



Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 01:37 PM JST

PDB ID : 6M62
EMDB ID : EMD-30108
Title : Cryo-Em structure of eukaryotic pre-60S ribosome subunit from *Saccharomyces cerevisiae* rpf2 delta 255-344 strain, C4 state.
Authors : Li, Y.; Micic, J.
Deposited on : 2020-03-12
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

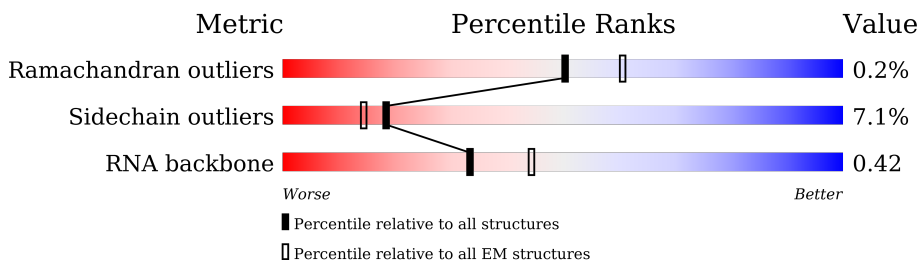
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



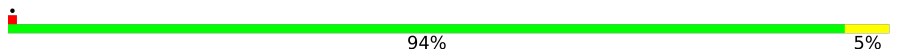

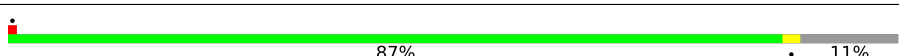
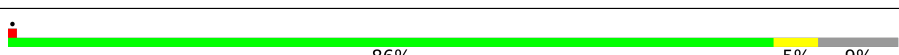
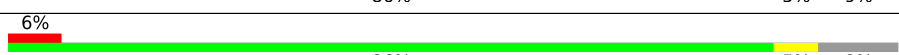

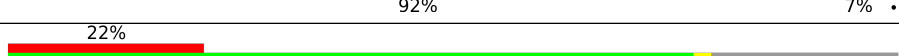

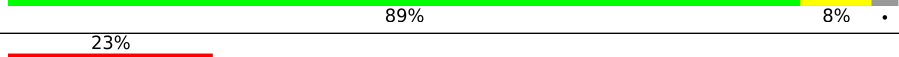


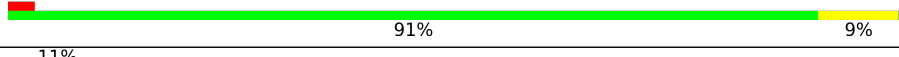
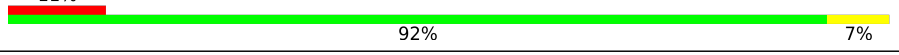
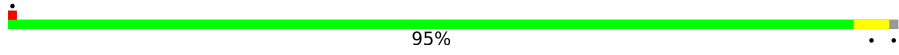
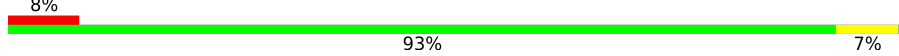

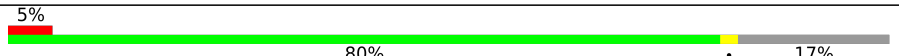
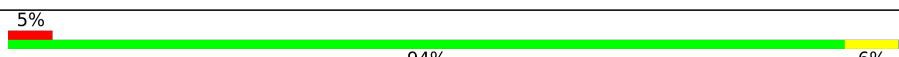
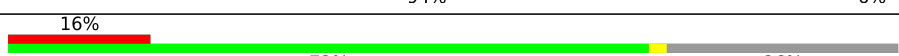


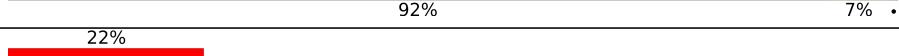
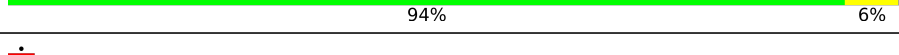
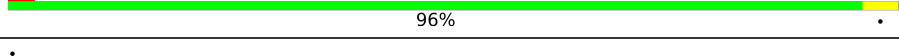
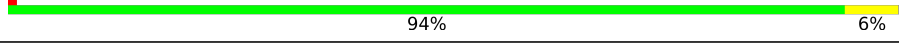
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	1	3396	
2	2	158	
3	3	121	
4	4	593	
5	5	120	
6	6	232	
7	A	254	
8	B	387	

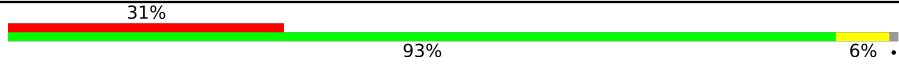
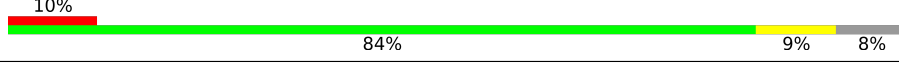
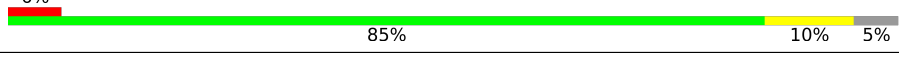
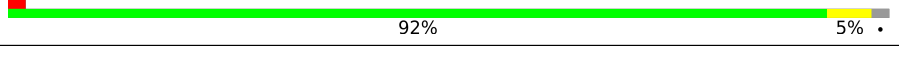
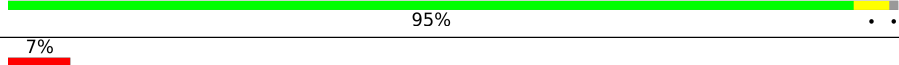
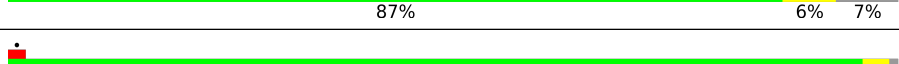
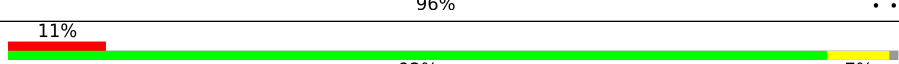
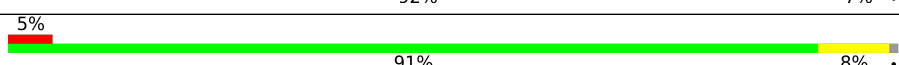
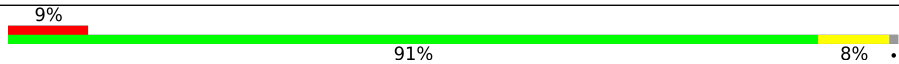
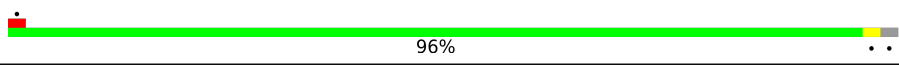

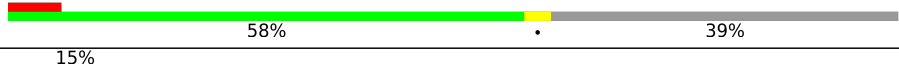
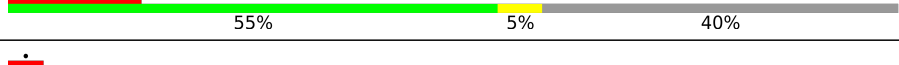
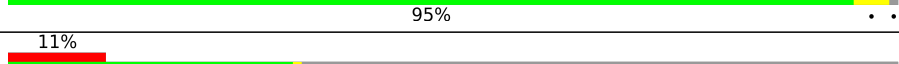
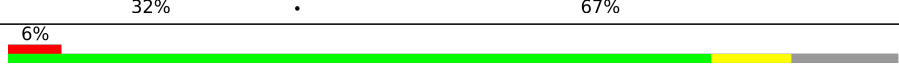
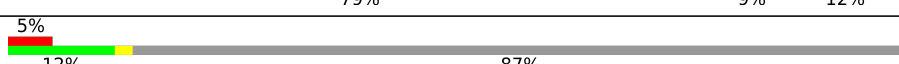


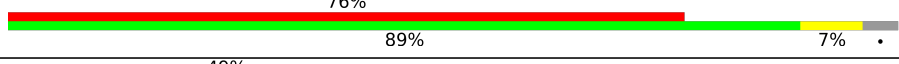
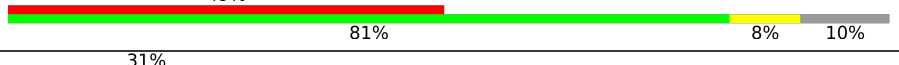

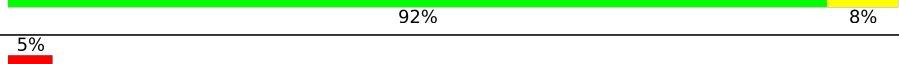
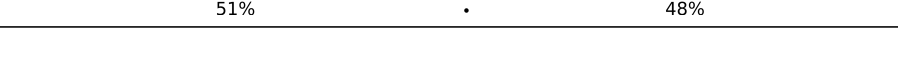


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Mol	Chain	Length	Quality of chain
9	C	362	
10	D	297	
11	E	176	
12	F	244	
13	G	256	
14	H	191	
15	I	166	
16	J	174	
17	K	376	
18	L	199	
19	M	138	
20	N	204	
21	O	199	
22	P	184	
23	Q	186	
24	R	189	
25	S	172	
26	T	160	
27	U	121	
28	V	137	
29	W	236	
30	X	142	
31	Y	127	
32	Z	136	
33	a	149	

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Mol	Chain	Length	Quality of chain
34	b	647	
35	c	105	
36	d	113	
37	e	130	
38	f	107	
39	g	121	
40	h	120	
41	i	100	
42	j	88	
43	k	78	
44	l	51	
45	m	486	
46	n	605	
47	o	220	
48	p	92	
49	q	455	
50	r	261	
51	s	520	
52	t	322	
53	u	199	
54	v	254	
55	w	203	
56	x	515	
57	y	245	
58	z	106	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 153289 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RDN25-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2972	63583	28398	11464	20749	2972	0	0

- Molecule 2 is a RNA chain called RDN58-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	158	3353	1500	586	1109	158	0	0

- Molecule 3 is a RNA chain called RDN5-2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	121	2579	1152	461	845	121	0	0

- Molecule 4 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	516	3999	2530	688	766	15	0	0

- Molecule 5 is a protein called rRNA-processing protein CGR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	73	645	395	133	114	3	0	0

- Molecule 6 is a RNA chain called ITS2-1 miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	6	65	1370	614	228	463	65	0	0

- Molecule 7 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A	213	1634	1023	326	284	1	0	0

- Molecule 8 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B	386	3081	1956	584	533	8	0	0

- Molecule 9 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	361	2749	1730	522	494	3	0	0

- Molecule 10 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	D	276	2211	1397	391	421	2	0	0

- Molecule 11 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	E	156	1239	800	222	216	1	0	0

- Molecule 12 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	F	222	1784	1151	324	308	1	0	0

- Molecule 13 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	G	233	1817	1159	326	329	3	0	0

- Molecule 14 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 15 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	131	Total	C	N	O	S	0	0
			1059	662	195	198	4		

- Molecule 16 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 17 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	256	Total	C	N	O	S	0	0
			2064	1332	342	387	3		

- Molecule 18 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	L	187	Total	C	N	O	0	0
			1499	934	307	258		

- Molecule 19 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 20 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 21 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	O	197	1555	1003	289	262	1	0	0

- Molecule 22 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	P	183	1442	896	287	259		0	0

- Molecule 23 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	Q	134	1035	659	196	179	1	0	0

- Molecule 24 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	R	156	1258	781	265	212		0	0

- Molecule 25 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	S	171	1437	925	266	243	3	0	0

- Molecule 26 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	T	119	943	595	180	165	3	0	0

- Molecule 27 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	U	106	844	545	138	161		0	0

- Molecule 28 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 29 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	234	Total	C	N	O	S	0	0
			1885	1194	323	362	6		

- Molecule 30 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	141	Total	C	N	O	S	0	0
			1100	705	196	197	2		

- Molecule 31 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 32 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 33 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	93	Total	C	N	O	S	0	0
			735	479	130	125	1		

- Molecule 34 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	642	Total	C	N	O	S	0	0
			5185	3251	938	970	26		

- Molecule 35 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 36 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 37 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 38 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 39 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 40 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 41 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 42 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 43 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	77	Total	C	N	O	S	0	0
			612	391	115	106			

- Molecule 44 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 45 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	453	Total	C	N	O	S	0	0
			3648	2308	657	674	9		

- Molecule 46 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	371	Total	C	N	O	S	0	0
			3030	1963	523	534	10		

- Molecule 47 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 48 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 49 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	151	Total	C	N	O	S	0	0
			1258	793	226	238	1		

- Molecule 50 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 51 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	69	Total	C	N	O	S	0	0
			573	359	113	98	3		

- Molecule 52 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	287	Total	C	N	O	S	0	0
			2306	1459	427	417	3		

- Molecule 53 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 54 is a protein called Ribosome biogenesis protein RPF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	v	245	Total	C	N	O	S	0	0
			1985	1275	344	353	13		

- Molecule 55 is a protein called Regulator of ribosome biosynthesis.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	w	182	Total	C	N	O	S	0	0
			1448	911	261	271	5		

- Molecule 56 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	x	395	3093	1941	559	573	20	0	0

- Molecule 57 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	y	244	1849	1146	319	377	7	0	0

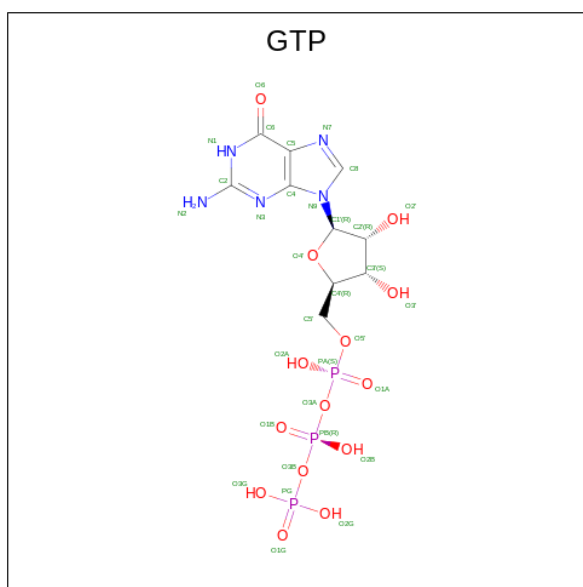
- Molecule 58 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	z	55	444	273	88	83	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
59	I	1	1	1	0
59	j	1	1	1	0
59	p	1	1	1	0
59	u	1	1	1	0

- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	b	1	32	10	5	14	3	0
60	m	1	32	10	5	14	3	0

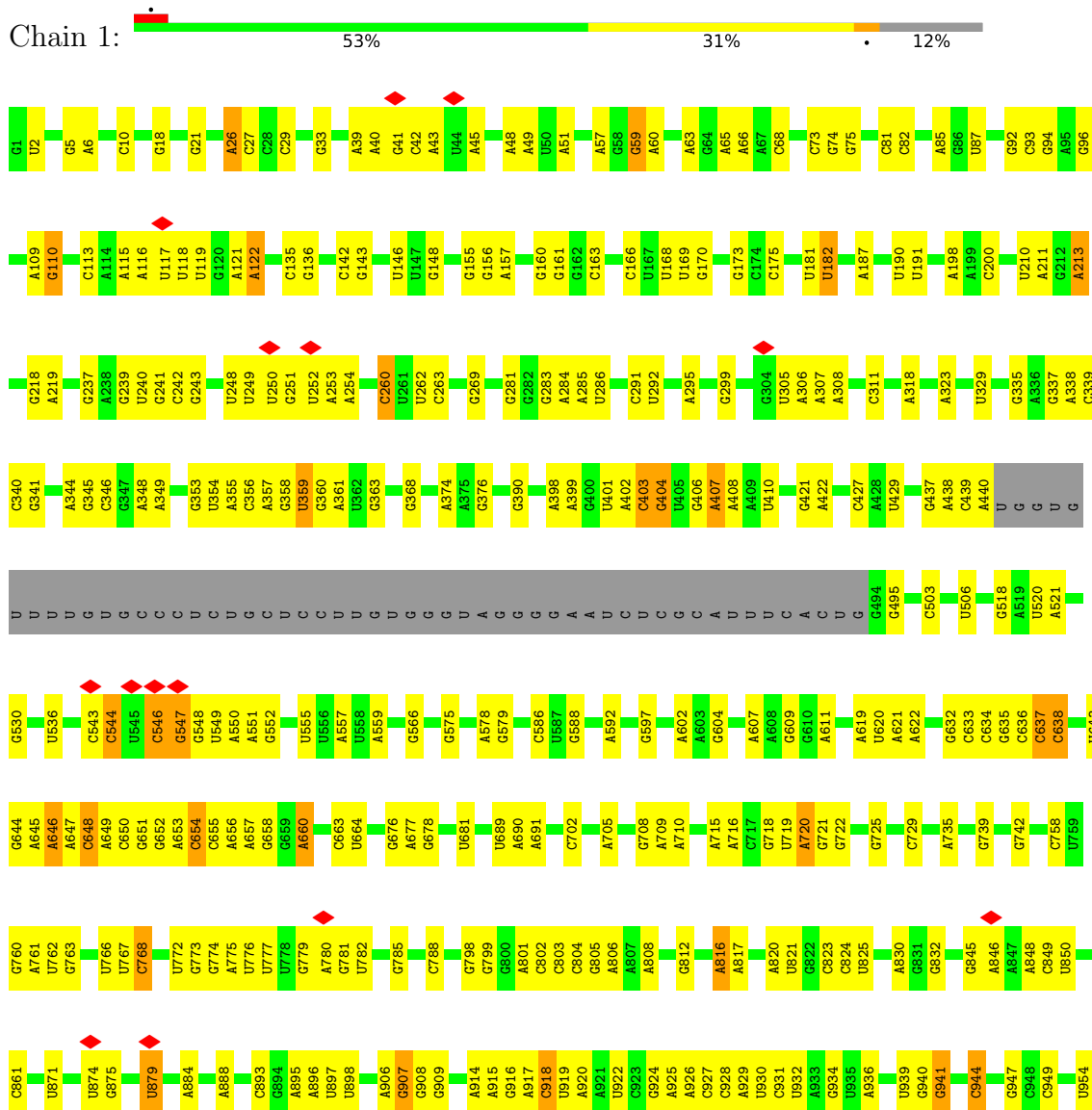
- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

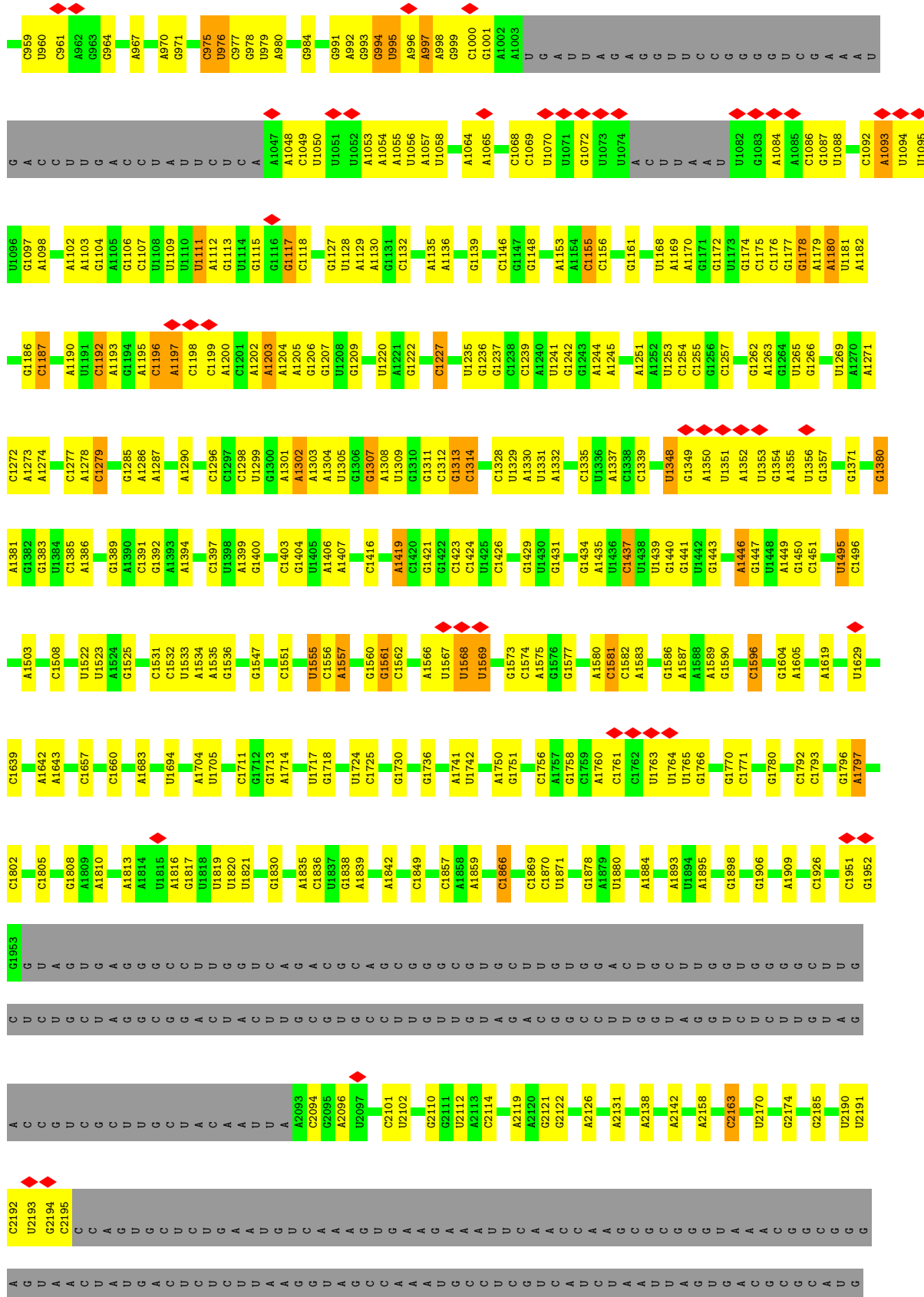
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
61	b	1	1	1	0
61	m	1	1	1	0

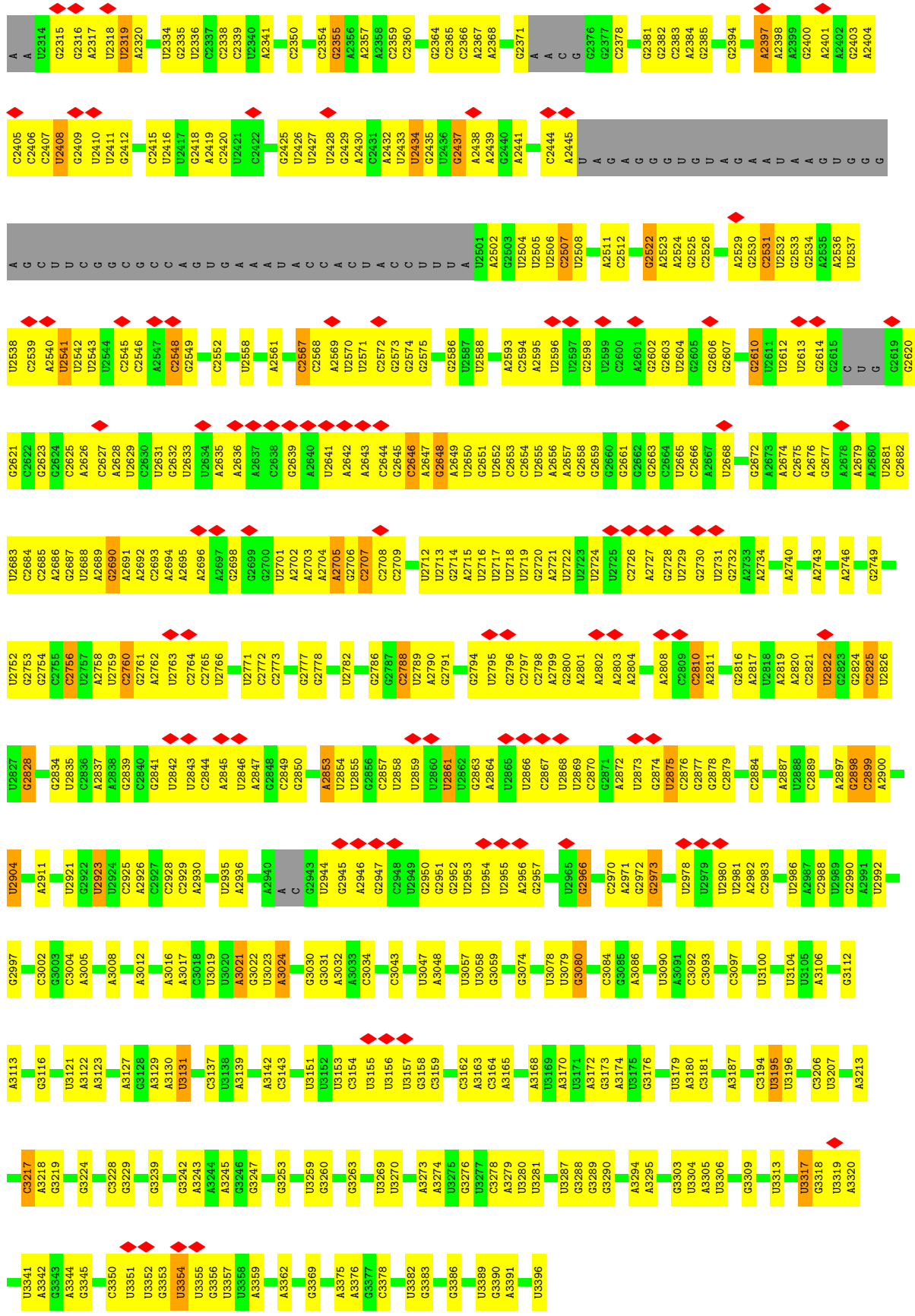
3 Residue-property plots i

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.

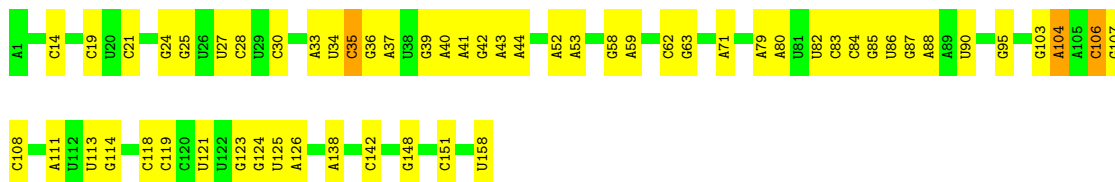
• Molecule 1: RDN25-1 rRNA



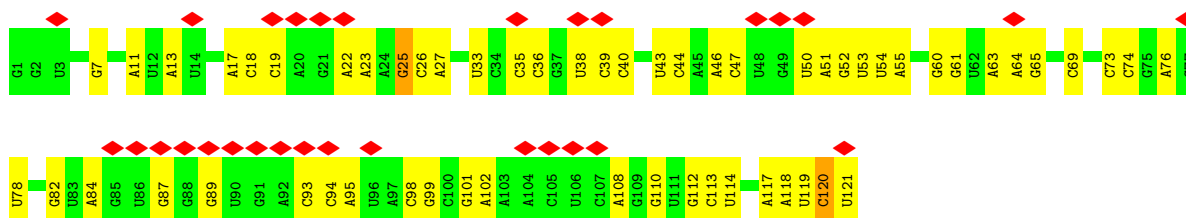




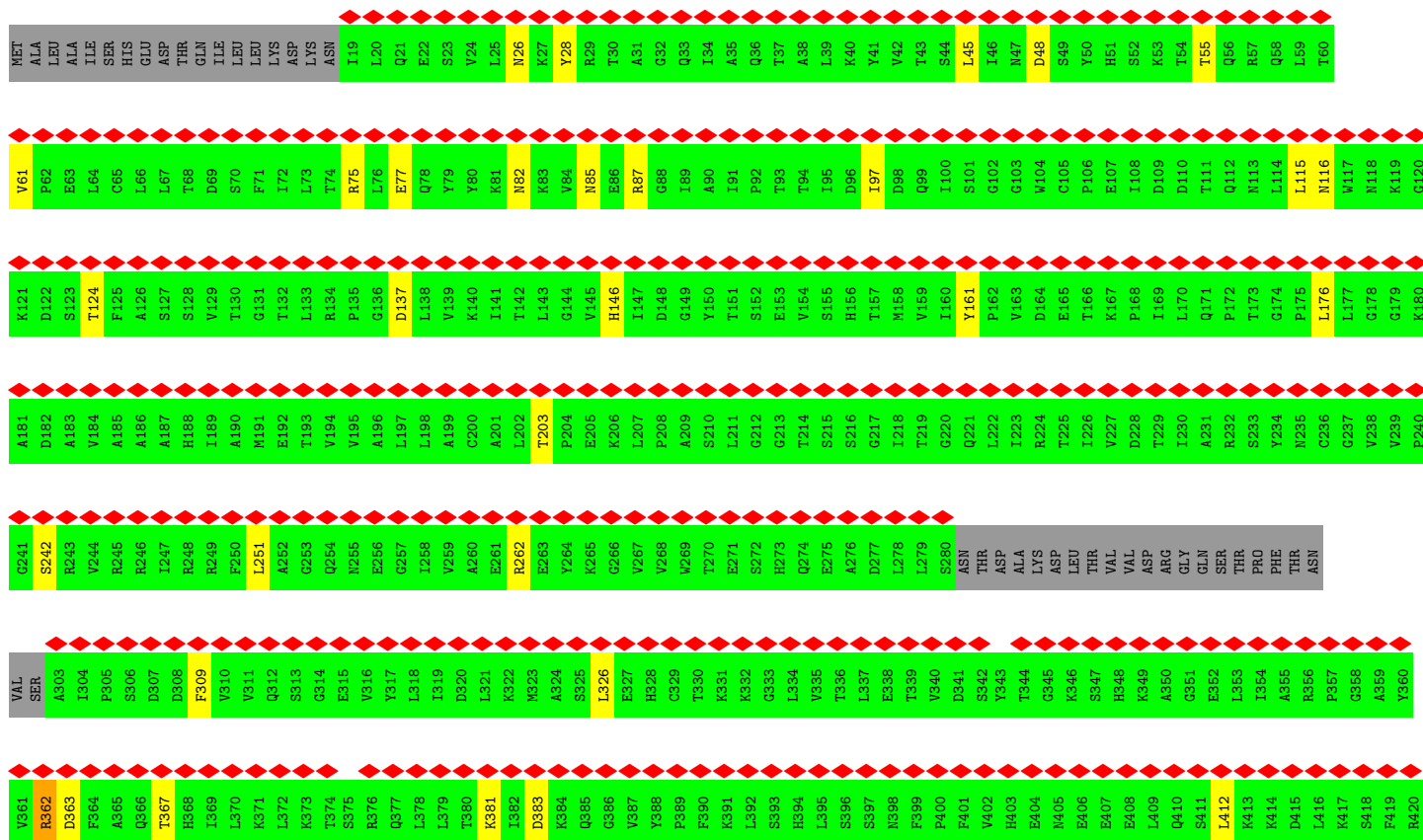
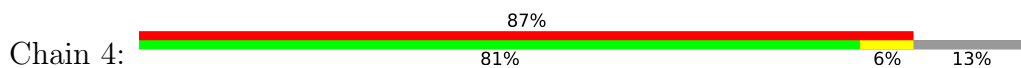
• Molecule 2: RDN58-1 rRNA

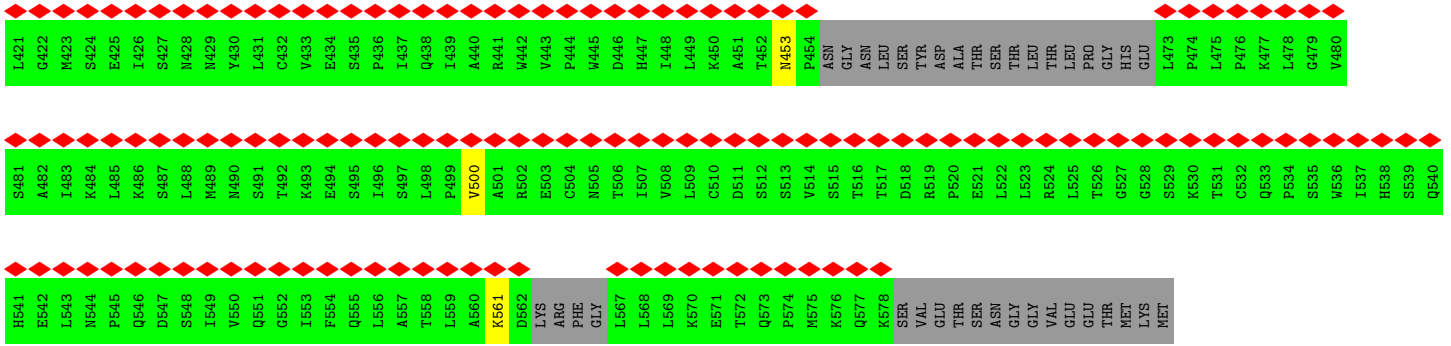


• Molecule 3: RDN5-2 rRNA

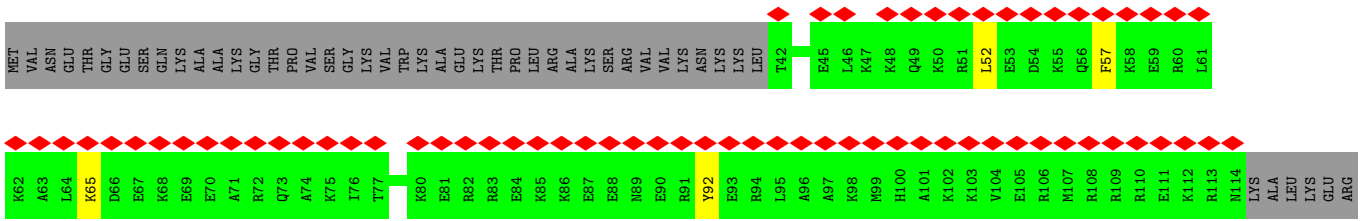


• Molecule 4: Probable metalloprotease ARX1

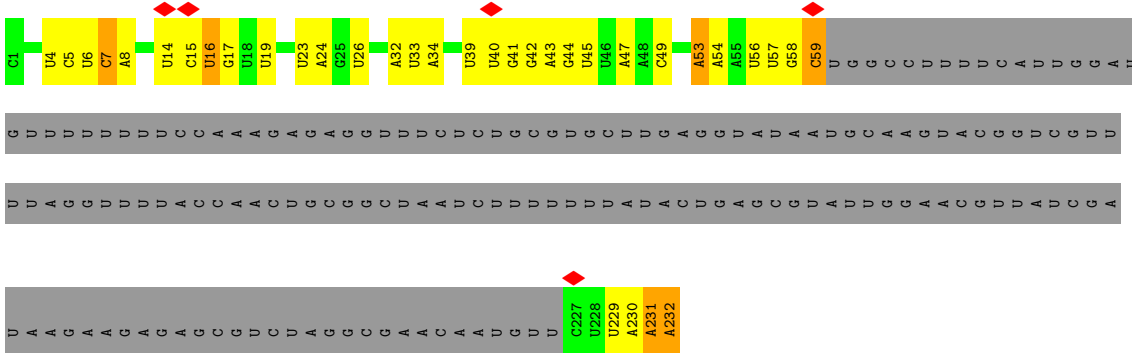




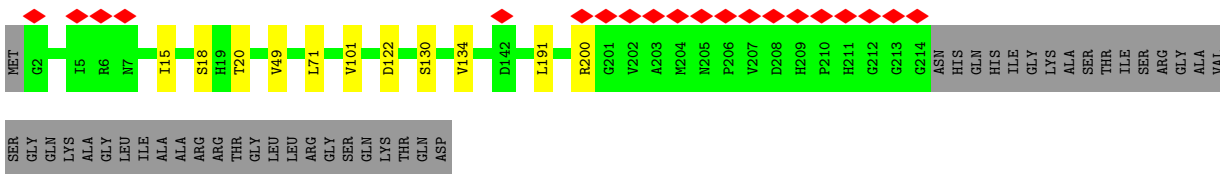
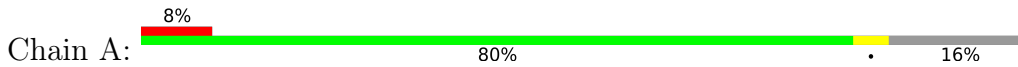
- Molecule 5: rRNA-processing protein CGR1



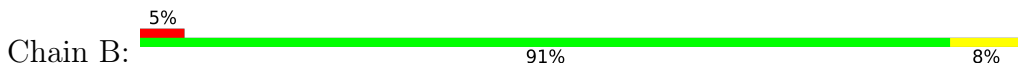
- Molecule 6: ITS2-1 miscRNA

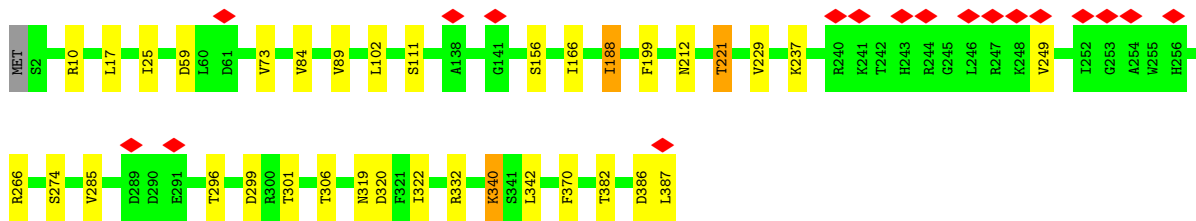


- Molecule 7: 60S ribosomal protein L2-A



- Molecule 8: 60S ribosomal protein L3

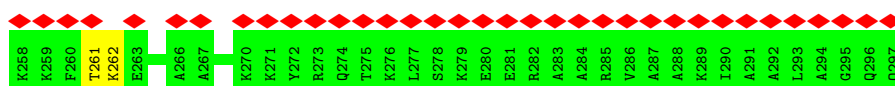
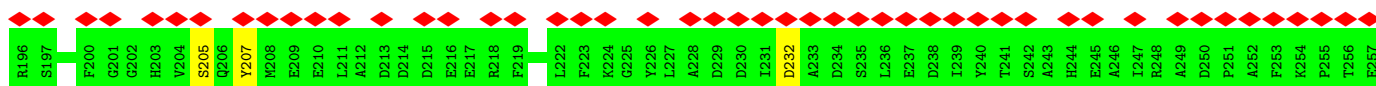
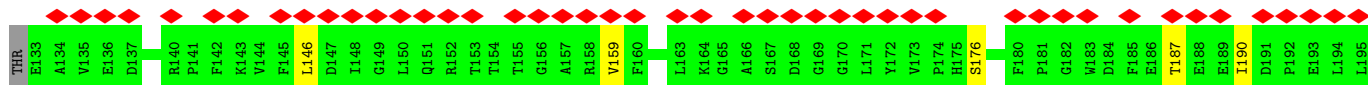
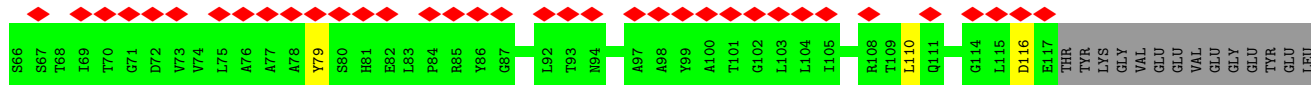
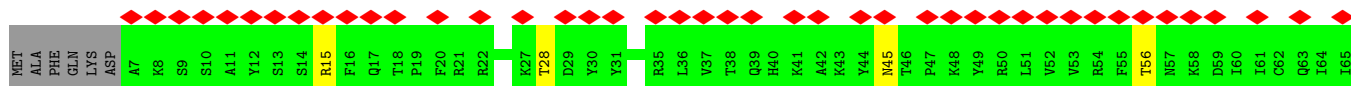
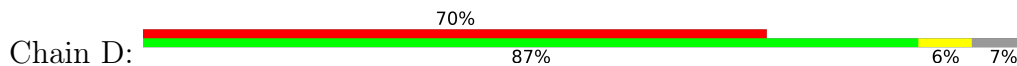




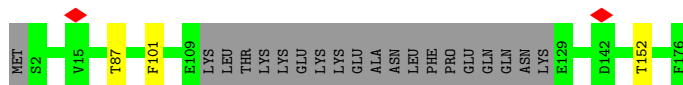
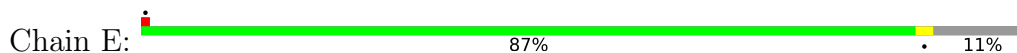
• Molecule 9: 60S ribosomal protein L4-A



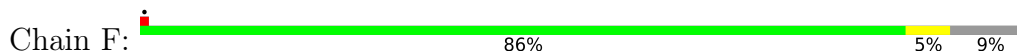
• Molecule 10: 60S ribosomal protein L5

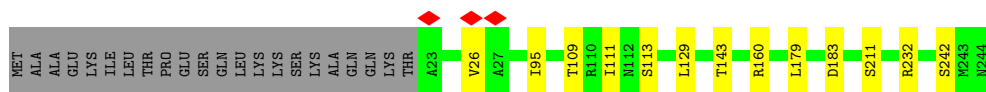


• Molecule 11: 60S ribosomal protein L6-A

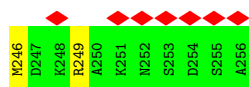
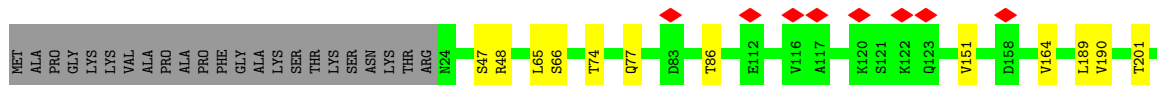
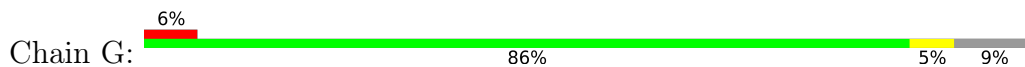


• Molecule 12: 60S ribosomal protein L7-A

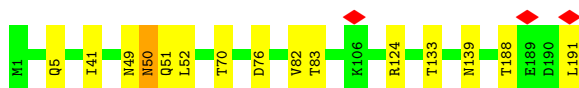
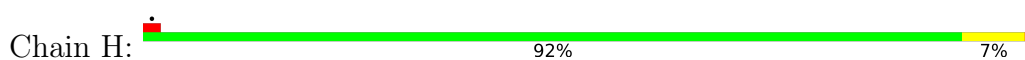




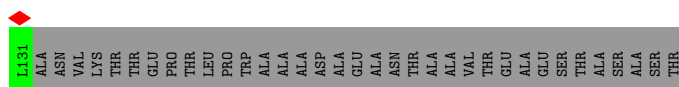
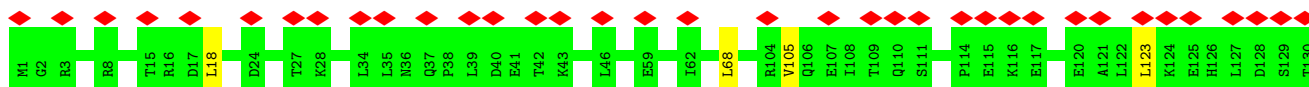
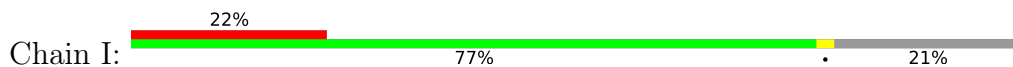
- Molecule 13: 60S ribosomal protein L8-A



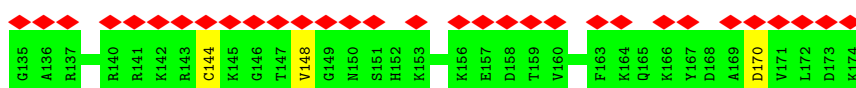
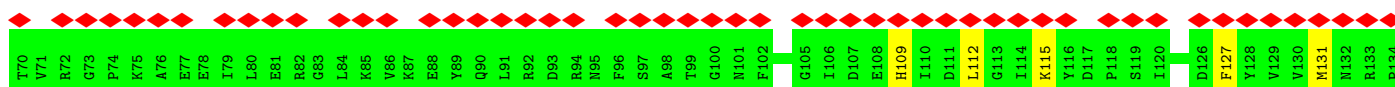
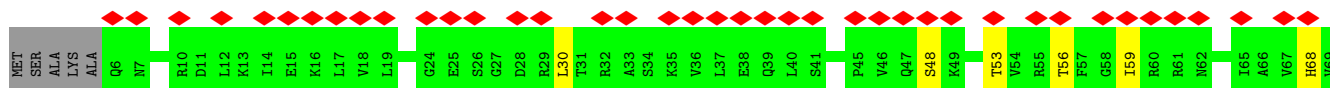
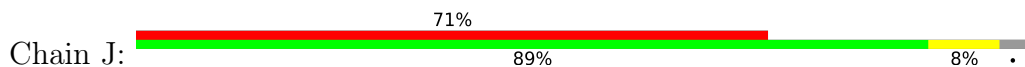
- Molecule 14: 60S ribosomal protein L9-A



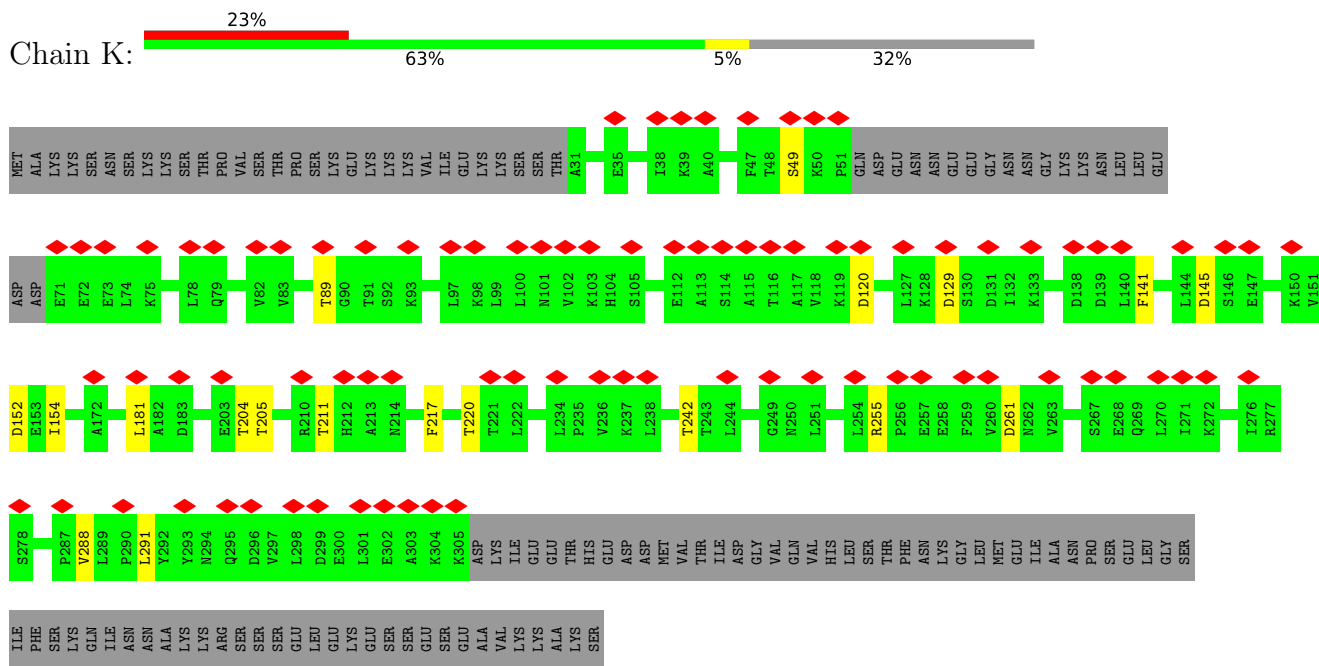
- Molecule 15: Bud site selection protein 20



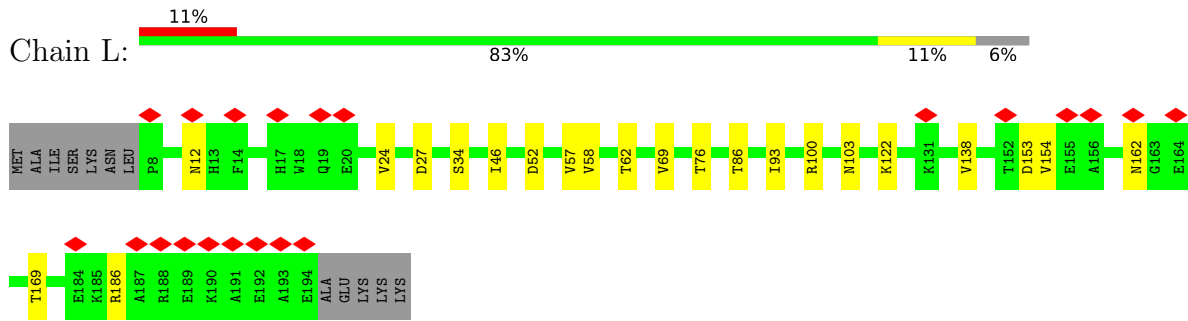
- Molecule 16: 60S ribosomal protein L11-A



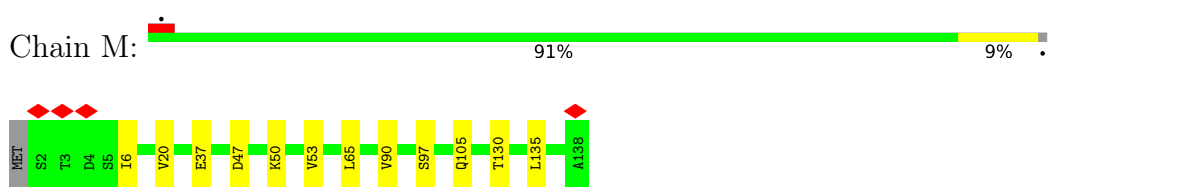
- Molecule 17: Proteasome-interacting protein CIC1



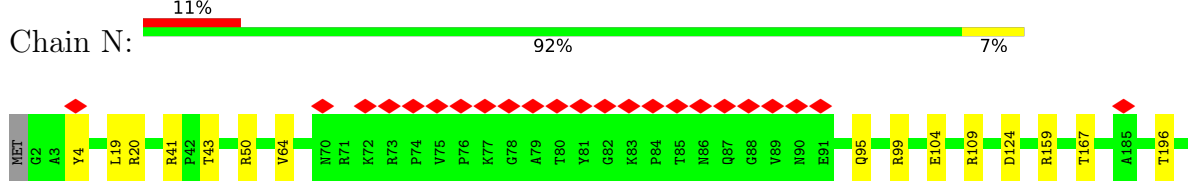
• Molecule 18: 60S ribosomal protein L13-A



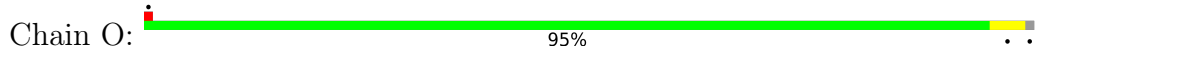
• Molecule 19: 60S ribosomal protein L14-A



• Molecule 20: 60S ribosomal protein L15-A

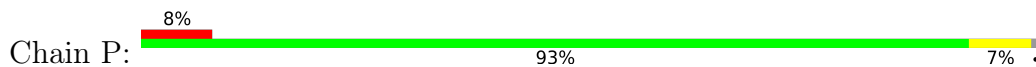


• Molecule 21: 60S ribosomal protein L16-A

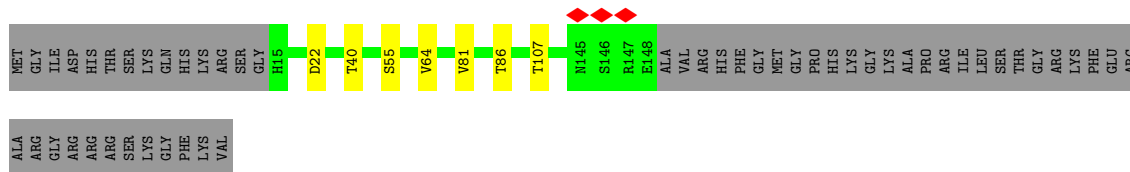




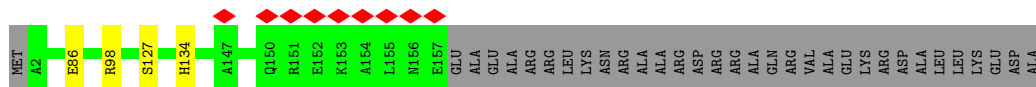
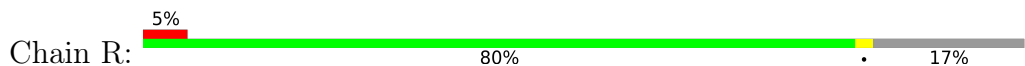
- Molecule 22: 60S ribosomal protein L17-A



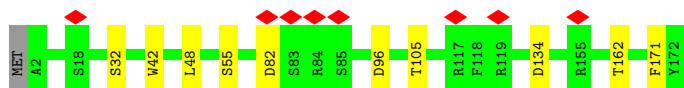
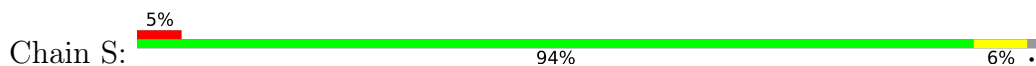
- Molecule 23: 60S ribosomal protein L18-A



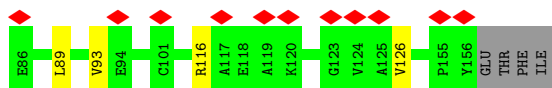
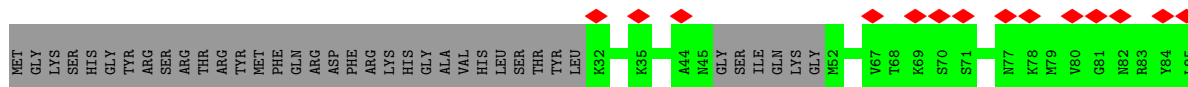
- Molecule 24: 60S ribosomal protein L19-A



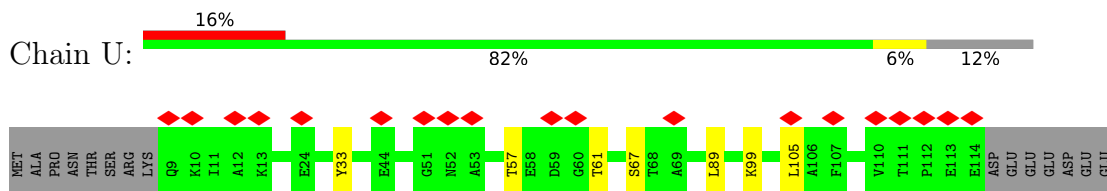
- Molecule 25: 60S ribosomal protein L20-A



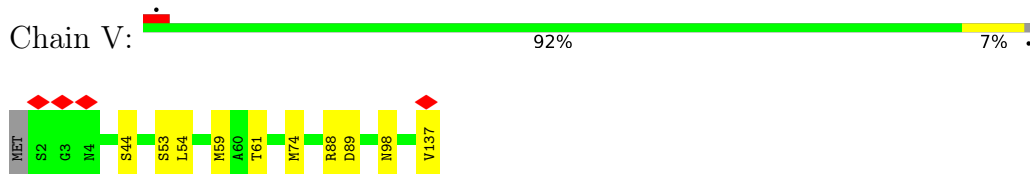
- Molecule 26: 60S ribosomal protein L21-A



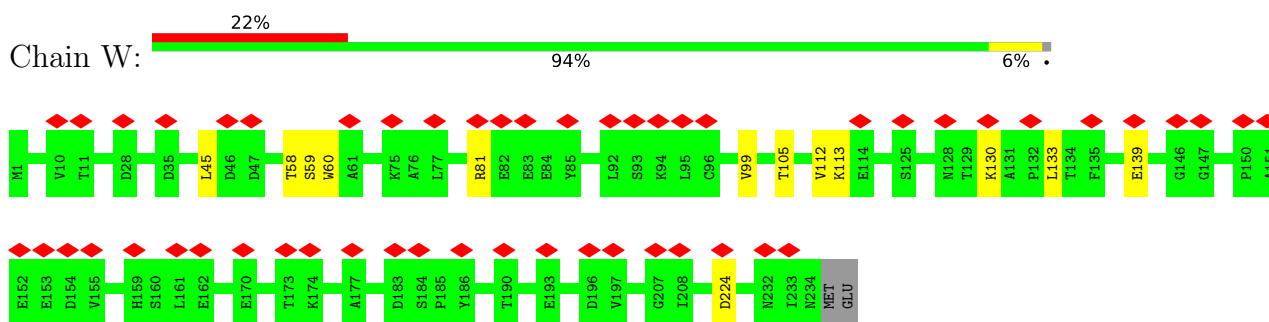
- Molecule 27: 60S ribosomal protein L22-A



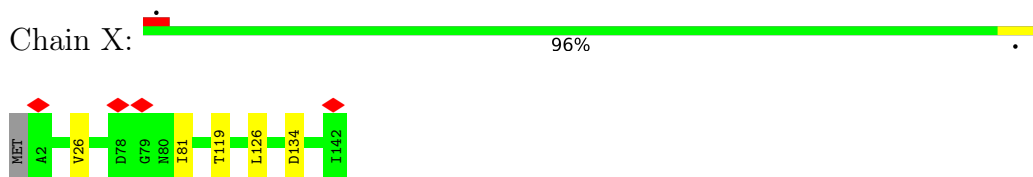
• Molecule 28: 60S ribosomal protein L23-A



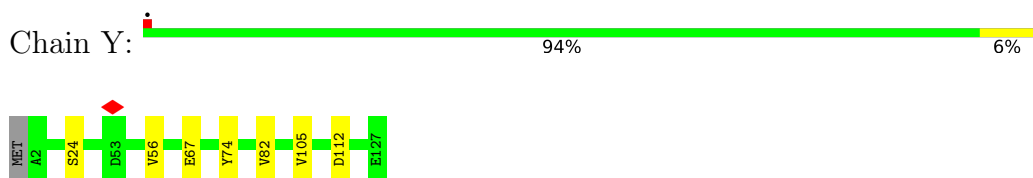
• Molecule 29: Ribosome assembly factor MRT4



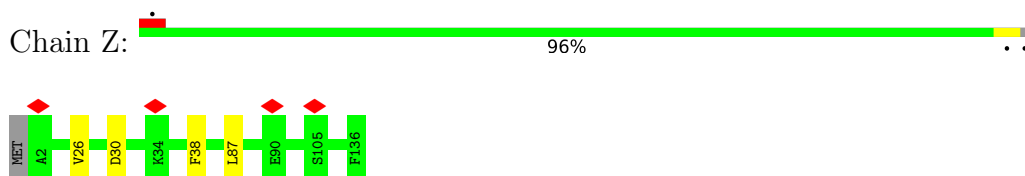
• Molecule 30: 60S ribosomal protein L25



• Molecule 31: 60S ribosomal protein L26-A

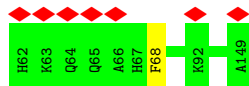
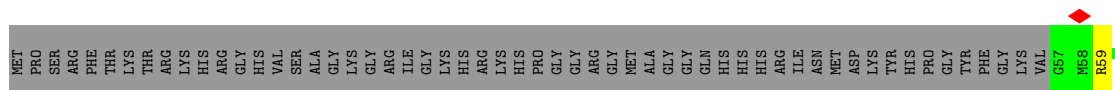


• Molecule 32: 60S ribosomal protein L27-A

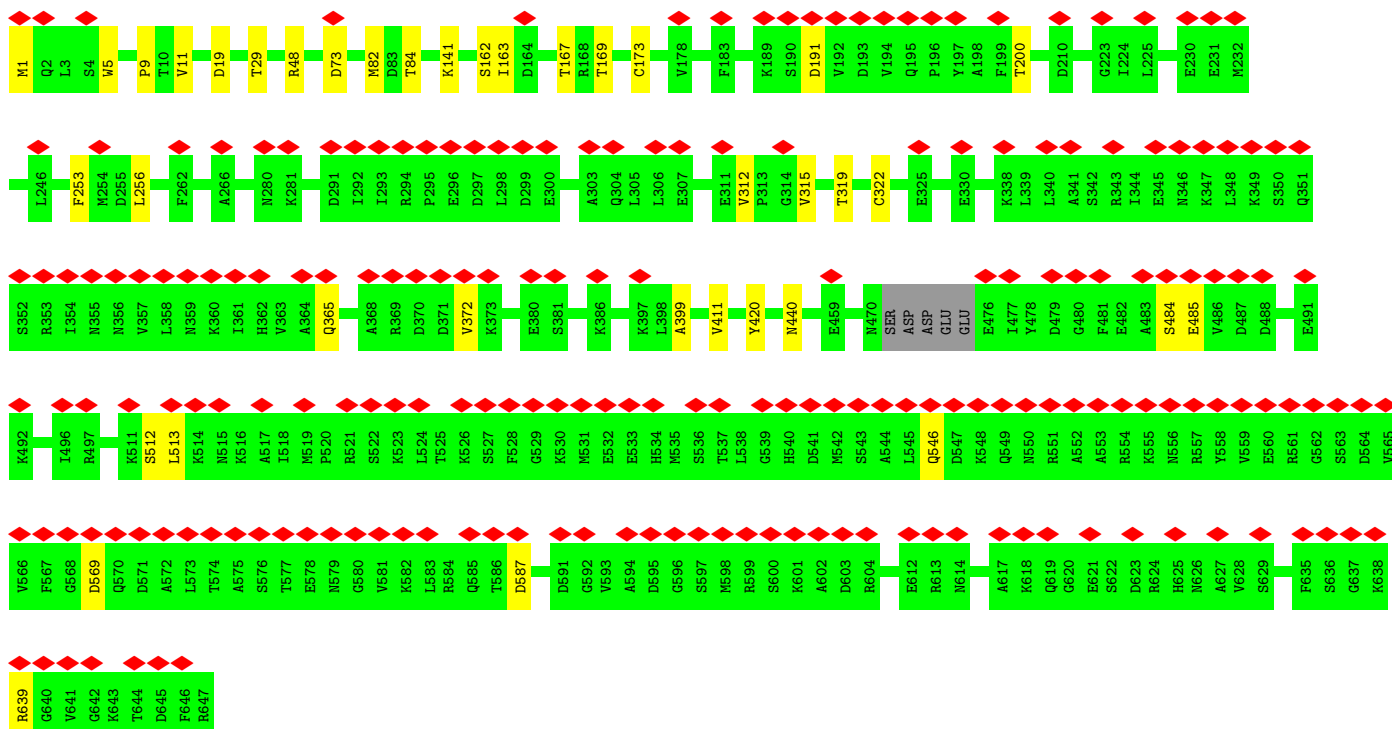
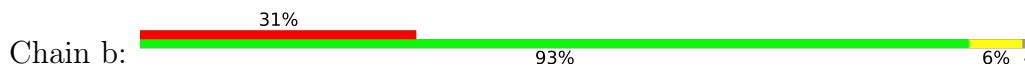


• Molecule 33: 60S ribosomal protein L28

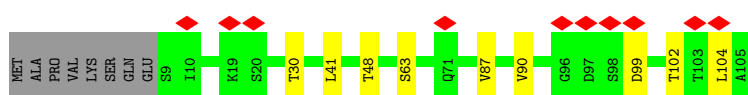
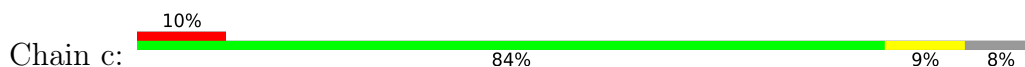




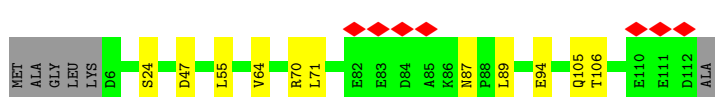
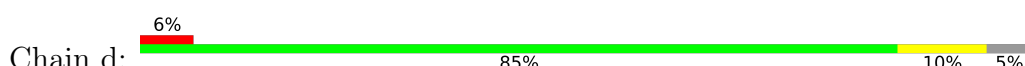
• Molecule 34: Nucleolar GTP-binding protein 1



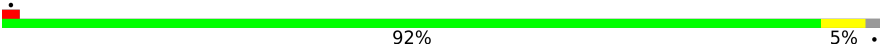
• Molecule 35: 60S ribosomal protein L30

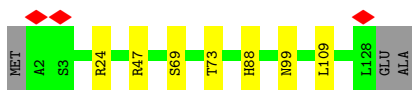


• Molecule 36: 60S ribosomal protein L31-A



• Molecule 37: 60S ribosomal protein L32

Chain e:  92% 5%




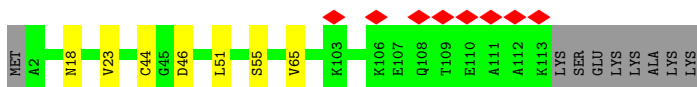
- Molecule 38: 60S ribosomal protein L33-A

Chain f:  95%



- Molecule 39: 60S ribosomal protein L34-A

Chain g:  7% 87% 6% 7%




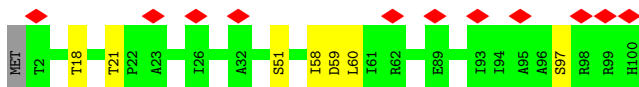
- Molecule 40: 60S ribosomal protein L35-A

Chain h:  96%




- Molecule 41: 60S ribosomal protein L36-A

Chain i:  11% 92% 7%

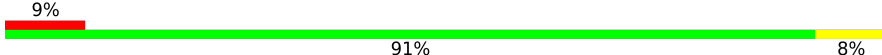


- Molecule 42: 60S ribosomal protein L37-A

Chain j:  5% 91% 8%

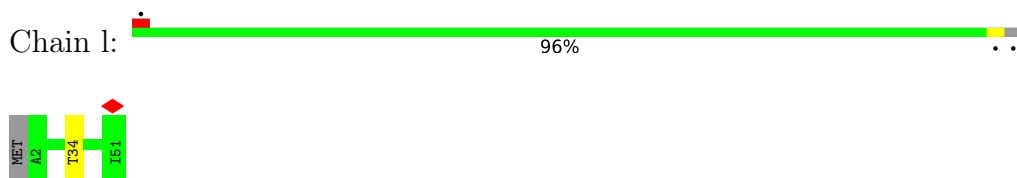


- Molecule 43: 60S ribosomal protein L38

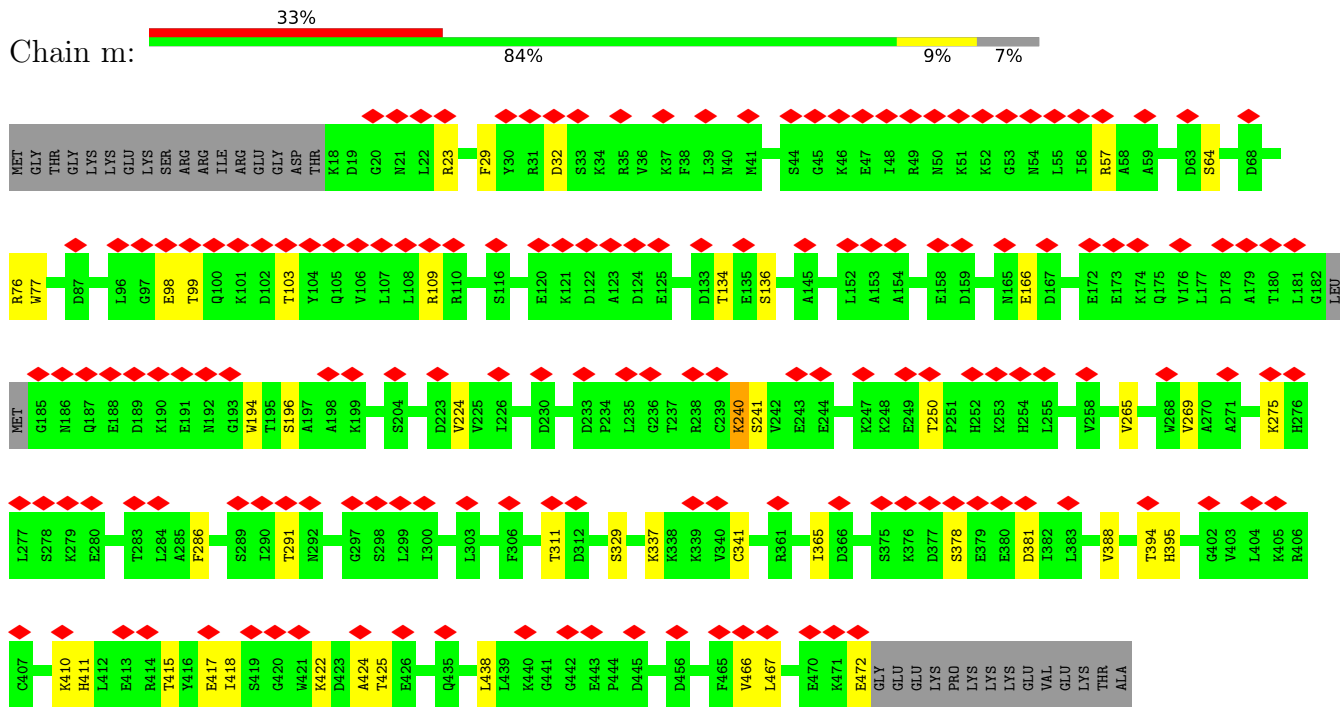
Chain k:  9% 91% 8%



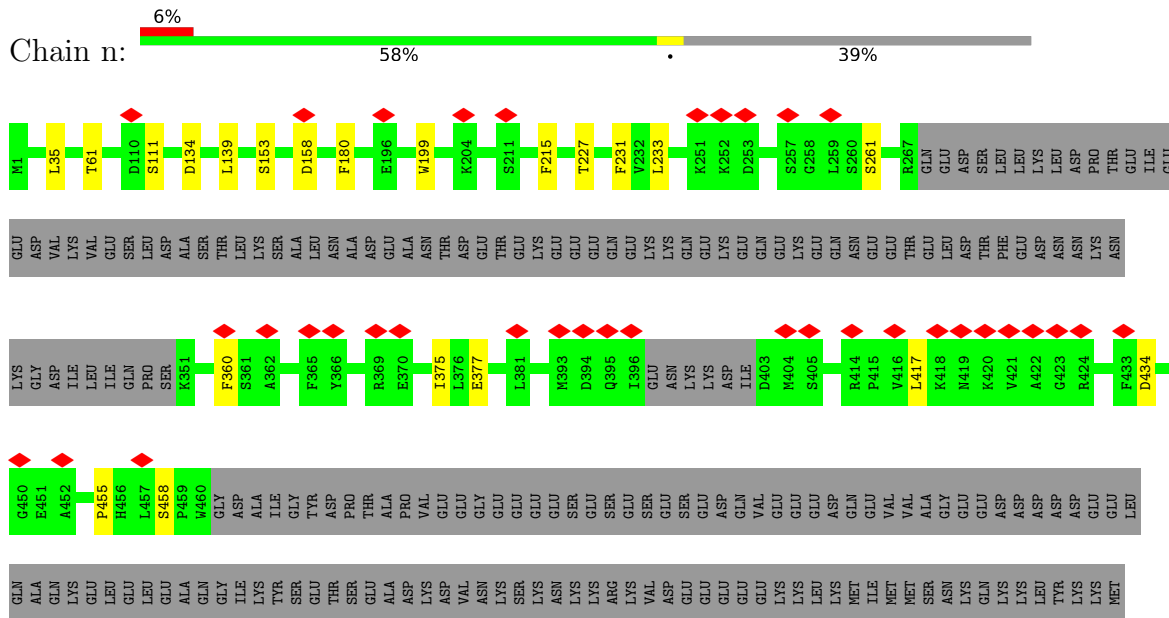
• Molecule 44: 60S ribosomal protein L39

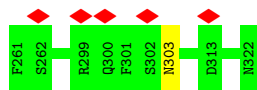


• Molecule 45: Nucleolar GTP-binding protein 2

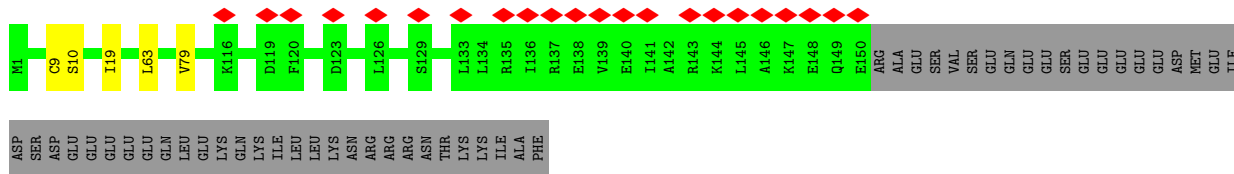
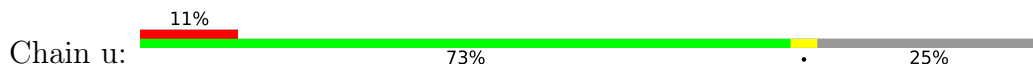


• Molecule 46: Pescadillo homolog

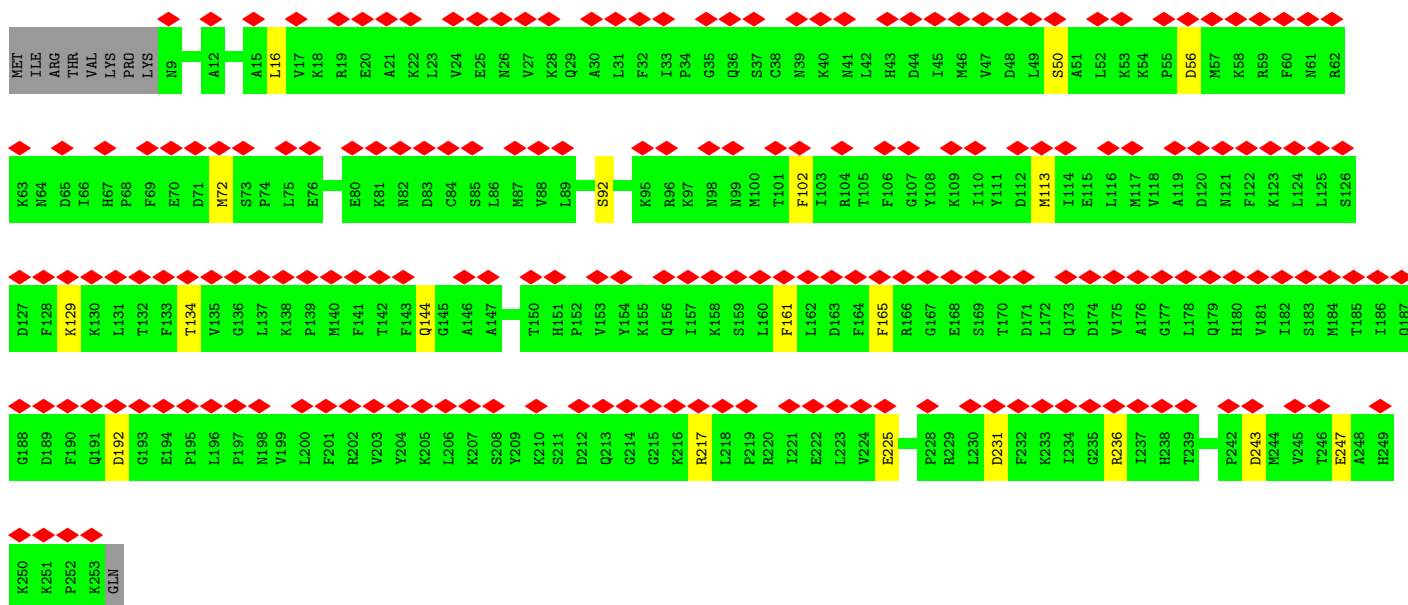
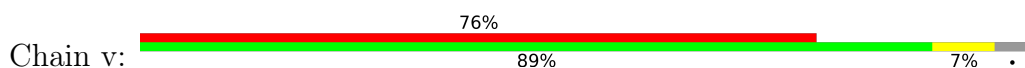




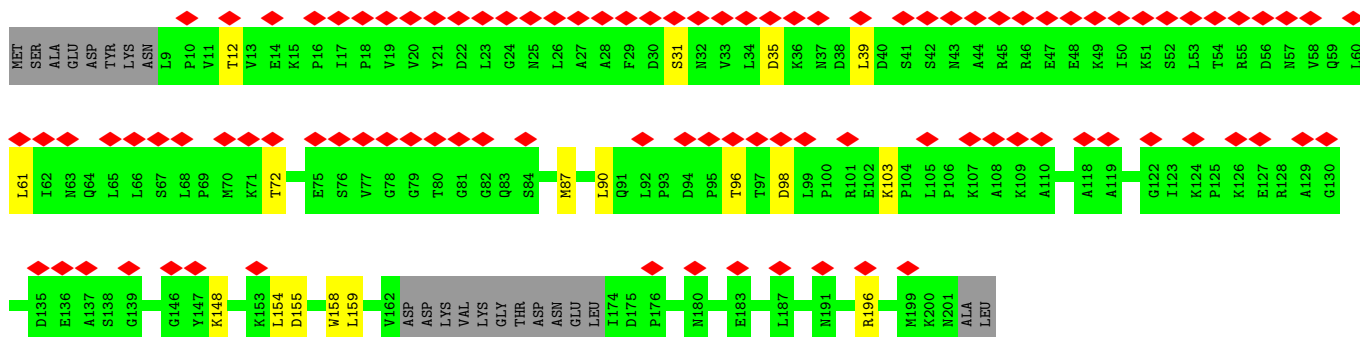
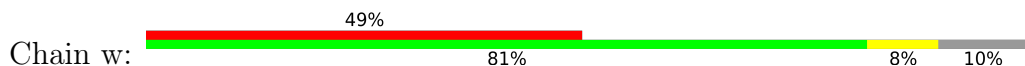
• Molecule 53: Ribosome biogenesis protein RLP24



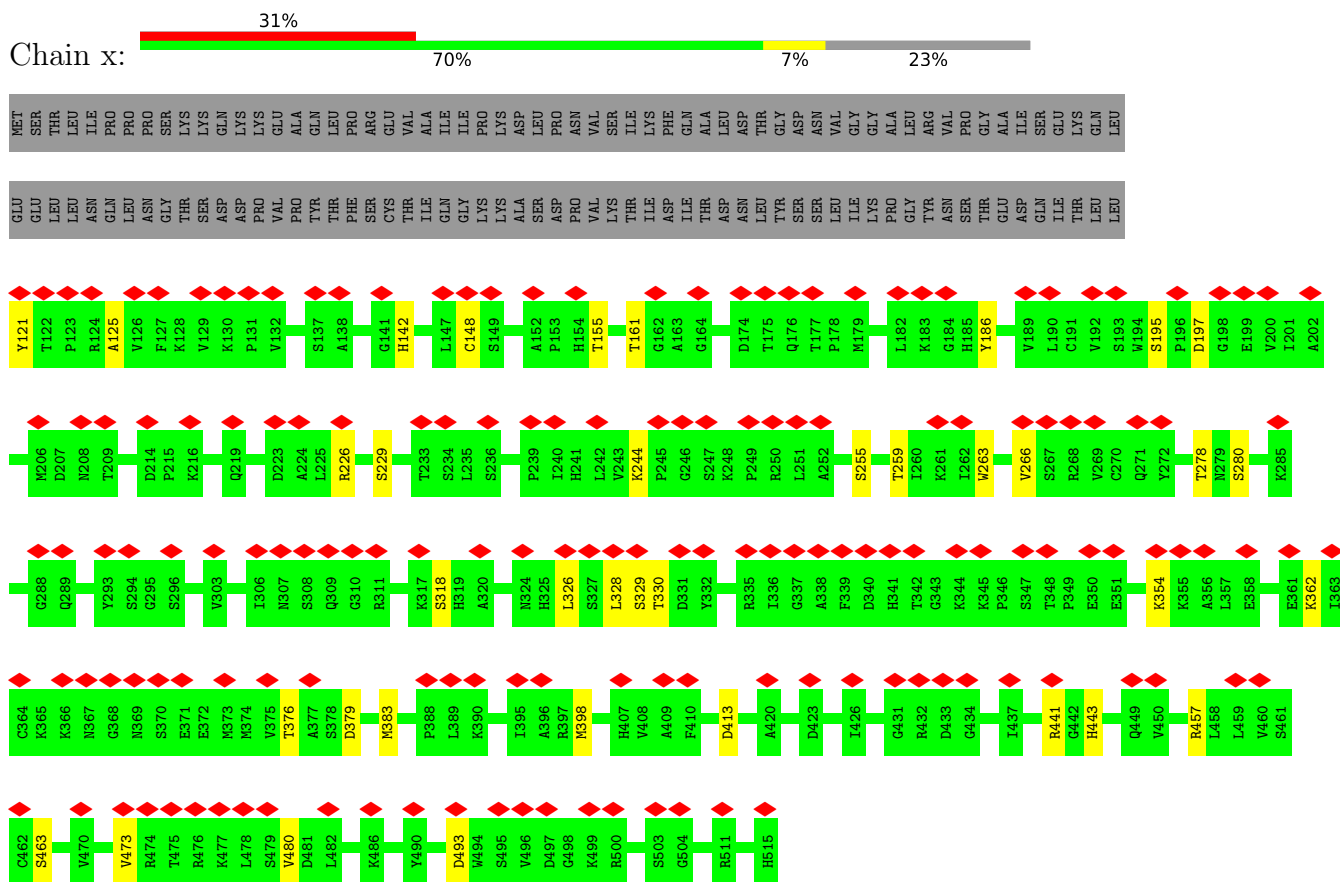
• Molecule 54: Ribosome biogenesis protein RPF2



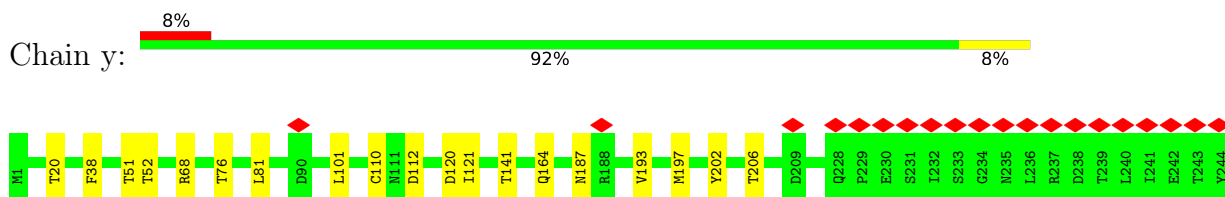
• Molecule 55: Regulator of ribosome biosynthesis



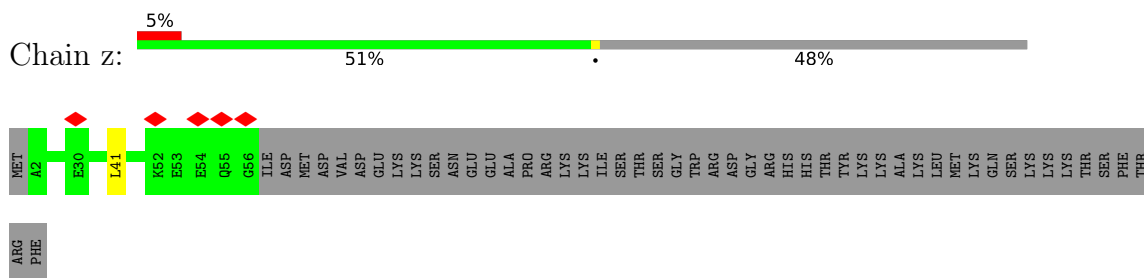
• Molecule 56: Ribosome assembly protein 4



• Molecule 57: Eukaryotic translation initiation factor 6



• Molecule 58: UPF0642 protein YBL028C



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53177	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.164	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	422.80002, 422.80002, 422.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.057, 1.057, 1.057	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	1.47	285/71167 (0.4%)	1.15	254/110944 (0.2%)
2	2	1.83	32/3746 (0.9%)	1.09	2/5832 (0.0%)
3	3	0.52	0/2883	1.11	12/4491 (0.3%)
4	4	0.32	0/4069	0.56	0/5520
5	5	0.32	0/649	0.52	0/848
6	6	0.73	0/1527	1.22	13/2371 (0.5%)
7	A	0.66	0/1666	0.58	0/2241
8	B	0.77	1/3152 (0.0%)	0.60	0/4239
9	C	0.76	0/2801	0.60	1/3792 (0.0%)
10	D	0.33	0/2257	0.52	0/3043
11	E	0.57	0/1260	0.55	0/1694
12	F	0.72	0/1821	0.56	0/2451
13	G	0.71	0/1849	0.62	0/2495
14	H	0.66	0/1539	0.60	0/2073
15	I	0.44	0/1075	0.54	0/1443
16	J	0.31	0/1374	0.53	0/1842
17	K	0.37	0/2098	0.54	0/2830
18	L	0.64	0/1524	0.58	0/2046
19	M	0.63	0/1074	0.56	0/1446
20	N	0.91	0/1757	0.63	0/2354
21	O	0.93	0/1585	0.62	0/2128
22	P	0.75	0/1465	0.59	0/1968
23	Q	0.64	0/1050	0.59	0/1419
24	R	0.59	0/1275	0.56	0/1702
25	S	0.68	0/1473	0.58	0/1980
26	T	0.44	0/957	0.54	0/1285
27	U	0.50	0/861	0.57	0/1167
28	V	0.64	0/1018	0.59	0/1369
29	W	0.39	0/1918	0.55	0/2586
30	X	0.74	0/1116	0.62	0/1503
31	Y	0.61	0/1004	0.56	0/1341
32	Z	0.56	0/1118	0.55	0/1497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.56	0/751	0.62	0/1013
34	b	0.46	0/5270	0.56	0/7080
35	c	0.53	0/751	0.55	0/1008
36	d	0.69	0/887	0.60	0/1191
37	e	0.86	0/1041	0.59	0/1394
38	f	0.93	0/868	0.59	0/1168
39	g	0.73	0/891	0.61	0/1191
40	h	0.67	0/978	0.58	0/1301
41	i	0.42	0/778	0.53	0/1034
42	j	0.99	0/696	0.61	0/923
43	k	0.49	0/618	0.55	0/826
44	l	0.65	0/443	0.54	0/588
45	m	0.41	0/3722	0.55	0/5017
46	n	0.56	0/3101	0.55	0/4187
47	o	0.48	1/1129 (0.1%)	0.56	0/1502
48	p	0.67	0/701	0.57	0/934
49	q	0.43	0/1279	0.54	0/1710
50	r	0.56	1/1892 (0.1%)	0.60	0/2528
51	s	0.45	0/577	0.54	0/752
52	t	0.43	0/2333	0.54	0/3128
53	u	0.58	0/1287	0.57	0/1711
54	v	0.34	0/2027	0.52	0/2718
55	w	0.35	0/1471	0.55	0/1980
56	x	0.36	0/3174	0.56	0/4305
57	y	0.52	0/1872	0.60	0/2548
58	z	0.50	0/445	0.57	0/585
All	All	1.10	320/163110 (0.2%)	0.92	282/236262 (0.1%)

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
4	4	0	3
8	B	0	2
9	C	0	1
12	F	0	1
16	J	0	1
18	L	0	1
28	V	0	1
36	d	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
45	m	0	6
46	n	0	1
47	o	0	1
50	r	0	1
53	u	0	1
56	x	0	1
All	All	0	22

All (320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1535	A	N9-C4	-8.03	1.33	1.37
1	1	655	C	N1-C6	-7.93	1.32	1.37
2	2	104	A	N3-C4	-7.66	1.30	1.34
1	1	824	C	N1-C6	-7.36	1.32	1.37
1	1	361	A	N9-C4	-7.34	1.33	1.37
1	1	929	A	N9-C4	-7.32	1.33	1.37
1	1	660	A	N9-C4	-7.28	1.33	1.37
1	1	635	G	N3-C4	-6.93	1.30	1.35
1	1	374	A	N9-C4	-6.91	1.33	1.37
1	1	213	A	N9-C4	-6.90	1.33	1.37
1	1	888	A	N9-C4	-6.83	1.33	1.37
1	1	2364	G	N9-C4	-6.76	1.32	1.38
1	1	340	C	N1-C6	-6.74	1.33	1.37
1	1	361	A	C5-C4	-6.71	1.34	1.38
1	1	1175	C	N1-C6	-6.65	1.33	1.37
1	1	927	C	N1-C6	-6.64	1.33	1.37
1	1	1869	C	N1-C6	-6.63	1.33	1.37
1	1	658	G	N9-C8	-6.51	1.33	1.37
1	1	907	G	C5-C4	-6.47	1.33	1.38
1	1	949	C	N1-C6	-6.46	1.33	1.37
1	1	1176	C	N1-C6	-6.45	1.33	1.37
1	1	1535	A	N3-C4	-6.42	1.30	1.34
1	1	804	C	N1-C6	-6.36	1.33	1.37
1	1	928	C	N1-C6	-6.36	1.33	1.37
2	2	19	C	N1-C6	-6.34	1.33	1.37
1	1	926	A	C6-N1	-6.31	1.31	1.35
1	1	1895	A	N9-C4	-6.28	1.34	1.37
1	1	10	C	N1-C6	-6.25	1.33	1.37
1	1	361	A	N7-C5	-6.25	1.35	1.39
1	1	658	G	C5-C4	-6.23	1.33	1.38
1	1	1435	A	C5-C4	-6.22	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	81	C	N1-C6	-6.19	1.33	1.37
1	1	2341	A	N9-C4	-6.19	1.34	1.37
1	1	3043	C	N1-C6	-6.18	1.33	1.37
1	1	1161	G	N7-C5	-6.15	1.35	1.39
1	1	1660	C	N1-C6	-6.13	1.33	1.37
1	1	341	G	C6-N1	-6.12	1.35	1.39
1	1	213	A	N3-C4	-6.12	1.31	1.34
1	1	1175	C	C2-N3	-6.11	1.30	1.35
1	1	803	C	N1-C6	-6.10	1.33	1.37
1	1	1859	A	N9-C4	-6.08	1.34	1.37
1	1	1586	G	C5-C4	-6.08	1.34	1.38
1	1	2988	C	N1-C6	-6.08	1.33	1.37
1	1	1403	C	N1-C6	-6.08	1.33	1.37
1	1	931	C	N1-C6	-6.08	1.33	1.37
1	1	1435	A	C6-N1	-6.02	1.31	1.35
1	1	3002	C	N1-C6	-6.02	1.33	1.37
2	2	14	C	N1-C6	-6.00	1.33	1.37
1	1	1898	G	C5-C4	-5.99	1.34	1.38
1	1	1381	A	N9-C4	-5.99	1.34	1.37
1	1	1380	G	C5-C4	-5.97	1.34	1.38
1	1	1146	C	N1-C6	-5.96	1.33	1.37
2	2	104	A	N9-C4	-5.96	1.34	1.37
1	1	1175	C	N3-C4	-5.92	1.29	1.33
1	1	926	A	N7-C5	-5.92	1.35	1.39
1	1	970	A	N9-C4	-5.92	1.34	1.37
1	1	664	U	N1-C2	-5.91	1.33	1.38
1	1	1335	C	N1-C6	-5.91	1.33	1.37
1	1	1857	C	N1-C6	-5.90	1.33	1.37
2	2	44	A	N9-C4	-5.89	1.34	1.37
8	B	340	LYS	CA-CB	-5.89	1.41	1.53
1	1	1176	C	N3-C4	-5.89	1.29	1.33
1	1	929	A	C5-C4	-5.87	1.34	1.38
1	1	1381	A	N3-C4	-5.87	1.31	1.34
2	2	30	C	N1-C6	-5.86	1.33	1.37
1	1	654	C	N1-C6	-5.86	1.33	1.37
2	2	142	C	N1-C6	-5.86	1.33	1.37
1	1	3034	C	N1-C6	-5.84	1.33	1.37
1	1	356	C	N1-C6	-5.84	1.33	1.37
1	1	1419	A	N3-C4	-5.84	1.31	1.34
1	1	2368	A	C5-C4	-5.83	1.34	1.38
1	1	802	C	N1-C6	-5.83	1.33	1.37
1	1	63	A	C6-N1	-5.82	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1435	A	N3-C4	-5.82	1.31	1.34
1	1	1535	A	C5-C4	-5.81	1.34	1.38
1	1	361	A	N3-C4	-5.80	1.31	1.34
1	1	2366	C	C4-C5	-5.79	1.38	1.43
1	1	652	G	C5-C4	-5.78	1.34	1.38
1	1	2383	C	N1-C6	-5.77	1.33	1.37
2	2	33	A	N9-C4	-5.76	1.34	1.37
1	1	57	A	N9-C4	-5.73	1.34	1.37
1	1	2359	C	N1-C6	-5.72	1.33	1.37
1	1	340	C	N3-C4	-5.71	1.29	1.33
1	1	1424	C	N1-C6	-5.71	1.33	1.37
1	1	51	A	N7-C5	-5.71	1.35	1.39
1	1	1312	C	N3-C4	-5.70	1.29	1.33
1	1	2354	C	N1-C6	-5.70	1.33	1.37
2	2	44	A	C5-C4	-5.68	1.34	1.38
1	1	360	G	N7-C5	-5.68	1.35	1.39
1	1	341	G	N1-C2	-5.67	1.33	1.37
1	1	2381	G	N7-C5	-5.67	1.35	1.39
1	1	3004	C	N1-C6	-5.67	1.33	1.37
1	1	634	C	N1-C6	-5.67	1.33	1.37
1	1	2367	A	N9-C4	-5.67	1.34	1.37
2	2	42	G	C5-C4	-5.66	1.34	1.38
1	1	2384	A	N9-C4	-5.66	1.34	1.37
1	1	2394	G	C5-C4	-5.66	1.34	1.38
1	1	788	C	N1-C6	-5.65	1.33	1.37
1	1	927	C	N1-C2	-5.65	1.34	1.40
1	1	1446	A	N9-C4	-5.64	1.34	1.37
1	1	930	U	N1-C2	-5.64	1.33	1.38
1	1	2338	C	N3-C4	-5.64	1.30	1.33
1	1	2350	C	N1-C6	-5.64	1.33	1.37
2	2	21	C	N1-C6	-5.63	1.33	1.37
1	1	344	A	C5-C4	-5.63	1.34	1.38
1	1	1311	G	N1-C2	-5.63	1.33	1.37
1	1	1328	C	N1-C6	-5.63	1.33	1.37
1	1	1385	C	N1-C6	-5.62	1.33	1.37
2	2	58	G	N9-C8	-5.62	1.33	1.37
1	1	1155	C	N1-C6	-5.61	1.33	1.37
1	1	408	A	N9-C4	-5.61	1.34	1.37
1	1	1301	A	N3-C4	-5.59	1.31	1.34
1	1	1337	A	N9-C4	-5.59	1.34	1.37
1	1	33	G	C5-C4	-5.58	1.34	1.38
1	1	920	A	N7-C5	-5.58	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	940	G	C5-C4	-5.57	1.34	1.38
1	1	656	A	N7-C5	-5.57	1.35	1.39
1	1	358	G	C5-C4	-5.57	1.34	1.38
1	1	1531	C	N1-C6	-5.56	1.33	1.37
1	1	663	C	N1-C6	-5.55	1.33	1.37
1	1	1535	A	C5-C6	-5.55	1.36	1.41
1	1	823	C	N1-C6	-5.55	1.33	1.37
1	1	635	G	N9-C4	-5.55	1.33	1.38
1	1	68	C	N1-C6	-5.54	1.33	1.37
2	2	24	G	C5-C4	-5.54	1.34	1.38
1	1	1406	A	N9-C4	-5.53	1.34	1.37
2	2	37	A	N3-C4	-5.53	1.31	1.34
1	1	2988	C	N1-C2	-5.52	1.34	1.40
1	1	403	C	N1-C6	-5.52	1.33	1.37
1	1	929	A	N3-C4	-5.51	1.31	1.34
1	1	1495	U	C2-N3	-5.51	1.33	1.37
1	1	702	C	N1-C6	-5.50	1.33	1.37
1	1	1371	G	C5-C4	-5.50	1.34	1.38
1	1	1429	G	C5-C4	-5.50	1.34	1.38
1	1	122	A	N3-C4	-5.50	1.31	1.34
1	1	345	G	C5-C4	-5.50	1.34	1.38
1	1	632	G	C5-C4	-5.49	1.34	1.38
1	1	1169	A	N7-C5	-5.49	1.35	1.39
2	2	41	A	C5-C4	-5.49	1.34	1.38
1	1	803	C	C4-C5	-5.48	1.38	1.43
1	1	346	C	N1-C6	-5.48	1.33	1.37
1	1	1534	A	N7-C5	-5.47	1.35	1.39
1	1	1301	A	N9-C4	-5.45	1.34	1.37
1	1	2365	C	N1-C6	-5.45	1.33	1.37
1	1	1495	U	N3-C4	-5.45	1.33	1.38
1	1	3047	U	N1-C2	-5.45	1.33	1.38
2	2	35	C	C4-C5	-5.45	1.38	1.43
1	1	1551	C	N1-C6	-5.44	1.33	1.37
1	1	59	G	C5-C4	-5.43	1.34	1.38
1	1	1440	G	C5-C4	-5.42	1.34	1.38
1	1	1313	G	C6-N1	-5.42	1.35	1.39
1	1	1314	C	C4-C5	-5.42	1.38	1.43
1	1	651	G	C5-C4	-5.42	1.34	1.38
1	1	2355	G	C5-C4	-5.42	1.34	1.38
1	1	3043	C	N3-C4	-5.42	1.30	1.33
1	1	1172	G	C6-N1	-5.41	1.35	1.39
1	1	635	G	C2-N3	-5.41	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	918	C	N1-C6	-5.41	1.33	1.37
1	1	906	A	N7-C5	-5.41	1.36	1.39
1	1	1419	A	C5-C4	-5.41	1.34	1.38
1	1	633	C	N1-C6	-5.40	1.33	1.37
1	1	1534	A	N9-C8	-5.39	1.33	1.37
1	1	1439	U	N1-C2	-5.39	1.33	1.38
1	1	586	C	N1-C6	-5.39	1.33	1.37
1	1	798	G	C5-C4	-5.39	1.34	1.38
1	1	3005	A	N3-C4	-5.39	1.31	1.34
1	1	3137	C	N1-C6	-5.39	1.33	1.37
1	1	2884	C	N1-C6	-5.38	1.33	1.37
1	1	1437	C	C4-C5	-5.38	1.38	1.43
1	1	374	A	N3-C4	-5.37	1.31	1.34
1	1	1148	G	C5-C4	-5.37	1.34	1.38
1	1	1195	A	N9-C4	-5.37	1.34	1.37
1	1	359	U	C2-N3	-5.37	1.33	1.37
1	1	1859	A	N3-C4	-5.37	1.31	1.34
1	1	318	A	N3-C4	-5.35	1.31	1.34
1	1	1202	A	N3-C4	-5.34	1.31	1.34
1	1	344	A	N3-C4	-5.34	1.31	1.34
1	1	360	G	N9-C8	-5.34	1.34	1.37
1	1	1407	A	C5-C4	-5.34	1.35	1.38
2	2	58	G	C6-N1	-5.33	1.35	1.39
1	1	804	C	N3-C4	-5.33	1.30	1.33
1	1	927	C	N3-C4	-5.33	1.30	1.33
50	r	185	THR	C-N	-5.33	1.21	1.34
1	1	1174	G	N7-C5	-5.33	1.36	1.39
2	2	104	A	C6-N1	-5.32	1.31	1.35
2	2	119	C	N1-C6	-5.32	1.33	1.37
1	1	1535	A	N7-C5	-5.31	1.36	1.39
1	1	410	U	N1-C2	-5.31	1.33	1.38
1	1	660	A	N3-C4	-5.31	1.31	1.34
1	1	3024	A	N9-C4	-5.31	1.34	1.37
1	1	944	C	N1-C6	-5.31	1.33	1.37
1	1	407	A	N9-C4	-5.30	1.34	1.37
2	2	28	C	N1-C6	-5.30	1.33	1.37
1	1	10	C	N3-C4	-5.30	1.30	1.33
1	1	2828	G	C5-C4	-5.30	1.34	1.38
1	1	926	A	C5-C4	-5.29	1.35	1.38
1	1	2382	G	C5-C4	-5.29	1.34	1.38
1	1	2360	C	N1-C6	-5.29	1.33	1.37
1	1	1496	C	C4-C5	-5.28	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	361	A	C5-C6	-5.28	1.36	1.41
1	1	805	G	C5-C4	-5.27	1.34	1.38
1	1	812	G	N9-C8	-5.27	1.34	1.37
1	1	1170	A	C5-C4	-5.27	1.35	1.38
1	1	427	C	N1-C6	-5.27	1.33	1.37
1	1	802	C	N3-C4	-5.26	1.30	1.33
1	1	349	A	C6-N1	-5.26	1.31	1.35
1	1	799	G	C8-N7	-5.26	1.27	1.30
1	1	816	A	C5-C4	-5.25	1.35	1.38
2	2	118	C	N1-C6	-5.25	1.33	1.37
1	1	404	G	N7-C5	-5.25	1.36	1.39
2	2	43	A	N9-C4	-5.25	1.34	1.37
1	1	2339	C	N1-C6	-5.24	1.34	1.37
1	1	407	A	N3-C4	-5.23	1.31	1.34
1	1	928	C	N1-C2	-5.23	1.34	1.40
1	1	660	A	C5-C6	-5.23	1.36	1.41
1	1	1557	A	N9-C4	-5.23	1.34	1.37
1	1	1423	C	N1-C6	-5.22	1.34	1.37
1	1	363	G	C5-C4	-5.22	1.34	1.38
1	1	337	G	N7-C5	-5.22	1.36	1.39
1	1	348	A	N9-C4	-5.22	1.34	1.37
1	1	353	G	C5-C4	-5.21	1.34	1.38
1	1	653	A	N7-C5	-5.21	1.36	1.39
1	1	1307	G	N7-C5	-5.21	1.36	1.39
1	1	3084	C	N1-C6	-5.21	1.34	1.37
2	2	33	A	C5-C4	-5.21	1.35	1.38
1	1	1426	C	N1-C6	-5.21	1.34	1.37
1	1	1407	A	N3-C4	-5.21	1.31	1.34
2	2	36	G	C5-C4	-5.21	1.34	1.38
2	2	27	U	N1-C2	-5.20	1.33	1.38
1	1	2119	A	N3-C4	-5.20	1.31	1.34
1	1	2366	C	N1-C6	-5.20	1.34	1.37
1	1	1423	C	C4-C5	-5.20	1.38	1.43
1	1	638	C	N1-C6	-5.20	1.34	1.37
1	1	355	A	C5-C4	-5.19	1.35	1.38
1	1	1389	G	C5-C4	-5.19	1.34	1.38
1	1	1451	C	N1-C6	-5.19	1.34	1.37
1	1	1339	C	N1-C6	-5.19	1.34	1.37
1	1	407	A	C6-N1	-5.18	1.31	1.35
1	1	941	G	C5-C4	-5.18	1.34	1.38
1	1	3005	A	N9-C4	-5.18	1.34	1.37
1	1	1587	A	C6-N1	-5.18	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1835	A	C6-N1	-5.17	1.31	1.35
1	1	3106	A	C6-N1	-5.17	1.31	1.35
2	2	106	C	N1-C6	-5.17	1.34	1.37
1	1	29	C	N1-C6	-5.17	1.34	1.37
1	1	893	C	N1-C6	-5.16	1.34	1.37
2	2	107	G	N7-C5	-5.16	1.36	1.39
1	1	213	A	C5-C4	-5.16	1.35	1.38
1	1	1168	U	N3-C4	-5.15	1.33	1.38
1	1	2378	C	N1-C6	-5.15	1.34	1.37
1	1	26	A	N7-C5	-5.15	1.36	1.39
1	1	919	U	C2-N3	-5.14	1.34	1.37
1	1	821	U	C2-N3	-5.14	1.34	1.37
1	1	825	U	N1-C2	-5.14	1.33	1.38
1	1	21	G	C5-C4	-5.13	1.34	1.38
1	1	1711	C	N1-C6	-5.13	1.34	1.37
1	1	1174	G	N9-C8	-5.12	1.34	1.37
1	1	1797	A	N7-C5	-5.12	1.36	1.39
1	1	335	G	C5-C4	-5.11	1.34	1.38
1	1	657	A	N9-C4	-5.11	1.34	1.37
1	1	3106	A	C5-C4	-5.11	1.35	1.38
2	2	33	A	N7-C5	-5.11	1.36	1.39
1	1	357	A	C5-C4	-5.11	1.35	1.38
1	1	1596	C	N1-C6	-5.11	1.34	1.37
1	1	408	A	C5-C4	-5.11	1.35	1.38
1	1	812	G	C5-C4	-5.11	1.34	1.38
1	1	1195	A	N3-C4	-5.11	1.31	1.34
1	1	1397	C	N1-C6	-5.11	1.34	1.37
1	1	1446	A	C5-C4	-5.11	1.35	1.38
2	2	41	A	N9-C4	-5.11	1.34	1.37
1	1	1870	C	N1-C6	-5.10	1.34	1.37
1	1	3097	C	N1-C6	-5.10	1.34	1.37
1	1	3008	A	N9-C4	-5.10	1.34	1.37
1	1	1179	A	N9-C4	-5.10	1.34	1.37
1	1	1187	C	N3-C4	-5.10	1.30	1.33
1	1	1407	A	N9-C4	-5.10	1.34	1.37
1	1	2357	A	N9-C4	-5.10	1.34	1.37
1	1	926	A	N3-C4	-5.10	1.31	1.34
1	1	2119	A	N9-C4	-5.10	1.34	1.37
1	1	506	U	N1-C2	-5.09	1.33	1.38
1	1	27	C	N1-C6	-5.08	1.34	1.37
1	1	82	C	N1-C6	-5.08	1.34	1.37
1	1	2355	G	N1-C2	-5.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	820	A	C5-C4	-5.08	1.35	1.38
1	1	3344	A	N9-C4	-5.08	1.34	1.37
1	1	356	C	C4-C5	-5.08	1.38	1.43
2	2	103	G	C5-C4	-5.08	1.34	1.38
1	1	1836	C	N1-C6	-5.07	1.34	1.37
1	1	1404	G	N9-C8	-5.07	1.34	1.37
1	1	355	A	C6-N1	-5.07	1.32	1.35
1	1	947	G	N9-C8	-5.07	1.34	1.37
1	1	110	G	N7-C5	-5.07	1.36	1.39
1	1	1441	G	C5-C4	-5.07	1.34	1.38
1	1	1586	G	N9-C8	-5.06	1.34	1.37
1	1	51	A	C5-C4	-5.05	1.35	1.38
1	1	359	U	N1-C2	-5.05	1.34	1.38
1	1	1532	C	N1-C6	-5.05	1.34	1.37
47	o	166	VAL	C-N	-5.05	1.22	1.34
1	1	1180	A	N9-C4	-5.05	1.34	1.37
1	1	3305	A	N9-C4	-5.05	1.34	1.37
1	1	1186	G	C5-C4	-5.04	1.34	1.38
1	1	341	G	C5-C4	-5.04	1.34	1.38
1	1	1313	G	C5-C4	-5.04	1.34	1.38
1	1	406	G	C5-C4	-5.03	1.34	1.38
1	1	898	U	N1-C2	-5.03	1.34	1.38
1	1	341	G	N9-C8	-5.03	1.34	1.37
1	1	928	C	N3-C4	-5.03	1.30	1.33
1	1	2367	A	C5-C4	-5.03	1.35	1.38
1	1	318	A	N9-C4	-5.02	1.34	1.37
1	1	1435	A	N9-C4	-5.01	1.34	1.37
2	2	37	A	C5-C4	-5.01	1.35	1.38
1	1	632	G	N9-C8	-5.01	1.34	1.37
1	1	2368	A	N9-C4	-5.01	1.34	1.37
1	1	655	C	N1-C2	-5.01	1.35	1.40
2	2	108	C	N1-C6	-5.01	1.34	1.37
1	1	1446	A	N3-C4	-5.01	1.31	1.34
1	1	1156	C	N1-C6	-5.00	1.34	1.37
1	1	1332	A	N7-C5	-5.00	1.36	1.39
1	1	1178	G	N1-C2	-5.00	1.33	1.37
1	1	1447	G	C5-C4	-5.00	1.34	1.38

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	994	G	O4'-C1'-N9	-10.02	100.19	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2548	C	N1-C2-O2	9.47	124.58	118.90
1	1	2760	C	C2-N1-C1'	9.25	128.98	118.80
1	1	2771	U	C2-N1-C1'	8.80	128.26	117.70
1	1	1561	G	O4'-C1'-N9	8.69	115.16	108.20
1	1	2708	C	N3-C2-O2	-8.64	115.86	121.90
1	1	2788	C	N1-C2-O2	8.56	124.04	118.90
1	1	2112	U	N3-C2-O2	-8.52	116.24	122.20
1	1	2428	U	N3-C2-O2	-8.43	116.30	122.20
1	1	2548	C	N3-C2-O2	-8.30	116.09	121.90
1	1	2760	C	N1-C2-O2	8.21	123.83	118.90
1	1	3354	U	N1-C2-O2	8.12	128.49	122.80
1	1	2861	U	C2-N1-C1'	8.06	127.37	117.70
1	1	3021	A	O4'-C1'-N9	7.97	114.57	108.20
1	1	2548	C	C2-N1-C1'	7.91	127.50	118.80
1	1	3354	U	C2-N1-C1'	7.83	127.10	117.70
1	1	2921	U	N1-C2-O2	7.80	128.26	122.80
1	1	2861	U	N1-C2-O2	7.77	128.24	122.80
1	1	2771	U	N1-C2-O2	7.75	128.23	122.80
1	1	1495	U	N1-C2-N3	7.67	119.50	114.90
1	1	543	C	C2-N1-C1'	7.65	127.22	118.80
1	1	2428	U	N1-C2-O2	7.64	128.15	122.80
1	1	2788	C	N3-C2-O2	-7.59	116.59	121.90
1	1	1279	C	C6-N1-C2	-7.54	117.28	120.30
1	1	2112	U	C2-N1-C1'	7.53	126.74	117.70
1	1	2112	U	N1-C2-O2	7.53	128.07	122.80
1	1	2898	G	C2-N3-C4	-7.50	108.15	111.90
1	1	3217	C	N1-C2-O2	7.46	123.38	118.90
1	1	2364	G	N3-C4-N9	-7.46	121.53	126.00
6	6	231	A	O4'-C1'-N9	7.46	114.16	108.20
1	1	635	G	N3-C4-N9	-7.37	121.58	126.00
1	1	1269	U	C2-N1-C1'	7.35	126.52	117.70
1	1	1416	C	N1-C2-O2	-7.35	114.49	118.90
1	1	2921	U	N3-C2-O2	-7.29	117.10	122.20
1	1	2663	G	N1-C6-O6	-7.25	115.55	119.90
6	6	33	U	C2-N1-C1'	7.25	126.40	117.70
1	1	2788	C	C2-N1-C1'	7.24	126.77	118.80
1	1	2364	G	N3-C4-C5	7.23	132.21	128.60
1	1	1117	G	O4'-C1'-N9	7.18	113.94	108.20
3	3	120	C	C6-N1-C2	-7.17	117.43	120.30
1	1	2707	C	N1-C2-O2	7.16	123.20	118.90
1	1	2861	U	N3-C2-O2	-7.16	117.19	122.20
1	1	2319	U	C2-N1-C1'	7.13	126.26	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3354	U	N3-C2-O2	-7.12	117.21	122.20
1	1	3016	A	O4'-C1'-N9	7.11	113.89	108.20
1	1	922	U	C2-N1-C1'	7.07	126.18	117.70
1	1	3217	C	N3-C2-O2	-7.01	116.99	121.90
6	6	7	C	O4'-C1'-N1	6.99	113.79	108.20
1	1	2319	U	C5-C6-N1	6.97	126.19	122.70
1	1	543	C	C6-N1-C1'	-6.96	112.45	120.80
1	1	976	U	C2-N1-C1'	6.95	126.05	117.70
1	1	2663	G	C5-C6-O6	6.93	132.76	128.60
6	6	232	A	O4'-C1'-N9	6.93	113.74	108.20
3	3	18	C	C5-C6-N1	6.93	124.46	121.00
1	1	1555	U	O4'-C1'-N1	6.90	113.72	108.20
1	1	2708	C	N1-C2-O2	6.87	123.02	118.90
1	1	1227	C	C2-N1-C1'	6.80	126.28	118.80
1	1	1495	U	C5-C6-N1	-6.77	119.31	122.70
1	1	3306	U	N3-C2-O2	-6.77	117.46	122.20
1	1	547	G	C5-C6-O6	6.75	132.65	128.60
1	1	1277	C	N3-C2-O2	-6.75	117.17	121.90
1	1	2810	C	C2-N1-C1'	6.74	126.22	118.80
1	1	2319	U	N1-C2-O2	6.71	127.50	122.80
1	1	1069	C	C2-N1-C1'	6.71	126.18	118.80
1	1	1093	A	O4'-C1'-N9	6.70	113.56	108.20
1	1	3019	U	N3-C2-O2	-6.70	117.51	122.20
1	1	2921	U	C2-N1-C1'	6.69	125.73	117.70
1	1	3008	A	O5'-P-OP1	-6.66	99.70	105.70
1	1	758	C	N3-C2-O2	-6.64	117.25	121.90
1	1	2411	U	C2-N1-C1'	6.63	125.66	117.70
3	3	120	C	N3-C2-O2	-6.62	117.27	121.90
1	1	976	U	N1-C2-O2	6.59	127.42	122.80
1	1	2760	C	C6-N1-C1'	-6.59	112.89	120.80
6	6	7	C	N1-C2-O2	6.58	122.85	118.90
1	1	678	G	C4-C5-N7	6.52	113.41	110.80
1	1	1069	C	C5-C6-N1	6.48	124.24	121.00
1	1	1196	C	C2-N1-C1'	6.48	125.93	118.80
1	1	1177	G	C8-N9-C1'	-6.47	118.59	127.00
6	6	59	C	C2-N1-C1'	6.47	125.92	118.80
1	1	2192	C	C2-N1-C1'	6.46	125.91	118.80
1	1	2411	U	C6-N1-C1'	-6.43	112.20	121.20
1	1	1111	U	N3-C2-O2	-6.42	117.71	122.20
3	3	18	C	C2-N1-C1'	6.41	125.85	118.80
1	1	2825	C	O4'-C1'-N1	6.40	113.32	108.20
1	1	1177	G	C4-N9-C1'	6.38	134.80	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2408	U	N3-C2-O2	-6.38	117.74	122.20
1	1	1312	C	C6-N1-C2	-6.36	117.76	120.30
1	1	2192	C	N1-C2-O2	6.35	122.71	118.90
1	1	997	A	C5-C6-N6	-6.35	118.62	123.70
1	1	2428	U	C2-N1-C1'	6.34	125.31	117.70
1	1	3116	G	N1-C6-O6	-6.34	116.09	119.90
1	1	1279	C	N3-C2-O2	-6.30	117.49	121.90
1	1	879	U	C2-N1-C1'	6.26	125.21	117.70
3	3	120	C	N1-C2-O2	6.25	122.65	118.90
1	1	548	G	C6-C5-N7	-6.24	126.66	130.40
1	1	2771	U	N3-C2-O2	-6.23	117.84	122.20
1	1	1269	U	N3-C2-O2	-6.21	117.85	122.20
1	1	2904	U	C2-N1-C1'	6.20	125.14	117.70
1	1	2567	C	C2-N1-C1'	6.18	125.60	118.80
1	1	544	C	C6-N1-C1'	6.17	128.21	120.80
1	1	2760	C	N3-C2-O2	-6.17	117.58	121.90
1	1	546	C	N1-C2-O2	6.16	122.60	118.90
1	1	1299	U	N3-C2-O2	-6.15	117.89	122.20
1	1	117	U	C2-N1-C1'	6.15	125.08	117.70
1	1	113	C	C6-N1-C2	-6.14	117.84	120.30
1	1	1197	A	C2-N3-C4	6.13	113.66	110.60
1	1	2760	C	C5-C6-N1	6.12	124.06	121.00
1	1	547	G	N9-C4-C5	6.09	107.84	105.40
1	1	1255	C	C2-N1-C1'	6.08	125.49	118.80
1	1	3318	G	N3-C4-C5	6.08	131.64	128.60
1	1	2705	A	N7-C8-N9	6.07	116.84	113.80
1	1	768	C	C6-N1-C2	-6.07	117.87	120.30
1	1	2163	C	C2-N1-C1'	6.07	125.47	118.80
1	1	2690	G	N3-C4-N9	-6.07	122.36	126.00
6	6	33	U	N1-C2-O2	6.06	127.05	122.80
1	1	1298	C	C6-N1-C2	-6.05	117.88	120.30
1	1	1771	C	N3-C2-O2	-6.04	117.67	121.90
2	2	107	G	C4-C5-N7	6.03	113.21	110.80
1	1	1192	C	C6-N1-C2	6.02	122.71	120.30
1	1	1569	U	C2-N1-C1'	5.98	124.88	117.70
1	1	544	C	C2-N1-C1'	-5.96	112.24	118.80
1	1	547	G	N1-C6-O6	-5.96	116.33	119.90
1	1	2771	U	C6-N1-C1'	-5.95	112.87	121.20
1	1	1255	C	C6-N1-C2	-5.95	117.92	120.30
1	1	87	U	N1-C2-O2	5.93	126.95	122.80
1	1	1307	G	P-O3'-C3'	5.92	126.81	119.70
1	1	1187	C	N3-C2-O2	-5.91	117.76	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2437	G	N3-C4-N9	-5.91	122.45	126.00
1	1	1495	U	C4-C5-C6	5.91	123.24	119.70
1	1	2756	C	N1-C2-O2	5.90	122.44	118.90
1	1	1496	C	C2-N1-C1'	5.89	125.28	118.80
1	1	1569	U	N1-C2-O2	5.89	126.92	122.80
1	1	2397	A	C8-N9-C4	5.88	108.15	105.80
1	1	2548	C	C6-N1-C2	-5.87	117.95	120.30
1	1	2531	C	C6-N1-C2	-5.85	117.96	120.30
1	1	1522	U	C2-N1-C1'	-5.83	110.70	117.70
1	1	546	C	C2-N1-C1'	5.82	125.21	118.80
1	1	922	U	C6-N1-C1'	-5.82	113.06	121.20
1	1	3278	C	N1-C2-O2	5.81	122.39	118.90
1	1	3217	C	C2-N1-C1'	5.79	125.17	118.80
1	1	3362	A	N7-C8-N9	5.78	116.69	113.80
1	1	2810	C	C6-N1-C1'	-5.75	113.90	120.80
1	1	548	G	N3-C4-N9	5.72	129.44	126.00
1	1	2923	U	C2-N1-C1'	5.72	124.56	117.70
1	1	2707	C	N3-C2-O2	-5.71	117.91	121.90
1	1	1857	C	C6-N1-C2	-5.70	118.02	120.30
1	1	1522	U	C5-C6-N1	-5.69	119.86	122.70
1	1	2507	C	N1-C2-O2	5.69	122.31	118.90
1	1	1302	A	C8-N9-C4	-5.68	103.53	105.80
6	6	33	U	N3-C2-O2	-5.67	118.23	122.20
1	1	2825	C	C2-N1-C1'	5.67	125.03	118.80
1	1	3362	A	O4'-C1'-N9	5.67	112.73	108.20
1	1	2966	G	N1-C6-O6	-5.66	116.50	119.90
1	1	2811	A	N1-C6-N6	5.66	122.00	118.60
1	1	995	U	C2-N1-C1'	5.66	124.49	117.70
1	1	2663	G	N1-C2-N2	-5.64	111.12	116.20
6	6	53	A	OP2-P-O3'	5.64	117.61	105.20
1	1	2771	U	C5-C6-N1	5.64	125.52	122.70
1	1	678	G	C6-C5-N7	-5.63	127.02	130.40
1	1	1581	C	N3-C4-C5	5.63	124.15	121.90
1	1	635	G	N3-C2-N2	-5.62	115.96	119.90
1	1	970	A	C2-N3-C4	-5.59	107.80	110.60
3	3	18	C	N1-C2-O2	5.59	122.25	118.90
1	1	2434	U	C2-N1-C1'	5.58	124.40	117.70
1	1	1111	U	N1-C2-O2	5.57	126.70	122.80
1	1	1302	A	C4-N9-C1'	5.55	136.28	126.30
1	1	2411	U	N1-C2-O2	5.54	126.68	122.80
6	6	232	A	C4-N9-C1'	5.54	136.28	126.30
1	1	2192	C	N3-C2-O2	-5.53	118.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	544	C	C5-C4-N4	5.52	124.07	120.20
1	1	2760	C	C6-N1-C2	-5.52	118.09	120.30
1	1	2899	C	C2-N1-C1'	5.52	124.87	118.80
1	1	1197	A	C8-N9-C4	-5.51	103.60	105.80
1	1	1314	C	C5-C6-N1	5.50	123.75	121.00
1	1	997	A	C5-C6-N1	5.50	120.45	117.70
3	3	114	U	C5-C6-N1	5.50	125.45	122.70
3	3	120	C	C5-C6-N1	5.50	123.75	121.00
1	1	2861	U	C6-N1-C1'	-5.49	113.51	121.20
1	1	975	C	N1-C2-O2	5.48	122.19	118.90
1	1	3195	U	C2-N1-C1'	5.48	124.28	117.70
1	1	2607	G	C4-N9-C1'	5.47	133.61	126.50
1	1	3131	U	C2-N1-C1'	5.47	124.26	117.70
1	1	637	C	C2-N1-C1'	5.46	124.81	118.80
1	1	971	G	N3-C2-N2	-5.46	116.08	119.90
1	1	546	C	N3-C2-O2	-5.45	118.09	121.90
1	1	3112	G	C4-C5-N7	5.44	112.98	110.80
1	1	3021	A	C6-C5-N7	-5.43	128.50	132.30
1	1	2690	G	C8-N9-C1'	5.43	134.06	127.00
9	C	182	LEU	CA-CB-CG	5.43	127.80	115.30
1	1	3048	A	O4'-C1'-N9	5.42	112.53	108.20
1	1	547	G	N3-C4-N9	-5.41	122.75	126.00
1	1	1269	U	N1-C2-O2	5.40	126.58	122.80
1	1	1227	C	N1-C2-O2	5.39	122.13	118.90
3	3	61	G	N3-C4-N9	5.38	129.23	126.00
1	1	1348	U	O4'-C1'-N1	5.37	112.50	108.20
1	1	2610	G	N3-C4-N9	-5.37	122.78	126.00
1	1	3116	G	C5-C6-O6	5.37	131.82	128.60
1	1	2541	U	P-O3'-C3'	5.37	126.14	119.70
1	1	1176	C	O5'-P-OP2	-5.36	100.88	105.70
1	1	291	C	N3-C2-O2	-5.35	118.15	121.90
1	1	63	A	N1-C6-N6	-5.35	115.39	118.60
6	6	53	A	P-O3'-C3'	5.35	126.12	119.70
1	1	260	C	C2-N1-C1'	5.35	124.68	118.80
3	3	25	G	N7-C8-N9	5.35	115.77	113.10
1	1	906	A	C5-C6-N6	-5.33	119.43	123.70
1	1	1604	G	C4-N9-C1'	5.32	133.41	126.50
1	1	3080	G	C6-C5-N7	-5.32	127.21	130.40
1	1	1139	G	C4-N9-C1'	5.31	133.40	126.50
1	1	1109	U	C2-N1-C1'	5.31	124.07	117.70
1	1	1805	C	C6-N1-C2	-5.31	118.18	120.30
1	1	1604	G	C8-N9-C1'	-5.30	120.11	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	3057	U	N3-C2-O2	-5.30	118.49	122.20
1	1	2548	C	C6-N1-C1'	-5.30	114.44	120.80
1	1	1866	C	N3-C2-O2	-5.29	118.19	121.90
1	1	1255	C	N1-C2-O2	5.29	122.08	118.90
6	6	32	A	C2-N3-C4	5.29	113.25	110.60
1	1	548	G	N9-C4-C5	-5.27	103.29	105.40
1	1	3306	U	C5-C4-O4	5.26	129.06	125.90
1	1	2412	G	C4-C5-N7	5.26	112.90	110.80
1	1	729	C	C2-N1-C1'	5.23	124.55	118.80
1	1	2904	U	C6-N1-C1'	-5.23	113.88	121.20
2	2	40	A	N1-C6-N6	-5.22	115.47	118.60
1	1	2822	U	C2-N1-C1'	5.22	123.96	117.70
1	1	2835	U	C5-C4-O4	-5.22	122.77	125.90
1	1	1568	U	P-O3'-C3'	5.21	125.95	119.70
1	1	2507	C	C2-N1-C1'	5.21	124.53	118.80
1	1	1525	G	C4-N9-C1'	5.20	133.27	126.50
1	1	976	U	N3-C2-O2	-5.20	118.56	122.20
1	1	2522	G	C8-N9-C1'	-5.20	120.24	127.00
1	1	113	C	C2-N1-C1'	5.20	124.51	118.80
1	1	2825	C	C6-N1-C1'	-5.19	114.57	120.80
1	1	2923	U	N1-C2-O2	5.19	126.43	122.80
1	1	678	G	N9-C4-C5	-5.17	103.33	105.40
1	1	1301	A	C5-N7-C8	-5.17	101.31	103.90
3	3	110	G	N3-C2-N2	-5.17	116.28	119.90
1	1	3317	U	C2-N1-C1'	5.16	123.89	117.70
1	1	976	U	C5-C6-N1	5.15	125.27	122.70
1	1	1296	C	C5-C6-N1	5.15	123.57	121.00
1	1	1495	U	N3-C2-O2	-5.15	118.60	122.20
1	1	720	A	P-O3'-C3'	5.14	125.87	119.70
1	1	2574	G	N3-C4-N9	5.14	129.08	126.00
1	1	2607	G	C8-N9-C1'	-5.14	120.32	127.00
1	1	3303	G	O4'-C1'-N9	5.14	112.31	108.20
1	1	845	G	N3-C4-C5	5.13	131.17	128.60
1	1	283	G	C2-N3-C4	5.12	114.46	111.90
3	3	25	G	C4-N9-C1'	5.12	133.15	126.50
1	1	895	A	C6-C5-N7	-5.12	128.72	132.30
1	1	1590	G	C4-C5-N7	5.11	112.84	110.80
1	1	3021	A	C4-N9-C1'	5.08	135.45	126.30
1	1	1139	G	C6-C5-N7	-5.08	127.35	130.40
1	1	3354	U	C6-N1-C1'	-5.07	114.10	121.20
1	1	1255	C	N3-C2-O2	-5.07	118.35	121.90
1	1	1437	C	C2-N1-C1'	5.07	124.38	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2507	C	C5-C6-N1	5.07	123.53	121.00
1	1	2788	C	C6-N1-C1'	-5.07	114.72	120.80
1	1	1279	C	C5-C6-N1	5.06	123.53	121.00
1	1	2973	G	C5-C6-O6	5.06	131.64	128.60
1	1	2853	A	C5-C6-N6	-5.05	119.66	123.70
1	1	3080	G	N3-C4-N9	5.05	129.03	126.00
1	1	548	G	C4-N9-C1'	5.05	133.07	126.50
1	1	1302	A	C4-C5-C6	5.05	119.53	117.00
1	1	646	A	N9-C1'-C2'	5.05	120.56	114.00
1	1	2853	A	C6-C5-N7	-5.05	128.77	132.30
1	1	922	U	N1-C2-O2	5.04	126.33	122.80
1	1	2598	G	N3-C4-N9	-5.04	122.98	126.00
1	1	182	U	C2-N1-C1'	5.04	123.74	117.70
1	1	1314	C	C6-N1-C2	-5.03	118.29	120.30
1	1	635	G	N3-C4-C5	5.03	131.12	128.60
1	1	2412	G	C6-C5-N7	-5.03	127.38	130.40
1	1	2648	G	N1-C6-O6	-5.03	116.88	119.90
1	1	3362	A	C5-N7-C8	-5.03	101.39	103.90
1	1	2682	C	N1-C2-O2	5.03	121.92	118.90
1	1	237	G	C6-C5-N7	-5.03	127.39	130.40
1	1	2646	C	N3-C2-O2	-5.03	118.38	121.90
1	1	2875	U	OP1-P-O3'	5.02	116.25	105.20
1	1	3139	A	O5'-P-OP1	-5.02	101.18	105.70
6	6	16	U	P-O3'-C3'	5.02	125.72	119.70
1	1	1203	A	C4-C5-N7	5.01	113.21	110.70
1	1	2567	C	C6-N1-C1'	-5.01	114.79	120.80
1	1	648	C	C6-N1-C2	-5.01	118.30	120.30
1	1	3058	U	C2-N1-C1'	5.01	123.71	117.70
1	1	2364	G	C2-N3-C4	-5.00	109.40	111.90

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	26	ASN	Peptide
4	4	362	ARG	Peptide
4	4	97	ILE	Peptide
8	B	221	THR	Peptide
8	B	340	LYS	Peptide
9	C	318	LEU	Peptide
12	F	232	ARG	Peptide
16	J	170	ASP	Peptide

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Mol	Chain	Res	Type	Group
18	L	46	ILE	Peptide
28	V	89	ASP	Peptide
36	d	87	ASN	Peptide
45	m	378	SER	Peptide
45	m	417	GLU	Peptide
45	m	422	LYS	Peptide
45	m	77	TRP	Peptide
45	m	98	GLU	Peptide
45	m	99	THR	Peptide
46	n	375	ILE	Peptide
47	o	171	ALA	Peptide
50	r	236	LYS	Peptide
53	u	79	VAL	Peptide
56	x	125	ALA	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	508/593 (86%)	423 (83%)	84 (16%)	1 (0%)	47	79
5	5	71/120 (59%)	69 (97%)	2 (3%)	0	100	100
7	A	211/254 (83%)	173 (82%)	38 (18%)	0	100	100
8	B	384/387 (99%)	322 (84%)	59 (15%)	3 (1%)	19	58
9	C	359/362 (99%)	297 (83%)	61 (17%)	1 (0%)	41	74
10	D	272/297 (92%)	223 (82%)	48 (18%)	1 (0%)	34	69
11	E	152/176 (86%)	137 (90%)	15 (10%)	0	100	100
12	F	220/244 (90%)	197 (90%)	23 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	G	231/256 (90%)	194 (84%)	37 (16%)	0	100	100
14	H	189/191 (99%)	161 (85%)	27 (14%)	1 (0%)	29	67
15	I	129/166 (78%)	113 (88%)	15 (12%)	1 (1%)	19	58
16	J	167/174 (96%)	134 (80%)	33 (20%)	0	100	100
17	K	252/376 (67%)	219 (87%)	33 (13%)	0	100	100
18	L	185/199 (93%)	151 (82%)	33 (18%)	1 (0%)	29	67
19	M	135/138 (98%)	119 (88%)	16 (12%)	0	100	100
20	N	201/204 (98%)	176 (88%)	24 (12%)	1 (0%)	29	67
21	O	195/199 (98%)	184 (94%)	11 (6%)	0	100	100
22	P	181/184 (98%)	156 (86%)	25 (14%)	0	100	100
23	Q	132/186 (71%)	116 (88%)	16 (12%)	0	100	100
24	R	154/189 (82%)	141 (92%)	13 (8%)	0	100	100
25	S	169/172 (98%)	141 (83%)	28 (17%)	0	100	100
26	T	115/160 (72%)	103 (90%)	12 (10%)	0	100	100
27	U	104/121 (86%)	89 (86%)	15 (14%)	0	100	100
28	V	134/137 (98%)	120 (90%)	14 (10%)	0	100	100
29	W	232/236 (98%)	201 (87%)	31 (13%)	0	100	100
30	X	139/142 (98%)	122 (88%)	17 (12%)	0	100	100
31	Y	124/127 (98%)	111 (90%)	13 (10%)	0	100	100
32	Z	133/136 (98%)	110 (83%)	23 (17%)	0	100	100
33	a	91/149 (61%)	74 (81%)	17 (19%)	0	100	100
34	b	638/647 (99%)	525 (82%)	110 (17%)	3 (0%)	29	67
35	c	95/105 (90%)	84 (88%)	11 (12%)	0	100	100
36	d	105/113 (93%)	87 (83%)	18 (17%)	0	100	100
37	e	125/130 (96%)	112 (90%)	13 (10%)	0	100	100
38	f	104/107 (97%)	91 (88%)	13 (12%)	0	100	100
39	g	110/121 (91%)	98 (89%)	12 (11%)	0	100	100
40	h	117/120 (98%)	110 (94%)	7 (6%)	0	100	100
41	i	97/100 (97%)	84 (87%)	13 (13%)	0	100	100
42	j	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
43	k	75/78 (96%)	69 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	l	48/51 (94%)	41 (85%)	7 (15%)	0	100	100
45	m	449/486 (92%)	358 (80%)	86 (19%)	5 (1%)	14	51
46	n	365/605 (60%)	307 (84%)	56 (15%)	2 (0%)	29	67
47	o	131/220 (60%)	106 (81%)	25 (19%)	0	100	100
48	p	89/92 (97%)	77 (86%)	12 (14%)	0	100	100
49	q	147/455 (32%)	120 (82%)	26 (18%)	1 (1%)	22	61
50	r	224/261 (86%)	185 (83%)	38 (17%)	1 (0%)	34	69
51	s	65/520 (12%)	57 (88%)	8 (12%)	0	100	100
52	t	283/322 (88%)	239 (84%)	42 (15%)	2 (1%)	22	61
53	u	148/199 (74%)	129 (87%)	19 (13%)	0	100	100
54	v	243/254 (96%)	201 (83%)	42 (17%)	0	100	100
55	w	178/203 (88%)	143 (80%)	35 (20%)	0	100	100
56	x	393/515 (76%)	316 (80%)	77 (20%)	0	100	100
57	y	242/245 (99%)	203 (84%)	39 (16%)	0	100	100
58	z	53/106 (50%)	51 (96%)	2 (4%)	0	100	100
All	All	10178/12418 (82%)	8645 (85%)	1509 (15%)	24 (0%)	50	79

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	4	PRO
20	N	95	GLN
34	b	9	PRO
34	b	399	ALA
46	n	153	SER
15	I	18	LEU
45	m	136	SER
52	t	58	ALA
4	4	363	ASP
8	B	342	LEU
10	D	261	THR
34	b	484	SER
45	m	240	LYS
45	m	424	ALA
50	r	147	TRP
52	t	247	VAL
14	H	50	ASN

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Mol	Chain	Res	Type
18	L	76	THR
45	m	241	SER
45	m	418	ILE
49	q	385	THR
46	n	455	PRO
8	B	166	ILE
8	B	188	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	
4	4	453/520 (87%)	422 (93%)	31 (7%)	16	49
5	5	67/106 (63%)	63 (94%)	4 (6%)	19	54
7	A	166/196 (85%)	155 (93%)	11 (7%)	16	51
8	B	322/323 (100%)	290 (90%)	32 (10%)	8	30
9	C	288/289 (100%)	272 (94%)	16 (6%)	21	57
10	D	227/245 (93%)	211 (93%)	16 (7%)	15	48
11	E	134/153 (88%)	131 (98%)	3 (2%)	52	79
12	F	186/205 (91%)	174 (94%)	12 (6%)	17	51
13	G	191/208 (92%)	177 (93%)	14 (7%)	14	46
14	H	171/171 (100%)	156 (91%)	15 (9%)	10	36
15	I	117/141 (83%)	114 (97%)	3 (3%)	46	76
16	J	147/150 (98%)	134 (91%)	13 (9%)	10	36
17	K	236/346 (68%)	217 (92%)	19 (8%)	11	42
18	L	149/159 (94%)	129 (87%)	20 (13%)	4	18
19	M	108/109 (99%)	96 (89%)	12 (11%)	6	25
20	N	175/176 (99%)	161 (92%)	14 (8%)	12	42
21	O	160/162 (99%)	152 (95%)	8 (5%)	24	60
22	P	145/146 (99%)	133 (92%)	12 (8%)	11	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	Q	110/151 (73%)	103 (94%)	7 (6%)	17	52
24	R	129/154 (84%)	125 (97%)	4 (3%)	40	72
25	S	155/156 (99%)	145 (94%)	10 (6%)	17	51
26	T	102/137 (74%)	98 (96%)	4 (4%)	32	67
27	U	93/107 (87%)	86 (92%)	7 (8%)	13	45
28	V	104/105 (99%)	95 (91%)	9 (9%)	10	37
29	W	211/213 (99%)	198 (94%)	13 (6%)	18	53
30	X	117/118 (99%)	112 (96%)	5 (4%)	29	64
31	Y	109/110 (99%)	102 (94%)	7 (6%)	17	52
32	Z	115/116 (99%)	111 (96%)	4 (4%)	36	69
33	a	76/119 (64%)	74 (97%)	2 (3%)	46	76
34	b	568/573 (99%)	533 (94%)	35 (6%)	18	53
35	c	81/88 (92%)	72 (89%)	9 (11%)	6	25
36	d	94/97 (97%)	84 (89%)	10 (11%)	6	27
37	e	109/111 (98%)	102 (94%)	7 (6%)	17	52
38	f	90/91 (99%)	86 (96%)	4 (4%)	28	64
39	g	95/103 (92%)	88 (93%)	7 (7%)	13	46
40	h	104/105 (99%)	100 (96%)	4 (4%)	33	67
41	i	81/82 (99%)	74 (91%)	7 (9%)	10	38
42	j	70/71 (99%)	63 (90%)	7 (10%)	7	30
43	k	68/69 (99%)	62 (91%)	6 (9%)	10	36
44	l	45/46 (98%)	44 (98%)	1 (2%)	52	79
45	m	400/428 (94%)	363 (91%)	37 (9%)	9	33
46	n	334/548 (61%)	316 (95%)	18 (5%)	22	58
47	o	118/199 (59%)	108 (92%)	10 (8%)	10	38
48	p	71/72 (99%)	67 (94%)	4 (6%)	21	57
49	q	140/420 (33%)	136 (97%)	4 (3%)	42	74
50	r	203/229 (89%)	182 (90%)	21 (10%)	7	29
51	s	62/445 (14%)	53 (86%)	9 (14%)	3	15
52	t	256/287 (89%)	245 (96%)	11 (4%)	29	64
53	u	133/180 (74%)	129 (97%)	4 (3%)	41	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	v	222/231 (96%)	203 (91%)	19 (9%)	10	38
55	w	161/179 (90%)	144 (89%)	17 (11%)	6	27
56	x	344/451 (76%)	308 (90%)	36 (10%)	7	28
57	y	210/211 (100%)	191 (91%)	19 (9%)	9	34
58	z	48/95 (50%)	47 (98%)	1 (2%)	53	79
All	All	8870/10702 (83%)	8236 (93%)	634 (7%)	18	47

All (634) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	4	28	TYR
4	4	45	LEU
4	4	48	ASP
4	4	55	THR
4	4	61	VAL
4	4	75	ARG
4	4	77	GLU
4	4	82	ASN
4	4	85	ASN
4	4	87	ARG
4	4	115	LEU
4	4	116	ASN
4	4	124	THR
4	4	137	ASP
4	4	146	HIS
4	4	161	TYR
4	4	176	LEU
4	4	203	THR
4	4	242	SER
4	4	251	LEU
4	4	262	ARG
4	4	309	PHE
4	4	326	LEU
4	4	362	ARG
4	4	367	THR
4	4	381	LYS
4	4	383	ASP
4	4	412	LEU
4	4	453	ASN
4	4	500	VAL

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Mol	Chain	Res	Type
4	4	561	LYS
5	5	52	LEU
5	5	57	PHE
5	5	65	LYS
5	5	92	TYR
7	A	15	ILE
7	A	18	SER
7	A	20	THR
7	A	49	VAL
7	A	71	LEU
7	A	101	VAL
7	A	122	ASP
7	A	130	SER
7	A	134	VAL
7	A	191	LEU
7	A	200	ARG
8	B	10	ARG
8	B	17	LEU
8	B	25	ILE
8	B	59	ASP
8	B	73	VAL
8	B	84	VAL
8	B	89	VAL
8	B	102	LEU
8	B	111	SER
8	B	156	SER
8	B	188	ILE
8	B	199	PHE
8	B	212	ASN
8	B	221	THR
8	B	229	VAL
8	B	237	LYS
8	B	249	VAL
8	B	266	ARG
8	B	274	SER
8	B	285	VAL
8	B	296	THR
8	B	299	ASP
8	B	301	THR
8	B	306	THR
8	B	319	ASN
8	B	320	ASP

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Mol	Chain	Res	Type
8	B	322	ILE
8	B	332	ARG
8	B	370	PHE
8	B	382	THR
8	B	386	ASP
8	B	387	LEU
9	C	16	THR
9	C	60	THR
9	C	93	MET
9	C	110	ASN
9	C	136	LEU
9	C	141	ARG
9	C	194	TYR
9	C	230	VAL
9	C	291	ASN
9	C	292	SER
9	C	306	THR
9	C	310	THR
9	C	334	PHE
9	C	341	SER
9	C	347	THR
9	C	349	THR
10	D	15	ARG
10	D	28	THR
10	D	45	ASN
10	D	56	THR
10	D	79	TYR
10	D	110	LEU
10	D	116	ASP
10	D	146	LEU
10	D	159	VAL
10	D	176	SER
10	D	187	THR
10	D	190	ILE
10	D	205	SER
10	D	207	TYR
10	D	232	ASP
10	D	262	LYS
11	E	87	THR
11	E	101	PHE
11	E	152	THR
12	F	26	VAL

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Mol	Chain	Res	Type
12	F	95	ILE
12	F	109	THR
12	F	111	ILE
12	F	113	SER
12	F	129	LEU
12	F	143	THR
12	F	160	ARG
12	F	179	LEU
12	F	183	ASP
12	F	211	SER
12	F	242	SER
13	G	47	SER
13	G	48	ARG
13	G	65	LEU
13	G	66	SER
13	G	74	THR
13	G	77	GLN
13	G	86	THR
13	G	151	VAL
13	G	164	VAL
13	G	189	LEU
13	G	190	VAL
13	G	201	THR
13	G	246	MET
13	G	249	ARG
14	H	5	GLN
14	H	41	ILE
14	H	49	ASN
14	H	50	ASN
14	H	51	GLN
14	H	52	LEU
14	H	70	THR
14	H	76	ASP
14	H	82	VAL
14	H	83	THR
14	H	124	ARG
14	H	133	THR
14	H	139	ASN
14	H	188	THR
14	H	191	LEU
15	I	68	LEU
15	I	105	VAL

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Mol	Chain	Res	Type
15	I	123	LEU
16	J	30	LEU
16	J	48	SER
16	J	53	THR
16	J	56	THR
16	J	59	ILE
16	J	68	HIS
16	J	109	HIS
16	J	112	LEU
16	J	115	LYS
16	J	127	PHE
16	J	131	MET
16	J	144	CYS
16	J	148	VAL
17	K	49	SER
17	K	89	THR
17	K	120	ASP
17	K	129	ASP
17	K	141	PHE
17	K	145	ASP
17	K	152	ASP
17	K	154	ILE
17	K	181	LEU
17	K	204	THR
17	K	205	THR
17	K	211	THR
17	K	217	PHE
17	K	220	THR
17	K	242	THR
17	K	255	ARG
17	K	261	ASP
17	K	288	VAL
17	K	291	LEU
18	L	12	ASN
18	L	24	VAL
18	L	27	ASP
18	L	34	SER
18	L	52	ASP
18	L	57	VAL
18	L	58	VAL
18	L	62	THR
18	L	69	VAL

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Mol	Chain	Res	Type
18	L	86	THR
18	L	93	ILE
18	L	100	ARG
18	L	103	ASN
18	L	122	LYS
18	L	138	VAL
18	L	153	ASP
18	L	154	VAL
18	L	162	ASN
18	L	169	THR
18	L	186	ARG
19	M	6	ILE
19	M	20	VAL
19	M	37	GLU
19	M	47	ASP
19	M	50	LYS
19	M	53	VAL
19	M	65	LEU
19	M	90	VAL
19	M	97	SER
19	M	105	GLN
19	M	130	THR
19	M	135	LEU
20	N	4	TYR
20	N	19	LEU
20	N	20	ARG
20	N	41	ARG
20	N	43	THR
20	N	50	ARG
20	N	64	VAL
20	N	99	ARG
20	N	104	GLU
20	N	109	ARG
20	N	124	ASP
20	N	159	ARG
20	N	167	THR
20	N	196	THR
21	O	34	VAL
21	O	48	PHE
21	O	84	LEU
21	O	117	ARG
21	O	138	LEU

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Mol	Chain	Res	Type
21	O	150	GLU
21	O	167	TYR
21	O	187	GLU
22	P	7	THR
22	P	29	THR
22	P	32	THR
22	P	36	ILE
22	P	42	THR
22	P	65	SER
22	P	87	SER
22	P	113	TYR
22	P	114	VAL
22	P	119	VAL
22	P	128	ARG
22	P	144	SER
23	Q	22	ASP
23	Q	40	THR
23	Q	55	SER
23	Q	64	VAL
23	Q	81	VAL
23	Q	86	THR
23	Q	107	THR
24	R	86	GLU
24	R	98	ARG
24	R	127	SER
24	R	134	HIS
25	S	32	SER
25	S	42	TRP
25	S	48	LEU
25	S	55	SER
25	S	82	ASP
25	S	96	ASP
25	S	105	THR
25	S	134	ASP
25	S	162	THR
25	S	171	PHE
26	T	89	LEU
26	T	93	VAL
26	T	116	ARG
26	T	126	VAL
27	U	33	TYR
27	U	57	THR

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Mol	Chain	Res	Type
27	U	61	THR
27	U	67	SER
27	U	89	LEU
27	U	99	LYS
27	U	105	LEU
28	V	44	SER
28	V	53	SER
28	V	54	LEU
28	V	59	MET
28	V	61	THR
28	V	74	MET
28	V	88	ARG
28	V	98	ASN
28	V	137	VAL
29	W	45	LEU
29	W	58	THR
29	W	59	SER
29	W	60	TRP
29	W	81	ARG
29	W	99	VAL
29	W	105	THR
29	W	112	VAL
29	W	113	LYS
29	W	130	LYS
29	W	133	LEU
29	W	139	GLU
29	W	224	ASP
30	X	26	VAL
30	X	81	ILE
30	X	119	THR
30	X	126	LEU
30	X	134	ASP
31	Y	24	SER
31	Y	56	VAL
31	Y	67	GLU
31	Y	74	TYR
31	Y	82	VAL
31	Y	105	VAL
31	Y	112	ASP
32	Z	26	VAL
32	Z	30	ASP
32	Z	38	PHE

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Mol	Chain	Res	Type
32	Z	87	LEU
33	a	59	ARG
33	a	68	PHE
34	b	1	MET
34	b	5	TRP
34	b	11	VAL
34	b	19	ASP
34	b	29	THR
34	b	48	ARG
34	b	73	ASP
34	b	82	MET
34	b	84	THR
34	b	141	LYS
34	b	162	SER
34	b	163	ILE
34	b	167	THR
34	b	169	THR
34	b	173	CYS
34	b	191	ASP
34	b	200	THR
34	b	253	PHE
34	b	256	LEU
34	b	312	VAL
34	b	315	VAL
34	b	319	THR
34	b	322	CYS
34	b	365	GLN
34	b	372	VAL
34	b	411	VAL
34	b	420	TYR
34	b	440	ASN
34	b	485	GLU
34	b	512	SER
34	b	513	LEU
34	b	546	GLN
34	b	569	ASP
34	b	587	ASP
34	b	639	ARG
35	c	30	THR
35	c	41	LEU
35	c	48	THR
35	c	63	SER

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Mol	Chain	Res	Type
35	c	87	VAL
35	c	90	VAL
35	c	99	ASP
35	c	102	THR
35	c	104	LEU
36	d	24	SER
36	d	47	ASP
36	d	55	LEU
36	d	64	VAL
36	d	70	ARG
36	d	71	LEU
36	d	89	LEU
36	d	94	GLU
36	d	105	GLN
36	d	106	THR
37	e	24	ARG
37	e	47	ARG
37	e	69	SER
37	e	73	THR
37	e	88	HIS
37	e	99	ASN
37	e	109	LEU
38	f	15	SER
38	f	22	VAL
38	f	37	THR
38	f	60	ARG
39	g	18	ASN
39	g	23	VAL
39	g	44	CYS
39	g	46	ASP
39	g	51	LEU
39	g	55	SER
39	g	65	VAL
40	h	11	THR
40	h	69	LEU
40	h	79	ASP
40	h	93	THR
41	i	18	THR
41	i	21	THR
41	i	51	SER
41	i	58	ILE
41	i	59	ASP

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Mol	Chain	Res	Type
41	i	60	LEU
41	i	97	SER
42	j	3	LYS
42	j	21	ARG
42	j	33	THR
42	j	45	ARG
42	j	59	THR
42	j	69	HIS
42	j	72	ARG
43	k	19	ASP
43	k	41	THR
43	k	53	THR
43	k	54	LEU
43	k	57	ASN
43	k	69	LEU
44	l	34	THR
45	m	23	ARG
45	m	29	PHE
45	m	32	ASP
45	m	57	ARG
45	m	64	SER
45	m	76	ARG
45	m	103	THR
45	m	109	ARG
45	m	134	THR
45	m	166	GLU
45	m	194	TRP
45	m	196	SER
45	m	224	VAL
45	m	240	LYS
45	m	250	THR
45	m	265	VAL
45	m	269	VAL
45	m	275	LYS
45	m	286	PHE
45	m	291	THR
45	m	311	THR
45	m	329	SER
45	m	337	LYS
45	m	341	CYS
45	m	365	ILE
45	m	381	ASP

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Mol	Chain	Res	Type
45	m	388	VAL
45	m	394	THR
45	m	395	HIS
45	m	410	LYS
45	m	411	HIS
45	m	415	THR
45	m	425	THR
45	m	438	LEU
45	m	466	VAL
45	m	467	LEU
45	m	472	GLU
46	n	35	LEU
46	n	61	THR
46	n	111	SER
46	n	134	ASP
46	n	139	LEU
46	n	158	ASP
46	n	180	PHE
46	n	199	TRP
46	n	215	PHE
46	n	227	THR
46	n	231	PHE
46	n	233	LEU
46	n	261	SER
46	n	360	PHE
46	n	377	GLU
46	n	417	LEU
46	n	434	ASP
46	n	458	SER
47	o	94	TYR
47	o	102	PHE
47	o	122	LEU
47	o	127	LYS
47	o	132	ARG
47	o	139	PHE
47	o	144	ASP
47	o	157	LEU
47	o	191	LYS
47	o	214	SER
48	p	41	PHE
48	p	56	THR
48	p	70	THR

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Mol	Chain	Res	Type
48	p	84	ARG
49	q	218	THR
49	q	240	LYS
49	q	244	GLU
49	q	271	ASP
50	r	18	LEU
50	r	43	THR
50	r	60	SER
50	r	92	LEU
50	r	119	SER
50	r	133	MET
50	r	152	THR
50	r	157	VAL
50	r	161	PHE
50	r	162	THR
50	r	163	ARG
50	r	194	PHE
50	r	205	GLN
50	r	208	MET
50	r	210	THR
50	r	212	LEU
50	r	241	LYS
50	r	248	GLU
50	r	251	ARG
50	r	260	LEU
50	r	261	VAL
51	s	1	MET
51	s	8	SER
51	s	10	ARG
51	s	13	THR
51	s	50	ILE
51	s	60	ILE
51	s	61	LEU
51	s	68	LYS
51	s	73	GLU
52	t	50	SER
52	t	97	LYS
52	t	99	PHE
52	t	130	ARG
52	t	134	THR
52	t	141	LEU
52	t	146	ARG

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Mol	Chain	Res	Type
52	t	167	ARG
52	t	187	LEU
52	t	210	LYS
52	t	303	ASN
53	u	9	CYS
53	u	10	SER
53	u	19	ILE
53	u	63	LEU
54	v	16	LEU
54	v	50	SER
54	v	56	ASP
54	v	72	MET
54	v	92	SER
54	v	102	PHE
54	v	113	MET
54	v	129	LYS
54	v	134	THR
54	v	144	GLN
54	v	161	PHE
54	v	165	PHE
54	v	192	ASP
54	v	217	ARG
54	v	225	GLU
54	v	231	ASP
54	v	236	ARG
54	v	243	ASP
54	v	247	GLU
55	w	12	THR
55	w	31	SER
55	w	35	ASP
55	w	39	LEU
55	w	61	LEU
55	w	72	THR
55	w	87	MET
55	w	90	LEU
55	w	96	THR
55	w	98	ASP
55	w	103	LYS
55	w	148	LYS
55	w	154	LEU
55	w	155	ASP
55	w	158	TRP

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Mol	Chain	Res	Type
55	w	159	LEU
55	w	196	ARG
56	x	121	TYR
56	x	142	HIS
56	x	148	CYS
56	x	155	THR
56	x	161	THR
56	x	186	TYR
56	x	195	SER
56	x	197	ASP
56	x	226	ARG
56	x	229	SER
56	x	244	LYS
56	x	255	SER
56	x	259	THR
56	x	263	TRP
56	x	266	VAL
56	x	278	THR
56	x	280	SER
56	x	318	SER
56	x	326	LEU
56	x	328	LEU
56	x	329	SER
56	x	330	THR
56	x	354	LYS
56	x	362	LYS
56	x	376	THR
56	x	379	ASP
56	x	383	MET
56	x	398	MET
56	x	413	ASP
56	x	441	ARG
56	x	443	HIS
56	x	457	ARG
56	x	463	SER
56	x	473	VAL
56	x	480	VAL
56	x	493	ASP
57	y	20	THR
57	y	38	PHE
57	y	51	THR
57	y	52	THR

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Mol	Chain	Res	Type
57	y	68	ARG
57	y	76	THR
57	y	81	LEU
57	y	101	LEU
57	y	110	CYS
57	y	112	ASP
57	y	120	ASP
57	y	121	ILE
57	y	141	THR
57	y	164	GLN
57	y	187	ASN
57	y	193	VAL
57	y	197	MET
57	y	202	TYR
57	y	206	THR
58	z	41	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	58	GLN
4	4	235	ASN
4	4	555	GLN
5	5	73	GLN
7	A	132	ASN
8	B	3	HIS
8	B	13	HIS
8	B	68	HIS
8	B	243	HIS
10	D	151	GLN
12	F	209	ASN
12	F	225	GLN
13	G	33	ASN
13	G	38	GLN
13	G	123	GLN
14	H	50	ASN
14	H	125	ASN
14	H	183	HIS
15	I	126	HIS
17	K	104	HIS
17	K	200	ASN
17	K	295	GLN

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Mol	Chain	Res	Type
18	L	106	GLN
19	M	41	GLN
20	N	87	GLN
22	P	10	ASN
24	R	134	HIS
25	S	88	HIS
25	S	108	GLN
28	V	81	GLN
29	W	91	GLN
29	W	159	HIS
32	Z	29	HIS
34	b	26	GLN
34	b	413	ASN
34	b	440	ASN
34	b	465	ASN
34	b	500	GLN
34	b	579	ASN
37	e	88	HIS
38	f	42	GLN
40	h	104	GLN
42	j	69	HIS
42	j	76	ASN
43	k	32	ASN
45	m	146	GLN
45	m	175	GLN
45	m	207	GLN
45	m	310	HIS
45	m	408	GLN
46	n	164	ASN
46	n	456	HIS
47	o	199	ASN
50	r	96	GLN
52	t	88	ASN
52	t	238	GLN
52	t	291	GLN
52	t	300	GLN
54	v	144	GLN
54	v	191	GLN
55	w	57	ASN
55	w	151	ASN
55	w	195	GLN
55	w	198	ASN

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Mol	Chain	Res	Type
56	x	176	GLN
56	x	325	HIS
56	x	443	HIS
57	y	82	GLN
57	y	86	ASN
57	y	164	GLN
57	y	170	GLN
57	y	178	GLN
58	z	31	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2962/3396 (87%)	915 (30%)	58 (1%)
2	2	157/158 (99%)	33 (21%)	2 (1%)
3	3	120/121 (99%)	54 (45%)	0
6	6	63/232 (27%)	33 (52%)	5 (7%)
All	All	3302/3907 (84%)	1035 (31%)	65 (1%)

All (1035) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	5	G
1	1	6	A
1	1	18	G
1	1	26	A
1	1	39	A
1	1	40	A
1	1	41	G
1	1	42	C
1	1	43	A
1	1	45	A
1	1	48	A
1	1	49	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	73	C
1	1	74	G

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Mol	Chain	Res	Type
1	1	75	G
1	1	85	A
1	1	92	G
1	1	93	C
1	1	94	G
1	1	96	G
1	1	109	A
1	1	110	G
1	1	115	A
1	1	116	A
1	1	118	U
1	1	119	U
1	1	121	A
1	1	122	A
1	1	135	C
1	1	136	G
1	1	142	C
1	1	143	G
1	1	146	U
1	1	148	G
1	1	155	G
1	1	156	G
1	1	157	A
1	1	160	G
1	1	161	G
1	1	163	C
1	1	166	C
1	1	168	U
1	1	169	U
1	1	170	G
1	1	173	G
1	1	175	C
1	1	181	U
1	1	182	U
1	1	187	A
1	1	190	U
1	1	191	U
1	1	198	A
1	1	200	C
1	1	210	U
1	1	211	A
1	1	213	A

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Mol	Chain	Res	Type
1	1	218	G
1	1	219	A
1	1	240	U
1	1	241	G
1	1	242	C
1	1	243	G
1	1	248	U
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	253	A
1	1	254	A
1	1	260	C
1	1	262	U
1	1	263	C
1	1	269	G
1	1	281	G
1	1	284	A
1	1	285	A
1	1	286	U
1	1	292	U
1	1	295	A
1	1	299	G
1	1	305	U
1	1	306	A
1	1	307	A
1	1	308	A
1	1	311	C
1	1	323	A
1	1	329	U
1	1	338	A
1	1	339	C
1	1	354	U
1	1	359	U
1	1	368	G
1	1	376	G
1	1	390	G
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A

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Mol	Chain	Res	Type
1	1	403	C
1	1	404	G
1	1	407	A
1	1	421	G
1	1	422	A
1	1	429	U
1	1	437	G
1	1	438	A
1	1	439	C
1	1	440	A
1	1	495	G
1	1	503	C
1	1	518	G
1	1	520	U
1	1	521	A
1	1	530	G
1	1	536	U
1	1	544	C
1	1	546	C
1	1	547	G
1	1	549	U
1	1	550	A
1	1	551	A
1	1	552	G
1	1	555	U
1	1	557	A
1	1	559	A
1	1	566	G
1	1	575	G
1	1	578	A
1	1	579	G
1	1	592	A
1	1	597	G
1	1	602	A
1	1	604	G
1	1	607	A
1	1	609	G
1	1	611	A
1	1	619	A
1	1	620	U
1	1	621	A
1	1	622	A

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Mol	Chain	Res	Type
1	1	636	C
1	1	637	C
1	1	638	C
1	1	643	U
1	1	644	G
1	1	645	A
1	1	646	A
1	1	647	A
1	1	648	C
1	1	649	A
1	1	650	C
1	1	654	C
1	1	660	A
1	1	676	G
1	1	677	A
1	1	681	U
1	1	689	U
1	1	690	A
1	1	691	A
1	1	705	A
1	1	708	G
1	1	709	A
1	1	710	A
1	1	715	A
1	1	716	A
1	1	718	G
1	1	719	U
1	1	720	A
1	1	721	G
1	1	722	G
1	1	725	G
1	1	735	A
1	1	739	G
1	1	742	G
1	1	760	G
1	1	762	U
1	1	763	G
1	1	766	U
1	1	767	U
1	1	768	C
1	1	772	U
1	1	773	G

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Mol	Chain	Res	Type
1	1	774	G
1	1	775	A
1	1	776	U
1	1	777	U
1	1	779	G
1	1	780	A
1	1	781	G
1	1	782	U
1	1	785	G
1	1	801	A
1	1	806	A
1	1	808	A
1	1	816	A
1	1	817	A
1	1	830	A
1	1	832	G
1	1	846	A
1	1	848	A
1	1	849	C
1	1	850	U
1	1	861	C
1	1	871	U
1	1	874	U
1	1	875	G
1	1	879	U
1	1	884	A
1	1	896	A
1	1	897	U
1	1	907	G
1	1	908	G
1	1	909	G
1	1	914	A
1	1	915	A
1	1	916	G
1	1	917	A
1	1	918	C
1	1	924	G
1	1	925	A
1	1	932	U
1	1	934	G
1	1	936	A
1	1	939	U

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Mol	Chain	Res	Type
1	1	941	G
1	1	944	C
1	1	954	U
1	1	959	C
1	1	960	U
1	1	961	C
1	1	964	G
1	1	967	A
1	1	975	C
1	1	976	U
1	1	977	C
1	1	978	G
1	1	979	U
1	1	980	A
1	1	984	G
1	1	991	G
1	1	992	A
1	1	993	G
1	1	994	G
1	1	995	U
1	1	996	A
1	1	997	A
1	1	998	A
1	1	999	G
1	1	1000	C
1	1	1001	G
1	1	1048	A
1	1	1049	C
1	1	1050	U
1	1	1053	A
1	1	1054	A
1	1	1055	A
1	1	1056	U
1	1	1057	A
1	1	1058	U
1	1	1064	A
1	1	1065	A
1	1	1068	C
1	1	1070	U
1	1	1072	G
1	1	1084	A
1	1	1086	C

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Mol	Chain	Res	Type
1	1	1087	G
1	1	1088	U
1	1	1092	C
1	1	1093	A
1	1	1094	U
1	1	1095	U
1	1	1097	G
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1106	G
1	1	1107	C
1	1	1111	U
1	1	1112	A
1	1	1113	G
1	1	1115	G
1	1	1117	G
1	1	1118	C
1	1	1127	G
1	1	1128	U
1	1	1129	A
1	1	1130	A
1	1	1132	C
1	1	1135	A
1	1	1136	A
1	1	1153	A
1	1	1155	C
1	1	1178	G
1	1	1180	A
1	1	1181	U
1	1	1182	A
1	1	1187	C
1	1	1190	A
1	1	1192	C
1	1	1193	A
1	1	1196	C
1	1	1197	A
1	1	1198	C
1	1	1199	C
1	1	1200	A
1	1	1203	A
1	1	1204	A

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Mol	Chain	Res	Type
1	1	1206	G
1	1	1207	G
1	1	1209	G
1	1	1220	U
1	1	1222	G
1	1	1227	C
1	1	1235	U
1	1	1236	G
1	1	1237	G
1	1	1239	C
1	1	1241	U
1	1	1242	G
1	1	1244	A
1	1	1245	A
1	1	1251	A
1	1	1253	U
1	1	1254	C
1	1	1257	C
1	1	1262	G
1	1	1263	A
1	1	1265	U
1	1	1266	G
1	1	1271	A
1	1	1272	C
1	1	1273	A
1	1	1274	A
1	1	1278	A
1	1	1279	C
1	1	1285	G
1	1	1286	A
1	1	1287	A
1	1	1290	A
1	1	1302	A
1	1	1303	A
1	1	1304	A
1	1	1305	U
1	1	1307	G
1	1	1308	A
1	1	1309	U
1	1	1313	G
1	1	1314	C
1	1	1330	A

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Mol	Chain	Res	Type
1	1	1331	U
1	1	1348	U
1	1	1349	G
1	1	1350	A
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1354	G
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1380	G
1	1	1383	G
1	1	1386	A
1	1	1391	C
1	1	1392	G
1	1	1394	A
1	1	1399	A
1	1	1400	G
1	1	1419	A
1	1	1421	G
1	1	1431	G
1	1	1434	G
1	1	1437	C
1	1	1443	G
1	1	1446	A
1	1	1449	A
1	1	1450	G
1	1	1495	U
1	1	1503	A
1	1	1508	C
1	1	1523	U
1	1	1533	U
1	1	1536	G
1	1	1547	G
1	1	1555	U
1	1	1556	C
1	1	1557	A
1	1	1560	G
1	1	1561	G
1	1	1562	C
1	1	1566	A

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Mol	Chain	Res	Type
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1573	G
1	1	1575	A
1	1	1577	G
1	1	1580	A
1	1	1581	C
1	1	1582	C
1	1	1583	A
1	1	1589	A
1	1	1596	C
1	1	1605	A
1	1	1619	A
1	1	1629	U
1	1	1639	C
1	1	1642	A
1	1	1643	A
1	1	1657	C
1	1	1683	A
1	1	1694	U
1	1	1704	A
1	1	1705	U
1	1	1713	G
1	1	1714	A
1	1	1717	U
1	1	1718	G
1	1	1724	U
1	1	1725	C
1	1	1730	G
1	1	1736	G
1	1	1741	A
1	1	1742	U
1	1	1750	A
1	1	1751	G
1	1	1756	C
1	1	1758	G
1	1	1760	A
1	1	1761	C
1	1	1763	U
1	1	1764	U
1	1	1765	U

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Mol	Chain	Res	Type
1	1	1766	G
1	1	1770	G
1	1	1780	G
1	1	1792	C
1	1	1793	C
1	1	1796	G
1	1	1797	A
1	1	1802	C
1	1	1808	G
1	1	1810	A
1	1	1813	A
1	1	1816	A
1	1	1817	G
1	1	1819	U
1	1	1820	U
1	1	1821	U
1	1	1830	G
1	1	1838	G
1	1	1839	A
1	1	1842	A
1	1	1849	C
1	1	1866	C
1	1	1871	U
1	1	1878	G
1	1	1880	U
1	1	1884	A
1	1	1893	A
1	1	1906	G
1	1	1909	A
1	1	1926	C
1	1	1951	C
1	1	1952	G
1	1	2094	C
1	1	2096	A
1	1	2101	C
1	1	2102	U
1	1	2110	G
1	1	2114	C
1	1	2121	G
1	1	2122	G
1	1	2126	A
1	1	2131	A

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Mol	Chain	Res	Type
1	1	2138	A
1	1	2142	A
1	1	2158	A
1	1	2163	C
1	1	2170	U
1	1	2174	G
1	1	2185	G
1	1	2190	U
1	1	2191	U
1	1	2193	U
1	1	2194	G
1	1	2195	C
1	1	2315	G
1	1	2316	G
1	1	2317	A
1	1	2318	U
1	1	2319	U
1	1	2320	A
1	1	2334	U
1	1	2335	G
1	1	2336	U
1	1	2355	G
1	1	2371	G
1	1	2385	G
1	1	2397	A
1	1	2398	A
1	1	2401	A
1	1	2403	G
1	1	2404	A
1	1	2405	C
1	1	2406	C
1	1	2407	C
1	1	2408	U
1	1	2409	G
1	1	2410	U
1	1	2415	C
1	1	2416	U
1	1	2418	G
1	1	2419	A
1	1	2420	C
1	1	2425	G
1	1	2426	U

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Mol	Chain	Res	Type
1	1	2427	U
1	1	2429	G
1	1	2430	A
1	1	2432	A
1	1	2433	U
1	1	2434	U
1	1	2435	G
1	1	2437	G
1	1	2438	A
1	1	2439	A
1	1	2441	A
1	1	2444	C
1	1	2445	A
1	1	2502	A
1	1	2504	U
1	1	2505	U
1	1	2506	U
1	1	2507	C
1	1	2508	U
1	1	2511	A
1	1	2512	C
1	1	2522	G
1	1	2523	A
1	1	2524	A
1	1	2525	G
1	1	2526	C
1	1	2529	A
1	1	2530	G
1	1	2531	C
1	1	2532	U
1	1	2533	G
1	1	2534	G
1	1	2536	A
1	1	2537	U
1	1	2538	U
1	1	2539	C
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2545	C
1	1	2546	C

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Mol	Chain	Res	Type
1	1	2548	C
1	1	2549	G
1	1	2552	C
1	1	2558	U
1	1	2561	A
1	1	2567	C
1	1	2568	C
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2575	G
1	1	2586	G
1	1	2588	U
1	1	2593	A
1	1	2594	C
1	1	2595	A
1	1	2596	U
1	1	2602	G
1	1	2603	G
1	1	2604	U
1	1	2606	G
1	1	2610	G
1	1	2612	U
1	1	2613	U
1	1	2614	G
1	1	2620	G
1	1	2621	G
1	1	2623	G
1	1	2625	C
1	1	2626	A
1	1	2627	C
1	1	2628	A
1	1	2629	U
1	1	2631	U
1	1	2632	G
1	1	2633	U
1	1	2635	A
1	1	2636	A
1	1	2639	G
1	1	2641	U

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Mol	Chain	Res	Type
1	1	2642	A
1	1	2643	A
1	1	2644	C
1	1	2645	G
1	1	2646	C
1	1	2647	A
1	1	2648	G
1	1	2649	A
1	1	2650	U
1	1	2652	U
1	1	2653	C
1	1	2654	C
1	1	2655	U
1	1	2656	A
1	1	2657	A
1	1	2659	G
1	1	2661	G
1	1	2665	U
1	1	2666	C
1	1	2668	U
1	1	2672	G
1	1	2674	A
1	1	2675	C
1	1	2676	A
1	1	2677	G
1	1	2679	A
1	1	2681	U
1	1	2683	U
1	1	2684	C
1	1	2685	C
1	1	2686	A
1	1	2687	G
1	1	2688	U
1	1	2689	A
1	1	2690	G
1	1	2691	A
1	1	2692	A
1	1	2693	C
1	1	2694	A
1	1	2695	A
1	1	2696	A
1	1	2698	G

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Mol	Chain	Res	Type
1	1	2701	U
1	1	2702	A
1	1	2703	A
1	1	2704	A
1	1	2705	A
1	1	2706	G
1	1	2707	C
1	1	2709	C
1	1	2712	U
1	1	2713	U
1	1	2714	G
1	1	2715	A
1	1	2716	U
1	1	2717	U
1	1	2718	U
1	1	2719	U
1	1	2720	G
1	1	2721	A
1	1	2722	U
1	1	2724	U
1	1	2726	C
1	1	2727	A
1	1	2728	G
1	1	2729	U
1	1	2730	G
1	1	2731	U
1	1	2732	G
1	1	2734	A
1	1	2740	A
1	1	2743	A
1	1	2746	A
1	1	2749	G
1	1	2752	U
1	1	2754	G
1	1	2756	C
1	1	2758	A
1	1	2759	U
1	1	2760	C
1	1	2761	G
1	1	2762	A
1	1	2763	U
1	1	2764	C

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Mol	Chain	Res	Type
1	1	2765	C
1	1	2766	U
1	1	2772	C
1	1	2773	C
1	1	2777	G
1	1	2778	G
1	1	2782	U
1	1	2786	G
1	1	2788	C
1	1	2789	U
1	1	2790	A
1	1	2791	G
1	1	2794	G
1	1	2795	U
1	1	2796	G
1	1	2797	C
1	1	2798	C
1	1	2799	A
1	1	2800	G
1	1	2801	A
1	1	2802	A
1	1	2803	A
1	1	2804	A
1	1	2808	A
1	1	2810	C
1	1	2816	G
1	1	2817	A
1	1	2819	A
1	1	2820	A
1	1	2821	C
1	1	2822	U
1	1	2824	G
1	1	2825	C
1	1	2826	U
1	1	2828	G
1	1	2834	G
1	1	2837	A
1	1	2839	G
1	1	2841	G
1	1	2842	U
1	1	2843	U
1	1	2844	C

Continued on next page...

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Mol	Chain	Res	Type
1	1	2845	A
1	1	2846	U
1	1	2847	A
1	1	2849	C
1	1	2850	G
1	1	2853	A
1	1	2854	U
1	1	2855	U
1	1	2857	C
1	1	2858	U
1	1	2859	U
1	1	2861	U
1	1	2863	G
1	1	2864	A
1	1	2866	U
1	1	2867	C
1	1	2868	U
1	1	2869	U
1	1	2870	C
1	1	2872	A
1	1	2873	U
1	1	2874	G
1	1	2875	U
1	1	2876	C
1	1	2877	G
1	1	2878	G
1	1	2879	C
1	1	2887	A
1	1	2889	C
1	1	2897	A
1	1	2898	G
1	1	2899	C
1	1	2900	A
1	1	2904	U
1	1	2911	A
1	1	2923	U
1	1	2925	C
1	1	2926	A
1	1	2928	C
1	1	2929	C
1	1	2930	A
1	1	2935	U

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Mol	Chain	Res	Type
1	1	2936	A
1	1	2944	U
1	1	2945	G
1	1	2946	A
1	1	2947	G
1	1	2950	G
1	1	2951	G
1	1	2952	G
1	1	2953	U
1	1	2954	U
1	1	2955	U
1	1	2956	A
1	1	2957	G
1	1	2966	G
1	1	2971	A
1	1	2972	G
1	1	2973	G
1	1	2978	U
1	1	2980	U
1	1	2981	U
1	1	2982	A
1	1	2983	C
1	1	2986	U
1	1	2990	G
1	1	2992	U
1	1	2997	G
1	1	3012	A
1	1	3017	A
1	1	3021	A
1	1	3022	G
1	1	3023	U
1	1	3024	A
1	1	3031	G
1	1	3032	A
1	1	3059	G
1	1	3074	G
1	1	3078	U
1	1	3079	U
1	1	3080	G
1	1	3086	A
1	1	3090	U
1	1	3092	C

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Mol	Chain	Res	Type
1	1	3093	C
1	1	3100	U
1	1	3104	U
1	1	3113	A
1	1	3121	U
1	1	3122	A
1	1	3123	A
1	1	3127	A
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3151	U
1	1	3153	U
1	1	3154	C
1	1	3155	U
1	1	3156	U
1	1	3157	U
1	1	3158	G
1	1	3159	C
1	1	3162	C
1	1	3163	A
1	1	3164	C
1	1	3165	A
1	1	3168	A
1	1	3170	A
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3187	A
1	1	3194	C
1	1	3195	U
1	1	3196	U
1	1	3206	C
1	1	3207	U
1	1	3213	A
1	1	3217	C

Continued on next page...

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Mol	Chain	Res	Type
1	1	3218	A
1	1	3219	G
1	1	3224	G
1	1	3228	C
1	1	3229	G
1	1	3239	G
1	1	3242	G
1	1	3243	A
1	1	3245	A
1	1	3247	G
1	1	3253	G
1	1	3259	U
1	1	3260	G
1	1	3263	G
1	1	3270	U
1	1	3273	A
1	1	3274	A
1	1	3276	G
1	1	3279	A
1	1	3280	U
1	1	3281	U
1	1	3287	U
1	1	3288	G
1	1	3289	G
1	1	3290	G
1	1	3294	A
1	1	3295	A
1	1	3304	U
1	1	3309	G
1	1	3313	U
1	1	3317	U
1	1	3319	U
1	1	3320	A
1	1	3341	U
1	1	3342	A
1	1	3345	G
1	1	3350	C
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3354	U
1	1	3355	U

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Mol	Chain	Res	Type
1	1	3356	G
1	1	3357	U
1	1	3359	A
1	1	3369	G
1	1	3375	A
1	1	3376	A
1	1	3378	C
1	1	3382	U
1	1	3383	G
1	1	3386	G
1	1	3389	U
1	1	3390	G
1	1	3391	A
1	1	3396	U
2	2	25	G
2	2	34	U
2	2	35	C
2	2	52	A
2	2	53	A
2	2	59	A
2	2	62	C
2	2	63	G
2	2	71	A
2	2	79	A
2	2	80	A
2	2	82	U
2	2	83	C
2	2	84	C
2	2	85	G
2	2	86	U
2	2	87	G
2	2	88	A
2	2	90	U
2	2	95	G
2	2	104	A
2	2	106	C
2	2	111	A
2	2	113	U
2	2	114	G
2	2	121	U
2	2	124	G
2	2	125	U

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Mol	Chain	Res	Type
2	2	126	A
2	2	138	A
2	2	148	G
2	2	151	C
2	2	158	U
3	3	7	G
3	3	11	A
3	3	13	A
3	3	17	A
3	3	19	C
3	3	22	A
3	3	23	A
3	3	25	G
3	3	26	C
3	3	27	A
3	3	33	U
3	3	35	C
3	3	36	C
3	3	38	U
3	3	39	C
3	3	40	C
3	3	43	U
3	3	44	C
3	3	46	A
3	3	47	C
3	3	50	U
3	3	51	A
3	3	52	G
3	3	53	U
3	3	54	U
3	3	55	A
3	3	60	G
3	3	63	A
3	3	64	A
3	3	65	G
3	3	69	C
3	3	73	C
3	3	74	C
3	3	76	A
3	3	78	U
3	3	82	G
3	3	84	A

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Mol	Chain	Res	Type
3	3	87	G
3	3	89	G
3	3	93	C
3	3	94	C
3	3	95	A
3	3	98	C
3	3	99	G
3	3	101	G
3	3	102	A
3	3	108	A
3	3	112	G
3	3	113	C
3	3	117	A
3	3	118	A
3	3	119	U
3	3	120	C
3	3	121	U
6	6	4	U
6	6	5	C
6	6	6	U
6	6	7	C
6	6	8	A
6	6	14	U
6	6	15	C
6	6	16	U
6	6	17	G
6	6	19	U
6	6	23	U
6	6	24	A
6	6	26	U
6	6	34	A
6	6	39	U
6	6	40	U
6	6	41	G
6	6	42	G
6	6	43	A
6	6	44	G
6	6	45	U
6	6	47	A
6	6	49	C
6	6	53	A
6	6	54	A

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Mol	Chain	Res	Type
6	6	56	U
6	6	57	U
6	6	58	G
6	6	59	C
6	6	229	U
6	6	230	A
6	6	231	A
6	6	232	A

All (65) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	40	A
1	1	160	G
1	1	239	G
1	1	284	A
1	1	305	U
1	1	588	G
1	1	637	C
1	1	645	A
1	1	646	A
1	1	649	A
1	1	720	A
1	1	761	A
1	1	849	C
1	1	916	G
1	1	976	U
1	1	1064	A
1	1	1097	G
1	1	1102	A
1	1	1103	A
1	1	1128	U
1	1	1205	A
1	1	1241	U
1	1	1302	A
1	1	1307	G
1	1	1329	U
1	1	1331	U
1	1	1355	A
1	1	1568	U
1	1	1574	C
1	1	2101	C

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Mol	Chain	Res	Type
1	1	2400	G
1	1	2432	A
1	1	2522	G
1	1	2537	U
1	1	2541	U
1	1	2593	A
1	1	2651	G
1	1	2655	U
1	1	2658	G
1	1	2693	C
1	1	2715	A
1	1	2728	G
1	1	2753	G
1	1	2824	G
1	1	2857	C
1	1	2866	U
1	1	2875	U
1	1	2950	G
1	1	2970	C
1	1	3030	G
1	1	3078	U
1	1	3121	U
1	1	3218	A
1	1	3228	C
1	1	3269	U
1	1	3341	U
1	1	3350	C
1	1	3351	U
2	2	39	G
2	2	123	G
6	6	16	U
6	6	23	U
6	6	53	A
6	6	56	U
6	6	57	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	GTP	b	701	61	26,34,34	1.20	1 (3%)	32,54,54	1.58	6 (18%)
60	GTP	m	501	61	26,34,34	1.31	2 (7%)	32,54,54	1.70	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	GTP	b	701	61	-	5/18/38/38	0/3/3/3
60	GTP	m	501	61	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	m	501	GTP	C5-C6	-4.45	1.38	1.47
60	b	701	GTP	C5-C6	-4.28	1.38	1.47
60	m	501	GTP	C2-N3	2.07	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	b	701	GTP	PA-O3A-PB	-4.17	118.51	132.83
60	m	501	GTP	PB-O3B-PG	-3.78	119.84	132.83
60	m	501	GTP	C5-C6-N1	3.45	120.04	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	b	701	GTP	C5-C6-N1	3.35	119.87	113.95
60	b	701	GTP	C8-N7-C5	3.27	109.22	102.99
60	m	501	GTP	C8-N7-C5	3.01	108.72	102.99
60	b	701	GTP	C2-N1-C6	-2.92	119.72	125.10
60	m	501	GTP	C2-N1-C6	-2.89	119.78	125.10
60	m	501	GTP	PA-O3A-PB	-2.84	123.08	132.83
60	b	701	GTP	PB-O3B-PG	-2.82	123.13	132.83
60	m	501	GTP	C3'-C2'-C1'	2.76	105.13	100.98
60	m	501	GTP	O6-C6-C5	-2.42	119.64	124.37
60	b	701	GTP	C3'-C2'-C1'	2.12	104.17	100.98
60	m	501	GTP	O2'-C2'-C3'	-2.01	105.31	111.82

There are no chirality outliers.

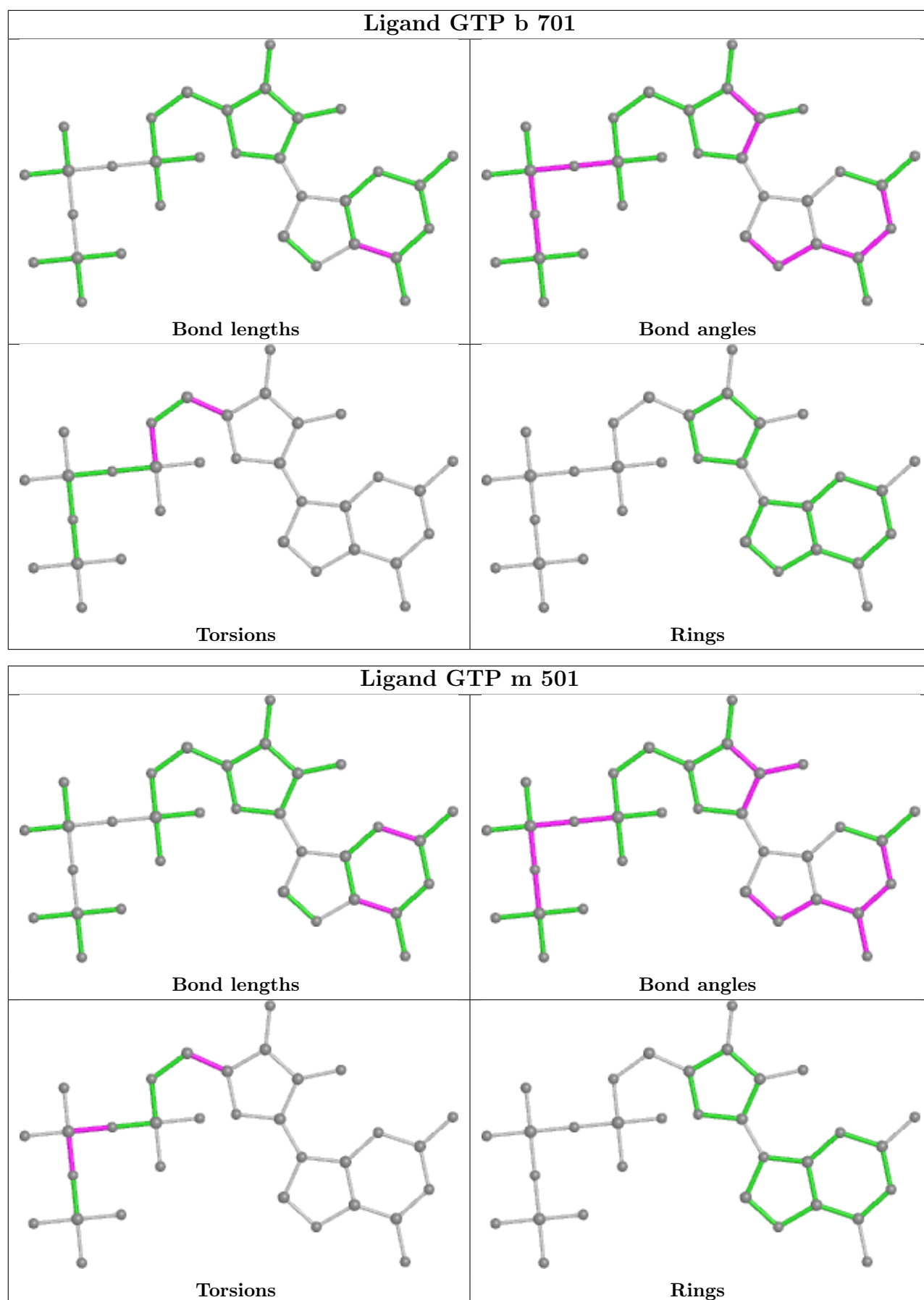
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	b	701	GTP	C5'-O5'-PA-O1A
60	b	701	GTP	C5'-O5'-PA-O2A
60	b	701	GTP	C3'-C4'-C5'-O5'
60	b	701	GTP	O4'-C4'-C5'-O5'
60	m	501	GTP	PA-O3A-PB-O3B
60	b	701	GTP	C5'-O5'-PA-O3A
60	m	501	GTP	O4'-C4'-C5'-O5'
60	m	501	GTP	PG-O3B-PB-O1B
60	m	501	GTP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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



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.

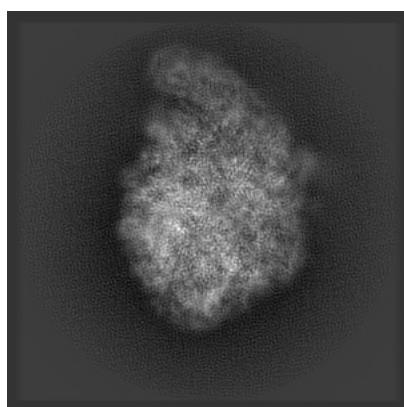
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30108. These allow visual inspection of the internal detail of the map and identification of artifacts.

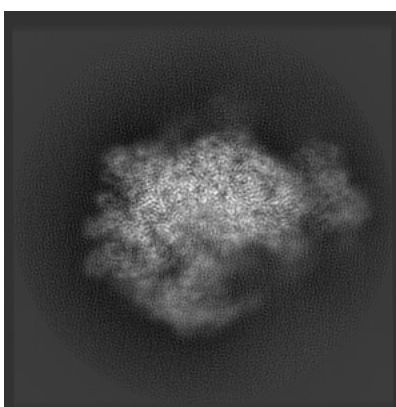
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

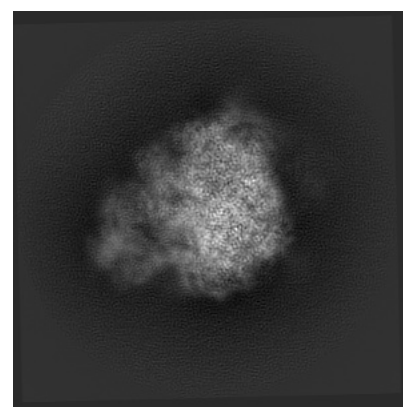
6.1.1 Primary map



X



Y

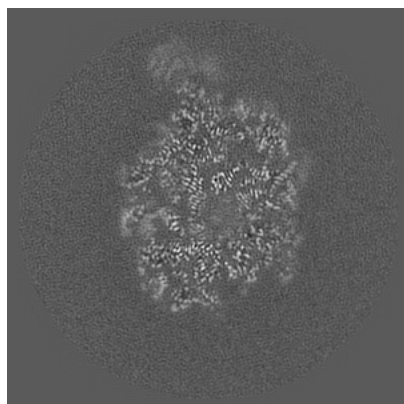


Z

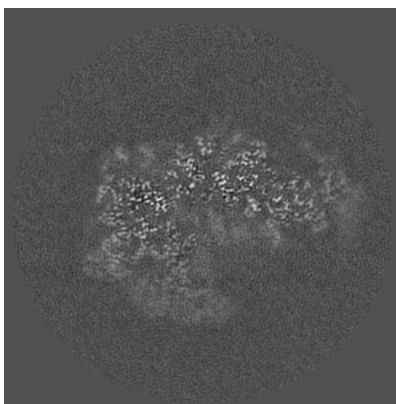
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

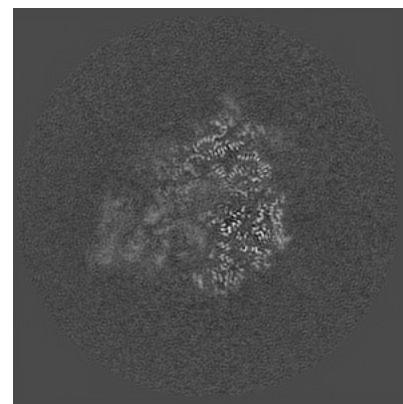
6.2.1 Primary map



X Index: 200



Y Index: 200

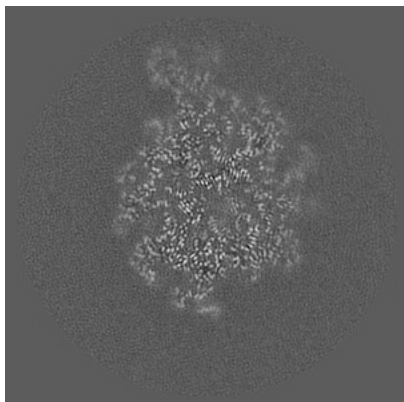


Z Index: 200

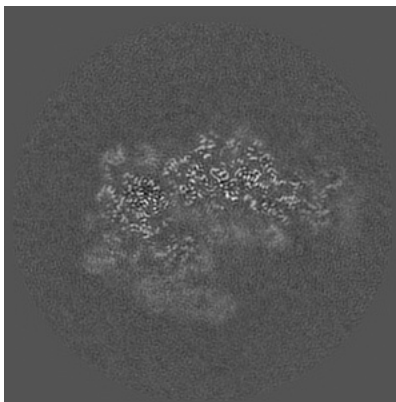
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

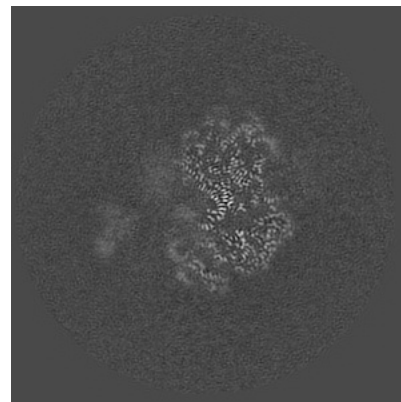
6.3.1 Primary map



X Index: 210



Y Index: 197



Z Index: 223

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

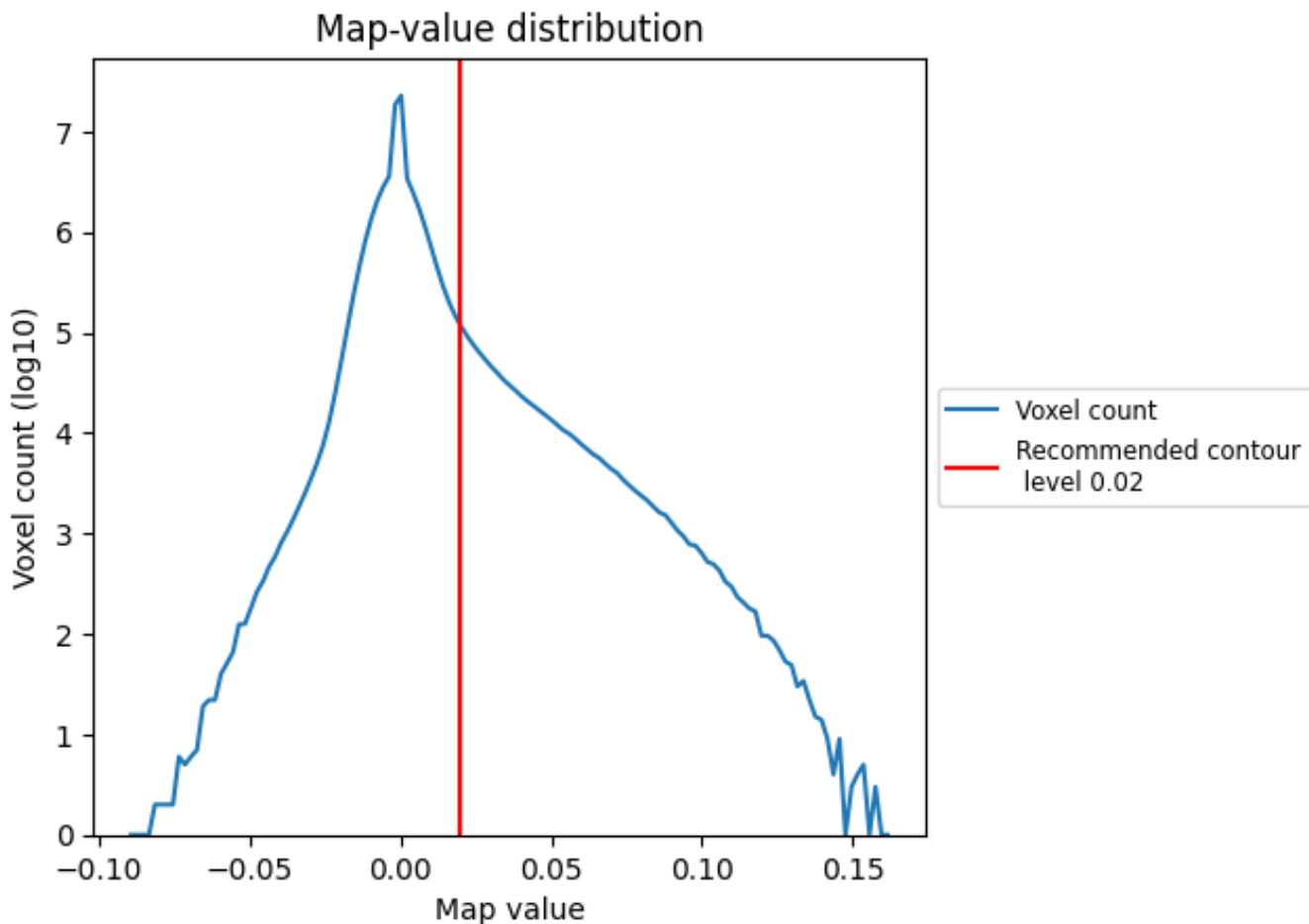
6.5 Mask visualisation

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

7 Map analysis [i](#)

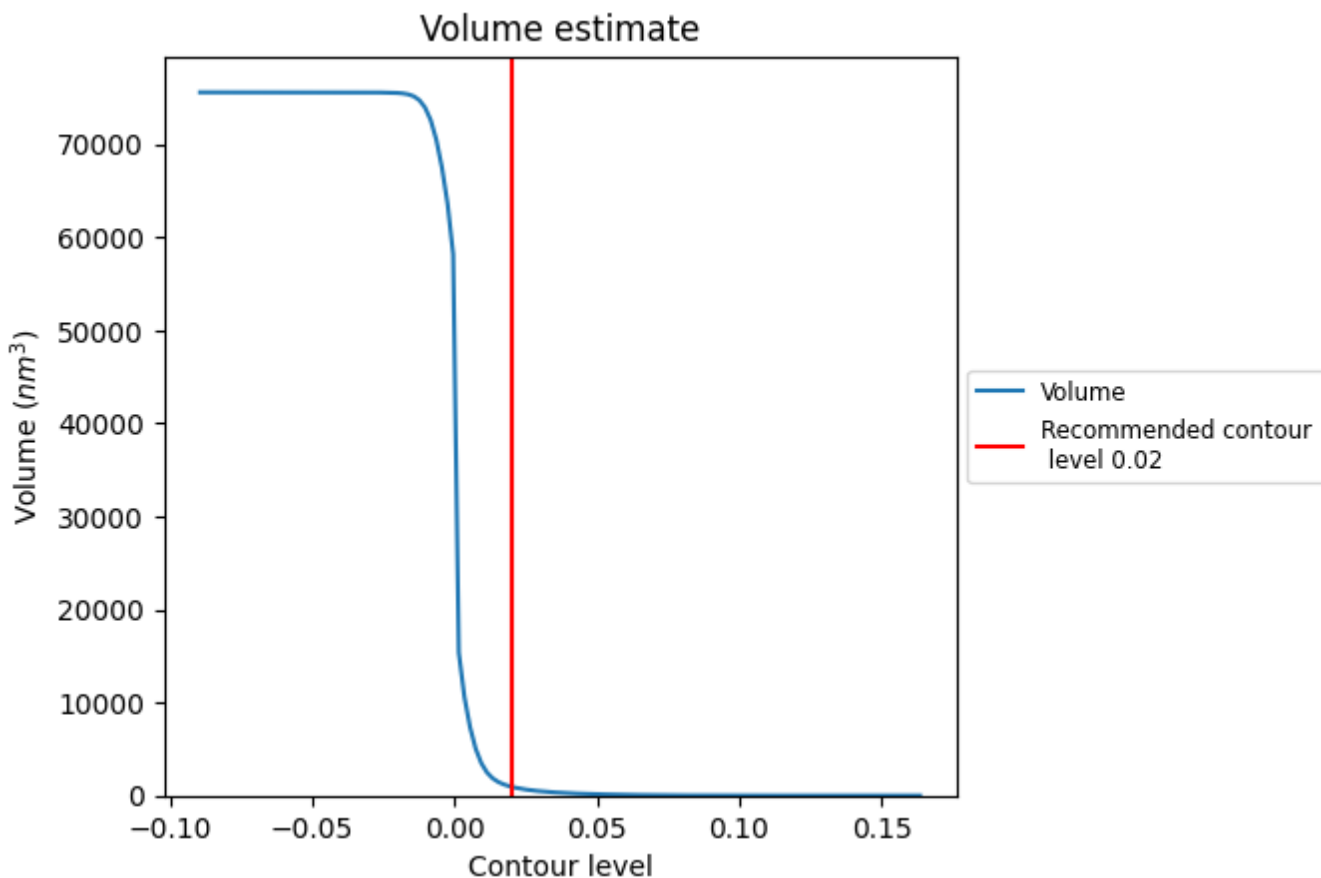
This section contains the results of statistical analysis of the map.

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.

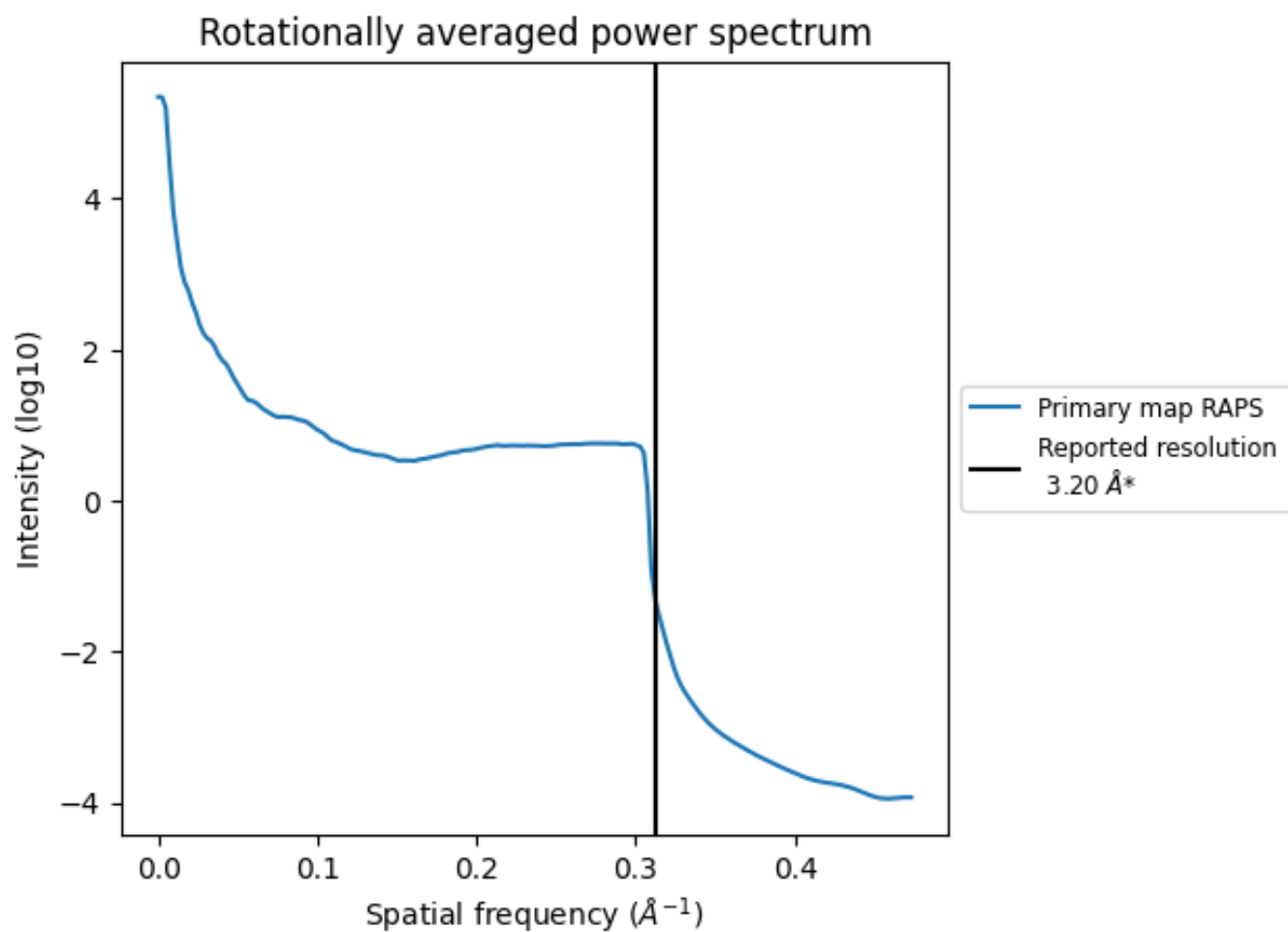
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 950 nm³; this corresponds to an approximate mass of 858 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 0.312 Å⁻¹

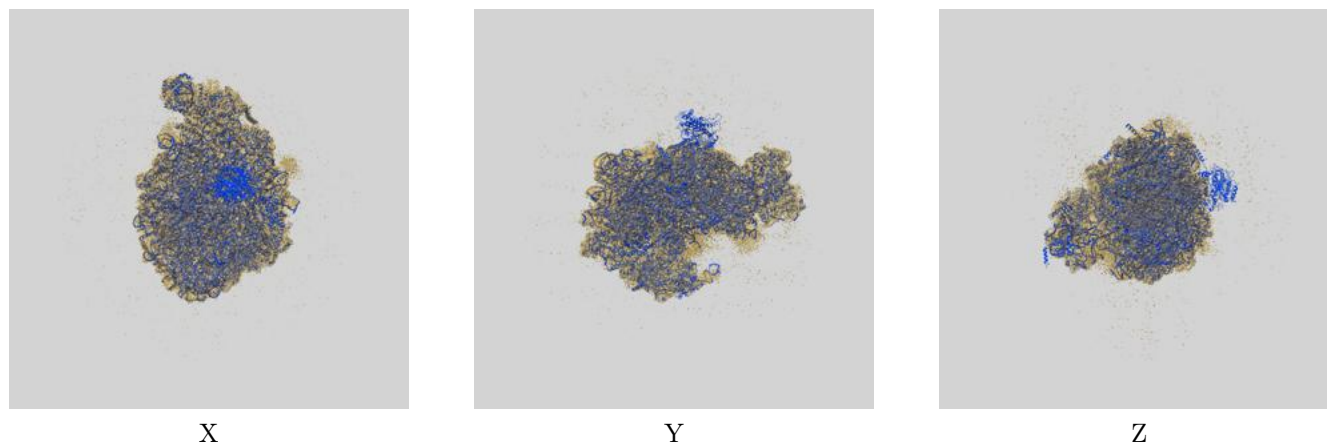
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

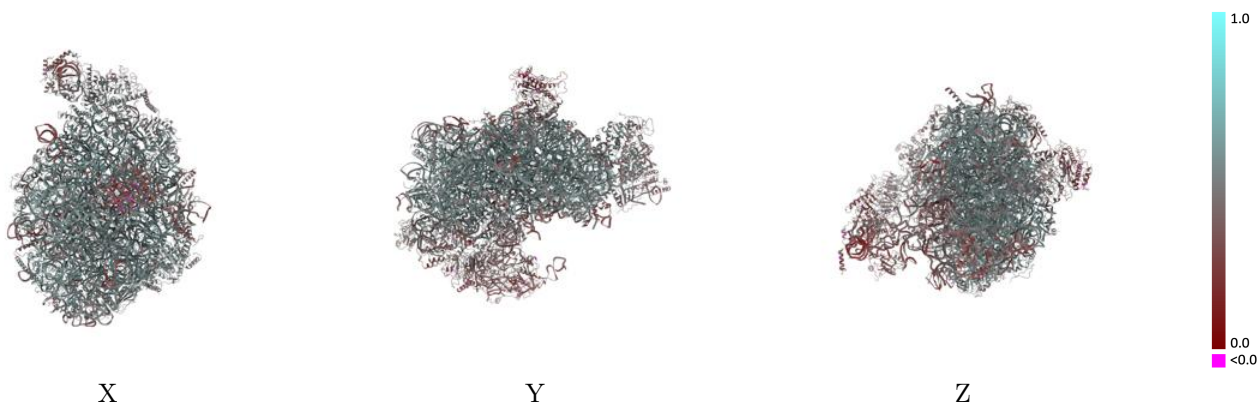
This section contains information regarding the fit between EMDB map EMD-30108 and PDB model 6M62. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



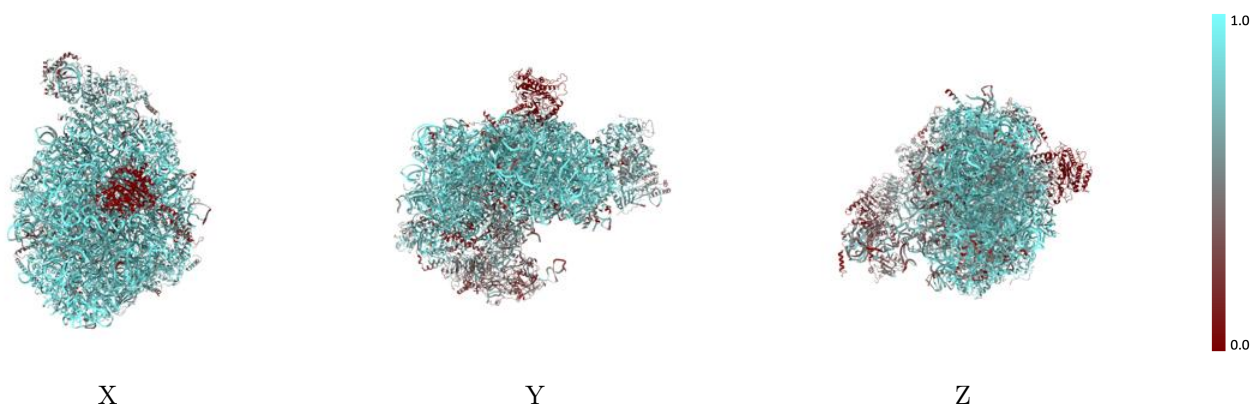
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



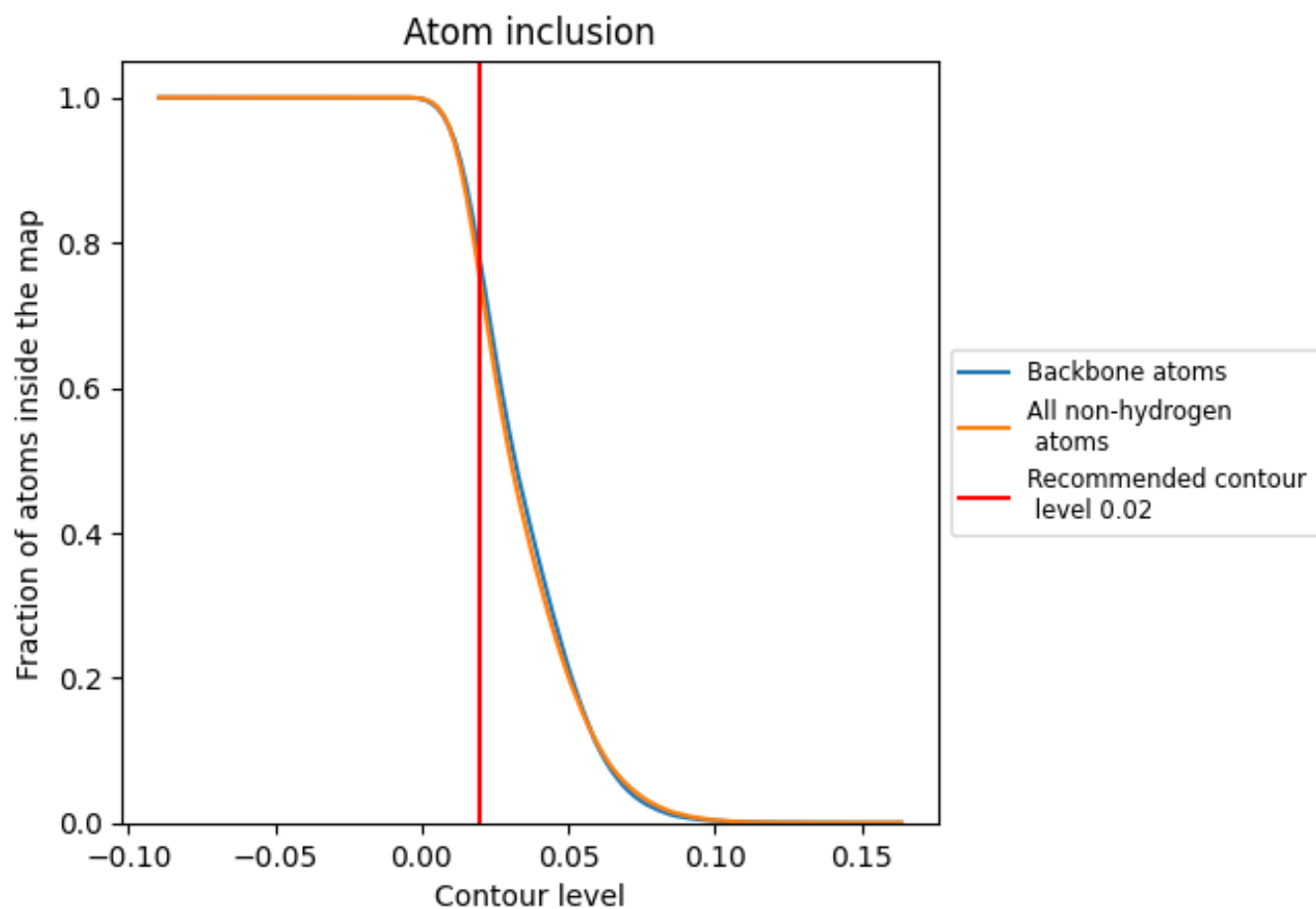
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

















































The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7478	 0.4890
1	 0.8740	 0.5000
2	 0.9565	 0.5640
3	 0.5204	 0.2580
4	 0.0373	 0.3610
5	 0.1163	 0.3560
6	 0.7431	 0.3920
A	 0.7901	 0.5510
B	 0.8515	 0.5600
C	 0.8664	 0.5630
D	 0.2647	 0.3260
E	 0.8129	 0.5210
F	 0.8639	 0.5550
G	 0.7972	 0.5310
H	 0.8322	 0.5470
I	 0.5333	 0.4990
J	 0.2776	 0.3250
K	 0.4985	 0.4020
L	 0.7685	 0.5200
M	 0.8537	 0.5470
N	 0.8149	 0.5530
O	 0.9115	 0.5790
P	 0.8195	 0.5550
Q	 0.8461	 0.5460
R	 0.8086	 0.5400
S	 0.8257	 0.5300
T	 0.6141	 0.4590
U	 0.6506	 0.4460
V	 0.8355	 0.5660
W	 0.5798	 0.4320
X	 0.8562	 0.5630
Y	 0.8385	 0.5520
Z	 0.8207	 0.5340
a	 0.7667	 0.4900
b	 0.5663	 0.4620



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Chain	Atom inclusion	Q-score
c	 0.7250	 0.5110
d	 0.8146	 0.5580
e	 0.8783	 0.5810
f	 0.9160	 0.5930
g	 0.8298	 0.5600
h	 0.8431	 0.5580
i	 0.6899	 0.4810
j	 0.9055	 0.5940
k	 0.7279	 0.5070
l	 0.8410	 0.5840
m	 0.4918	 0.4490
n	 0.7123	 0.5030
o	 0.5788	 0.4420
p	 0.8075	 0.5450
q	 0.5497	 0.4670
r	 0.7404	 0.5170
s	 0.5358	 0.5010
t	 0.6297	 0.4750
u	 0.7461	 0.5000
v	 0.2513	 0.3450
w	 0.4101	 0.4000
x	 0.4724	 0.3840
y	 0.7391	 0.5050
z	 0.7350	 0.5190