Full wwPDB EM Validation Report (i)

May 18, 2024 – 02:47 pm BST

PDB ID	:	6R6P
EMDB ID	:	EMD-4737
Title	:	Structure of XBP1u-paused ribosome nascent chain complex (rotated state)
Authors	:	Shanmuganathan, V.; Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2019-03-27
Resolution	:	3.10 Å(reported)

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

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

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

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

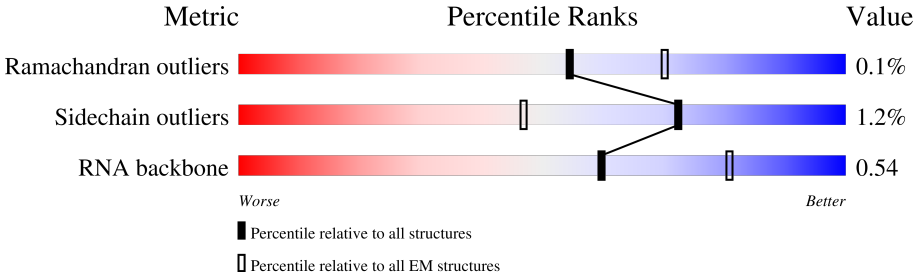
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	5	3662	16% 74% 23% •
2	7	120	• 85% 14% •
3	8	156	12% 72% 26% •
4	A	244	• 98% •
5	B	394	• 98% •
6	C	362	6% 99% •
7	D	292	8% 100%
8	E	248	20% 94% • 5%

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Mol	Chain	Length	Quality of chain
9	F	225	6% 100%
10	G	241	18% 98%
11	H	190	7% 99%
12	I	213	94%
13	J	169	11% 99%
14	L	210	15% 99%
15	M	138	6% 100%
16	N	203	100%
17	O	199	97%
18	P	153	99%
19	Q	187	100%
20	R	180	17% 98%
21	S	175	99%
22	T	159	8% 99%
23	U	99	15% 99%
24	V	131	99%
25	W	63	5% 98%
26	X	119	7% 99%
27	Y	134	7% 99%
28	Z	135	10% 98%
29	a	147	100%
30	b	75	24% 99%
31	c	94	6% 99%
32	d	107	9% 98%
33	e	128	99%

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Mol	Chain	Length	Quality of chain
34	f	109	5% 98%
35	g	114	7% 98%
36	h	122	6% 99%
37	i	102	11% 99%
38	j	86	98%
39	k	69	25% 99%
40	l	50	94% 6%
41	m	52	6% 100%
42	n	23	13% 100%
43	o	104	12% 96%
44	p	91	7% 98%
45	r	125	8% 95%
46	s	198	98% 99%
47	t	163	100% 98%
48	1	24	8% 96%
49	2	76	66% 67% 30%
50	3	75	27% 79% 20%
51	K	1698	18% 76% 22%
52	q	217	40% 100%
53	u	213	21% 99%
54	v	221	34% 99%
55	x	262	56% 99%
56	z	237	54% 99%
57	y	189	60% 97%
58	CC	206	39% 99%

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Mol	Chain	Length	Quality of chain
59	XX	185	53% 98%
60	EE	151	27% 93% 5%
61	QQ	149	28% 99%
62	MM	136	20% 99%
63	UU	142	54% 98%
64	YY	132	70% 100%
65	HH	83	45% 99%
66	TT	129	24% 100%
67	VV	141	8% 99%
68	NN	124	63% 99%
69	ZZ	101	23% 100%
70	JJ	83	41% 99%
71	AA	55	67% 96%
72	DD	228	62% 98%
73	BB	191	44% 97%
74	SS	96	73% 99%
75	RR	117	94% 99%
76	9	120	39% 98%
77	II	144	39% 99%
78	PP	141	50% 99%
79	GG	100	71% 99%
80	OO	75	55% 100%
81	FF	62	61% 98%
82	w	55	29% 100%
83	0	68	85% 99%

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Mol	Chain	Length	Quality of chain
84	6	313	94% 99%
85	4	10	10% 50% 50%

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 218067 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3662	78486	34947	14363	25515	3661	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	7	120	2558	1141	456	842	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	8	156	3314	1480	585	1094	155	0	0

- Molecule 4 is a protein called uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	244	1868	1171	382	309	6	0	0

- Molecule 5 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	394	3148	2007	591	537	13	0	0

- Molecule 6 is a protein called uL4.

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

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	292	2386	1509	437	426	14	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	236	1898	1215	362	318	3	0	0

- Molecule 9 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	225	1870	1202	358	301	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	175	ALA	THR	conflict	UNP G1SV32
F	185	GLY	ASN	conflict	UNP G1SV32
F	202	ARG	HIS	conflict	UNP G1SV32
F	233	GLU	GLY	conflict	UNP G1SV32

- Molecule 10 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	241	1934	1233	371	326	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	GLY	CYS	conflict	UNP G1STW0

- Molecule 11 is a protein called uL6.

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

- Molecule 12 is a protein called Ribosomal protein L10 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	204	1655	1051	319	272	13	0	0

- Molecule 13 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	J	169	1353	855	252	240	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	L	210	1703	1065	354	280	4	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	47	ALA	-	insertion	UNP G1TPV0
L	48	PRO	-	insertion	UNP G1TPV0
L	49	ARG	-	insertion	UNP G1TPV0
L	50	PRO	-	insertion	UNP G1TPV0
L	51	ALA	-	insertion	UNP G1TPV0
L	52	SER	-	insertion	UNP G1TPV0
L	53	GLY	-	insertion	UNP G1TPV0
L	54	PRO	-	insertion	UNP G1TPV0
L	55	LEU	-	insertion	UNP G1TPV0

- Molecule 15 is a protein called Ribosomal protein L14.

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

- Molecule 16 is a protein called Ribosomal protein L15.

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

- Molecule 17 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	O	199	1638	1056	321	256	5	0	0

- Molecule 18 is a protein called uL22.

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

- Molecule 19 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Q	187	1506	941	311	249	5	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	6	ARG	LEU	conflict	UNP G1TX70
Q	14	ARG	TRP	conflict	UNP G1TX70
Q	23	ILE	MET	conflict	UNP G1TX70
Q	24	TYR	CYS	conflict	UNP G1TX70
Q	38	ARG	HIS	conflict	UNP G1TX70
Q	57	ASN	LYS	conflict	UNP G1TX70
Q	66	MET	VAL	conflict	UNP G1TX70
Q	74	GLY	ASP	conflict	UNP G1TX70
Q	75	ARG	PRO	conflict	UNP G1TX70
Q	77	GLY	ASN	conflict	UNP G1TX70
Q	106	SER	THR	conflict	UNP G1TX70
Q	110	ARG	HIS	conflict	UNP G1TX70
Q	117	GLY	GLU	conflict	UNP G1TX70
Q	124	ASP	HIS	conflict	UNP G1TX70
Q	134	CYS	ARG	conflict	UNP G1TX70
Q	150	ARG	GLN	conflict	UNP G1TX70
Q	172	ARG	GLY	conflict	UNP G1TX70
Q	184	ARG	TRP	conflict	UNP G1TX70

- Molecule 20 is a protein called eL19.

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

- Molecule 21 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	S	175	1454	925	284	235	10	0	0

- Molecule 22 is a protein called eL21.

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

- Molecule 23 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	U	99	808	518	141	147	2	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	32	GLY	ARG	conflict	UNP G1TSG1
U	36	ALA	GLU	conflict	UNP G1TSG1
U	39	PHE	SER	conflict	UNP G1TSG1
U	54	GLY	ARG	conflict	UNP G1TSG1
U	60	VAL	ALA	conflict	UNP G1TSG1
U	97	ARG	HIS	conflict	UNP G1TSG1

- Molecule 24 is a protein called uL14.

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

- Molecule 25 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	W	63	528	337	103	85	3	0	0

- Molecule 26 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	119	976	624	183	168	1	0	0

- Molecule 27 is a protein called Ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called uL15.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	75	609	378	130	98	3	0	0

- Molecule 31 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	94	732	465	130	131	6	0	0

- Molecule 32 is a protein called eL31.

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

- Molecule 33 is a protein called eL32.

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

- Molecule 34 is a protein called eL33.

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

- Molecule 35 is a protein called eL34.

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

- Molecule 36 is a protein called uL29.

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

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

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

- Molecule 38 is a protein called Ribosomal protein L37.

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

- Molecule 39 is a protein called eL38.

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

- Molecule 40 is a protein called ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l	50	444	281	98	64	1	0	0

- Molecule 41 is a protein called eL40.

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

- Molecule 42 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	n	23	222	134	61	25	2	0	0

- Molecule 43 is a protein called eL42.

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

- Molecule 44 is a protein called ribosomal protein eL43.

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

- Molecule 45 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	r	125	1001	621	206	168	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	s	198	1523	969	265	280	9	0	0

- Molecule 47 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	t	163	1238	773	230	230	5	0	0

- Molecule 48 is a protein called X-box-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	1	24	204	137	35	30	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	255	ALA	SER	conflict	UNP P17861

- Molecule 49 is a RNA chain called A/P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	2	76	1614	722	287	530	75	0	0

- Molecule 50 is a RNA chain called P/E-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	3	75	1597	714	287	522	74	0	0

- Molecule 51 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	K	1698	36248	16180	6508	11863	1697	0	0

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called 40S ribosomal protein S3a.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called 40S ribosomal protein S4.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	25	GLY	SER	conflict	UNP G1TK17
x	51	ARG	LYS	conflict	UNP G1TK17
x	78	THR	ALA	conflict	UNP G1TK17
x	156	VAL	MET	conflict	UNP G1TK17

- Molecule 56 is a protein called 40S ribosomal protein S6.

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

- Molecule 57 is a protein called 40S ribosomal protein S7.

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

- Molecule 58 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 59 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 60 is a protein called Ribosomal protein S11.

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

- Molecule 61 is a protein called ribosomal protein uS15.

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

- Molecule 62 is a protein called uS11.

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

- Molecule 63 is a protein called Ribosomal protein S16.

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

- Molecule 64 is a protein called eS17.

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

- Molecule 65 is a protein called eS21.

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

- Molecule 66 is a protein called Ribosomal protein S15a.

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

- Molecule 67 is a protein called Ribosomal protein S23.

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

- Molecule 68 is a protein called eS24.

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

- Molecule 69 is a protein called eS26.

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

- Molecule 70 is a protein called 40S ribosomal protein S27.

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

- Molecule 71 is a protein called 40S ribosomal protein S30.

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

- Molecule 72 is a protein called Ribosomal protein S3.

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

- Molecule 73 is a protein called Ribosomal protein S5.

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

- Molecule 74 is a protein called eS10.

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

- Molecule 75 is a protein called 40S ribosomal protein S12.

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

- Molecule 76 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	9	120	997	635	187	168	7	0	0

- Molecule 77 is a protein called uS13.

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

- Molecule 78 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
PP	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 79 is a protein called uS10.

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

- Molecule 80 is a protein called ribosomal protein eS25.

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

- Molecule 81 is a protein called Ribosomal protein S28.

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

- Molecule 82 is a protein called S29.

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

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	0	68	555	351	103	94	7	0	0

- Molecule 84 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	6	313	2436	1535	424	465	12	0	0

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
85	4	10	211	95	37	69	10	0	0

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
86	5	148	148	148	0
86	7	4	4	4	0
86	8	1	1	1	0
86	I	1	1	1	0
86	P	1	1	1	0
86	Q	1	1	1	0
86	V	1	1	1	0
86	e	1	1	1	0
86	g	1	1	1	0

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

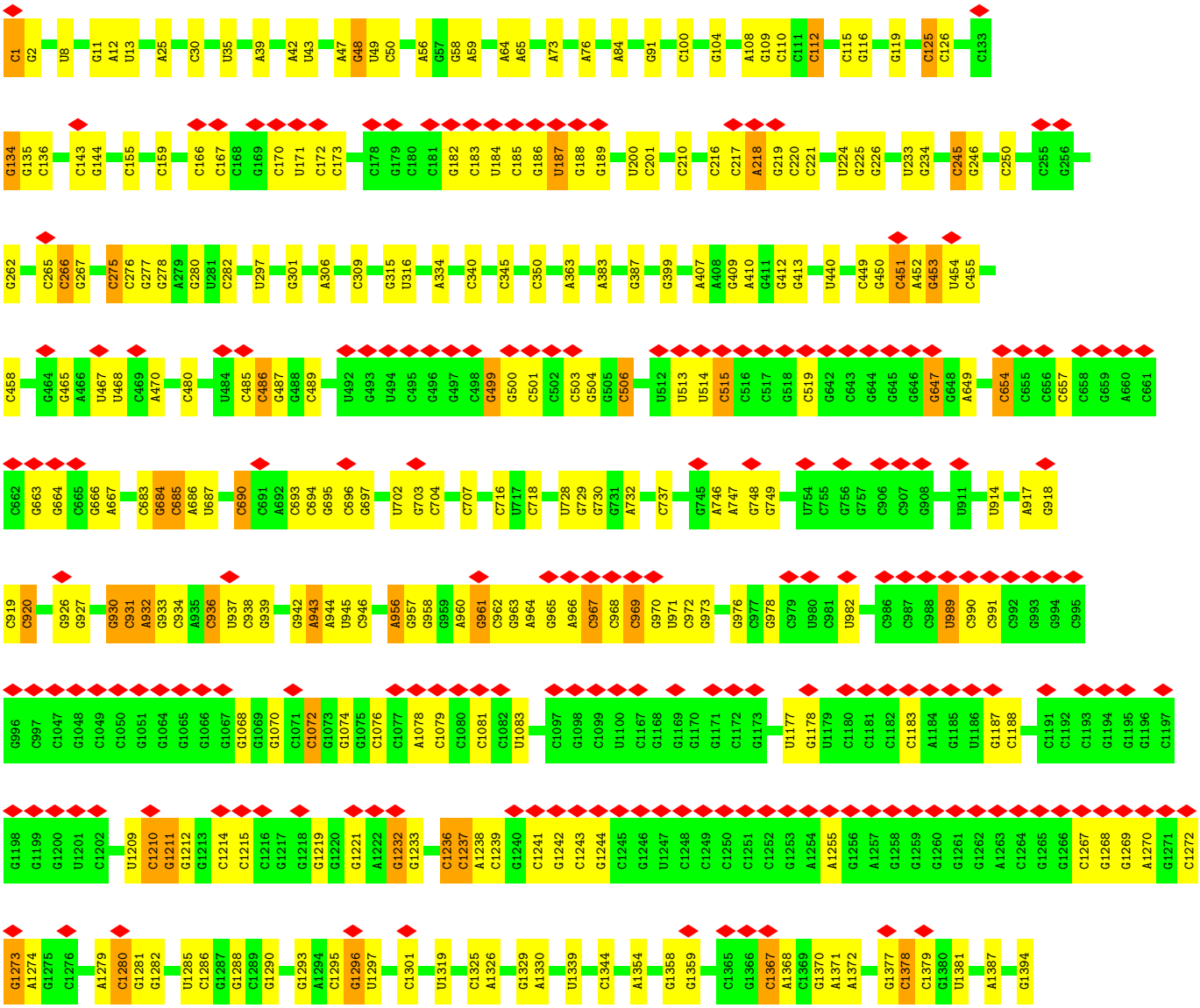
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
87	g	1	1	1	0
87	j	1	1	1	0
87	m	1	1	1	0
87	o	1	1	1	0
87	p	1	1	1	0

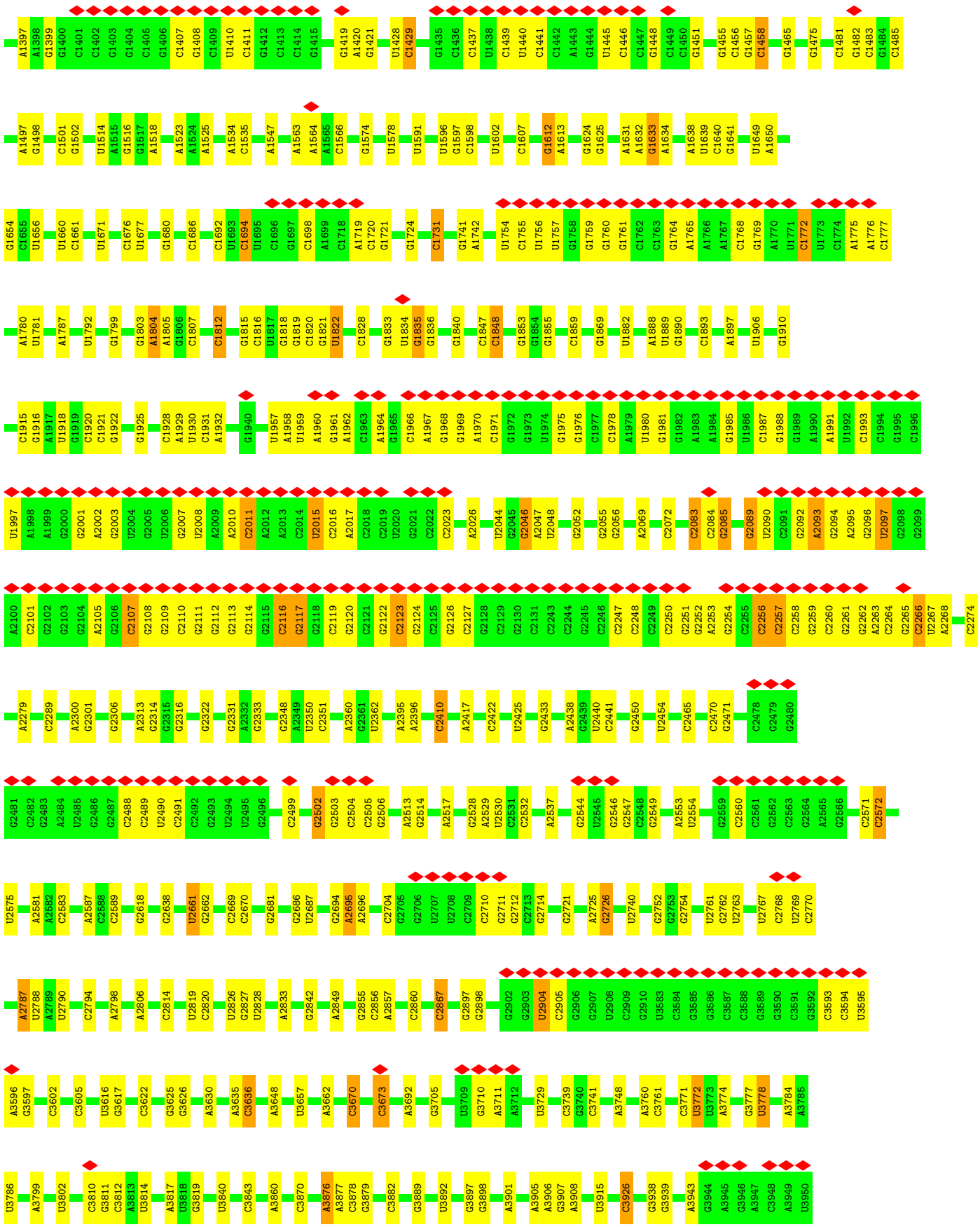
3 Residue-property plots (i)

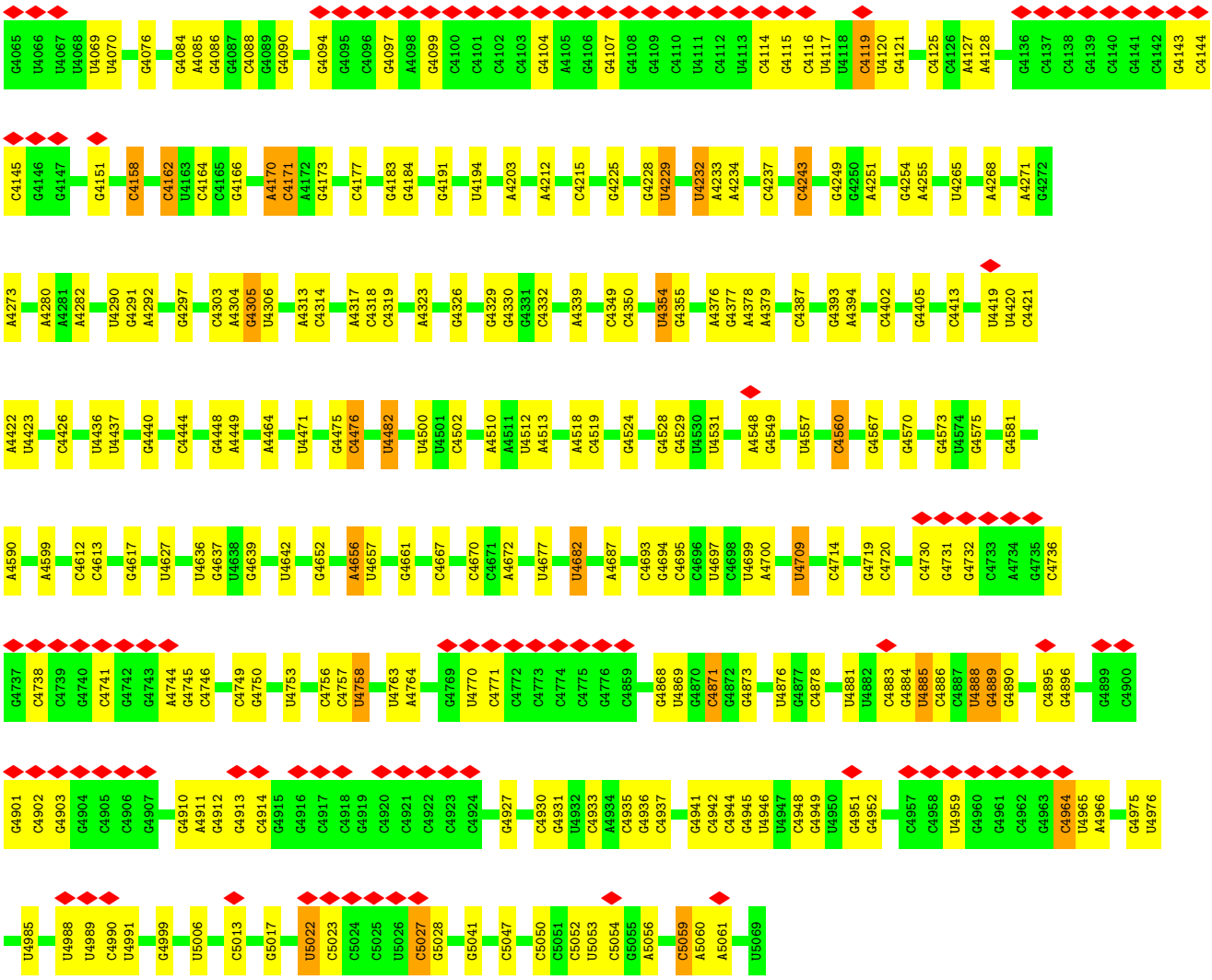
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 28S ribosomal RNA

Chain 5:

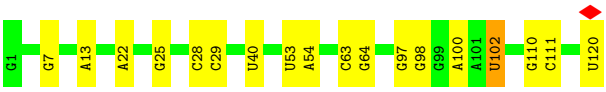



A1397 A1398 G1399 G1400 C1401 C1402 G1403 G1404 C1405 C1406 C1407 G1408 C1409 U1410 C1411 G1412 C1413 C1414 G1415 G1419 A1420 G1421 U1428 C1429 G1435 C1436 C1437 U1438 C1439 U1440 C1441 C1442 A1443 G1444 U1445 C1446 C1447 G1448 C1449 C1450 G1451 G1455 C1456 G1457 C1458 G1465 G1475 C1481 G1482 C1483 G1484 C1485
A1497 G1498 C1501 G1502 U1514 A1515 G1516 G1517 A1518 A1523 A1524 A1525 A1534 C1535 A1547 A1563 A1564 A1565 C1566 G1574 U1578 U1591 U1596 G1597 C1598 U1602 C1607 G1612 A1613 G1624 G1625 A1631 A1632 G1633 A1634 A1638 U1639 C1640 G1641 U1649 A1650
G1654 C1655 U1656 U1660 C1661 U1671 C1676 U1677 G1680 C1686 C1692 U1693 C1694 U1695 C1696 G1697 C1698 A1699 C1718 A1719 C1720 G1721 G1724 C1731 G1741 A1742 U1754 C1755 U1756 U1757 G1758 G1759 G1760 G1761 C1762 C1763 G1764 A1765 A1766 A1767 C1768 G1769 A1770 U1771 C1772 U1773 C1774 A1775 A1776 C1777
A1780 U1781 A1787 U1792 G1799 G1803 A1804 A1805 G1806 C1807 C1812 G1815 C1816 U1817 G1818 G1819 C1820 G1821 U1822 C1828 G1833 U1834 G1835 G1836 G1840 C1847 C1848 G1853 G1854 G1855 C1859 G1869 U1882 A1888 U1889 G1890 C1893 A1897 U1906 G1910
C1915 G1916 A1917 U1918 G1919 C1920 C1921 G1922 G1925 C1928 A1929 U1930 C1931 A1932 G1940 U1957 A1958 U1959 A1960 G1961 A1962 C1963 A1964 G1965 C1966 A1967 G1968 G1969 A1970 C1971 G1972 G1973 U1974 G1975 G1976 C1977 C1978 A1979 U1980 G1981 G1982 A1983 A1984 G1985 U1986 C1987 G1988 G1989 A1990 A1991 U1992 C1993 C1994 G1995 C1996
U1997 A1998 A1999 G2000 G2001 A2002 G2003 U2004 G2005 U2006 G2007 U2008 A2009 A2010 C2011 A2012 A2013 C2014 U2015 C2016 A2017 C2018 C2019 U2020 G2021 C2022 C2023 A2026 U2044 G2045 G2046 A2047 U2048 G2052 G2055 G2056 A2069 C2072 C2083 C2084 G2085 G2089 U2090 C2091 G2092 A2093 G2094 A2095 G2096 U2097 G2098 G2099
A2100 C2101 G2102 G2103 G2104 A2105 C2106 C2107 G2108 G2109 C2110 G2111 G2112 G2113 G2114 G2115 C2116 G2117 G2118 C2119 G2120 C2121 G2122 C2123 G2124 C2125 G2126 C2127 G2128 C2129 G2130 C2131 C2243 C2244 G2245 C2246 C2247 C2248 C2249 C2250 G2251 G2252 A2253 G2254 C2255 C2256 C2257 C2258 G2259 C2260 G2261 G2262 A2263 C2264 G2265 C2266 U2267 A2268 C2274
A2279 C2289 A2300 G2301 G2306 A2313 G2314 G2315 G2316 G2322 G2331 A2332 G2333 G2348 A2349 U2350 C2351 A2360 G2361 U2362 A2395 A2396 C2410 A2417 C2422 U2425 G2433 A2438 G2439 U2440 C2441 G2450 U2454 C2465 C2470 G2471 C2478 G2479 G2480
G2481 C2482 G2483 A2484 U2485 G2486 G2487 C2488 C2489 U2490 C2491 C2492 G2493 U2494 U2495 G2496 C2499 G2502 G2503 C2504 C2505 G2506 A2513 G2514 A2517 G2528 A2529 U2530 C2531 C2532 A2537 G2544 U2545 G2546 G2547 C2548 G2549 A2553 U2554 G2559 C2560 C2561 G2562 G2563 G2564 A2565 G2566 C2571 C2572
U2575 A2581 A2582 C2583 A2587 C2588 C2589 G2618 G2638 U2661 G2662 C2669 C2670 G2681 G2686 U2687 G2694 A2695 A2696 C2704 G2705 G2706 U2707 U2708 C2709 C2710 G2711 G2712 C2713 G2714 G2721 A2725 G2726 U2740 G2752 G2753 G2754 U2761 G2762 U2763 U2767 C2768 U2769 C2770
A2787 U2788 A2789 U2790 C2794 A2798 A2806 C2814 U2819 C2820 U2826 G2827 U2828 A2833 G2842 A2849 G2855 C2856 A2857 C2860 C2867 G2897 G2898 G2902 G2903 U2904 C2905 G2906 G2907 U2908 C2909 G2910 U3583 C3584 G3585 G3586 C3587 C3588 G3589 G3590 C3591 G3592 C3593 C3594 U3595
A3596 G3597 C3602 C3605 U3616 G3617 C3622 G3625 G3626 A3630 A3635 C3636 A3648 U3657 A3662 C3670 C3673 A3692 G3705 U3709 G3710 A3711 A3712 U3729 C3739 G3740 C3741 A3748 A3760 C3761 C3771 U3772 U3773 A3774 G3777 U3778 A3784 A3785
U3786 A3799 U3802 C3810 G3811 C3812 A3813 U3814 A3817 U3818 G3819 U3840 C3843 A3860 C3870 A3876 A3877 C3878 G3879 C3882 G3889 U3892 G3897 G3898 A3901 A3905 A3906 G3907 A3908 U3915 C3926 G3938 G3939 A3943 G3944 A3945 G3946 A3947 C3948 A3949 U3950



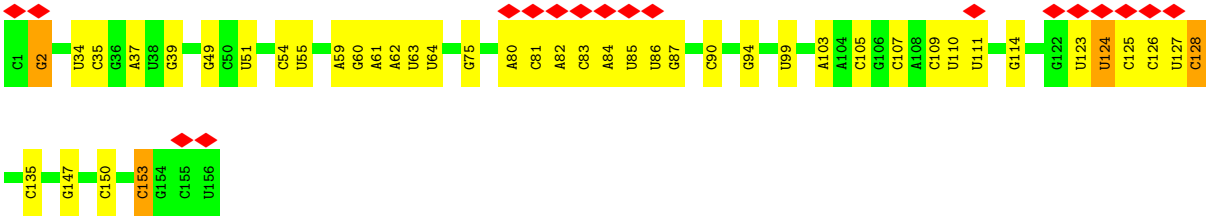
- Molecule 2: 5S ribosomal RNA

Chain 7:



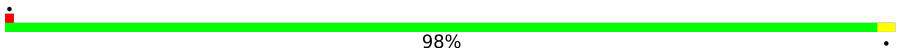
- Molecule 3: 5.8S ribosomal RNA

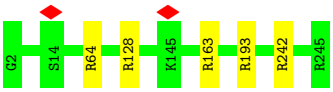
Chain 8:



- Molecule 4: uL2

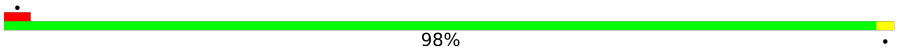
Chain A:

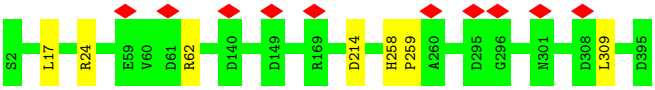




• Molecule 5: uL3

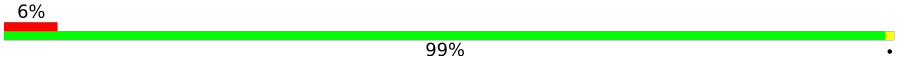
Chain B:

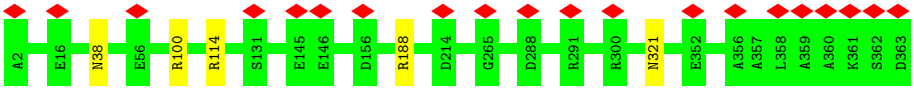




• Molecule 6: uL4

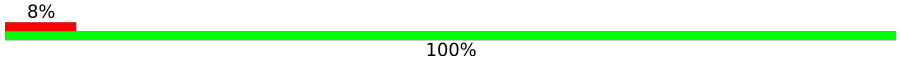
Chain C:

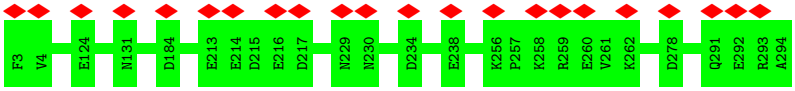




• Molecule 7: 60S ribosomal protein L5

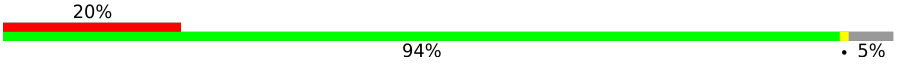
Chain D:

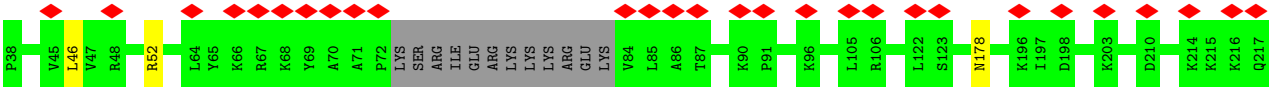


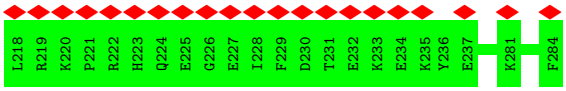


• Molecule 8: 60S ribosomal protein L6

Chain E:

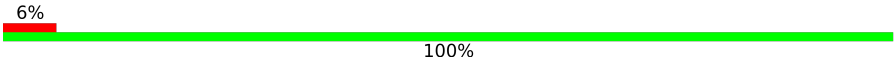


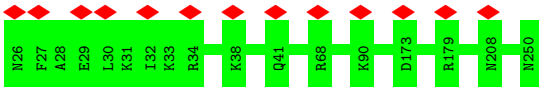




• Molecule 9: uL30

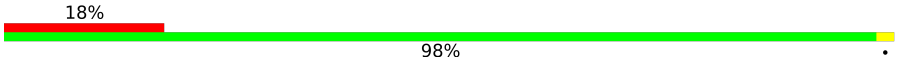
Chain F:





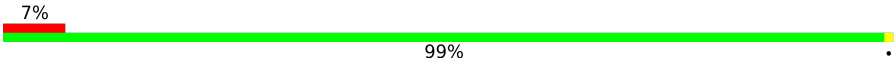
• Molecule 10: eL8

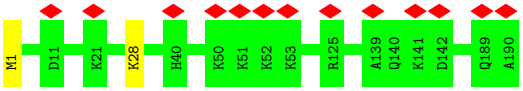
Chain G:



• Molecule 11: uL6

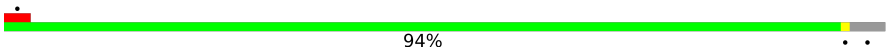
Chain H:

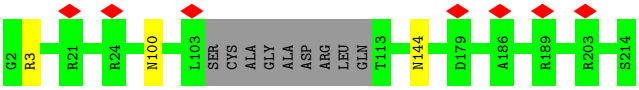




• Molecule 12: Ribosomal protein L10 (Predicted)

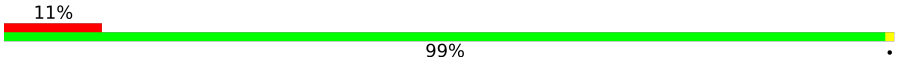
Chain I:

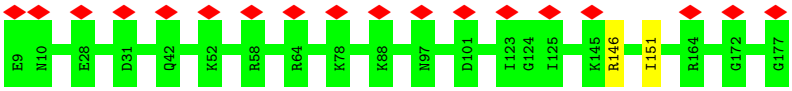




• Molecule 13: uL5

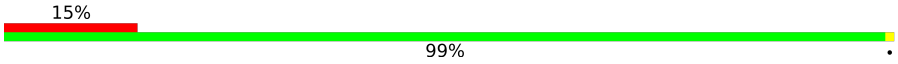
Chain J:

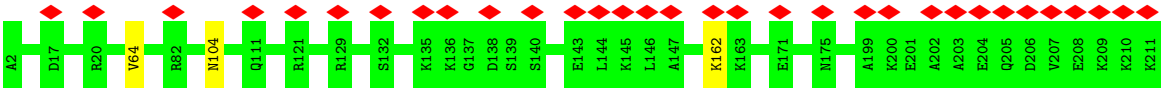




• Molecule 14: 60S ribosomal protein L13

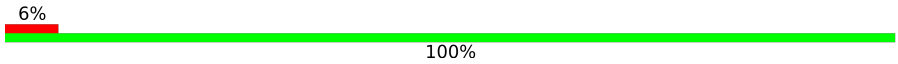
Chain L:

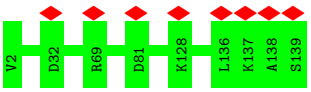




• Molecule 15: Ribosomal protein L14

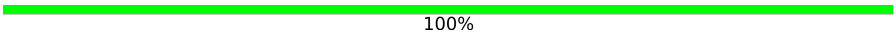
Chain M:

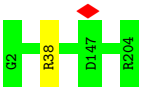




• Molecule 16: Ribosomal protein L15

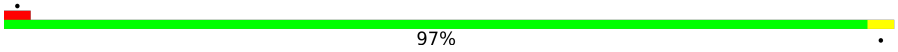
Chain N:





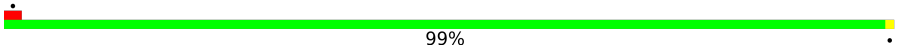
• Molecule 17: uL13

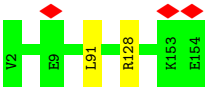
Chain O:



• Molecule 18: uL22

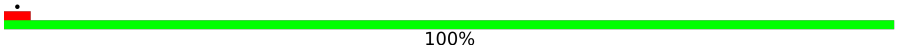
Chain P:

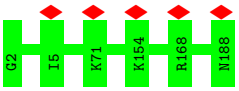




• Molecule 19: eL18

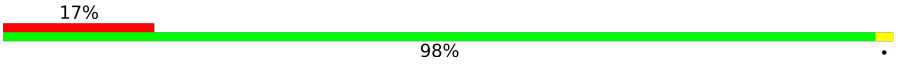
Chain Q:

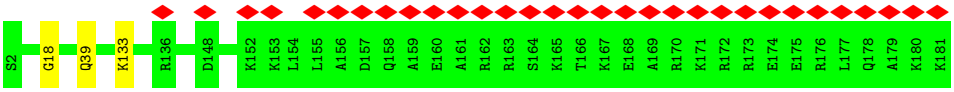




• Molecule 20: eL19

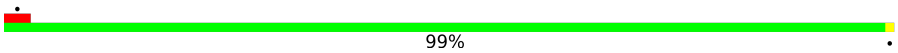
Chain R:

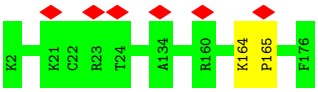




• Molecule 21: eL20

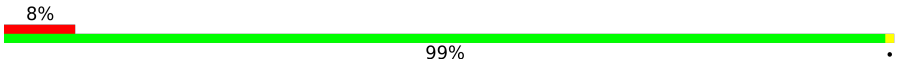
Chain S:

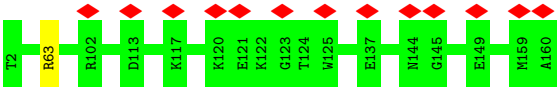




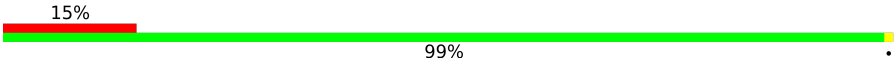
• Molecule 22: eL21

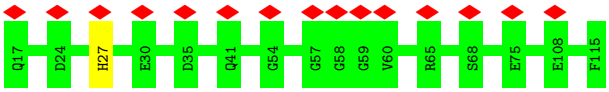
Chain T:



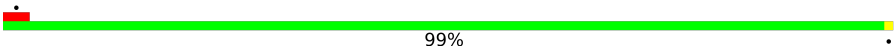


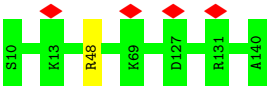
• Molecule 23: Ribosomal protein L22

Chain U: 

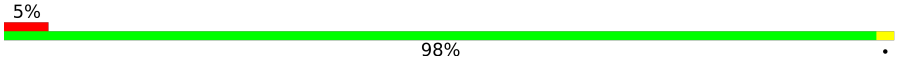


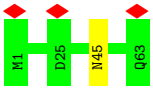
• Molecule 24: uL14

Chain V: 

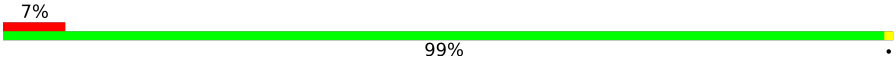


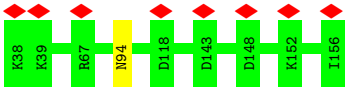
• Molecule 25: Ribosomal protein L24

Chain W: 

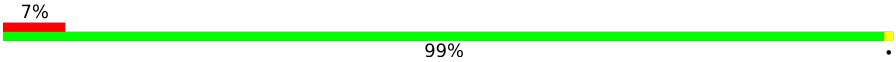


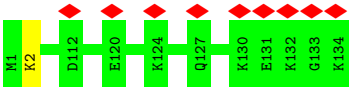
• Molecule 26: uL23

Chain X: 

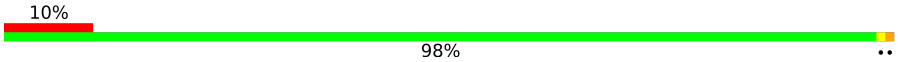


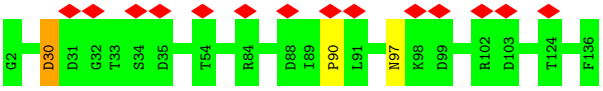
• Molecule 27: Ribosomal protein L26

Chain Y: 

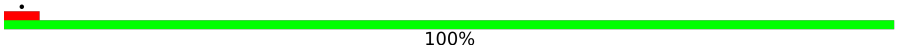


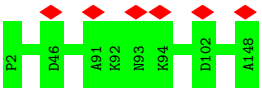
• Molecule 28: 60S ribosomal protein L27

Chain Z: 



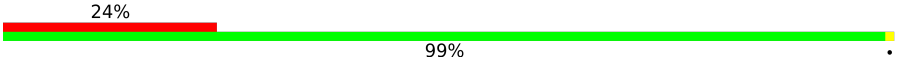
• Molecule 29: uL15

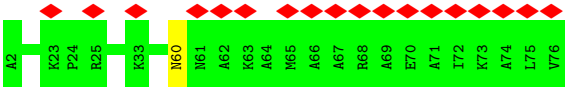
Chain a: 



- Molecule 30: 60S ribosomal protein L29

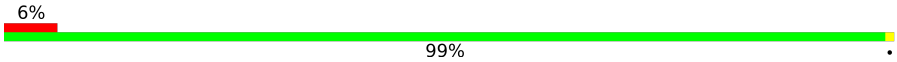
Chain b:

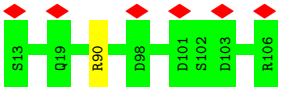




- Molecule 31: eL30

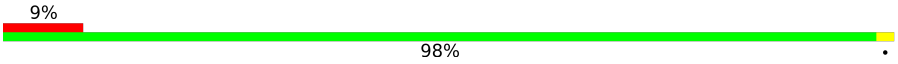
Chain c:

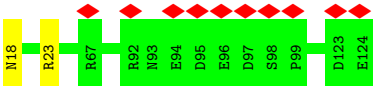




- Molecule 32: eL31

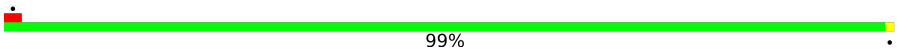
Chain d:

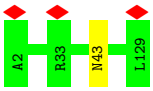




- Molecule 33: eL32

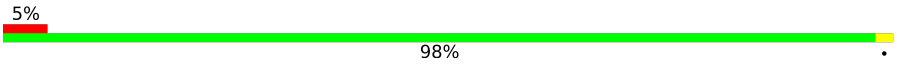
Chain e:

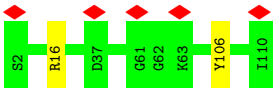




- Molecule 34: eL33

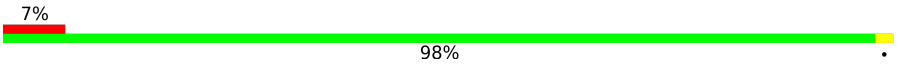
Chain f:

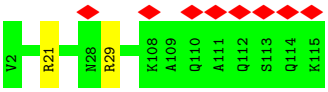




- Molecule 35: eL34

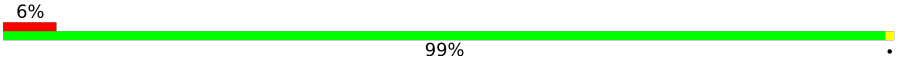
Chain g:

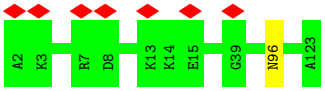




- Molecule 36: uL29

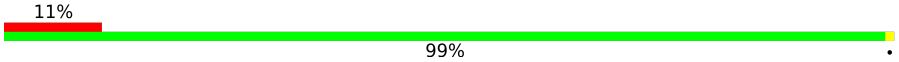
Chain h:

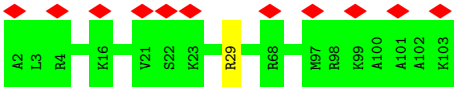




• Molecule 37: 60S ribosomal protein L36

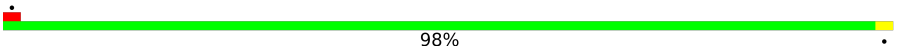
Chain i:

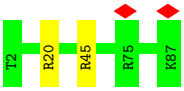




• Molecule 38: Ribosomal protein L37

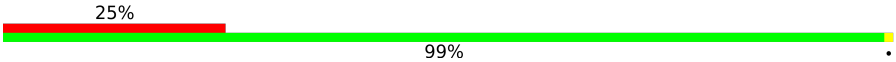
Chain j:

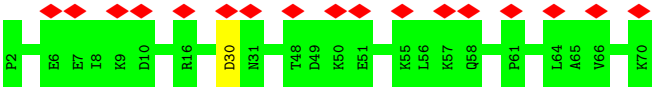




• Molecule 39: eL38

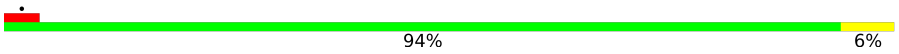
Chain k:

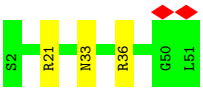




• Molecule 40: ribosomal protein eL39

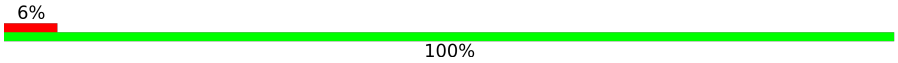
Chain l:

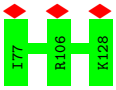




• Molecule 41: eL40

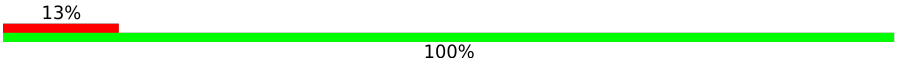
Chain m:

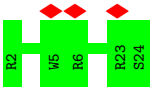




• Molecule 42: 60s ribosomal protein l41

Chain n:





• Molecule 43: eL42

Chain o: 12% 96%

V2 R9 K30 D31 S32 D42 K58 R69 N76 C77 R78 M82 H90 D96 K97 K98 R99 K100 G101 I104 Q105

• Molecule 44: ribosomal protein eL43

Chain p: 7% 98%

A2 R17 R49 R85 E88 L89 K90 D91 Q92

• Molecule 45: eL28

Chain r: 8% 95%

S2 N12 K19 R20 N21 N31 A55 D56 G57 K58 S68 R71 M83 R87 R119 V124 M125 V126

• Molecule 46: 60S acidic ribosomal protein P0

Chain s: 98% 99%

D5 R6 A7 T8 W9 K10 S11 N12 Y13 F14 L15 K16 I17 I18 Q19 L20 L21 D22 D23 Y24 P25 K26 C27 F28 I29 V30 G31 A32 D33 N34 V35 G36 S37 K38 Q39 M40 Q41 Q42 I43 R44 M45 S46 L47 R48 G49 K50 A51 V52 V53 L54 M55 G56 K57 N58 T59 M60 M61 R62 K63 A64

I65 R66 G67 H68 L69 E70 N71 N72 P73 A74 L75 E76 K77 L78 L79 P80 H81 I82 R83 G84 N85 V86 G87 F88 V89 F90 T91 K92 E93 D94 L95 T96 E97 I98 R99 D100 M101 L102 L103 A104 N105 K106 V107 P108 A109 A110 A111 R112 A113 G114 A115 I116 A117 P118 C119 E120 V121 T122 V123 P124

A125 Q126 N127 T128 G129 L130 G131 P132 E133 K134 T135 S136 F137 F138 Q139 A140 L141 G142 I143 T144 T145 K146 I147 S148 R149 G150 T151 I152 E153 I154 L155 S156 D157 V158 Q159 L160 I161 K162 T163 G164 D165 K166 V167 G168 A169 S170 E171 A172 T173 L174 L175 N176 M177 L178 N179 I180 S181 P182 F183 S184

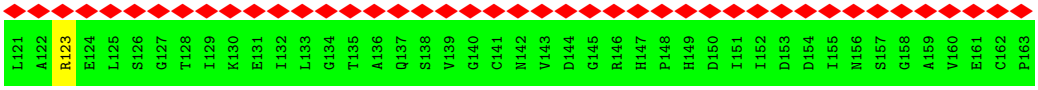
F185 G186 L187 I188 I189 Q190 Q191 V192 F193 D194 N195 G196 S197 I198 Y199 N200 P201 E202

• Molecule 47: Ribosomal protein L12

Chain t: 100% 98%

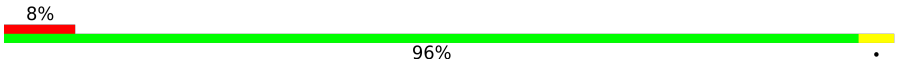
M1 P2 P3 K4 F5 D6 P7 N8 E9 I10 K11 V12 V13 Y14 L15 R16 C17 T18 G19 G20 E21 V22 G23 A24 T25 S26 A27 L28 A29 P30 K31 I32 G33 P34 L35 G36 L37 S38 P39 K40 K41 V42 G43 D44 D45 I46 A47 K48 A49 T50 G51 D52 W53 K54 G55 L56 R57 I58 T59 V60

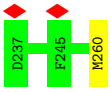
K61 L62 T63 I64 Q65 N66 R67 Q68 A69 Q70 I71 E72 V73 V74 P75 S76 A77 S78 A79 L80 I81 I82 K83 A84 L85 K86 E87 P88 P89 R90 D91 R92 K93 K94 Q95 K96 N97 I98 K99 H100 S101 G102 N103 I104 T105 F106 D107 E108 I109 V110 N111 I112 A113 R114 Q115 M116 R117 H118 R119 S120



• Molecule 48: X-box-binding protein 1

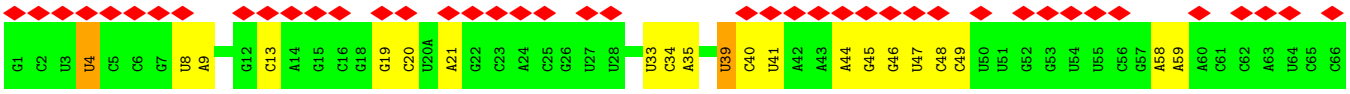
Chain 1:

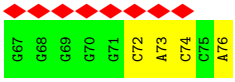




• Molecule 49: A/P-tRNA

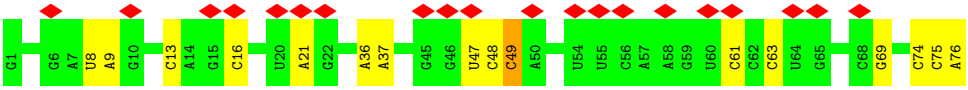
Chain 2:





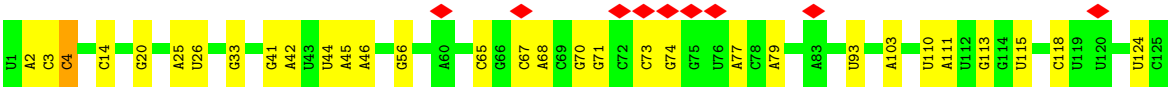
• Molecule 50: P/E-tRNA

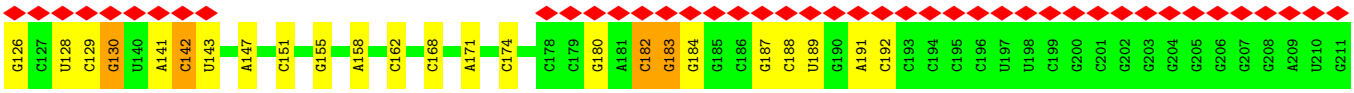
Chain 3:

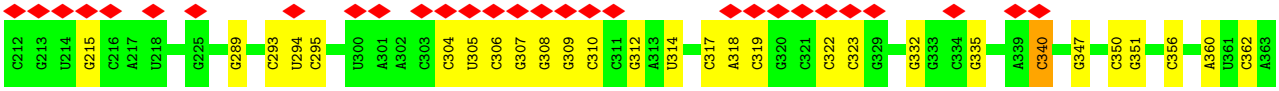


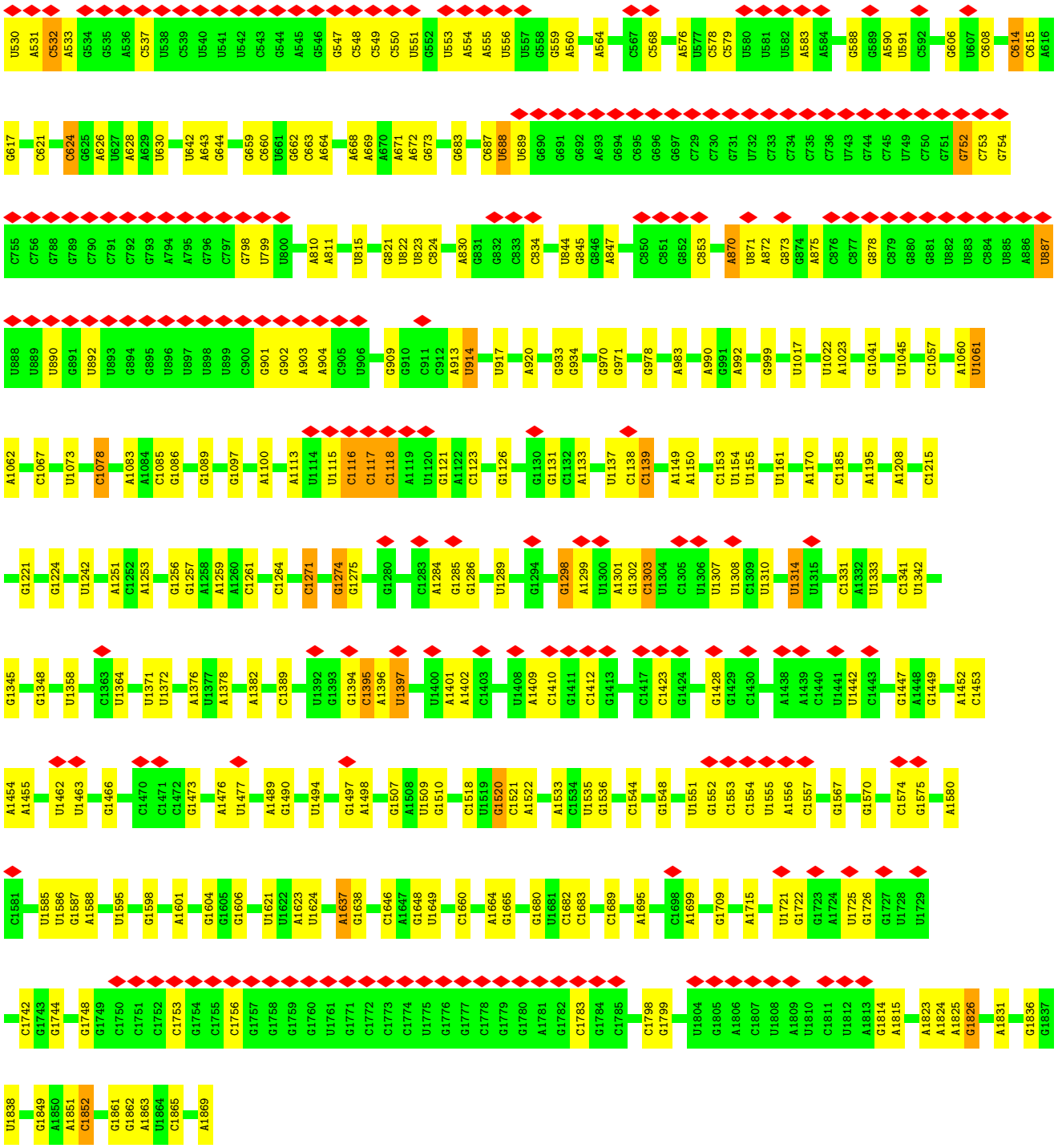
• Molecule 51: 18S rRNA

Chain K:



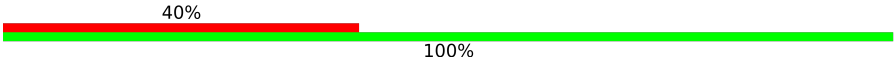


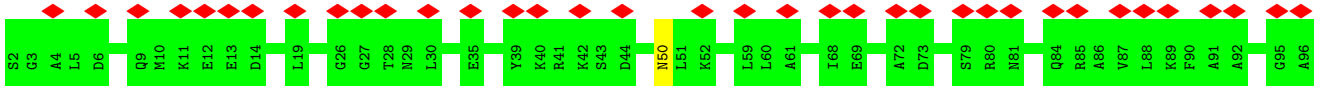


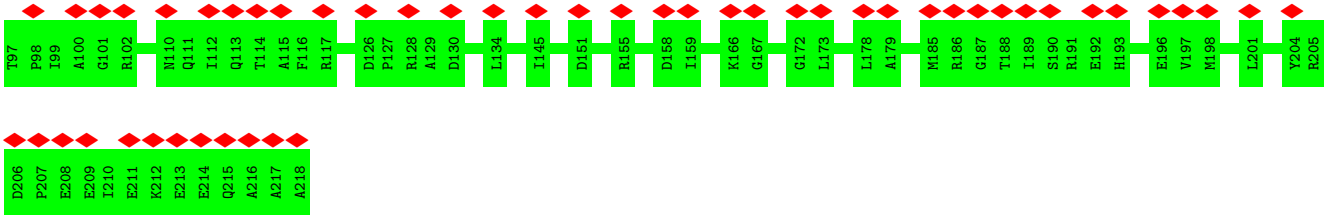


- Molecule 52: uS2

Chain q:

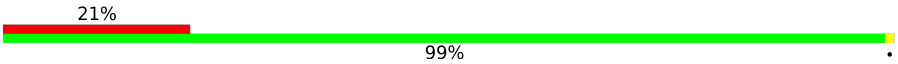


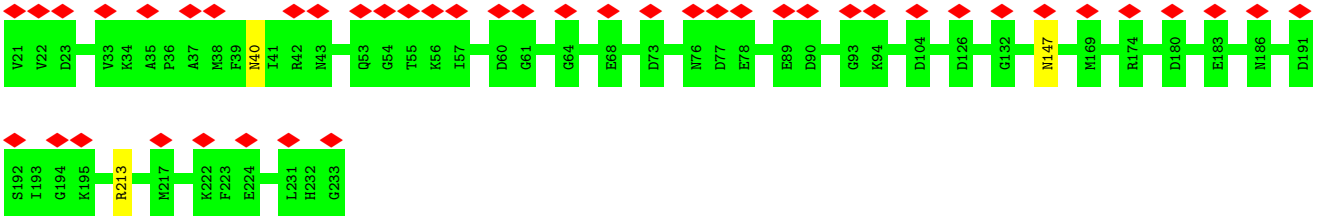




• Molecule 53: 40S ribosomal protein S3a

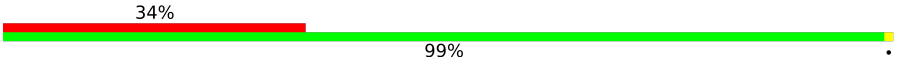
Chain u:

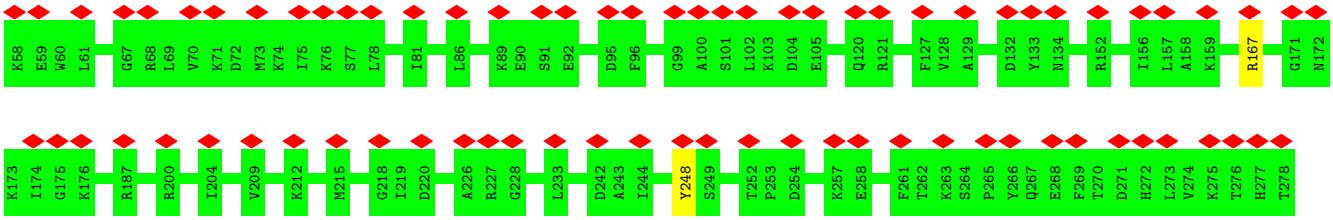




• Molecule 54: uS5

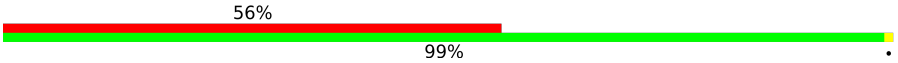
Chain v:

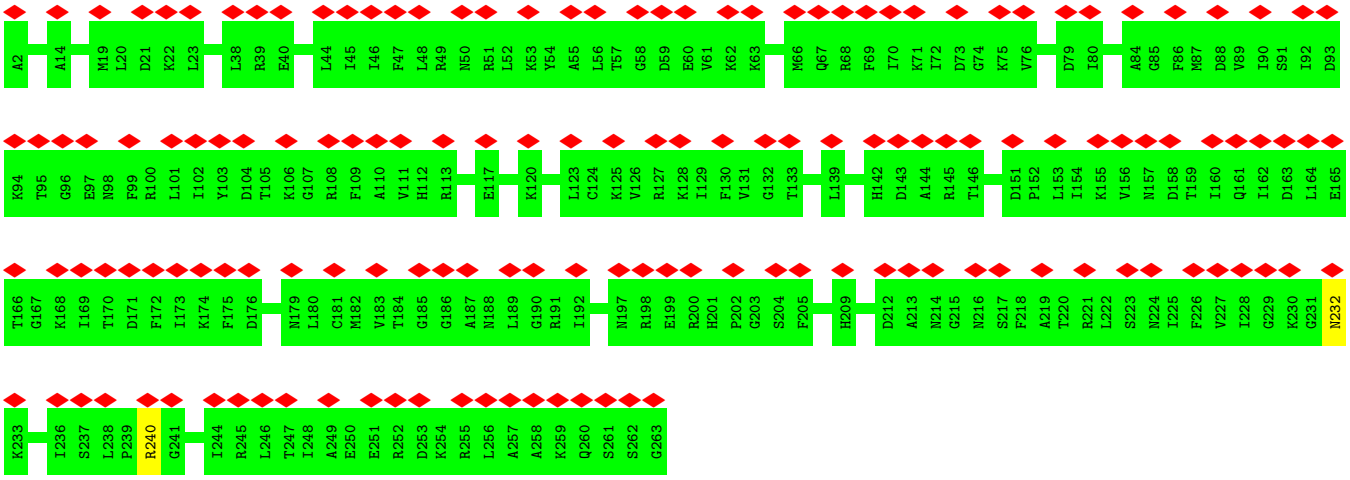




• Molecule 55: 40S ribosomal protein S4

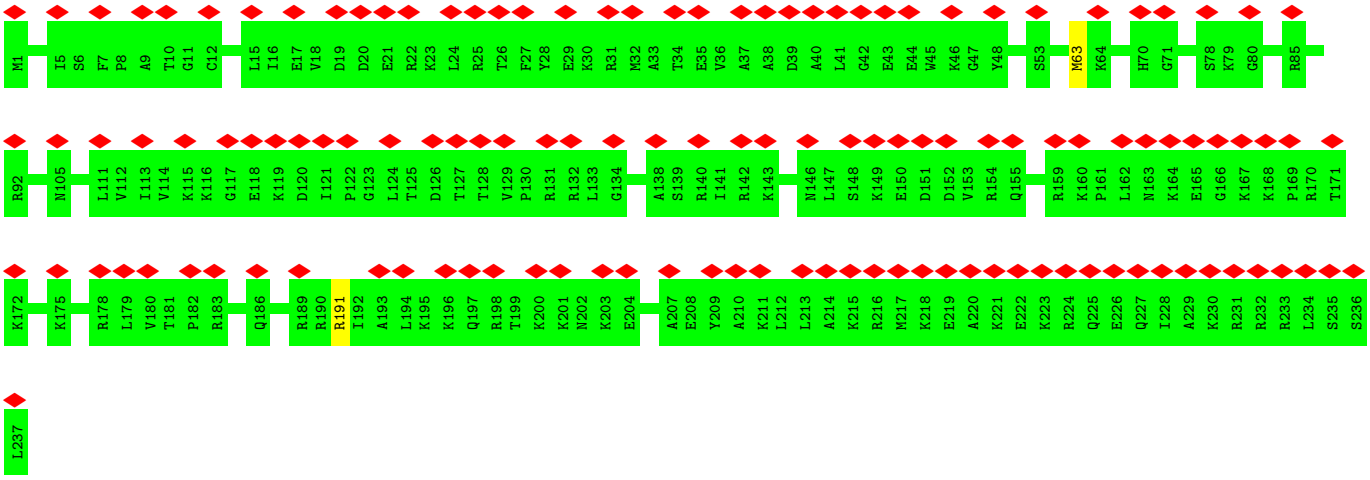
Chain x:





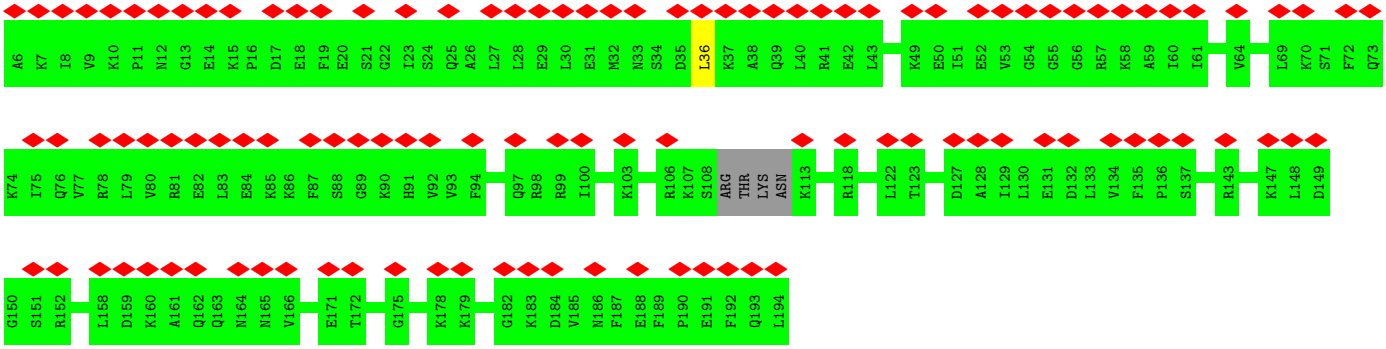
• Molecule 56: 40S ribosomal protein S6

Chain z: 54% 99%



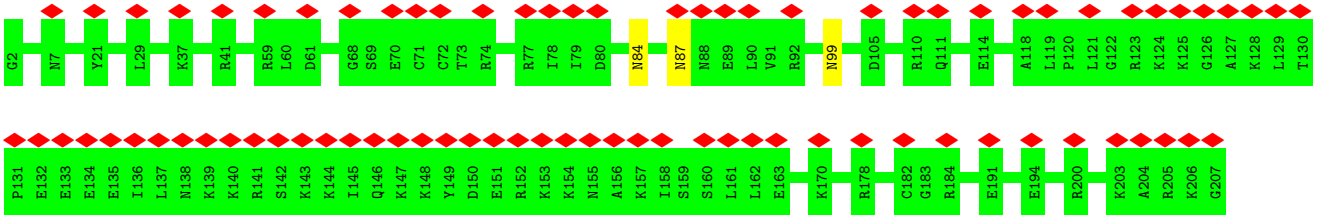
- Molecule 57: 40S ribosomal protein S7

Chain y: 60% 97%



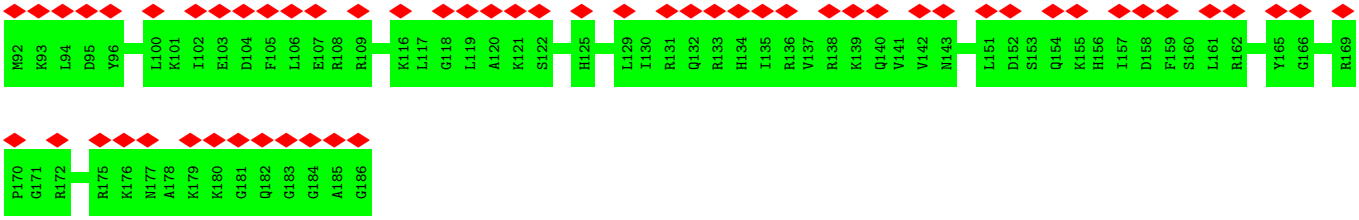
- Molecule 58: 40S ribosomal protein S8

Chain CC: 39% 99%



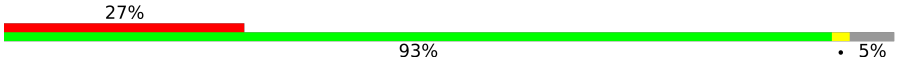
- Molecule 59: Ribosomal protein S9 (Predicted)

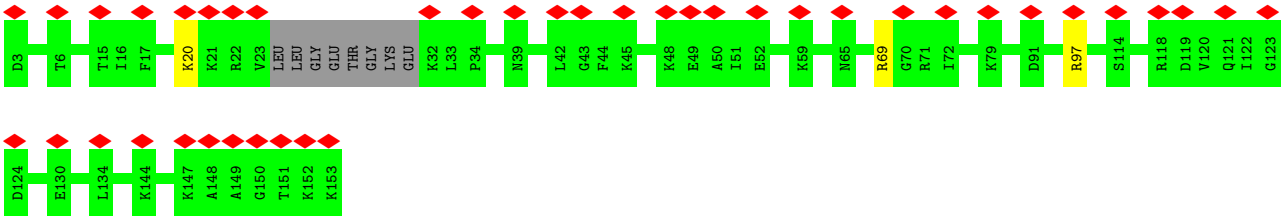
Chain XX: 53% 98%



- Molecule 60: Ribosomal protein S11

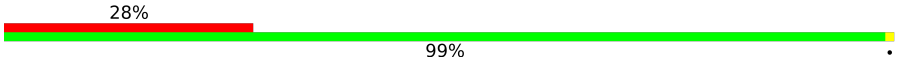
Chain EE:

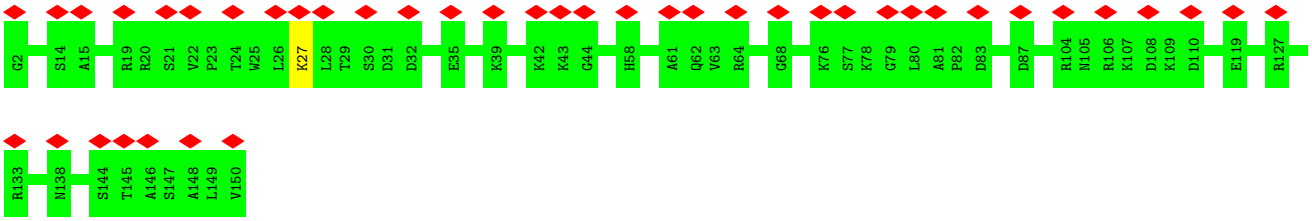




- Molecule 61: ribosomal protein uS15

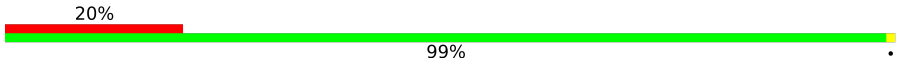
Chain QQ:

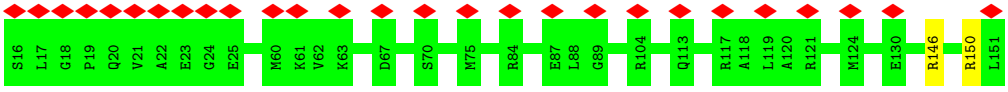




- Molecule 62: uS11

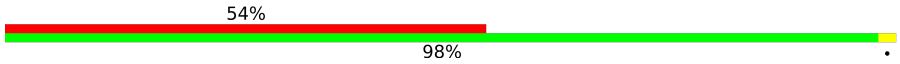
Chain MM:

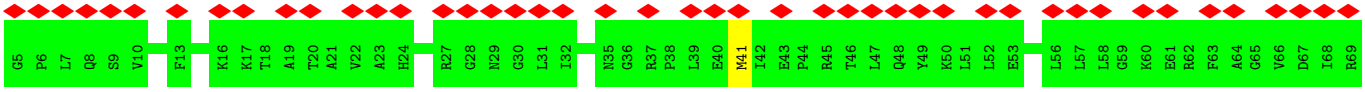


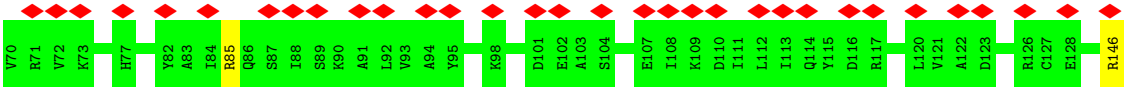


- Molecule 63: Ribosomal protein S16

Chain UU:

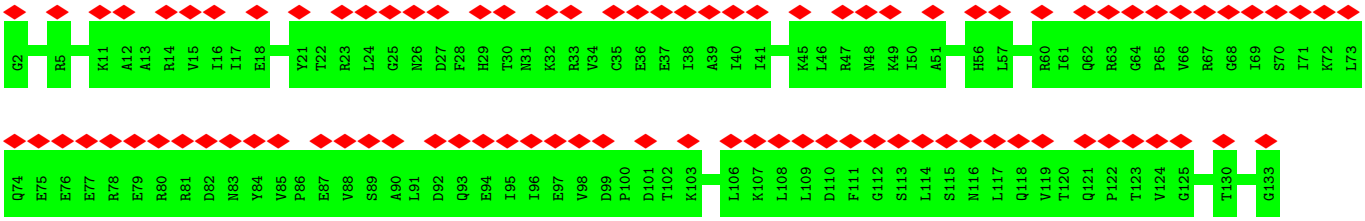






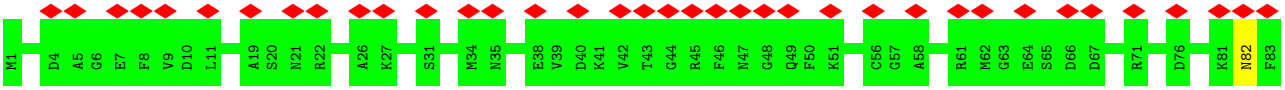
- Molecule 64: eS17

Chain YY: 70% 100%



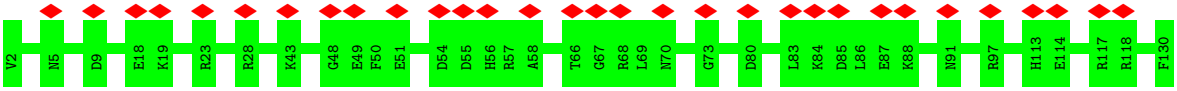
- Molecule 65: eS21

Chain HH: 45% 99%



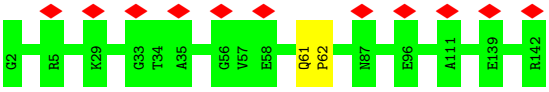
- Molecule 66: Ribosomal protein S15a

Chain TT: 24% 100%



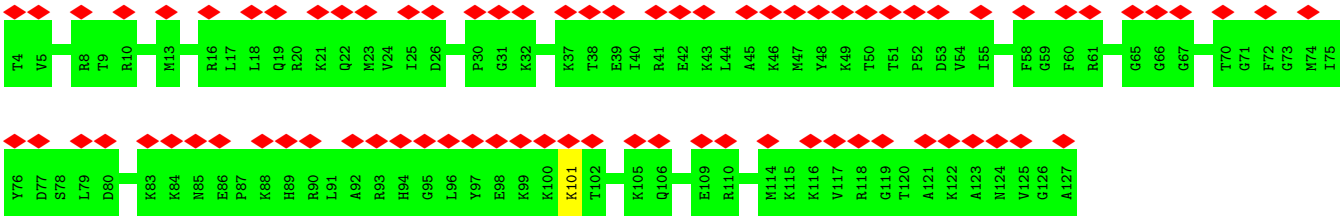
- Molecule 67: Ribosomal protein S23

Chain VV: 8% 99%



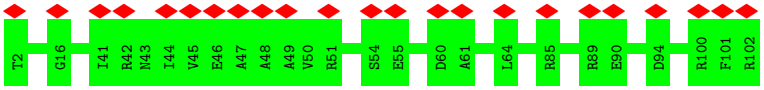
- Molecule 68: eS24

Chain NN: 63% 99%



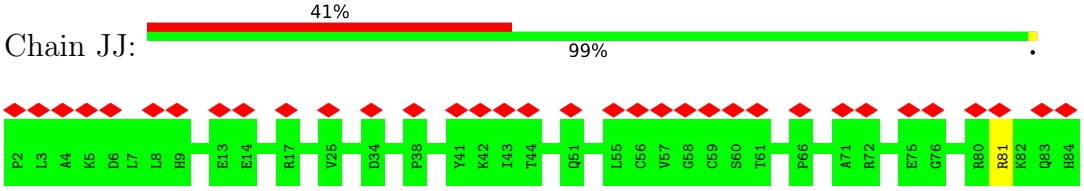
- Molecule 69: eS26

Chain ZZ: 23% 100%



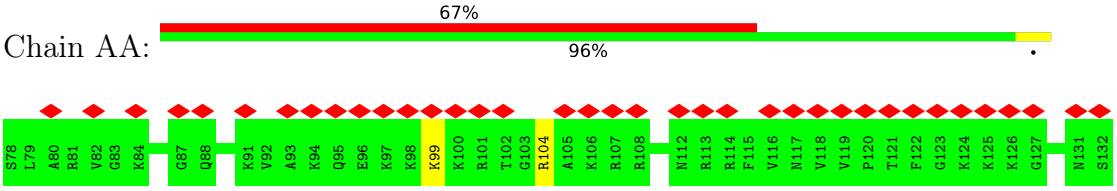
- Molecule 70: 40S ribosomal protein S27

Chain JJ:



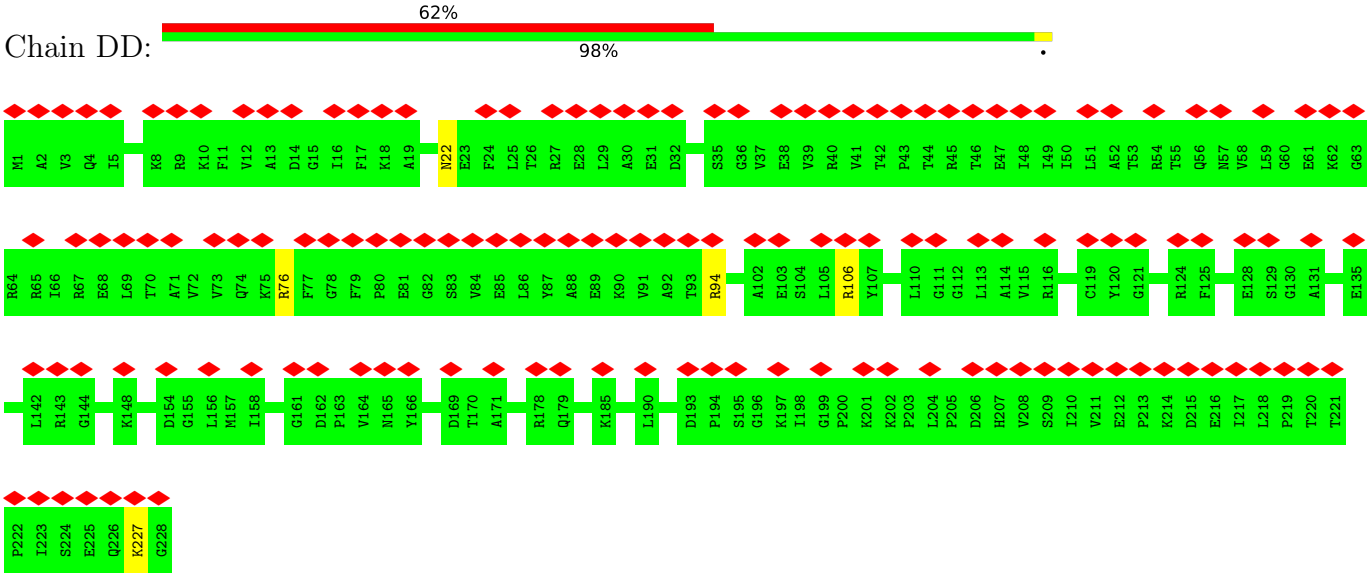
- Molecule 71: 40S ribosomal protein S30

Chain AA:



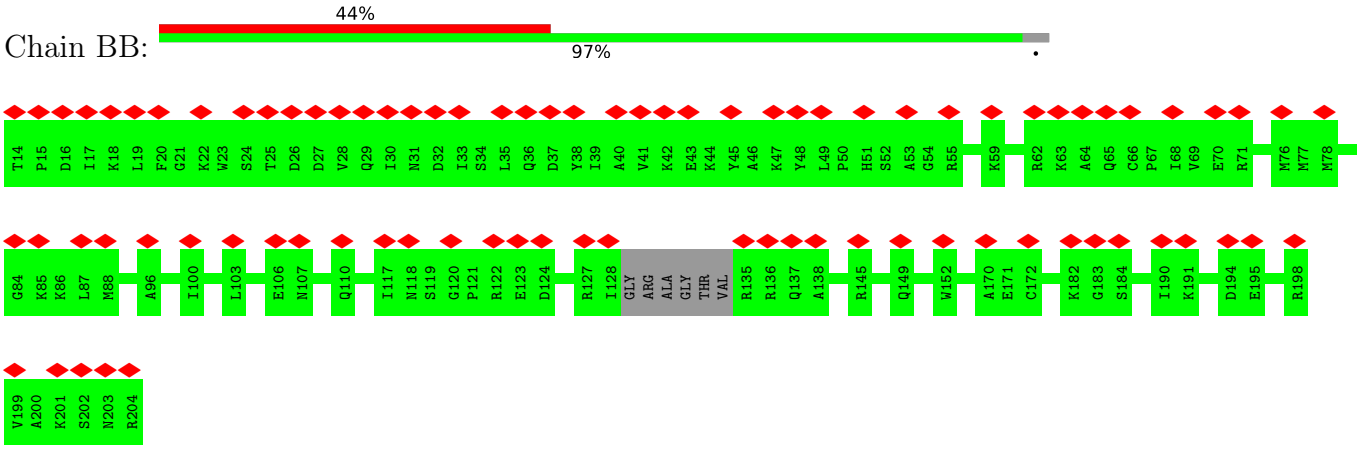
- Molecule 72: Ribosomal protein S3

Chain DD:



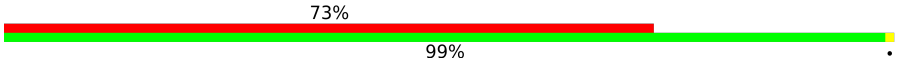
- Molecule 73: Ribosomal protein S5

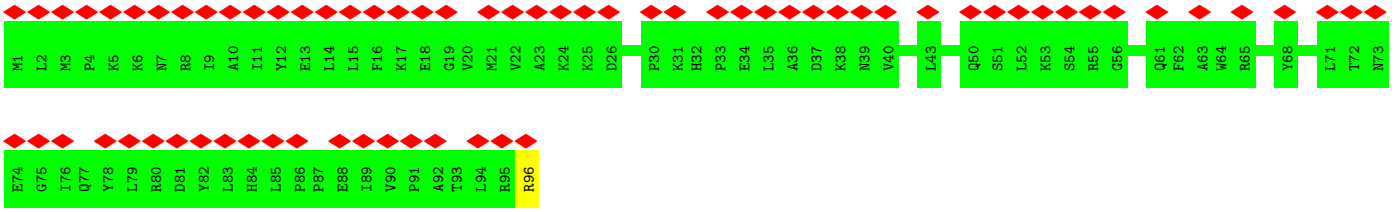
Chain BB:



- Molecule 74: eS10

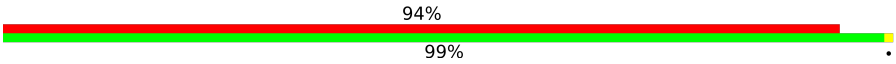
Chain SS:

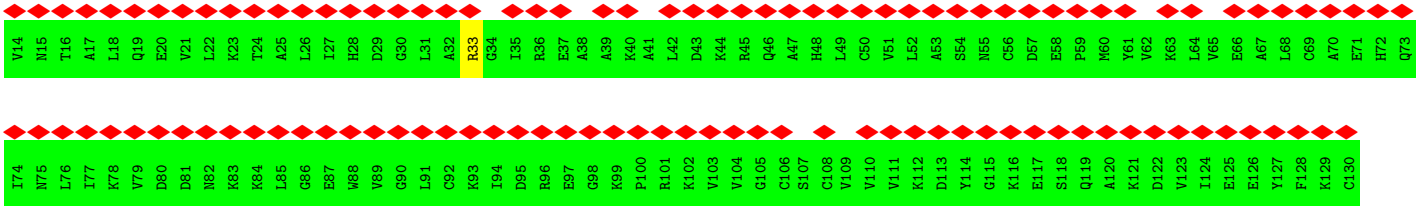




- Molecule 75: 40S ribosomal protein S12

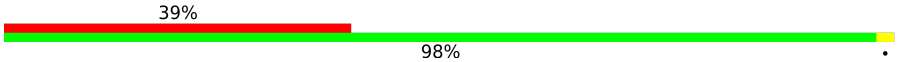
Chain RR:

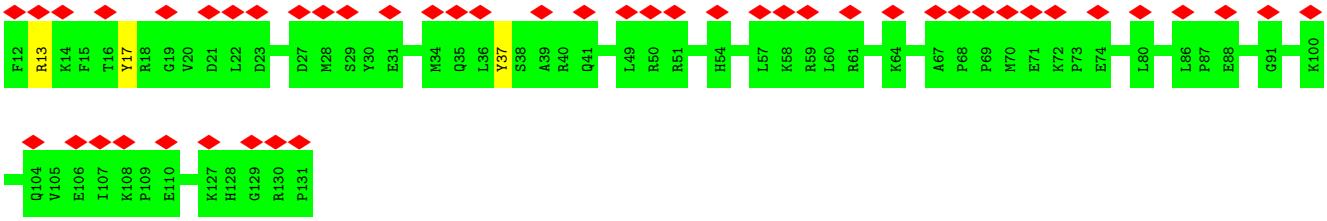




- Molecule 76: uS14

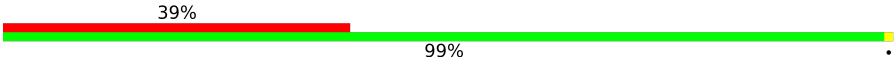
Chain 9:

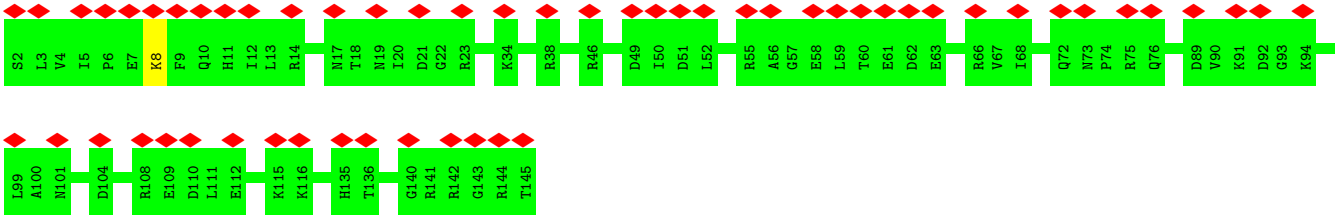




- Molecule 77: uS13

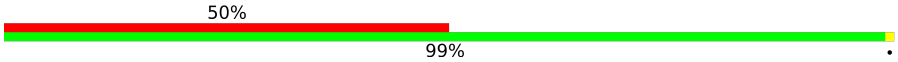
Chain II:

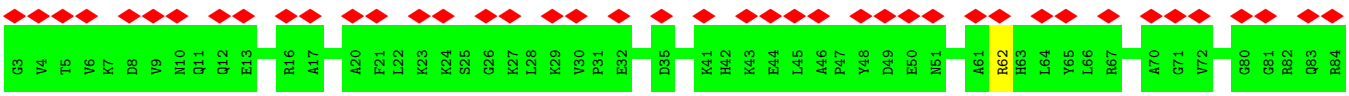


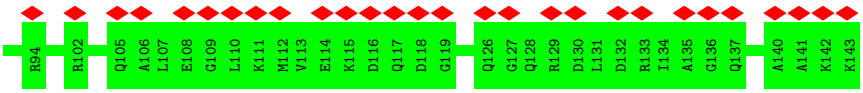


- Molecule 78: eS19

Chain PP:

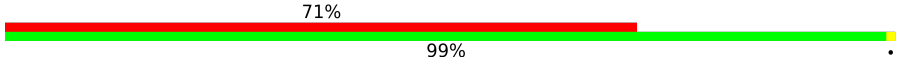


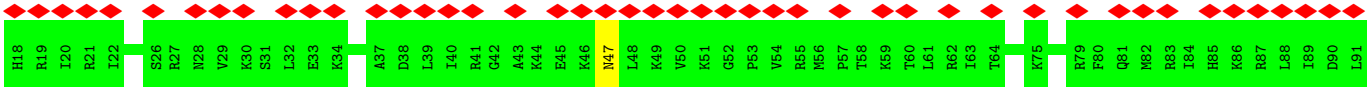


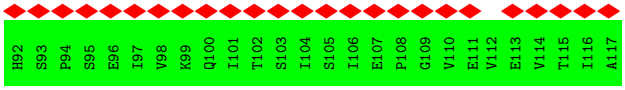


- Molecule 79: uS10

Chain GG:

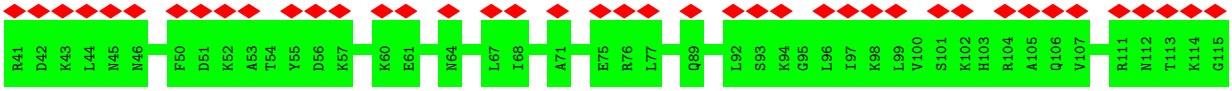






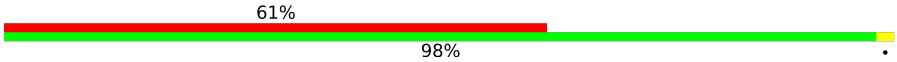
- Molecule 80: ribosomal protein eS25

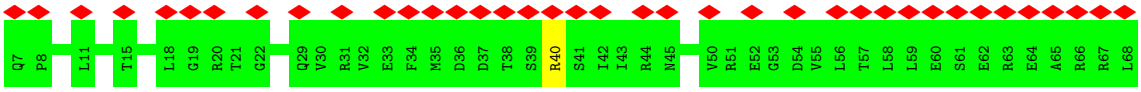
Chain OO:



- Molecule 81: Ribosomal protein S28

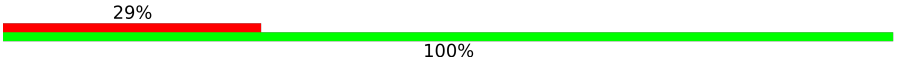
Chain FF:

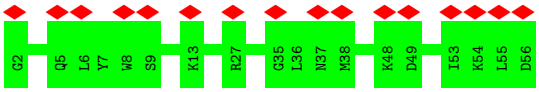




- Molecule 82: S29

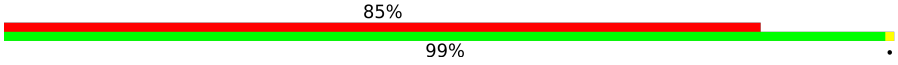
Chain w:

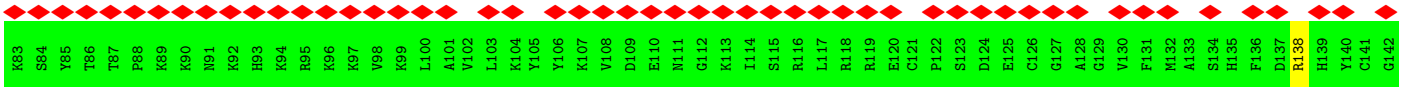


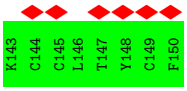


- Molecule 83: eS31

Chain 0:







- Molecule 84: ribosomal protein RACK1

Chain 6: 94% 99%

T2 E3 Q4 M5 T6 L7 R8 G9 T10 L11 K12 G13 H14 N15 G16 W17 V18 T19 Q20 I21 A22 T23 T24 P25 Q26 F27 P28 D29 M30 I31 L32 S33 A34 S35 R36 D37 K38 T39 I40 I41 M42 W43 K44 L45 T46 R47 D48 E49 T50 N51 Y52 G53 I54 P55 Q56 R57 A58 L59 R60 G61

H62 S63 H64 F65 V66 S67 D68 V69 V70 I71 S72 S73 D74 G75 Q76 F77 A78 L79 S80 G81 S82 W83 D84 G85 T86 L87 R88 L89 W90 D91 L92 T93 T94 G95 T96 T97 T98 R99 R100 F101 V102 G103 H104 T105 K106 D107 V108 L109 S110 V111 A112 F113 S114 S115 D116 N117 R118 Q119 I120 V121

S122 G123 S124 R125 D126 K127 T128 I129 K130 L131 W132 N133 T134 L135 G136 V137 C138 K139 Y140 T141 V142 Q143 D144 E145 S146 H147 S148 E149 W150 C153 V154 R155 F156 S157 P158 N159 S160 S161 N162 P163 I164 I165 V166 S167 C168 G169 W170 D171 K172 L173 V174 K175 V176 W177 N178 L179 A180 N181 C182

K183 L184 K185 T186 N187 H188 I189 G190 H191 T192 G193 Y194 L195 N196 T197 V198 T199 V200 S201 P202 D203 G204 S205 L206 C207 A208 S209 G210 G211 K212 D213 G214 Q215 A216 M217 L218 W219 D220 L221 N222 E223 G224 K225 H226 L227 Y228 T229 L230 D231 G232 G233 D234 I235 I236 N237 A238 L239 C240 F241 S242

P243 N244 R245 Y246 W247 L248 C249 A250 A251 T252 G253 P254 S255 I256 K257 I258 W259 D260 L261 E262 G263 K264 I265 I266 V267 D268 E269 L270 K271 Q272 E273 V274 I275 S276 T277 S278 S279 K280 A281 E282 P283 P284 Q285 C286 T287 S288 L289 A290 W291 S292 A293 D294 G295 Q296 T297 L298 F299 A300 G301 Y302

T303 D304 N305 L306 V307 R308 V309 W310 Q311 V312 T313 I314

- Molecule 85: mRNA

Chain 4: 10% 50% 50%

C43 C44 A45 U46 A49 U50 G51 A52

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94923	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.741	Depositor
Minimum map value	-0.435	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	5	0.31	1/87794 (0.0%)	1.05	383/136953 (0.3%)
2	7	0.28	0/2858	0.99	6/4455 (0.1%)
3	8	0.32	0/3701	1.06	10/5766 (0.2%)
4	A	0.29	0/1906	0.55	0/2556
5	B	0.27	0/3216	0.55	2/4311 (0.0%)
6	C	0.26	0/2937	0.51	0/3946
7	D	0.26	0/2432	0.50	0/3257
8	E	0.26	0/1936	0.61	1/2600 (0.0%)
9	F	0.28	0/1905	0.51	0/2539
10	G	0.27	0/1967	0.55	1/2647 (0.0%)
11	H	0.27	0/1535	0.54	0/2063
12	I	0.27	0/1693	0.49	0/2260
13	J	0.27	0/1376	0.56	0/1841
14	L	0.27	0/1734	0.53	0/2317
15	M	0.27	0/1158	0.52	0/1547
16	N	0.27	0/1746	0.51	0/2338
17	O	0.28	0/1671	0.51	0/2234
18	P	0.33	0/1268	0.53	1/1700 (0.1%)
19	Q	0.25	0/1530	0.53	0/2041
20	R	0.27	0/1524	0.54	0/2013
21	S	0.27	0/1493	0.51	0/2002
22	T	0.27	0/1326	0.49	0/1770
23	U	0.27	0/822	0.53	0/1103
24	V	0.28	0/993	0.56	0/1332
25	W	0.27	0/541	0.50	0/720
26	X	0.25	0/993	0.51	0/1334
27	Y	0.26	0/1132	0.50	0/1504
28	Z	0.28	0/1130	0.55	1/1507 (0.1%)
29	a	0.29	0/1191	0.51	0/1590
30	b	0.25	0/619	0.46	0/818
31	c	0.28	0/742	0.51	0/996
32	d	0.28	0/903	0.51	0/1216

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.27	0/1071	0.49	0/1429
34	f	0.27	0/895	0.58	0/1198
35	g	0.26	0/916	0.55	0/1220
36	h	0.26	0/1021	0.51	0/1348
37	i	0.26	0/841	0.52	0/1112
38	j	0.26	0/720	0.51	0/952
39	k	0.30	0/575	0.70	1/761 (0.1%)
40	l	0.26	0/454	0.47	0/599
41	m	0.28	0/435	0.54	0/575
42	n	0.25	0/223	0.45	0/284
43	o	0.27	0/864	0.59	0/1140
44	p	0.26	0/718	0.54	0/953
45	r	0.29	0/1017	0.67	1/1364 (0.1%)
46	s	0.27	0/1547	0.52	0/2088
47	t	0.32	0/1257	0.65	0/1697
48	1	0.50	0/216	0.56	0/298
49	2	0.28	0/1802	0.95	6/2804 (0.2%)
50	3	0.27	0/1783	1.00	3/2773 (0.1%)
51	K	0.29	1/40530 (0.0%)	1.04	165/63160 (0.3%)
52	q	0.26	0/1747	0.50	0/2374
53	u	0.25	0/1756	0.53	0/2350
54	v	0.27	0/1753	0.51	0/2369
55	x	0.25	0/2118	0.51	0/2849
56	z	0.25	0/1946	0.48	0/2590
57	y	0.26	0/1510	0.52	1/2022 (0.0%)
58	CC	0.25	0/1715	0.49	0/2287
59	XX	0.25	0/1550	0.50	0/2069
60	EE	0.26	0/1195	0.50	0/1597
61	QQ	0.25	0/1226	0.46	0/1649
62	MM	0.26	0/1029	0.51	0/1380
63	UU	0.26	0/1146	0.50	0/1534
64	YY	0.24	0/1082	0.46	0/1452
65	HH	0.27	0/643	0.52	0/860
66	TT	0.27	0/1051	0.51	0/1406
67	VV	0.26	0/1116	0.53	0/1490
68	NN	0.26	0/1028	0.48	0/1366
69	ZZ	0.26	0/828	0.49	0/1109
70	JJ	0.25	0/665	0.48	0/891
71	AA	0.26	0/447	0.46	0/587
72	DD	0.27	0/1796	0.54	0/2417
73	BB	0.26	0/1492	0.49	0/2005
74	SS	0.27	0/834	0.55	0/1125
75	RR	0.26	0/918	0.56	0/1233

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	9	0.26	0/1017	0.50	0/1358
77	II	0.27	0/1208	0.53	0/1618
78	PP	0.26	0/1115	0.50	0/1493
79	GG	0.25	0/805	0.50	0/1081
80	OO	0.24	0/604	0.51	0/810
81	FF	0.24	0/490	0.48	0/656
82	w	0.26	0/470	0.46	0/623
83	0	0.25	0/567	0.48	0/753
84	6	0.25	0/2493	0.53	0/3394
85	4	0.45	0/235	1.14	1/363 (0.3%)
All	All	0.29	2/234252 (0.0%)	0.89	583/344191 (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
5	B	0	2
20	R	0	1
21	S	0	1
23	U	0	1
34	f	0	1
67	VV	0	2
76	9	0	2
All	All	0	10

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	967	C	N3-C4	-5.24	1.30	1.33
51	K	1520	G	N9-C4	5.10	1.42	1.38

All (583) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	961	G	N1-C6-O6	-19.59	108.15	119.90
1	5	967	C	N3-C4-N4	-19.03	104.68	118.00
1	5	967	C	C5-C4-N4	16.73	131.91	120.20
1	5	961	G	C5-C6-O6	13.97	136.98	128.60
1	5	931	C	N1-C2-O2	13.86	127.22	118.90
1	5	931	C	C2-N1-C1'	13.23	133.35	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1072	C	N1-C2-O2	12.14	126.19	118.90
1	5	1072	C	C2-N1-C1'	11.32	131.25	118.80
1	5	931	C	N3-C2-O2	-10.89	114.27	121.90
51	K	1520	G	N3-C4-C5	-10.11	123.55	128.60
1	5	4420	U	C2-N1-C1'	10.01	129.72	117.70
1	5	4420	U	N1-C2-O2	10.01	129.80	122.80
51	K	1123	C	N1-C2-O2	9.79	124.77	118.90
1	5	100	C	C2-N1-C1'	9.70	129.47	118.80
51	K	853	C	C2-N1-C1'	9.36	129.09	118.80
51	K	1139	C	N1-C2-O2	9.35	124.51	118.90
1	5	1072	C	N3-C2-O2	-9.25	115.42	121.90
51	K	1261	C	N1-C2-O2	9.16	124.40	118.90
1	5	931	C	C6-N1-C1'	-9.12	109.85	120.80
1	5	4420	U	N3-C2-O2	-9.11	115.82	122.20
51	K	1520	G	C2-N3-C4	9.10	116.45	111.90
51	K	1078	C	N1-C2-O2	8.95	124.27	118.90
1	5	449	C	N1-C2-O2	8.90	124.24	118.90
1	5	4749	C	C2-N1-C1'	8.89	128.58	118.80
1	5	4749	C	N1-C2-O2	8.87	124.22	118.90
51	K	1078	C	C2-N1-C1'	8.85	128.54	118.80
51	K	1123	C	N3-C2-O2	-8.82	115.73	121.90
1	5	4413	C	C2-N1-C1'	8.77	128.45	118.80
1	5	931	C	C6-N1-C2	-8.77	116.79	120.30
51	K	853	C	N1-C2-O2	8.72	124.13	118.90
1	5	100	C	N1-C2-O2	8.54	124.03	118.90
51	K	1453	C	N1-C2-O2	8.44	123.96	118.90
51	K	1453	C	C2-N1-C1'	8.38	128.02	118.80
1	5	4119	C	N1-C2-O2	8.36	123.92	118.90
51	K	174	C	N3-C2-O2	-8.21	116.15	121.90
39	k	30	ASP	CB-CG-OD1	8.19	125.67	118.30
1	5	1381	U	C2-N1-C1'	8.13	127.45	117.70
1	5	1639	U	C2-N1-C1'	8.12	127.45	117.70
1	5	4119	C	C2-N1-C1'	8.11	127.72	118.80
1	5	1822	U	N1-C2-O2	8.04	128.43	122.80
1	5	972	C	N1-C2-O2	8.02	123.71	118.90
51	K	1261	C	C2-N1-C1'	8.00	127.60	118.80
1	5	1072	C	C6-N1-C1'	-7.98	111.22	120.80
1	5	4413	C	N1-C2-O2	7.98	123.69	118.90
51	K	1520	G	N3-C4-N9	7.96	130.78	126.00
51	K	1139	C	C2-N1-C1'	7.93	127.52	118.80
1	5	3594	C	N1-C2-O2	7.87	123.62	118.90
1	5	4413	C	N3-C2-O2	-7.86	116.39	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	449	C	C2-N1-C1'	7.85	127.44	118.80
1	5	1822	U	N3-C2-O2	-7.84	116.71	122.20
51	K	1139	C	N3-C2-O2	-7.84	116.41	121.90
51	K	1364	U	N1-C2-O2	7.82	128.27	122.80
51	K	1271	C	N1-C2-O2	7.77	123.56	118.90
1	5	499	G	C4-N9-C1'	7.76	136.59	126.50
1	5	453	G	C4-N9-C1'	7.73	136.55	126.50
1	5	3636	C	N3-C2-O2	-7.73	116.49	121.90
1	5	2023	C	N1-C2-O2	7.71	123.52	118.90
1	5	453	G	N3-C4-C5	-7.63	124.78	128.60
1	5	1236	C	N3-C2-O2	-7.63	116.56	121.90
3	8	128	C	N1-C2-O2	7.62	123.47	118.90
1	5	499	G	N3-C4-N9	7.60	130.56	126.00
51	K	1078	C	C6-N1-C2	-7.58	117.27	120.30
51	K	1261	C	N3-C2-O2	-7.56	116.61	121.90
51	K	1364	U	C2-N1-C1'	7.54	126.75	117.70
1	5	2499	C	N1-C2-O2	7.53	123.42	118.90
1	5	453	G	N3-C4-N9	7.53	130.52	126.00
1	5	687	U	N1-C2-O2	7.52	128.06	122.80
1	5	1639	U	N1-C2-O2	7.50	128.05	122.80
1	5	100	C	N3-C2-O2	-7.47	116.67	121.90
1	5	2015	U	C2'-C3'-O3'	7.46	125.91	109.50
51	K	1298	G	C4-N9-C1'	7.44	136.17	126.50
1	5	931	C	C5-C6-N1	7.38	124.69	121.00
51	K	1078	C	N3-C2-O2	-7.32	116.78	121.90
1	5	4305	G	C4-N9-C1'	7.31	136.00	126.50
51	K	578	C	N1-C2-O2	7.30	123.28	118.90
51	K	1298	G	N3-C4-N9	7.29	130.37	126.00
1	5	2097	U	C2-N1-C1'	7.27	126.42	117.70
1	5	1381	U	N1-C2-O2	7.26	127.88	122.80
1	5	961	G	N9-C4-C5	-7.25	102.50	105.40
51	K	183	G	C4-N9-C1'	7.25	135.92	126.50
1	5	1237	C	N1-C2-O2	7.25	123.25	118.90
51	K	1261	C	C6-N1-C2	-7.25	117.40	120.30
1	5	2097	U	N1-C2-O2	7.23	127.86	122.80
51	K	1303	C	N1-C2-O2	7.22	123.23	118.90
1	5	2819	U	N3-C2-O2	-7.21	117.15	122.20
1	5	2256	C	P-O3'-C3'	7.17	128.31	119.70
51	K	1298	G	N3-C4-C5	-7.17	125.01	128.60
1	5	2499	C	N3-C2-O2	-7.14	116.90	121.90
1	5	956	A	P-O3'-C3'	7.13	128.25	119.70
51	K	1364	U	N3-C2-O2	-7.10	117.23	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2046	G	P-O3'-C3'	7.09	128.21	119.70
1	5	1612	G	N3-C4-N9	7.08	130.25	126.00
1	5	2107	C	P-O3'-C3'	7.08	128.20	119.70
1	5	5027	C	P-O3'-C3'	7.08	128.19	119.70
51	K	1303	C	C2-N1-C1'	7.07	126.57	118.80
1	5	1772	C	N3-C2-O2	-7.06	116.96	121.90
51	K	293	C	N1-C2-O2	7.04	123.13	118.90
1	5	1076	C	C2-N1-C1'	7.03	126.54	118.80
51	K	1139	C	C6-N1-C2	-7.03	117.49	120.30
1	5	1072	C	C6-N1-C2	-7.02	117.49	120.30
1	5	4889	G	P-O3'-C3'	7.01	128.12	119.70
51	K	130	G	C4-N9-C1'	7.01	135.62	126.50
1	5	4749	C	N3-C2-O2	-7.00	117.00	121.90
1	5	687	U	N3-C2-O2	-6.98	117.32	122.20
1	5	1822	U	C2-N1-C1'	6.98	126.07	117.70
1	5	4413	C	O4'-C1'-N1	6.97	113.78	108.20
1	5	1772	C	N1-C2-O2	6.96	123.08	118.90
1	5	2695	A	P-O3'-C3'	6.96	128.05	119.70
51	K	1520	G	C4-N9-C1'	6.95	135.54	126.50
51	K	853	C	N3-C2-O2	-6.95	117.03	121.90
1	5	1639	U	N3-C2-O2	-6.92	117.36	122.20
1	5	449	C	N3-C2-O2	-6.89	117.07	121.90
51	K	130	G	N3-C4-N9	6.88	130.13	126.00
51	K	1624	U	C2-N1-C1'	6.88	125.95	117.70
1	5	1612	G	N3-C4-C5	-6.87	125.17	128.60
1	5	4757	C	C2-N1-C1'	6.86	126.34	118.80
1	5	4413	C	C6-N1-C2	-6.85	117.56	120.30
1	5	1481	C	N1-C2-O2	6.84	123.00	118.90
1	5	499	G	N3-C4-C5	-6.84	125.18	128.60
51	K	688	U	P-O3'-C3'	6.83	127.89	119.70
51	K	1274	G	C4-N9-C1'	6.82	135.36	126.50
1	5	4871	C	C2-N1-C1'	6.79	126.27	118.80
1	5	3636	C	N1-C2-O2	6.79	122.97	118.90
51	K	1624	U	N3-C2-O2	-6.78	117.45	122.20
51	K	1057	C	C2-N1-C1'	6.77	126.25	118.80
1	5	2257	C	P-O3'-C3'	6.76	127.82	119.70
51	K	1298	G	C8-N9-C1'	-6.76	118.21	127.00
1	5	499	G	C8-N9-C1'	-6.76	118.21	127.00
1	5	2528	G	C4-N9-C1'	6.76	135.28	126.50
1	5	1236	C	N1-C2-O2	6.74	122.95	118.90
1	5	972	C	N3-C2-O2	-6.74	117.19	121.90
1	5	4709	U	C2-N1-C1'	6.71	125.75	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4757	C	N1-C2-O2	6.71	122.92	118.90
1	5	4871	C	N1-C2-O2	6.69	122.92	118.90
1	5	3594	C	N3-C2-O2	-6.69	117.22	121.90
51	K	1453	C	N3-C2-O2	-6.68	117.22	121.90
1	5	3594	C	C6-N1-C2	-6.68	117.63	120.30
1	5	2528	G	N3-C4-N9	6.67	130.00	126.00
1	5	1612	G	C4-N9-C1'	6.67	135.17	126.50
49	2	4	U	N1-C2-O2	6.67	127.47	122.80
1	5	685	C	N1-C2-O2	6.66	122.89	118.90
1	5	4423	U	C2-N1-C1'	6.66	125.69	117.70
1	5	956	A	OP2-P-O3'	6.65	119.84	105.20
1	5	4714	C	N1-C2-O2	6.65	122.89	118.90
1	5	48	G	P-O3'-C3'	6.63	127.65	119.70
1	5	100	C	C6-N1-C1'	-6.61	112.86	120.80
51	K	1123	C	C2-N1-C1'	6.59	126.04	118.80
51	K	853	C	C6-N1-C1'	-6.58	112.90	120.80
1	5	1686	C	N1-C2-O2	6.58	122.85	118.90
1	5	100	C	C6-N1-C2	-6.58	117.67	120.30
1	5	2097	U	N3-C2-O2	-6.57	117.60	122.20
51	K	130	G	N3-C4-C5	-6.57	125.32	128.60
51	K	183	G	N3-C4-C5	-6.56	125.32	128.60
1	5	3741	C	N3-C2-O2	-6.55	117.32	121.90
1	5	4888	U	P-O3'-C3'	6.54	127.55	119.70
5	B	309	LEU	CA-CB-CG	6.53	130.32	115.30
51	K	1852	C	N1-C2-O2	6.52	122.81	118.90
1	5	4502	C	N1-C2-O2	6.52	122.81	118.90
1	5	2820	C	N1-C2-O2	6.52	122.81	118.90
51	K	1123	C	C6-N1-C2	-6.51	117.69	120.30
1	5	4171	C	N1-C2-O2	6.51	122.81	118.90
1	5	4305	G	N3-C4-N9	6.50	129.90	126.00
51	K	1689	C	C2-N1-C1'	6.50	125.95	118.80
1	5	50	C	N1-C2-O2	6.49	122.79	118.90
1	5	961	G	N3-C4-N9	6.49	129.90	126.00
1	5	2465	C	N1-C2-O2	6.49	122.79	118.90
1	5	1792	U	C2-N1-C1'	6.49	125.48	117.70
1	5	1481	C	C2-N1-C1'	6.48	125.93	118.80
1	5	4420	U	C6-N1-C1'	-6.48	112.13	121.20
1	5	4736	C	N1-C2-O2	6.47	122.78	118.90
1	5	1686	C	N3-C2-O2	-6.46	117.38	121.90
1	5	2011	C	N1-C2-O2	6.46	122.78	118.90
1	5	453	G	C8-N9-C1'	-6.46	118.61	127.00
1	5	4119	C	N3-C2-O2	-6.46	117.38	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	K	752	G	P-O3'-C3'	6.45	127.44	119.70
51	K	1274	G	N3-C4-N9	6.45	129.87	126.00
51	K	1274	G	N3-C4-C5	-6.44	125.38	128.60
1	5	4758	U	C2-N1-C1'	6.44	125.43	117.70
51	K	340	C	N1-C2-O2	6.43	122.76	118.90
1	5	489	C	N1-C2-O2	6.41	122.75	118.90
1	5	2023	C	C2-N1-C1'	6.41	125.85	118.80
51	K	1624	U	N1-C2-O2	6.40	127.28	122.80
1	5	1731	C	C2-N1-C1'	6.39	125.83	118.80
1	5	2819	U	N1-C2-O2	6.38	127.27	122.80
1	5	4305	G	N3-C4-C5	-6.37	125.41	128.60
1	5	1072	C	C5-C6-N1	6.37	124.18	121.00
1	5	2661	U	P-O3'-C3'	6.35	127.32	119.70
1	5	4946	U	N1-C2-O2	6.35	127.24	122.80
1	5	4229	U	N3-C2-O2	-6.35	117.76	122.20
51	K	183	G	N3-C4-N9	6.35	129.81	126.00
1	5	969	C	O4'-C1'-N1	6.33	113.27	108.20
51	K	356	C	C2-N1-C1'	6.33	125.77	118.80
1	5	4232	U	P-O3'-C3'	6.32	127.29	119.70
51	K	1689	C	N1-C2-O2	6.32	122.69	118.90
51	K	4	C	C2-N1-C1'	6.32	125.75	118.80
1	5	1812	C	C2-N1-C1'	6.32	125.75	118.80
1	5	2116	C	P-O3'-C3'	6.30	127.26	119.70
1	5	2528	G	N3-C4-C5	-6.30	125.45	128.60
1	5	1632	A	C2-N3-C4	6.29	113.74	110.60
1	5	4758	U	N1-C2-O2	6.27	127.19	122.80
1	5	1378	C	C6-N1-C2	-6.27	117.79	120.30
1	5	4237	C	C2-N1-C1'	6.27	125.69	118.80
1	5	1237	C	N3-C2-O2	-6.26	117.52	121.90
1	5	3594	C	C2-N1-C1'	6.26	125.69	118.80
1	5	4158	C	N3-C2-O2	-6.24	117.53	121.90
1	5	112	C	C2-N1-C1'	6.24	125.66	118.80
1	5	2465	C	N3-C2-O2	-6.22	117.55	121.90
1	5	1847	C	C2-N1-C1'	6.21	125.64	118.80
1	5	4749	C	C6-N1-C1'	-6.19	113.37	120.80
51	K	1271	C	N3-C2-O2	-6.19	117.57	121.90
51	K	1637	A	P-O3'-C3'	6.19	127.13	119.70
51	K	1057	C	N1-C2-O2	6.18	122.61	118.90
3	8	128	C	N3-C2-O2	-6.18	117.58	121.90
1	5	961	G	C4-C5-N7	6.17	113.27	110.80
51	K	1520	G	C8-N9-C4	-6.17	103.93	106.40
1	5	1210	C	C2-N1-C1'	6.17	125.59	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2023	C	N3-C2-O2	-6.17	117.58	121.90
49	2	49	C	N1-C2-O2	6.15	122.59	118.90
51	K	118	C	N1-C2-O2	6.13	122.58	118.90
1	5	4305	G	C8-N9-C1'	-6.13	119.04	127.00
51	K	531	A	P-O3'-C3'	6.12	127.04	119.70
1	5	4881	U	C2-N1-C1'	6.11	125.03	117.70
49	2	4	U	N3-C2-O2	-6.09	117.94	122.20
51	K	1078	C	C5-C6-N1	6.09	124.04	121.00
1	5	989	U	N1-C2-O2	6.08	127.05	122.80
51	K	1271	C	C2-N1-C1'	6.07	125.48	118.80
51	K	151	C	N1-C2-O2	6.07	122.54	118.90
1	5	1807	C	C2-N1-C1'	6.07	125.48	118.80
1	5	3636	C	C6-N1-C2	-6.07	117.87	120.30
1	5	685	C	C2-N1-C1'	6.05	125.45	118.80
1	5	687	U	C2-N1-C1'	6.05	124.96	117.70
1	5	1210	C	N1-C2-O2	6.05	122.53	118.90
51	K	293	C	C2-N1-C1'	6.05	125.45	118.80
1	5	1692	C	C2-N1-C1'	6.04	125.44	118.80
1	5	1381	U	N3-C2-O2	-6.03	117.98	122.20
51	K	578	C	N3-C2-O2	-6.03	117.68	121.90
1	5	1485	C	C2-N1-C1'	6.02	125.42	118.80
51	K	1118	C	C2-N1-C1'	6.01	125.41	118.80
2	7	29	C	C2-N1-C1'	6.00	125.40	118.80
18	P	91	LEU	CA-CB-CG	6.00	129.10	115.30
51	K	14	C	C2-N1-C1'	6.00	125.40	118.80
51	K	183	G	C8-N9-C1'	-5.99	119.21	127.00
51	K	1423	C	N1-C2-O2	5.99	122.49	118.90
1	5	2867	C	C2-N1-C1'	5.98	125.38	118.80
1	5	1273	G	C4-N9-C1'	5.98	134.27	126.50
51	K	130	G	C8-N9-C1'	-5.97	119.24	127.00
1	5	972	C	C6-N1-C2	-5.97	117.91	120.30
1	5	684	G	P-O3'-C3'	5.96	126.86	119.70
51	K	1389	C	N1-C2-O2	5.96	122.48	118.90
51	K	624	C	C6-N1-C2	-5.95	117.92	120.30
1	5	1081	C	C2-N1-C1'	5.94	125.33	118.80
1	5	2266	C	P-O3'-C3'	5.94	126.83	119.70
1	5	4177	C	C2-N1-C1'	5.94	125.33	118.80
51	K	824	C	N1-C2-O2	5.94	122.46	118.90
51	K	659	G	C4-N9-C1'	5.94	134.22	126.50
1	5	3741	C	N1-C2-O2	5.93	122.46	118.90
1	5	4215	C	N1-C2-O2	5.93	122.46	118.90
51	K	174	C	N1-C2-O2	5.92	122.45	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1485	C	N1-C2-O2	5.92	122.45	118.90
3	8	153	C	C2-N1-C1'	5.92	125.31	118.80
1	5	3778	U	N1-C2-O2	5.91	126.94	122.80
1	5	4476	C	C2-N1-C1'	5.91	125.31	118.80
1	5	4423	U	N3-C2-O2	-5.91	118.06	122.20
1	5	4656	A	P-O3'-C3'	5.91	126.79	119.70
1	5	4736	C	N3-C2-O2	-5.89	117.78	121.90
1	5	2093	A	P-O3'-C3'	5.89	126.77	119.70
1	5	4354	U	P-O3'-C3'	5.89	126.77	119.70
51	K	1358	U	N3-C2-O2	-5.89	118.08	122.20
51	K	1518	C	C2-N1-C1'	5.89	125.28	118.80
1	5	4423	U	N1-C2-O2	5.89	126.92	122.80
51	K	356	C	N1-C2-O2	5.88	122.43	118.90
1	5	930	G	P-O3'-C3'	5.88	126.75	119.70
1	5	4413	C	C6-N1-C1'	-5.88	113.75	120.80
1	5	4229	U	N1-C2-O2	5.87	126.91	122.80
51	K	1117	C	N1-C2-O2	5.87	122.42	118.90
1	5	4420	U	C5-C6-N1	5.86	125.63	122.70
3	8	124	U	P-O3'-C3'	5.86	126.73	119.70
1	5	2274	C	C2-N1-C1'	5.85	125.23	118.80
51	K	815	U	N3-C2-O2	-5.85	118.11	122.20
1	5	1835	G	P-O3'-C3'	5.84	126.71	119.70
51	K	1303	C	N3-C2-O2	-5.84	117.81	121.90
1	5	1671	U	N3-C2-O2	-5.84	118.11	122.20
1	5	3876	A	P-O3'-C3'	5.84	126.71	119.70
1	5	3739	C	N1-C2-O2	5.83	122.40	118.90
1	5	2117	G	C4-N9-C1'	5.83	134.08	126.50
1	5	2528	G	C8-N9-C1'	-5.83	119.42	127.00
1	5	4749	C	C6-N1-C2	-5.82	117.97	120.30
1	5	506	C	C2-N1-C1'	5.82	125.20	118.80
1	5	134	G	P-O3'-C3'	5.82	126.68	119.70
1	5	4952	G	N3-C4-C5	-5.81	125.69	128.60
51	K	1660	C	C2-N1-C1'	5.81	125.19	118.80
1	5	920	C	C2-N1-C1'	5.81	125.19	118.80
1	5	4758	U	N3-C2-O2	-5.81	118.14	122.20
1	5	115	C	C2-N1-C1'	5.79	125.16	118.80
1	5	4402	C	N1-C2-O2	5.79	122.37	118.90
1	5	2123	C	P-O3'-C3'	5.78	126.64	119.70
1	5	449	C	C6-N1-C2	-5.78	117.99	120.30
51	K	579	C	N1-C2-O2	5.78	122.37	118.90
51	K	1271	C	C6-N1-C2	-5.77	117.99	120.30
1	5	155	C	N3-C2-O2	-5.76	117.86	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4964	C	N1-C2-O2	5.76	122.36	118.90
1	5	1381	U	C6-N1-C1'	-5.76	113.14	121.20
1	5	4303	C	C2-N1-C1'	5.76	125.14	118.80
1	5	245	C	P-O3'-C3'	5.76	126.61	119.70
1	5	1273	G	N3-C4-C5	-5.76	125.72	128.60
1	5	1074	G	N3-C4-N9	5.75	129.45	126.00
51	K	1453	C	C6-N1-C2	-5.75	118.00	120.30
51	K	1709	G	C4-N9-C1'	5.75	133.97	126.50
1	5	1804	A	P-O3'-C3'	5.75	126.60	119.70
1	5	458	C	N1-C2-O2	5.75	122.35	118.90
51	K	1261	C	C5-C6-N1	5.74	123.87	121.00
51	K	853	C	C6-N1-C2	-5.73	118.01	120.30
1	5	1428	U	N1-C2-O2	5.72	126.81	122.80
1	5	1273	G	N3-C4-N9	5.72	129.43	126.00
1	5	1792	U	N3-C2-O2	-5.72	118.19	122.20
1	5	4682	U	N1-C2-O2	5.72	126.80	122.80
49	2	4	U	C2-N1-C1'	5.72	124.56	117.70
1	5	1367	C	C2-N1-C1'	5.71	125.08	118.80
51	K	465	A	P-O3'-C3'	5.71	126.55	119.70
51	K	1358	U	N1-C2-O2	5.71	126.80	122.80
1	5	1792	U	N1-C2-O2	5.70	126.79	122.80
51	K	1274	G	C8-N9-C1'	-5.70	119.59	127.00
2	7	28	C	N1-C2-O2	5.70	122.32	118.90
1	5	451	C	P-O3'-C3'	5.69	126.53	119.70
51	K	614	C	P-O3'-C3'	5.69	126.53	119.70
1	5	4881	U	N1-C2-O2	5.69	126.78	122.80
1	5	1848	C	N1-C2-O2	5.69	122.31	118.90
57	y	36	LEU	CA-CB-CG	5.69	128.38	115.30
1	5	690	C	N1-C2-O2	5.68	122.31	118.90
1	5	943	A	P-O3'-C3'	5.68	126.52	119.70
1	5	4170	A	P-O3'-C3'	5.68	126.52	119.70
51	K	1453	C	C6-N1-C1'	-5.68	113.98	120.80
1	5	967	C	N1-C2-O2	5.67	122.30	118.90
1	5	1612	G	C8-N9-C1'	-5.67	119.63	127.00
1	5	1671	U	N1-C2-O2	5.67	126.77	122.80
1	5	4946	U	N3-C2-O2	-5.66	118.24	122.20
51	K	182	C	P-O3'-C3'	5.66	126.49	119.70
1	5	1429	C	N1-C2-O2	5.66	122.30	118.90
1	5	4612	C	N1-C2-O2	5.66	122.29	118.90
1	5	4482	U	N3-C2-O2	-5.65	118.25	122.20
51	K	531	A	OP1-P-O3'	5.65	117.63	105.20
51	K	4	C	N1-C2-O2	5.65	122.29	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	4682	U	N3-C2-O2	-5.64	118.25	122.20
1	5	4119	C	C6-N1-C1'	-5.64	114.03	120.80
1	5	4952	G	N3-C4-N9	5.63	129.38	126.00
1	5	1076	C	N1-C2-O2	5.62	122.28	118.90
51	K	1289	U	N1-C2-O2	5.62	126.74	122.80
51	K	870	A	P-O3'-C3'	5.61	126.43	119.70
1	5	4682	U	C2-N1-C1'	5.61	124.43	117.70
51	K	1742	C	C2-N1-C1'	5.61	124.97	118.80
1	5	4714	C	N3-C2-O2	-5.60	117.98	121.90
1	5	1232	G	P-O3'-C3'	5.60	126.42	119.70
1	5	690	C	C2-N1-C1'	5.60	124.96	118.80
51	K	1057	C	N3-C2-O2	-5.59	117.99	121.90
1	5	218	A	P-O3'-C3'	5.59	126.41	119.70
1	5	2083	C	P-O3'-C3'	5.58	126.40	119.70
1	5	1079	C	N1-C2-O2	5.58	122.25	118.90
51	K	1022	U	C2-N1-C1'	5.58	124.40	117.70
51	K	1116	C	N1-C2-O2	5.58	122.25	118.90
51	K	1078	C	C6-N1-C1'	-5.57	114.12	120.80
1	5	2820	C	N3-C2-O2	-5.56	118.01	121.90
1	5	972	C	C2-N1-C1'	5.55	124.90	118.80
1	5	1598	C	N1-C2-O2	5.54	122.23	118.90
1	5	4964	C	N3-C2-O2	-5.54	118.02	121.90
1	5	2410	C	C2-N1-C1'	5.53	124.89	118.80
1	5	2560	C	C2-N1-C1'	5.53	124.88	118.80
1	5	3657	U	N3-C2-O2	-5.53	118.33	122.20
51	K	1826	G	N3-C4-N9	5.53	129.32	126.00
1	5	1378	C	C5-C6-N1	5.52	123.76	121.00
1	5	2023	C	C6-N1-C2	-5.52	118.09	120.30
51	K	1551	U	C2-N1-C1'	5.52	124.33	117.70
51	K	1826	G	C4-N9-C1'	5.52	133.68	126.50
1	5	221	C	C2-N1-C1'	5.50	124.86	118.80
1	5	453	G	C2-N3-C4	5.50	114.65	111.90
1	5	1893	C	C2-N1-C1'	5.50	124.86	118.80
51	K	1073	U	N3-C2-O2	-5.50	118.35	122.20
1	5	4237	C	C6-N1-C2	-5.50	118.10	120.30
51	K	151	C	C2-N1-C1'	5.49	124.84	118.80
1	5	2704	C	N1-C2-O2	5.47	122.19	118.90
1	5	1359	G	C4-N9-C1'	5.46	133.60	126.50
1	5	1929	A	C4-N9-C1'	5.45	136.12	126.30
1	5	4952	G	C4-N9-C1'	5.45	133.59	126.50
1	5	2787	A	C2-N3-C4	5.45	113.33	110.60
1	5	1359	G	N7-C8-N9	5.45	115.82	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2085	G	C4-N9-C1'	5.45	133.58	126.50
1	5	155	C	N1-C2-O2	5.44	122.17	118.90
1	5	685	C	N3-C2-O2	-5.44	118.09	121.90
50	3	49	C	N1-C2-O2	5.44	122.16	118.90
1	5	961	G	C8-N9-C1'	-5.43	119.93	127.00
51	K	151	C	C6-N1-C2	-5.43	118.13	120.30
1	5	4757	C	N3-C2-O2	-5.43	118.10	121.90
51	K	427	U	C2-N1-C1'	5.43	124.21	117.70
1	5	4560	C	N1-C2-O2	5.42	122.16	118.90
1	5	4627	U	N1-C2-O2	5.42	126.60	122.80
1	5	4749	C	O4'-C1'-N1	5.42	112.54	108.20
1	5	4171	C	N3-C2-O2	-5.42	118.11	121.90
1	5	100	C	O4'-C1'-N1	5.41	112.53	108.20
51	K	1709	G	N3-C4-N9	5.41	129.24	126.00
1	5	989	U	N3-C2-O2	-5.41	118.42	122.20
1	5	1458	C	N1-C2-O2	5.41	122.14	118.90
1	5	2117	G	N3-C4-C5	-5.41	125.90	128.60
1	5	2117	G	N3-C4-N9	5.41	129.24	126.00
1	5	2083	C	OP2-P-O3'	5.40	117.08	105.20
1	5	4482	U	N1-C2-O2	5.40	126.58	122.80
85	4	44	C	N1-C2-O2	5.40	122.14	118.90
1	5	4243	C	C6-N1-C2	-5.40	118.14	120.30
51	K	1298	G	O4'-C1'-N9	-5.39	103.89	108.20
1	5	2256	C	N1-C2-O2	5.39	122.14	118.90
1	5	1339	U	N1-C2-O2	5.39	126.57	122.80
1	5	2454	U	N3-C2-O2	-5.38	118.43	122.20
5	B	214	ASP	CB-CG-OD1	5.38	123.14	118.30
2	7	28	C	N3-C2-O2	-5.38	118.14	121.90
3	8	128	C	C2-N1-C1'	5.38	124.71	118.80
1	5	3772	U	C2-N1-C1'	5.37	124.15	117.70
51	K	168	C	N1-C2-O2	5.37	122.12	118.90
51	K	1118	C	N1-C2-O2	5.37	122.12	118.90
1	5	1656	U	N1-C2-O2	5.36	126.55	122.80
1	5	2470	C	N1-C2-O2	5.36	122.12	118.90
1	5	4171	C	C6-N1-C2	-5.36	118.16	120.30
1	5	1929	A	C2-N3-C4	5.36	113.28	110.60
1	5	1	C	P-O3'-C3'	5.35	126.12	119.70
1	5	3778	U	N3-C2-O2	-5.35	118.45	122.20
1	5	5022	U	P-O3'-C3'	5.35	126.12	119.70
51	K	1314	U	C2-N1-C1'	5.35	124.12	117.70
1	5	2072	C	C6-N1-C2	-5.35	118.16	120.30
1	5	4881	U	N3-C2-O2	-5.34	118.46	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	2257	C	OP1-P-O3'	5.34	116.95	105.20
1	5	245	C	N1-C2-O2	5.34	122.10	118.90
1	5	4502	C	N3-C2-O2	-5.34	118.16	121.90
51	K	624	C	C5-C6-N1	5.33	123.67	121.00
1	5	449	C	C6-N1-C1'	-5.33	114.40	120.80
1	5	48	G	OP2-P-O3'	5.33	116.92	105.20
1	5	1367	C	N1-C2-O2	5.33	122.10	118.90
51	K	1395	C	P-O3'-C3'	5.33	126.09	119.70
1	5	4177	C	C6-N1-C2	-5.32	118.17	120.30
2	7	29	C	N1-C2-O2	5.32	122.09	118.90
1	5	1848	C	C2-N1-C1'	5.32	124.65	118.80
1	5	961	G	N1-C2-N3	-5.32	120.71	123.90
51	K	630	U	C2-N1-C1'	5.31	124.07	117.70
1	5	4171	C	C2-N1-C1'	5.31	124.64	118.80
1	5	1915	C	N1-C2-O2	5.31	122.08	118.90
51	K	537	C	C2-N1-C1'	5.30	124.63	118.80
51	K	1057	C	C6-N1-C2	-5.30	118.18	120.30
1	5	647	G	C4-N9-C1'	5.30	133.39	126.50
51	K	14	C	C6-N1-C2	-5.30	118.18	120.30
51	K	823	U	C2-N1-C1'	5.30	124.06	117.70
51	K	532	C	P-O3'-C3'	5.30	126.06	119.70
1	5	2661	U	OP1-P-O3'	5.29	116.85	105.20
1	5	1639	U	C6-N1-C1'	-5.29	113.79	121.20
1	5	2904	U	C2-N1-C1'	5.29	124.05	117.70
1	5	2726	G	C4-N9-C1'	5.29	133.38	126.50
1	5	489	C	N3-C2-O2	-5.29	118.20	121.90
1	5	3622	C	N1-C2-O2	5.29	122.07	118.90
1	5	2704	C	C2-N1-C1'	5.29	124.61	118.80
51	K	1073	U	N1-C2-O2	5.28	126.49	122.80
1	5	1853	G	C4-N9-C1'	5.27	133.35	126.50
51	K	1139	C	C5-C6-N1	5.27	123.64	121.00
1	5	458	C	C2-N1-C1'	5.27	124.59	118.80
51	K	340	C	N3-C2-O2	-5.27	118.21	121.90
51	K	369	C	N1-C2-O2	5.26	122.06	118.90
1	5	961	G	C5-C6-N1	5.26	114.13	111.50
1	5	1686	C	C6-N1-C2	-5.26	118.20	120.30
1	5	30	C	C2-N1-C1'	5.25	124.58	118.80
1	5	2499	C	C6-N1-C2	-5.25	118.20	120.30
51	K	983	A	N3-C4-N9	5.25	131.60	127.40
1	5	654	C	C6-N1-C2	-5.25	118.20	120.30
1	5	3778	U	C2-N1-C1'	5.25	124.00	117.70
1	5	4162	C	N1-C2-O2	5.25	122.05	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1241	C	OP1-P-O3'	5.24	116.74	105.20
1	5	3772	U	N3-C2-O2	-5.24	118.53	122.20
51	K	1061	U	P-O3'-C3'	5.24	125.98	119.70
1	5	3772	U	N1-C2-O2	5.23	126.46	122.80
1	5	50	C	N3-C2-O2	-5.23	118.24	121.90
1	5	3673	C	N1-C2-O2	5.23	122.04	118.90
1	5	266	C	O5'-P-OP2	-5.23	101.00	105.70
1	5	1211	G	P-O3'-C3'	5.22	125.97	119.70
1	5	1807	C	N1-C2-O2	5.22	122.03	118.90
1	5	4871	C	C6-N1-C1'	-5.22	114.53	120.80
51	K	815	U	N1-C2-O2	5.22	126.45	122.80
1	5	1214	C	N1-C2-O2	5.22	122.03	118.90
51	K	142	C	N1-C2-O2	5.22	122.03	118.90
1	5	3670	C	N1-C2-O2	5.21	122.03	118.90
51	K	1518	C	N1-C2-O2	5.21	122.03	118.90
51	K	1798	C	C6-N1-C2	-5.21	118.21	120.30
1	5	1339	U	N3-C2-O2	-5.21	118.55	122.20
51	K	1364	U	C5-C6-N1	5.21	125.31	122.70
51	K	659	G	C8-N9-C1'	-5.21	120.23	127.00
1	5	2011	C	N3-C2-O2	-5.21	118.25	121.90
8	E	46	LEU	CA-CB-CG	5.21	127.28	115.30
1	5	932	A	C4-N9-C1'	5.20	135.66	126.30
1	5	3926	C	C2-N1-C1'	5.20	124.52	118.80
1	5	2362	U	N3-C2-O2	-5.20	118.56	122.20
1	5	1859	C	N1-C2-O2	5.19	122.02	118.90
1	5	2860	C	N1-C2-O2	5.19	122.02	118.90
51	K	1397	U	N3-C2-O2	-5.19	118.56	122.20
3	8	54	C	N1-C2-O2	5.19	122.01	118.90
1	5	1325	C	N1-C2-O2	5.18	122.01	118.90
1	5	2096	G	C4-N9-C1'	5.18	133.24	126.50
1	5	1633	G	P-O3'-C3'	5.18	125.92	119.70
51	K	1389	C	N3-C2-O2	-5.18	118.27	121.90
1	5	2089	G	N3-C4-N9	5.18	129.11	126.00
28	Z	30	ASP	CB-CG-OD1	5.17	122.96	118.30
1	5	486	C	P-O3'-C3'	5.17	125.91	119.70
1	5	1428	U	N3-C2-O2	-5.17	118.58	122.20
51	K	183	G	C2-N3-C4	5.17	114.49	111.90
51	K	1289	U	N3-C2-O2	-5.17	118.58	122.20
51	K	1624	U	O4'-C1'-N1	5.17	112.34	108.20
1	5	3882	C	C2-N1-C1'	5.17	124.49	118.80
1	5	2502	G	P-O3'-C3'	5.17	125.90	119.70
1	5	4942	C	C2-N1-C1'	5.17	124.48	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	657	C	N3-C2-O2	-5.16	118.29	121.90
1	5	2096	G	N3-C4-C5	-5.16	126.02	128.60
45	r	20	ARG	CA-CB-CG	5.16	124.75	113.40
50	3	8	U	C2-N1-C1'	5.16	123.89	117.70
1	5	1241	C	P-O3'-C3'	5.16	125.89	119.70
51	K	1331	C	N1-C2-O2	5.16	121.99	118.90
1	5	690	C	C6-N1-C2	-5.15	118.24	120.30
51	K	293	C	N3-C2-O2	-5.15	118.29	121.90
51	K	687	C	N1-C2-O2	5.15	121.99	118.90
1	5	125	C	P-O3'-C3'	5.15	125.88	119.70
51	K	1709	G	N3-C4-C5	-5.14	126.03	128.60
3	8	135	C	C2-N1-C1'	5.14	124.45	118.80
1	5	218	A	OP1-P-O3'	5.13	116.50	105.20
2	7	28	C	C6-N1-C2	-5.13	118.25	120.30
51	K	914	U	C2-N1-C1'	5.13	123.86	117.70
51	K	93	U	N1-C2-O2	5.13	126.39	122.80
1	5	4119	C	C6-N1-C2	-5.13	118.25	120.30
51	K	1397	U	N1-C2-O2	5.13	126.39	122.80
1	5	515	C	C5-C6-N1	5.12	123.56	121.00
1	5	1848	C	C6-N1-C2	-5.12	118.25	120.30
3	8	2	G	C4-N9-C1'	5.11	133.15	126.50
3	8	64	U	N3-C2-O2	-5.11	118.62	122.20
1	5	250	C	C2-N1-C1'	5.11	124.42	118.80
1	5	2532	C	C2-N1-C1'	5.11	124.42	118.80
1	5	2572	C	C2-N1-C1'	5.11	124.42	118.80
1	5	3594	C	C5-C6-N1	5.10	123.55	121.00
51	K	295	C	C2-N1-C1'	5.10	124.41	118.80
1	5	1816	C	C5-C6-N1	5.10	123.55	121.00
1	5	2362	U	N1-C2-O2	5.09	126.37	122.80
1	5	2856	C	N1-C2-O2	5.09	121.96	118.90
1	5	2502	G	OP1-P-O3'	5.09	116.40	105.20
1	5	275	C	P-O3'-C3'	5.09	125.81	119.70
51	K	1595	U	N1-C2-O2	5.09	126.36	122.80
1	5	1296	G	P-O3'-C3'	5.09	125.80	119.70
1	5	1731	C	C5-C6-N1	5.09	123.54	121.00
1	5	4237	C	C5-C6-N1	5.09	123.54	121.00
1	5	489	C	C2-N1-C1'	5.08	124.39	118.80
51	K	442	C	C5-C6-N1	5.08	123.54	121.00
51	K	1389	C	C2-N1-C1'	5.08	124.39	118.80
1	5	5027	C	N1-C2-O2	5.07	121.94	118.90
50	3	74	C	C2-N1-C1'	5.07	124.38	118.80
3	8	55	U	N3-C2-O2	-5.07	118.65	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	5	1694	C	C6-N1-C2	-5.07	118.27	120.30
1	5	515	C	C2-N1-C1'	5.06	124.37	118.80
1	5	4627	U	N3-C2-O2	-5.06	118.66	122.20
1	5	187	U	P-O3'-C3'	5.06	125.77	119.70
1	5	2410	C	C6-N1-C2	-5.06	118.28	120.30
49	2	33	U	C2-N1-C1'	5.06	123.77	117.70
51	K	887	U	C2-N1-C1'	5.06	123.77	117.70
1	5	2274	C	C6-N1-C2	-5.06	118.28	120.30
1	5	647	G	N3-C4-N9	5.05	129.03	126.00
1	5	919	C	C2-N1-C1'	5.05	124.36	118.80
1	5	1656	U	N3-C2-O2	-5.05	118.67	122.20
1	5	5059	C	P-O3'-C3'	5.04	125.75	119.70
1	5	1280	C	C6-N1-C2	-5.04	118.28	120.30
1	5	4613	C	N1-C2-O2	5.04	121.92	118.90
1	5	506	C	C5-C6-N1	5.04	123.52	121.00
51	K	578	C	C6-N1-C2	-5.03	118.29	120.30
1	5	4885	U	P-O3'-C3'	5.02	125.72	119.70
1	5	1295	C	C2-N1-C1'	5.02	124.32	118.80
51	K	1798	C	C5-C6-N1	5.02	123.51	121.00
49	2	39	U	P-O3'-C3'	5.02	125.72	119.70
51	K	1067	C	C2-N1-C1'	5.02	124.32	118.80
1	5	936	C	N1-C2-O2	5.01	121.91	118.90
1	5	2008	U	C2-N1-C1'	5.01	123.72	117.70
10	G	146	LEU	CA-CB-CG	5.01	126.83	115.30
2	7	102	U	N1-C2-O2	5.01	126.31	122.80
51	K	1185	C	N1-C2-O2	5.01	121.91	118.90
51	K	1649	U	N1-C2-O2	5.01	126.31	122.80
1	5	2410	C	C5-C6-N1	5.01	123.50	121.00
1	5	282	C	N1-C2-O2	5.01	121.90	118.90
51	K	1271	C	C5-C6-N1	5.01	123.50	121.00
1	5	4194	U	C2-N1-C1'	5.00	123.71	117.70

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
76	9	17	TYR	Peptide
76	9	37	TYR	Peptide
5	B	17	LEU	Peptide
5	B	258	HIS	Peptide
20	R	18	GLY	Peptide
21	S	164	LYS	Peptide

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Mol	Chain	Res	Type	Group
23	U	27	HIS	Peptide
67	VV	61	GLN	Mainchain,Peptide
34	f	106	TYR	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	242/244 (99%)	222 (92%)	20 (8%)	0	100	100
5	B	392/394 (100%)	370 (94%)	21 (5%)	1 (0%)	41	73
6	C	360/362 (99%)	338 (94%)	22 (6%)	0	100	100
7	D	290/292 (99%)	273 (94%)	17 (6%)	0	100	100
8	E	232/248 (94%)	195 (84%)	37 (16%)	0	100	100
9	F	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
10	G	239/241 (99%)	213 (89%)	26 (11%)	0	100	100
11	H	188/190 (99%)	174 (93%)	14 (7%)	0	100	100
12	I	200/213 (94%)	192 (96%)	8 (4%)	0	100	100
13	J	167/169 (99%)	155 (93%)	12 (7%)	0	100	100
14	L	208/210 (99%)	190 (91%)	17 (8%)	1 (0%)	29	64
15	M	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
16	N	201/203 (99%)	190 (94%)	11 (6%)	0	100	100
17	O	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
18	P	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
19	Q	185/187 (99%)	176 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	R	178/180 (99%)	170 (96%)	8 (4%)	0	100	100
21	S	173/175 (99%)	164 (95%)	8 (5%)	1 (1%)	25	59
22	T	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
23	U	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
24	V	129/131 (98%)	120 (93%)	9 (7%)	0	100	100
25	W	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
26	X	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
27	Y	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
28	Z	133/135 (98%)	122 (92%)	9 (7%)	2 (2%)	10	39
29	a	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
30	b	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
31	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
32	d	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
33	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
34	f	107/109 (98%)	99 (92%)	8 (8%)	0	100	100
35	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
36	h	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
37	i	100/102 (98%)	92 (92%)	8 (8%)	0	100	100
38	j	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
39	k	67/69 (97%)	59 (88%)	8 (12%)	0	100	100
40	l	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
41	m	50/52 (96%)	50 (100%)	0	0	100	100
42	n	21/23 (91%)	21 (100%)	0	0	100	100
43	o	102/104 (98%)	94 (92%)	7 (7%)	1 (1%)	15	49
44	p	89/91 (98%)	84 (94%)	5 (6%)	0	100	100
45	r	123/125 (98%)	110 (89%)	11 (9%)	2 (2%)	9	37
46	s	196/198 (99%)	178 (91%)	18 (9%)	0	100	100
47	t	161/163 (99%)	124 (77%)	36 (22%)	1 (1%)	25	59
48	1	22/24 (92%)	21 (96%)	1 (4%)	0	100	100
52	q	215/217 (99%)	204 (95%)	11 (5%)	0	100	100
53	u	211/213 (99%)	199 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	v	219/221 (99%)	213 (97%)	6 (3%)	0	100	100
55	x	260/262 (99%)	247 (95%)	13 (5%)	0	100	100
56	z	235/237 (99%)	232 (99%)	3 (1%)	0	100	100
57	y	181/189 (96%)	172 (95%)	9 (5%)	0	100	100
58	CC	204/206 (99%)	189 (93%)	15 (7%)	0	100	100
59	XX	183/185 (99%)	178 (97%)	5 (3%)	0	100	100
60	EE	139/151 (92%)	131 (94%)	8 (6%)	0	100	100
61	QQ	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
62	MM	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
63	UU	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
64	YY	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
65	HH	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
66	TT	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
67	VV	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	57
68	NN	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
69	ZZ	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
70	JJ	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
71	AA	53/55 (96%)	52 (98%)	1 (2%)	0	100	100
72	DD	226/228 (99%)	221 (98%)	5 (2%)	0	100	100
73	BB	181/191 (95%)	170 (94%)	11 (6%)	0	100	100
74	SS	94/96 (98%)	88 (94%)	6 (6%)	0	100	100
75	RR	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
76	9	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
77	II	142/144 (99%)	129 (91%)	13 (9%)	0	100	100
78	PP	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
79	GG	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
80	OO	73/75 (97%)	70 (96%)	3 (4%)	0	100	100
81	FF	60/62 (97%)	60 (100%)	0	0	100	100
82	w	53/55 (96%)	53 (100%)	0	0	100	100
83	0	66/68 (97%)	61 (92%)	5 (8%)	0	100	100
84	6	311/313 (99%)	289 (93%)	22 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11507/11712 (98%)	10831 (94%)	666 (6%)	10 (0%)	54 83

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	L	64	VAL
67	VV	62	PRO
43	o	97	LYS
45	r	19	LYS
45	r	21	ASN
28	Z	30	ASP
47	t	3	PRO
21	S	165	PRO
28	Z	90	PRO
5	B	259	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	A	187/187 (100%)	182 (97%)	5 (3%)	44 74
5	B	336/342 (98%)	334 (99%)	2 (1%)	86 94
6	C	302/302 (100%)	297 (98%)	5 (2%)	60 83
7	D	247/247 (100%)	247 (100%)	0	100 100
8	E	208/221 (94%)	206 (99%)	2 (1%)	76 90
9	F	194/195 (100%)	194 (100%)	0	100 100
10	G	206/206 (100%)	201 (98%)	5 (2%)	49 76
11	H	169/169 (100%)	167 (99%)	2 (1%)	71 88
12	I	174/180 (97%)	171 (98%)	3 (2%)	60 83
13	J	142/142 (100%)	140 (99%)	2 (1%)	67 86
14	L	176/176 (100%)	174 (99%)	2 (1%)	73 89
15	M	117/117 (100%)	117 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	171/171 (100%)	170 (99%)	1 (1%)	86	94
17	O	171/171 (100%)	165 (96%)	6 (4%)	36	68
18	P	134/134 (100%)	133 (99%)	1 (1%)	84	93
19	Q	163/163 (100%)	163 (100%)	0	100	100
20	R	159/159 (100%)	157 (99%)	2 (1%)	69	87
21	S	156/156 (100%)	156 (100%)	0	100	100
22	T	139/139 (100%)	138 (99%)	1 (1%)	84	93
23	U	89/89 (100%)	89 (100%)	0	100	100
24	V	101/101 (100%)	100 (99%)	1 (1%)	76	90
25	W	55/55 (100%)	54 (98%)	1 (2%)	59	82
26	X	107/107 (100%)	106 (99%)	1 (1%)	78	91
27	Y	124/124 (100%)	123 (99%)	1 (1%)	81	92
28	Z	117/117 (100%)	116 (99%)	1 (1%)	78	91
29	a	119/119 (100%)	119 (100%)	0	100	100
30	b	62/62 (100%)	61 (98%)	1 (2%)	62	84
31	c	79/79 (100%)	78 (99%)	1 (1%)	69	87
32	d	98/98 (100%)	96 (98%)	2 (2%)	55	80
33	e	114/114 (100%)	113 (99%)	1 (1%)	78	91
34	f	88/88 (100%)	87 (99%)	1 (1%)	73	89
35	g	98/98 (100%)	96 (98%)	2 (2%)	55	80
36	h	109/109 (100%)	108 (99%)	1 (1%)	78	91
37	i	86/86 (100%)	85 (99%)	1 (1%)	71	88
38	j	73/73 (100%)	71 (97%)	2 (3%)	44	74
39	k	64/64 (100%)	64 (100%)	0	100	100
40	l	47/47 (100%)	44 (94%)	3 (6%)	17	48
41	m	48/48 (100%)	48 (100%)	0	100	100
42	n	22/22 (100%)	22 (100%)	0	100	100
43	o	92/92 (100%)	89 (97%)	3 (3%)	38	69
44	p	74/74 (100%)	72 (97%)	2 (3%)	44	74
45	r	109/109 (100%)	105 (96%)	4 (4%)	34	66
46	s	166/166 (100%)	165 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	t	136/136 (100%)	133 (98%)	3 (2%)	52	78
48	1	22/22 (100%)	21 (96%)	1 (4%)	27	60
52	q	180/181 (99%)	179 (99%)	1 (1%)	86	94
53	u	194/194 (100%)	191 (98%)	3 (2%)	65	85
54	v	187/187 (100%)	185 (99%)	2 (1%)	73	89
55	x	224/224 (100%)	222 (99%)	2 (1%)	78	91
56	z	207/207 (100%)	205 (99%)	2 (1%)	76	90
57	y	165/169 (98%)	165 (100%)	0	100	100
58	CC	178/178 (100%)	175 (98%)	3 (2%)	60	83
59	XX	161/161 (100%)	158 (98%)	3 (2%)	57	81
60	EE	130/136 (96%)	127 (98%)	3 (2%)	50	77
61	QQ	130/130 (100%)	129 (99%)	1 (1%)	81	92
62	MM	106/106 (100%)	104 (98%)	2 (2%)	57	81
63	UU	117/117 (100%)	114 (97%)	3 (3%)	46	74
64	YY	119/119 (100%)	119 (100%)	0	100	100
65	HH	67/67 (100%)	66 (98%)	1 (2%)	65	85
66	TT	112/112 (100%)	112 (100%)	0	100	100
67	VV	113/113 (100%)	113 (100%)	0	100	100
68	NN	107/107 (100%)	106 (99%)	1 (1%)	78	91
69	ZZ	88/88 (100%)	88 (100%)	0	100	100
70	JJ	75/75 (100%)	74 (99%)	1 (1%)	69	87
71	AA	46/46 (100%)	44 (96%)	2 (4%)	29	62
72	DD	190/190 (100%)	185 (97%)	5 (3%)	46	74
73	BB	158/161 (98%)	158 (100%)	0	100	100
74	SS	87/87 (100%)	86 (99%)	1 (1%)	73	89
75	RR	99/99 (100%)	98 (99%)	1 (1%)	76	90
76	9	109/109 (100%)	108 (99%)	1 (1%)	78	91
77	II	125/125 (100%)	124 (99%)	1 (1%)	81	92
78	PP	111/111 (100%)	110 (99%)	1 (1%)	78	91
79	GG	92/92 (100%)	91 (99%)	1 (1%)	73	89
80	OO	66/66 (100%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
81	FF	55/55 (100%)	54 (98%)	1 (2%)	59	82
82	w	48/48 (100%)	48 (100%)	0	100	100
83	0	61/61 (100%)	60 (98%)	1 (2%)	62	84
84	6	272/272 (100%)	270 (99%)	2 (1%)	84	93
All	All	10029/10069 (100%)	9911 (99%)	118 (1%)	72	88

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	64	ARG
4	A	128	ARG
4	A	163	ARG
4	A	193	ARG
4	A	242	ARG
5	B	24	ARG
5	B	62	ARG
6	C	38	ASN
6	C	100	ARG
6	C	114	ARG
6	C	188	ARG
6	C	321	ASN
8	E	52	ARG
8	E	178	ASN
10	G	38	ASN
10	G	81	ASN
10	G	189	ARG
10	G	196	ARG
10	G	240	ASN
11	H	1	MET
11	H	28	LYS
12	I	3	ARG
12	I	100	ASN
12	I	144	ASN
13	J	146	ARG
13	J	151	ILE
14	L	104	ASN
14	L	162	LYS
16	N	38	ARG
17	O	12	ARG
17	O	65	ASN
17	O	94	ARG

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Mol	Chain	Res	Type
17	O	117	ARG
17	O	187	LYS
17	O	191	ARG
18	P	128	ARG
20	R	39	GLN
20	R	133	LYS
22	T	63	ARG
24	V	48	ARG
25	W	45	ASN
26	X	94	ASN
27	Y	2	LYS
28	Z	97	ASN
30	b	60	ASN
31	c	90	ARG
32	d	18	ASN
32	d	23	ARG
33	e	43	ASN
34	f	16	ARG
35	g	21	ARG
35	g	29	ARG
36	h	96	ASN
37	i	29	ARG
38	j	20	ARG
38	j	45	ARG
40	l	21	ARG
40	l	33	ASN
40	l	36	ARG
43	o	9	ARG
43	o	69	ARG
43	o	82	MET
44	p	17	ARG
44	p	49	ARG
45	r	12	ASN
45	r	21	ASN
45	r	31	ASN
45	r	83	ASN
46	s	62	ARG
47	t	1	MET
47	t	40	LYS
47	t	123	ARG
48	1	260	MET
52	q	50	ASN

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Mol	Chain	Res	Type
53	u	40	ASN
53	u	147	ASN
53	u	213	ARG
54	v	167	ARG
54	v	248	TYR
55	x	232	ASN
55	x	240	ARG
56	z	63	MET
56	z	191	ARG
58	CC	84	ASN
58	CC	87	ASN
58	CC	99	ASN
59	XX	69	ARG
59	XX	70	ARG
59	XX	79	ARG
60	EE	20	LYS
60	EE	69	ARG
60	EE	97	ARG
61	QQ	27	LYS
62	MM	146	ARG
62	MM	150	ARG
63	UU	41	MET
63	UU	85	ARG
63	UU	146	ARG
65	HH	82	ASN
68	NN	101	LYS
70	JJ	81	ARG
71	AA	99	LYS
71	AA	104	ARG
72	DD	22	ASN
72	DD	76	ARG
72	DD	94	ARG
72	DD	106	ARG
72	DD	227	LYS
74	SS	96	ARG
75	RR	33	ARG
76	9	13	ARG
77	II	8	LYS
78	PP	62	ARG
79	GG	47	ASN
81	FF	40	ARG
83	0	138	ARG

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Mol	Chain	Res	Type
84	6	159	ASN
84	6	178	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
5	B	167	GLN
5	B	204	GLN
5	B	245	HIS
5	B	302	ASN
5	B	354	GLN
6	C	38	ASN
6	C	50	GLN
7	D	225	GLN
8	E	178	ASN
8	E	275	ASN
8	E	280	HIS
9	F	41	GLN
9	F	112	GLN
9	F	133	ASN
10	G	38	ASN
10	G	46	GLN
10	G	81	ASN
10	G	112	GLN
10	G	240	ASN
11	H	8	GLN
11	H	39	ASN
12	I	95	HIS
12	I	144	ASN
14	L	19	GLN
16	N	181	HIS
16	N	201	HIS
17	O	50	ASN
17	O	65	ASN
17	O	199	HIS
18	P	75	GLN
18	P	80	GLN
20	R	58	HIS
20	R	130	ASN
21	S	50	GLN
21	S	163	HIS
22	T	3	ASN

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Mol	Chain	Res	Type
22	T	95	HIS
22	T	127	GLN
24	V	77	HIS
25	W	17	HIS
25	W	45	ASN
26	X	93	ASN
26	X	94	ASN
26	X	111	GLN
28	Z	97	ASN
29	a	14	HIS
31	c	15	ASN
31	c	51	ASN
32	d	18	ASN
32	d	30	HIS
33	e	43	ASN
33	e	52	GLN
34	f	80	ASN
34	f	99	HIS
35	g	100	GLN
35	g	112	GLN
36	h	63	GLN
36	h	96	ASN
40	l	33	ASN
44	p	92	GLN
45	r	12	ASN
45	r	21	ASN
45	r	31	ASN
45	r	83	ASN
46	s	191	GLN
48	1	253	GLN
52	q	50	ASN
52	q	111	GLN
52	q	141	ASN
53	u	101	HIS
53	u	124	HIS
53	u	147	ASN
53	u	157	GLN
54	v	113	GLN
54	v	272	HIS
55	x	36	HIS
55	x	67	GLN
55	x	232	ASN

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Mol	Chain	Res	Type
56	z	81	HIS
56	z	202	ASN
57	y	186	ASN
58	CC	84	ASN
58	CC	87	ASN
58	CC	88	ASN
58	CC	99	ASN
58	CC	138	ASN
58	CC	165	GLN
60	EE	83	GLN
62	MM	94	HIS
63	UU	11	GLN
63	UU	35	ASN
63	UU	80	GLN
63	UU	97	GLN
64	YY	62	GLN
65	HH	47	ASN
65	HH	82	ASN
66	TT	113	HIS
68	NN	15	ASN
68	NN	63	HIS
71	AA	117	ASN
72	DD	22	ASN
73	BB	114	ASN
74	SS	44	HIS
75	RR	48	HIS
75	RR	82	ASN
76	9	41	GLN
79	GG	47	ASN
81	FF	29	GLN
84	6	159	ASN
84	6	178	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3649/3662 (99%)	841 (23%)	72 (1%)
2	7	119/120 (99%)	16 (13%)	0
3	8	155/156 (99%)	40 (25%)	1 (0%)
49	2	74/76 (97%)	23 (31%)	1 (1%)
50	3	72/75 (96%)	13 (18%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	K	1686/1698 (99%)	352 (20%)	22 (1%)
85	4	9/10 (90%)	4 (44%)	0
All	All	5764/5797 (99%)	1289 (22%)	97 (1%)

All (1289) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	2	G
1	5	8	U
1	5	11	G
1	5	12	A
1	5	13	U
1	5	25	A
1	5	35	U
1	5	39	A
1	5	42	A
1	5	43	U
1	5	47	A
1	5	48	G
1	5	49	U
1	5	56	A
1	5	58	G
1	5	59	A
1	5	64	A
1	5	65	A
1	5	73	A
1	5	76	A
1	5	84	A
1	5	91	G
1	5	104	G
1	5	108	A
1	5	109	G
1	5	110	C
1	5	112	C
1	5	116	G
1	5	119	G
1	5	126	C
1	5	134	G
1	5	135	G
1	5	136	C
1	5	143	C
1	5	144	G

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Mol	Chain	Res	Type
1	5	159	C
1	5	166	C
1	5	167	C
1	5	171	U
1	5	172	C
1	5	173	C
1	5	182	G
1	5	183	C
1	5	184	U
1	5	185	C
1	5	186	G
1	5	187	U
1	5	188	G
1	5	189	G
1	5	200	U
1	5	201	C
1	5	210	C
1	5	216	C
1	5	217	C
1	5	218	A
1	5	219	G
1	5	220	C
1	5	224	U
1	5	225	G
1	5	226	G
1	5	233	U
1	5	234	G
1	5	246	G
1	5	262	G
1	5	265	C
1	5	266	C
1	5	267	G
1	5	276	C
1	5	277	G
1	5	278	G
1	5	280	G
1	5	297	U
1	5	301	G
1	5	306	A
1	5	309	C
1	5	315	G
1	5	316	U

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Mol	Chain	Res	Type
1	5	334	A
1	5	340	C
1	5	345	C
1	5	350	C
1	5	363	A
1	5	383	A
1	5	387	G
1	5	399	G
1	5	407	A
1	5	409	G
1	5	410	A
1	5	412	G
1	5	413	G
1	5	440	U
1	5	450	G
1	5	451	C
1	5	452	A
1	5	453	G
1	5	454	U
1	5	455	C
1	5	465	G
1	5	467	U
1	5	468	U
1	5	470	A
1	5	480	C
1	5	485	C
1	5	486	C
1	5	487	G
1	5	499	G
1	5	500	G
1	5	501	C
1	5	503	C
1	5	504	G
1	5	506	C
1	5	513	U
1	5	514	U
1	5	515	C
1	5	519	C
1	5	647	G
1	5	649	A
1	5	654	C
1	5	663	G

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Mol	Chain	Res	Type
1	5	664	G
1	5	666	G
1	5	667	A
1	5	683	C
1	5	684	G
1	5	685	C
1	5	686	A
1	5	690	C
1	5	694	C
1	5	695	G
1	5	696	C
1	5	697	G
1	5	702	U
1	5	703	G
1	5	704	C
1	5	707	C
1	5	716	C
1	5	718	C
1	5	728	U
1	5	729	G
1	5	730	G
1	5	732	A
1	5	737	C
1	5	746	A
1	5	747	A
1	5	748	G
1	5	749	G
1	5	914	U
1	5	917	A
1	5	918	G
1	5	920	C
1	5	926	G
1	5	927	G
1	5	930	G
1	5	931	C
1	5	932	A
1	5	933	G
1	5	934	C
1	5	936	C
1	5	937	U
1	5	938	C
1	5	939	G

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Mol	Chain	Res	Type
1	5	942	G
1	5	944	A
1	5	945	U
1	5	946	C
1	5	957	G
1	5	958	G
1	5	960	A
1	5	961	G
1	5	962	C
1	5	963	G
1	5	964	A
1	5	965	G
1	5	966	A
1	5	967	C
1	5	968	C
1	5	969	C
1	5	970	G
1	5	971	U
1	5	973	G
1	5	976	G
1	5	978	G
1	5	982	U
1	5	989	U
1	5	990	C
1	5	991	C
1	5	1068	G
1	5	1070	G
1	5	1072	C
1	5	1078	A
1	5	1083	U
1	5	1177	U
1	5	1178	G
1	5	1183	C
1	5	1187	G
1	5	1188	C
1	5	1209	U
1	5	1210	C
1	5	1211	G
1	5	1212	G
1	5	1215	C
1	5	1219	G
1	5	1221	G

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Mol	Chain	Res	Type
1	5	1233	G
1	5	1237	C
1	5	1238	A
1	5	1239	C
1	5	1242	G
1	5	1243	C
1	5	1244	G
1	5	1255	A
1	5	1267	C
1	5	1268	G
1	5	1269	G
1	5	1270	A
1	5	1272	C
1	5	1273	G
1	5	1274	A
1	5	1279	A
1	5	1280	C
1	5	1281	G
1	5	1282	G
1	5	1285	U
1	5	1286	C
1	5	1288	G
1	5	1290	G
1	5	1293	G
1	5	1297	U
1	5	1301	C
1	5	1319	U
1	5	1326	A
1	5	1330	A
1	5	1344	C
1	5	1354	A
1	5	1358	G
1	5	1367	C
1	5	1368	A
1	5	1370	G
1	5	1371	A
1	5	1372	A
1	5	1377	G
1	5	1378	C
1	5	1379	C
1	5	1387	A
1	5	1394	G

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Mol	Chain	Res	Type
1	5	1397	A
1	5	1399	G
1	5	1408	G
1	5	1410	U
1	5	1411	C
1	5	1419	G
1	5	1420	A
1	5	1421	G
1	5	1429	C
1	5	1437	C
1	5	1439	C
1	5	1440	U
1	5	1441	C
1	5	1445	U
1	5	1446	C
1	5	1448	G
1	5	1451	G
1	5	1456	C
1	5	1457	G
1	5	1458	C
1	5	1465	G
1	5	1475	G
1	5	1482	G
1	5	1483	C
1	5	1497	A
1	5	1498	G
1	5	1501	C
1	5	1502	G
1	5	1514	U
1	5	1516	G
1	5	1518	A
1	5	1523	A
1	5	1525	A
1	5	1534	A
1	5	1535	C
1	5	1547	A
1	5	1563	A
1	5	1564	A
1	5	1566	C
1	5	1574	G
1	5	1578	U
1	5	1591	U

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Mol	Chain	Res	Type
1	5	1596	U
1	5	1597	G
1	5	1602	U
1	5	1607	C
1	5	1612	G
1	5	1613	A
1	5	1624	G
1	5	1625	G
1	5	1631	A
1	5	1633	G
1	5	1634	A
1	5	1638	A
1	5	1640	C
1	5	1641	G
1	5	1649	U
1	5	1650	A
1	5	1654	G
1	5	1660	U
1	5	1661	C
1	5	1676	C
1	5	1677	U
1	5	1680	G
1	5	1694	C
1	5	1698	C
1	5	1719	A
1	5	1720	C
1	5	1721	G
1	5	1724	G
1	5	1731	C
1	5	1741	G
1	5	1742	A
1	5	1754	U
1	5	1755	C
1	5	1756	U
1	5	1757	U
1	5	1759	G
1	5	1760	G
1	5	1761	G
1	5	1764	G
1	5	1765	A
1	5	1768	C
1	5	1769	G

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Mol	Chain	Res	Type
1	5	1772	C
1	5	1775	A
1	5	1776	A
1	5	1777	C
1	5	1780	A
1	5	1781	U
1	5	1787	A
1	5	1799	G
1	5	1803	G
1	5	1804	A
1	5	1805	A
1	5	1812	C
1	5	1815	G
1	5	1819	G
1	5	1820	C
1	5	1821	G
1	5	1822	U
1	5	1828	C
1	5	1833	G
1	5	1834	U
1	5	1835	G
1	5	1836	G
1	5	1840	G
1	5	1848	C
1	5	1855	G
1	5	1869	G
1	5	1882	U
1	5	1888	A
1	5	1889	U
1	5	1890	G
1	5	1897	A
1	5	1906	U
1	5	1910	G
1	5	1916	G
1	5	1918	U
1	5	1920	C
1	5	1921	C
1	5	1922	G
1	5	1925	G
1	5	1928	C
1	5	1930	U
1	5	1931	C

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Mol	Chain	Res	Type
1	5	1932	A
1	5	1957	U
1	5	1958	A
1	5	1959	U
1	5	1960	A
1	5	1961	G
1	5	1962	A
1	5	1964	A
1	5	1966	C
1	5	1967	A
1	5	1968	G
1	5	1969	G
1	5	1970	A
1	5	1971	C
1	5	1975	G
1	5	1976	G
1	5	1978	C
1	5	1980	U
1	5	1981	G
1	5	1985	G
1	5	1987	C
1	5	1988	G
1	5	1991	A
1	5	1993	C
1	5	1997	U
1	5	2001	G
1	5	2002	A
1	5	2003	G
1	5	2007	G
1	5	2010	A
1	5	2011	C
1	5	2016	C
1	5	2017	A
1	5	2026	A
1	5	2044	U
1	5	2047	A
1	5	2048	U
1	5	2052	G
1	5	2055	G
1	5	2056	G
1	5	2069	A
1	5	2084	C

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Mol	Chain	Res	Type
1	5	2085	G
1	5	2089	G
1	5	2090	U
1	5	2092	G
1	5	2093	A
1	5	2094	G
1	5	2095	A
1	5	2097	U
1	5	2101	C
1	5	2105	A
1	5	2107	C
1	5	2108	G
1	5	2109	G
1	5	2110	C
1	5	2111	G
1	5	2112	G
1	5	2113	G
1	5	2114	G
1	5	2116	C
1	5	2117	G
1	5	2119	C
1	5	2120	G
1	5	2122	G
1	5	2123	C
1	5	2124	G
1	5	2126	G
1	5	2127	C
1	5	2247	C
1	5	2248	C
1	5	2250	C
1	5	2251	G
1	5	2252	G
1	5	2253	A
1	5	2254	G
1	5	2257	C
1	5	2258	C
1	5	2259	G
1	5	2260	C
1	5	2261	G
1	5	2263	A
1	5	2264	C
1	5	2265	G

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Mol	Chain	Res	Type
1	5	2266	C
1	5	2267	U
1	5	2268	A
1	5	2279	A
1	5	2289	C
1	5	2300	A
1	5	2301	G
1	5	2306	G
1	5	2313	A
1	5	2314	G
1	5	2316	G
1	5	2322	G
1	5	2331	G
1	5	2333	G
1	5	2348	G
1	5	2350	U
1	5	2351	C
1	5	2360	A
1	5	2395	A
1	5	2396	A
1	5	2410	C
1	5	2417	A
1	5	2422	C
1	5	2425	U
1	5	2433	G
1	5	2438	A
1	5	2440	U
1	5	2441	C
1	5	2450	G
1	5	2471	G
1	5	2488	C
1	5	2489	C
1	5	2490	U
1	5	2491	C
1	5	2503	G
1	5	2504	C
1	5	2505	C
1	5	2506	G
1	5	2513	A
1	5	2514	G
1	5	2517	A
1	5	2529	A

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Mol	Chain	Res	Type
1	5	2530	U
1	5	2537	A
1	5	2544	G
1	5	2546	G
1	5	2547	G
1	5	2549	G
1	5	2553	A
1	5	2554	U
1	5	2571	C
1	5	2572	C
1	5	2575	U
1	5	2581	A
1	5	2583	C
1	5	2587	A
1	5	2589	C
1	5	2618	G
1	5	2638	G
1	5	2661	U
1	5	2662	G
1	5	2669	C
1	5	2670	C
1	5	2681	G
1	5	2686	G
1	5	2687	U
1	5	2694	G
1	5	2695	A
1	5	2696	A
1	5	2710	C
1	5	2711	G
1	5	2712	G
1	5	2714	G
1	5	2721	G
1	5	2725	A
1	5	2726	G
1	5	2740	U
1	5	2752	G
1	5	2754	G
1	5	2761	U
1	5	2762	G
1	5	2763	U
1	5	2767	U
1	5	2768	C

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Mol	Chain	Res	Type
1	5	2769	U
1	5	2770	C
1	5	2787	A
1	5	2788	U
1	5	2790	U
1	5	2794	C
1	5	2798	A
1	5	2806	A
1	5	2814	C
1	5	2826	U
1	5	2827	G
1	5	2828	U
1	5	2833	A
1	5	2842	G
1	5	2849	A
1	5	2855	G
1	5	2857	A
1	5	2867	C
1	5	2897	G
1	5	2898	G
1	5	2904	U
1	5	2905	C
1	5	3593	C
1	5	3595	U
1	5	3596	A
1	5	3597	G
1	5	3602	C
1	5	3605	C
1	5	3616	U
1	5	3617	G
1	5	3625	G
1	5	3626	G
1	5	3630	A
1	5	3635	A
1	5	3636	C
1	5	3648	A
1	5	3662	A
1	5	3670	C
1	5	3673	C
1	5	3692	A
1	5	3705	G
1	5	3710	G

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Mol	Chain	Res	Type
1	5	3711	A
1	5	3729	U
1	5	3748	A
1	5	3760	A
1	5	3761	C
1	5	3772	U
1	5	3774	A
1	5	3777	G
1	5	3778	U
1	5	3784	A
1	5	3786	U
1	5	3799	A
1	5	3802	U
1	5	3810	C
1	5	3811	G
1	5	3812	C
1	5	3814	U
1	5	3817	A
1	5	3819	G
1	5	3840	U
1	5	3843	C
1	5	3860	A
1	5	3870	C
1	5	3876	A
1	5	3877	A
1	5	3878	C
1	5	3879	G
1	5	3889	G
1	5	3892	U
1	5	3897	G
1	5	3898	G
1	5	3901	A
1	5	3905	A
1	5	3906	A
1	5	3907	G
1	5	3908	A
1	5	3915	U
1	5	3926	C
1	5	3938	G
1	5	3939	G
1	5	3943	A
1	5	4069	U

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Mol	Chain	Res	Type
1	5	4070	U
1	5	4076	G
1	5	4084	G
1	5	4085	A
1	5	4086	G
1	5	4088	C
1	5	4090	G
1	5	4094	G
1	5	4097	G
1	5	4099	G
1	5	4104	G
1	5	4107	G
1	5	4114	C
1	5	4115	G
1	5	4116	C
1	5	4117	U
1	5	4119	C
1	5	4120	U
1	5	4121	G
1	5	4125	C
1	5	4127	A
1	5	4128	A
1	5	4143	G
1	5	4144	C
1	5	4145	C
1	5	4151	G
1	5	4158	C
1	5	4162	C
1	5	4164	C
1	5	4166	G
1	5	4170	A
1	5	4171	C
1	5	4173	G
1	5	4183	G
1	5	4184	G
1	5	4191	G
1	5	4203	A
1	5	4212	A
1	5	4225	G
1	5	4228	G
1	5	4229	U
1	5	4233	A

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Mol	Chain	Res	Type
1	5	4234	A
1	5	4243	C
1	5	4249	G
1	5	4251	A
1	5	4254	G
1	5	4255	A
1	5	4265	U
1	5	4268	A
1	5	4271	A
1	5	4273	A
1	5	4280	A
1	5	4282	A
1	5	4290	U
1	5	4291	G
1	5	4292	A
1	5	4297	G
1	5	4304	A
1	5	4305	G
1	5	4306	U
1	5	4313	A
1	5	4314	C
1	5	4317	A
1	5	4318	C
1	5	4319	C
1	5	4323	A
1	5	4326	G
1	5	4329	G
1	5	4330	G
1	5	4332	C
1	5	4339	A
1	5	4349	C
1	5	4350	C
1	5	4354	U
1	5	4355	G
1	5	4376	A
1	5	4377	G
1	5	4378	A
1	5	4379	A
1	5	4387	C
1	5	4393	G
1	5	4394	A
1	5	4405	G

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Mol	Chain	Res	Type
1	5	4419	U
1	5	4421	C
1	5	4422	A
1	5	4426	C
1	5	4436	U
1	5	4437	U
1	5	4440	G
1	5	4444	C
1	5	4448	G
1	5	4449	A
1	5	4464	A
1	5	4471	U
1	5	4475	G
1	5	4476	C
1	5	4482	U
1	5	4500	U
1	5	4510	A
1	5	4512	U
1	5	4513	A
1	5	4518	A
1	5	4519	C
1	5	4524	G
1	5	4528	G
1	5	4529	G
1	5	4531	U
1	5	4548	A
1	5	4549	G
1	5	4557	U
1	5	4560	C
1	5	4567	G
1	5	4570	G
1	5	4573	G
1	5	4575	G
1	5	4581	G
1	5	4590	A
1	5	4599	A
1	5	4617	G
1	5	4636	U
1	5	4637	G
1	5	4639	G
1	5	4642	U
1	5	4652	G

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Mol	Chain	Res	Type
1	5	4656	A
1	5	4657	U
1	5	4661	G
1	5	4667	C
1	5	4670	C
1	5	4672	A
1	5	4677	U
1	5	4682	U
1	5	4687	A
1	5	4693	C
1	5	4694	G
1	5	4695	C
1	5	4697	U
1	5	4700	A
1	5	4709	U
1	5	4719	G
1	5	4720	C
1	5	4730	C
1	5	4731	G
1	5	4732	G
1	5	4738	C
1	5	4741	C
1	5	4744	A
1	5	4745	G
1	5	4746	C
1	5	4750	G
1	5	4753	U
1	5	4756	C
1	5	4758	U
1	5	4763	U
1	5	4764	A
1	5	4770	U
1	5	4771	C
1	5	4868	G
1	5	4869	U
1	5	4871	C
1	5	4873	G
1	5	4876	U
1	5	4878	C
1	5	4883	C
1	5	4884	G
1	5	4886	C

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Mol	Chain	Res	Type
1	5	4889	G
1	5	4890	G
1	5	4895	C
1	5	4896	G
1	5	4901	G
1	5	4902	C
1	5	4903	G
1	5	4910	G
1	5	4911	A
1	5	4912	G
1	5	4913	G
1	5	4914	C
1	5	4927	G
1	5	4930	C
1	5	4931	G
1	5	4933	C
1	5	4936	G
1	5	4937	C
1	5	4941	G
1	5	4944	C
1	5	4945	G
1	5	4949	G
1	5	4951	G
1	5	4959	U
1	5	4964	C
1	5	4965	U
1	5	4966	A
1	5	4975	G
1	5	4976	U
1	5	4985	U
1	5	4988	U
1	5	4989	U
1	5	4990	C
1	5	4991	U
1	5	4999	G
1	5	5006	U
1	5	5013	C
1	5	5017	G
1	5	5023	C
1	5	5027	C
1	5	5028	G
1	5	5041	G

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Mol	Chain	Res	Type
1	5	5047	C
1	5	5050	C
1	5	5052	C
1	5	5053	U
1	5	5054	C
1	5	5056	A
1	5	5060	A
1	5	5061	A
2	7	7	G
2	7	13	A
2	7	22	A
2	7	25	G
2	7	40	U
2	7	53	U
2	7	54	A
2	7	63	C
2	7	64	G
2	7	97	G
2	7	98	G
2	7	100	A
2	7	102	U
2	7	110	G
2	7	111	C
2	7	120	U
3	8	2	G
3	8	34	U
3	8	35	C
3	8	37	A
3	8	39	G
3	8	49	G
3	8	51	U
3	8	59	A
3	8	60	G
3	8	61	A
3	8	62	A
3	8	63	U
3	8	75	G
3	8	80	A
3	8	81	C
3	8	82	A
3	8	83	C
3	8	84	A

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Mol	Chain	Res	Type
3	8	85	U
3	8	86	U
3	8	87	G
3	8	90	C
3	8	94	G
3	8	99	U
3	8	103	A
3	8	105	C
3	8	107	C
3	8	109	C
3	8	110	U
3	8	111	U
3	8	114	G
3	8	123	U
3	8	124	U
3	8	125	C
3	8	126	C
3	8	127	U
3	8	128	C
3	8	147	G
3	8	150	C
3	8	153	C
49	2	4	U
49	2	8	U
49	2	9	A
49	2	13	C
49	2	19	G
49	2	20	C
49	2	21	A
49	2	34	C
49	2	35	A
49	2	39	U
49	2	40	C
49	2	41	U
49	2	44	A
49	2	45	G
49	2	46	G
49	2	47	U
49	2	48	C
49	2	58	A
49	2	59	A
49	2	72	C

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Mol	Chain	Res	Type
49	2	73	A
49	2	74	C
49	2	76	A
50	3	9	A
50	3	13	C
50	3	16	C
50	3	21	A
50	3	37	A
50	3	47	U
50	3	48	C
50	3	49	C
50	3	61	C
50	3	63	C
50	3	69	G
50	3	75	C
50	3	76	A
51	K	2	A
51	K	3	C
51	K	4	C
51	K	20	G
51	K	25	A
51	K	26	U
51	K	33	G
51	K	41	G
51	K	42	A
51	K	44	U
51	K	45	A
51	K	46	A
51	K	56	G
51	K	65	C
51	K	67	C
51	K	68	A
51	K	70	G
51	K	71	G
51	K	73	C
51	K	74	G
51	K	77	A
51	K	79	A
51	K	103	A
51	K	111	A
51	K	113	G
51	K	115	U

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Mol	Chain	Res	Type
51	K	124	U
51	K	126	G
51	K	128	U
51	K	129	C
51	K	130	G
51	K	141	A
51	K	142	C
51	K	143	U
51	K	147	A
51	K	155	G
51	K	158	A
51	K	162	C
51	K	171	A
51	K	180	G
51	K	182	C
51	K	183	G
51	K	184	G
51	K	187	G
51	K	188	C
51	K	189	U
51	K	191	A
51	K	192	C
51	K	215	G
51	K	289	G
51	K	294	U
51	K	304	C
51	K	305	U
51	K	306	C
51	K	307	G
51	K	308	G
51	K	309	G
51	K	310	C
51	K	312	G
51	K	314	U
51	K	317	C
51	K	318	A
51	K	319	C
51	K	323	C
51	K	332	G
51	K	335	G
51	K	340	C
51	K	347	G

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Mol	Chain	Res	Type
51	K	350	C
51	K	351	G
51	K	360	A
51	K	362	C
51	K	364	A
51	K	368	U
51	K	369	C
51	K	370	G
51	K	381	C
51	K	385	G
51	K	386	C
51	K	398	A
51	K	400	C
51	K	408	A
51	K	409	C
51	K	417	C
51	K	418	A
51	K	421	G
51	K	426	A
51	K	435	A
51	K	438	G
51	K	448	A
51	K	450	C
51	K	455	A
51	K	464	A
51	K	465	A
51	K	466	G
51	K	471	G
51	K	472	C
51	K	473	A
51	K	474	G
51	K	476	A
51	K	482	G
51	K	487	U
51	K	492	C
51	K	525	A
51	K	530	U
51	K	532	C
51	K	533	A
51	K	547	G
51	K	548	C
51	K	549	C

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Mol	Chain	Res	Type
51	K	550	C
51	K	551	U
51	K	554	A
51	K	555	A
51	K	556	U
51	K	559	G
51	K	560	A
51	K	564	A
51	K	568	C
51	K	576	A
51	K	583	A
51	K	588	G
51	K	590	A
51	K	591	U
51	K	606	G
51	K	608	C
51	K	614	C
51	K	615	C
51	K	617	G
51	K	621	C
51	K	624	C
51	K	626	A
51	K	628	A
51	K	643	A
51	K	644	G
51	K	660	C
51	K	662	G
51	K	663	C
51	K	664	A
51	K	668	A
51	K	669	A
51	K	671	A
51	K	672	A
51	K	673	G
51	K	683	G
51	K	688	U
51	K	689	U
51	K	752	G
51	K	753	C
51	K	754	G
51	K	798	G
51	K	799	U

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Mol	Chain	Res	Type
51	K	810	A
51	K	811	A
51	K	821	G
51	K	822	U
51	K	830	A
51	K	834	C
51	K	844	U
51	K	845	G
51	K	847	A
51	K	870	A
51	K	871	U
51	K	872	A
51	K	873	G
51	K	875	A
51	K	878	G
51	K	887	U
51	K	890	U
51	K	892	U
51	K	901	G
51	K	903	A
51	K	904	A
51	K	909	G
51	K	913	A
51	K	914	U
51	K	917	U
51	K	920	A
51	K	933	G
51	K	934	G
51	K	970	G
51	K	971	G
51	K	978	G
51	K	990	A
51	K	992	A
51	K	999	G
51	K	1017	U
51	K	1023	A
51	K	1041	G
51	K	1045	U
51	K	1060	A
51	K	1061	U
51	K	1062	A
51	K	1078	C

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Mol	Chain	Res	Type
51	K	1083	A
51	K	1085	C
51	K	1086	G
51	K	1089	G
51	K	1097	G
51	K	1100	A
51	K	1113	A
51	K	1115	U
51	K	1116	C
51	K	1117	C
51	K	1118	C
51	K	1121	G
51	K	1126	G
51	K	1131	G
51	K	1133	A
51	K	1138	C
51	K	1139	C
51	K	1149	A
51	K	1150	A
51	K	1153	C
51	K	1154	U
51	K	1155	U
51	K	1161	U
51	K	1170	A
51	K	1195	A
51	K	1208	A
51	K	1215	C
51	K	1221	G
51	K	1224	G
51	K	1242	U
51	K	1251	A
51	K	1253	A
51	K	1256	G
51	K	1257	G
51	K	1259	A
51	K	1264	C
51	K	1271	C
51	K	1274	G
51	K	1275	G
51	K	1284	A
51	K	1285	G
51	K	1286	G

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Mol	Chain	Res	Type
51	K	1298	G
51	K	1299	A
51	K	1301	A
51	K	1302	G
51	K	1303	C
51	K	1307	U
51	K	1308	U
51	K	1310	U
51	K	1314	U
51	K	1333	U
51	K	1341	C
51	K	1342	U
51	K	1345	G
51	K	1348	G
51	K	1371	U
51	K	1372	U
51	K	1376	A
51	K	1378	A
51	K	1382	A
51	K	1394	G
51	K	1395	C
51	K	1396	A
51	K	1397	U
51	K	1401	A
51	K	1402	A
51	K	1409	A
51	K	1410	C
51	K	1412	C
51	K	1428	G
51	K	1442	U
51	K	1447	G
51	K	1449	G
51	K	1452	A
51	K	1454	A
51	K	1455	A
51	K	1462	U
51	K	1463	U
51	K	1466	G
51	K	1473	G
51	K	1476	A
51	K	1477	U
51	K	1489	A

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Mol	Chain	Res	Type
51	K	1490	G
51	K	1494	U
51	K	1497	G
51	K	1498	A
51	K	1507	G
51	K	1509	U
51	K	1510	G
51	K	1521	C
51	K	1522	A
51	K	1533	A
51	K	1535	U
51	K	1536	G
51	K	1544	C
51	K	1548	G
51	K	1552	G
51	K	1553	C
51	K	1554	C
51	K	1555	U
51	K	1556	A
51	K	1557	C
51	K	1567	G
51	K	1570	G
51	K	1574	C
51	K	1575	G
51	K	1580	A
51	K	1585	U
51	K	1586	U
51	K	1587	G
51	K	1588	A
51	K	1598	G
51	K	1601	A
51	K	1604	G
51	K	1606	G
51	K	1621	U
51	K	1623	A
51	K	1637	A
51	K	1638	G
51	K	1646	C
51	K	1648	G
51	K	1664	A
51	K	1665	G
51	K	1680	G

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Mol	Chain	Res	Type
51	K	1682	C
51	K	1683	C
51	K	1695	A
51	K	1699	A
51	K	1715	A
51	K	1721	U
51	K	1722	G
51	K	1725	U
51	K	1726	G
51	K	1744	G
51	K	1748	G
51	K	1753	C
51	K	1756	C
51	K	1783	C
51	K	1799	G
51	K	1814	G
51	K	1815	A
51	K	1823	A
51	K	1824	A
51	K	1825	A
51	K	1826	G
51	K	1831	A
51	K	1836	G
51	K	1838	U
51	K	1849	G
51	K	1851	A
51	K	1852	C
51	K	1861	G
51	K	1862	G
51	K	1863	A
51	K	1865	C
51	K	1869	A
85	4	45	A
85	4	46	U
85	4	49	A
85	4	50	U

All (97) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	1	C
1	5	48	G

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Mol	Chain	Res	Type
1	5	125	C
1	5	134	G
1	5	170	C
1	5	187	U
1	5	216	C
1	5	218	A
1	5	245	C
1	5	265	C
1	5	275	C
1	5	451	C
1	5	454	U
1	5	486	C
1	5	684	G
1	5	693	C
1	5	930	G
1	5	943	A
1	5	956	A
1	5	989	U
1	5	1211	G
1	5	1232	G
1	5	1236	C
1	5	1238	A
1	5	1296	G
1	5	1329	G
1	5	1407	C
1	5	1440	U
1	5	1455	G
1	5	1633	G
1	5	1804	A
1	5	1818	G
1	5	1835	G
1	5	2015	U
1	5	2017	A
1	5	2046	G
1	5	2083	C
1	5	2089	G
1	5	2093	A
1	5	2107	C
1	5	2116	C
1	5	2123	C
1	5	2256	C
1	5	2257	C

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Mol	Chain	Res	Type
1	5	2260	C
1	5	2262	G
1	5	2266	C
1	5	2502	G
1	5	2661	U
1	5	2695	A
1	5	3625	G
1	5	3771	C
1	5	3876	A
1	5	4119	C
1	5	4170	A
1	5	4232	U
1	5	4354	U
1	5	4448	G
1	5	4528	G
1	5	4548	A
1	5	4656	A
1	5	4699	U
1	5	4719	G
1	5	4885	U
1	5	4888	U
1	5	4889	G
1	5	4935	C
1	5	4948	C
1	5	5022	U
1	5	5027	C
1	5	5059	C
1	5	5060	A
3	8	124	U
49	2	39	U
50	3	36	A
51	K	110	U
51	K	182	C
51	K	304	C
51	K	305	U
51	K	322	C
51	K	434	G
51	K	465	A
51	K	532	C
51	K	553	U
51	K	614	C
51	K	642	U

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Mol	Chain	Res	Type
51	K	688	U
51	K	752	G
51	K	798	G
51	K	870	A
51	K	902	G
51	K	1061	U
51	K	1137	U
51	K	1395	C
51	K	1520	G
51	K	1637	A
51	K	1664	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 164 ligands modelled in this entry, 164 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	12
51	K	11
50	3	2
49	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	697:G	O3'	729:C	P	18.34
1	K	756:C	O3'	788:G	P	17.89
1	K	1761:U	O3'	1771:G	P	17.79
1	5	4776:G	O3'	4859:C	P	17.38
1	5	757:G	O3'	906:C	P	17.23
1	5	2910:G	O3'	3583:U	P	17.01
1	5	519:C	O3'	642:G	P	17.00
1	K	834:C	O3'	841:G	P	16.21
1	K	323:C	O3'	329:G	P	15.96
1	K	1417:C	O3'	1423:C	P	15.13
1	5	3950:U	O3'	4065:G	P	14.95
1	5	997:C	O3'	1047:C	P	14.50
1	5	2131:C	O3'	2243:C	P	14.18
1	K	130:G	O3'	140:U	P	14.04
1	5	1051:G	O3'	1064:G	P	10.03
1	K	745:C	O3'	749:U	P	7.98
1	K	225:G	O3'	287:U	P	7.30
1	K	736:C	O3'	743:U	P	6.33
1	3	19:G	O3'	20:U	P	6.15
1	2	16:C	O3'	18:G	P	5.67
1	5	1699:A	O3'	1718:C	P	5.39
1	3	16:C	O3'	18:U	P	5.26
1	K	1432:U	O3'	1438:A	P	4.82
1	5	1840:G	O3'	1842:G	P	4.76
1	5	1100:U	O3'	1167:C	P	4.13
1	5	1222:A	O3'	1232:G	P	3.81

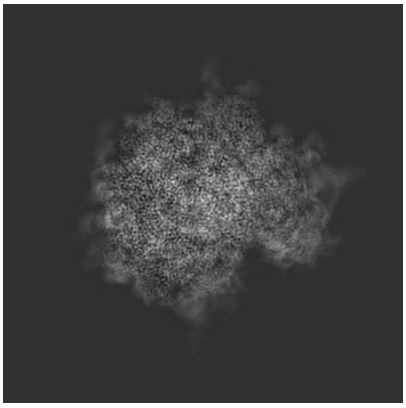
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4737. These allow visual inspection of the internal detail of the map and identification of artifacts.

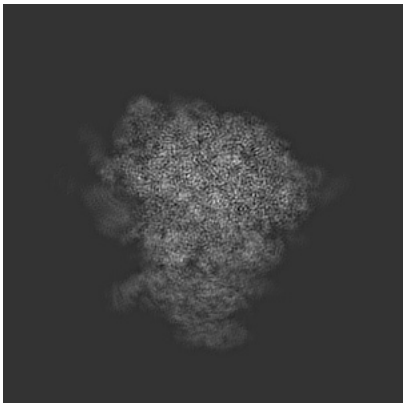
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

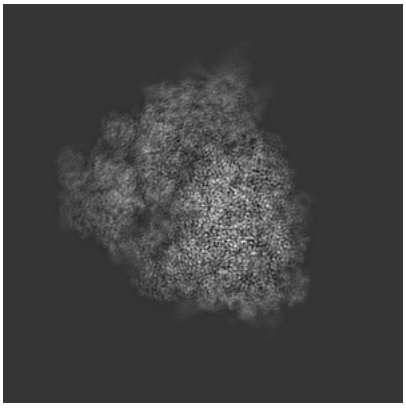
6.1.1 Primary map



X



Y

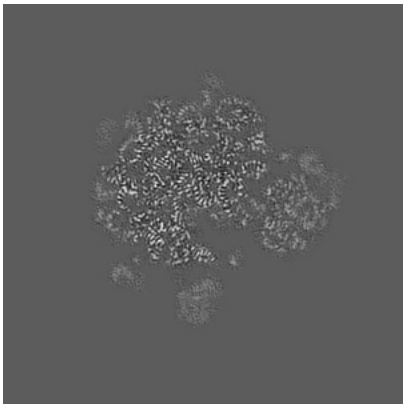


Z

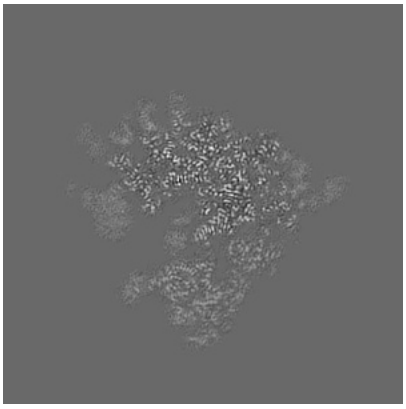
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

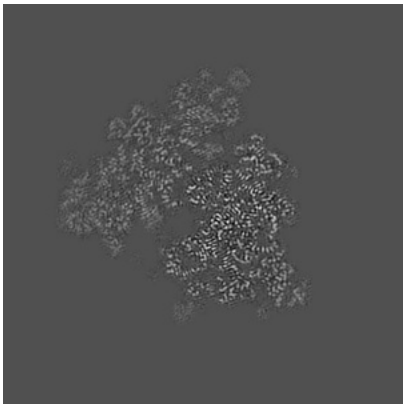
6.2.1 Primary map



X Index: 198



Y Index: 198

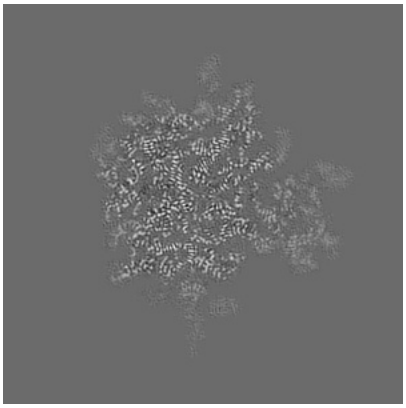


Z Index: 198

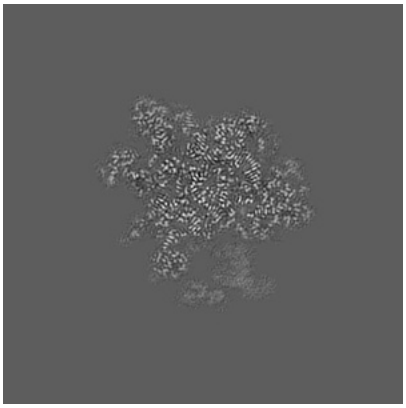
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

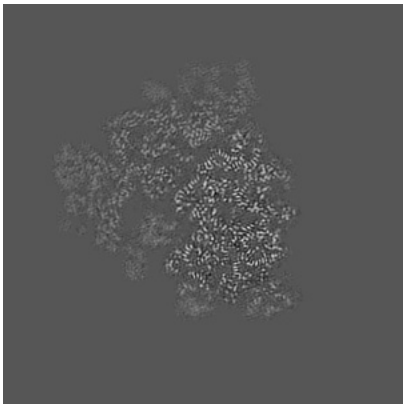
6.3.1 Primary map



X Index: 215



Y Index: 154

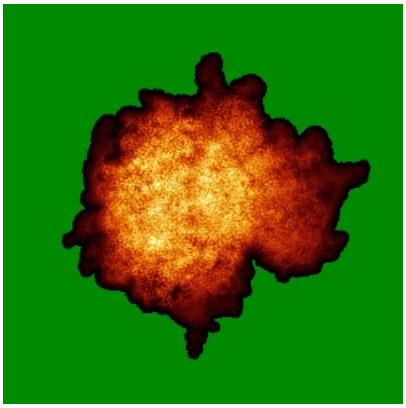


Z Index: 212

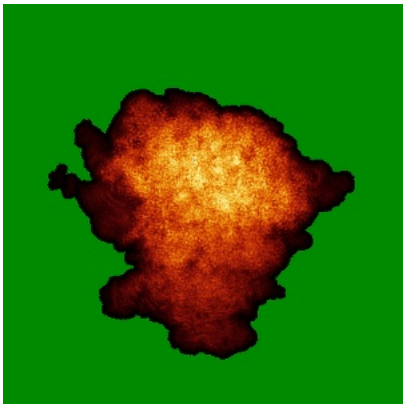
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

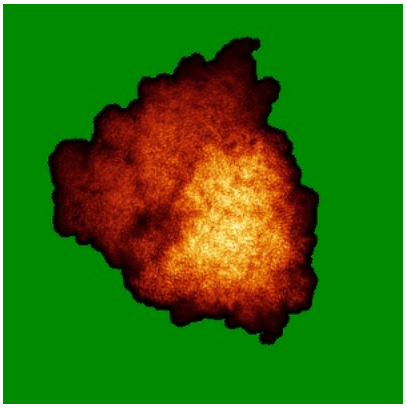
6.4.1 Primary map



X



Y

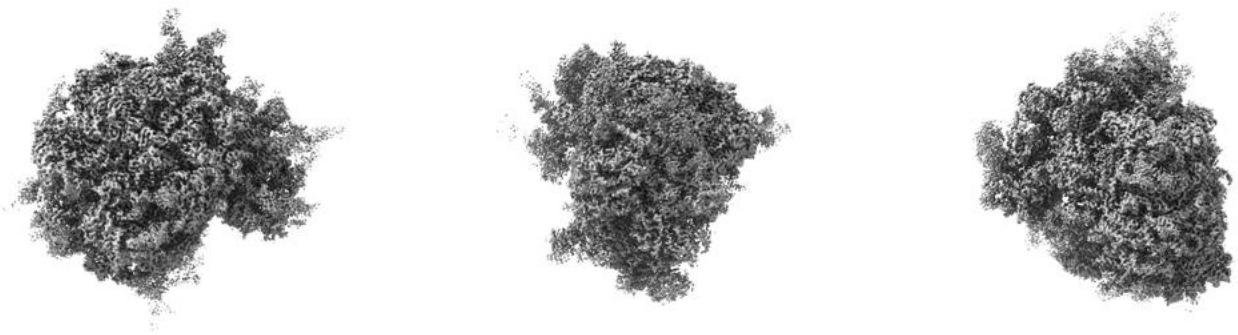


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

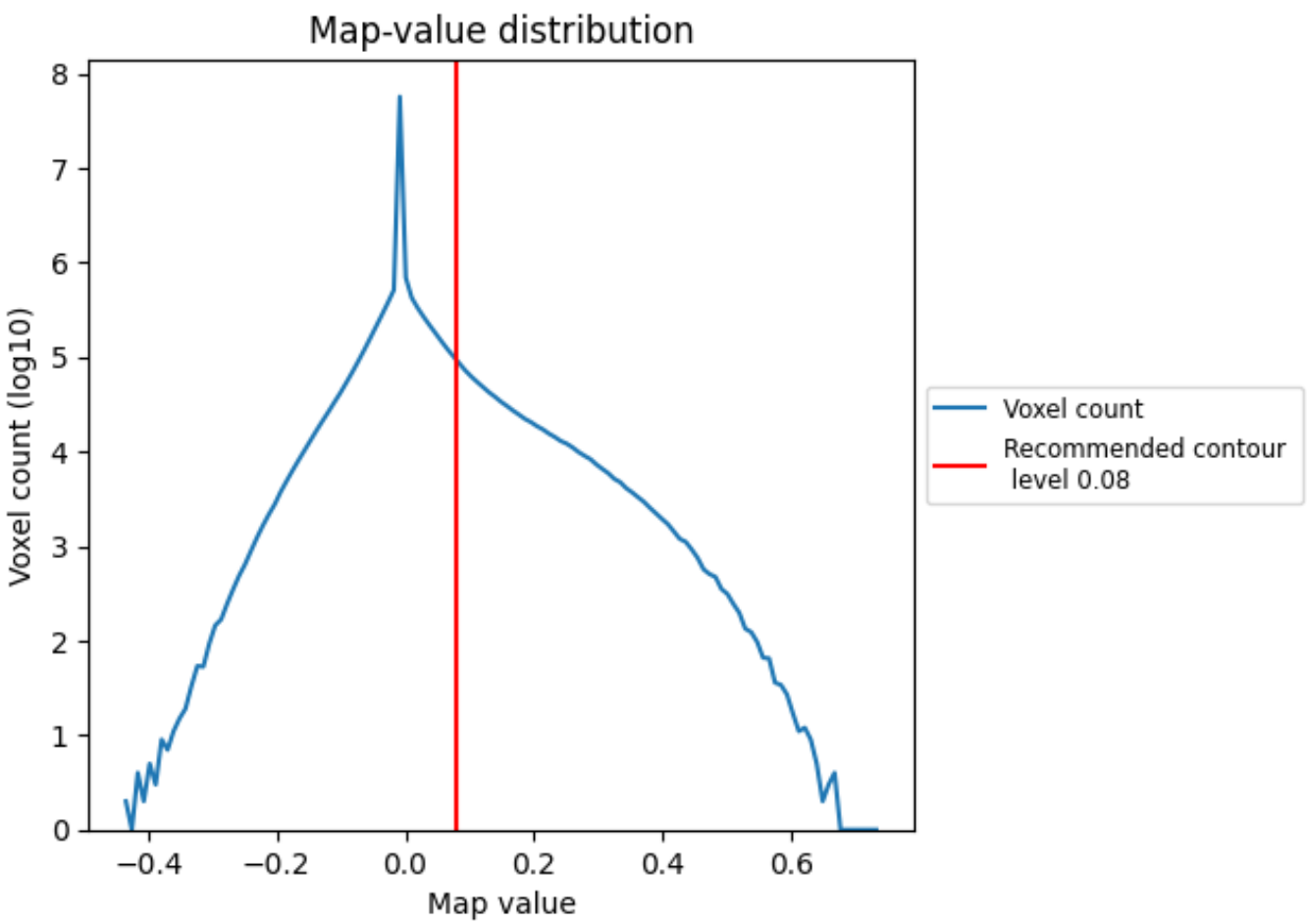
6.6 Mask visualisation (i)

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

7 Map analysis (i)

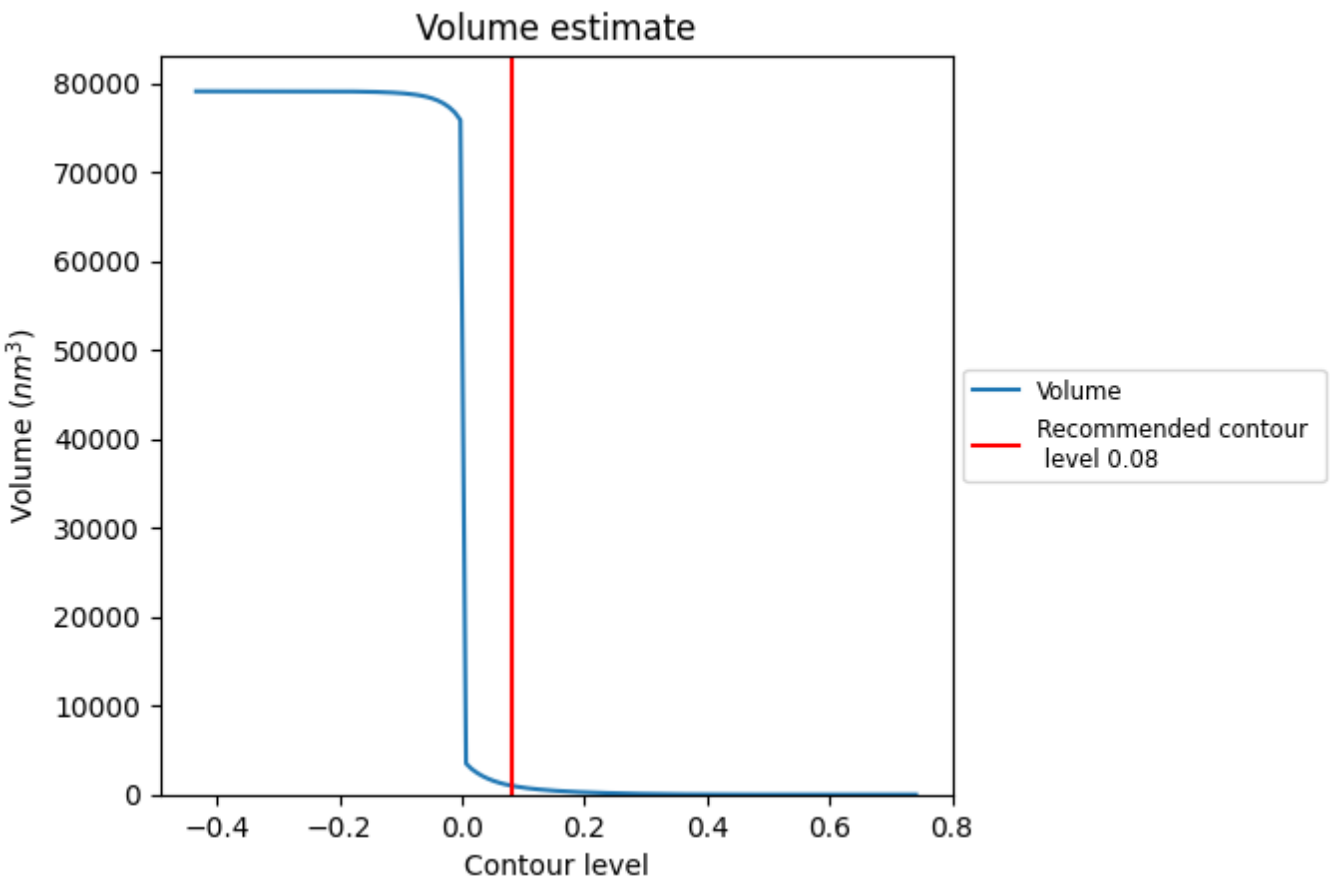
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

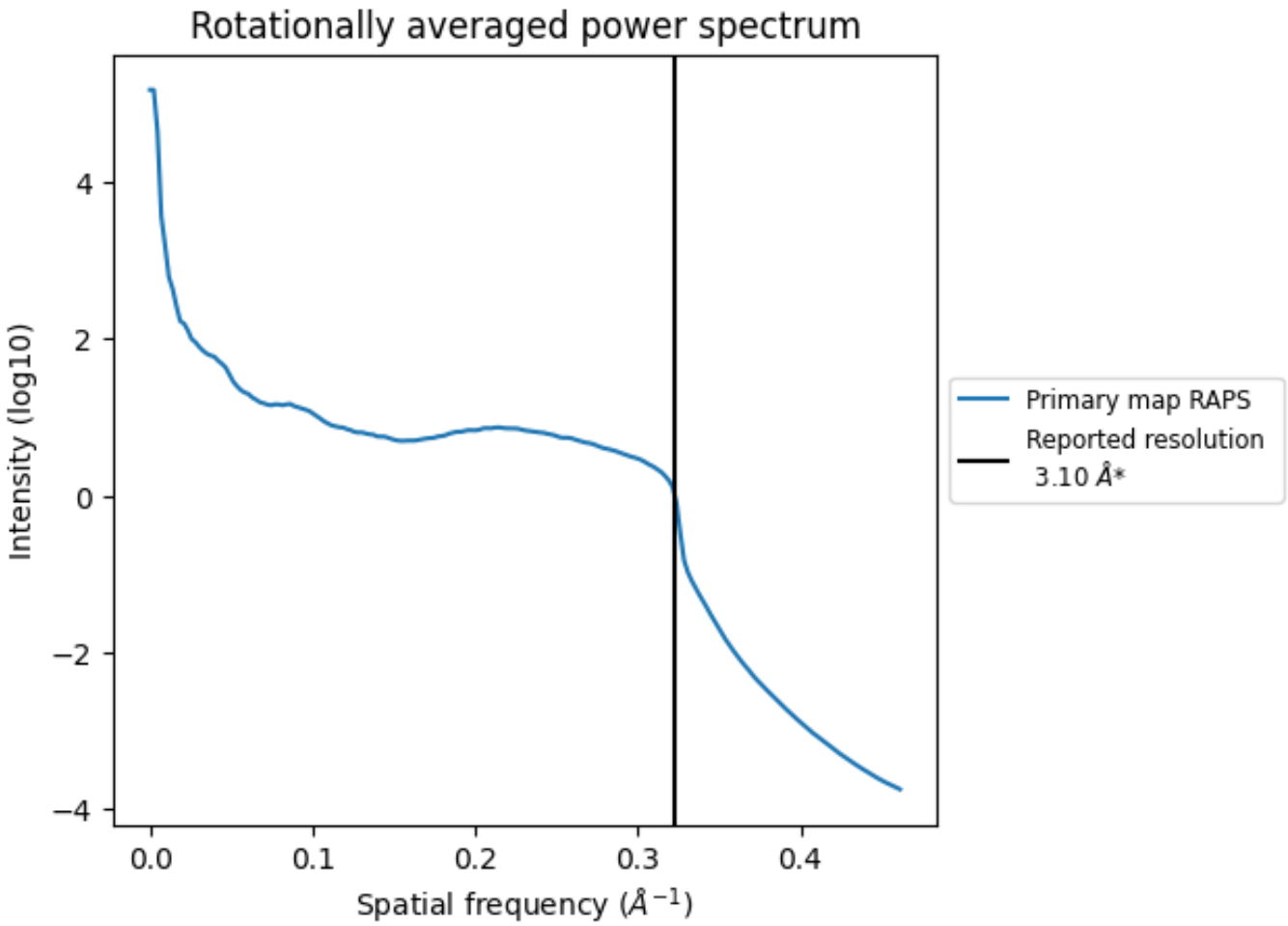
7.2 Volume estimate (i)



The volume at the recommended contour level is 1009 nm^3; this corresponds to an approximate mass of 911 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)

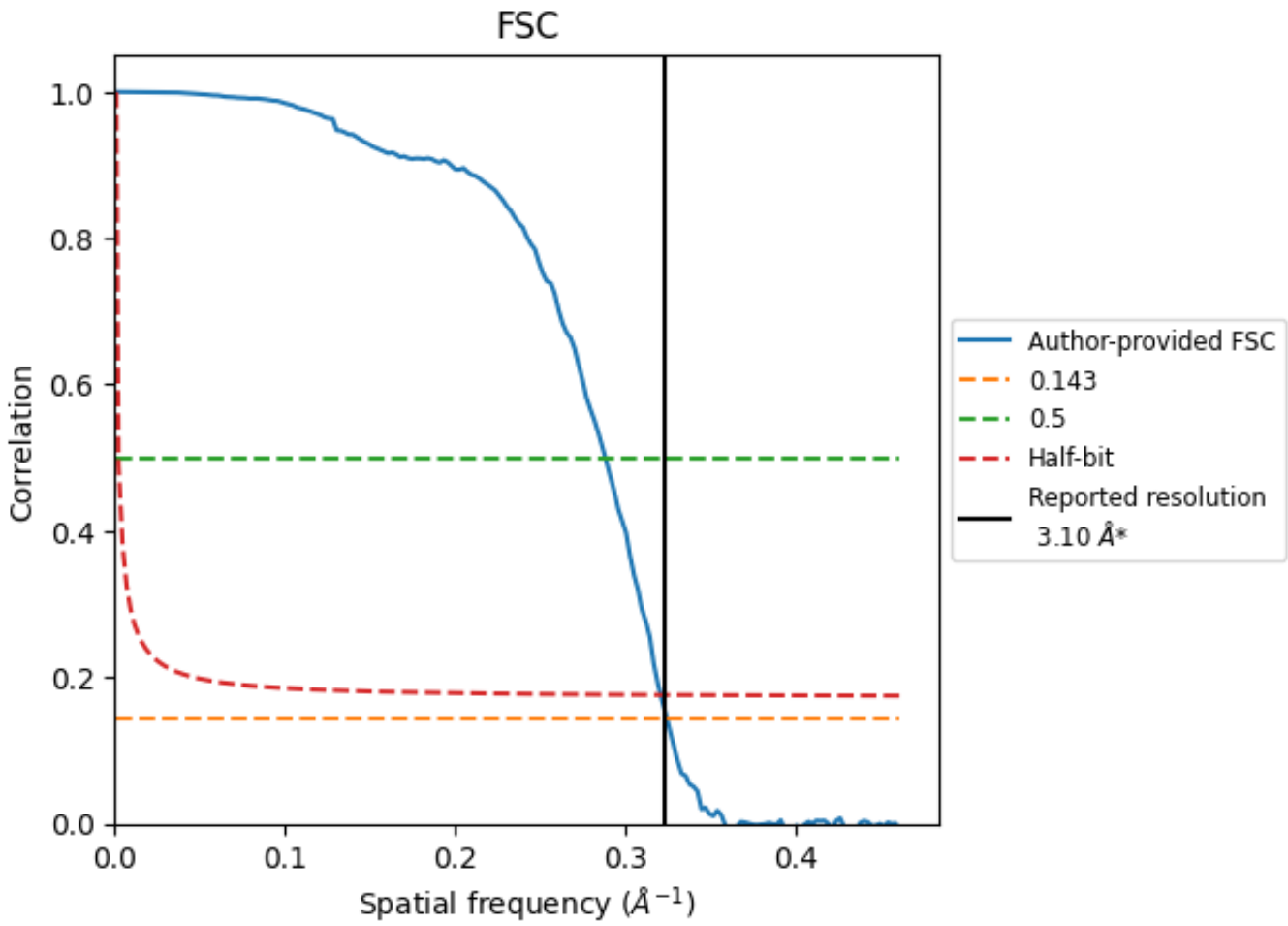


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

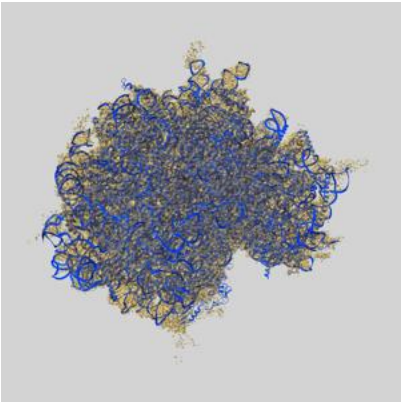
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.47	3.12
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

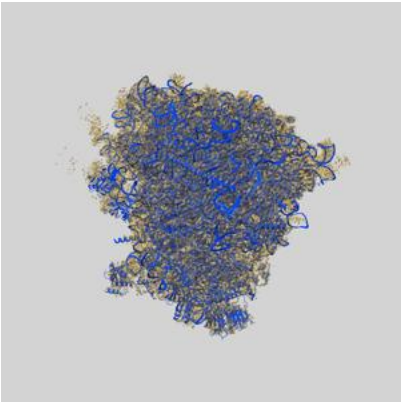
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4737 and PDB model 6R6P. Per-residue inclusion information can be found in section 3 on page 22.

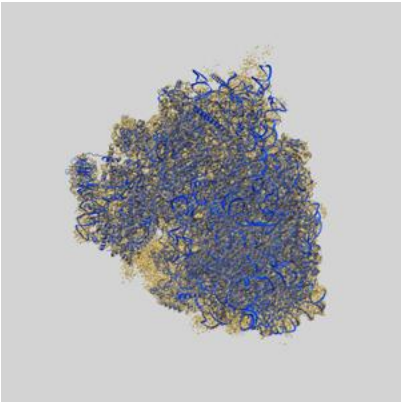
9.1 Map-model overlay (i)



X



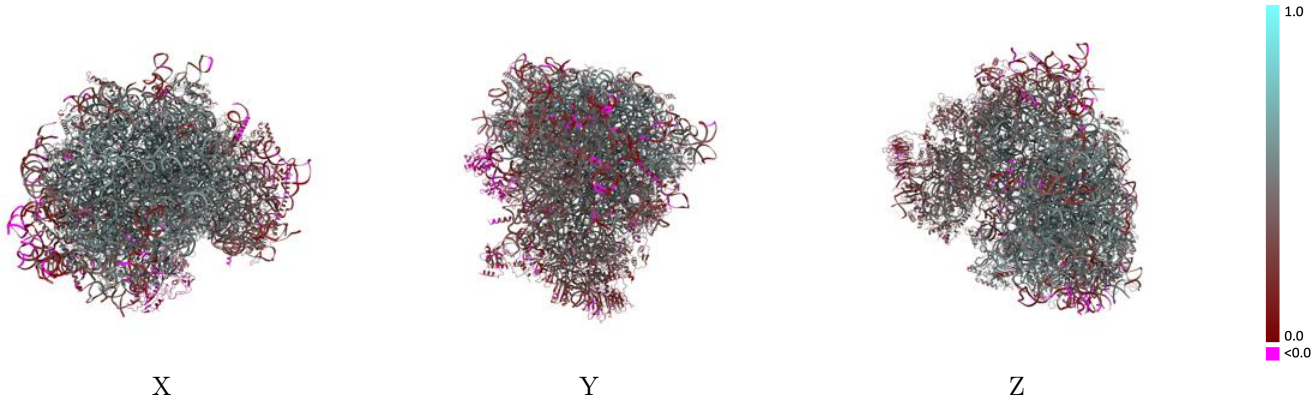
Y



Z

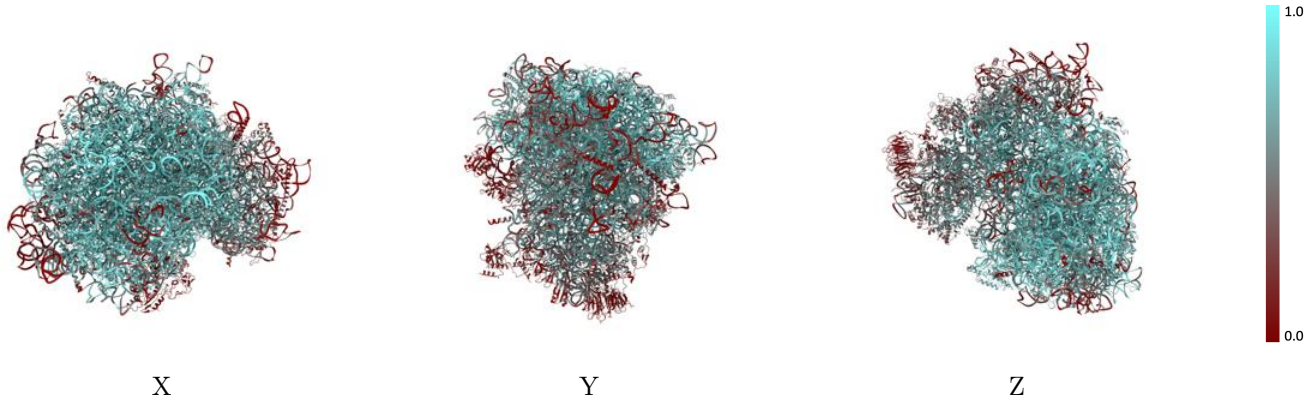
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



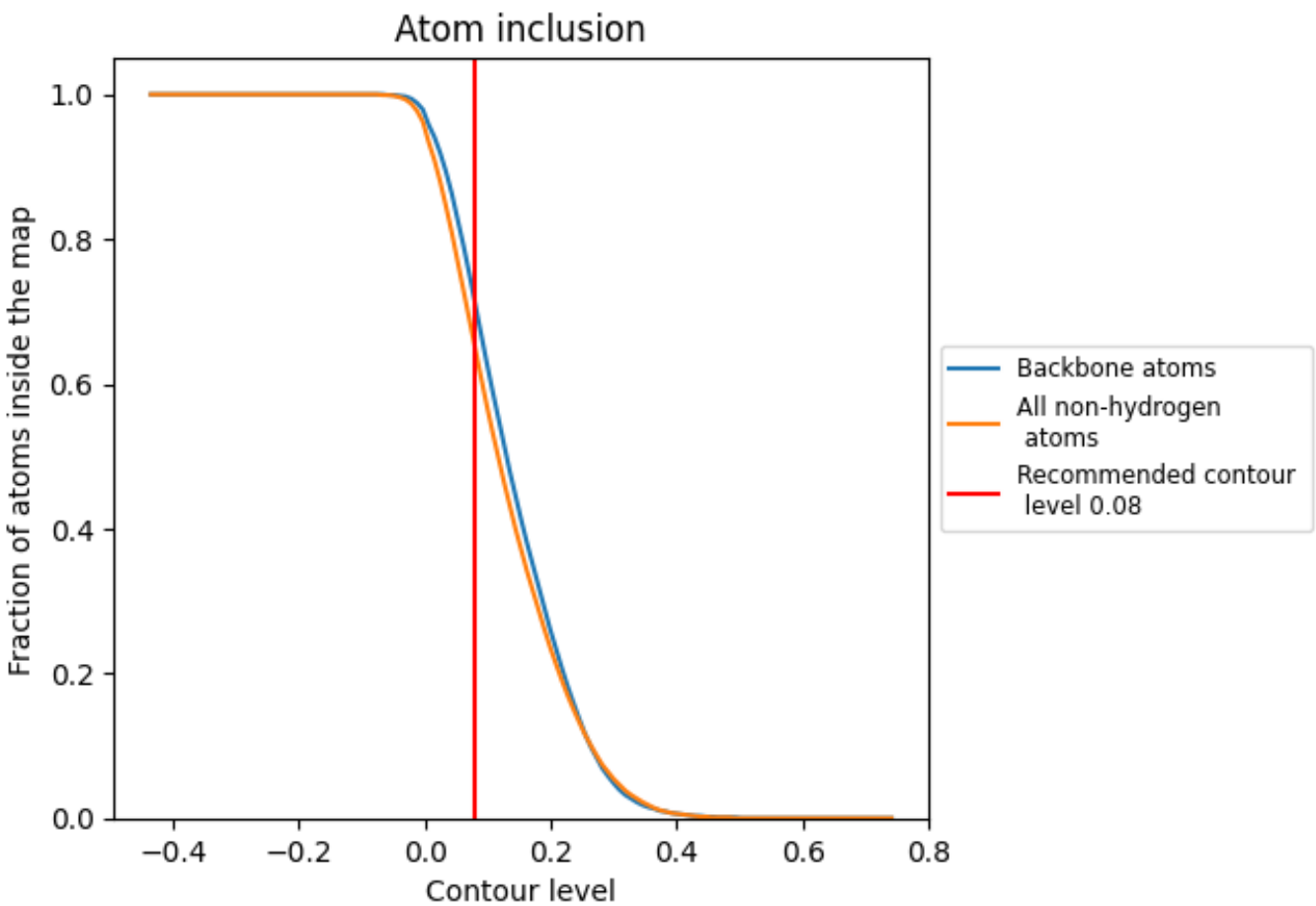
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6500	0.4290
0	0.1780	0.1670
1	0.7040	0.5380
2	0.3430	0.3240
3	0.5530	0.3530
4	0.7010	0.4530
5	0.7440	0.4610
6	0.1380	0.1930
7	0.8890	0.5500
8	0.7930	0.4960
9	0.4740	0.3200
A	0.7800	0.5370
AA	0.3170	0.2900
B	0.7660	0.5170
BB	0.4130	0.3620
C	0.7480	0.5000
CC	0.4470	0.3500
D	0.7170	0.4640
DD	0.3250	0.2960
E	0.6050	0.3850
EE	0.5460	0.4230
F	0.7450	0.4970
FF	0.3080	0.3270
G	0.6090	0.4330
GG	0.2690	0.2660
H	0.7120	0.4930
HH	0.4470	0.3600
I	0.7480	0.4990
II	0.4830	0.3640
J	0.6650	0.4450
JJ	0.4440	0.3590
K	0.6400	0.4080
L	0.6620	0.4540
M	0.7150	0.4840
MM	0.5320	0.4100

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Chain	Atom inclusion	Q-score
N	0.7990	0.5320
NN	0.3690	0.3220
O	0.7670	0.5070
OO	0.3770	0.3290
P	0.7800	0.5280
PP	0.4100	0.3310
Q	0.7630	0.5060
QQ	0.5520	0.4270
R	0.6160	0.4080
RR	0.1330	0.1510
S	0.7710	0.5060
SS	0.3080	0.2490
T	0.7070	0.4840
TT	0.5400	0.4080
U	0.5900	0.4060
UU	0.3760	0.3380
V	0.7500	0.5240
VV	0.6160	0.4600
W	0.7390	0.5150
X	0.6910	0.4870
XX	0.4230	0.3350
Y	0.7250	0.4770
YY	0.3250	0.2980
Z	0.6840	0.4500
ZZ	0.5450	0.4200
a	0.7830	0.5220
b	0.6090	0.3960
c	0.6900	0.4770
d	0.6990	0.4890
e	0.7740	0.5300
f	0.7800	0.5240
g	0.7050	0.4910
h	0.7180	0.4760
i	0.6630	0.4640
j	0.7790	0.5150
k	0.5760	0.4060
l	0.7380	0.5060
m	0.7520	0.4900
n	0.6320	0.4310
o	0.7030	0.4880
p	0.7050	0.5120
q	0.4620	0.3600

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Chain	Atom inclusion	Q-score
r	0.7310	0.4760
s	0.0300	0.0030
t	0.0070	0.0090
u	0.5460	0.4130
v	0.4690	0.3530
w	0.5150	0.3870
x	0.3910	0.3360
y	0.3560	0.2900
z	0.3640	0.2960