
44	2	1358	C
44	2	1359	C
44	2	1360	G
44	2	1361	U
44	2	1366	C
44	2	1367	A
44	2	1368	A
44	2	1372	A
44	2	1374	G
44	2	1376	G
44	2	1377	A
44	2	1378	A
44	2	1384	G
44	2	1388	G
44	2	1389	C
44	2	1390	U
44	2	1392	G
44	2	1393	C
44	2	1398	C
44	2	1399	G
44	2	1400	A
44	2	1401	G
44	2	1402	G
44	2	1406	G
44	2	1409	C
44	2	1410	C
44	2	1412	G
44	2	1416	C

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Mol	Chain	Res	Type
44	2	1417	C
44	2	1418	U
44	2	1419	C
44	2	1420	U
44	2	1421	C
44	2	1422	C
44	2	1423	A
44	2	1424	G
44	2	1426	C
44	2	1428	G
44	2	1433	G
44	2	1434	G
44	2	1436	G
44	2	1438	A
44	2	1444	G
44	2	1445	G
44	2	1446	C
44	2	1449	G
44	2	1452	U
44	2	1454	G
44	2	1455	C
44	2	1459	C
44	2	1460	C
44	2	1461	G
44	2	1463	G
44	2	1464	C
44	2	1465	C
44	2	1466	G
44	2	1467	G
44	2	1468	G
44	2	1471	G
44	2	1476	A
44	2	1477	G
44	2	1478	C
44	2	1479	A
44	2	1480	C
44	2	1481	G
44	2	1482	A
44	2	1483	G
44	2	1484	C
44	2	1487	A
44	2	1488	C

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Mol	Chain	Res	Type
44	2	1493	U
44	2	1495	G
44	2	1498	C
44	2	1499	C
44	2	1500	C
44	2	1502	A
44	2	1503	A
44	2	1504	A
44	2	1505	G
44	2	1513	A
44	2	1518	G
44	2	1520	C
44	2	1521	U
44	2	1522	G
44	2	1523	G
44	2	1524	G
44	2	1526	A
44	2	1530	C
44	2	1531	G
44	2	1532	A
44	2	1533	A
44	2	1537	A
44	2	1540	G
44	2	1541	G
44	2	1542	A
44	2	1543	A
44	2	1544	A
44	2	1545	C
44	2	1550	G
44	2	1553	G
44	2	1554	A
44	2	1555	G
44	2	1556	G
44	2	1557	U
44	2	1558	C
44	2	1561	U
44	2	1567	U
44	2	1570	U
44	2	1571	G
44	2	1572	A
44	2	1573	C
44	2	1574	G

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Mol	Chain	Res	Type
44	2	1575	U
44	2	1576	G
44	2	1580	A
44	2	1582	C
44	2	1583	G
44	2	1585	U
44	2	1590	C
44	2	1591	G
44	2	1593	C
44	2	1595	U
44	2	1596	G
44	2	1597	G
44	2	1599	U
44	2	1600	A
44	2	1603	G
44	2	1604	G
44	2	1607	C
44	2	1609	A
44	2	1610	A
44	2	1611	A
44	2	1612	G
44	2	1613	A
44	2	1614	C
44	2	1615	U
44	2	1616	A
44	2	1617	A
44	2	1620	G
44	2	1623	C
44	2	1629	A
44	2	1630	G
44	2	1631	U
44	2	1633	G
44	2	1635	U
44	2	1637	G
44	2	1639	U
44	2	1640	C
44	2	1644	C
44	2	1648	A
44	2	1649	G
44	2	1650	U
44	2	1651	U
44	2	1653	C

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Mol	Chain	Res	Type
44	2	1654	C
44	2	1655	C
44	2	1656	U
44	2	1657	C
44	2	1658	A
44	2	1659	G
44	2	1660	G
44	2	1661	A
44	2	1663	A
44	2	1666	U
44	2	1667	G
44	2	1669	C
44	2	1671	C
44	2	1672	U
44	2	1673	C
44	2	1701	C
44	2	1703	G
44	2	1704	U
44	2	1706	U
44	2	1709	U
44	2	1710	C
44	2	1711	C
44	2	1712	G
44	2	1713	G
44	2	1714	U
44	2	1715	A
44	2	1719	C
44	2	1721	A
44	2	1725	A
44	2	1726	U
44	2	1727	U
44	2	1729	G
44	2	1730	A
44	2	1732	G
44	2	1733	U
44	2	1734	C
44	2	1736	U
44	2	1737	G
44	2	1743	G
44	2	1744	A
44	2	1745	A
44	2	1746	A

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Mol	Chain	Res	Type
44	2	1747	C
44	2	1749	A
44	2	1752	U
44	2	1754	A
44	2	1755	A
44	2	1757	C
44	2	1758	U
44	2	1759	A
44	2	1760	U
44	2	1761	U
44	2	1766	A
44	2	1768	C
44	2	1772	A
44	2	1773	A
44	2	1775	U
44	2	1779	U
44	2	1780	A
44	2	1781	A
44	2	1783	A
44	2	1784	A
44	2	1785	G
44	2	1786	C
44	2	1787	C
44	2	1789	G
44	2	1790	G
44	2	1792	U
44	2	1793	C
44	2	1794	G
44	2	1795	C
44	2	1796	U
44	2	1797	G
44	2	1798	G
44	2	1799	C
44	2	1800	G
44	2	1801	U
44	2	1802	G
44	2	1804	A
44	2	1805	G
44	2	1806	C
44	2	1809	G
44	2	1810	G
44	2	1811	G

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Mol	Chain	Res	Type
44	2	1813	G
44	2	1815	A
44	2	1816	A
44	2	1818	G
44	2	1820	G
44	2	1821	A
44	2	1822	G
44	2	1825	C
44	2	1829	G
44	2	1832	G
44	2	1833	G
44	2	1835	C
44	2	1836	A
44	2	1839	U
44	2	1840	U
44	2	1844	U
44	2	1845	A
44	2	1846	A
44	2	1847	G
44	2	1848	C
44	2	1849	A
44	2	1852	A
44	2	1853	C
44	2	1855	G
44	2	1856	G
44	2	1857	C
44	2	1859	C
44	2	1860	U
44	2	1861	G
44	2	1865	G
44	2	1867	U
44	2	1868	G
44	2	1869	A
44	2	1870	A
44	2	1871	C
44	2	1873	G
44	2	1874	A
44	2	1875	A
44	2	1876	C
44	2	1877	G
44	2	1879	C
44	2	1880	G

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Mol	Chain	Res	Type
44	2	1881	G
44	2	1883	U
44	2	1884	U
44	2	1885	A
44	2	1886	A
44	2	1891	C
44	2	1893	C
44	2	1894	G
44	2	1895	A
44	2	1896	U
44	2	1897	G
44	2	1898	C
44	2	1899	C
44	2	1900	G
44	2	1901	A
44	2	1903	G
44	2	1911	G
44	2	1912	A
44	2	1917	A
44	2	1918	G
44	2	1919	A
44	2	1920	A
44	2	1924	G
44	2	1925	U
44	2	1926	G
44	2	1929	G
44	2	1930	G
44	2	1931	U
44	2	1935	U
44	2	1936	A
44	2	1939	G
44	2	1941	C
44	2	1942	A
44	2	2000	C
44	2	2001	C
44	2	2002	G
44	2	2004	A
44	2	2005	U
44	2	2006	C
44	2	2007	A
44	2	2009	C
44	2	2010	U

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Mol	Chain	Res	Type
44	2	2011	A
44	2	2012	G
44	2	2013	C
44	2	2014	C
44	2	2016	U
44	2	2020	A
44	2	2022	U
44	2	2023	G
44	2	2024	G
44	2	2025	A
44	2	2026	U
44	2	2027	G
44	2	2029	C
44	2	2030	G
44	2	2031	C
44	2	2032	U
44	2	2033	G
44	2	2035	A
44	2	2037	C
44	2	2039	U
44	2	2040	C
44	2	2041	G
44	2	2042	G
44	2	2043	G
44	2	2044	C
44	2	2046	C
44	2	2047	A
44	2	2048	U
44	2	2049	A
44	2	2050	C
44	2	2052	C
44	2	2056	C
44	2	2057	G
44	2	2061	C
44	2	2062	C
44	2	2064	G
44	2	2251	G
44	2	2254	G
44	2	2255	A
44	2	2257	U
44	2	2258	A
44	2	2259	G

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Mol	Chain	Res	Type
44	2	2260	G
44	2	2263	G
44	2	2264	G
44	2	2265	C
44	2	2266	C
44	2	2267	G
44	2	2268	C
44	2	2269	U
44	2	2270	G
44	2	2271	C
44	2	2273	G
44	2	2274	U
44	2	2275	G
44	2	2276	A
44	2	2277	G
44	2	2279	C
44	2	2280	U
44	2	2282	G
44	2	2283	A
44	2	2284	A
44	2	2288	U
44	2	2289	A
44	2	2290	G
44	2	2293	C
44	2	2294	G
44	2	2295	C
44	2	2296	G
44	2	2297	G
44	2	2298	G
44	2	2301	C
44	2	2302	G
44	2	2304	G
44	2	2306	G
44	2	2307	G
44	2	2308	A
44	2	2309	G
44	2	2310	G
44	2	2311	C
44	2	2315	C
44	2	2320	G
44	2	2321	U
44	2	2322	G

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Mol	Chain	Res	Type
44	2	2325	G
44	2	2326	A
44	2	2328	C
44	2	2329	U
44	2	2331	G
44	2	2332	G
44	2	2333	U
44	2	2334	G
44	2	2337	A
44	2	2344	A
44	2	2345	A
44	2	2346	U
44	2	2347	A
44	2	2348	U
44	2	2351	A
44	2	2353	A
44	2	2354	C
44	2	2355	G
44	2	2358	A
44	2	2359	A
44	2	2360	C
44	2	2361	U
44	2	2362	U
44	2	2367	G
44	2	2368	G
44	2	2369	C
44	2	2370	C
44	2	2371	G
44	2	2372	A
44	2	2373	A
44	2	2374	G
44	2	2376	G
44	2	2379	G
44	2	2380	A
44	2	2381	A
44	2	2384	G
44	2	2385	U
44	2	2386	U
44	2	2387	C
44	2	2388	C
44	2	2392	U
44	2	2393	G

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Mol	Chain	Res	Type
44	2	2394	A
44	2	2395	A
44	2	2396	C
44	2	2397	A
44	2	2398	G
44	2	2399	C
44	2	2400	A
44	2	2402	U
44	2	2403	U
44	2	2405	A
44	2	2407	C
44	2	2411	G
44	2	2412	G
44	2	2414	C
44	2	2415	A
44	2	2416	G
44	2	2418	C
44	2	2421	U
44	2	2424	U
44	2	2426	A
44	2	2427	G
44	2	2429	G
44	2	2430	A
44	2	2431	U
44	2	2433	G
44	2	2435	C
44	2	2436	G
44	2	2437	A
44	2	2440	G
44	2	2442	C
44	2	2443	G
44	2	2444	U
44	2	2445	U
44	2	2446	C
44	2	2447	C
44	2	2448	G
44	2	2449	A
44	2	2450	A
44	2	2451	G
44	2	2452	G
44	2	2453	G
44	2	2455	C

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Mol	Chain	Res	Type
44	2	2456	G
44	2	2457	G
44	2	2458	G
44	2	2462	U
44	2	2463	G
44	2	2464	G
44	2	2465	C
44	2	2466	C
44	2	2467	U
44	2	2468	C
44	2	2469	C
44	2	2477	U
44	2	2479	G
44	2	2480	G
44	2	2481	C
44	2	2482	C
44	2	2483	G
44	2	2484	A
44	2	2486	C
44	2	2490	A
44	2	2492	G
44	2	2494	A
44	2	2496	U
44	2	2499	G
44	2	2502	U
44	2	2503	C
44	2	2504	A
44	2	2507	U
44	2	2508	C
44	2	2509	C
44	2	2510	C
44	2	2511	C
44	2	2519	G
44	2	2521	G
44	2	2524	G
44	2	2525	C
44	2	2526	G
44	2	2527	G
44	2	2528	A
44	2	2529	G
44	2	2531	U
44	2	2532	G

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Mol	Chain	Res	Type
44	2	2537	C
44	2	2538	C
44	2	2544	G
44	2	2548	C
44	2	2549	C
44	2	2550	A
44	2	2552	U
44	2	2553	G
44	2	2554	C
44	2	2556	G
44	2	2557	U
44	2	2559	A
44	2	2560	C
44	2	2561	G
44	2	2562	C
44	2	2563	G
44	2	2564	A
44	2	2565	C
44	2	2566	C
44	2	2567	G
44	2	2574	G
44	2	2575	A
44	2	2576	G
44	2	2577	A
44	2	2578	A
44	2	2579	G
44	2	2582	G
44	2	2587	G
44	2	2588	A
44	2	2589	G
44	2	2590	C
44	2	2592	C
44	2	2593	C
44	2	2594	G
44	2	2596	G
44	2	2597	G
44	2	2598	A
44	2	2599	G
44	2	2601	G
44	2	2602	U
44	2	2603	U
44	2	2604	C

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Mol	Chain	Res	Type
44	2	2607	U
44	2	2608	U
44	2	2609	U
44	2	2613	U
44	2	2624	A
44	2	2625	G
44	2	2627	G
44	2	2628	C
44	2	2629	G
44	2	2630	C
44	2	2631	C
44	2	2632	C
44	2	2633	U
44	2	2635	G
44	2	2636	A
44	2	2639	G
44	2	2641	G
44	2	2642	U
44	2	2646	C
44	2	2647	C
44	2	2648	C
44	2	2651	A
44	2	2652	G
44	2	2653	A
44	2	2654	G
44	2	2658	G
44	2	2661	C
44	2	2663	G
44	2	2664	U
44	2	2665	G
44	2	2666	C
44	2	2669	U
44	2	2671	G
44	2	2672	A
44	2	2673	A
44	2	2674	A
44	2	2676	C
44	2	2677	G
44	2	2678	U
44	2	2682	G
44	2	2683	G
44	2	2684	U

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Mol	Chain	Res	Type
44	2	2685	U
44	2	2686	C
44	2	2687	C
44	2	2689	G
44	2	2692	G
44	2	2696	C
44	2	2698	G
44	2	2700	U
44	2	2701	G
44	2	2702	A
44	2	2703	G
44	2	2704	C
44	2	2705	U
44	2	2706	C
44	2	2707	U
44	2	2709	G
44	2	2710	C
44	2	2711	U
44	2	2715	C
44	2	2716	C
44	2	2717	U
44	2	2718	U
44	2	2719	G
44	2	2720	A
44	2	2729	G
44	2	2731	G
44	2	2732	A
44	2	2733	G
44	2	2734	A
44	2	2735	G
44	2	2736	G
44	2	2739	G
44	2	2740	U
44	2	2741	A
44	2	2742	A
44	2	2745	C
44	2	2746	U
44	2	2750	G
44	2	2751	C
44	2	2752	C
44	2	2755	G
44	2	2759	U

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Mol	Chain	Res	Type
44	2	2761	C
44	2	2762	C
44	2	2764	A
44	2	2765	U
44	2	2766	A
44	2	2767	U
44	2	2771	C
44	2	2772	A
44	2	2774	C
44	2	2775	A
44	2	2778	U
44	2	2780	U
44	2	2782	C
44	2	2783	A
44	2	2789	A
44	2	2791	C
44	2	2792	A
44	2	2794	C
44	2	2796	U
44	2	2801	C
44	2	2802	A
44	2	2803	U
44	2	2804	G
44	2	2805	U
44	2	2806	U
44	2	2807	G
44	2	2810	A
44	2	2811	C
44	2	2812	A
44	2	2815	G
44	2	2817	A
44	2	2818	G
44	2	2823	G
44	2	2826	A
44	2	2827	A
44	2	2828	G
44	2	2831	G
44	2	2832	G
44	2	2833	C
44	2	2835	A
44	2	2837	C
44	2	2839	G

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Mol	Chain	Res	Type
44	2	2840	G
44	2	2843	C
44	2	2844	C
44	2	2845	G
44	2	2846	U
44	2	2847	A
44	2	2848	A
44	2	2852	C
44	2	2853	G
44	2	2854	G
44	2	2857	U
44	2	2858	A
44	2	2860	G
44	2	2861	G
44	2	2863	U
44	2	2864	U
44	2	2867	C
44	2	2868	U
44	2	2869	C
44	2	2871	A
44	2	2873	G
44	2	2877	U
44	2	2878	G
44	2	2879	G
44	2	3567	C
44	2	3568	A
44	2	3570	C
44	2	3574	C
44	2	3575	U
44	2	3578	G
44	2	3579	A
44	2	3583	G
44	2	3584	G
44	2	3585	U
44	2	3586	G
44	2	3587	C
44	2	3588	G
44	2	3590	A
44	2	3594	G
44	2	3595	G
44	2	3597	G
44	2	3599	A

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Mol	Chain	Res	Type
44	2	3600	U
44	2	3602	C
44	2	3603	G
44	2	3604	A
44	2	3605	C
44	2	3610	U
44	2	3611	A
44	2	3612	A
44	2	3613	U
44	2	3617	A
44	2	3618	A
44	2	3619	C
44	2	3622	A
44	2	3624	C
44	2	3626	U
44	2	3627	C
44	2	3631	A
44	2	3634	G
44	2	3635	C
44	2	3636	C
44	2	3641	G
44	2	3642	C
44	2	3643	G
44	2	3646	U
44	2	3649	U
44	2	3650	G
44	2	3651	A
44	2	3652	C
44	2	3653	G
44	2	3654	C
44	2	3655	G
44	2	3657	U
44	2	3658	G
44	2	3661	A
44	2	3662	U
44	2	3664	U
44	2	3665	C
44	2	3666	U
44	2	3667	G
44	2	3668	C
44	2	3675	C
44	2	3676	U

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Mol	Chain	Res	Type
44	2	3678	U
44	2	3679	G
44	2	3680	A
44	2	3681	A
44	2	3682	U
44	2	3683	G
44	2	3684	U
44	2	3685	C
44	2	3686	A
44	2	3693	A
44	2	3695	A
44	2	3696	A
44	2	3697	A
44	2	3700	C
44	2	3706	A
44	2	3710	C
44	2	3717	A
44	2	3720	G
44	2	3722	G
44	2	3723	G
44	2	3724	G
44	2	3725	A
44	2	3726	G
44	2	3727	U
44	2	3728	A
44	2	3729	A
44	2	3730	C
44	2	3732	A
44	2	3733	U
44	2	3734	G
44	2	3736	C
44	2	3737	U
44	2	3741	U
44	2	3743	A
44	2	3744	A
44	2	3746	G
44	2	3749	G
44	2	3750	C
44	2	3751	C
44	2	3753	A
44	2	3754	A
44	2	3755	U

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Mol	Chain	Res	Type
44	2	3756	G
44	2	3759	U
44	2	3761	G
44	2	3764	A
44	2	3765	U
44	2	3767	U
44	2	3768	A
44	2	3769	A
44	2	3770	U
44	2	3771	U
44	2	3772	A
44	2	3776	A
44	2	3778	G
44	2	3779	C
44	2	3780	G
44	2	3781	C
44	2	3782	A
44	2	3786	A
44	2	3787	U
44	2	3788	G
44	2	3792	G
44	2	3793	A
44	2	3797	A
44	2	3798	G
44	2	3799	A
44	2	3800	U
44	2	3801	U
44	2	3802	C
44	2	3803	C
44	2	3807	U
44	2	3808	G
44	2	3809	U
44	2	3814	A
44	2	3815	C
44	2	3819	C
44	2	3826	G
44	2	3830	A
44	2	3833	C
44	2	3834	A
44	2	3836	A
44	2	3837	G
44	2	3838	C

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Mol	Chain	Res	Type
44	2	3845	A
44	2	3846	A
44	2	3847	C
44	2	3848	G
44	2	3850	G
44	2	3852	U
44	2	3854	G
44	2	3856	C
44	2	3857	G
44	2	3858	G
44	2	3859	A
44	2	3863	A
44	2	3866	G
44	2	3867	G
44	2	3870	A
44	2	3871	A
44	2	3872	A
44	2	3873	G
44	2	3874	A
44	2	3875	A
44	2	3876	G
44	2	3877	A
44	2	3879	C
44	2	3883	U
44	2	3884	U
44	2	3885	G
44	2	3887	G
44	2	3888	C
44	2	3890	U
44	2	3891	G
44	2	3894	U
44	2	3895	C
44	2	3897	A
44	2	3898	G
44	2	3905	A
44	2	3907	G
44	2	3908	G
44	2	3910	G
44	2	3911	A
44	2	3913	G
44	2	3914	A
44	2	3919	U

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Mol	Chain	Res	Type
44	2	3922	G
44	2	3923	A
44	2	3924	G
44	2	3925	G
44	2	3926	U
44	2	3927	G
44	2	3931	A
44	2	3933	U
44	2	3934	A
44	2	3936	G
44	2	3938	G
44	2	3941	A
44	2	3942	G
44	2	3943	G
44	2	3945	C
44	2	4007	G
44	2	4008	C
44	2	4009	C
44	2	4011	G
44	2	4012	U
44	2	4015	A
44	2	4018	A
44	2	4024	A
44	2	4025	C
44	2	4026	U
44	2	4027	C
44	2	4029	G
44	2	4032	C
44	2	4033	G
44	2	4036	U
44	2	4037	U
44	2	4041	A
44	2	4044	G
44	2	4045	A
44	2	4046	C
44	2	4047	C
44	2	4050	G
44	2	4051	U
44	2	4052	G
44	2	4053	A
44	2	4054	G
44	2	4055	G

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Mol	Chain	Res	Type
44	2	4056	C
44	2	4057	G
44	2	4059	G
44	2	4060	G
44	2	4063	G
44	2	4066	A
44	2	4068	C
44	2	4069	C
44	2	4070	C
44	2	4071	G
44	2	4073	G
44	2	4074	G
44	2	4079	C
44	2	4080	U
44	2	4081	C
44	2	4082	G
44	2	4083	C
44	2	4084	U
44	2	4085	U
44	2	4086	C
44	2	4087	U
44	2	4089	G
44	2	4090	C
44	2	4092	C
44	2	4093	C
44	2	4094	A
44	2	4101	C
44	2	4103	C
44	2	4105	C
44	2	4106	G
44	2	4108	C
44	2	4109	C
44	2	4111	G
44	2	4117	A
44	2	4118	C
44	2	4119	C
44	2	4120	C
44	2	4121	G
44	2	4122	C
44	2	4123	U
44	2	4124	C
44	2	4126	G

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Mol	Chain	Res	Type
44	2	4129	G
44	2	4130	A
44	2	4131	C
44	2	4135	G
44	2	4137	C
44	2	4138	A
44	2	4142	G
44	2	4143	G
44	2	4144	G
44	2	4145	G
44	2	4151	G
44	2	4155	G
44	2	4156	G
44	2	4159	C
44	2	4163	A
44	2	4164	C
44	2	4165	A
44	2	4166	C
44	2	4168	U
44	2	4174	A
44	2	4175	C
44	2	4176	G
44	2	4177	G
44	2	4179	A
44	2	4180	A
44	2	4181	C
44	2	4182	G
44	2	4185	G
44	2	4186	G
44	2	4187	U
44	2	4188	G
44	2	4189	U
44	2	4190	C
44	2	4191	C
44	2	4192	U
44	2	4193	A
44	2	4194	A
44	2	4195	G
44	2	4199	A
44	2	4200	G
44	2	4201	C
44	2	4210	G

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Mol	Chain	Res	Type
44	2	4211	A
44	2	4212	C
44	2	4214	G
44	2	4215	A
44	2	4226	G
44	2	4227	G
44	2	4231	A
44	2	4232	G
44	2	4233	A
44	2	4234	A
44	2	4236	G
44	2	4237	G
44	2	4239	A
44	2	4240	A
44	2	4241	A
44	2	4242	A
44	2	4245	U
44	2	4247	G
44	2	4250	U
44	2	4251	G
44	2	4252	A
44	2	4253	U
44	2	4254	C
44	2	4255	U
44	2	4256	U
44	2	4261	U
44	2	4262	U
44	2	4263	C
44	2	4264	A
44	2	4265	G
44	2	4266	U
44	2	4267	A
44	2	4269	G
44	2	4270	A
44	2	4271	A
44	2	4273	A
44	2	4276	G
44	2	4277	A
44	2	4279	C
44	2	4280	G
44	2	4283	A
44	2	4286	G

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Mol	Chain	Res	Type
44	2	4287	C
44	2	4288	G
44	2	4289	G
44	2	4290	G
44	2	4291	G
44	2	4292	C
44	2	4293	C
44	2	4297	C
44	2	4298	G
44	2	4301	C
44	2	4303	U
44	2	4304	U
44	2	4305	C
44	2	4306	U
44	2	4308	A
44	2	4309	C
44	2	4313	U
44	2	4314	U
44	2	4315	G
44	2	4316	G
44	2	4317	G
44	2	4319	U
44	2	4321	U
44	2	4324	G
44	2	4326	A
44	2	4327	G
44	2	4328	G
44	2	4329	A
44	2	4331	G
44	2	4333	G
44	2	4335	C
44	2	4336	A
44	2	4337	G
44	2	4338	A
44	2	4339	A
44	2	4341	A
44	2	4342	G
44	2	4345	A
44	2	4346	C
44	2	4347	C
44	2	4348	A
44	2	4350	A

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Mol	Chain	Res	Type
44	2	4353	G
44	2	4354	A
44	2	4355	U
44	2	4357	A
44	2	4359	U
44	2	4362	C
44	2	4363	U
44	2	4366	U
44	2	4367	G
44	2	4370	G
44	2	4372	C
44	2	4373	C
44	2	4375	A
44	2	4376	G
44	2	4377	C
44	2	4379	U
44	2	4380	U
44	2	4382	A
44	2	4383	U
44	2	4384	A
44	2	4386	C
44	2	4387	G
44	2	4388	A
44	2	4389	C
44	2	4390	G
44	2	4394	C
44	2	4396	U
44	2	4397	U
44	2	4401	A
44	2	4404	C
44	2	4406	U
44	2	4407	C
44	2	4408	G
44	2	4409	A
44	2	4410	U
44	2	4411	G
44	2	4412	U
44	2	4413	C
44	2	4415	G
44	2	4416	C
44	2	4420	U
44	2	4421	C

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Mol	Chain	Res	Type
44	2	4422	C
44	2	4423	U
44	2	4424	A
44	2	4425	U
44	2	4426	C
44	2	4431	U
44	2	4433	A
44	2	4434	A
44	2	4435	G
44	2	4437	A
44	2	4438	G
44	2	4448	A
44	2	4449	G
44	2	4451	G
44	2	4452	U
44	2	4453	U
44	2	4454	G
44	2	4455	G
44	2	4456	A
44	2	4457	U
44	2	4458	U
44	2	4459	G
44	2	4460	U
44	2	4461	U
44	2	4465	C
44	2	4466	C
44	2	4470	A
44	2	4472	U
44	2	4473	A
44	2	4474	G
44	2	4477	A
44	2	4478	A
44	2	4479	C
44	2	4480	G
44	2	4482	G
44	2	4483	A
44	2	4484	G
44	2	4488	G
44	2	4489	G
44	2	4491	U
44	2	4492	U
44	2	4494	G

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Mol	Chain	Res	Type
44	2	4498	G
44	2	4499	U
44	2	4500	C
44	2	4502	U
44	2	4503	G
44	2	4505	G
44	2	4507	C
44	2	4508	A
44	2	4509	G
44	2	4510	G
44	2	4512	U
44	2	4515	U
44	2	4516	U
44	2	4519	A
44	2	4520	C
44	2	4521	C
44	2	4522	C
44	2	4525	C
44	2	4526	U
44	2	4527	G
44	2	4528	A
44	2	4529	U
44	2	4530	G
44	2	4532	U
44	2	4533	G
44	2	4534	U
44	2	4535	G
44	2	4536	U
44	2	4538	G
44	2	4539	U
44	2	4541	G
44	2	4543	C
44	2	4544	A
44	2	4545	U
44	2	4549	A
44	2	4550	A
44	2	4551	U
44	2	4552	C
44	2	4557	U
44	2	4558	C
44	2	4560	G
44	2	4561	U

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Mol	Chain	Res	Type
44	2	4562	A
44	2	4563	C
44	2	4566	G
44	2	4567	A
44	2	4568	G
44	2	4569	G
44	2	4570	A
44	2	4577	G
44	2	4578	G
44	2	4579	U
44	2	4580	U
44	2	4583	G
44	2	4584	A
44	2	4586	A
44	2	4587	U
44	2	4592	U
44	2	4594	U
44	2	4595	A
44	2	4596	U
44	2	4597	G
44	2	4598	U
44	2	4599	G
44	2	4600	C
44	2	4601	U
44	2	4602	U
44	2	4604	G
44	2	4609	G
44	2	4610	G
44	2	4612	G
44	2	4613	C
44	2	4615	A
44	2	4616	A
44	2	4617	U
44	2	4618	G
44	2	4621	G
44	2	4622	C
44	2	4628	U
44	2	4629	A
44	2	4630	C
44	2	4632	A
44	2	4636	G
44	2	4637	U

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Mol	Chain	Res	Type
44	2	4638	G
44	2	4639	G
44	2	4640	G
44	2	4641	A
44	2	4642	U
44	2	4643	U
44	2	4646	G
44	2	4651	A
44	2	4654	G
44	2	4655	C
44	2	4657	U
44	2	4658	C
44	2	4659	U
44	2	4660	A
44	2	4661	A
44	2	4664	C
44	2	4665	A
44	2	4668	A
44	2	4669	U
44	2	4671	C
44	2	4672	C
44	2	4675	C
44	2	4676	C
44	2	4678	G
44	2	4679	G
44	2	4680	C
44	2	4681	G
44	2	4682	A
44	2	4684	C
44	2	4688	A
44	2	4689	C
44	2	4690	G
44	2	4691	G
44	2	4692	C
44	2	4693	A
44	2	4694	G
44	2	4696	G
44	2	4698	C
44	2	4699	G
44	2	4700	C
44	2	4701	G
44	2	4706	C

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Mol	Chain	Res	Type
44	2	4710	G
44	2	4711	U
44	2	4712	U
44	2	4713	G
44	2	4714	G
44	2	4716	C
44	2	4718	C
44	2	4719	G
44	2	4720	G
44	2	4721	A
44	2	4723	A
44	2	4724	G
44	2	4725	C
44	2	4726	C
44	2	4733	C
44	2	4734	C
44	2	4735	G
44	2	4736	C
44	2	4739	G
44	2	4740	U
44	2	4741	C
44	2	4742	C
44	2	4746	C
44	2	4803	C
44	2	4804	G
44	2	4807	C
44	2	4808	C
44	2	4809	G
44	2	4812	A
44	2	4813	C
44	2	4814	C
44	2	4815	G
44	2	4816	G
44	2	4822	G
44	2	4824	U
44	2	4825	G
44	2	4826	C
44	2	4827	G
44	2	4828	G
44	2	4829	A
44	2	4831	U
44	2	4832	G

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Mol	Chain	Res	Type
44	2	4834	C
44	2	4836	U
44	2	4838	C
44	2	4839	G
44	2	4840	U
44	2	4844	G
44	2	4847	A
44	2	4848	A
44	2	4849	A
44	2	4850	C
44	2	4851	G
44	2	4852	G
44	2	4853	G
44	2	4854	G
44	2	4855	C
44	2	4856	G
44	2	4857	C
44	2	4858	G
44	2	4862	G
44	2	4863	G
44	2	4867	G
44	2	4868	G
44	2	4875	C
44	2	4879	C
44	2	4880	U
44	2	4881	C
44	2	4882	G
44	2	4883	C
44	2	4892	C
44	2	4893	A
44	2	4894	C
44	2	4895	C
44	2	4896	G
44	2	4897	C
44	2	4898	A
44	2	4899	C
44	2	4900	G
44	2	4901	U
44	2	4902	U
44	2	4903	C
44	2	4904	G
44	2	4905	U

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Mol	Chain	Res	Type
44	2	4906	G
44	2	4919	C
44	2	4921	A
44	2	4923	A
44	2	4924	C
44	2	4930	G
44	2	4931	U
44	2	4932	A
44	2	4940	U
44	2	4943	U
44	2	4944	U
44	2	4945	C
44	2	4946	U
44	2	4947	G
44	2	4949	G
44	2	4955	G
44	2	4956	U
44	2	4958	U
44	2	4959	C
44	2	4960	G
44	2	4962	A
44	2	4963	C
44	2	4968	C
44	2	4969	A
44	2	4972	G
44	2	4974	A
44	2	4975	G
44	2	4976	C
44	2	4978	C
44	2	4979	C
44	2	4980	C
44	2	4981	U
44	2	4982	C
44	2	4983	G
44	2	4985	U
44	2	4986	G
44	2	4988	G
44	2	4995	U
44	2	4996	G
44	2	4998	A
44	2	5002	C
44	2	5003	A

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Mol	Chain	Res	Type
44	2	5005	C
44	2	5009	C
44	2	5010	G
44	2	5015	A
44	2	5016	A
44	2	5017	G
44	2	5018	G
44	2	5019	G
44	2	5020	U
44	2	5021	U
45	3	4	C
45	3	6	C
45	3	7	U
45	3	8	U
45	3	9	A
45	3	10	G
45	3	12	G
45	3	13	G
45	3	14	U
45	3	16	G
45	3	20	A
45	3	23	C
45	3	24	G
45	3	25	G
45	3	26	C
45	3	28	C
45	3	30	U
45	3	32	C
45	3	34	U
45	3	38	U
45	3	43	A
45	3	47	C
45	3	49	G
45	3	51	U
45	3	52	A
45	3	58	G
45	3	59	A
45	3	61	A
45	3	62	A
45	3	63	U
45	3	69	U
45	3	71	A

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Mol	Chain	Res	Type
45	3	72	A
45	3	75	G
45	3	76	C
45	3	77	A
45	3	78	G
45	3	80	A
45	3	81	C
45	3	82	A
45	3	83	C
45	3	84	A
45	3	85	U
45	3	86	U
45	3	89	U
45	3	94	G
45	3	95	A
45	3	103	A
45	3	104	A
45	3	105	C
45	3	106	G
45	3	107	C
45	3	109	C
45	3	111	U
45	3	112	G
45	3	114	G
45	3	117	C
45	3	120	G
45	3	122	G
45	3	123	U
45	3	124	U
45	3	125	C
45	3	126	C
45	3	128	C
45	3	129	C
45	3	130	C
45	3	131	G
45	3	137	A
45	3	138	C
45	3	140	C
45	3	141	C
45	3	143	G
45	3	144	U
45	3	146	U

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Mol	Chain	Res	Type
45	3	147	G
45	3	148	A
45	3	149	G
45	3	150	C
45	3	151	G
45	3	156	U
45	3	157	U
46	4	3	C
46	4	6	C
46	4	7	G
46	4	9	C
46	4	10	C
46	4	11	A
46	4	12	U
46	4	13	A
46	4	15	C
46	4	19	C
46	4	22	A
46	4	27	G
46	4	28	C
46	4	29	C
46	4	30	C
46	4	33	U
46	4	34	C
46	4	35	U
46	4	36	C
46	4	40	U
46	4	41	G
46	4	46	C
46	4	47	G
46	4	48	G
46	4	49	A
46	4	53	U
46	4	54	A
46	4	55	A
46	4	56	G
46	4	57	C
46	4	58	A
46	4	61	G
46	4	62	U
46	4	63	C
46	4	64	G

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Mol	Chain	Res	Type
46	4	65	G
46	4	67	C
46	4	68	C
46	4	69	U
46	4	73	U
46	4	74	A
46	4	75	G
46	4	76	U
46	4	77	A
46	4	79	U
46	4	81	G
46	4	85	G
46	4	86	G
46	4	87	G
46	4	89	G
46	4	91	C
46	4	94	C
46	4	95	C
46	4	96	U
46	4	97	G
46	4	99	G
46	4	100	A
46	4	101	A
46	4	103	A
46	4	105	C
46	4	107	G
46	4	108	G
46	4	109	U
46	4	110	G
46	4	113	G
46	4	116	G
46	4	117	G
46	4	118	C

All (340) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	2	13	U
44	2	14	C
44	2	19	G
44	2	48	G
44	2	64	A

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Mol	Chain	Res	Type
44	2	69	A
44	2	70	A
44	2	96	U
44	2	156	C
44	2	181	U
44	2	188	G
44	2	192	C
44	2	193	C
44	2	196	G
44	2	207	C
44	2	212	C
44	2	215	A
44	2	216	G
44	2	221	U
44	2	229	G
44	2	266	C
44	2	287	A
44	2	292	G
44	2	300	C
44	2	328	U
44	2	331	C
44	2	333	G
44	2	334	C
44	2	342	C
44	2	371	U
44	2	379	A
44	2	381	C
44	2	386	A
44	2	398	A
44	2	402	G
44	2	424	A
44	2	433	G
44	2	441	G
44	2	443	A
44	2	444	G
44	2	458	U
44	2	459	U
44	2	460	C
44	2	461	A
44	2	462	A
44	2	473	G
44	2	474	G

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Mol	Chain	Res	Type
44	2	477	C
44	2	482	G
44	2	633	G
44	2	658	G
44	2	717	G
44	2	718	G
44	2	719	G
44	2	720	A
44	2	721	A
44	2	727	G
44	2	736	G
44	2	897	U
44	2	914	G
44	2	916	A
44	2	927	A
44	2	928	A
44	2	939	G
44	2	941	G
44	2	943	G
44	2	944	A
44	2	947	G
44	2	957	G
44	2	959	C
44	2	967	C
44	2	973	U
44	2	974	C
44	2	1082	U
44	2	1147	C
44	2	1177	C
44	2	1193	G
44	2	1196	C
44	2	1197	G
44	2	1204	G
44	2	1205	U
44	2	1207	C
44	2	1208	U
44	2	1209	C
44	2	1211	C
44	2	1216	C
44	2	1217	C
44	2	1218	A
44	2	1219	C

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Mol	Chain	Res	Type
44	2	1249	G
44	2	1280	G
44	2	1282	U
44	2	1293	C
44	2	1299	U
44	2	1304	A
44	2	1340	G
44	2	1349	C
44	2	1357	G
44	2	1358	C
44	2	1360	G
44	2	1367	A
44	2	1377	A
44	2	1388	G
44	2	1400	A
44	2	1421	C
44	2	1423	A
44	2	1444	G
44	2	1453	C
44	2	1458	G
44	2	1475	G
44	2	1476	A
44	2	1478	C
44	2	1481	G
44	2	1497	A
44	2	1502	A
44	2	1523	G
44	2	1530	C
44	2	1532	A
44	2	1553	G
44	2	1554	A
44	2	1604	G
44	2	1612	G
44	2	1619	C
44	2	1628	U
44	2	1639	U
44	2	1659	G
44	2	1673	C
44	2	1703	G
44	2	1732	G
44	2	1744	A
44	2	1745	A

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Mol	Chain	Res	Type
44	2	1756	C
44	2	1783	A
44	2	1786	C
44	2	1802	G
44	2	1805	G
44	2	1836	A
44	2	1846	A
44	2	1855	G
44	2	1859	C
44	2	1860	U
44	2	1868	G
44	2	1870	A
44	2	1874	A
44	2	1883	U
44	2	1885	A
44	2	1900	G
44	2	1916	C
44	2	1918	G
44	2	1924	G
44	2	1930	G
44	2	2000	C
44	2	2003	A
44	2	2006	C
44	2	2009	C
44	2	2011	A
44	2	2023	G
44	2	2024	G
44	2	2034	G
44	2	2046	C
44	2	2048	U
44	2	2270	G
44	2	2294	G
44	2	2309	G
44	2	2310	G
44	2	2324	A
44	2	2333	U
44	2	2347	A
44	2	2348	U
44	2	2358	A
44	2	2360	C
44	2	2369	C
44	2	2371	G

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Mol	Chain	Res	Type
44	2	2373	A
44	2	2375	U
44	2	2394	A
44	2	2395	A
44	2	2396	C
44	2	2405	A
44	2	2411	G
44	2	2415	A
44	2	2450	A
44	2	2454	A
44	2	2465	C
44	2	2481	C
44	2	2489	A
44	2	2502	U
44	2	2508	C
44	2	2548	C
44	2	2551	G
44	2	2561	G
44	2	2564	A
44	2	2606	C
44	2	2607	U
44	2	2650	G
44	2	2673	A
44	2	2684	U
44	2	2702	A
44	2	2703	G
44	2	2716	C
44	2	2718	U
44	2	2735	G
44	2	2740	U
44	2	2741	A
44	2	2745	C
44	2	2749	C
44	2	2802	A
44	2	2803	U
44	2	2838	C
44	2	3578	G
44	2	3583	G
44	2	3584	G
44	2	3585	U
44	2	3648	U
44	2	3666	U

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Mol	Chain	Res	Type
44	2	3684	U
44	2	3696	A
44	2	3724	G
44	2	3727	U
44	2	3729	A
44	2	3733	U
44	2	3743	A
44	2	3753	A
44	2	3754	A
44	2	3769	A
44	2	3770	U
44	2	3802	C
44	2	3821	A
44	2	3845	A
44	2	3865	C
44	2	3866	G
44	2	3873	G
44	2	3876	G
44	2	3887	G
44	2	3907	G
44	2	3926	U
44	2	3933	U
44	2	4017	U
44	2	4033	G
44	2	4043	U
44	2	4044	G
44	2	4081	C
44	2	4083	C
44	2	4084	U
44	2	4085	U
44	2	4088	G
44	2	4091	G
44	2	4105	C
44	2	4117	A
44	2	4122	C
44	2	4130	A
44	2	4155	G
44	2	4181	C
44	2	4211	A
44	2	4226	G
44	2	4236	G
44	2	4252	A

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Mol	Chain	Res	Type
44	2	4254	C
44	2	4292	C
44	2	4336	A
44	2	4338	A
44	2	4354	A
44	2	4374	A
44	2	4387	G
44	2	4388	A
44	2	4396	U
44	2	4408	G
44	2	4409	A
44	2	4433	A
44	2	4437	A
44	2	4454	G
44	2	4455	G
44	2	4485	C
44	2	4515	U
44	2	4533	G
44	2	4551	U
44	2	4561	U
44	2	4562	A
44	2	4566	G
44	2	4596	U
44	2	4597	G
44	2	4609	G
44	2	4616	A
44	2	4628	U
44	2	4636	G
44	2	4637	U
44	2	4659	U
44	2	4660	A
44	2	4675	C
44	2	4680	C
44	2	4688	A
44	2	4690	G
44	2	4692	C
44	2	4693	A
44	2	4699	G
44	2	4711	U
44	2	4712	U
44	2	4717	U
44	2	4723	A

Continued on next page...

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Mol	Chain	Res	Type
44	2	4733	C
44	2	4740	U
44	2	4807	C
44	2	4813	C
44	2	4823	G
44	2	4824	U
44	2	4825	G
44	2	4827	G
44	2	4829	A
44	2	4837	U
44	2	4847	A
44	2	4848	A
44	2	4849	A
44	2	4854	G
44	2	4862	G
44	2	4867	G
44	2	4895	C
44	2	4930	G
44	2	4943	U
44	2	4944	U
44	2	4977	U
44	2	4978	C
44	2	4980	C
44	2	5002	C
44	2	5004	G
44	2	5019	G
45	3	22	U
45	3	71	A
45	3	84	A
45	3	105	C
45	3	111	U
45	3	125	C
46	4	12	U
46	4	26	C
46	4	54	A
46	4	63	C
46	4	74	A
46	4	75	G
46	4	90	A
46	4	108	G
46	4	109	U

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

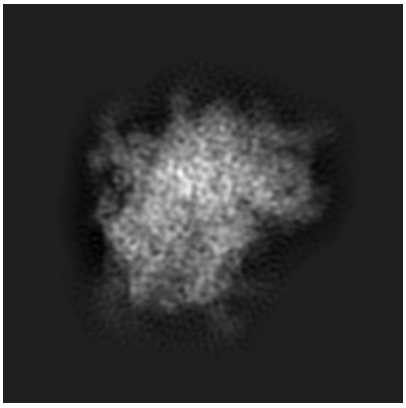
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-2813. These allow visual inspection of the internal detail of the map and identification of artifacts.

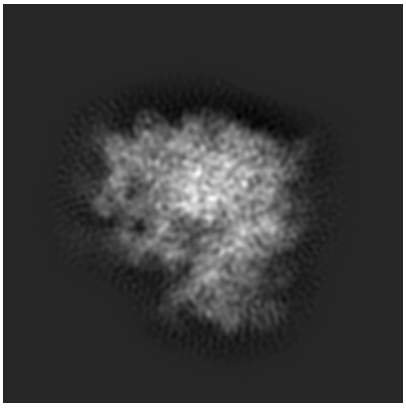
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

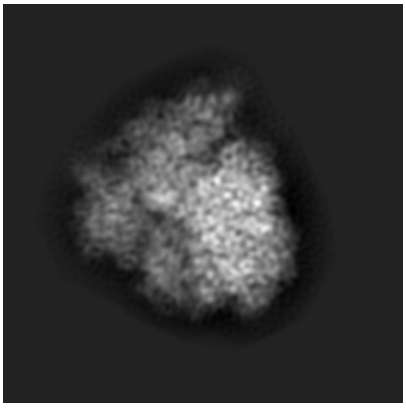
6.1.1 Primary map



X



Y

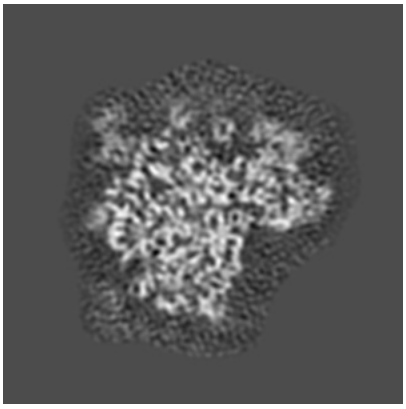


Z

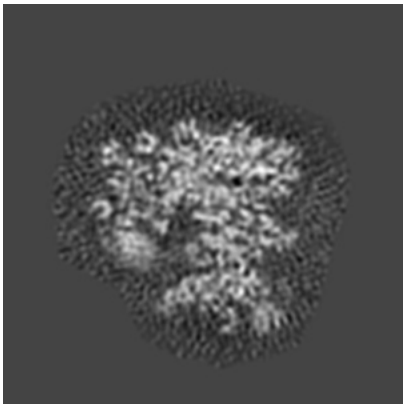
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

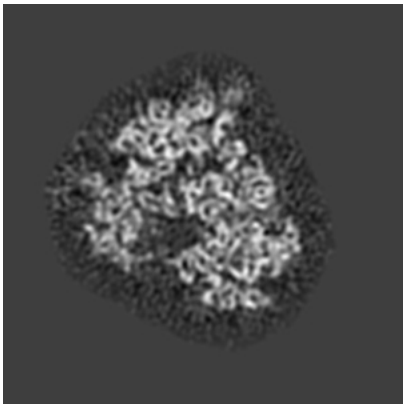
6.2.1 Primary map



X Index: 150



Y Index: 150

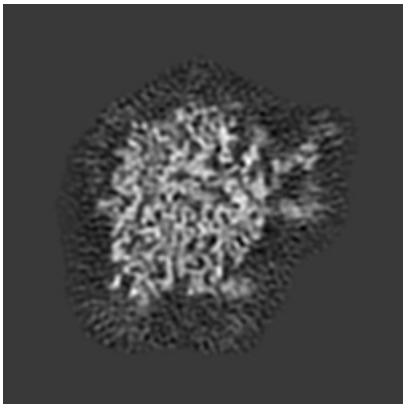


Z Index: 150

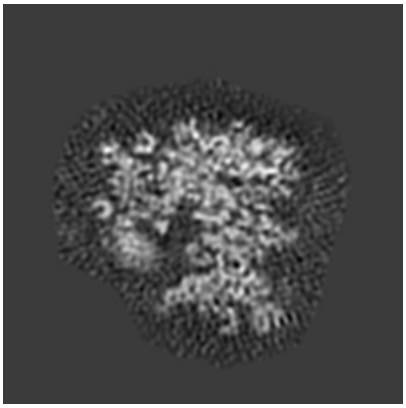
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

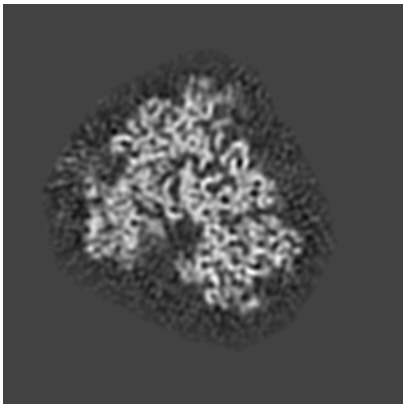
6.3.1 Primary map



X Index: 172



Y Index: 149



Z Index: 154

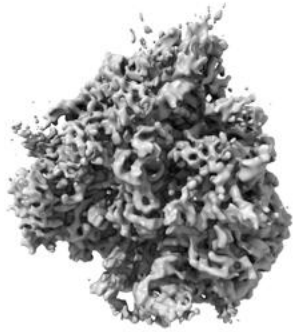
The images above show the largest variance slices of the map in three orthogonal directions.

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

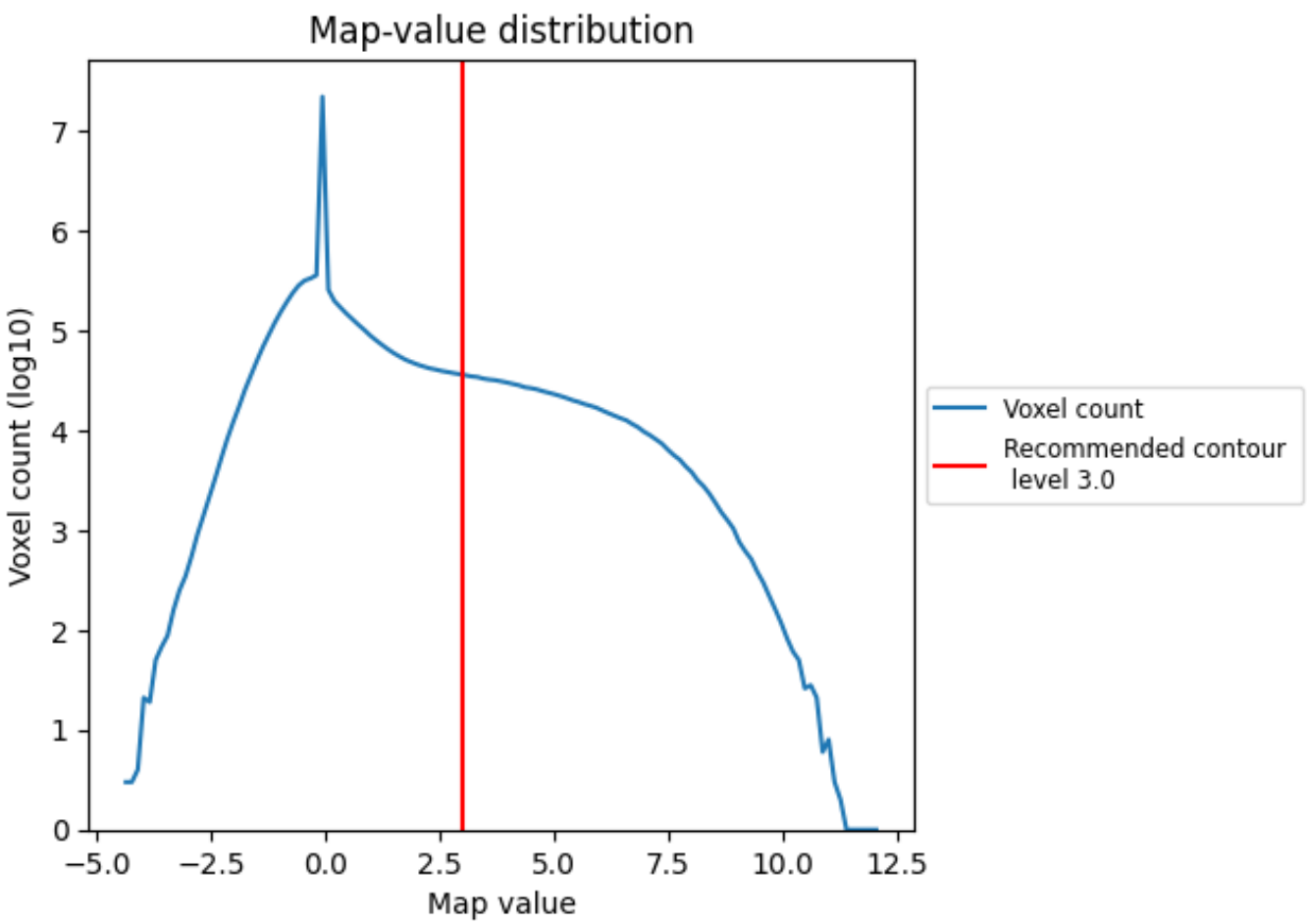
6.5 Mask visualisation (i)

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

7 Map analysis (i)

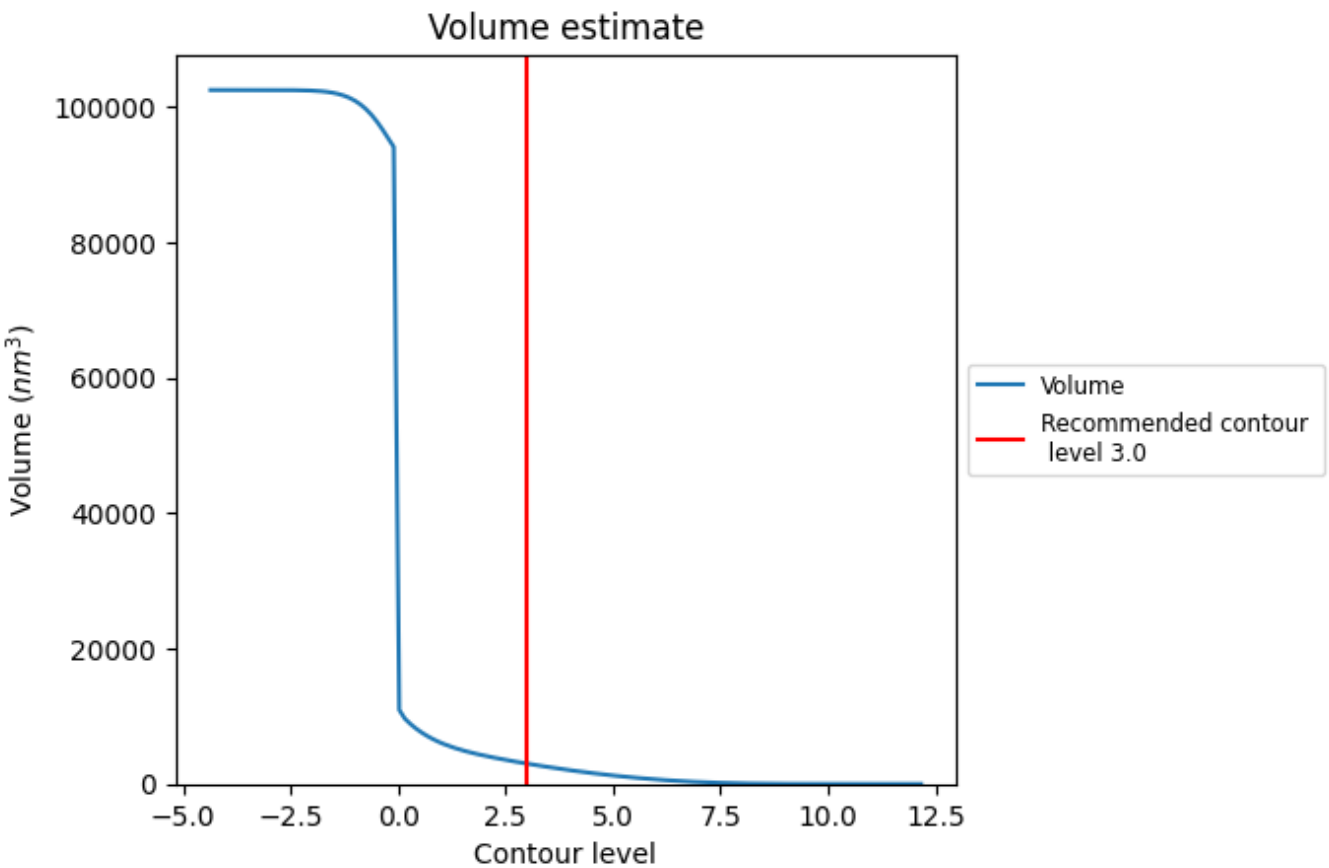
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

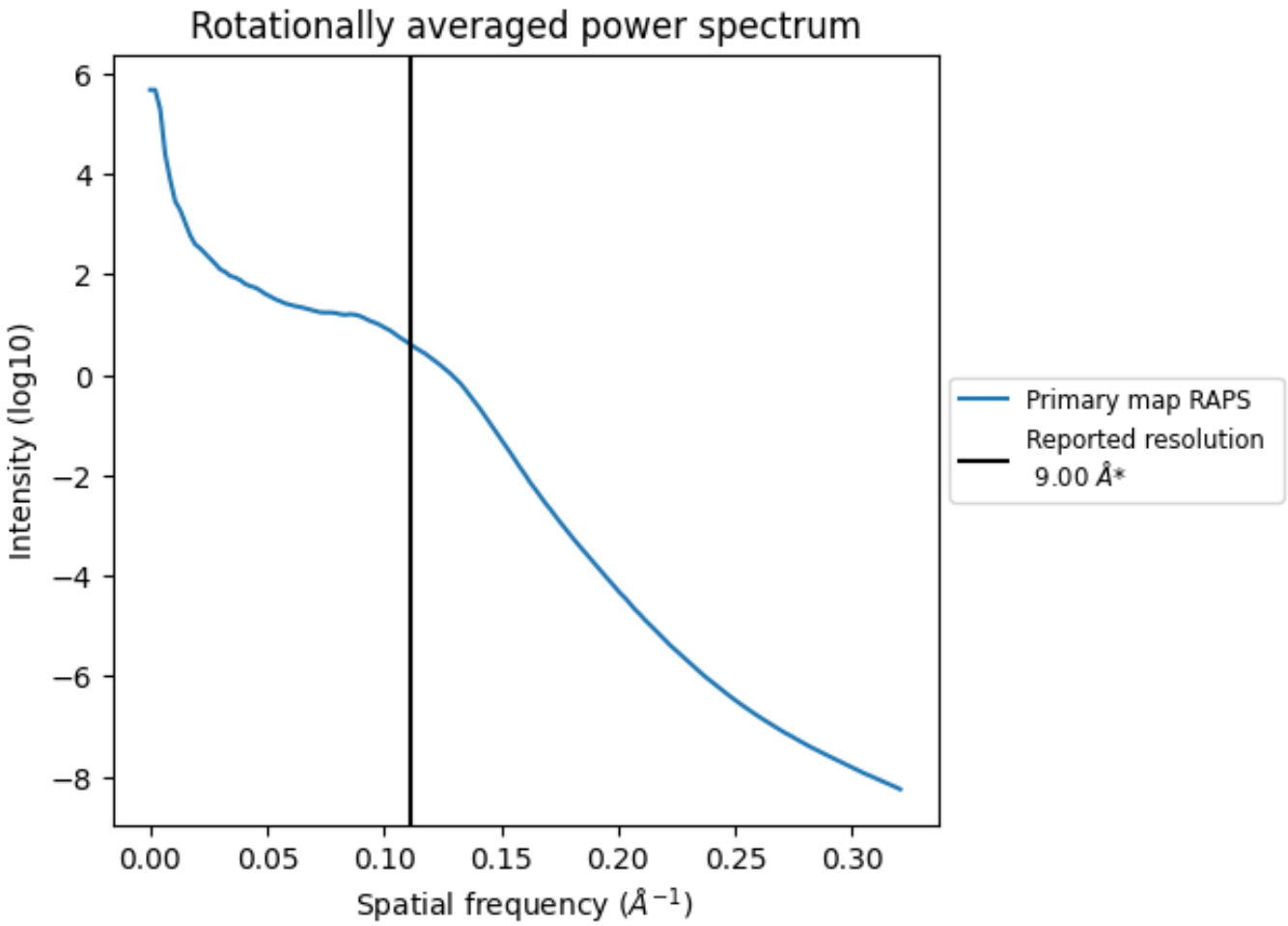
7.2 Volume estimate (i)



The volume at the recommended contour level is 3001 nm^3; this corresponds to an approximate mass of 2711 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 0.111 Å^{-1}

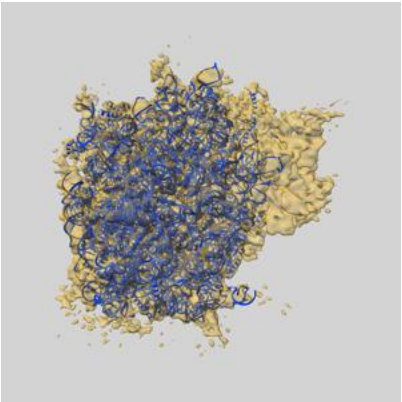
8 Fourier-Shell correlation (i)

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

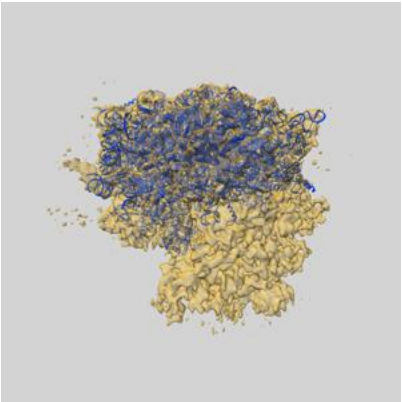
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2813 and PDB model 4D67. Per-residue inclusion information can be found in section 3 on page 12.

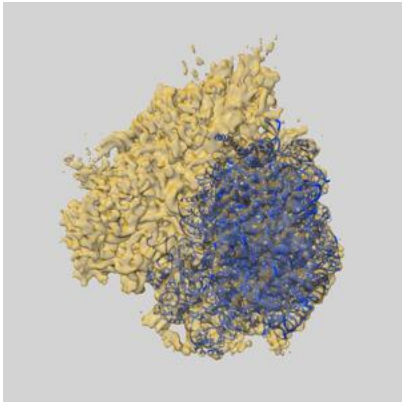
9.1 Map-model overlay (i)



X



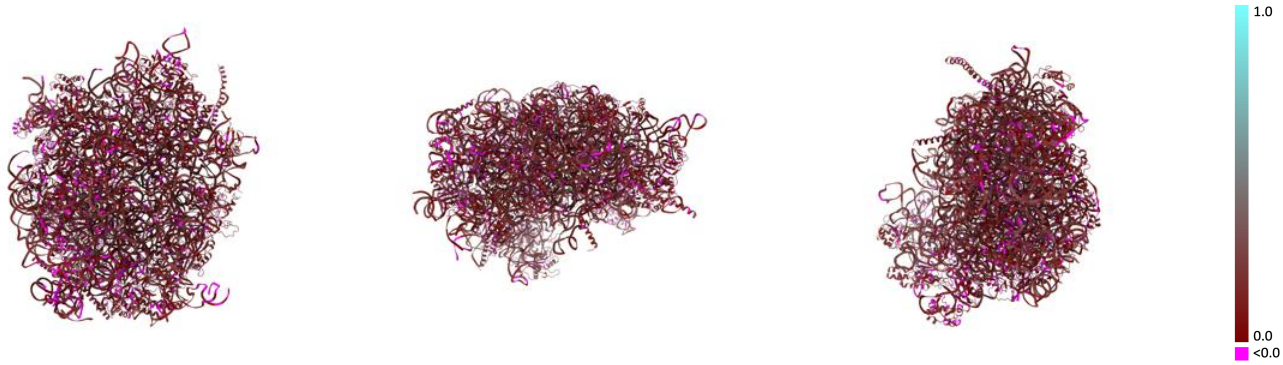
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

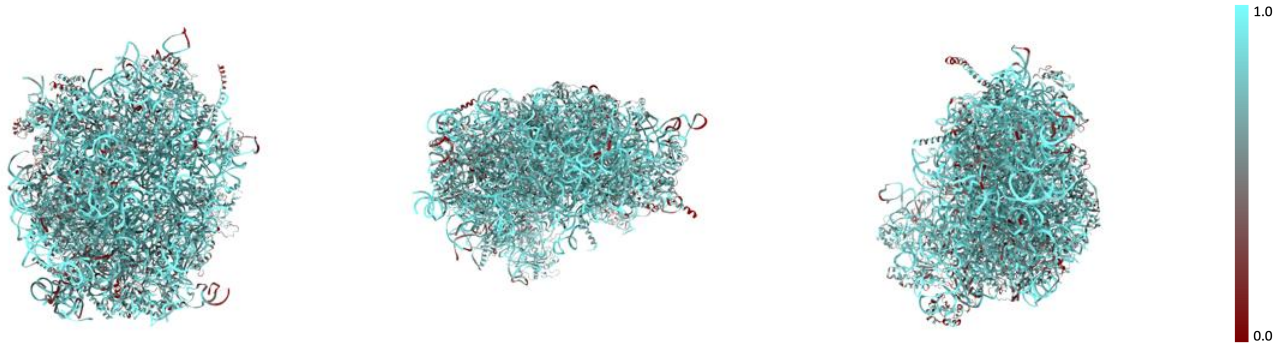
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

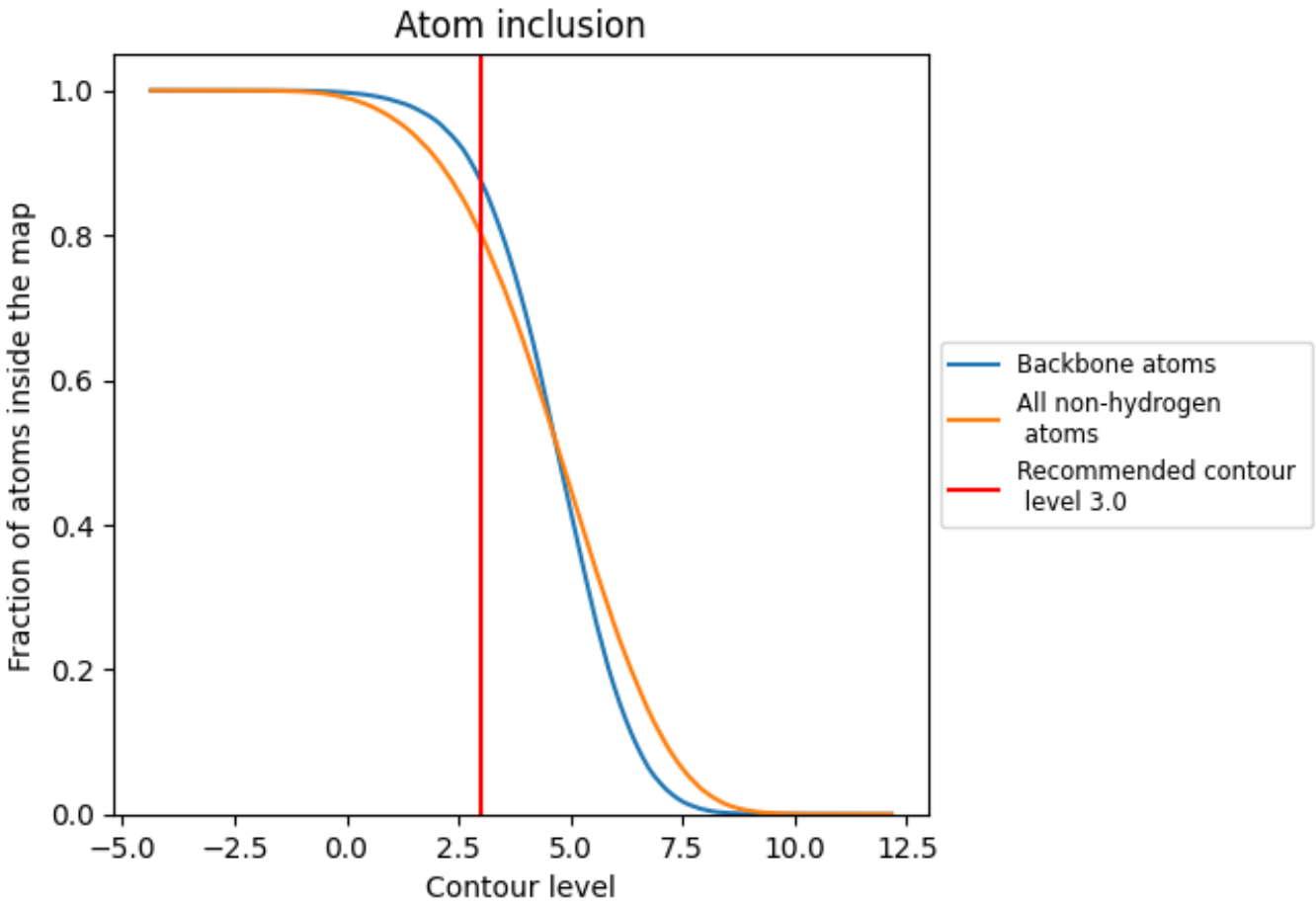
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8017	0.1420
2	0.8832	0.1660
3	0.9034	0.1700
4	0.9464	0.1820
A	0.6614	0.0870
B	0.6850	0.0980
C	0.6880	0.0900
D	0.6678	0.1060
E	0.6065	0.0930
F	0.6514	0.1020
G	0.6606	0.1250
H	0.7154	0.1300
I	0.6587	0.1180
J	0.7328	0.1140
L	0.6353	0.1020
M	0.7013	0.1110
N	0.6779	0.0780
O	0.6871	0.1080
P	0.6970	0.0890
Q	0.6583	0.0980
R	0.6724	0.1170
S	0.6818	0.1090
T	0.6656	0.1050
U	0.6230	0.1370
V	0.6312	0.1120
W	0.6863	0.1100
X	0.6350	0.1070
Y	0.7014	0.1080
Z	0.6833	0.1160
a	0.6758	0.1000
b	0.7040	0.1090
c	0.6306	0.1200
d	0.7102	0.1200
e	0.6483	0.1020
f	0.6594	0.0700

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Chain	Atom inclusion	Q-score
g	0.6828	0.0980
h	0.6622	0.1140
i	0.6596	0.1260
j	0.7534	0.0940
k	0.5881	0.1300
l	0.7630	0.1260
m	0.6981	0.1130
n	0.6468	0.1010
o	0.5865	0.0950
p	0.6623	0.1090
t	0.6670	0.0860
u	0.4884	0.0770