



## Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 10:58 PM EST

PDB ID : 5T2A  
EMDB ID : EMD-8343  
Title : CryoEM structure of the Leishmania donovani 80S ribosome at 2.9 Angstrom resolution  
Authors : Zhang, X.; Lai, M.; Zhou, Z.H.  
Deposited on : 2016-08-23  
Resolution : 2.90 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](mailto: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>.

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

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

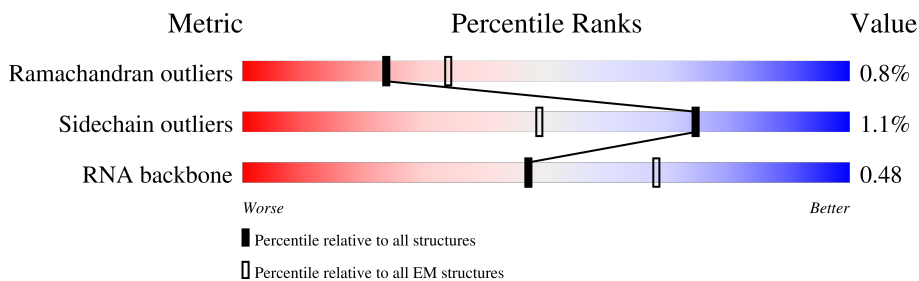
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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  $\geq 3$ , 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	A	1781	
2	B	1465	
3	C	262	
4	D	120	
5	E	213	
6	F	73	
7	G	183	
8	H	127	

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Mol	Chain	Length	Quality of chain
9	I	198	20% 94% 5% ..
10	J	213	29% 97% ..
11	K	188	52% 88% . 11%
12	L	220	17% 80% . 19%
13	M	222	17% 96% .
14	N	175	36% 93% . . .
15	O	204	7% 97% .
16	P	166	7% 92% . 7%
17	Q	179	13% 98% ..
18	R	245	24% 79% . 20%
19	S	159	21% 97% . .
20	T	129	32% 94% . 5%
21	U	139	9% 99% .
22	V	145	17% 82% . 17%
23	W	124	9% 51% . 48%
24	X	143	15% 82% . 16%
25	Y	134	26% 98% ..
26	Z	145	17% 97% . . .
27	a	147	29% 97% . . .
28	b	70	26% 96% . .
29	c	260	7% 94% . . . .
30	d	419	10% 94% . 5%
31	e	104	15% 84% 5% . 10%
32	f	183	8% 60% 40%
33	g	133	19% 95% . .

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Mol	Chain	Length	Quality of chain
34	h	168	15% 73% 26%
35	i	127	30% 98% ..
36	j	144	13% 90% .. 8%
37	k	105	44% 93% 6%
38	l	83	6% 93% ..
39	m	92	14% 98% ..
40	n	83	29% 89% 10%
41	o	51	10% 98% .
42	p	373	23% 96% ..
43	q	128	5% 40% 59%
44	r	106	19% 86% .. 9%
45	s	305	28% 87% 13%
46	t	195	17% 67% .. 30%
47	u	252	17% 88% 10%
48	v	348	21% 66% 34%
49	w	190	13% 97% ..
50	0	264	30% 80% .. 16%
51	1	273	21% 92% 5%
52	2	2205	26% 47% 29% 6% 18%
53	3	249	53% 98% ..
54	4	200	32% 96% ..
55	5	220	11% 79% 17%
56	6	190	17% 84% .. 14%
57	7	312	99% 95% ..
58	8	57	63% 58% 9% 33%

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Mol	Chain	Length	Quality of chain
59	AC	246	
60	AD	153	
61	AE	173	
62	AG	151	
63	AH	144	
64	AI	152	
65	AJ	130	
66	AK	149	
67	AL	143	
68	AM	153	
69	AN	190	
70	AO	179	
71	AP	265	
72	AQ	116	
73	AR	164	
74	AS	143	
75	AT	137	
76	AV	112	
77	AW	86	
78	AX	219	
79	AY	66	
80	AZ	87	

## 2 Entry composition [i](#)

There are 80 unique types of molecules in this entry. The entry contains 200172 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 LSU-alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1603	34365	15347	6297	11118	1603	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	761	U	A	conflict	GB 322500086
A	1393	G	A	conflict	GB 322500086
A	?	-	A	deletion	GB 322500086

- Molecule 2 is a RNA chain called LSU-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	1064	22723	10152	4100	7407	1064	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	162	3449	1542	615	1130	162	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	141	C	U	conflict	GB 79677111
C	182	G	A	conflict	GB 79677111
C	185	C	G	conflict	GB 79677111
C	226	A	U	conflict	GB 79677111
C	228	C	U	conflict	GB 79677111
C	246	C	U	conflict	GB 79677111

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	119	2531	1132	452	828	119	0	0

- Molecule 5 is a RNA chain called srRNA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	169	3589	1604	626	1190	169	0	0

- Molecule 6 is a RNA chain called srRNA3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	F	71	1508	676	273	488	71	0	0

- Molecule 7 is a RNA chain called srRNA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	G	183	3911	1744	704	1280	183	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	169	U	A	conflict	GB 5019758
G	171	U	A	conflict	GB 5019758

- Molecule 8 is a RNA chain called srRNA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	H	93	1996	889	369	645	93	0	0

- Molecule 9 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	197	1539	968	307	258	6	0	0

- Molecule 10 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	211	1704	1071	338	279	16	0	0

- Molecule 11 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	167	1339	844	249	238	8	0	0

- Molecule 12 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	179	1435	901	296	230	8	0	0

- Molecule 13 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	221	1780	1126	354	293	7	0	0

- Molecule 14 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	168	1336	832	265	231	8	0	0

- Molecule 15 is a protein called eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	203	1714	1080	362	264	8	0	0

- Molecule 16 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	155	1245	776	246	212	11	0	1

- Molecule 17 is a protein called eL20.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	178	1456	927	280	244	5	0	0

- Molecule 18 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	196	1646	1010	360	271	5	0	0

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	158	1261	803	245	208	5	0	0

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	123	997	642	179	173	3	0	1

- Molecule 21 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	137	1035	653	195	181	6	0	0

- Molecule 22 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	120	963	611	182	169	1	0	0

- Molecule 23 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	65	563	368	110	81	4	0	0

- Molecule 24 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	120	Total	C	N	O	S	0	0
			965	601	201	159	4		

- Molecule 25 is a protein called eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	133	Total	C	N	O	S	0	0
			1079	688	215	173	3		

- Molecule 26 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	144	Total	C	N	O	S	0	0
			1126	708	226	186	6		

- Molecule 27 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	146	Total	C	N	O	S	0	0
			1140	698	243	194	5		

- Molecule 28 is a protein called eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	69	Total	C	N	O	0	0
			554	339	127	88		

- Molecule 29 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	253	Total	C	N	O	S	0	1
			1921	1193	392	326	10		

- Molecule 30 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	399	Total	C	N	O	S	0	0
			3183	2003	629	538	13		

- Molecule 31 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	94	Total	C	N	O	S	0	0
			720	448	131	136	5		

- Molecule 32 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	110	Total	C	N	O	S	0	0
			878	561	166	149	2		

- Molecule 33 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	129	Total	C	N	O	S	0	0
			1050	664	209	174	3		

- Molecule 34 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	124	Total	C	N	O	S	0	0
			1014	624	221	163	6		

- Molecule 35 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	126	Total	C	N	O	S	0	0
			1056	658	218	176	4		

- Molecule 36 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	132	Total	C	N	O	S	0	0
			1060	663	221	171	5		

- Molecule 37 is a protein called eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	99	Total	C	N	O	S	0	0
			787	497	160	128	2		

- Molecule 38 is a protein called eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	81	Total	C	N	O	S	0	0
			674	410	154	104	6		

- Molecule 39 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	91	Total	C	N	O	S	0	0
			712	443	146	117	6		

- Molecule 40 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	75	Total	C	N	O	S	0	0
			605	383	118	101	3		

- Molecule 41 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	50	Total	C	N	O	S	0	0
			450	291	95	63	1		

- Molecule 42 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	365	Total	C	N	O	S	0	1
			2825	1761	563	486	15		

- Molecule 43 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	52	Total	C	N	O	S	0	0
			425	266	88	64	7		

- Molecule 44 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	96	Total	C	N	O	S	0	0
			779	493	157	124	5		

- Molecule 45 is a protein called uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	266	Total	C	N	O	S	0	0
			2094	1334	397	357	6		

- Molecule 46 is a protein called eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	137	Total	C	N	O	S	0	0
			1054	668	197	187	2		

- Molecule 47 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	228	Total	C	N	O	S	0	0
			1857	1180	358	308	11		

- Molecule 48 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	230	Total	C	N	O	S	0	0
			1850	1160	368	315	7		

- Molecule 49 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	187	Total	C	N	O	S	0	0
			1484	938	273	267	6		

- Molecule 50 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	0	221	Total	C	N	O	S	0	0
			1786	1121	338	316	11		

- Molecule 51 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	258	Total	C	N	O	S	0	0
			2037	1291	387	350	9		

- Molecule 52 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	2	1814	38724	17307	6969	12635	1813	0	0

- Molecule 53 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	3	249	1994	1243	409	339	3	0	0

- Molecule 54 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	4	200	1667	1059	324	276	8	0	0

- Molecule 55 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	5	183	1473	921	308	242	2	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	220	ARG	LYS	conflict	UNP E9BH78

- Molecule 56 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	6	164	1362	862	265	227	8	0	0

- Molecule 57 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	7	308	2394	1500	426	456	12	0	0

- Molecule 58 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	8	38	Total	C	N	O	S	0	0
			314	194	63	52	5		

- Molecule 59 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AC	203	Total	C	N	O	S	0	0
			1622	1033	294	283	12		

- Molecule 60 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AD	93	Total	C	N	O	S	0	0
			767	491	136	133	7		

- Molecule 61 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AE	140	Total	C	N	O	S	0	0
			1148	725	229	189	5		

- Molecule 62 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AG	141	Total	C	N	O	S	0	0
			1157	730	229	190	8		

- Molecule 63 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AH	136	Total	C	N	O	S	0	0
			1023	631	200	184	8		

- Molecule 64 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AI	121	Total	C	N	O	S	0	0
			984	626	188	166	4		

- Molecule 65 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	AJ	129	1020	646	188	178	8	0	0

- Molecule 66 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	AK	140	1108	710	206	189	3	0	0

- Molecule 67 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	AL	121	983	613	192	173	5	0	0

- Molecule 68 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	AM	148	1186	743	237	202	4	0	0

- Molecule 69 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	AN	190	1493	927	287	271	8	0	0

- Molecule 70 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	AO	145	1150	729	224	193	4	0	0

- Molecule 71 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	AP	224	1722	1096	304	312	10	0	1

- Molecule 72 is a protein called uS10.



Mol	Chain	Residues	Atoms					AltConf	Trace
72	AQ	102	Total	C	N	O	S	0	0
			807	504	148	153	2		

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	AR	83	Total	C	N	O	S	0	0
			630	388	116	122	4		

- Molecule 74 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	AS	142	Total	C	N	O	S	0	0
			1114	703	222	187	2		

- Molecule 75 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AT	126	Total	C	N	O	S	0	0
			1033	661	198	172	2		

- Molecule 76 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AV	104	Total	C	N	O	S	0	0
			828	515	175	130	8		

- Molecule 77 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AW	82	Total	C	N	O	S	0	0
			646	396	128	114	8		

- Molecule 78 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AX	203	Total	C	N	O	S	0	0
			1595	1003	295	284	13		

- Molecule 79 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	AY	56	452	285	94	72	1	0	0

- Molecule 80 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	AZ	68	526	319	106	97	4	0	0

### 3 Residue-property plots i

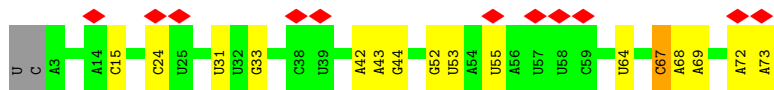
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: LSU-alpha

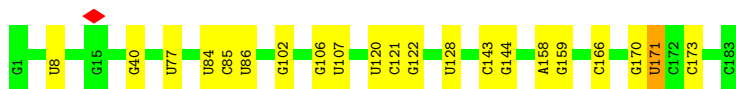
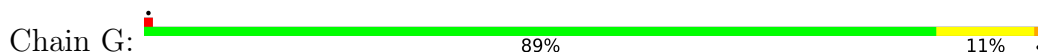




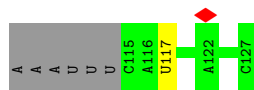
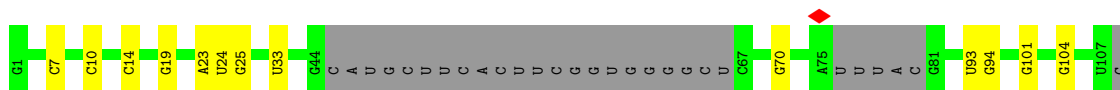




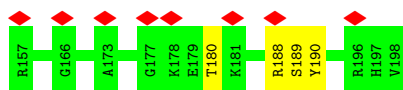
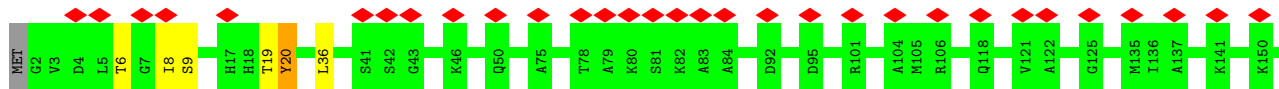
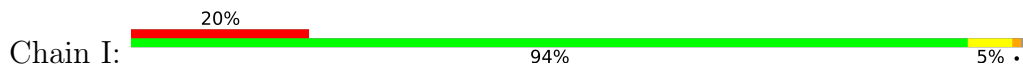
• Molecule 7: srRNA2



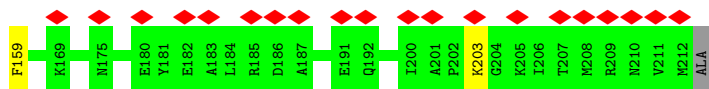
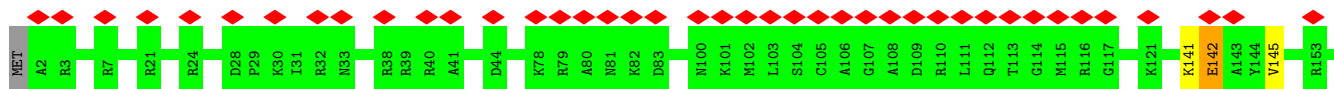
• Molecule 8: srRNA4



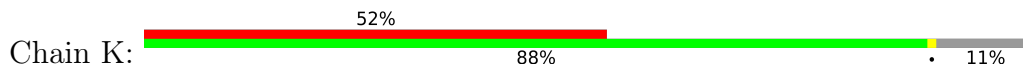
• Molecule 9: eL18

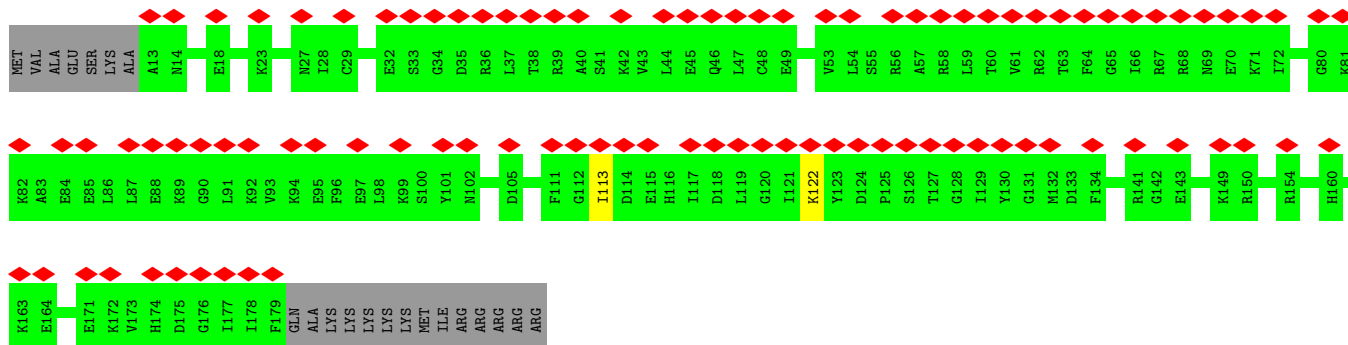


• Molecule 10: uL16

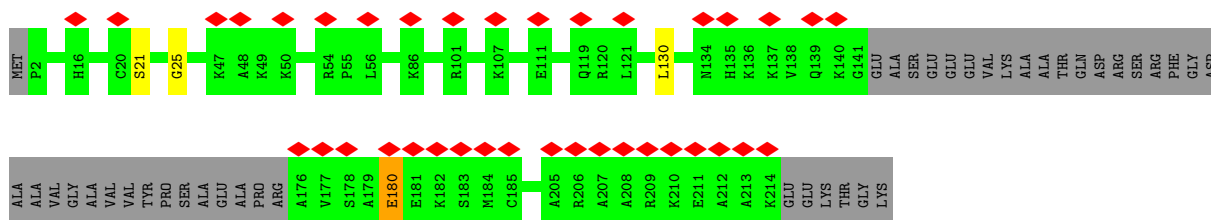
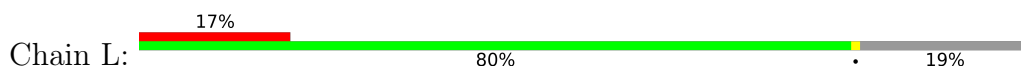


• Molecule 11: uL5

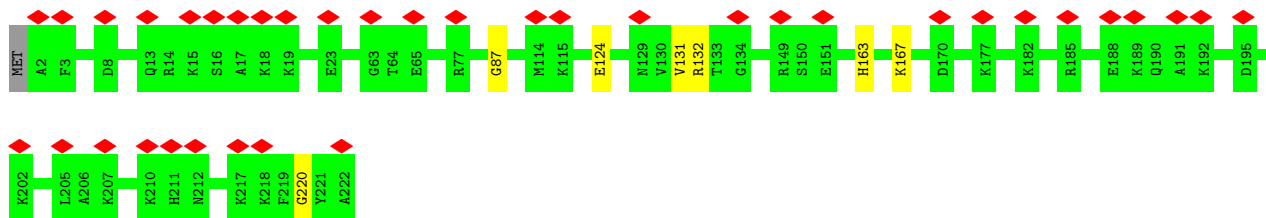




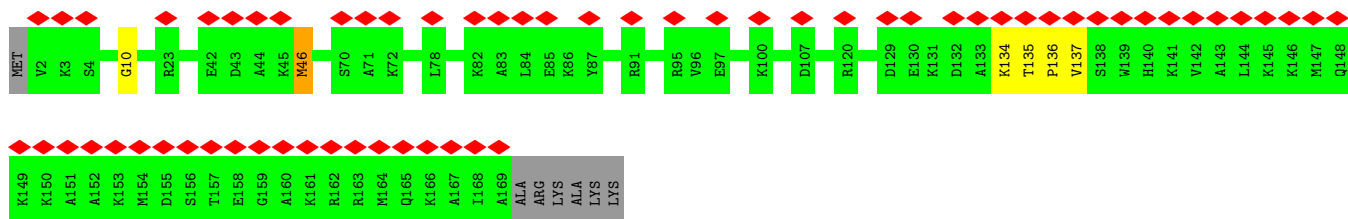
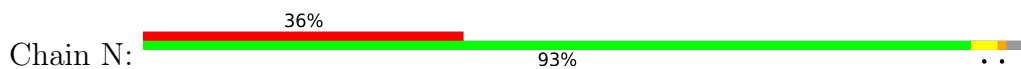
• Molecule 12: eL13



• Molecule 13: uL13

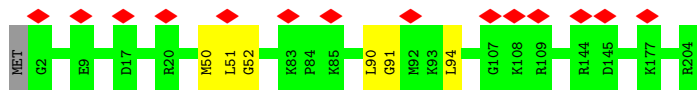


• Molecule 14: eL14

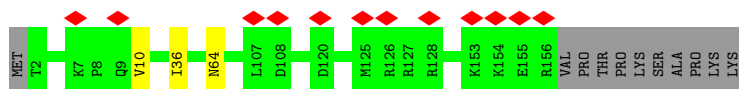
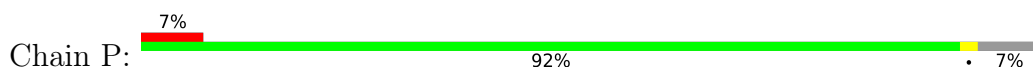


• Molecule 15: eL15

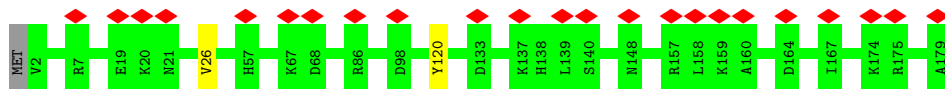




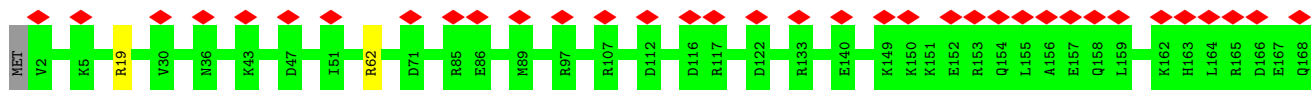
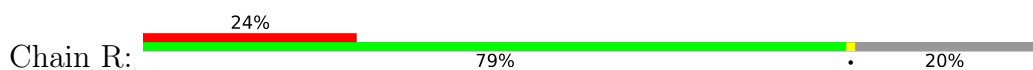
• Molecule 16: uL22



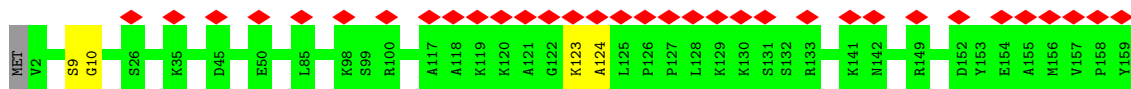
• Molecule 17: eL20



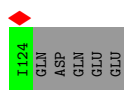
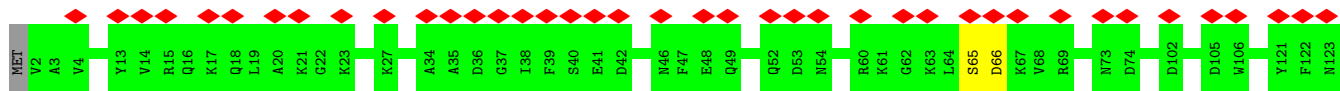
• Molecule 18: eL19



• Molecule 19: eL21

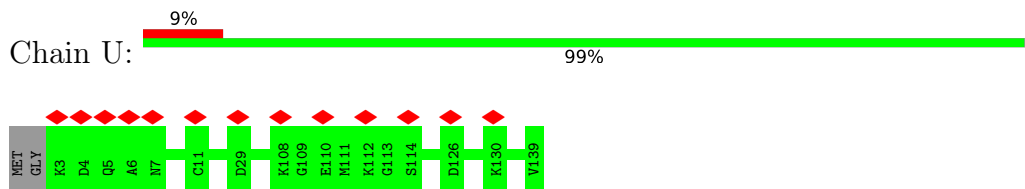


• Molecule 20: eL22

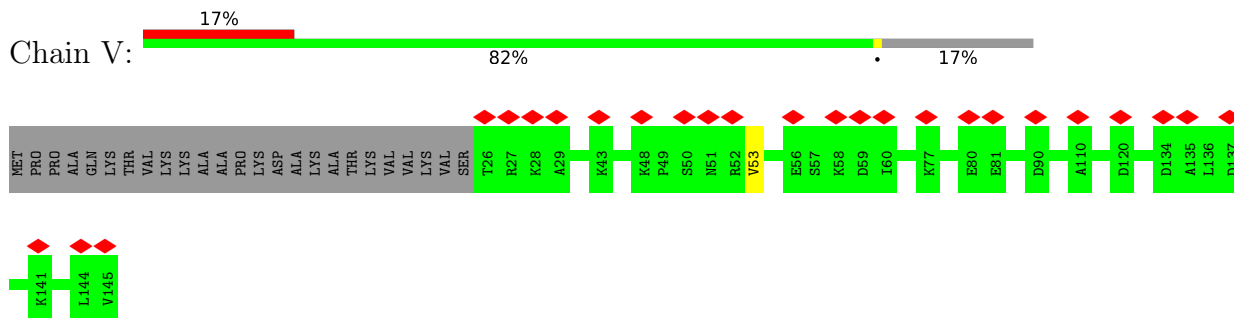




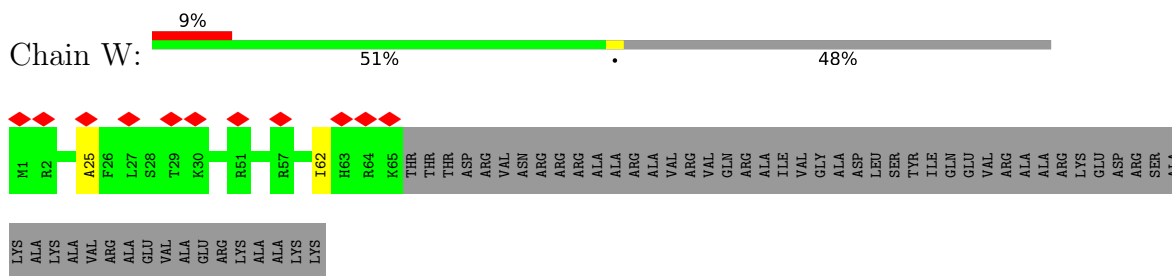
• Molecule 21: uL14



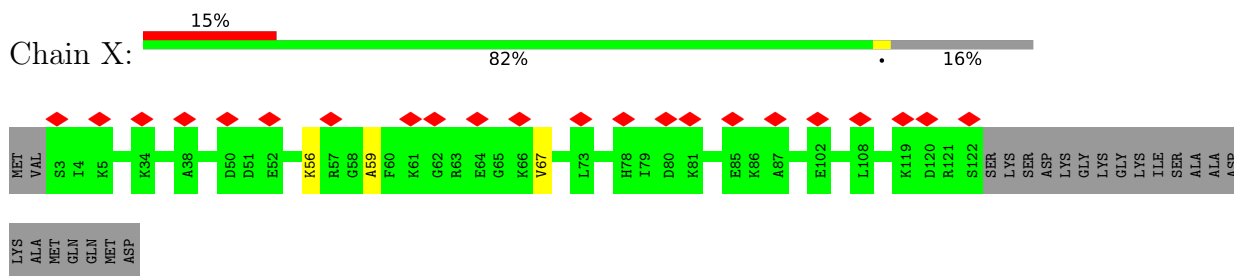
• Molecule 22: uL23



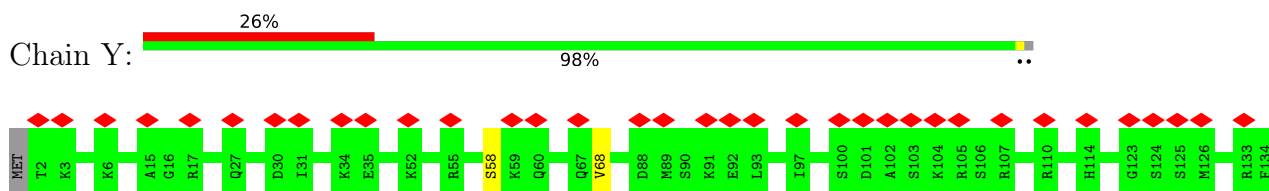
• Molecule 23: eL24



• Molecule 24: uL24

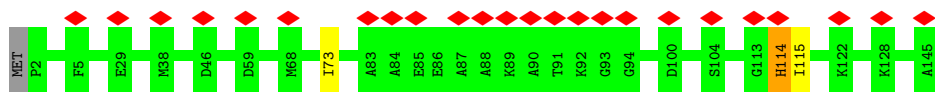


• Molecule 25: eL27

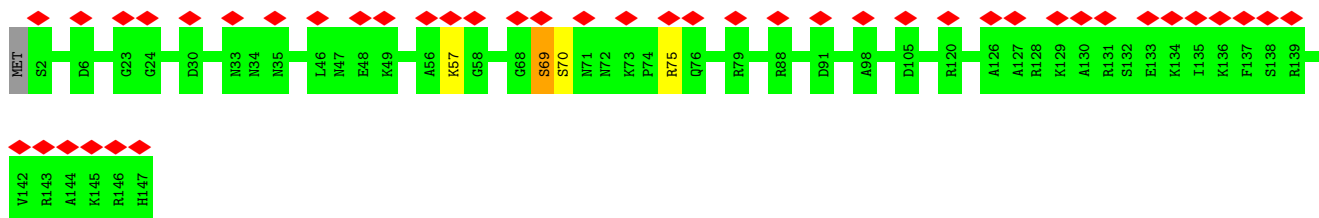


• Molecule 26: uL15

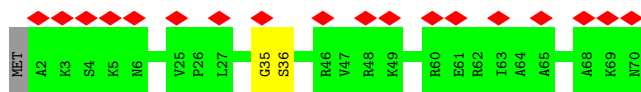




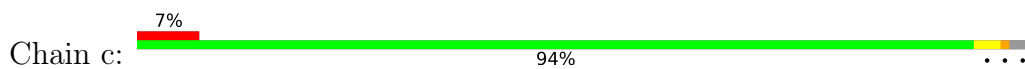
• Molecule 27: eL28



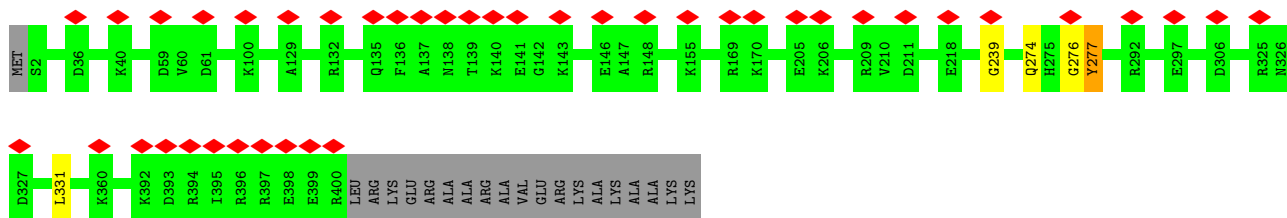
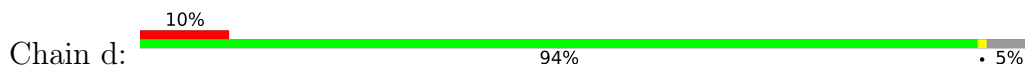
• Molecule 28: eL29



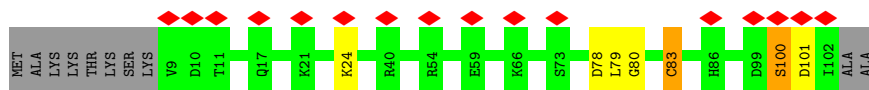
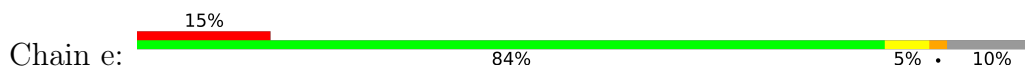
• Molecule 29: uL2



• Molecule 30: uL3

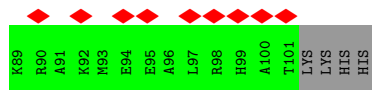


• Molecule 31: eL30

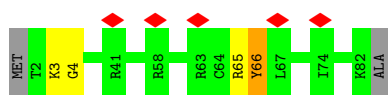
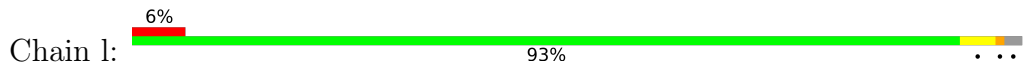


• Molecule 32: eL31

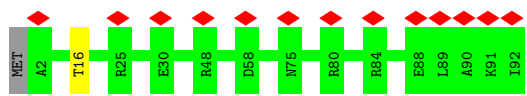




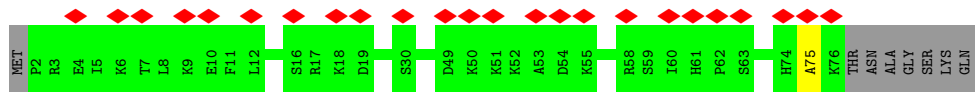
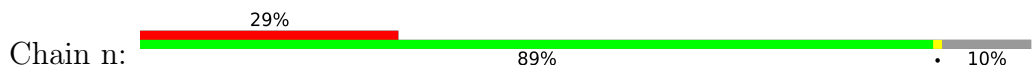
• Molecule 38: eL37



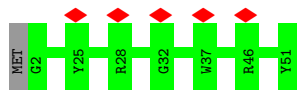
• Molecule 39: eL43



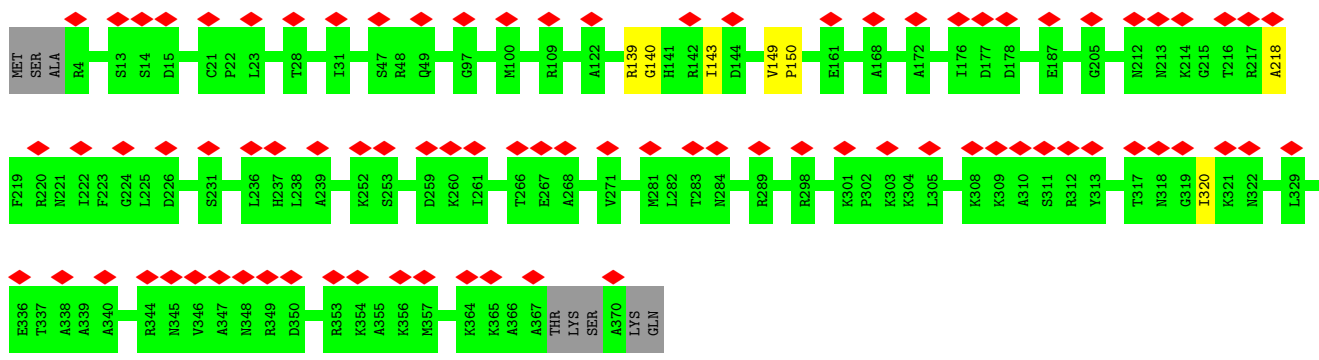
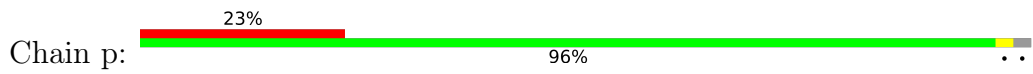
• Molecule 40: eL38



• Molecule 41: eL39

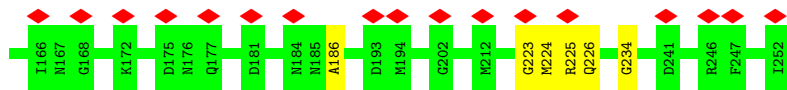


• Molecule 42: uL4

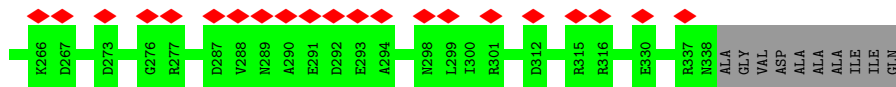
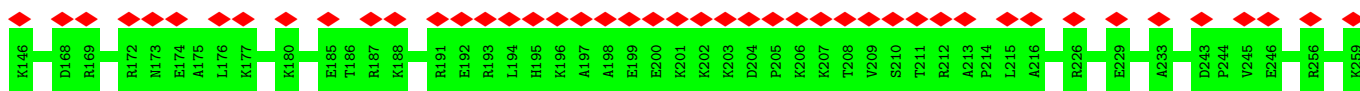
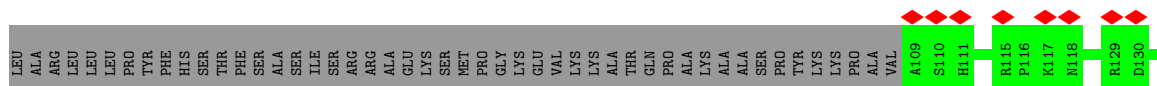
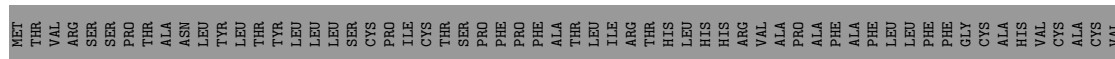


• Molecule 43: eL40

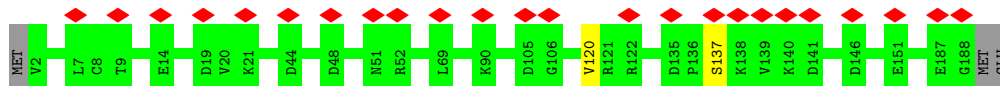




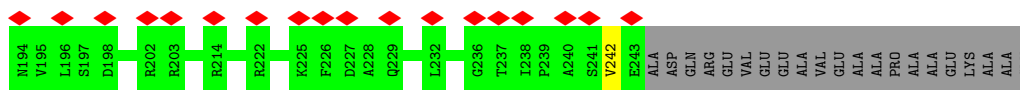
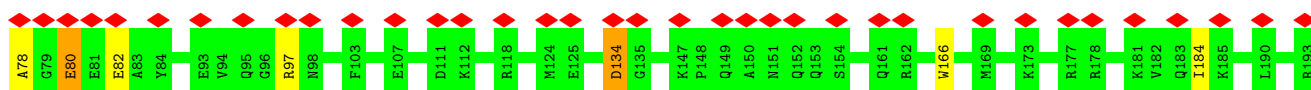
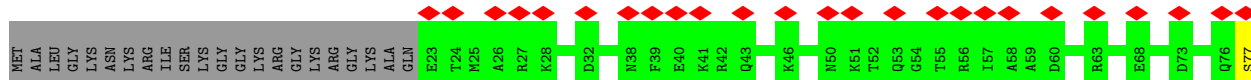
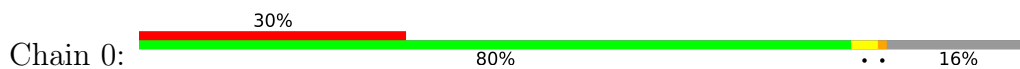
• Molecule 48: eL8



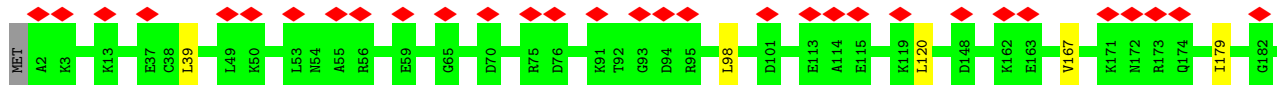
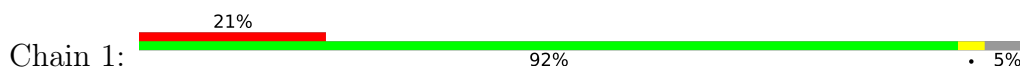
• Molecule 49: uL6

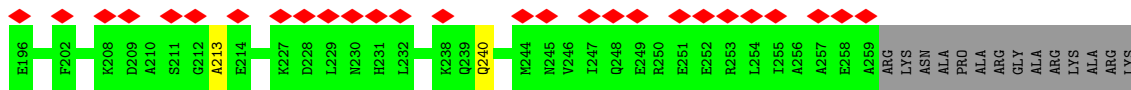


• Molecule 50: eS1

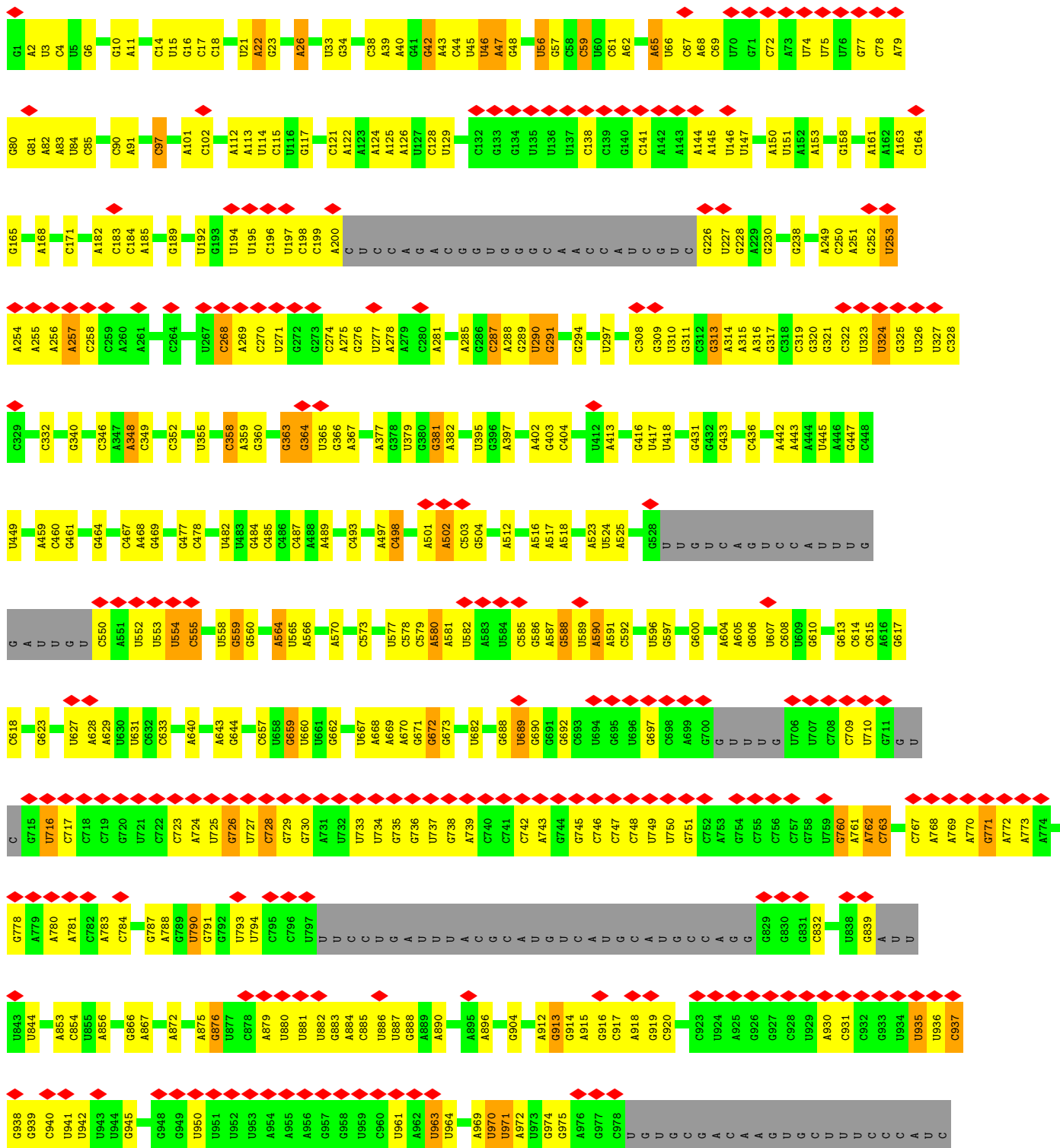


• Molecule 51: eS4



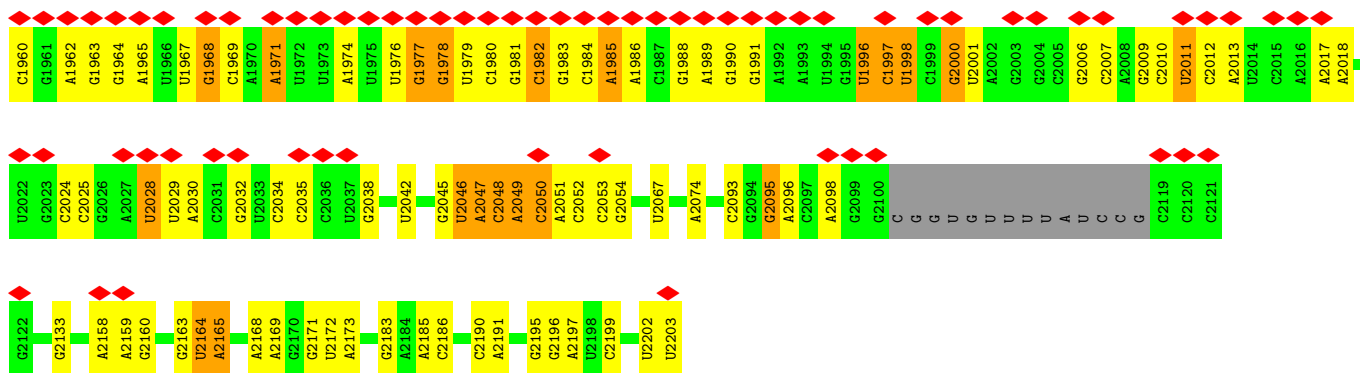


• Molecule 52: 18S rRNA

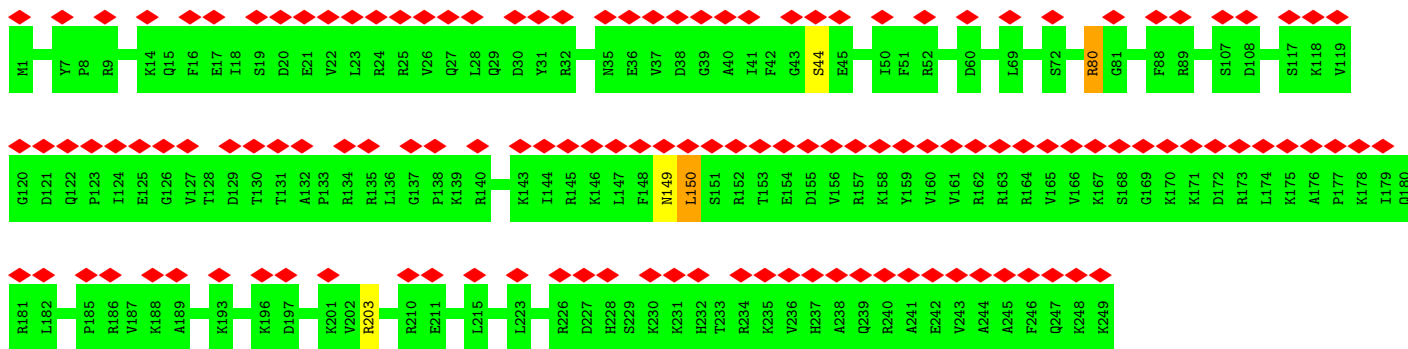




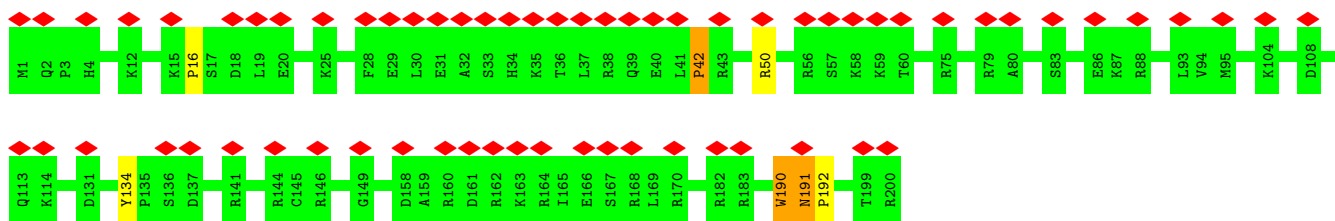




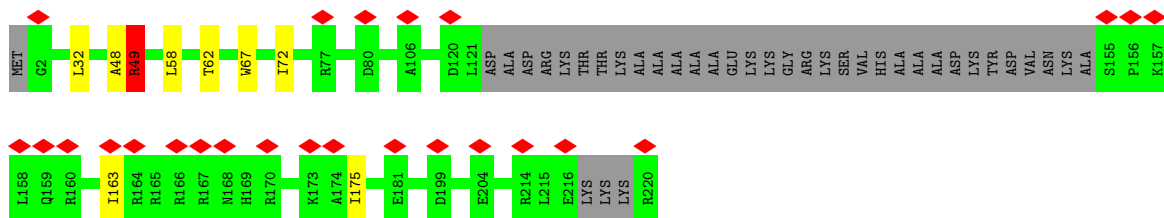
• Molecule 53: eS6



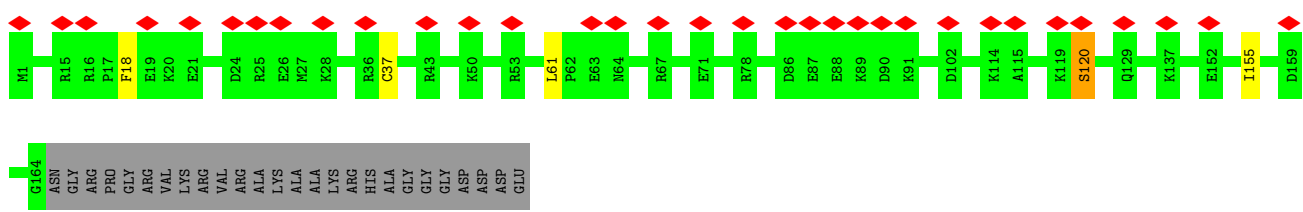
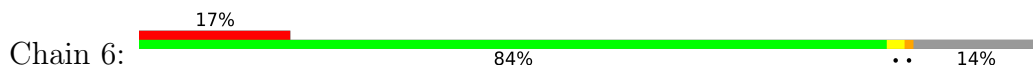
• Molecule 54: eS7



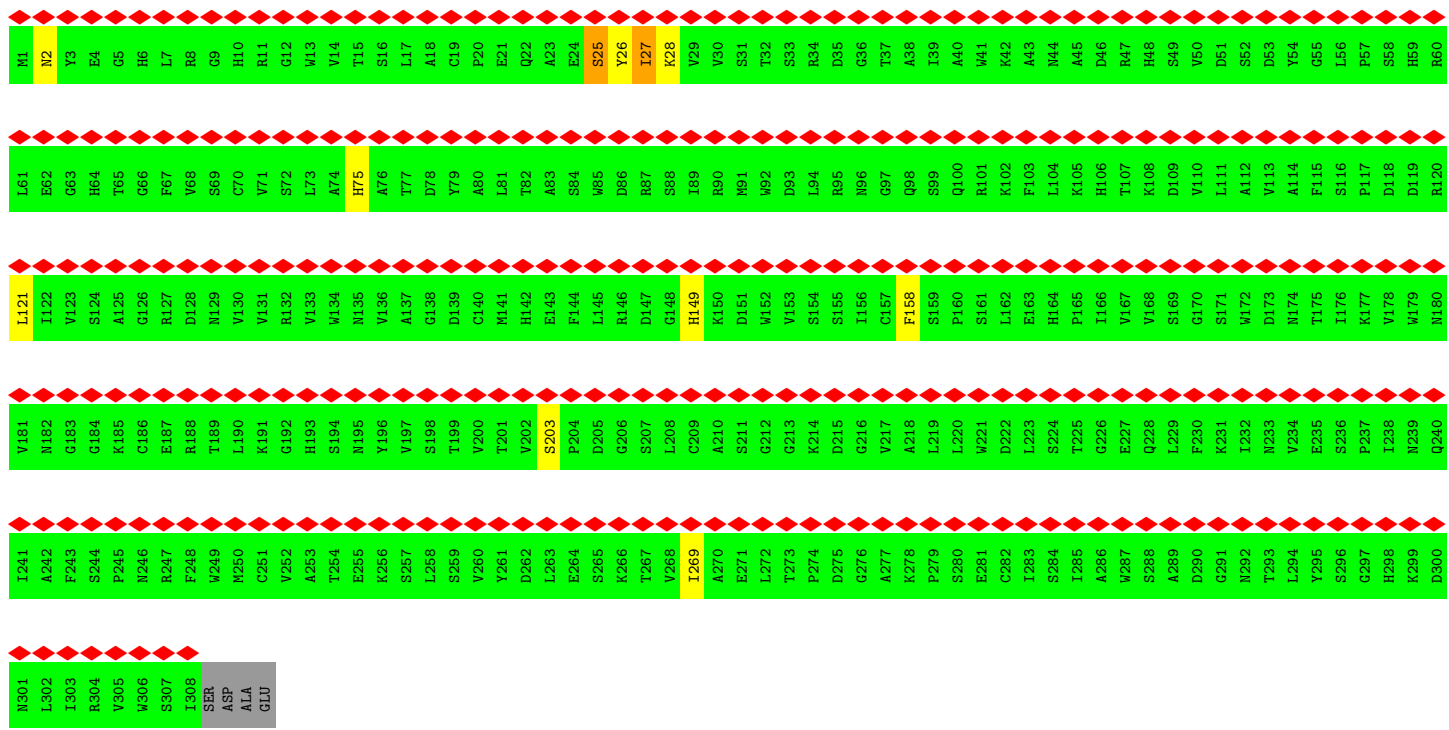
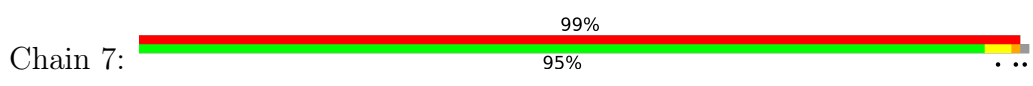
• Molecule 55: eS8



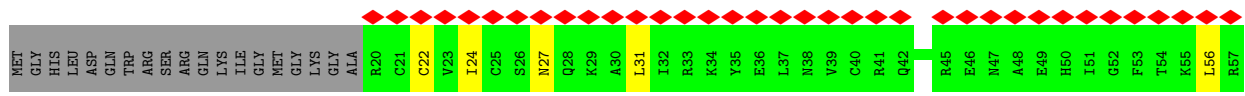
• Molecule 56: uS4



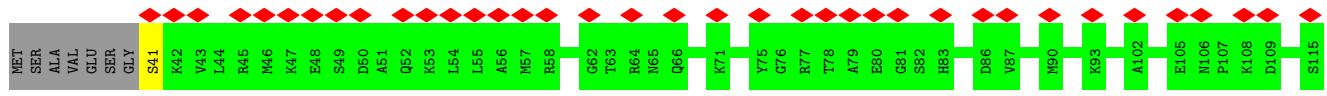
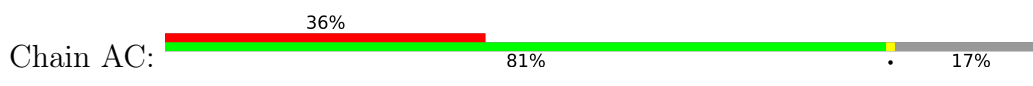
• Molecule 57: RACK1

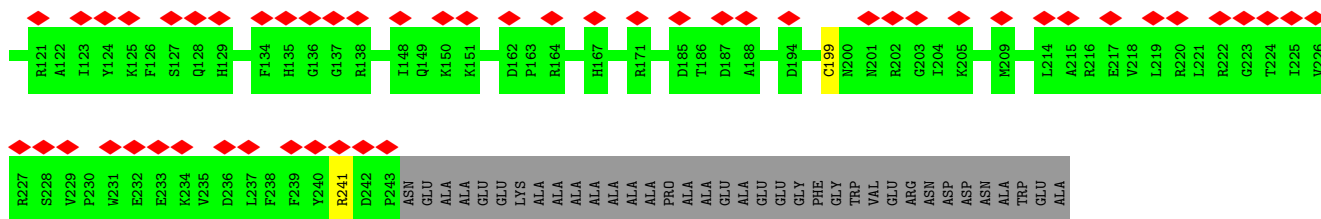


• Molecule 58: uS14

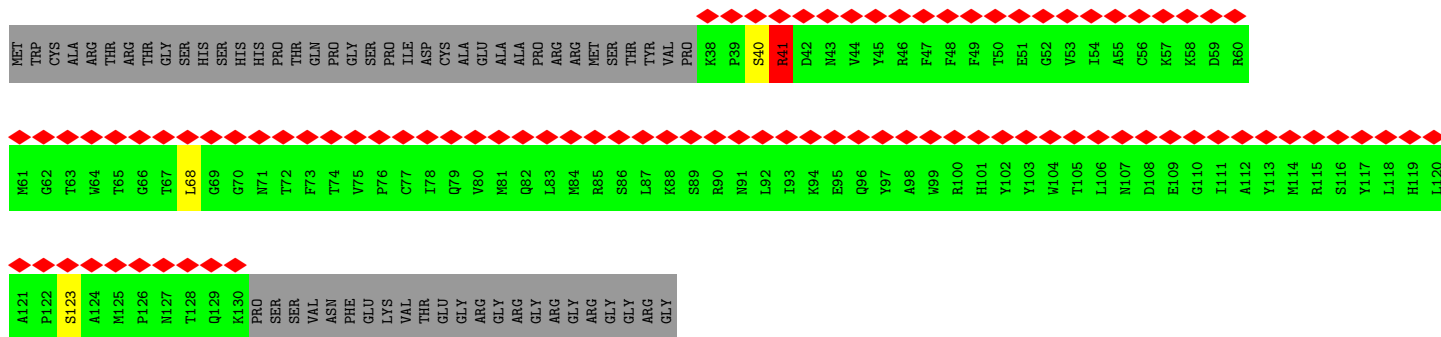


• Molecule 59: uS2

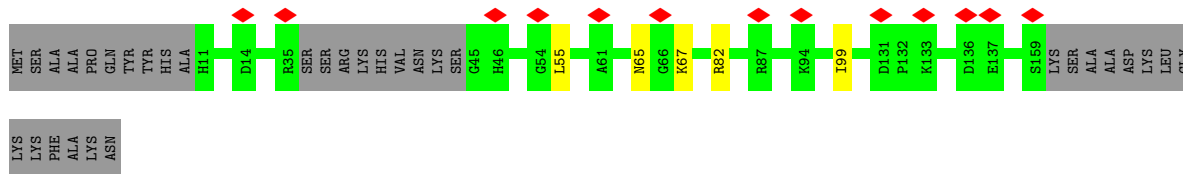
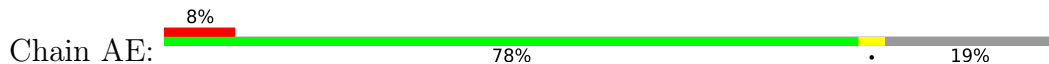




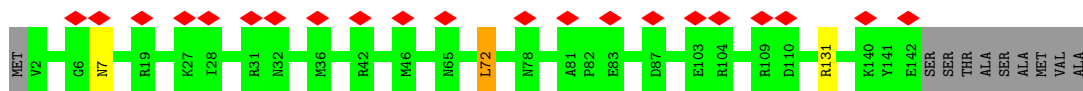
• Molecule 60: eS10



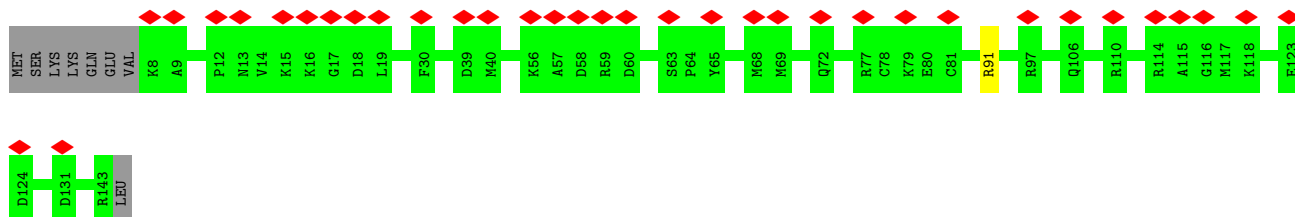
• Molecule 61: uS17



• Molecule 62: uS15

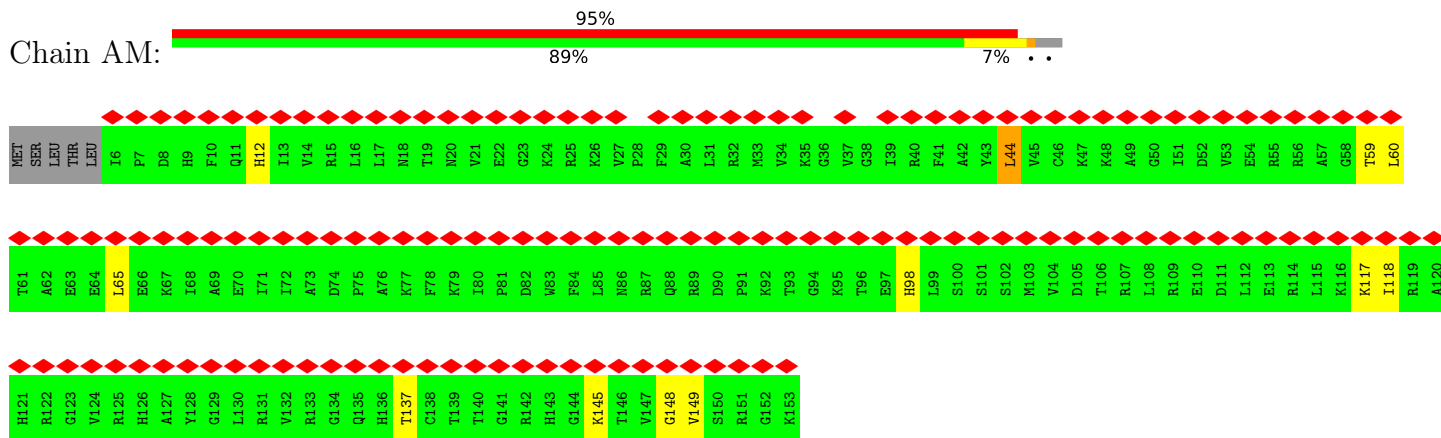


• Molecule 63: uS11





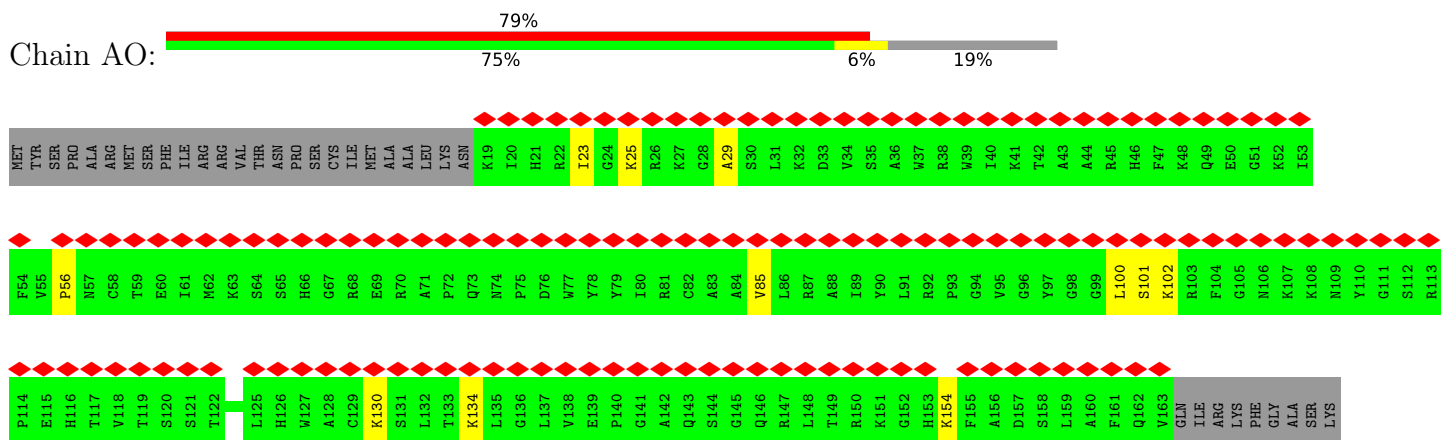
• Molecule 68: uS13



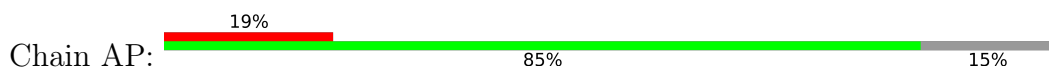
• Molecule 69: uS7

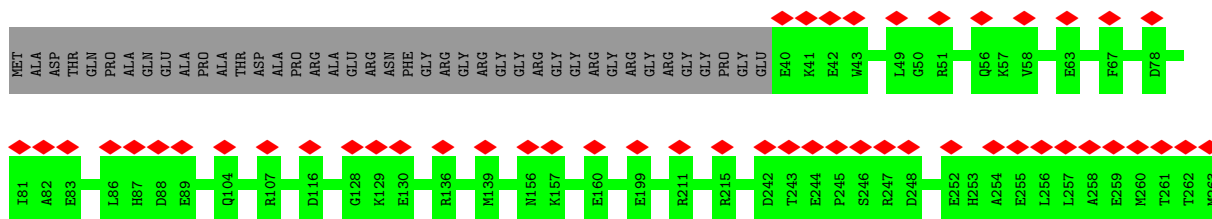


• Molecule 70: eS19

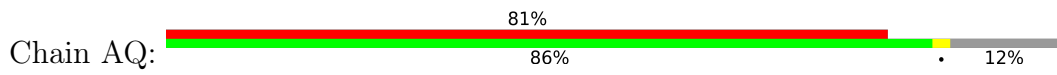


• Molecule 71: uS5

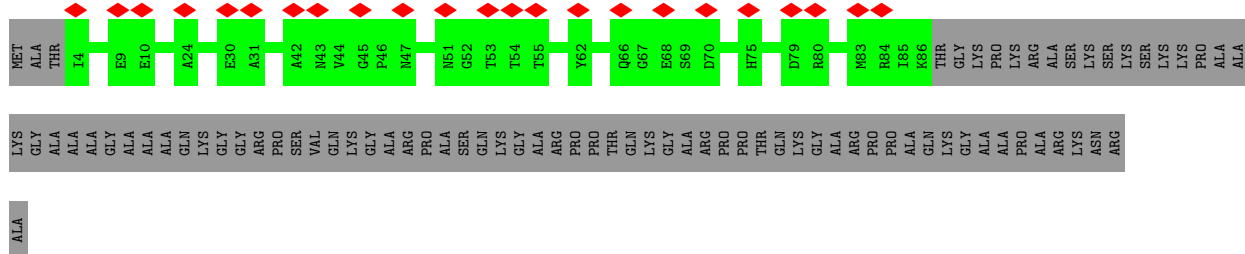




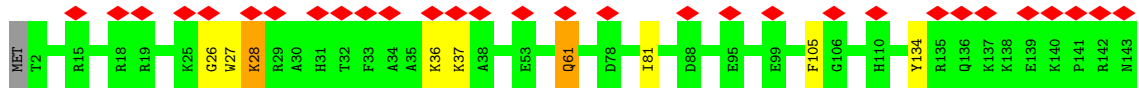
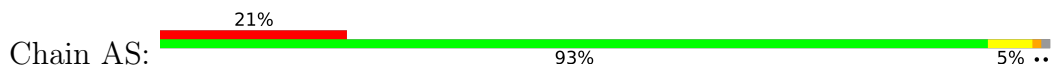
• Molecule 72: uS10



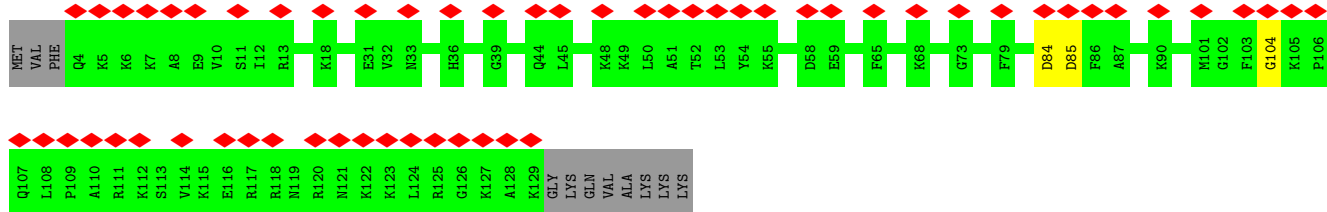
• Molecule 73: eS21



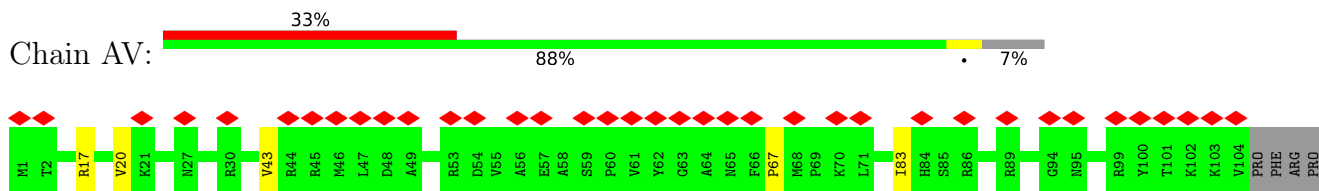
• Molecule 74: uS12



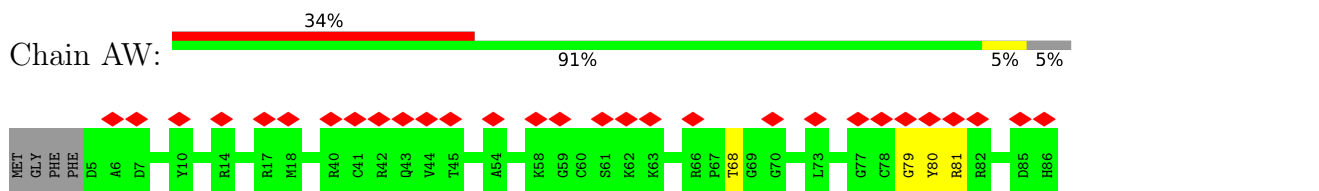
• Molecule 75: eS24



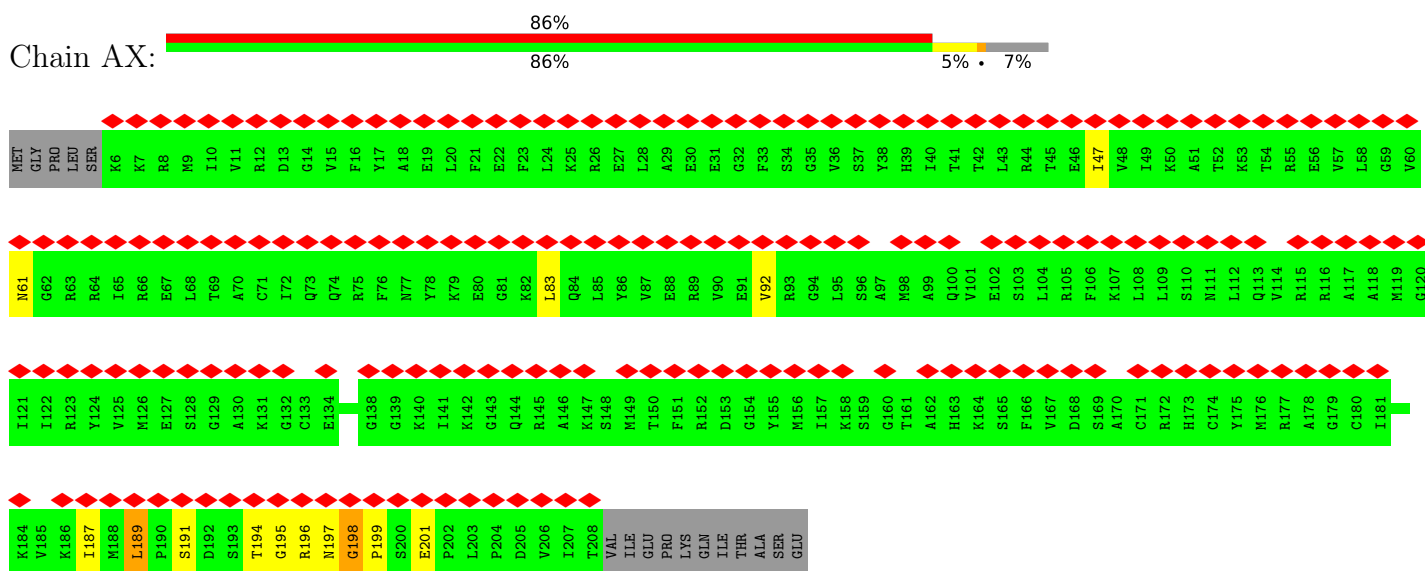
• Molecule 76: eS26



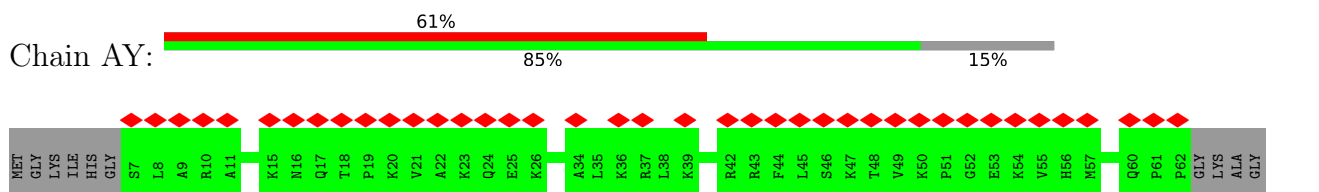
• Molecule 77: eS27



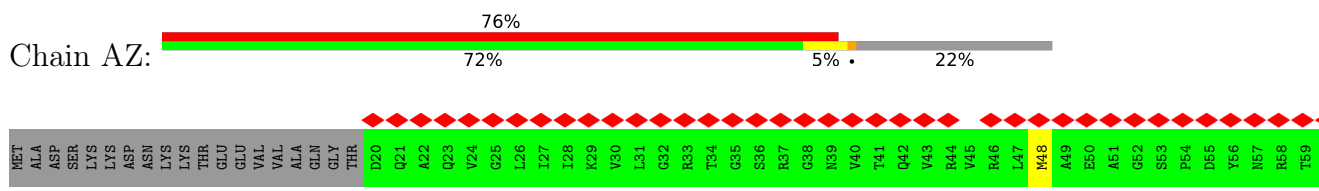
• Molecule 78: uS3



• Molecule 79: eS30



• Molecule 80: eS28



Y61	Y62	Y63	Y64	Y65	Y66	Y67	Y68	Y69	Y70	Y71	Y72	Y73	Y74	Y75	Y76	Y77	Y78	Y79	Y80	Y81	Y82	Y83	Y84	Y85	Y86	Y87
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213108	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	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	0.039	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	317.31998, 317.31998, 317.31998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.7932999, 0.7932999, 0.7932999	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.03	0/38479	0.88	24/59984 (0.0%)
2	B	1.05	0/25421	0.84	8/39614 (0.0%)
3	C	0.98	1/3855 (0.0%)	0.89	2/6002 (0.0%)
4	D	0.93	0/2829	0.79	0/4405
5	E	1.01	0/4004	0.83	1/6223 (0.0%)
6	F	0.84	0/1686	0.86	1/2623 (0.0%)
7	G	1.11	0/4373	0.88	8/6817 (0.1%)
8	H	1.15	0/2230	0.88	2/3470 (0.1%)
9	I	0.60	1/1564 (0.1%)	0.75	2/2092 (0.1%)
10	J	0.53	0/1737	0.62	0/2324
11	K	0.42	0/1362	0.56	0/1821
12	L	0.52	0/1463	0.60	2/1952 (0.1%)
13	M	0.59	0/1815	0.67	3/2436 (0.1%)
14	N	0.51	0/1355	0.66	3/1814 (0.2%)
15	O	0.65	2/1754 (0.1%)	0.71	5/2342 (0.2%)
16	P	0.61	0/1269	0.62	0/1700
17	Q	0.61	0/1490	0.60	0/2007
18	R	0.50	0/1665	0.54	0/2206
19	S	0.58	0/1290	0.71	2/1734 (0.1%)
20	T	0.52	0/1013	0.61	1/1350 (0.1%)
21	U	0.64	0/1052	0.64	0/1417
22	V	0.50	0/978	0.58	0/1318
23	W	0.65	0/584	0.53	0/785
24	X	0.54	0/980	0.67	0/1308
25	Y	0.56	0/1100	0.57	0/1470
26	Z	0.57	0/1153	0.72	2/1541 (0.1%)
27	a	0.47	0/1157	0.65	2/1548 (0.1%)
28	b	0.41	0/565	0.62	1/754 (0.1%)
29	c	0.69	2/1961 (0.1%)	0.72	1/2630 (0.0%)
30	d	0.64	0/3250	0.69	4/4368 (0.1%)
31	e	0.57	0/730	0.77	3/988 (0.3%)
32	f	0.55	0/893	0.61	0/1196
33	g	0.57	0/1071	0.71	1/1432 (0.1%)
34	h	0.57	0/1030	0.62	0/1369

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	i	0.45	0/1067	0.59	1/1416 (0.1%)
36	j	0.63	0/1082	0.68	1/1454 (0.1%)
37	k	0.42	0/802	0.50	0/1073
38	l	0.64	1/688 (0.1%)	0.87	2/918 (0.2%)
39	m	0.63	0/724	0.66	0/964
40	n	0.54	0/614	0.58	1/818 (0.1%)
41	o	0.58	0/463	0.65	0/617
42	p	0.53	0/2874	0.67	3/3865 (0.1%)
43	q	0.61	0/431	0.66	1/572 (0.2%)
44	r	0.59	1/792 (0.1%)	0.69	2/1046 (0.2%)
45	s	0.49	0/2129	0.58	1/2846 (0.0%)
46	t	0.57	0/1074	0.78	5/1454 (0.3%)
47	u	0.57	0/1891	0.61	2/2531 (0.1%)
48	v	0.48	0/1878	0.57	0/2524
49	w	0.56	0/1504	0.64	0/2024
50	0	0.70	0/1811	0.76	4/2438 (0.2%)
51	1	0.80	0/2076	0.78	1/2799 (0.0%)
52	2	1.66	86/43318 (0.2%)	1.27	315/67487 (0.5%)
53	3	0.66	1/2019 (0.0%)	0.77	3/2694 (0.1%)
54	4	0.76	0/1697	0.88	4/2276 (0.2%)
55	5	0.89	2/1494 (0.1%)	1.01	7/2000 (0.3%)
56	6	0.75	1/1389 (0.1%)	0.73	1/1866 (0.1%)
57	7	0.46	1/2454 (0.0%)	0.75	6/3337 (0.2%)
58	8	0.73	0/317	1.00	3/421 (0.7%)
59	AC	0.68	0/1656	0.69	0/2238
60	AD	0.47	0/788	0.91	3/1064 (0.3%)
61	AE	0.98	0/1171	0.75	1/1570 (0.1%)
62	AG	0.83	0/1180	0.80	1/1581 (0.1%)
63	AH	0.78	0/1038	0.80	1/1392 (0.1%)
64	AI	1.11	1/1006 (0.1%)	0.94	8/1351 (0.6%)
65	AJ	0.94	2/1037 (0.2%)	0.89	1/1391 (0.1%)
66	AK	0.54	0/1128	0.82	3/1515 (0.2%)
67	AL	0.52	0/993	0.69	0/1322
68	AM	0.50	0/1206	0.88	2/1615 (0.1%)
69	AN	0.48	0/1516	0.75	2/2034 (0.1%)
70	AO	0.51	0/1180	0.78	1/1585 (0.1%)
71	AP	0.80	0/1758	0.76	0/2380
72	AQ	0.51	0/817	0.75	0/1107
73	AR	0.67	0/639	0.72	0/866
74	AS	0.81	0/1134	0.89	3/1517 (0.2%)
75	AT	0.68	0/1054	0.70	0/1405
76	AV	0.69	0/845	0.76	0/1130
77	AW	1.25	2/658 (0.3%)	0.80	1/883 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
78	AX	0.56	0/1616	0.83	6/2159 (0.3%)
79	AY	0.54	0/460	0.73	0/611
80	AZ	0.60	1/528 (0.2%)	0.83	1/705 (0.1%)
All	All	1.06	105/215154 (0.0%)	0.92	475/315901 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	I	0	1
13	M	0	2
16	P	0	2
20	T	0	1
23	W	0	1
24	X	0	1
28	b	0	1
29	c	0	1
31	e	0	1
37	k	0	1
38	l	0	3
39	m	0	1
47	u	0	1
50	0	0	1
53	3	0	1
54	4	0	1
55	5	0	2
57	7	0	1
58	8	0	1
59	AC	0	3
61	AE	0	1
62	AG	0	3
64	AI	0	3
66	AK	0	1
67	AL	0	1
68	AM	0	7
69	AN	0	4
70	AO	0	6
72	AQ	0	1
75	AT	0	2
77	AW	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
78	AX	0	1
All	All	0	58

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	2	1864	C	N3-C4	80.83	1.90	1.33
52	2	1864	C	C2-N3	72.70	1.94	1.35
52	2	1864	C	N1-C6	69.47	1.78	1.37
52	2	1864	C	N1-C2	48.39	1.88	1.40
52	2	1864	C	C4-C5	48.22	1.81	1.43
52	2	1864	C	C5-C6	44.65	1.70	1.34
52	2	1954	U	O3'-P	38.92	2.07	1.61
64	AI	135	HIS	CB-CG	30.36	2.04	1.50
77	AW	80	TYR	C-N	-20.26	0.87	1.34
52	2	1954	U	C3'-O3'	19.37	1.69	1.42
77	AW	79	GLY	C-N	15.09	1.68	1.34
29	c	246	ILE	C-N	-14.26	1.01	1.34
15	O	51	LEU	C-N	9.04	1.49	1.33
52	2	1956	G	N7-C5	-9.04	1.33	1.39
15	O	50	MET	C-N	-8.01	1.15	1.34
9	I	20	TYR	C-N	7.84	1.52	1.34
52	2	969	A	N9-C4	-7.78	1.33	1.37
29	c	247	ARG	C-N	7.74	1.47	1.33
80	AZ	85	ARG	C-N	7.69	1.51	1.34
52	2	1899	A	C1'-N9	-7.08	1.36	1.46
52	2	1956	G	N9-C8	-7.07	1.32	1.37
52	2	913	G	N9-C4	-6.80	1.32	1.38
52	2	1645	G	N3-C4	-6.62	1.30	1.35
38	1	66	TYR	C-N	-6.58	1.19	1.34
55	5	49	ARG	C-N	-6.48	1.21	1.33
52	2	1525	A	N7-C5	-6.41	1.35	1.39
52	2	1977	G	C1'-N9	-6.39	1.38	1.46
52	2	640	A	N9-C4	-6.38	1.34	1.37
52	2	590	A	N9-C4	-6.33	1.34	1.37
52	2	1971	A	C1'-N9	-6.31	1.38	1.46
52	2	969	A	N3-C4	-6.29	1.31	1.34
52	2	1934	C	C1'-N1	6.27	1.58	1.48
52	2	97	C	N1-C6	-6.25	1.33	1.37
52	2	2168	A	N9-C4	-6.19	1.34	1.37
3	C	153	A	N9-C4	-6.11	1.34	1.37
52	2	153	A	N9-C4	-6.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	2	1678	G	N3-C4	-6.01	1.31	1.35
52	2	1480	G	C5-C4	-5.99	1.34	1.38
44	r	77	CYS	CB-SG	-5.97	1.72	1.81
52	2	315	A	N9-C4	-5.93	1.34	1.37
52	2	1864	C	P-O5'	5.92	1.65	1.59
52	2	1459	C	N3-C4	-5.90	1.29	1.33
52	2	1935	C	C1'-N1	5.88	1.57	1.48
52	2	381	G	C5-C4	-5.87	1.34	1.38
52	2	1459	C	N1-C6	-5.81	1.33	1.37
52	2	726	G	C1'-N9	-5.80	1.38	1.46
65	AJ	72	CYS	CB-SG	-5.80	1.72	1.81
52	2	1438	A	N3-C4	-5.74	1.31	1.34
52	2	771	G	N9-C4	-5.72	1.33	1.38
52	2	2049	A	N9-C4	-5.71	1.34	1.37
52	2	1645	G	N9-C4	-5.71	1.33	1.38
56	6	37	CYS	CB-SG	-5.67	1.72	1.81
52	2	1864	C	C5'-C4'	5.64	1.58	1.51
52	2	2173	A	N9-C4	-5.62	1.34	1.37
52	2	1955	G	N7-C5	-5.60	1.35	1.39
52	2	1413	A	N9-C4	-5.58	1.34	1.37
52	2	1182	A	N9-C4	-5.58	1.34	1.37
52	2	969	A	N7-C5	-5.57	1.35	1.39
52	2	1223	C	N1-C6	-5.56	1.33	1.37
52	2	348	A	N9-C4	-5.54	1.34	1.37
52	2	124	A	N9-C4	-5.54	1.34	1.37
52	2	1239	A	N3-C4	-5.53	1.31	1.34
52	2	1282	A	N9-C4	-5.52	1.34	1.37
52	2	1872	A	N9-C4	-5.49	1.34	1.37
52	2	1132	G	N3-C4	-5.42	1.31	1.35
52	2	1438	A	C6-N1	-5.42	1.31	1.35
52	2	22	A	N9-C4	-5.41	1.34	1.37
52	2	1678	G	N9-C4	-5.41	1.33	1.38
52	2	597	G	N9-C4	-5.41	1.33	1.38
52	2	670	A	N9-C4	-5.40	1.34	1.37
52	2	489	A	N9-C4	-5.39	1.34	1.37
52	2	1112	A	N9-C4	-5.38	1.34	1.37
52	2	1651	G	C5-C4	-5.37	1.34	1.38
52	2	1458	U	N1-C2	-5.37	1.33	1.38
52	2	969	A	C5-C6	-5.36	1.36	1.41
52	2	517	A	N9-C4	-5.35	1.34	1.37
52	2	377	A	N9-C4	-5.34	1.34	1.37
57	7	203	SER	C-N	-5.32	1.24	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	2	682	U	N1-C2	-5.29	1.33	1.38
65	AJ	81	CYS	CB-SG	-5.26	1.73	1.81
52	2	2190	C	N1-C6	-5.25	1.34	1.37
52	2	359	A	N3-C4	-5.24	1.31	1.34
52	2	1275	C	N1-C6	-5.24	1.34	1.37
52	2	436	C	N3-C4	-5.24	1.30	1.33
52	2	379	U	C2-N3	-5.21	1.34	1.37
52	2	771	G	N3-C4	-5.16	1.31	1.35
52	2	1215	U	N1-C2	-5.14	1.33	1.38
52	2	1497	A	N9-C4	-5.12	1.34	1.37
52	2	26	A	C5-C4	-5.12	1.35	1.38
52	2	16	G	C5-C4	-5.09	1.34	1.38
52	2	40	A	C5-C4	-5.06	1.35	1.38
52	2	2191	A	N9-C4	-5.06	1.34	1.37
52	2	121	C	N1-C6	-5.06	1.34	1.37
52	2	358	C	N1-C6	-5.05	1.34	1.37
52	2	2190	C	C4-C5	-5.05	1.39	1.43
52	2	1123	G	N9-C8	-5.04	1.34	1.37
53	3	80	ARG	CB-CG	-5.04	1.39	1.52
55	5	48	ALA	C-N	-5.04	1.22	1.34
52	2	1264	C	N1-C6	-5.02	1.34	1.37
52	2	1965	A	N9-C4	-5.02	1.34	1.37
52	2	670	A	N3-C4	-5.02	1.31	1.34
52	2	1481	A	N9-C4	-5.02	1.34	1.37
52	2	16	G	N3-C4	-5.01	1.31	1.35
52	2	397	A	N3-C4	-5.01	1.31	1.34
52	2	1108	A	N9-C4	-5.01	1.34	1.37

All (475) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	2	971	U	O5'-P-OP2	-31.09	73.39	110.70
52	2	1954	U	P-O3'-C3'	28.04	153.35	119.70
52	2	1818	U	O5'-P-OP2	-26.60	78.78	110.70
52	2	1818	U	O5'-P-OP1	-22.31	83.92	110.70
52	2	971	U	O5'-P-OP1	-21.05	85.44	110.70
55	5	49	ARG	O-C-N	-20.08	89.07	123.20
52	2	1577	G	N7-C8-N9	16.50	121.35	113.10
52	2	1818	U	OP1-P-OP2	16.10	143.75	119.60
52	2	1577	G	C8-N9-C4	-15.47	100.21	106.40
52	2	1577	G	C4-N9-C1'	13.33	143.83	126.50
52	2	1955	G	O5'-P-OP2	-13.07	93.94	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	t	108	ARG	C-N-CD	-13.04	91.91	120.60
52	2	970	U	OP2-P-O3'	-12.83	76.97	105.20
52	2	1817	U	OP2-P-O3'	-12.81	77.02	105.20
52	2	971	U	OP1-P-OP2	12.71	138.67	119.60
52	2	1875	A	C8-N9-C4	-12.64	100.74	105.80
64	AI	131	ARG	N-CA-C	-12.64	76.87	111.00
54	4	191	ASN	C-N-CD	-12.33	93.47	120.60
38	1	66	TYR	O-C-N	-12.25	103.11	122.70
52	2	1817	U	OP1-P-O3'	-11.89	79.05	105.20
52	2	970	U	OP1-P-O3'	-11.84	79.16	105.20
30	d	239	GLY	C-N-CA	-11.63	92.62	121.70
52	2	550	C	N1-C2-O2	11.61	125.86	118.90
52	2	771	G	N3-C4-N9	-11.47	119.12	126.00
60	AD	40	SER	N-CA-C	-11.42	80.16	111.00
52	2	1605	U	OP1-P-O3'	-11.31	80.31	105.20
52	2	1796	U	OP1-P-O3'	-11.21	80.53	105.20
52	2	2028	U	OP1-P-O3'	-11.15	80.67	105.20
52	2	1955	G	N7-C8-N9	11.05	118.63	113.10
52	2	1788	G	OP1-P-O3'	-10.98	81.05	105.20
52	2	2028	U	OP2-P-O3'	-10.80	81.43	105.20
52	2	56	U	C2-N1-C1'	10.64	130.47	117.70
31	e	83	CYS	N-CA-C	-10.32	83.13	111.00
52	2	1796	U	OP2-P-O3'	-10.32	82.49	105.20
52	2	1875	A	N7-C8-N9	10.32	118.96	113.80
52	2	1605	U	OP2-P-O3'	-10.27	82.61	105.20
52	2	1955	G	C8-N9-C4	-10.11	102.35	106.40
52	2	1864	C	C4-C5-C6	10.06	122.43	117.40
38	1	65	ARG	C-N-CA	-9.98	96.75	121.70
52	2	1577	G	C5-N7-C8	-9.96	99.32	104.30
52	2	2050	C	N1-C2-O2	9.90	124.84	118.90
52	2	1955	G	OP1-P-OP2	-9.79	104.91	119.60
64	AI	135	HIS	CA-CB-CG	9.53	129.79	113.60
52	2	1955	G	O5'-P-OP1	-9.50	97.15	105.70
52	2	1577	G	C6-C5-N7	-9.36	124.78	130.40
52	2	1956	G	C4-N9-C1'	9.17	138.42	126.50
52	2	550	C	N3-C2-O2	-9.14	115.50	121.90
26	Z	114	HIS	O-C-N	-9.00	108.30	122.70
52	2	1788	G	OP2-P-O3'	-8.95	85.51	105.20
60	AD	68	LEU	N-CA-C	8.95	135.16	111.00
63	AH	91	ARG	NE-CZ-NH1	-8.91	115.85	120.30
52	2	1956	G	C4-C5-C6	8.88	124.13	118.80
52	2	364	G	O4'-C1'-N9	8.87	115.29	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	AK	122	LEU	C-N-CA	-8.86	99.54	121.70
15	O	51	LEU	N-CA-C	-8.86	87.08	111.00
52	2	1863	A	P-O3'-C3'	8.81	130.27	119.70
52	2	56	U	C6-N1-C1'	-8.79	108.89	121.20
52	2	1960	C	O5'-P-OP1	-8.78	97.80	105.70
29	c	214	GLY	N-CA-C	8.74	134.94	113.10
52	2	1864	C	O4'-C1'-N1	8.72	115.18	108.20
52	2	1843	U	N3-C2-O2	-8.70	116.11	122.20
52	2	1955	G	C6-C5-N7	-8.67	125.20	130.40
52	2	1206	C	C2-N1-C1'	8.64	128.31	118.80
52	2	1954	U	OP2-P-O3'	8.63	124.19	105.20
52	2	2029	U	N3-C2-O2	-8.59	116.19	122.20
52	2	1864	C	N3-C4-C5	-8.59	118.46	121.90
52	2	1577	G	C8-N9-C1'	-8.55	115.89	127.00
52	2	2050	C	C2-N1-C1'	8.54	128.19	118.80
52	2	550	C	C2-N1-C1'	8.53	128.19	118.80
52	2	1816	U	C2-N1-C1'	8.49	127.89	117.70
52	2	913	G	N3-C4-C5	8.46	132.83	128.60
52	2	1843	U	N1-C2-O2	8.42	128.69	122.80
52	2	1645	G	C2-N3-C4	-8.33	107.74	111.90
45	s	126	ASP	N-CA-C	-8.31	88.55	111.00
52	2	364	G	O5'-P-OP1	-8.31	98.22	105.70
52	2	2029	U	N1-C2-O2	8.31	128.62	122.80
52	2	771	G	N3-C2-N2	-8.29	114.10	119.90
52	2	1678	G	N3-C4-N9	-8.27	121.04	126.00
52	2	913	G	N3-C4-N9	-8.23	121.06	126.00
52	2	1956	G	C6-C5-N7	-8.13	125.52	130.40
70	AO	100	LEU	CA-CB-CG	8.11	133.96	115.30
52	2	1864	C	N1-C2-N3	-8.08	113.54	119.20
52	2	56	U	C5-C6-N1	8.06	126.73	122.70
52	2	771	G	N3-C4-C5	8.03	132.62	128.60
74	AS	28	LYS	N-CA-C	-7.99	89.42	111.00
52	2	1875	A	C5'-C4'-O4'	-7.99	99.51	109.10
52	2	1997	C	C2-N1-C1'	7.97	127.57	118.80
46	t	67	GLY	N-CA-C	-7.94	93.24	113.10
52	2	1956	G	C8-N9-C1'	-7.94	116.67	127.00
52	2	969	A	C2-N3-C4	-7.94	106.63	110.60
52	2	2029	U	C2-N1-C1'	7.89	127.17	117.70
52	2	1997	C	N1-C2-O2	7.86	123.61	118.90
53	3	150	LEU	N-CA-C	7.83	132.15	111.00
52	2	1967	U	N1-C2-O2	7.79	128.25	122.80
52	2	1930	G	C4-C5-N7	7.78	113.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	761	U	C2-N1-C1'	7.68	126.91	117.70
51	1	120	LEU	CA-CB-CG	7.67	132.93	115.30
52	2	1789	A	OP1-P-OP2	7.63	131.05	119.60
44	r	17	CYS	CA-CB-SG	7.62	127.72	114.00
52	2	1525	A	C4-C5-C6	7.62	120.81	117.00
52	2	1955	G	C4-N9-C1'	7.61	136.39	126.50
52	2	46	U	C2-N1-C1'	7.60	126.82	117.70
52	2	1443	U	N3-C2-O2	-7.57	116.90	122.20
52	2	760	G	C5-C6-N1	7.57	115.28	111.50
7	G	85	C	N3-C2-O2	-7.55	116.61	121.90
52	2	1997	C	O5'-P-OP1	-7.54	98.92	105.70
7	G	85	C	N1-C2-O2	7.47	123.38	118.90
77	AW	79	GLY	O-C-N	-7.46	110.77	122.70
52	2	1955	G	N3-C4-C5	-7.44	124.88	128.60
52	2	1518	G	O4'-C1'-N9	7.44	114.15	108.20
52	2	1577	G	N1-C6-O6	7.42	124.36	119.90
33	g	102	GLY	N-CA-C	7.38	131.55	113.10
1	A	461	G	N3-C4-N9	-7.37	121.58	126.00
52	2	1678	G	N3-C2-N2	-7.36	114.75	119.90
52	2	2050	C	N3-C2-O2	-7.35	116.75	121.90
57	7	27	ILE	N-CA-C	7.35	130.85	111.00
52	2	2046	U	C5-C6-N1	7.35	126.37	122.70
15	O	51	LEU	O-C-N	7.32	135.65	123.20
52	2	502	A	N1-C2-N3	7.30	132.95	129.30
52	2	904	G	C6-C5-N7	-7.28	126.03	130.40
52	2	1950	C	C5-C6-N1	7.26	124.63	121.00
52	2	771	G	C4-N9-C1'	-7.25	117.08	126.50
69	AN	88	LEU	CA-CB-CG	7.24	131.94	115.30
64	AI	133	VAL	N-CA-C	7.23	130.53	111.00
13	M	220	GLY	N-CA-C	7.23	131.18	113.10
19	S	123	LYS	N-CA-C	-7.23	91.48	111.00
55	5	49	ARG	CA-C-N	7.22	130.65	116.20
52	2	1956	G	N3-C4-C5	-7.19	125.00	128.60
55	5	67	TRP	CA-CB-CG	7.19	127.36	113.70
52	2	1797	G	OP1-P-OP2	7.18	130.37	119.60
52	2	771	G	N9-C4-C5	7.17	108.27	105.40
52	2	1606	C	OP1-P-OP2	7.15	130.32	119.60
52	2	771	G	C8-N9-C1'	7.13	136.28	127.00
7	G	85	C	C2-N1-C1'	7.12	126.63	118.80
52	2	38	C	C5-C6-N1	-7.12	117.44	121.00
52	2	1850	U	N3-C2-O2	-7.10	117.23	122.20
52	2	1955	G	N3-C4-N9	7.10	130.26	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	2	1874	A	O4'-C1'-N9	7.08	113.86	108.20
52	2	1956	G	N3-C4-N9	7.08	130.25	126.00
52	2	1930	G	C5-C6-O6	-7.07	124.36	128.60
52	2	2050	C	C6-N1-C1'	-7.04	112.35	120.80
52	2	59	C	O4'-C1'-N1	6.97	113.78	108.20
52	2	1968	G	O4'-C1'-N9	6.96	113.77	108.20
52	2	1967	U	N3-C2-O2	-6.96	117.33	122.20
62	AG	72	LEU	CA-CB-CG	6.95	131.29	115.30
1	A	461	G	N3-C4-C5	6.95	132.07	128.60
52	2	1930	G	N1-C6-O6	6.91	124.04	119.90
52	2	1206	C	N3-C2-O2	-6.88	117.08	121.90
19	S	10	GLY	C-N-CA	-6.85	104.57	121.70
52	2	728	C	C2-N1-C1'	6.85	126.33	118.80
52	2	1529	U	O4'-C1'-N1	6.84	113.67	108.20
52	2	1206	C	N1-C2-O2	6.83	123.00	118.90
42	p	140	GLY	C-N-CA	-6.80	104.70	121.70
31	e	100	SER	N-CA-C	-6.80	92.65	111.00
52	2	763	C	N3-C2-O2	-6.79	117.15	121.90
52	2	1239	A	C2-N3-C4	-6.72	107.24	110.60
52	2	1860	G	N3-C4-N9	-6.71	121.97	126.00
52	2	324	U	N1-C2-O2	6.71	127.50	122.80
2	B	980	U	N3-C2-O2	-6.69	117.51	122.20
58	8	31	LEU	CA-CB-CG	6.69	130.69	115.30
52	2	2164	U	P-O3'-C3'	6.68	127.72	119.70
52	2	1955	G	O4'-C1'-N9	6.66	113.53	108.20
30	d	276	GLY	N-CA-C	6.66	129.75	113.10
58	8	24	ILE	CG1-CB-CG2	-6.66	96.76	111.40
9	I	36	LEU	CA-CB-CG	6.62	130.51	115.30
52	2	1864	C	C6-N1-C2	6.61	122.94	120.30
52	2	1816	U	C6-N1-C1'	-6.60	111.96	121.20
52	2	2029	U	OP1-P-OP2	6.60	129.50	119.60
1	A	814	C	N3-C2-O2	-6.57	117.30	121.90
78	AX	198	GLY	C-N-CD	-6.57	106.14	120.60
50	0	134	ASP	N-CA-C	-6.56	93.28	111.00
52	2	1577	G	N3-C4-C5	-6.55	125.32	128.60
52	2	1930	G	C6-C5-N7	-6.55	126.47	130.40
52	2	1954	U	O3'-P-O5'	6.53	116.40	104.00
52	2	559	G	O4'-C1'-N9	6.51	113.41	108.20
52	2	1791	U	P-O3'-C3'	6.51	127.51	119.70
52	2	42	G	P-O3'-C3'	6.51	127.51	119.70
1	A	186	G	N3-C4-C5	6.50	131.85	128.60
52	2	1997	C	C6-N1-C1'	-6.50	113.00	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	2	1434	C	C2-N1-C1'	6.49	125.94	118.80
52	2	1872	A	C2-N3-C4	-6.49	107.36	110.60
52	2	1985	A	N1-C6-N6	-6.47	114.72	118.60
52	2	1930	G	N9-C4-C5	-6.46	102.82	105.40
7	G	85	C	C6-N1-C2	-6.45	117.72	120.30
2	B	1453	C	C5-C6-N1	6.42	124.21	121.00
52	2	904	G	C4-N9-C1'	6.41	134.83	126.50
1	A	186	G	N3-C4-N9	-6.38	122.17	126.00
52	2	1978	G	C8-N9-C1'	6.36	135.27	127.00
43	q	110	CYS	CA-CB-SG	6.34	125.41	114.00
78	AX	199	PRO	N-CA-C	6.33	128.54	112.10
30	d	277	TYR	CA-CB-CG	6.32	125.41	113.40
52	2	1964	G	C2-N3-C4	-6.32	108.74	111.90
1	A	761	U	N1-C2-O2	6.30	127.21	122.80
52	2	1183	G	N3-C4-N9	-6.29	122.23	126.00
52	2	1525	A	C6-C5-N7	-6.28	127.91	132.30
52	2	290	U	N3-C2-O2	-6.27	117.81	122.20
52	2	1908	C	C2-N1-C1'	6.26	125.69	118.80
52	2	38	C	C4-C5-C6	6.26	120.53	117.40
52	2	963	U	OP1-P-O3'	6.26	118.98	105.20
52	2	1239	A	N1-C2-N3	6.26	132.43	129.30
52	2	56	U	C4-C5-C6	-6.25	115.95	119.70
52	2	56	U	O5'-P-OP2	6.25	118.20	110.70
52	2	1949	U	P-O3'-C3'	6.25	127.20	119.70
52	2	1416	A	O5'-P-OP1	-6.24	100.08	105.70
52	2	1860	G	N3-C4-C5	6.23	131.71	128.60
52	2	1181	C	C2-N1-C1'	6.22	125.64	118.80
52	2	1104	A	N7-C8-N9	6.21	116.91	113.80
52	2	716	U	C2'-C3'-O3'	6.16	123.56	113.70
52	2	1876	U	P-O5'-C5'	6.16	130.75	120.90
52	2	1869	A	C5-C6-N1	6.16	120.78	117.70
54	4	190	TRP	N-CA-C	6.15	127.61	111.00
52	2	1850	U	N1-C2-O2	6.15	127.10	122.80
52	2	762	A	OP1-P-OP2	-6.14	110.38	119.60
52	2	1881	G	N3-C4-N9	6.14	129.68	126.00
52	2	493	C	C6-N1-C2	6.13	122.75	120.30
52	2	1678	G	N9-C4-C5	6.13	107.85	105.40
52	2	1106	U	C3'-C2'-C1'	6.13	106.40	101.50
80	AZ	85	ARG	C-N-CA	6.12	137.01	121.70
52	2	1400	C	C5-C6-N1	-6.12	117.94	121.00
52	2	1967	U	C2-N1-C1'	6.12	125.04	117.70
31	e	80	GLY	C-N-CA	-6.11	106.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	0	78	ALA	N-CA-C	6.10	127.48	111.00
52	2	1843	U	C2-N1-C1'	6.10	125.02	117.70
26	Z	114	HIS	CA-C-N	6.10	130.62	117.20
52	2	10	G	C4-N9-C1'	6.09	134.42	126.50
52	2	1864	C	C5'-C4'-O4'	6.08	116.40	109.10
52	2	2030	A	N1-C2-N3	6.08	132.34	129.30
52	2	1548	A	O4'-C1'-N9	6.08	113.06	108.20
30	d	331	LEU	CA-CB-CG	6.07	129.27	115.30
1	A	367	A	C2-N3-C4	-6.07	107.57	110.60
52	2	550	C	C6-N1-C1'	-6.06	113.53	120.80
52	2	10	G	C8-N9-C1'	-6.06	119.13	127.00
52	2	1955	G	C5-C6-O6	-6.04	124.98	128.60
2	B	1452	G	C4-N9-C1'	6.02	134.33	126.50
52	2	153	A	O5'-P-OP1	-6.02	100.28	105.70
52	2	416	G	C8-N9-C1'	-6.02	119.17	127.00
15	O	91	GLY	C-N-CA	-6.02	106.65	121.70
60	AD	41	ARG	C-N-CA	-6.02	106.66	121.70
52	2	1527	C	C6-N1-C2	-6.01	117.90	120.30
64	AI	134	LEU	N-CA-C	6.00	127.20	111.00
52	2	363	G	OP1-P-O3'	6.00	118.40	105.20
52	2	38	C	N1-C2-O2	-5.99	115.30	118.90
52	2	1576	G	P-O3'-C3'	5.97	126.86	119.70
54	4	50	ARG	NE-CZ-NH1	-5.96	117.32	120.30
47	u	223	GLY	N-CA-C	5.95	127.96	113.10
9	I	20	TYR	O-C-N	5.94	132.21	122.70
52	2	1525	A	C8-N9-C4	-5.94	103.42	105.80
52	2	1206	C	C6-N1-C1'	-5.93	113.68	120.80
52	2	2011	U	P-O3'-C3'	5.93	126.81	119.70
52	2	1955	G	C5-N7-C8	-5.92	101.34	104.30
52	2	319	C	N3-C2-O2	5.92	126.04	121.90
53	3	80	ARG	CG-CD-NE	-5.91	99.38	111.80
52	2	1570	C	C6-N1-C2	5.89	122.66	120.30
7	G	166	C	C2-N1-C1'	5.89	125.28	118.80
61	AE	55	LEU	CA-CB-CG	-5.88	101.77	115.30
52	2	969	A	C5-N7-C8	-5.88	100.96	103.90
78	AX	189	LEU	N-CA-C	-5.87	95.15	111.00
15	O	94	LEU	CA-CB-CG	5.87	128.79	115.30
8	H	7	C	C2-N1-C1'	5.86	125.25	118.80
52	2	1627	G	P-O3'-C3'	5.86	126.74	119.70
1	A	761	U	N3-C2-O2	-5.85	118.10	122.20
46	t	107	GLN	N-CA-C	5.85	126.80	111.00
52	2	1239	A	O4'-C1'-N9	5.84	112.88	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	2	1875	A	N9-C4-C5	5.84	108.14	105.80
52	2	1577	G	C5-C6-O6	-5.84	125.10	128.60
40	n	75	ALA	N-CA-C	-5.82	95.30	111.00
52	2	1796	U	C5-C6-N1	5.82	125.61	122.70
52	2	1930	G	O4'-C1'-N9	-5.79	103.57	108.20
52	2	771	G	C6-C5-N7	5.79	133.87	130.40
7	G	171	U	C2-N1-C1'	5.79	124.64	117.70
1	A	360	U	C2-N1-C1'	5.78	124.64	117.70
74	AS	61	GLN	C-N-CD	5.78	140.54	128.40
12	L	25	GLY	N-CA-C	5.78	127.54	113.10
52	2	1104	A	C8-N9-C4	-5.77	103.49	105.80
57	7	25	SER	N-CA-C	5.77	126.57	111.00
74	AS	26	GLY	N-CA-C	-5.76	98.70	113.10
52	2	253	U	OP1-P-O3'	5.76	117.86	105.20
52	2	1378	U	P-O3'-C3'	5.76	126.61	119.70
52	2	1525	A	N7-C8-N9	5.76	116.68	113.80
52	2	1584	A	N9-C1'-C2'	-5.76	105.67	112.00
52	2	1996	U	C5-C6-N1	-5.75	119.82	122.70
52	2	257	A	OP1-P-O3'	5.75	117.85	105.20
52	2	1955	G	N1-C6-O6	5.75	123.35	119.90
52	2	1645	G	N1-C2-N3	5.75	127.35	123.90
52	2	1577	G	C4-C5-C6	5.74	122.24	118.80
52	2	790	U	P-O3'-C3'	5.73	126.57	119.70
52	2	1206	C	C6-N1-C2	-5.72	118.01	120.30
52	2	659	G	O4'-C1'-N9	5.71	112.77	108.20
52	2	672	G	N3-C4-C5	5.71	131.46	128.60
55	5	58	LEU	CA-CB-CG	5.71	128.44	115.30
52	2	689	U	N1-C2-O2	5.70	126.79	122.80
57	7	27	ILE	C-N-CA	5.70	135.96	121.70
52	2	1982	C	C5-C6-N1	5.70	123.85	121.00
52	2	597	G	N3-C4-C5	5.69	131.45	128.60
52	2	1400	C	OP1-P-OP2	-5.69	111.07	119.60
44	r	74	CYS	CA-CB-SG	5.68	124.23	114.00
52	2	771	G	C4-C5-N7	-5.68	108.53	110.80
65	AJ	28	ARG	C-N-CD	5.68	140.33	128.40
1	A	461	G	C2-N3-C4	-5.68	109.06	111.90
52	2	1434	C	O4'-C1'-N1	5.68	112.74	108.20
1	A	447	G	O4'-C1'-N9	5.65	112.72	108.20
52	2	1148	G	O4'-C1'-N9	5.64	112.72	108.20
52	2	1964	G	N1-C2-N3	5.64	127.29	123.90
52	2	46	U	C6-N1-C1'	-5.64	113.30	121.20
53	3	203	ARG	NE-CZ-NH1	-5.63	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	U	O4'-C1'-N1	5.63	112.71	108.20
52	2	416	G	C4-N9-C1'	5.62	133.81	126.50
52	2	689	U	C2-N1-C1'	5.62	124.45	117.70
52	2	1685	A	C2-N3-C4	5.62	113.41	110.60
56	6	61	LEU	CA-CB-CG	5.62	128.23	115.30
52	2	1983	G	N3-C4-C5	5.62	131.41	128.60
12	L	130	LEU	C-N-CA	-5.61	107.67	121.70
52	2	1943	A	C8-N9-C4	-5.61	103.56	105.80
52	2	1998	U	C2-N1-C1'	-5.61	110.97	117.70
52	2	1580	G	C4-N9-C1'	-5.60	119.22	126.50
52	2	1791	U	OP2-P-O3'	5.59	117.50	105.20
52	2	1556	A	P-O3'-C3'	5.59	126.41	119.70
52	2	313	G	C4-N9-C1'	5.58	133.75	126.50
52	2	2029	U	C6-N1-C1'	-5.57	113.40	121.20
57	7	121	LEU	CA-CB-CG	5.57	128.11	115.30
52	2	913	G	C2-N3-C4	-5.57	109.12	111.90
52	2	1982	C	C2-N1-C1'	5.56	124.92	118.80
52	2	555	C	C6-N1-C2	-5.56	118.08	120.30
52	2	1645	G	N3-C4-N9	-5.55	122.67	126.00
52	2	692	G	N3-C4-C5	5.54	131.37	128.60
47	u	234	GLY	N-CA-C	-5.54	99.25	113.10
57	7	158	PHE	N-CA-C	-5.53	96.07	111.00
36	j	14	LEU	CA-CB-CG	5.52	128.00	115.30
42	p	150	PRO	N-CA-C	-5.52	97.74	112.10
50	0	166	TRP	CA-CB-CG	5.52	124.19	113.70
1	A	367	A	N1-C2-N3	5.52	132.06	129.30
52	2	618	C	O5'-P-OP1	-5.52	100.73	105.70
52	2	1996	U	C6-N1-C2	5.52	124.31	121.00
52	2	1645	G	N3-C4-C5	5.52	131.36	128.60
52	2	2048	C	C2-N1-C1'	5.51	124.87	118.80
52	2	47	A	P-O3'-C3'	5.51	126.31	119.70
68	AM	44	LEU	CA-CB-CG	5.51	127.97	115.30
52	2	1525	A	N1-C6-N6	5.50	121.90	118.60
52	2	1876	U	C6-N1-C2	-5.50	117.70	121.00
52	2	316	A	O5'-P-OP2	-5.50	100.75	105.70
14	N	46	MET	N-CA-C	-5.49	96.18	111.00
52	2	1572	G	O4'-C1'-N9	-5.48	103.81	108.20
2	B	958	U	N1-C2-O2	5.47	126.63	122.80
52	2	573	C	C6-N1-C2	-5.46	118.11	120.30
78	AX	83	LEU	CB-CG-CD2	-5.46	101.73	111.00
52	2	1897	C	P-O3'-C3'	5.44	126.23	119.70
64	AI	131	ARG	C-N-CD	5.44	139.82	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	2	1955	G	C4-C5-C6	5.43	122.06	118.80
14	N	10	GLY	C-N-CA	-5.43	108.13	121.70
27	a	70	SER	N-CA-C	-5.43	96.34	111.00
52	2	728	C	N1-C2-O2	5.43	122.16	118.90
52	2	2165	A	O5'-P-OP1	-5.42	100.82	105.70
52	2	1577	G	C4-C5-N7	5.42	112.97	110.80
52	2	667	U	OP2-P-O3'	5.41	117.10	105.20
27	a	69	SER	N-CA-C	5.41	125.61	111.00
66	AK	46	LEU	C-N-CD	5.41	139.76	128.40
1	A	203	C	N3-C2-O2	-5.40	118.12	121.90
52	2	1103	G	P-O3'-C3'	5.40	126.18	119.70
52	2	38	C	C2-N3-C4	-5.39	117.20	119.90
6	F	67	C	N1-C2-O2	5.39	122.14	118.90
58	8	56	LEU	CA-CB-CG	-5.39	102.90	115.30
68	AM	149	VAL	CA-CB-CG2	5.39	118.99	110.90
52	2	1104	A	P-O3'-C3'	5.39	126.16	119.70
52	2	771	G	N1-C2-N2	5.38	121.04	116.20
13	M	124	GLU	C-N-CA	-5.37	111.02	122.30
52	2	1864	C	N1-C2-O2	5.37	122.12	118.90
64	AI	84	LYS	C-N-CA	5.37	135.12	121.70
1	A	761	U	C6-N1-C1'	-5.36	113.69	121.20
52	2	1863	A	N1-C6-N6	-5.36	115.38	118.60
52	2	1576	G	N3-C4-C5	-5.36	125.92	128.60
52	2	1881	G	C6-C5-N7	-5.36	127.19	130.40
52	2	2000	G	P-O3'-C3'	5.35	126.12	119.70
52	2	1950	C	C4-C5-C6	-5.35	114.73	117.40
52	2	1576	G	C4-C5-C6	5.34	122.01	118.80
64	AI	84	LYS	N-CA-C	5.34	125.41	111.00
52	2	596	U	N1-C2-O2	-5.33	119.07	122.80
52	2	46	U	N1-C2-O2	5.33	126.53	122.80
5	E	73	C	C2-N1-C1'	5.32	124.66	118.80
2	B	283	C	N3-C2-O2	-5.32	118.17	121.90
52	2	1606	C	N1-C2-O2	5.31	122.09	118.90
52	2	896	A	O4'-C1'-N9	5.31	112.45	108.20
52	2	876	G	C4-N9-C1'	5.30	133.39	126.50
78	AX	61	ASN	N-CA-C	-5.30	96.69	111.00
52	2	268	C	OP1-P-O3'	5.30	116.86	105.20
1	A	203	C	C6-N1-C2	-5.29	118.18	120.30
1	A	814	C	C2-N1-C1'	5.29	124.62	118.80
52	2	937	C	P-O3'-C3'	5.29	126.05	119.70
52	2	2046	U	C6-N1-C2	-5.29	117.83	121.00
52	2	1580	G	OP1-P-O3'	5.29	116.83	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	t	67	GLY	C-N-CD	5.28	139.49	128.40
2	B	320	U	C2-N1-C1'	5.28	124.03	117.70
52	2	65	A	C2-N3-C4	-5.28	107.96	110.60
52	2	38	C	C2-N1-C1'	-5.28	113.00	118.80
55	5	72	ILE	CG1-CB-CG2	-5.27	99.80	111.40
52	2	21	U	C5-C6-N1	5.27	125.34	122.70
52	2	1577	G	N9-C1'-C2'	5.27	120.85	114.00
52	2	1789	A	P-O3'-C3'	5.27	126.02	119.70
52	2	1881	G	C4-N9-C1'	5.26	133.34	126.50
52	2	1982	C	C6-N1-C2	-5.26	118.20	120.30
52	2	287	C	P-O3'-C3'	5.25	126.00	119.70
1	A	967	G	C4-C5-N7	5.25	112.90	110.80
52	2	416	G	C6-C5-N7	-5.25	127.25	130.40
64	AI	135	HIS	ND1-CG-CD2	-5.24	98.66	106.00
52	2	56	U	N1-C2-O2	5.24	126.47	122.80
52	2	340	G	O5'-P-OP1	-5.24	100.99	105.70
52	2	588	G	O4'-C1'-N9	5.24	112.39	108.20
52	2	935	U	OP1-P-O3'	5.23	116.71	105.20
52	2	1606	C	N3-C2-O2	-5.22	118.24	121.90
52	2	324	U	N3-C2-O2	-5.21	118.55	122.20
52	2	1581	A	O4'-C1'-N9	-5.21	104.03	108.20
52	2	2095	G	P-O3'-C3'	5.21	125.95	119.70
52	2	124	A	C8-N9-C4	5.21	107.88	105.80
52	2	1978	G	C4-N9-C1'	-5.20	119.74	126.50
52	2	257	A	P-O3'-C3'	5.20	125.94	119.70
3	C	101	C	C5-C6-N1	5.18	123.59	121.00
52	2	2047	A	C4-N9-C1'	-5.18	116.98	126.30
55	5	48	ALA	C-N-CA	5.18	134.65	121.70
7	G	171	U	C5-C6-N1	5.17	125.29	122.70
52	2	1576	G	N3-C4-N9	5.17	129.10	126.00
52	2	550	C	C6-N1-C2	-5.16	118.24	120.30
52	2	253	U	P-O3'-C3'	5.15	125.88	119.70
69	AN	43	GLN	C-N-CA	-5.15	108.82	121.70
42	p	149	VAL	C-N-CD	5.15	139.21	128.40
2	B	714	A	N1-C6-N6	-5.15	115.51	118.60
1	A	437	A	C2-N3-C4	-5.14	108.03	110.60
3	C	174	A	C2-N3-C4	-5.14	108.03	110.60
1	A	813	C	C2-N1-C1'	5.13	124.44	118.80
52	2	1854	C	OP2-P-O3'	5.13	116.48	105.20
7	G	166	C	N3-C2-O2	-5.13	118.31	121.90
52	2	1925	G	N3-C4-N9	-5.13	122.92	126.00
52	2	1830	A	P-O3'-C3'	5.12	125.84	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	2	564	A	OP1-P-O3'	5.12	116.46	105.20
52	2	950	U	N3-C2-O2	-5.12	118.62	122.20
8	H	7	C	N3-C2-O2	-5.12	118.32	121.90
52	2	904	G	C8-N9-C1'	-5.10	120.37	127.00
50	0	80	GLU	N-CA-C	5.10	124.77	111.00
52	2	1816	U	N1-C2-O2	5.10	126.37	122.80
52	2	1957	G	C8-N9-C4	-5.10	104.36	106.40
1	A	276	C	C2-N1-C1'	5.09	124.40	118.80
52	2	1251	G	N3-C4-C5	5.09	131.15	128.60
54	4	134	TYR	C-N-CD	-5.09	109.40	120.60
52	2	1148	G	N7-C8-N9	5.08	115.64	113.10
52	2	1239	A	C5-N7-C8	-5.08	101.36	103.90
66	AK	69	LEU	CA-CB-CG	-5.08	103.61	115.30
2	B	958	U	N3-C2-O2	-5.08	118.64	122.20
20	T	65	SER	C-N-CA	-5.08	109.00	121.70
52	2	1699	G	P-O3'-C3'	5.08	125.79	119.70
46	t	23	SER	C-N-CD	5.07	139.05	128.40
52	2	1606	C	P-O3'-C3'	5.07	125.78	119.70
78	AX	195	GLY	N-CA-C	-5.07	100.43	113.10
52	2	2164	U	OP2-P-O3'	5.07	116.34	105.20
52	2	1890	A	N1-C6-N6	-5.06	115.56	118.60
1	A	813	C	N3-C2-O2	-5.06	118.36	121.90
15	O	52	GLY	C-N-CA	-5.06	109.06	121.70
28	b	36	SER	N-CA-C	-5.06	97.35	111.00
52	2	291	G	O5'-P-OP1	-5.06	101.15	105.70
52	2	1875	A	C2-N3-C4	5.05	113.13	110.60
52	2	689	U	N3-C2-O2	-5.05	118.66	122.20
1	A	931	G	C4-N9-C1'	5.05	133.06	126.50
35	i	39	GLY	N-CA-C	5.05	125.72	113.10
52	2	1661	U	N3-C2-O2	-5.04	118.67	122.20
52	2	1854	C	P-O3'-C3'	5.04	125.75	119.70
13	M	87	GLY	C-N-CD	5.04	138.99	128.40
52	2	580	A	P-O3'-C3'	5.04	125.75	119.70
52	2	1132	G	N3-C4-N9	-5.04	122.98	126.00
55	5	62	THR	C-N-CA	-5.03	111.74	122.30
14	N	135	THR	C-N-CD	5.02	138.95	128.40
52	2	672	G	C2-N3-C4	-5.02	109.39	111.90
52	2	1576	G	C4-N9-C1'	5.02	133.03	126.50
52	2	1678	G	N3-C4-C5	5.01	131.11	128.60
57	7	27	ILE	CA-C-N	-5.01	106.17	117.20
52	2	498	C	C6-N1-C2	-5.01	118.30	120.30
52	2	554	U	P-O3'-C3'	5.01	125.71	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	2	672	G	C4-C5-N7	5.01	112.80	110.80
52	2	1400	C	C4-C5-C6	5.00	119.90	117.40

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	0	82	GLU	Peptide
53	3	149	ASN	Mainchain
54	4	42	PRO	Peptide
55	5	49	ARG	Mainchain,Peptide
57	7	2	ASN	Peptide
58	8	22	CYS	Peptide
59	AC	199	CYS	Peptide
59	AC	241	ARG	Peptide
59	AC	41	SER	Peptide
61	AE	82	ARG	Peptide
62	AG	131	ARG	Peptide
62	AG	7	ASN	Peptide
62	AG	72	LEU	Peptide
64	AI	107	HIS	Peptide
64	AI	124	GLY	Peptide
64	AI	43	LEU	Peptide
66	AK	32	GLN	Peptide
67	AL	85	ALA	Peptide
68	AM	117	LYS	Peptide
68	AM	118	ILE	Peptide
68	AM	12	HIS	Peptide
68	AM	137	THR	Peptide
68	AM	145	LYS	Peptide
68	AM	148	GLY	Peptide
68	AM	98	HIS	Peptide
69	AN	152	LEU	Peptide
69	AN	26	ASP	Peptide
69	AN	31	THR	Peptide
69	AN	88	LEU	Peptide
70	AO	101	SER	Peptide
70	AO	102	LYS	Peptide
70	AO	130	LYS	Peptide
70	AO	154	LYS	Peptide
70	AO	25	LYS	Peptide
70	AO	56	PRO	Peptide

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Mol	Chain	Res	Type	Group
72	AQ	24	ARG	Peptide
75	AT	104	GLY	Peptide
75	AT	84	ASP	Peptide
77	AW	68	THR	Peptide
78	AX	198	GLY	Peptide
9	I	180	THR	Peptide
13	M	132	ARG	Peptide
13	M	163	HIS	Peptide
16	P	36	ILE	Peptide
16	P	64	ASN	Peptide
20	T	66	ASP	Peptide
23	W	25	ALA	Peptide
24	X	56	LYS	Mainchain
28	b	35	GLY	Peptide
29	c	195	CYS	Peptide
31	e	78	ASP	Mainchain
37	k	12	ALA	Peptide
38	l	3	LYS	Peptide
38	l	4	GLY	Peptide
38	l	66	TYR	Mainchain
39	m	16	THR	Peptide
47	u	186	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	
9	I	195/198 (98%)	180 (92%)	12 (6%)	3 (2%)	10	34
10	J	209/213 (98%)	193 (92%)	13 (6%)	3 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	165/188 (88%)	152 (92%)	12 (7%)	1 (1%)	25	58
12	L	175/220 (80%)	159 (91%)	14 (8%)	2 (1%)	14	42
13	M	219/222 (99%)	212 (97%)	6 (3%)	1 (0%)	29	61
14	N	166/175 (95%)	153 (92%)	12 (7%)	1 (1%)	25	58
15	O	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
16	P	153/166 (92%)	145 (95%)	7 (5%)	1 (1%)	22	54
17	Q	176/179 (98%)	163 (93%)	11 (6%)	2 (1%)	14	42
18	R	194/245 (79%)	193 (100%)	1 (0%)	0	100	100
19	S	156/159 (98%)	144 (92%)	11 (7%)	1 (1%)	25	58
20	T	121/129 (94%)	116 (96%)	5 (4%)	0	100	100
21	U	135/139 (97%)	126 (93%)	9 (7%)	0	100	100
22	V	118/145 (81%)	106 (90%)	11 (9%)	1 (1%)	19	51
23	W	63/124 (51%)	61 (97%)	2 (3%)	0	100	100
24	X	118/143 (82%)	111 (94%)	5 (4%)	2 (2%)	9	31
25	Y	131/134 (98%)	124 (95%)	6 (5%)	1 (1%)	19	51
26	Z	142/145 (98%)	125 (88%)	14 (10%)	3 (2%)	7	26
27	a	144/147 (98%)	134 (93%)	9 (6%)	1 (1%)	22	54
28	b	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
29	c	251/260 (96%)	229 (91%)	20 (8%)	2 (1%)	19	51
30	d	397/419 (95%)	376 (95%)	20 (5%)	1 (0%)	41	71
31	e	92/104 (88%)	88 (96%)	4 (4%)	0	100	100
32	f	108/183 (59%)	102 (94%)	6 (6%)	0	100	100
33	g	127/133 (96%)	119 (94%)	8 (6%)	0	100	100
34	h	122/168 (73%)	117 (96%)	4 (3%)	1 (1%)	19	51
35	i	124/127 (98%)	117 (94%)	6 (5%)	1 (1%)	19	51
36	j	130/144 (90%)	119 (92%)	11 (8%)	0	100	100
37	k	97/105 (92%)	94 (97%)	3 (3%)	0	100	100
38	l	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
39	m	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
40	n	73/83 (88%)	70 (96%)	3 (4%)	0	100	100
41	o	48/51 (94%)	45 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	p	362/373 (97%)	340 (94%)	20 (6%)	2 (1%)	25	58
43	q	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
44	r	94/106 (89%)	85 (90%)	8 (8%)	1 (1%)	14	42
45	s	258/305 (85%)	246 (95%)	12 (5%)	0	100	100
46	t	133/195 (68%)	123 (92%)	8 (6%)	2 (2%)	10	34
47	u	226/252 (90%)	209 (92%)	16 (7%)	1 (0%)	34	66
48	v	228/348 (66%)	218 (96%)	10 (4%)	0	100	100
49	w	185/190 (97%)	173 (94%)	11 (6%)	1 (0%)	29	61
50	0	219/264 (83%)	208 (95%)	10 (5%)	1 (0%)	29	61
51	1	256/273 (94%)	231 (90%)	22 (9%)	3 (1%)	13	40
53	3	247/249 (99%)	236 (96%)	10 (4%)	1 (0%)	34	66
54	4	198/200 (99%)	183 (92%)	11 (6%)	4 (2%)	7	27
55	5	178/220 (81%)	160 (90%)	16 (9%)	2 (1%)	14	42
56	6	162/190 (85%)	151 (93%)	9 (6%)	2 (1%)	13	40
57	7	306/312 (98%)	275 (90%)	28 (9%)	3 (1%)	15	45
58	8	36/57 (63%)	30 (83%)	5 (14%)	1 (3%)	5	19
59	AC	201/246 (82%)	193 (96%)	8 (4%)	0	100	100
60	AD	91/153 (60%)	78 (86%)	11 (12%)	2 (2%)	6	24
61	AE	136/173 (79%)	131 (96%)	4 (3%)	1 (1%)	22	54
62	AG	139/151 (92%)	133 (96%)	6 (4%)	0	100	100
63	AH	134/144 (93%)	126 (94%)	8 (6%)	0	100	100
64	AI	119/152 (78%)	102 (86%)	17 (14%)	0	100	100
65	AJ	127/130 (98%)	120 (94%)	6 (5%)	1 (1%)	19	51
66	AK	138/149 (93%)	118 (86%)	16 (12%)	4 (3%)	4	18
67	AL	119/143 (83%)	108 (91%)	8 (7%)	3 (2%)	5	21
68	AM	146/153 (95%)	125 (86%)	21 (14%)	0	100	100
69	AN	188/190 (99%)	165 (88%)	21 (11%)	2 (1%)	14	42
70	AO	143/179 (80%)	114 (80%)	25 (18%)	4 (3%)	5	19
71	AP	222/265 (84%)	216 (97%)	6 (3%)	0	100	100
72	AQ	100/116 (86%)	86 (86%)	13 (13%)	1 (1%)	15	45
73	AR	81/164 (49%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
74	AS	140/143 (98%)	132 (94%)	5 (4%)	3 (2%)	7	26
75	AT	124/137 (90%)	117 (94%)	6 (5%)	1 (1%)	19	51
76	AV	102/112 (91%)	90 (88%)	8 (8%)	4 (4%)	3	12
77	AW	80/86 (93%)	76 (95%)	4 (5%)	0	100	100
78	AX	201/219 (92%)	179 (89%)	17 (8%)	5 (2%)	5	21
79	AY	54/66 (82%)	48 (89%)	6 (11%)	0	100	100
80	AZ	66/87 (76%)	60 (91%)	4 (6%)	2 (3%)	4	17
All	All	10774/12317 (88%)	9993 (93%)	696 (6%)	85 (1%)	24	51

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	142	GLU
10	J	145	VAL
12	L	21	SER
24	X	59	ALA
26	Z	114	HIS
26	Z	115	ILE
29	c	150	LEU
30	d	277	TYR
34	h	63	ILE
35	i	42	GLU
44	r	95	ASP
46	t	69	MET
47	u	226	GLN
50	0	242	VAL
54	4	192	PRO
57	7	28	LYS
58	8	27	ASN
65	AJ	29	PRO
66	AK	40	VAL
66	AK	119	ASP
72	AQ	107	VAL
74	AS	27	TRP
74	AS	61	GLN
75	AT	85	ASP
78	AX	187	ILE
78	AX	191	SER
78	AX	197	ASN
80	AZ	86	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	I	190	TYR
14	N	136	PRO
17	Q	120	TYR
26	Z	73	ILE
27	a	57	LYS
61	AE	67	LYS
66	AK	61	VAL
69	AN	64	PHE
70	AO	23	ILE
80	AZ	85	ARG
19	S	124	ALA
29	c	214	GLY
46	t	24	PRO
51	1	240	GLN
57	7	75	HIS
60	AD	41	ARG
66	AK	37	VAL
70	AO	134	LYS
22	V	53	VAL
55	5	32	LEU
60	AD	123	SER
67	AL	118	ARG
70	AO	29	ALA
70	AO	85	VAL
76	AV	17	ARG
9	I	6	THR
9	I	8	ILE
12	L	180	GLU
51	1	213	ALA
53	3	80	ARG
56	6	120	SER
74	AS	134	TYR
42	p	218	ALA
56	6	155	ILE
24	X	67	VAL
54	4	42	PRO
54	4	191	ASN
57	7	269	ILE
67	AL	95	ILE
76	AV	20	VAL
76	AV	67	PRO
78	AX	47	ILE

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Mol	Chain	Res	Type
49	w	120	VAL
54	4	16	PRO
11	K	113	ILE
25	Y	68	VAL
42	p	143	ILE
67	AL	85	ALA
76	AV	43	VAL
78	AX	92	VAL
10	J	159	PHE
13	M	131	VAL
17	Q	26	VAL
51	1	167	VAL
55	5	175	ILE
69	AN	133	VAL
16	P	10	VAL

### 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	
9	I	163/164 (99%)	158 (97%)	5 (3%)	40	74
10	J	178/179 (99%)	175 (98%)	3 (2%)	60	86
11	K	145/163 (89%)	144 (99%)	1 (1%)	84	95
12	L	152/182 (84%)	151 (99%)	1 (1%)	84	95
13	M	188/189 (100%)	187 (100%)	1 (0%)	88	96
14	N	139/144 (96%)	136 (98%)	3 (2%)	52	81
15	O	179/180 (99%)	178 (99%)	1 (1%)	86	96
16	P	133/144 (92%)	133 (100%)	0	100	100
17	Q	156/158 (99%)	156 (100%)	0	100	100
18	R	168/196 (86%)	166 (99%)	2 (1%)	71	91
19	S	132/133 (99%)	131 (99%)	1 (1%)	81	94
20	T	107/114 (94%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	U	110/111 (99%)	110 (100%)	0	100	100
22	V	103/123 (84%)	103 (100%)	0	100	100
23	W	60/104 (58%)	59 (98%)	1 (2%)	60	86
24	X	103/121 (85%)	103 (100%)	0	100	100
25	Y	114/115 (99%)	113 (99%)	1 (1%)	78	93
26	Z	114/115 (99%)	114 (100%)	0	100	100
27	a	118/119 (99%)	116 (98%)	2 (2%)	60	86
28	b	57/58 (98%)	57 (100%)	0	100	100
29	c	198/204 (97%)	193 (98%)	5 (2%)	47	78
30	d	337/351 (96%)	336 (100%)	1 (0%)	92	98
31	e	82/90 (91%)	77 (94%)	5 (6%)	18	48
32	f	97/156 (62%)	97 (100%)	0	100	100
33	g	113/117 (97%)	111 (98%)	2 (2%)	59	85
34	h	107/145 (74%)	107 (100%)	0	100	100
35	i	116/117 (99%)	116 (100%)	0	100	100
36	j	109/121 (90%)	107 (98%)	2 (2%)	59	85
37	k	81/87 (93%)	81 (100%)	0	100	100
38	l	69/70 (99%)	69 (100%)	0	100	100
39	m	73/74 (99%)	73 (100%)	0	100	100
40	n	68/74 (92%)	68 (100%)	0	100	100
41	o	46/47 (98%)	46 (100%)	0	100	100
42	p	295/302 (98%)	293 (99%)	2 (1%)	84	95
43	q	46/113 (41%)	46 (100%)	0	100	100
44	r	83/92 (90%)	80 (96%)	3 (4%)	35	69
45	s	209/242 (86%)	208 (100%)	1 (0%)	88	96
46	t	111/152 (73%)	110 (99%)	1 (1%)	78	93
47	u	190/209 (91%)	187 (98%)	3 (2%)	62	86
48	v	196/292 (67%)	196 (100%)	0	100	100
49	w	169/172 (98%)	168 (99%)	1 (1%)	86	96
50	0	194/222 (87%)	189 (97%)	5 (3%)	46	77
51	1	215/225 (96%)	212 (99%)	3 (1%)	67	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	3	208/208 (100%)	206 (99%)	2 (1%)	76	92
54	4	186/186 (100%)	185 (100%)	1 (0%)	88	96
55	5	149/176 (85%)	147 (99%)	2 (1%)	69	90
56	6	147/164 (90%)	145 (99%)	2 (1%)	67	89
57	7	263/266 (99%)	259 (98%)	4 (2%)	65	87
58	8	35/49 (71%)	35 (100%)	0	100	100
59	AC	177/202 (88%)	177 (100%)	0	100	100
60	AD	82/129 (64%)	81 (99%)	1 (1%)	71	91
61	AE	124/150 (83%)	122 (98%)	2 (2%)	62	86
62	AG	125/132 (95%)	125 (100%)	0	100	100
63	AH	105/113 (93%)	105 (100%)	0	100	100
64	AI	104/130 (80%)	102 (98%)	2 (2%)	57	84
65	AJ	110/111 (99%)	105 (96%)	5 (4%)	27	61
66	AK	113/120 (94%)	108 (96%)	5 (4%)	28	61
67	AL	107/123 (87%)	107 (100%)	0	100	100
68	AM	125/130 (96%)	121 (97%)	4 (3%)	39	73
69	AN	159/159 (100%)	158 (99%)	1 (1%)	86	96
70	AO	118/147 (80%)	118 (100%)	0	100	100
71	AP	184/209 (88%)	184 (100%)	0	100	100
72	AQ	94/104 (90%)	94 (100%)	0	100	100
73	AR	68/119 (57%)	68 (100%)	0	100	100
74	AS	115/116 (99%)	110 (96%)	5 (4%)	29	62
75	AT	111/120 (92%)	111 (100%)	0	100	100
76	AV	87/93 (94%)	86 (99%)	1 (1%)	73	92
77	AW	72/75 (96%)	71 (99%)	1 (1%)	67	89
78	AX	171/185 (92%)	167 (98%)	4 (2%)	50	80
79	AY	49/54 (91%)	49 (100%)	0	100	100
80	AZ	57/74 (77%)	54 (95%)	3 (5%)	22	54
All	All	9268/10330 (90%)	9167 (99%)	101 (1%)	74	92

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	9	SER
9	I	19	THR
9	I	20	TYR
9	I	188	ARG
9	I	189	SER
10	J	141	LYS
10	J	142	GLU
10	J	203	LYS
11	K	122	LYS
12	L	180	GLU
13	M	167	LYS
14	N	46	MET
14	N	134	LYS
14	N	137	VAL
15	O	90	LEU
18	R	19	ARG
18	R	62	ARG
19	S	9	SER
23	W	62	ILE
25	Y	58	SER
27	a	69	SER
27	a	75	ARG
29	c	136	ILE
29	c	149	LYS
29	c	150	LEU
29	c	174	ARG
29	c	187	TYR
30	d	274	GLN
31	e	24	LYS
31	e	79	LEU
31	e	83	CYS
31	e	100	SER
31	e	101	ASP
33	g	129	LYS
33	g	130	LEU
36	j	14	LEU
36	j	126	VAL
42	p	139	ARG
42	p	320	ILE
44	r	77	CYS
44	r	95	ASP
44	r	96	LYS
45	s	126	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
46	t	107	GLN
47	u	25	ARG
47	u	224	MET
47	u	225	ARG
49	w	137	SER
50	0	77	SER
50	0	80	GLU
50	0	97	ARG
50	0	134	ASP
50	0	184	ILE
51	1	39	LEU
51	1	98	LEU
51	1	179	ILE
53	3	44	SER
53	3	150	LEU
54	4	190	TRP
55	5	49	ARG
55	5	163	ILE
56	6	18	PHE
56	6	120	SER
57	7	25	SER
57	7	26	TYR
57	7	27	ILE
57	7	149	HIS
60	AD	41	ARG
61	AE	65	ASN
61	AE	99	ILE
64	AI	84	LYS
64	AI	134	LEU
65	AJ	5	SER
65	AJ	28	ARG
65	AJ	47	ILE
65	AJ	50	PHE
65	AJ	130	TYR
66	AK	36	LYS
66	AK	37	VAL
66	AK	46	LEU
66	AK	119	ASP
66	AK	122	LEU
68	AM	44	LEU
68	AM	59	THR
68	AM	60	LEU

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Mol	Chain	Res	Type
68	AM	65	LEU
69	AN	63	MET
74	AS	28	LYS
74	AS	36	LYS
74	AS	37	LYS
74	AS	81	ILE
74	AS	105	PHE
76	AV	83	ILE
77	AW	81	ARG
78	AX	189	LEU
78	AX	194	THR
78	AX	196	ARG
78	AX	201	GLU
80	AZ	48	MET
80	AZ	84	ARG
80	AZ	87	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
9	I	45	ASN
10	J	71	GLN
10	J	100	ASN
11	K	157	HIS
12	L	6	ASN
12	L	117	ASN
13	M	129	ASN
14	N	49	HIS
14	N	51	GLN
15	O	95	ASN
15	O	196	ASN
16	P	3	HIS
16	P	97	ASN
17	Q	110	HIS
17	Q	145	HIS
17	Q	155	GLN
18	R	137	ASN
18	R	169	ASN
20	T	75	ASN
21	U	49	ASN
23	W	14	HIS
24	X	111	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	Y	21	HIS
25	Y	77	HIS
25	Y	117	GLN
26	Z	11	GLN
26	Z	60	HIS
26	Z	114	HIS
27	a	33	ASN
27	a	42	HIS
28	b	6	ASN
29	c	139	HIS
29	c	215	ASN
30	d	261	HIS
30	d	274	GLN
30	d	352	GLN
30	d	378	GLN
32	f	120	ASN
33	g	28	GLN
34	h	7	GLN
34	h	13	HIS
34	h	123	ASN
39	m	37	HIS
40	n	74	HIS
42	p	145	ASN
42	p	237	HIS
42	p	306	GLN
43	q	90	ASN
43	q	109	ASN
44	r	59	HIS
44	r	82	GLN
45	s	35	GLN
45	s	39	GLN
45	s	201	HIS
46	t	60	ASN
47	u	120	GLN
47	u	185	ASN
47	u	226	GLN
47	u	245	ASN
48	v	111	HIS
48	v	123	GLN
49	w	77	GLN
50	0	75	ASN
50	0	102	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	0	104	HIS
50	0	151	ASN
51	1	5	HIS
51	1	33	HIS
51	1	68	HIS
51	1	142	HIS
51	1	230	ASN
51	1	231	HIS
53	3	10	ASN
53	3	15	GLN
53	3	180	GLN
54	4	34	HIS
54	4	178	GLN
54	4	196	GLN
55	5	88	ASN
56	6	3	ASN
56	6	122	HIS
56	6	130	GLN
57	7	10	HIS
57	7	75	HIS
57	7	149	HIS
57	7	195	ASN
57	7	233	ASN
57	7	298	HIS
57	7	301	ASN
58	8	27	ASN
58	8	47	ASN
58	8	50	HIS
59	AC	129	HIS
59	AC	149	GLN
59	AC	168	GLN
59	AC	200	ASN
60	AD	101	HIS
61	AE	20	GLN
61	AE	65	ASN
61	AE	107	HIS
62	AG	78	ASN
62	AG	123	HIS
63	AH	13	ASN
63	AH	36	HIS
63	AH	84	ASN
63	AH	87	HIS

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Mol	Chain	Res	Type
64	AI	51	ASN
64	AI	55	HIS
64	AI	86	HIS
65	AJ	56	HIS
66	AK	38	ASN
66	AK	80	GLN
66	AK	100	GLN
66	AK	103	HIS
68	AM	12	HIS
68	AM	86	ASN
68	AM	126	HIS
68	AM	136	HIS
69	AN	165	ASN
70	AO	46	HIS
70	AO	66	HIS
71	AP	112	ASN
71	AP	217	HIS
72	AQ	89	HIS
73	AR	23	HIS
74	AS	73	GLN
74	AS	77	ASN
74	AS	110	HIS
75	AT	4	GLN
75	AT	27	GLN
75	AT	95	ASN
77	AW	86	HIS
78	AX	111	ASN
78	AX	144	GLN
80	AZ	39	ASN
80	AZ	42	GLN
80	AZ	63	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1591/1781 (89%)	282 (17%)	1 (0%)
2	B	1058/1465 (72%)	162 (15%)	7 (0%)
3	C	160/262 (61%)	24 (15%)	1 (0%)
4	D	118/120 (98%)	10 (8%)	0
5	E	163/213 (76%)	20 (12%)	0
52	2	1801/2205 (81%)	656 (36%)	162 (8%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	F	70/73 (95%)	16 (22%)	1 (1%)
7	G	182/183 (99%)	18 (9%)	1 (0%)
8	H	89/127 (70%)	13 (14%)	0
All	All	5232/6429 (81%)	1201 (22%)	173 (3%)

All (1201) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	G
1	A	20	G
1	A	24	A
1	A	28	G
1	A	38	A
1	A	41	A
1	A	43	A
1	A	47	C
1	A	58	A
1	A	62	G
1	A	63	A
1	A	64	A
1	A	65	A
1	A	66	A
1	A	70	C
1	A	71	C
1	A	72	G
1	A	73	U
1	A	82	C
1	A	84	G
1	A	85	U
1	A	87	A
1	A	91	G
1	A	103	G
1	A	108	G
1	A	114	G
1	A	119	C
1	A	122	A
1	A	127	G
1	A	131	U
1	A	140	U
1	A	141	U
1	A	154	A
1	A	158	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	188	A
1	A	189	A
1	A	190	U
1	A	191	U
1	A	192	C
1	A	196	C
1	A	203	C
1	A	205	A
1	A	206	A
1	A	216	G
1	A	219	U
1	A	220	A
1	A	223	A
1	A	234	G
1	A	236	G
1	A	248	A
1	A	251	A
1	A	255	G
1	A	256	U
1	A	258	A
1	A	267	A
1	A	279	G
1	A	280	A
1	A	281	G
1	A	323	U
1	A	332	A
1	A	336	U
1	A	342	G
1	A	343	U
1	A	367	A
1	A	368	G
1	A	369	A
1	A	372	A
1	A	376	A
1	A	391	A
1	A	410	U
1	A	411	U
1	A	413	A
1	A	415	A
1	A	417	G
1	A	426	A
1	A	428	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	440	A
1	A	443	A
1	A	444	C
1	A	454	U
1	A	463	C
1	A	464	A
1	A	477	C
1	A	485	A
1	A	486	C
1	A	488	G
1	A	493	A
1	A	494	A
1	A	506	G
1	A	520	G
1	A	523	G
1	A	536	G
1	A	539	C
1	A	541	A
1	A	546	G
1	A	547	U
1	A	551	A
1	A	554	A
1	A	555	U
1	A	557	U
1	A	558	U
1	A	569	G
1	A	570	A
1	A	571	A
1	A	572	A
1	A	573	U
1	A	575	A
1	A	582	U
1	A	583	A
1	A	584	U
1	A	588	A
1	A	611	C
1	A	612	G
1	A	617	G
1	A	621	U
1	A	625	C
1	A	632	A
1	A	641	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	644	G
1	A	668	C
1	A	681	A
1	A	692	A
1	A	709	A
1	A	716	A
1	A	719	U
1	A	720	A
1	A	721	U
1	A	726	G
1	A	729	A
1	A	735	U
1	A	748	A
1	A	750	G
1	A	753	A
1	A	754	G
1	A	759	A
1	A	760	A
1	A	761	U
1	A	762	A
1	A	763	U
1	A	769	U
1	A	770	G
1	A	771	U
1	A	800	U
1	A	803	C
1	A	828	U
1	A	832	G
1	A	836	G
1	A	850	G
1	A	868	A
1	A	888	A
1	A	902	C
1	A	912	C
1	A	925	U
1	A	930	U
1	A	931	G
1	A	948	U
1	A	958	G
1	A	959	G
1	A	960	A
1	A	965	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	966	A
1	A	967	G
1	A	968	A
1	A	975	G
1	A	988	G
1	A	995	C
1	A	1004	G
1	A	1005	U
1	A	1011	U
1	A	1012	C
1	A	1025	G
1	A	1029	G
1	A	1030	U
1	A	1031	A
1	A	1032	G
1	A	1033	A
1	A	1045	G
1	A	1092	U
1	A	1098	A
1	A	1114	A
1	A	1116	A
1	A	1122	U
1	A	1123	G
1	A	1128	A
1	A	1132	A
1	A	1133	A
1	A	1134	C
1	A	1135	U
1	A	1141	G
1	A	1148	A
1	A	1150	A
1	A	1151	A
1	A	1155	A
1	A	1156	A
1	A	1160	G
1	A	1161	A
1	A	1174	G
1	A	1188	G
1	A	1200	A
1	A	1201	U
1	A	1211	A
1	A	1217	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1218	A
1	A	1225	U
1	A	1235	A
1	A	1238	C
1	A	1240	U
1	A	1242	U
1	A	1254	C
1	A	1257	U
1	A	1261	U
1	A	1263	A
1	A	1270	U
1	A	1271	G
1	A	1349	A
1	A	1367	U
1	A	1369	G
1	A	1371	U
1	A	1375	G
1	A	1378	U
1	A	1379	A
1	A	1389	A
1	A	1390	G
1	A	1392	G
1	A	1393	G
1	A	1394	U
1	A	1401	U
1	A	1404	U
1	A	1412	G
1	A	1413	U
1	A	1420	G
1	A	1422	A
1	A	1426	A
1	A	1440	A
1	A	1445	U
1	A	1446	A
1	A	1447	G
1	A	1466	G
1	A	1467	G
1	A	1468	C
1	A	1472	G
1	A	1490	A
1	A	1492	G
1	A	1506	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1509	G
1	A	1521	G
1	A	1523	G
1	A	1525	A
1	A	1526	G
1	A	1528	U
1	A	1529	C
1	A	1542	G
1	A	1547	G
1	A	1559	A
1	A	1571	U
1	A	1588	G
1	A	1591	C
1	A	1617	C
1	A	1618	U
1	A	1630	U
1	A	1633	U
1	A	1634	C
1	A	1647	C
1	A	1656	A
1	A	1663	U
1	A	1664	G
1	A	1665	U
1	A	1668	G
1	A	1669	G
1	A	1670	A
1	A	1671	A
1	A	1679	G
1	A	1680	U
1	A	1726	C
1	A	1727	U
1	A	1741	A
1	A	1746	A
1	A	1747	C
1	A	1749	U
1	A	1764	A
1	A	1766	A
1	A	1768	G
2	B	22	U
2	B	24	A
2	B	28	C
2	B	30	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	60	C
2	B	61	A
2	B	62	U
2	B	68	A
2	B	71	G
2	B	74	C
2	B	79	A
2	B	89	G
2	B	96	A
2	B	283	C
2	B	297	U
2	B	300	C
2	B	305	G
2	B	314	A
2	B	327	A
2	B	328	A
2	B	332	A
2	B	341	A
2	B	352	U
2	B	353	G
2	B	390	A
2	B	391	A
2	B	408	U
2	B	427	A
2	B	432	G
2	B	439	A
2	B	455	G
2	B	456	G
2	B	462	A
2	B	464	A
2	B	481	U
2	B	490	G
2	B	491	C
2	B	493	U
2	B	496	A
2	B	498	G
2	B	517	U
2	B	519	U
2	B	530	U
2	B	548	U
2	B	556	A
2	B	558	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	576	G
2	B	580	A
2	B	585	A
2	B	586	G
2	B	587	A
2	B	594	U
2	B	595	G
2	B	598	U
2	B	607	A
2	B	618	G
2	B	625	G
2	B	697	U
2	B	698	A
2	B	706	A
2	B	714	A
2	B	739	G
2	B	740	C
2	B	741	U
2	B	742	G
2	B	900	A
2	B	942	G
2	B	946	U
2	B	947	G
2	B	948	U
2	B	949	U
2	B	955	A
2	B	969	G
2	B	970	G
2	B	977	G
2	B	1014	G
2	B	1015	U
2	B	1018	U
2	B	1019	A
2	B	1020	A
2	B	1037	A
2	B	1039	A
2	B	1040	G
2	B	1044	U
2	B	1052	A
2	B	1054	A
2	B	1059	A
2	B	1067	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	1068	A
2	B	1075	U
2	B	1077	G
2	B	1082	A
2	B	1083	C
2	B	1092	G
2	B	1093	U
2	B	1117	G
2	B	1119	C
2	B	1125	A
2	B	1135	A
2	B	1143	G
2	B	1152	A
2	B	1170	G
2	B	1173	A
2	B	1174	G
2	B	1175	A
2	B	1177	U
2	B	1184	C
2	B	1188	G
2	B	1191	A
2	B	1195	C
2	B	1213	G
2	B	1218	C
2	B	1219	A
2	B	1234	U
2	B	1245	G
2	B	1246	A
2	B	1249	U
2	B	1261	A
2	B	1268	C
2	B	1273	C
2	B	1278	G
2	B	1309	C
2	B	1310	A
2	B	1316	C
2	B	1321	G
2	B	1322	C
2	B	1328	U
2	B	1345	A
2	B	1357	C
2	B	1364	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	1366	G
2	B	1369	G
2	B	1372	A
2	B	1373	A
2	B	1377	C
2	B	1379	A
2	B	1382	A
2	B	1384	A
2	B	1385	A
2	B	1386	G
2	B	1387	A
2	B	1388	U
2	B	1389	U
2	B	1390	A
2	B	1391	U
2	B	1392	C
2	B	1398	A
2	B	1399	A
2	B	1404	G
2	B	1410	G
2	B	1412	C
2	B	1414	G
2	B	1423	U
2	B	1436	C
2	B	1437	G
2	B	1439	U
2	B	1440	G
2	B	1449	U
2	B	1450	U
2	B	1451	G
2	B	1452	G
2	B	1456	U
3	C	103	A
3	C	113	U
3	C	137	G
3	C	138	C
3	C	140	G
3	C	150	A
3	C	153	A
3	C	154	G
3	C	162	A
3	C	173	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	175	U
3	C	177	U
3	C	178	A
3	C	179	A
3	C	185	C
3	C	187	A
3	C	194	A
3	C	196	C
3	C	201	A
3	C	202	C
3	C	210	G
3	C	215	A
3	C	226	A
3	C	248	U
4	D	8	G
4	D	34	U
4	D	50	A
4	D	51	A
4	D	54	U
4	D	65	A
4	D	98	G
4	D	101	A
4	D	111	G
4	D	120	C
5	E	31	C
5	E	49	G
5	E	99	G
5	E	106	U
5	E	107	U
5	E	108	A
5	E	121	U
5	E	122	U
5	E	146	A
5	E	147	A
5	E	148	A
5	E	179	U
5	E	180	G
5	E	189	G
5	E	192	U
5	E	193	U
5	E	196	A
5	E	199	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	207	G
5	E	210	G
6	F	15	C
6	F	24	C
6	F	31	U
6	F	33	G
6	F	42	A
6	F	43	A
6	F	44	G
6	F	52	G
6	F	53	U
6	F	55	U
6	F	64	U
6	F	67	C
6	F	68	A
6	F	69	A
6	F	72	A
6	F	73	A
7	G	8	U
7	G	40	G
7	G	77	U
7	G	84	U
7	G	86	U
7	G	102	G
7	G	106	G
7	G	107	U
7	G	120	U
7	G	121	C
7	G	122	G
7	G	128	U
7	G	144	G
7	G	158	A
7	G	159	G
7	G	170	G
7	G	171	U
7	G	173	C
8	H	10	C
8	H	14	C
8	H	19	G
8	H	23	A
8	H	24	U
8	H	25	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	33	U
8	H	70	G
8	H	93	U
8	H	94	G
8	H	101	G
8	H	104	G
8	H	117	U
52	2	2	A
52	2	3	U
52	2	4	C
52	2	6	G
52	2	11	A
52	2	14	C
52	2	15	U
52	2	17	C
52	2	18	C
52	2	22	A
52	2	23	G
52	2	26	A
52	2	33	U
52	2	34	G
52	2	39	A
52	2	42	G
52	2	43	A
52	2	44	C
52	2	45	U
52	2	46	U
52	2	47	A
52	2	48	G
52	2	56	U
52	2	57	G
52	2	59	C
52	2	61	C
52	2	62	A
52	2	65	A
52	2	66	U
52	2	67	C
52	2	68	A
52	2	69	C
52	2	72	C
52	2	74	U
52	2	75	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	77	G
52	2	78	C
52	2	79	A
52	2	80	G
52	2	81	G
52	2	82	A
52	2	83	A
52	2	84	U
52	2	85	C
52	2	90	C
52	2	91	A
52	2	97	C
52	2	101	A
52	2	102	C
52	2	112	A
52	2	113	A
52	2	115	C
52	2	117	G
52	2	122	A
52	2	125	A
52	2	126	A
52	2	128	C
52	2	129	U
52	2	138	C
52	2	141	C
52	2	144	A
52	2	145	A
52	2	146	U
52	2	147	U
52	2	150	A
52	2	151	U
52	2	158	G
52	2	161	A
52	2	163	A
52	2	164	C
52	2	165	G
52	2	168	A
52	2	171	C
52	2	183	C
52	2	184	C
52	2	185	A
52	2	189	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	192	U
52	2	194	U
52	2	195	U
52	2	197	U
52	2	198	C
52	2	199	C
52	2	200	A
52	2	227	U
52	2	228	G
52	2	230	G
52	2	238	G
52	2	249	A
52	2	250	C
52	2	251	A
52	2	252	G
52	2	253	U
52	2	254	A
52	2	255	A
52	2	256	A
52	2	257	A
52	2	258	C
52	2	268	C
52	2	269	A
52	2	270	C
52	2	271	U
52	2	275	A
52	2	277	U
52	2	278	A
52	2	281	A
52	2	285	A
52	2	287	C
52	2	288	A
52	2	290	U
52	2	291	G
52	2	294	G
52	2	308	C
52	2	309	G
52	2	310	U
52	2	311	G
52	2	313	G
52	2	314	A
52	2	317	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	320	G
52	2	321	G
52	2	322	C
52	2	323	U
52	2	324	U
52	2	326	U
52	2	327	U
52	2	328	C
52	2	332	C
52	2	346	C
52	2	348	A
52	2	349	C
52	2	352	C
52	2	355	U
52	2	358	C
52	2	360	G
52	2	363	G
52	2	364	G
52	2	365	U
52	2	366	G
52	2	367	A
52	2	381	G
52	2	382	A
52	2	395	U
52	2	403	G
52	2	404	C
52	2	413	A
52	2	417	U
52	2	418	U
52	2	431	G
52	2	433	G
52	2	442	A
52	2	443	A
52	2	445	U
52	2	447	G
52	2	449	U
52	2	459	A
52	2	461	G
52	2	464	G
52	2	467	C
52	2	468	A
52	2	469	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	477	G
52	2	478	C
52	2	482	U
52	2	484	G
52	2	485	C
52	2	487	C
52	2	497	A
52	2	498	C
52	2	501	A
52	2	502	A
52	2	503	C
52	2	504	G
52	2	512	A
52	2	516	A
52	2	518	A
52	2	523	A
52	2	524	U
52	2	525	A
52	2	552	U
52	2	553	U
52	2	555	C
52	2	558	U
52	2	559	G
52	2	560	G
52	2	565	U
52	2	566	A
52	2	570	A
52	2	577	U
52	2	578	C
52	2	579	C
52	2	580	A
52	2	581	A
52	2	582	U
52	2	585	C
52	2	587	A
52	2	588	G
52	2	589	U
52	2	590	A
52	2	591	A
52	2	592	C
52	2	600	G
52	2	604	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	605	A
52	2	606	G
52	2	607	U
52	2	608	C
52	2	610	G
52	2	613	G
52	2	614	C
52	2	615	C
52	2	617	G
52	2	623	G
52	2	627	U
52	2	628	A
52	2	629	A
52	2	631	U
52	2	633	C
52	2	643	A
52	2	644	G
52	2	657	C
52	2	659	G
52	2	660	U
52	2	662	G
52	2	668	A
52	2	669	A
52	2	671	G
52	2	672	G
52	2	673	G
52	2	688	G
52	2	689	U
52	2	690	G
52	2	697	G
52	2	710	U
52	2	717	C
52	2	723	C
52	2	724	A
52	2	725	U
52	2	726	G
52	2	727	U
52	2	728	C
52	2	729	G
52	2	730	G
52	2	733	U
52	2	734	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	735	G
52	2	736	G
52	2	737	U
52	2	738	G
52	2	739	A
52	2	742	C
52	2	743	A
52	2	745	G
52	2	746	C
52	2	747	C
52	2	748	C
52	2	749	U
52	2	750	U
52	2	751	G
52	2	760	G
52	2	761	A
52	2	762	A
52	2	763	C
52	2	768	A
52	2	769	A
52	2	770	A
52	2	771	G
52	2	772	A
52	2	773	A
52	2	778	G
52	2	780	A
52	2	781	A
52	2	784	C
52	2	788	A
52	2	790	U
52	2	791	G
52	2	793	U
52	2	794	U
52	2	832	C
52	2	839	G
52	2	844	U
52	2	853	A
52	2	854	C
52	2	856	A
52	2	866	G
52	2	867	A
52	2	872	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	875	A
52	2	876	G
52	2	879	A
52	2	881	U
52	2	882	U
52	2	883	G
52	2	884	A
52	2	886	U
52	2	887	U
52	2	888	G
52	2	890	A
52	2	912	A
52	2	913	G
52	2	914	G
52	2	915	A
52	2	916	G
52	2	917	C
52	2	918	A
52	2	919	G
52	2	920	C
52	2	930	A
52	2	931	C
52	2	936	U
52	2	937	C
52	2	938	G
52	2	939	G
52	2	940	C
52	2	941	U
52	2	942	U
52	2	945	G
52	2	961	U
52	2	964	U
52	2	970	U
52	2	971	U
52	2	972	A
52	2	974	G
52	2	975	G
52	2	1093	C
52	2	1097	C
52	2	1099	C
52	2	1101	A
52	2	1103	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1104	A
52	2	1105	A
52	2	1106	U
52	2	1107	G
52	2	1109	A
52	2	1119	U
52	2	1120	U
52	2	1121	C
52	2	1123	G
52	2	1129	A
52	2	1130	A
52	2	1133	U
52	2	1139	G
52	2	1145	A
52	2	1159	U
52	2	1160	A
52	2	1161	G
52	2	1162	A
52	2	1165	G
52	2	1166	C
52	2	1168	C
52	2	1173	A
52	2	1175	G
52	2	1180	A
52	2	1181	C
52	2	1182	A
52	2	1187	A
52	2	1189	G
52	2	1191	A
52	2	1192	U
52	2	1197	C
52	2	1198	A
52	2	1199	A
52	2	1206	C
52	2	1207	U
52	2	1213	A
52	2	1239	A
52	2	1240	A
52	2	1242	A
52	2	1244	G
52	2	1250	A
52	2	1251	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1252	A
52	2	1268	C
52	2	1272	A
52	2	1273	A
52	2	1275	C
52	2	1279	G
52	2	1287	U
52	2	1293	G
52	2	1299	C
52	2	1378	U
52	2	1379	A
52	2	1399	A
52	2	1402	G
52	2	1416	A
52	2	1434	C
52	2	1438	A
52	2	1443	U
52	2	1444	U
52	2	1445	U
52	2	1446	G
52	2	1447	A
52	2	1450	U
52	2	1451	U
52	2	1452	A
52	2	1454	A
52	2	1462	G
52	2	1463	G
52	2	1466	G
52	2	1467	A
52	2	1492	A
52	2	1504	G
52	2	1508	G
52	2	1509	G
52	2	1512	C
52	2	1514	A
52	2	1516	A
52	2	1517	A
52	2	1518	G
52	2	1519	A
52	2	1522	U
52	2	1524	G
52	2	1525	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1528	G
52	2	1529	U
52	2	1530	G
52	2	1531	C
52	2	1536	U
52	2	1537	A
52	2	1539	U
52	2	1540	U
52	2	1545	U
52	2	1547	A
52	2	1548	A
52	2	1549	C
52	2	1550	A
52	2	1551	C
52	2	1552	G
52	2	1553	G
52	2	1554	G
52	2	1555	G
52	2	1556	A
52	2	1557	A
52	2	1558	C
52	2	1559	U
52	2	1560	U
52	2	1562	A
52	2	1568	U
52	2	1571	G
52	2	1573	A
52	2	1575	A
52	2	1576	G
52	2	1577	G
52	2	1580	G
52	2	1581	A
52	2	1582	G
52	2	1583	G
52	2	1584	A
52	2	1585	U
52	2	1587	G
52	2	1597	G
52	2	1598	U
52	2	1599	G
52	2	1601	U
52	2	1605	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1607	U
52	2	1608	C
52	2	1609	G
52	2	1610	A
52	2	1611	U
52	2	1612	U
52	2	1619	A
52	2	1622	G
52	2	1623	U
52	2	1624	G
52	2	1627	G
52	2	1628	C
52	2	1629	A
52	2	1638	U
52	2	1639	U
52	2	1640	U
52	2	1655	U
52	2	1660	U
52	2	1661	U
52	2	1668	U
52	2	1669	U
52	2	1675	A
52	2	1686	U
52	2	1687	C
52	2	1700	U
52	2	1701	A
52	2	1711	A
52	2	1712	U
52	2	1774	A
52	2	1776	U
52	2	1777	C
52	2	1783	U
52	2	1786	G
52	2	1790	U
52	2	1791	U
52	2	1792	C
52	2	1793	C
52	2	1795	U
52	2	1796	U
52	2	1797	G
52	2	1801	U
52	2	1802	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1809	G
52	2	1812	G
52	2	1813	A
52	2	1814	A
52	2	1815	A
52	2	1816	U
52	2	1817	U
52	2	1818	U
52	2	1826	C
52	2	1828	G
52	2	1830	A
52	2	1831	G
52	2	1835	U
52	2	1836	G
52	2	1838	G
52	2	1839	A
52	2	1842	C
52	2	1844	C
52	2	1846	U
52	2	1847	C
52	2	1848	A
52	2	1849	A
52	2	1850	U
52	2	1851	G
52	2	1854	C
52	2	1855	U
52	2	1861	A
52	2	1862	C
52	2	1863	A
52	2	1864	C
52	2	1865	G
52	2	1866	C
52	2	1867	G
52	2	1874	A
52	2	1875	A
52	2	1876	U
52	2	1877	G
52	2	1878	U
52	2	1879	C
52	2	1880	A
52	2	1881	G
52	2	1882	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1883	G
52	2	1884	A
52	2	1885	G
52	2	1887	A
52	2	1888	C
52	2	1890	A
52	2	1895	A
52	2	1896	A
52	2	1897	C
52	2	1898	G
52	2	1899	A
52	2	1908	C
52	2	1909	C
52	2	1912	C
52	2	1913	U
52	2	1914	U
52	2	1915	G
52	2	1916	A
52	2	1917	U
52	2	1918	C
52	2	1919	A
52	2	1920	A
52	2	1921	A
52	2	1929	G
52	2	1931	A
52	2	1932	A
52	2	1933	A
52	2	1934	C
52	2	1935	C
52	2	1936	C
52	2	1938	G
52	2	1942	C
52	2	1943	A
52	2	1944	U
52	2	1945	A
52	2	1946	G
52	2	1947	A
52	2	1948	C
52	2	1949	U
52	2	1950	C
52	2	1951	A
52	2	1952	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1953	U
52	2	1954	U
52	2	1955	G
52	2	1957	G
52	2	1959	C
52	2	1962	A
52	2	1963	G
52	2	1968	G
52	2	1969	C
52	2	1971	A
52	2	1974	A
52	2	1976	U
52	2	1977	G
52	2	1978	G
52	2	1979	U
52	2	1980	C
52	2	1981	G
52	2	1982	C
52	2	1984	C
52	2	1985	A
52	2	1986	A
52	2	1988	G
52	2	1989	A
52	2	1990	G
52	2	1991	G
52	2	1997	C
52	2	1998	U
52	2	2000	G
52	2	2001	U
52	2	2007	C
52	2	2010	C
52	2	2011	U
52	2	2012	C
52	2	2013	A
52	2	2017	A
52	2	2018	A
52	2	2025	C
52	2	2028	U
52	2	2032	G
52	2	2035	C
52	2	2038	G
52	2	2042	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	2045	G
52	2	2047	A
52	2	2048	C
52	2	2049	A
52	2	2050	C
52	2	2051	A
52	2	2053	C
52	2	2054	G
52	2	2067	U
52	2	2074	A
52	2	2093	C
52	2	2095	G
52	2	2096	A
52	2	2098	A
52	2	2133	G
52	2	2158	A
52	2	2159	A
52	2	2160	G
52	2	2163	G
52	2	2164	U
52	2	2165	A
52	2	2169	A
52	2	2171	G
52	2	2172	U
52	2	2183	G
52	2	2185	A
52	2	2186	C
52	2	2195	G
52	2	2196	G
52	2	2197	A
52	2	2199	C
52	2	2202	U
52	2	2203	U

All (173) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1010	C
2	B	78	C
2	B	946	U
2	B	1173	A
2	B	1385	A

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	1390	A
2	B	1391	U
2	B	1450	U
3	C	174	A
6	F	72	A
7	G	143	C
52	2	42	G
52	2	44	C
52	2	46	U
52	2	47	A
52	2	56	U
52	2	65	A
52	2	68	A
52	2	74	U
52	2	78	C
52	2	83	A
52	2	91	A
52	2	112	A
52	2	114	U
52	2	125	A
52	2	128	C
52	2	144	A
52	2	146	U
52	2	182	A
52	2	194	U
52	2	196	C
52	2	198	C
52	2	226	G
52	2	250	C
52	2	251	A
52	2	252	G
52	2	253	U
52	2	254	A
52	2	256	A
52	2	257	A
52	2	268	C
52	2	270	C
52	2	274	C
52	2	276	G
52	2	277	U
52	2	287	C
52	2	289	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	290	U
52	2	297	U
52	2	325	G
52	2	348	A
52	2	363	G
52	2	364	G
52	2	366	G
52	2	402	A
52	2	460	C
52	2	554	U
52	2	564	A
52	2	579	C
52	2	580	A
52	2	581	A
52	2	586	G
52	2	591	A
52	2	604	A
52	2	709	C
52	2	716	U
52	2	724	A
52	2	726	G
52	2	761	A
52	2	762	A
52	2	767	C
52	2	770	A
52	2	772	A
52	2	780	A
52	2	783	A
52	2	787	G
52	2	790	U
52	2	880	U
52	2	885	C
52	2	886	U
52	2	887	U
52	2	913	G
52	2	914	G
52	2	915	A
52	2	917	C
52	2	918	A
52	2	930	A
52	2	935	U
52	2	937	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	963	U
52	2	970	U
52	2	1092	A
52	2	1098	U
52	2	1100	U
52	2	1103	G
52	2	1104	A
52	2	1106	U
52	2	1165	G
52	2	1271	C
52	2	1378	U
52	2	1443	U
52	2	1445	U
52	2	1516	A
52	2	1517	A
52	2	1521	G
52	2	1529	U
52	2	1536	U
52	2	1539	U
52	2	1547	A
52	2	1550	A
52	2	1553	G
52	2	1554	G
52	2	1555	G
52	2	1556	A
52	2	1572	G
52	2	1575	A
52	2	1576	G
52	2	1577	G
52	2	1580	G
52	2	1581	A
52	2	1606	C
52	2	1611	U
52	2	1623	U
52	2	1627	G
52	2	1628	C
52	2	1639	U
52	2	1699	G
52	2	1700	U
52	2	1789	A
52	2	1791	U
52	2	1792	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	2	1813	A
52	2	1816	U
52	2	1817	U
52	2	1829	C
52	2	1830	A
52	2	1835	U
52	2	1837	U
52	2	1841	G
52	2	1846	U
52	2	1849	A
52	2	1854	C
52	2	1861	A
52	2	1882	U
52	2	1889	A
52	2	1896	A
52	2	1897	C
52	2	1898	G
52	2	1917	U
52	2	1928	G
52	2	1930	G
52	2	1931	A
52	2	1937	C
52	2	1950	C
52	2	1952	C
52	2	1968	G
52	2	1981	G
52	2	1996	U
52	2	1997	C
52	2	2000	G
52	2	2006	G
52	2	2009	G
52	2	2011	U
52	2	2012	C
52	2	2024	C
52	2	2034	C
52	2	2046	U
52	2	2047	A
52	2	2050	C
52	2	2052	C
52	2	2053	C
52	2	2095	G
52	2	2164	U

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
52	2	2
77	AW	2
38	l	1
15	O	1
29	c	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1972:U	O3'	1973:U	P	6.52
1	2	1954:U	O3'	1955:G	P	2.07
1	AW	79:GLY	C	80:TYR	N	1.68
1	l	66:TYR	C	67:LEU	N	1.18
1	O	50:MET	C	51:LEU	N	1.15
1	c	246:ILE	C	247:ARG	N	1.01
1	AW	80:TYR	C	81:ARG	N	0.87

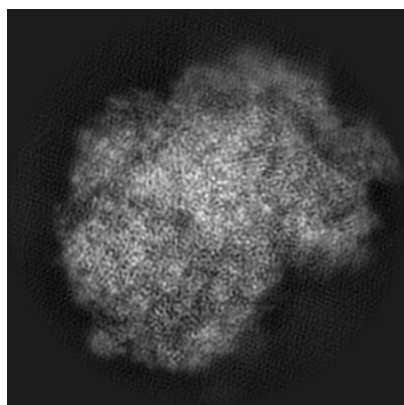
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8343. These allow visual inspection of the internal detail of the map and identification of artifacts.

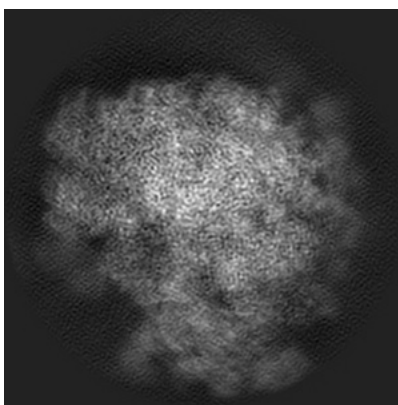
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

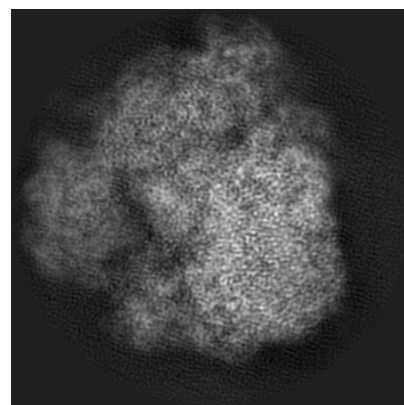
#### 6.1.1 Primary map



X



Y

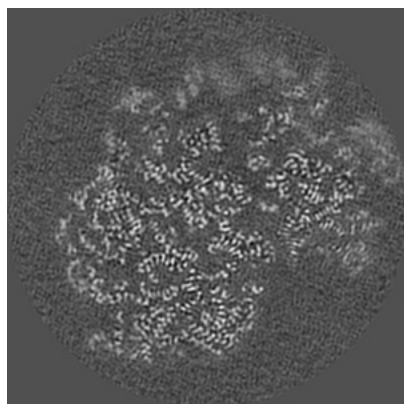


Z

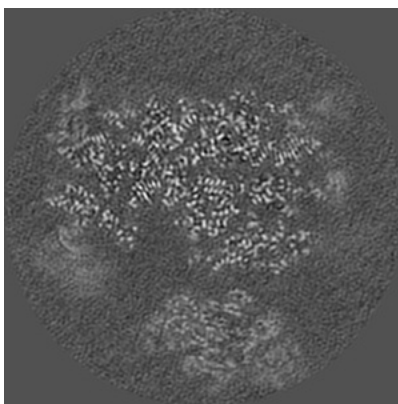
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

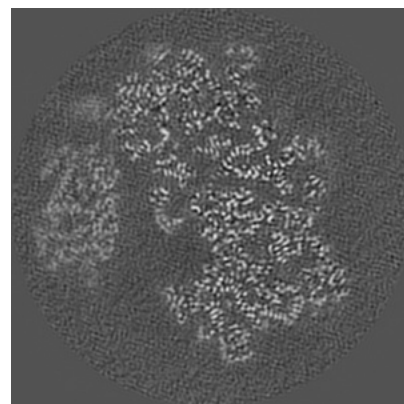
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

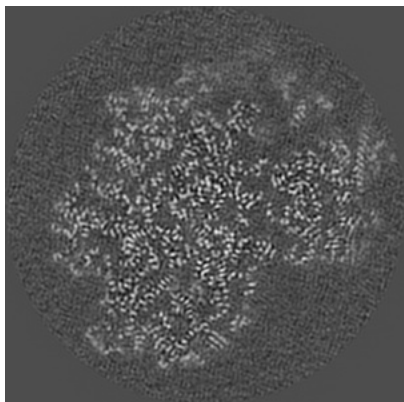


Z Index: 200

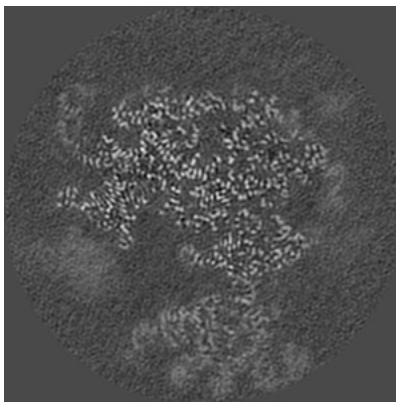
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

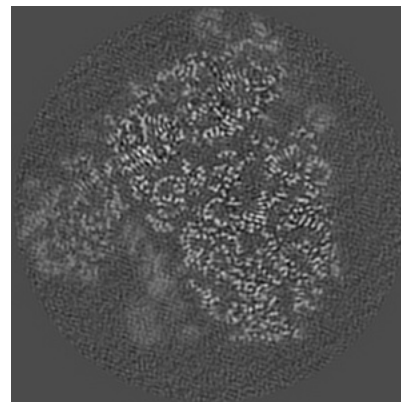
### 6.3.1 Primary map



X Index: 214



Y Index: 211

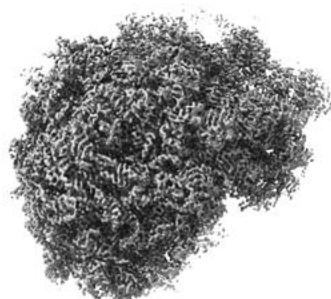


Z Index: 231

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

## 6.4 Orthogonal surface views [i](#)

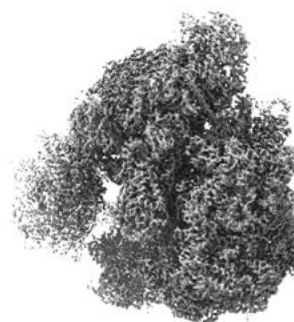
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

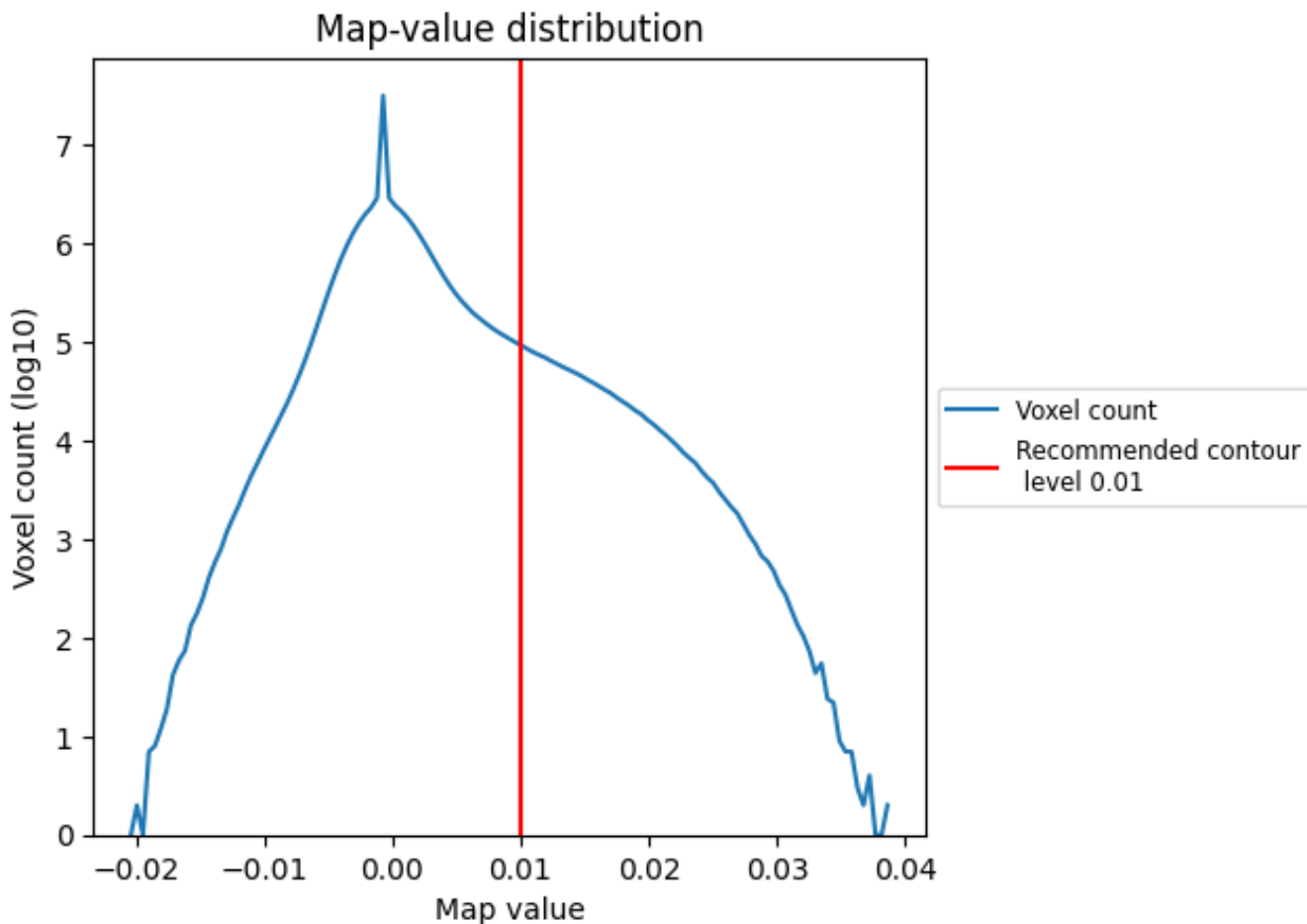
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

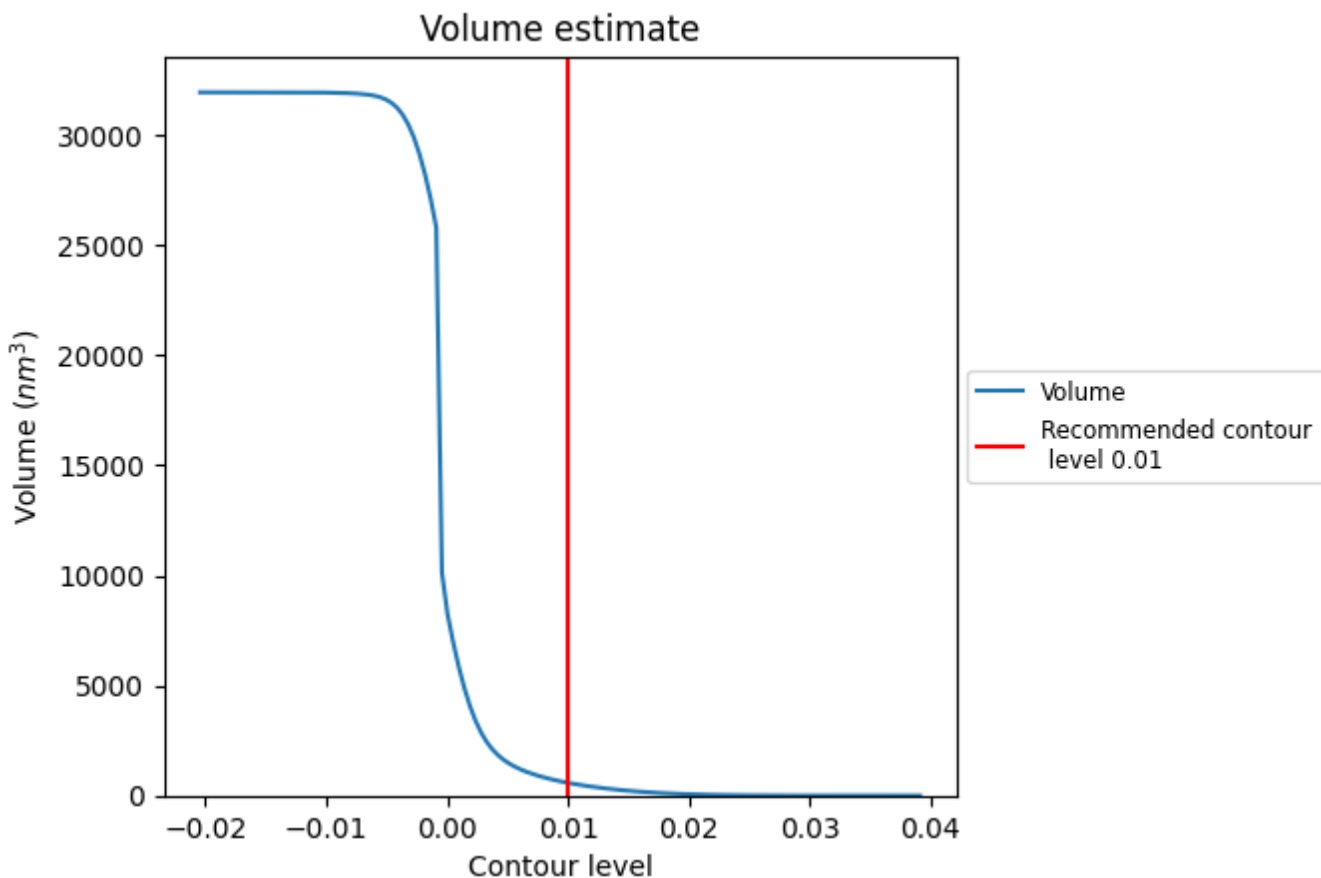
This section contains the results of statistical analysis of the map.

### 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](#)

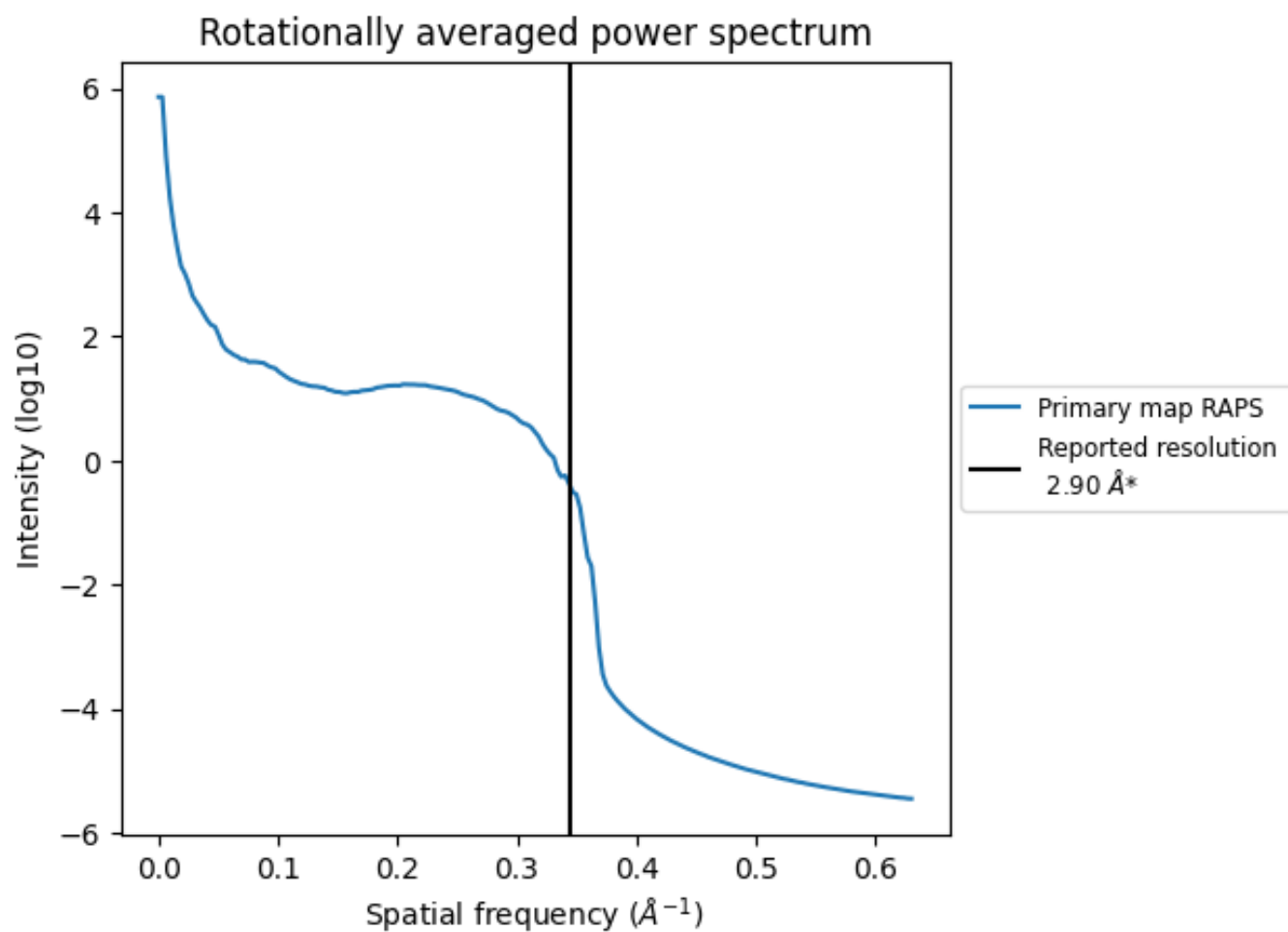


The volume at the recommended contour level is 580 nm<sup>3</sup>; this corresponds to an approximate mass of 524 kDa.

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 0.345 Å<sup>-1</sup>

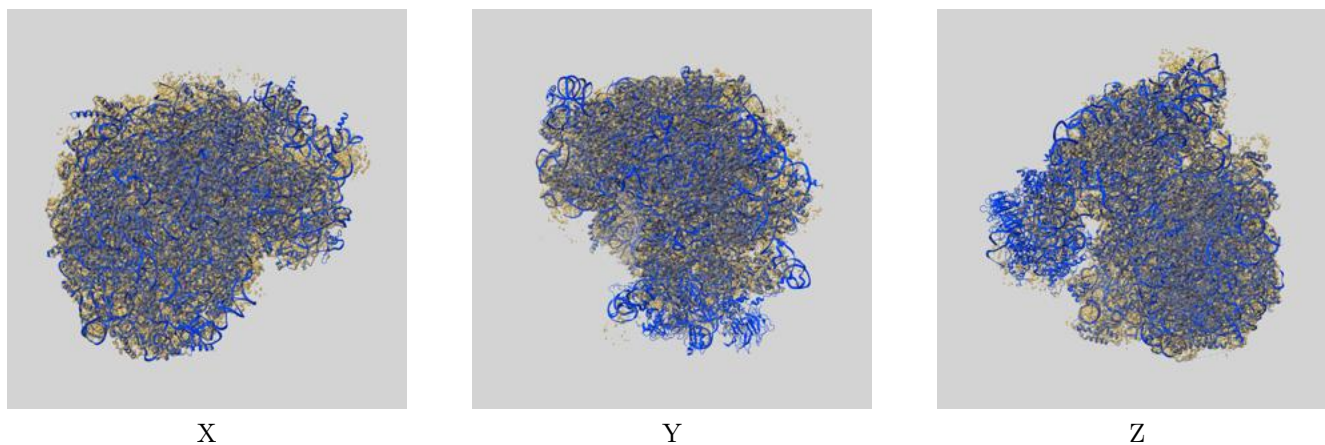
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

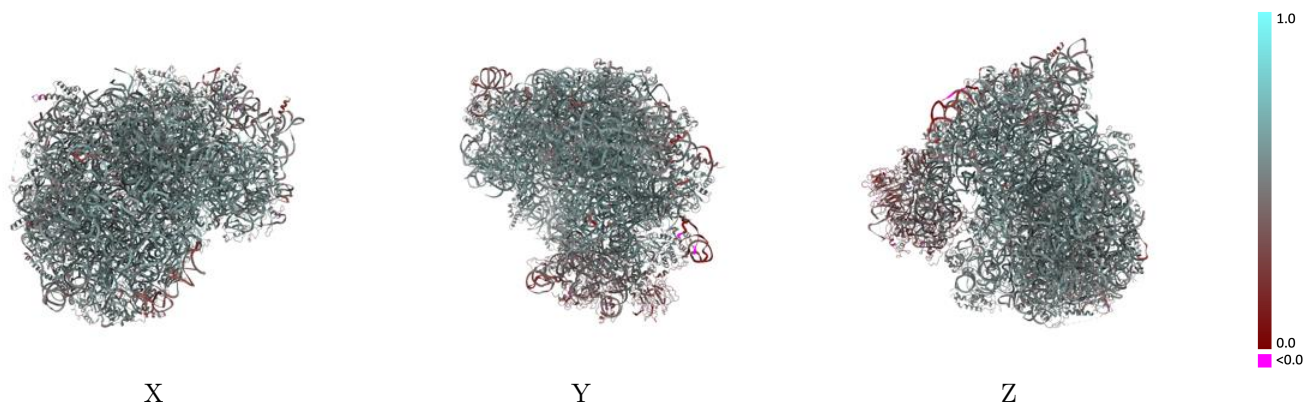
This section contains information regarding the fit between EMDB map EMD-8343 and PDB model 5T2A. Per-residue inclusion information can be found in section 3 on page 19.

### 9.1 Map-model overlay [i](#)



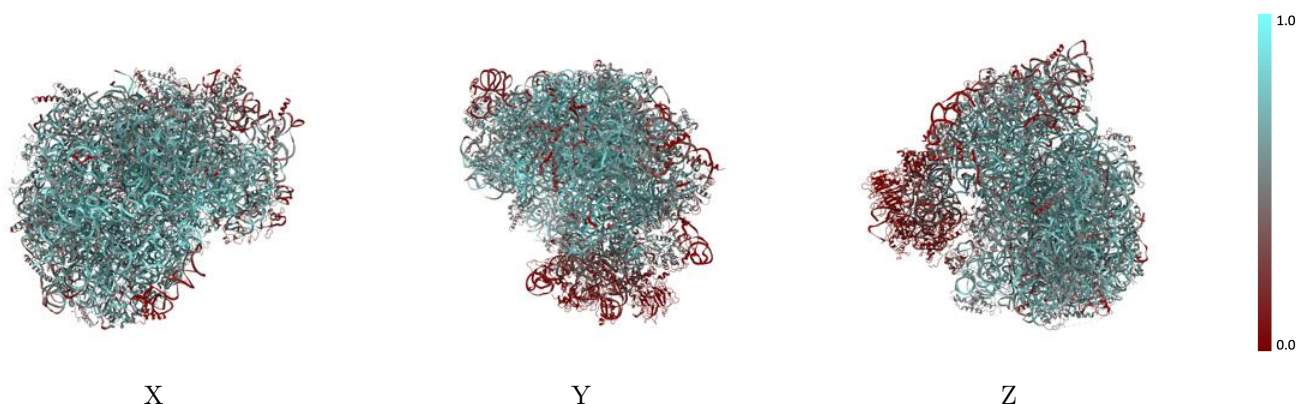
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



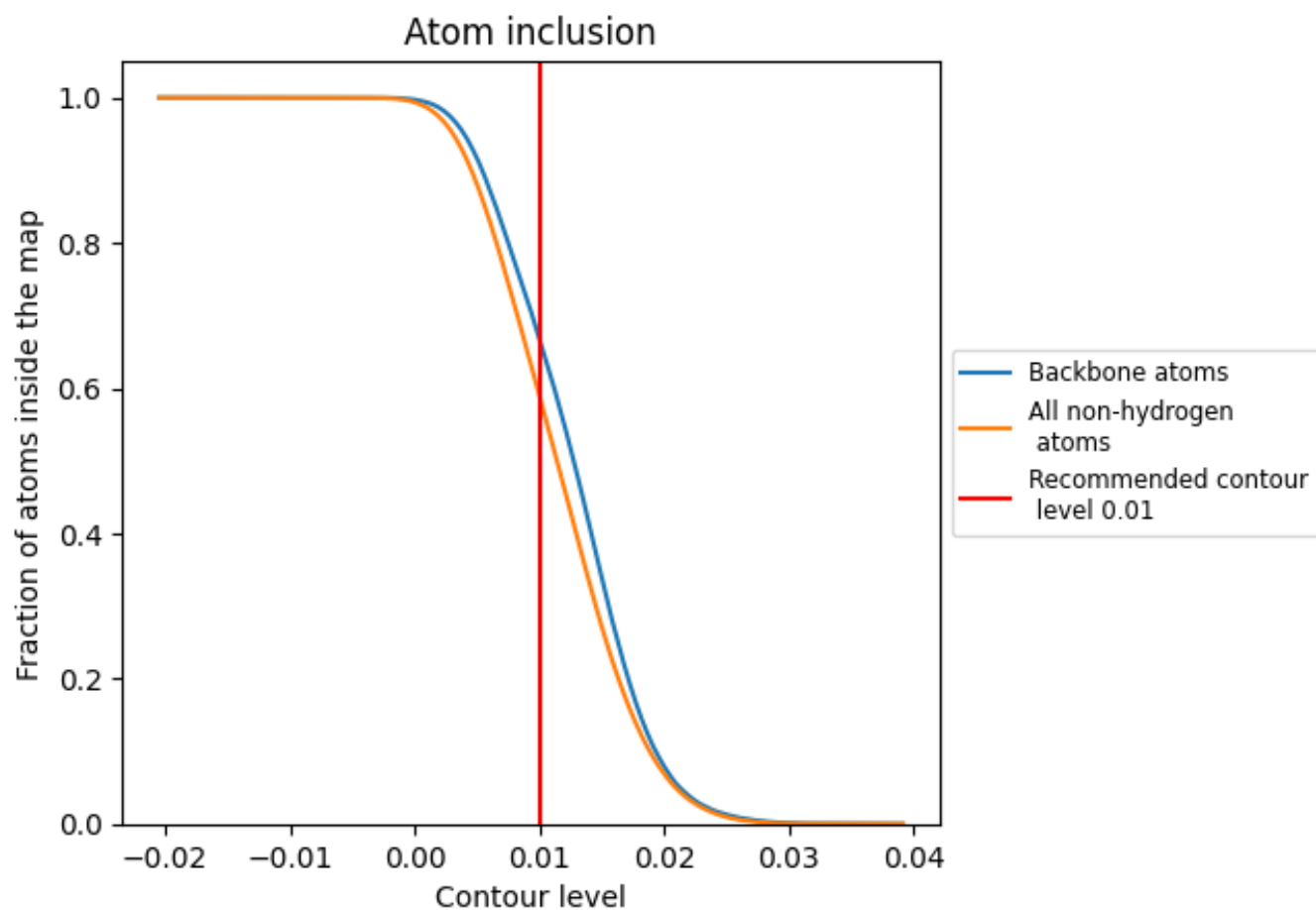
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 59% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5906	 0.5270
0	 0.4870	 0.5380
1	 0.5749	 0.5500
2	 0.5652	 0.5170
3	 0.3751	 0.4970
4	 0.4882	 0.5230
5	 0.6080	 0.5580
6	 0.5709	 0.5410
7	 0.0120	 0.3000
8	 0.1848	 0.4210
A	 0.7310	 0.5530
AC	 0.4354	 0.5100
AD	 0.0417	 0.3510
AE	 0.6514	 0.5800
AG	 0.6002	 0.5550
AH	 0.5066	 0.5350
AI	 0.0251	 0.3360
AJ	 0.6247	 0.5560
AK	 0.0971	 0.3800
AL	 0.1209	 0.4060
AM	 0.0602	 0.2810
AN	 0.0663	 0.4100
AO	 0.0933	 0.3020
AP	 0.5462	 0.5370
AQ	 0.0953	 0.3610
AR	 0.5048	 0.5220
AS	 0.5747	 0.5450
AT	 0.3946	 0.5170
AV	 0.4817	 0.5210
AW	 0.5064	 0.5350
AX	 0.1402	 0.4060
AY	 0.2779	 0.4900
AZ	 0.0828	 0.3970
B	 0.7220	 0.5550
C	 0.6959	 0.5260



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Chain	Atom inclusion	Q-score
D	 0.7294	 0.5450
E	 0.7225	 0.5630
F	 0.6247	 0.5290
G	 0.8077	 0.5870
H	 0.8136	 0.5920
I	 0.5681	 0.5280
J	 0.5369	 0.5240
K	 0.3566	 0.4740
L	 0.5427	 0.5060
M	 0.5964	 0.5520
N	 0.4571	 0.4860
O	 0.6253	 0.5490
P	 0.6678	 0.5560
Q	 0.6303	 0.5640
R	 0.5434	 0.5340
S	 0.5566	 0.5280
T	 0.4897	 0.5240
U	 0.6660	 0.5740
V	 0.5545	 0.5270
W	 0.6660	 0.5680
X	 0.5785	 0.5310
Y	 0.5476	 0.5340
Z	 0.6171	 0.5510
a	 0.5314	 0.5130
b	 0.5605	 0.5210
c	 0.6439	 0.5610
d	 0.6572	 0.5620
e	 0.5467	 0.5370
f	 0.6414	 0.5550
g	 0.5905	 0.5430
h	 0.5864	 0.5450
i	 0.5084	 0.5100
j	 0.6245	 0.5510
k	 0.4423	 0.4950
l	 0.6751	 0.5540
m	 0.6111	 0.5560
n	 0.5212	 0.5150
o	 0.6098	 0.5530
p	 0.5512	 0.5170
q	 0.6348	 0.5550
r	 0.5507	 0.5370
s	 0.4956	 0.5110

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Chain	Atom inclusion	Q-score
t	■ 0.5391	■ 0.5230
u	■ 0.5777	■ 0.5330
v	■ 0.4810	■ 0.5010
w	■ 0.6073	■ 0.5500