



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 06:01 pm GMT

PDB ID : 5IT7
EMDB ID : EMD-8123
Title : Structure of the *Kluyveromyces lactis* 80S ribosome in complex with the cricket paralysis virus IRES and eEF2
Authors : Murray, J.; Savva, C.G.; Shin, B.S.; Dever, T.E.; Ramakrishnan, V.; Fernandez, I.S.
Deposited on : 2016-03-16
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

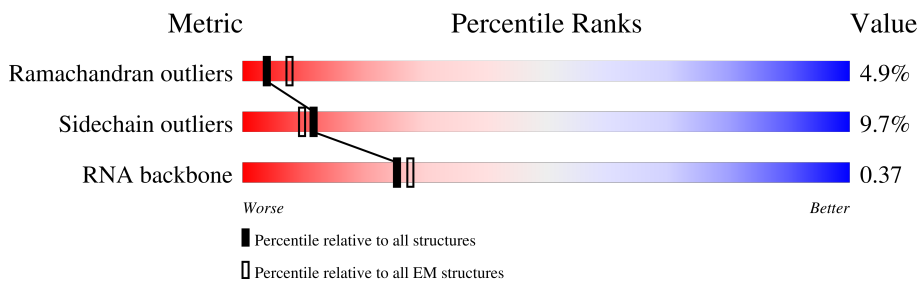
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	5	3270	 6% 68% 31%
2	7	121	 80% 20%
3	8	157	 75% 24%
4	AA	249	 88% 11%
5	BB	384	 82% 17%
6	CC	360	 82% 16%
7	DD	295	 8% 86% 13%
8	EE	170	 9% 82% 12% 5%

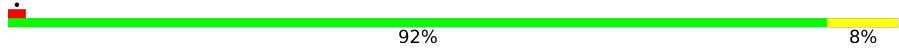

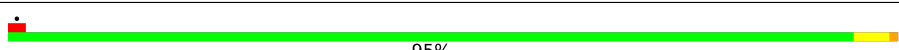
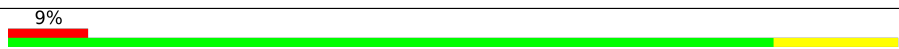

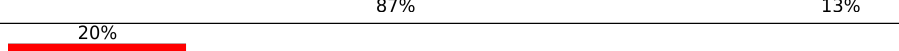
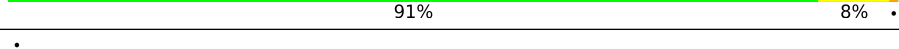

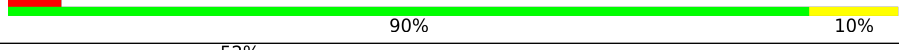
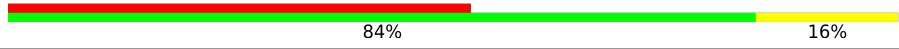





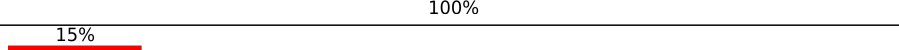





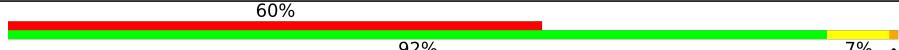

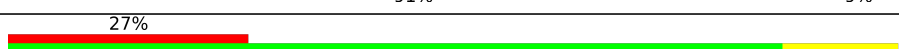
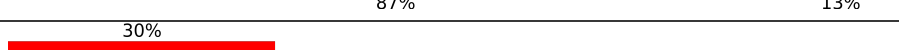
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Mol	Chain	Length	Quality of chain
9	FF	222	85% 14%
10	GG	233	89% 11% 7%
11	HH	191	90% 10% 6%
12	II	216	85% 11%
13	JJ	168	86% 14% 12%
14	LL	197	89% 11% 11%
15	MM	136	85% 14% 5%
16	NN	202	90% 10%
17	OO	198	56% 40% 9%
18	PP	180	87% 12% 9%
19	QQ	184	92% 8%
20	RR	188	94% 6% 13%
21	SS	169	91% 9%
22	TT	158	85% 13%
23	UU	100	100%
24	VV	132	88% 12% 7%
25	WW	62	97% 5%
26	XX	121	87% 13% 7%
27	YY	125	92% 6%
28	ZZ	134	87% 12% 7%
29	aa	147	85% 15%
30	bb	57	95% 5% 7%
31	cc	97	93% 7% 8%
32	dd	106	89% 11% 8%
33	ee	122	94% 6% 5%

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Mol	Chain	Length	Quality of chain
34	ff	105	 92% 8%
35	gg	121	 13% 91% 8%
36	hh	116	 95%
37	ii	98	 9% 86% 14%
38	jj	85	 87% 13%
39	kk	76	 20% 91% 8%
40	ll	49	 88% 12%
41	mm	51	 6% 90% 10%
42	nn	25	 52% 84% 16%
43	oo	101	 9% 87% 12%
44	pp	87	 5% 77% 18% 5%
45	qq	217	 78% 83% 14%
46	rr	195	 77% 85% 14%
47	KK	147	 80% 100%
48	A	206	 15% 86% 13%
49	B	214	 31% 89% 9%
50	C	217	 7% 83% 15%
51	D	223	 48% 88% 12%
52	E	260	 14% 86% 13%
53	F	206	 60% 92% 7%
54	G	226	 47% 91% 9%
55	H	184	 27% 87% 13%
56	I	200	 30% 82% 11% 6%
57	J	182	 14% 86% 13%
58	K	96	 63% 89% 9%

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Mol	Chain	Length	Quality of chain
59	L	155	24% 88% 11%
60	M	122	93% 93% 7%
61	N	150	16% 89% 11%
62	O	127	20% 89% 11%
63	P	123	64% 82% 17%
64	Q	141	48% 91% 9%
65	R	129	46% 88% 12%
66	S	145	71% 86% 14%
67	T	143	48% 94% 6%
68	U	106	58% 93% 7%
69	V	87	11% 84% 16%
70	W	129	83% 83% 16%
71	X	145	9% 84% 14%
72	Y	134	28% 87% 13%
73	Z	70	53% 93% 6%
74	a	100	19% 72% 23%
75	b	82	28% 91% 7%
76	c	63	52% 95% 5%
77	d	53	23% 94% 6%
78	e	55	38% 89% 11%
79	f	69	83% 78% 17%
80	g	324	68% 90% 7%
81	2	1798	16% 54% 44%
82	4	190	59% 52% 46%
83	1	827	44% 84% 13%

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 215768 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 DNA/RNA hybrid called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	5	3270	69896	31222	12579	22825	3270	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	121	2579	1152	461	845	121	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	157	3326	1488	573	1108	157	0	0

- Molecule 4 is a protein called KLLA0D16027p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AA	249	1892	1176	385	330	1	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BB	384	3064	1946	580	533	5	0	0

- Molecule 6 is a protein called KLLA0B07139p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CC	359	2731	1715	522	491	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	3	ARG	ILE	conflict	UNP Q6CW41

- Molecule 7 is a protein called KLLA0D06941p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	DD	295	2384	1510	417	456	1	0	0

- Molecule 8 is a protein called KLLA0B04686p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	EE	161	1300	834	243	223	0	0

- Molecule 9 is a protein called KLLA0D03410p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	FF	222	1774	1138	319	316	1	0	0

- Molecule 10 is a protein called KLLA0E00573p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	GG	233	1817	1160	324	330	3	0	0

- Molecule 11 is a protein called KLLA0F04499p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	HH	191	1528	965	277	284	2	0	0

- Molecule 12 is a protein called KLLA0D05643p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	II	207	1690	1074	319	292	5	0	0

- Molecule 13 is a protein called KLLA0F08261p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	JJ	168	1349	845	255	245	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LL	197	1581	988	317	276		0	0

- Molecule 15 is a protein called KLLA0B13409p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	MM	136	1045	666	196	183		0	0

- Molecule 16 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	NN	202	1709	1069	359	280	1	0	0

- Molecule 17 is a protein called KLLA0F04675p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	OO	198	1571	1013	290	267	1	196	0

- Molecule 18 is a protein called KLLA0A06336p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	PP	180	1432	885	287	260		0	0

- Molecule 19 is a protein called KLLA0A07227p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	QQ	184	1444	911	290	243		0	0

- Molecule 20 is a protein called KLLA0E12453p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	RR	188	1522	933	328	259	2	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	SS	169	1416	916	259	238	3	0	0

- Molecule 22 is a protein called KLLA0E23651p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	TT	158	1262	797	240	220	5	0	0

- Molecule 23 is a protein called KLLA0D05181p.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	UU	100	807	524	131	152	0	0

- Molecule 24 is a protein called KLLA0E06997p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	VV	132	976	612	182	174	8	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	WW	62	515	330	103	82	0	0

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	XX	121	964	620	169	174	1	0	0

- Molecule 27 is a protein called KLLA0B05742p.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	YY	125	Total	C	N	O	0	0
			992	622	189	181		

- Molecule 28 is a protein called KLLA0E03455p.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	ZZ	134	Total	C	N	O	0	0
			1089	708	199	182		

- Molecule 29 is a protein called RPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	aa	147	Total	C	N	O	S	0	0
			1156	740	225	189	2		

- Molecule 30 is a protein called KLLA0D16071p.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	bb	57	Total	C	N	O	0	0
			458	287	99	72		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	cc	97	Total	C	N	O	S	0	0
			740	477	125	137	1		

- Molecule 32 is a protein called KLLA0B02937p.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	dd	106	Total	C	N	O	S	0	0
			869	553	167	147	2		

- Molecule 33 is a protein called KLLA0E06843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	ee	122	Total	C	N	O	S	0	0
			980	618	198	162	2		

- Molecule 34 is a protein called KLLA0D07405p.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	ff	105	Total	C	N	O	S	0	0
			837	531	161	144	1		

- Molecule 35 is a protein called KLLA0C08371p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	gg	121	Total	C	N	O	S	0	0
			951	591	192	167	1		

- Molecule 36 is a protein called KLLA0F05247p.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	hh	116	Total	C	N	O	0	0
			961	608	187	166		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	ii	98	Total	C	N	O	S	0	0
			766	479	155	131	1		

- Molecule 38 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	jj	85	Total	C	N	O	S	0	0
			675	410	148	111	6		

- Molecule 39 is a protein called KLLA0C18216p.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	kk	76	Total	C	N	O	0	0
			619	398	114	107		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	ll	49	Total	C	N	O	S	0	0
			428	266	96	64	2		

- Molecule 41 is a protein called Ubiquitin fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	mm	51	Total	C	N	O	S	0	0
			410	254	85	66	5		

- Molecule 42 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	nn	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 43 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	oo	101	Total	C	N	O	S	0	0
			814	509	163	136	6		

- Molecule 44 is a protein called KLLA0E05941p.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	pp	87	Total	C	N	O	S	0	0
			660	404	133	117	6		

- Molecule 45 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	qq	217	Total	C	N	O	S	0	0
			1721	1100	300	312	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
qq	11	GLU	ASP	conflict	UNP Q6CWR9
qq	12	HIS	ASN	conflict	UNP Q6CWR9
qq	152	ARG	LYS	conflict	UNP Q6CWR9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	rr	195	Total	C	N	O	S	0	0
			1508	968	258	278	4		

- Molecule 47 is a protein called uL11.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	KK	147	Total	C	N	O		
			735	441	147	147	0	0

- Molecule 48 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A	206	Total	C	N	O	S		
			1616	1035	285	294	2	0	0

- Molecule 49 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B	214	Total	C	N	O	S		
			1722	1089	313	317	3	0	0

- Molecule 50 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	C	217	Total	C	N	O	S		
			1629	1041	287	297	4	0	0

- Molecule 51 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	D	223	Total	C	N	O	S		
			1744	1108	313	318	5	0	0

- Molecule 52 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	E	260	Total	C	N	O	S		
			2078	1322	393	359	4	0	0

- Molecule 53 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	F	206	Total	C	N	O	S		
			1609	1008	298	300	3	0	0

- Molecule 54 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	G	226	1812	1134	348	326	4	0	0

- Molecule 55 is a protein called KLLA0C13519p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	H	184	1483	950	270	263		0	0

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	I	188	1493	926	301	265	1	0	0

- Molecule 57 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	J	182	1471	929	287	254	1	0	0

- Molecule 58 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	K	96	809	533	129	146	1	0	0

- Molecule 59 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	L	155	1248	798	237	210	3	0	0

- Molecule 60 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
60	M	122	922	575	167	180	0	0

- Molecule 61 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	N	150	1187	756	223	206	2	0	0

- Molecule 62 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	O	127	942	578	188	173	3	0	0

- Molecule 63 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	P	123	980	628	179	168	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	130	ALA	-	expression tag	UNP Q6CKV4

- Molecule 64 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
64	Q	141	1105	709	204	192	0	0

- Molecule 65 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	R	129	1031	641	193	194	3	0	0

- Molecule 66 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	S	145	1193	741	240	210	2	0	0

- Molecule 67 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 68 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 69 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 70 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 71 is a protein called RPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	X	145	Total	C	N	O	S	0	0
			1127	713	219	192	3		

- Molecule 72 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
72	Y	134	Total	C	N	O	0	0
			1061	665	207	189		

- Molecule 73 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Z	70	Total	C	N	O	S	0	0
			558	355	104	98	1		

- Molecule 74 is a protein called KLLA0D05115p.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	a	100	Total	C	N	O	S	0	0
			798	491	170	131	6		

- Molecule 75 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	b	82	Total	C	N	O	S	0	0
			617	384	113	114	6		

- Molecule 76 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	c	63	Total	C	N	O	S	0	0
			494	305	98	90	1		

- Molecule 77 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	d	53	Total	C	N	O	S	0	0
			446	280	89	76	1		

- Molecule 78 is a protein called KLLA0C04809p.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	e	55	Total	C	N	O	S	0	0
			443	276	90	76	1		

- Molecule 79 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 80 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 81 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
81	2	1780	37797	16892	6658	12467	1780	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	676	G	U	conflict	GB 49642208
2	678	U	G	conflict	GB 49642208

- Molecule 82 is DNA/RNA hybrid called cricket paralysis virus IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
82	4	190	3950	1768	667	1325	190	0	0

- Molecule 83 is a protein called Eft2p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	1	827	6421	4070	1106	1216	29	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	310	GLU	ASP	conflict	UNP W7R097

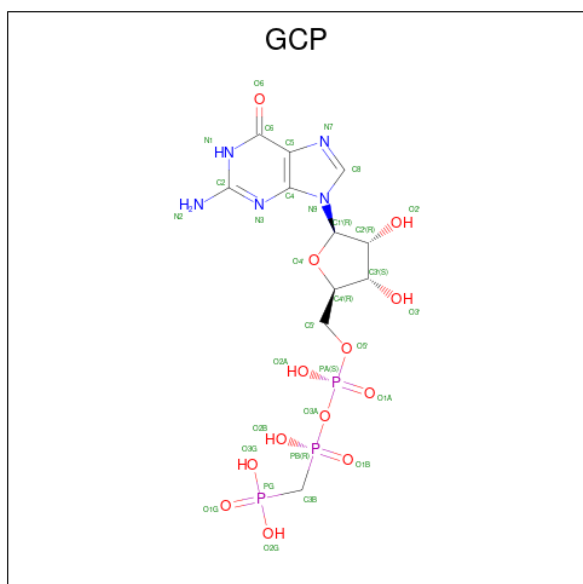
- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	5	2	Total 2	Mg 2	0
84	N	1	Total 1	Mg 1	0
84	f	1	Total 1	Mg 1	0
84	2	75	Total 75	Mg 75	0
84	1	1	Total 1	Mg 1	0

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

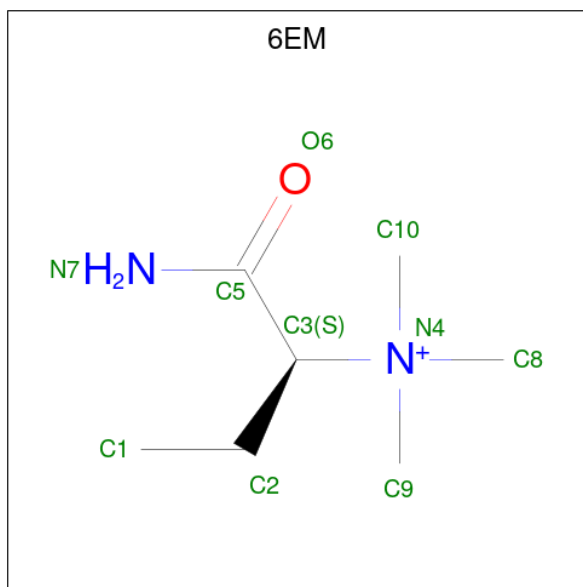
Mol	Chain	Residues	Atoms	AltConf
85	jj	1	Total Zn 1 1	0
85	mm	1	Total Zn 1 1	0
85	oo	1	Total Zn 1 1	0
85	a	1	Total Zn 1 1	0
85	b	1	Total Zn 1 1	0
85	f	1	Total Zn 1 1	0

- Molecule 86 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
86	1	1	Total C N O P 32 11 5 13 3	0

- Molecule 87 is (2S)-1-amino-N,N,N-trimethyl-1-oxobutan-2-aminium (three-letter code: 6EM) (formula: $C_7H_{17}N_2O$).

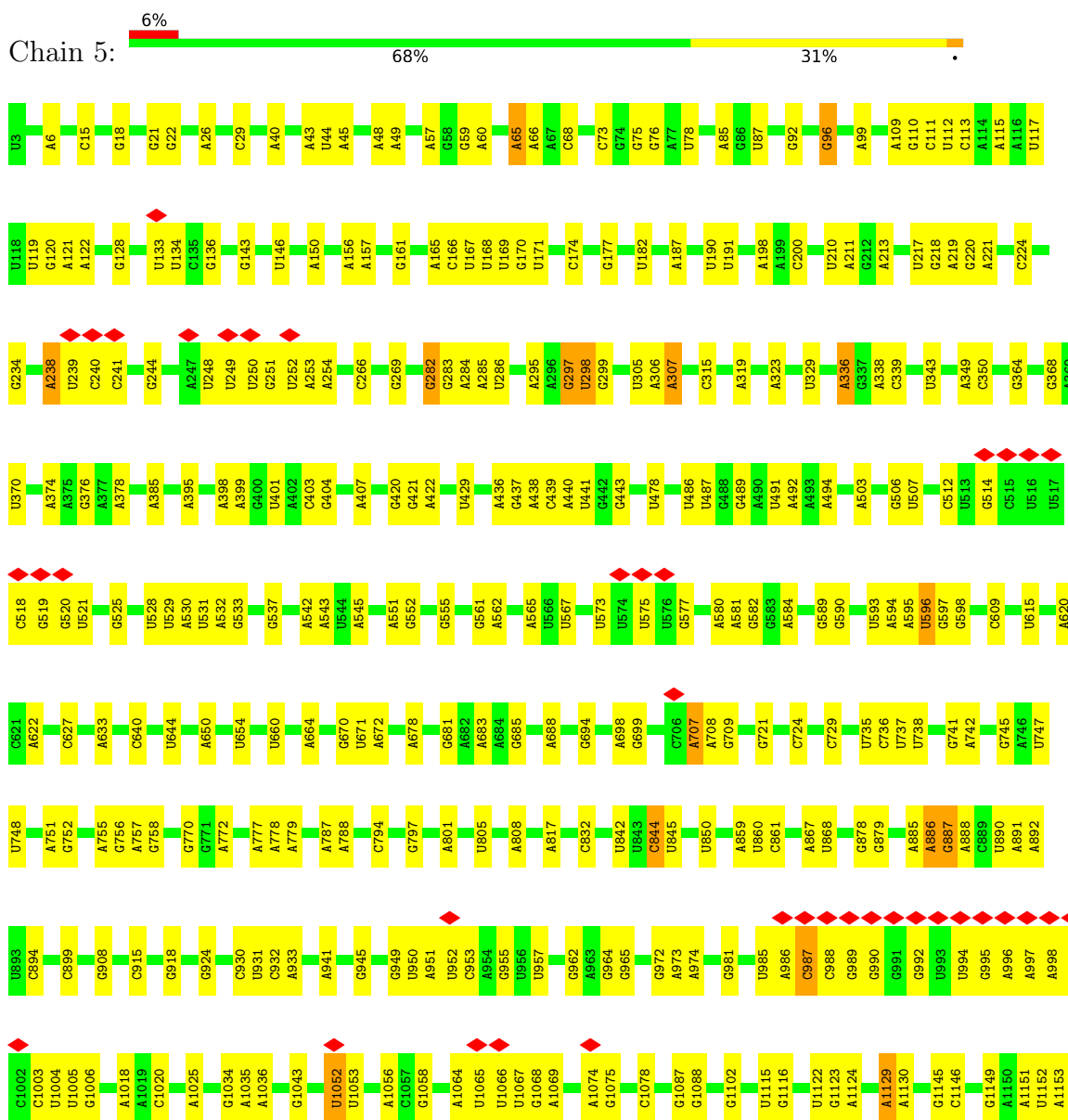


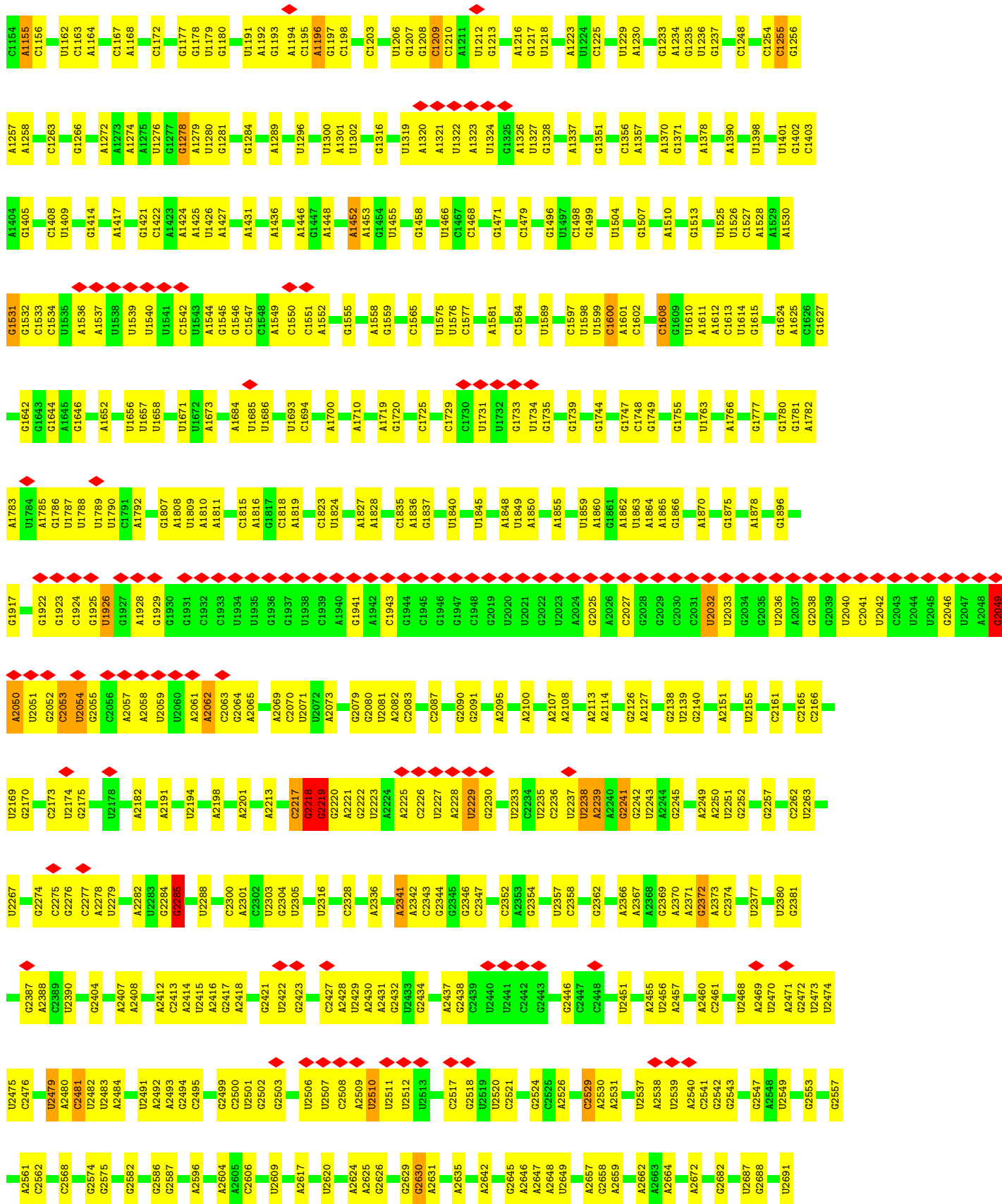
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
87	1	1	10	7	2	1	0

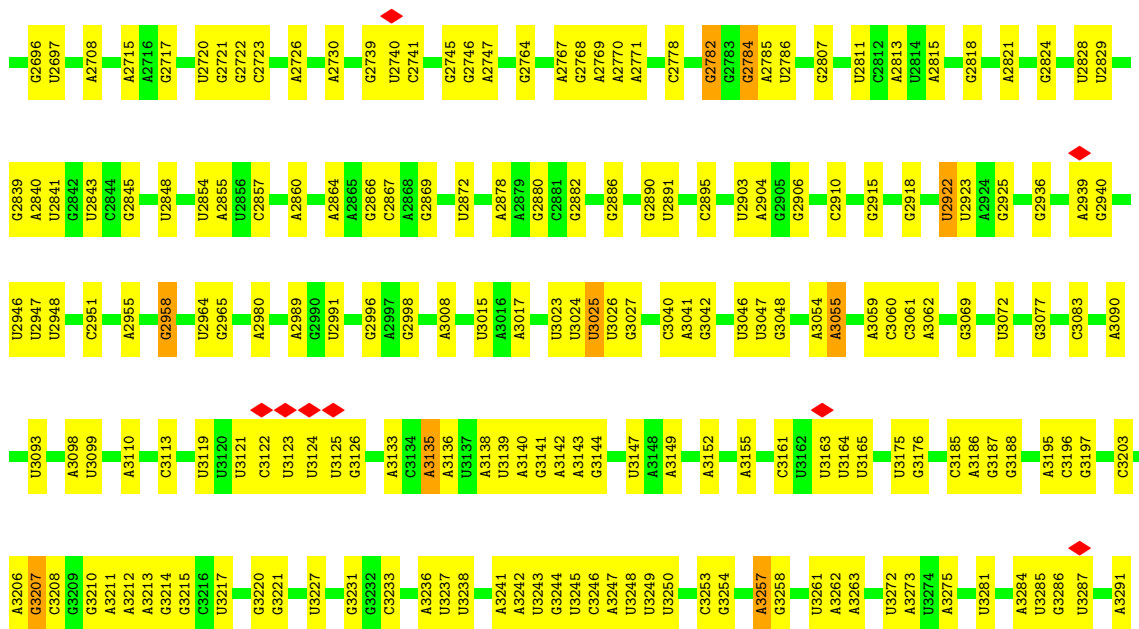
3 Residue-property plots

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.

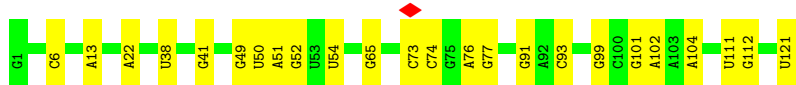
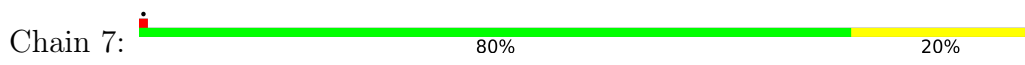
- Molecule 1: 25S ribosomal RNA



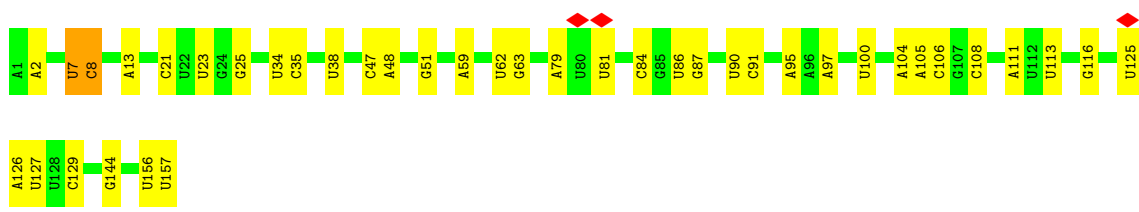
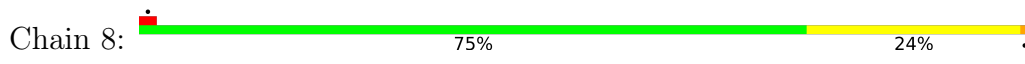




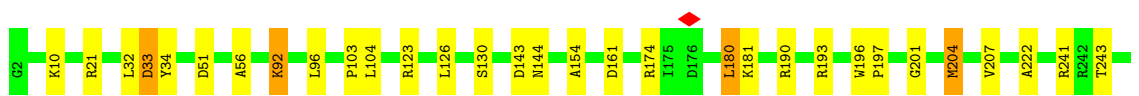
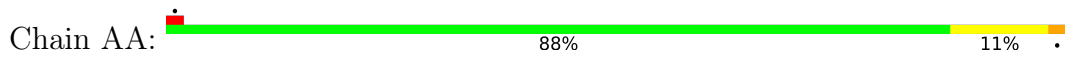
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5.8S ribosomal RNA

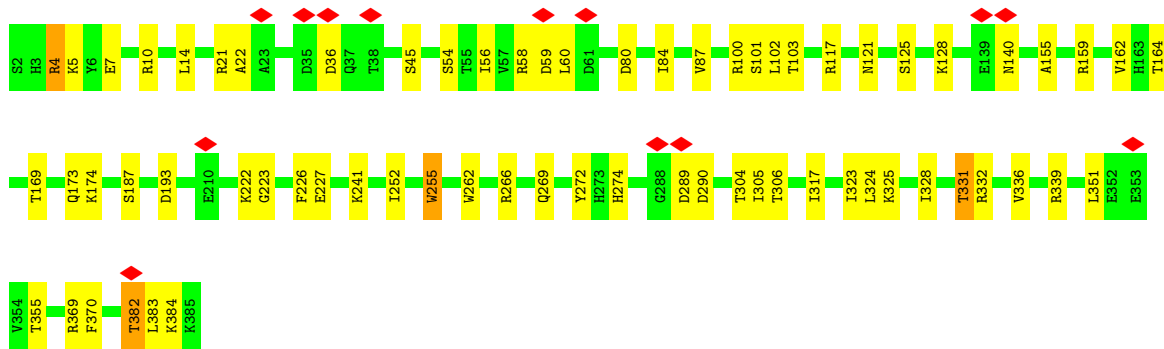
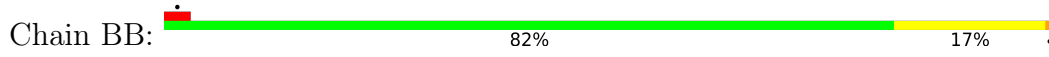


• Molecule 4: KLLA0D16027p

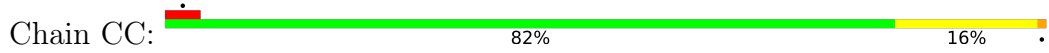




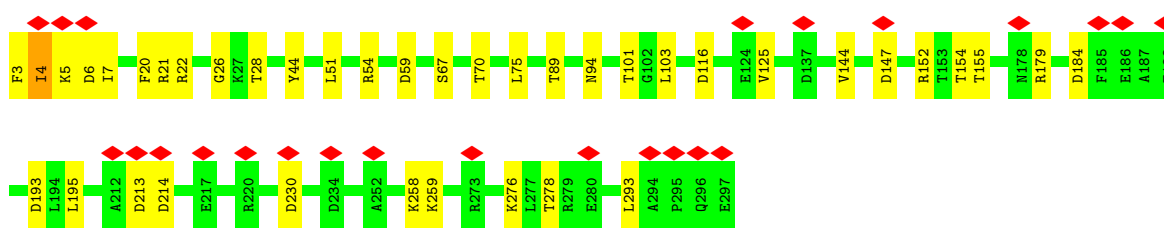
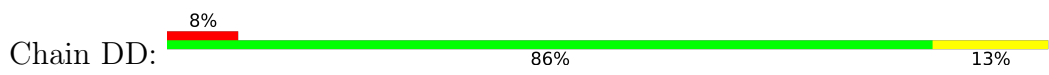
• Molecule 5: 60S ribosomal protein L3



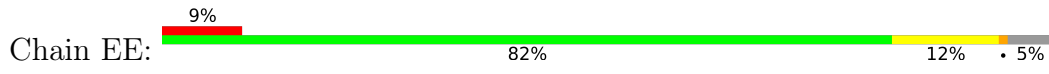
• Molecule 6: KLLA0B07139p

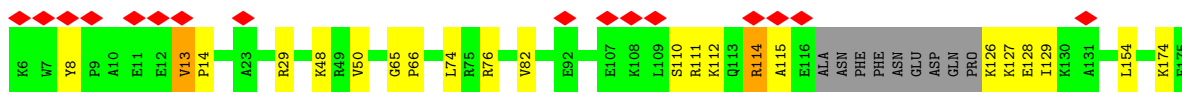


• Molecule 7: KLLA0D06941p

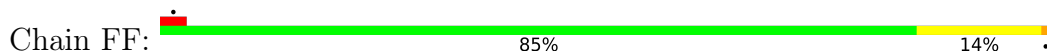


• Molecule 8: KLLA0B04686p

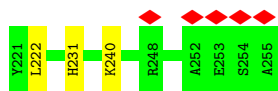
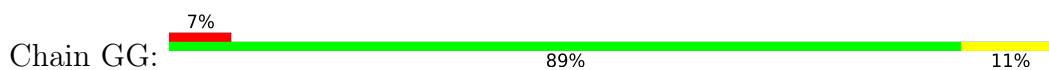




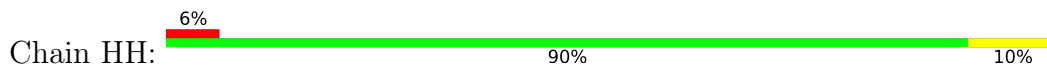
• Molecule 9: KLLA0D03410p



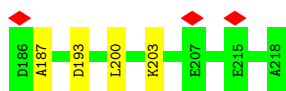
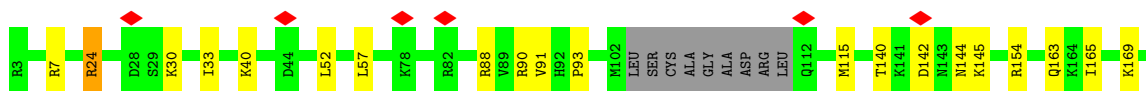
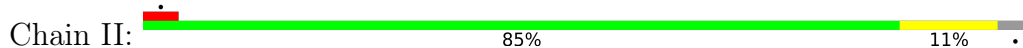
• Molecule 10: KLLA0E00573p



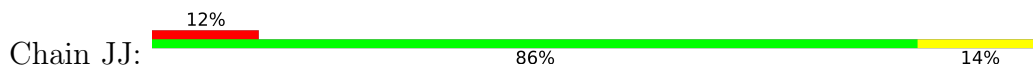
• Molecule 11: KLLA0F04499p

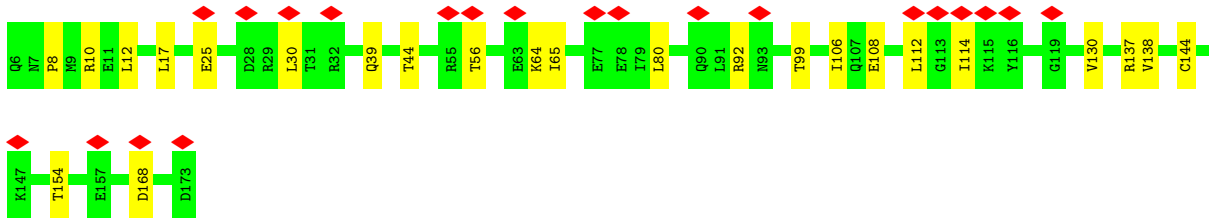


• Molecule 12: KLLA0D05643p

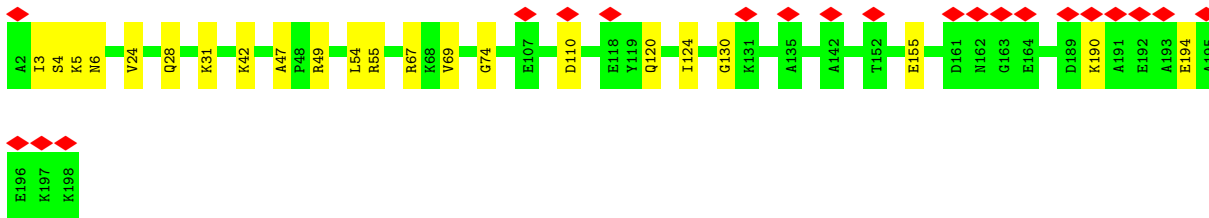
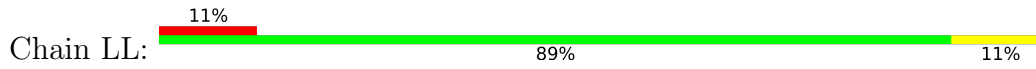


• Molecule 13: KLLA0F08261p

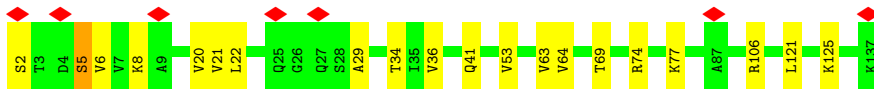
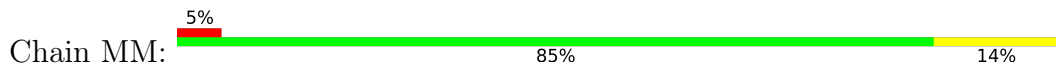




- Molecule 14: 60S ribosomal protein L13



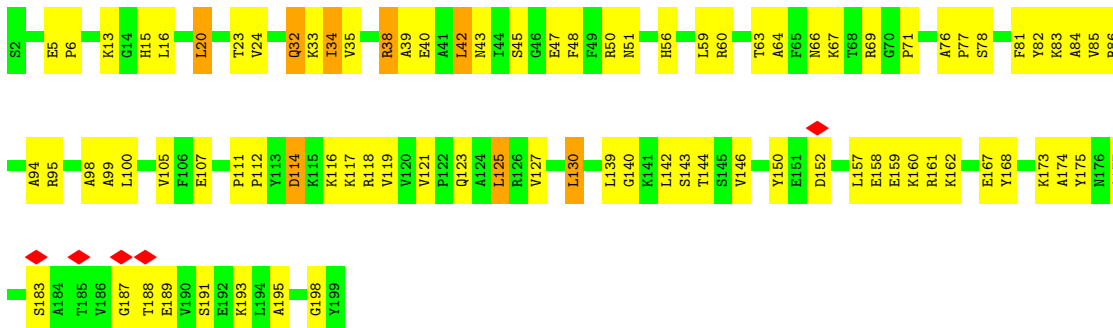
- Molecule 15: KLLA0B13409p



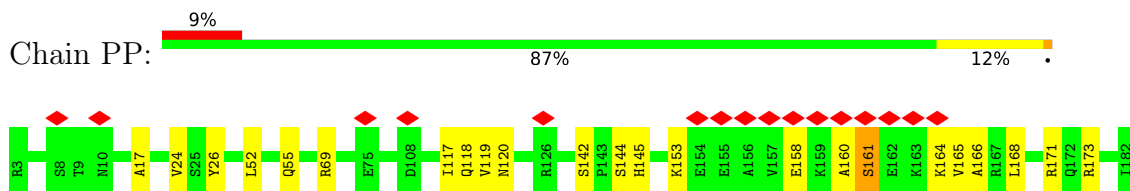
- Molecule 16: Ribosomal protein L15



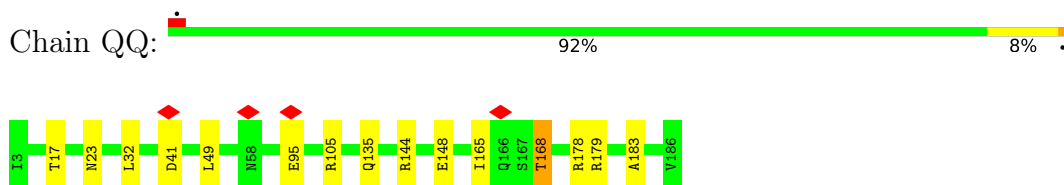
- Molecule 17: KLLA0F04675p



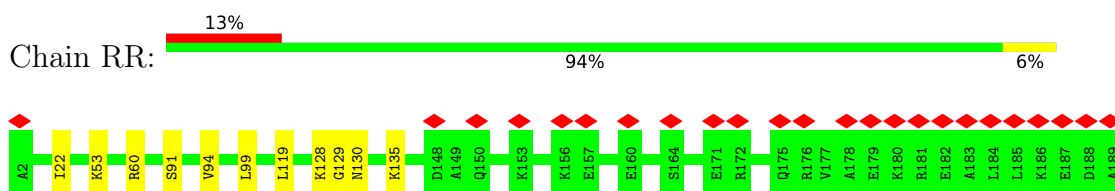
- Molecule 18: KLLA0A06336p



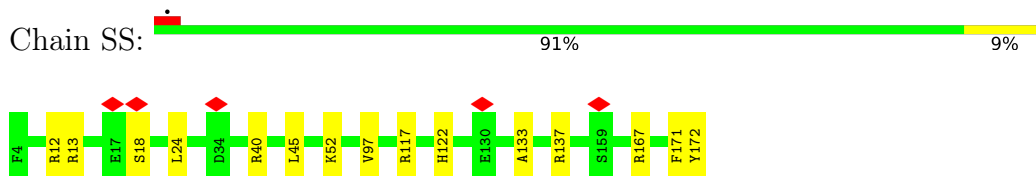
- Molecule 19: KLLA0A07227p



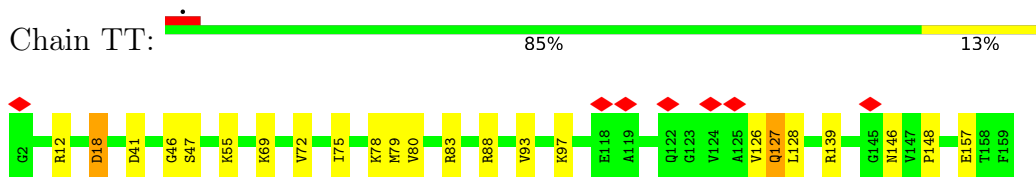
- Molecule 20: KLLA0E12453p



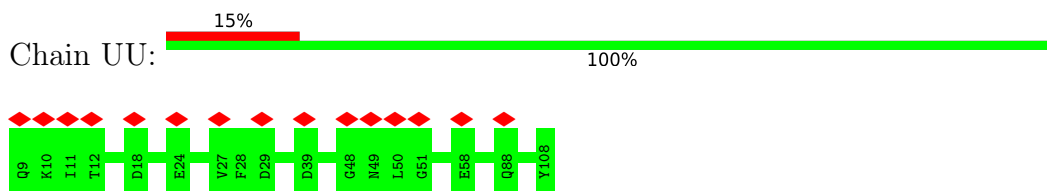
- Molecule 21: 60S ribosomal protein L20



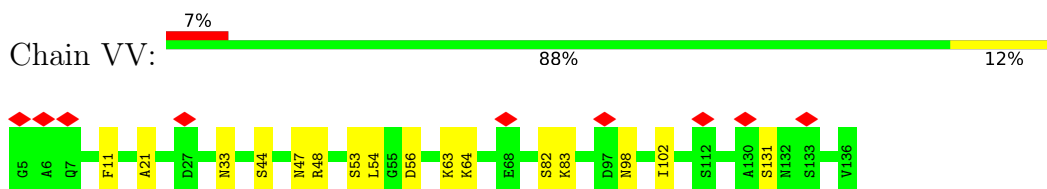
- Molecule 22: KLLA0E23651p



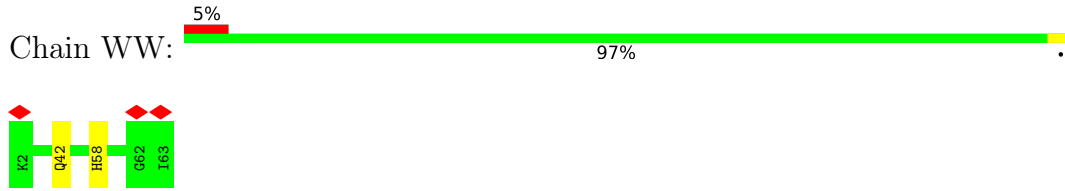
- Molecule 23: KLLA0D05181p



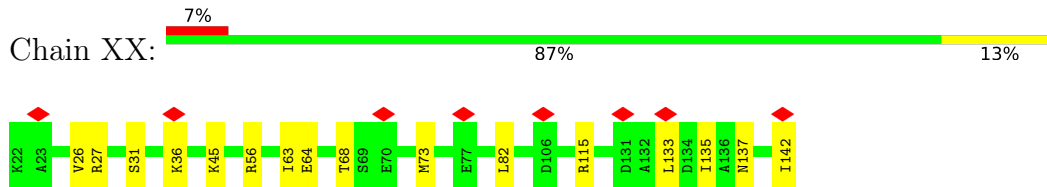
- Molecule 24: KLLA0E06997p



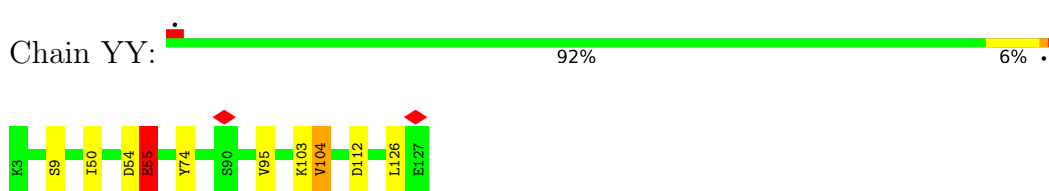
- Molecule 25: 60S ribosomal protein L24



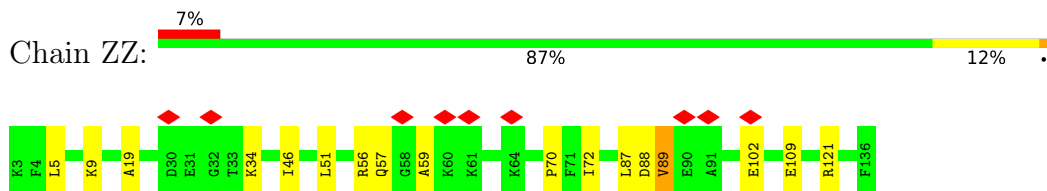
- Molecule 26: 60S ribosomal protein L25



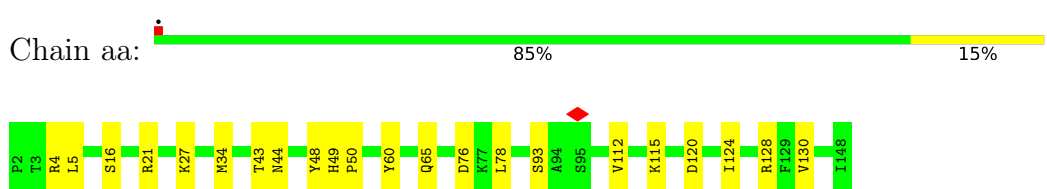
- Molecule 27: KLLA0B05742p



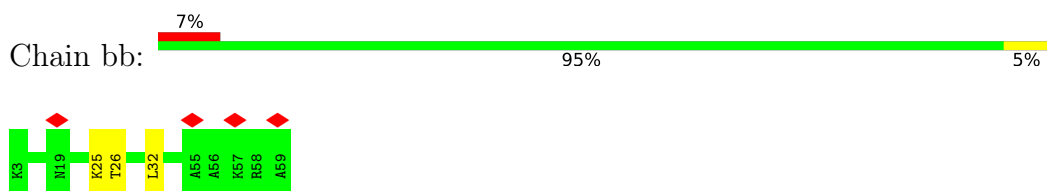
- Molecule 28: KLLA0E03455p



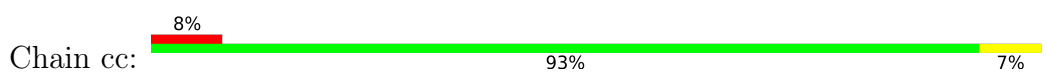
- Molecule 29: RPL28

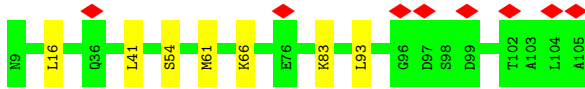


- Molecule 30: KLLA0D16071p

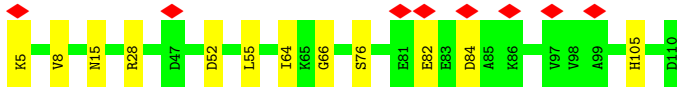
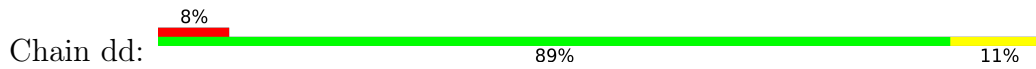


- Molecule 31: 60S ribosomal protein L30

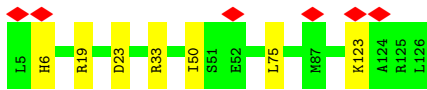




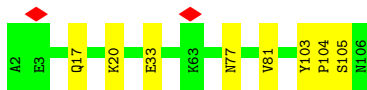
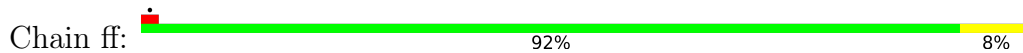
- Molecule 32: KLLA0B02937p



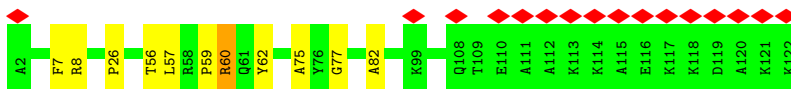
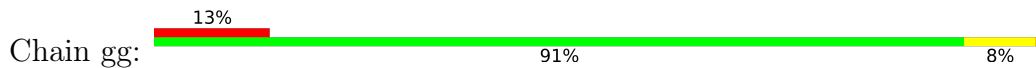
- Molecule 33: KLLA0E06843p



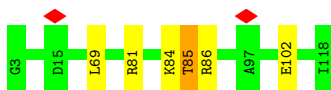
- Molecule 34: KLLA0D07405p



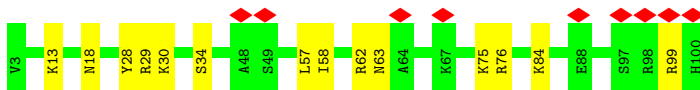
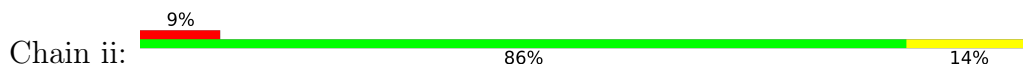
- Molecule 35: KLLA0C08371p



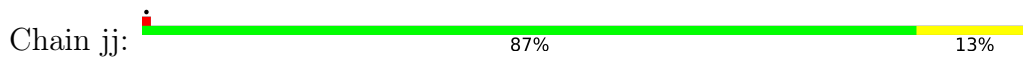
- Molecule 36: KLLA0F05247p



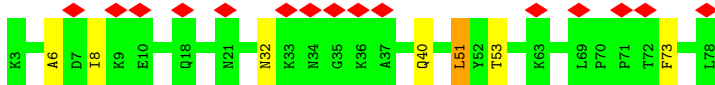
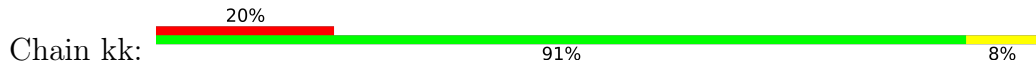
- Molecule 37: 60S ribosomal protein L36



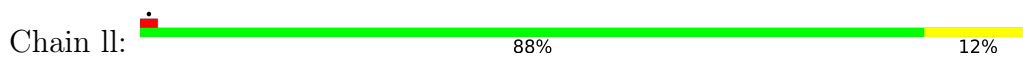
- Molecule 38: Ribosomal protein L37



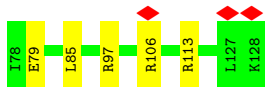
- Molecule 39: KLLA0C18216p



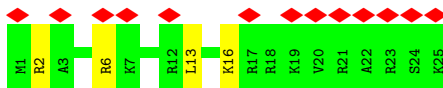
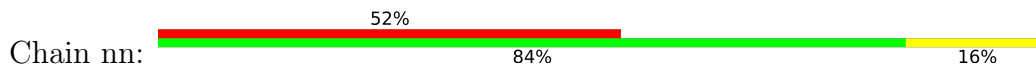
- Molecule 40: 60S ribosomal protein L39



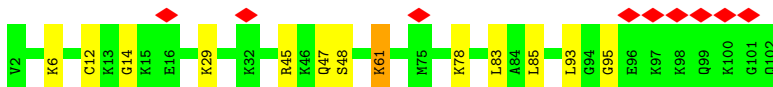
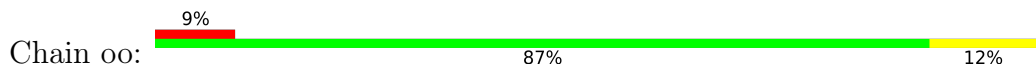
- Molecule 41: Ubiquitin fusion protein



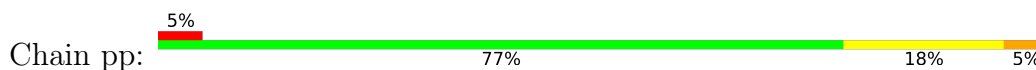
- Molecule 42: 60S ribosomal protein L41-A

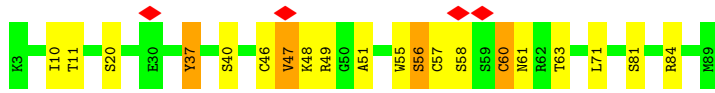


- Molecule 43: 60S ribosomal protein L44

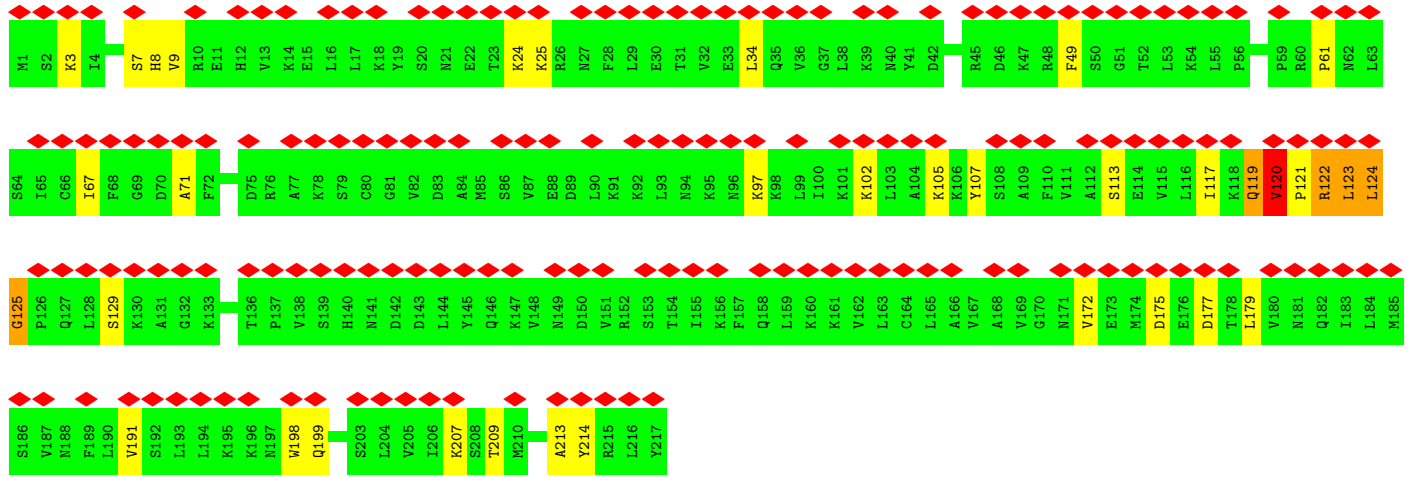
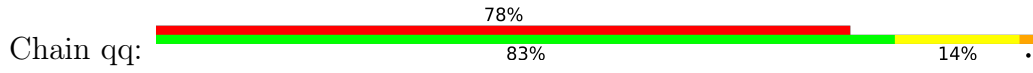


- Molecule 44: KLLA0E05941p

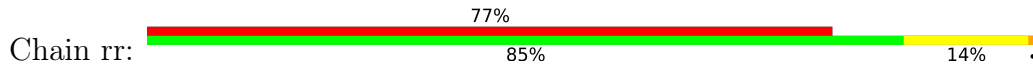




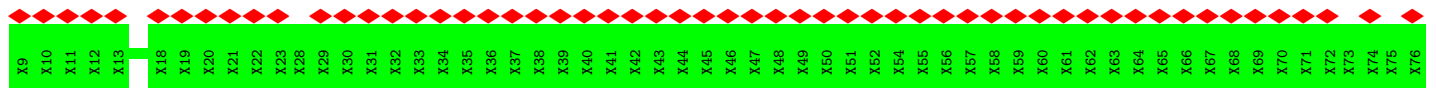
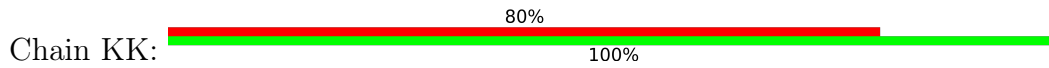
• Molecule 45: Ribosomal protein

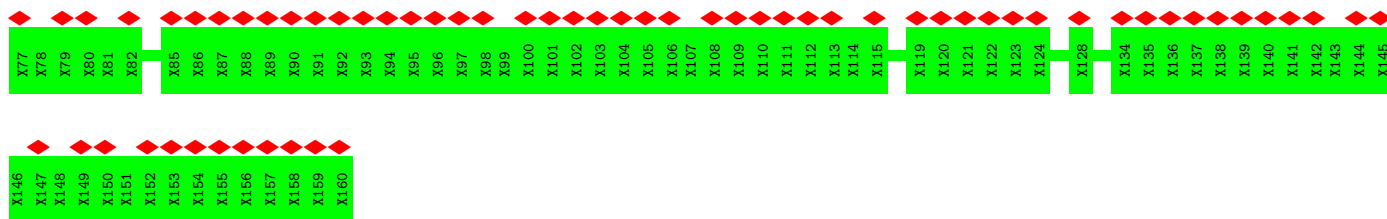


• Molecule 46: 60S acidic ribosomal protein P0

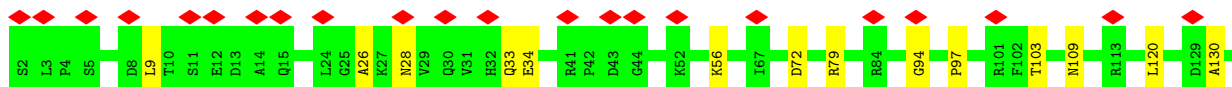
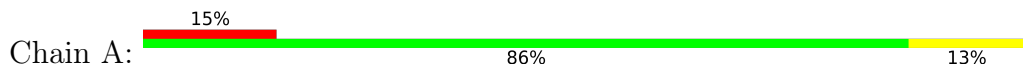


• Molecule 47: uL11

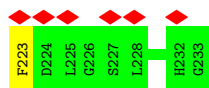
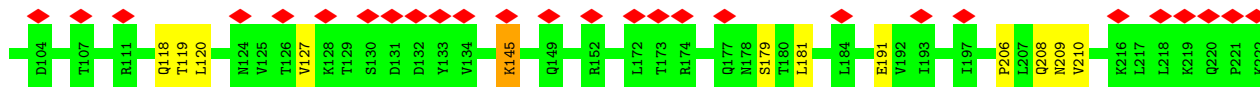
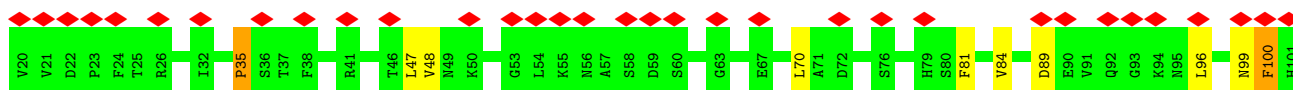
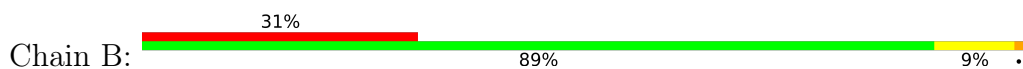




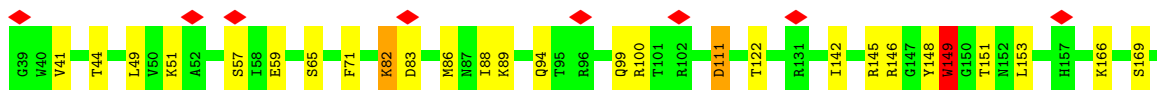
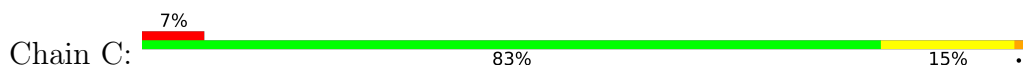
- Molecule 48: 40S ribosomal protein S0



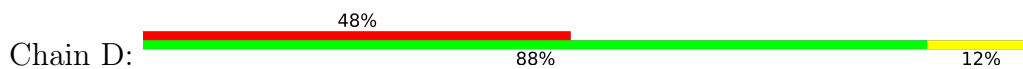
- Molecule 49: 40S ribosomal protein S1

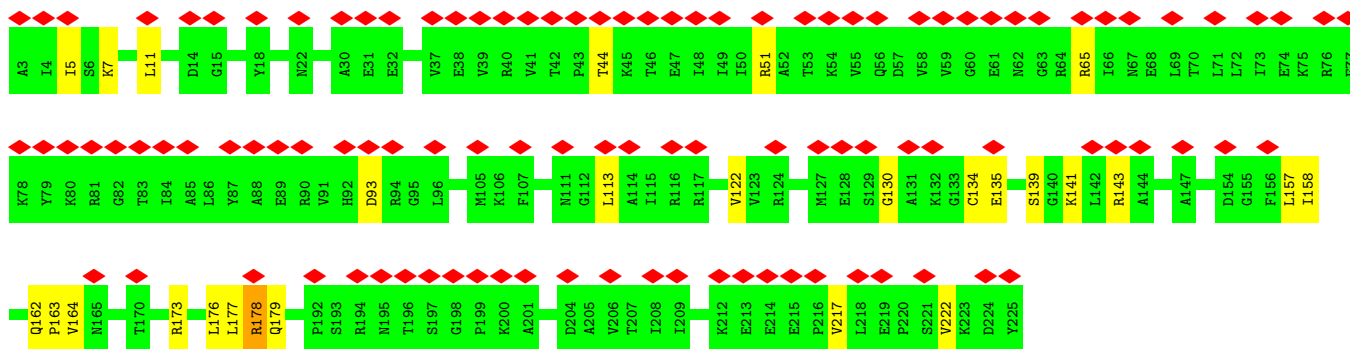


- Molecule 50: KLLA0F09812p

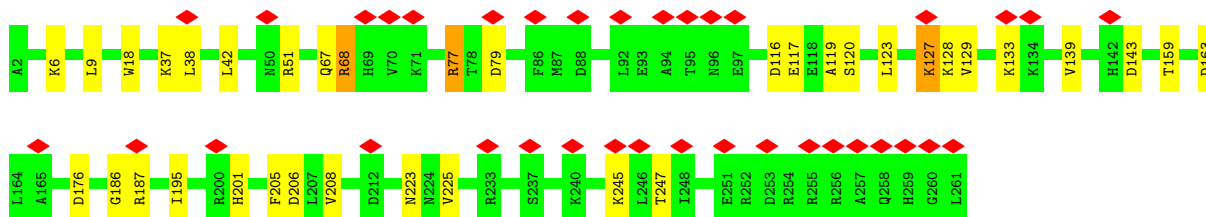
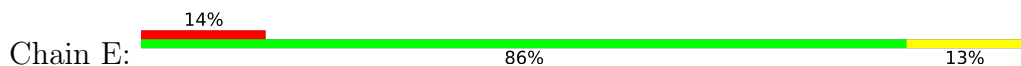


- Molecule 51: KLLA0D08305p

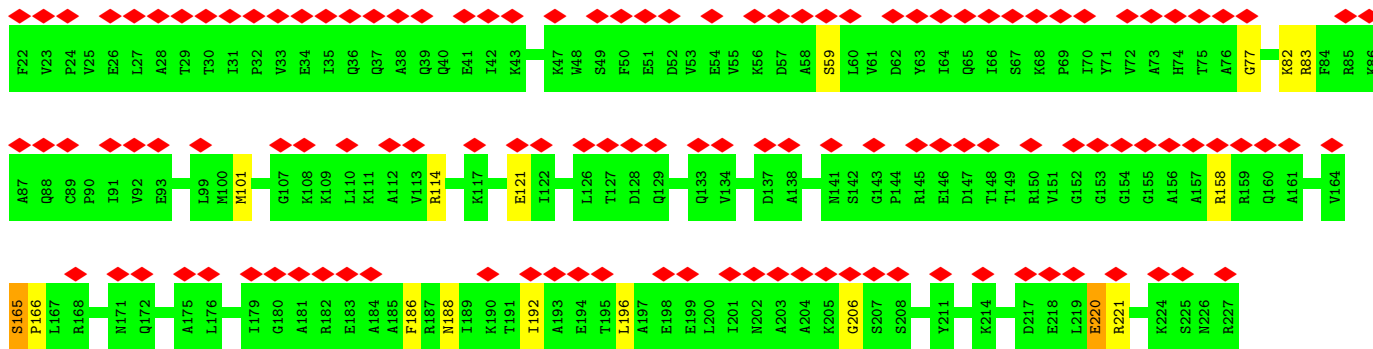
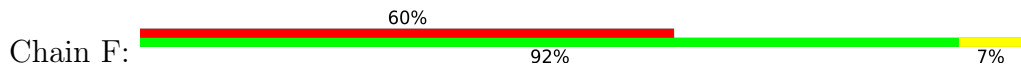




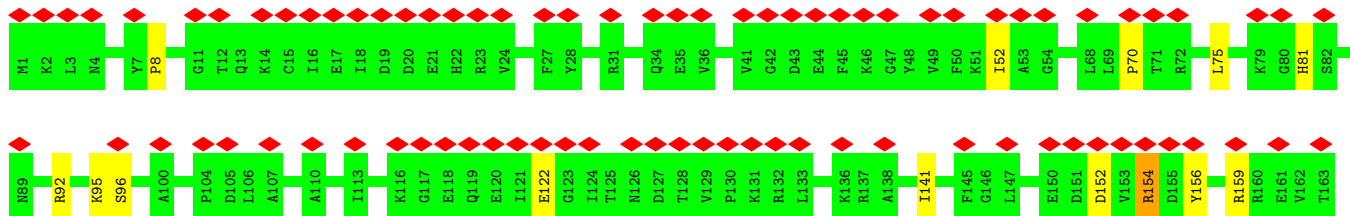
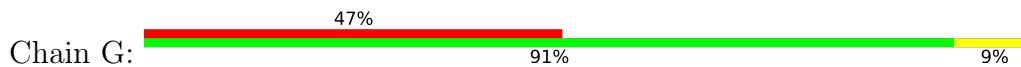
• Molecule 52: 40S ribosomal protein S4

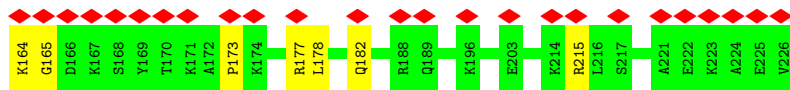


• Molecule 53: KLLA0D10659p

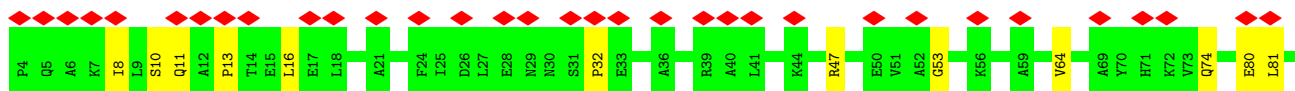
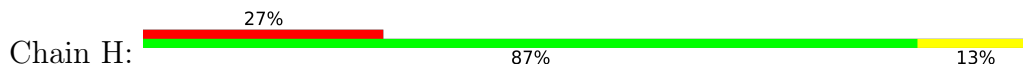


• Molecule 54: 40S ribosomal protein S6

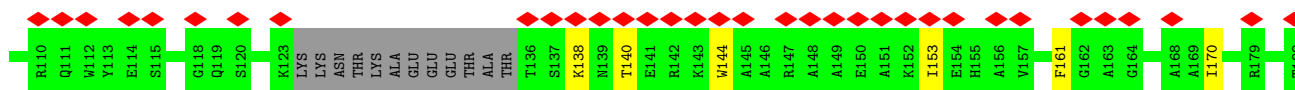
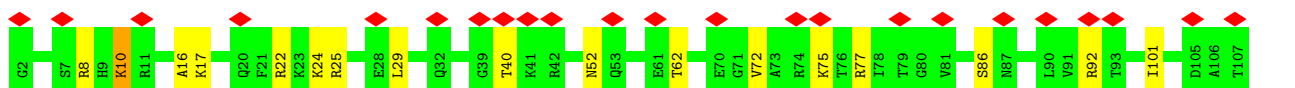
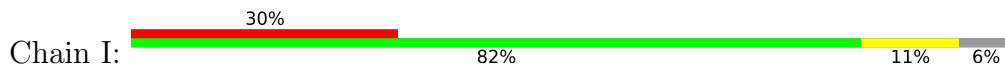




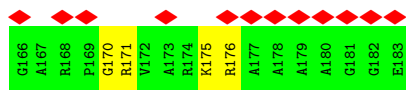
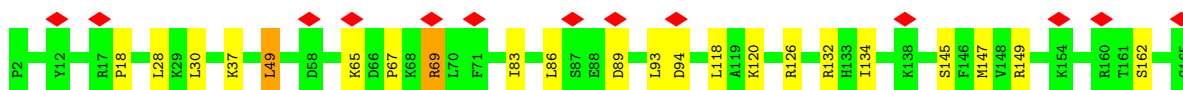
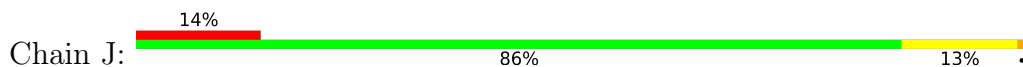
• Molecule 55: KLLA0C13519p



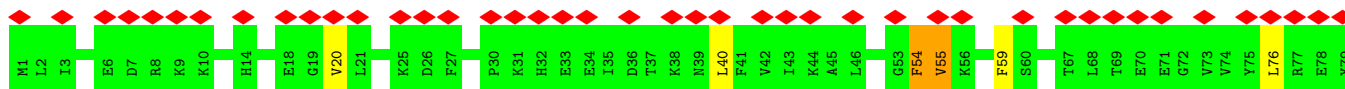
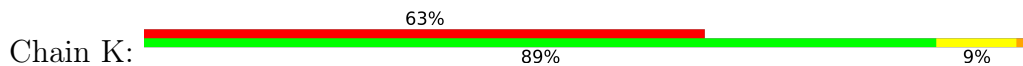
• Molecule 56: 40S ribosomal protein S8

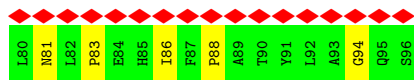


• Molecule 57: KLLA0E23673p

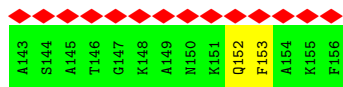
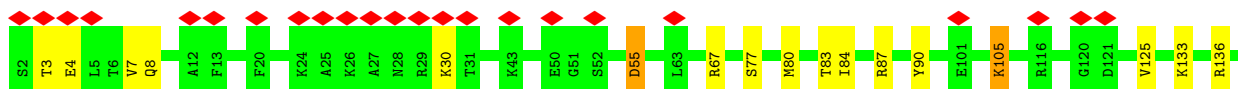
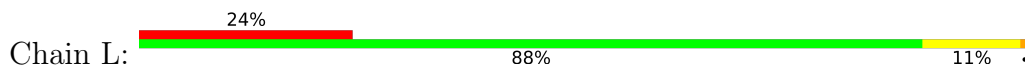


• Molecule 58: KLLA0B08173p

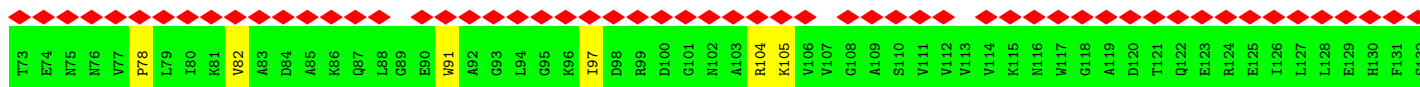
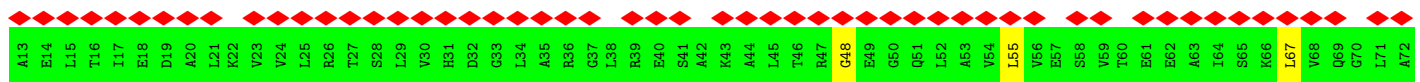




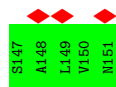
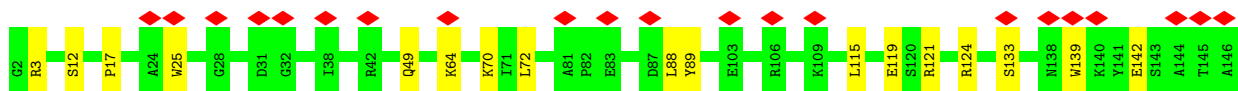
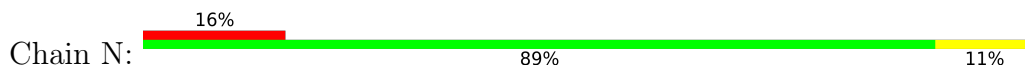
• Molecule 59: KLLA0A10483p



• Molecule 60: 40S ribosomal protein S12



• Molecule 61: KLLA0F18040p

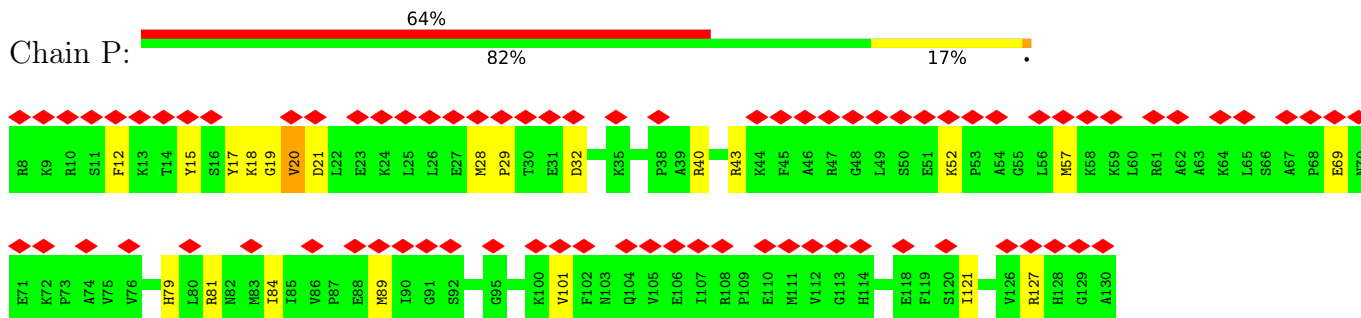


• Molecule 62: 40S ribosomal protein S14

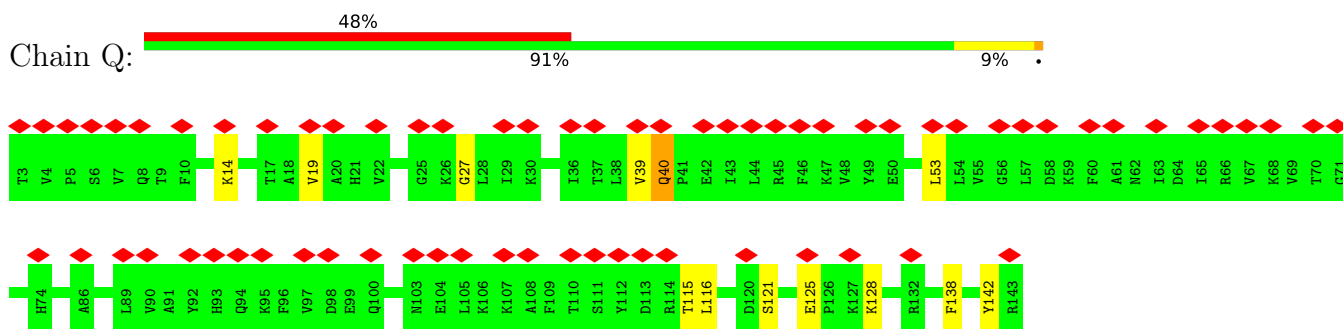


L137

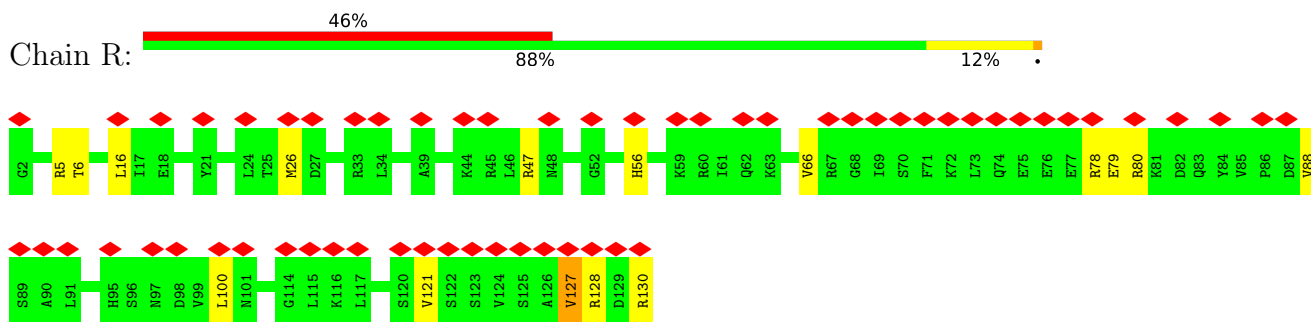
• Molecule 63: KLLA0F07843p



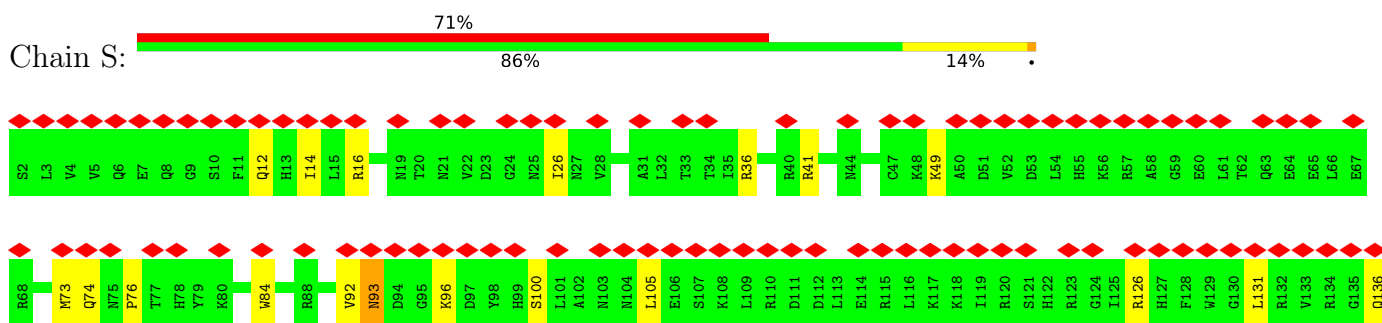
• Molecule 64: 40S ribosomal protein S16

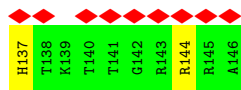


• Molecule 65: KLLA0B01474p

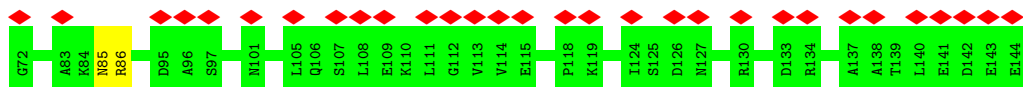
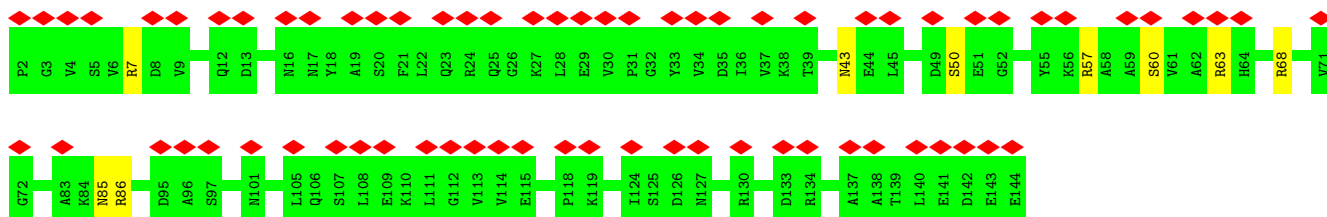
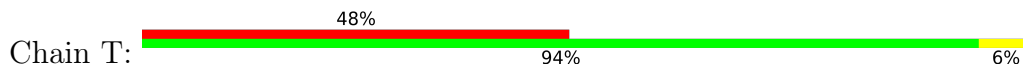


• Molecule 66: KLLA0B01562p

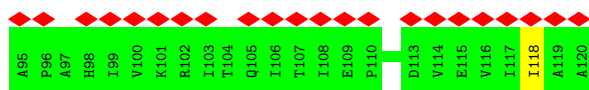
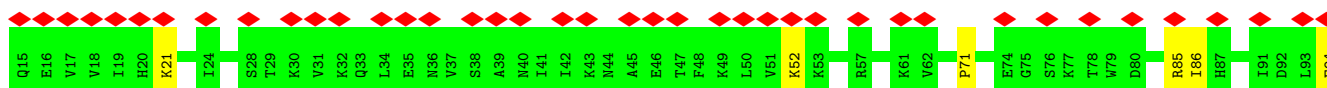
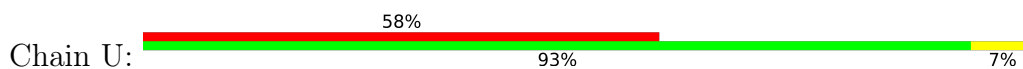




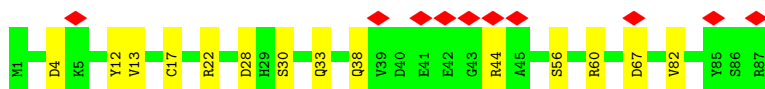
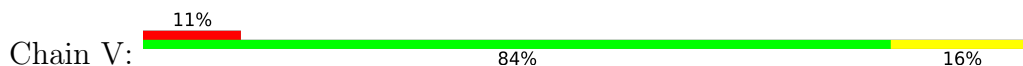
- Molecule 67: KLLA0A07194p



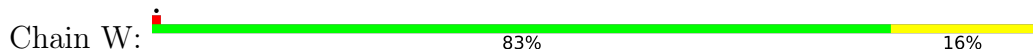
- Molecule 68: KLLA0F25542p



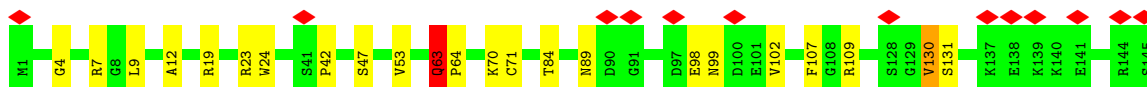
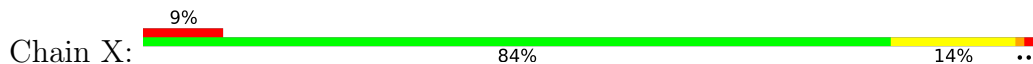
- Molecule 69: 40S ribosomal protein S21



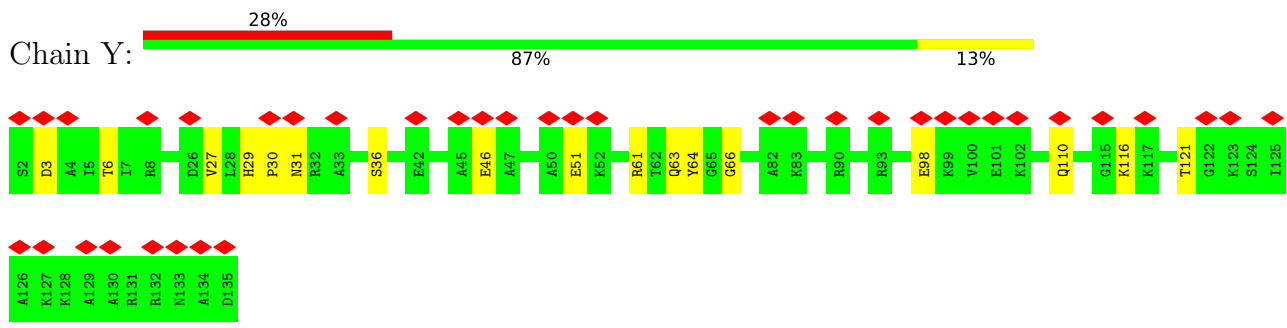
- Molecule 70: 40S ribosomal protein S22



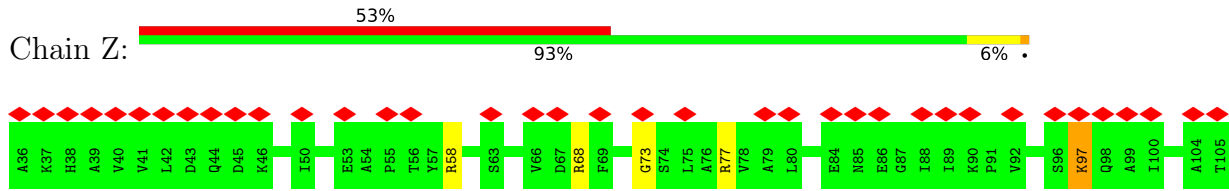
- Molecule 71: RPS23



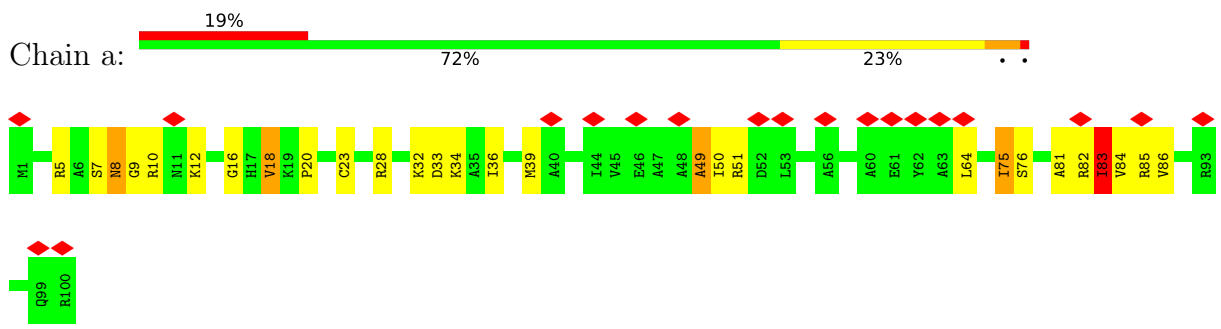
- Molecule 72: 40S ribosomal protein S24



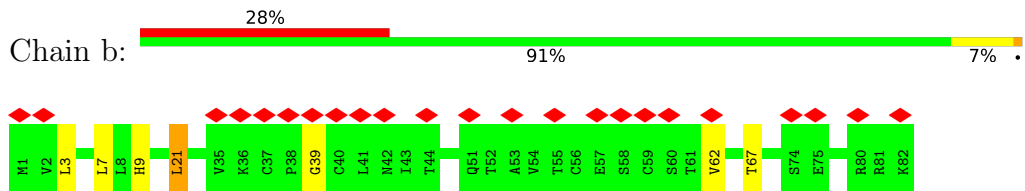
• Molecule 73: KLLA0B06182p



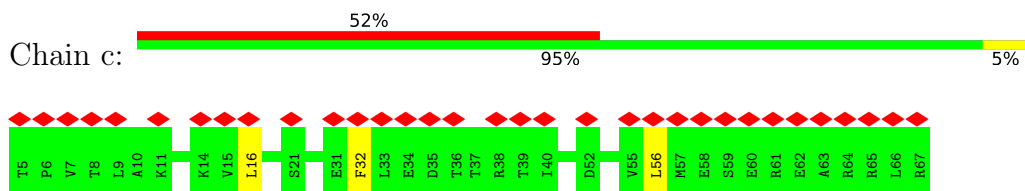
• Molecule 74: KLLA0D05115p



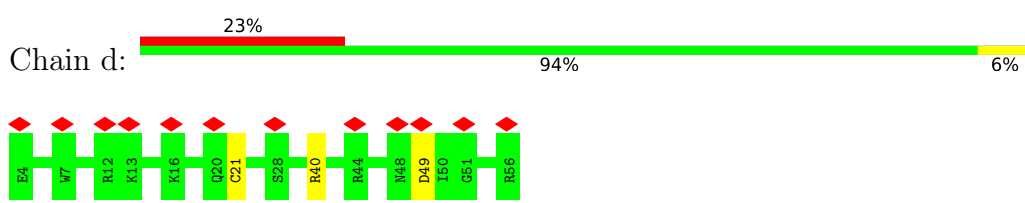
• Molecule 75: 40S ribosomal protein S27



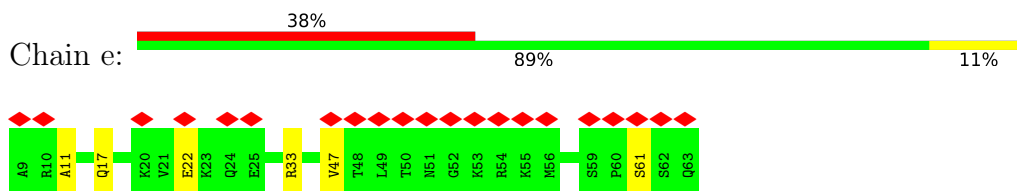
• Molecule 76: 40S ribosomal protein S28



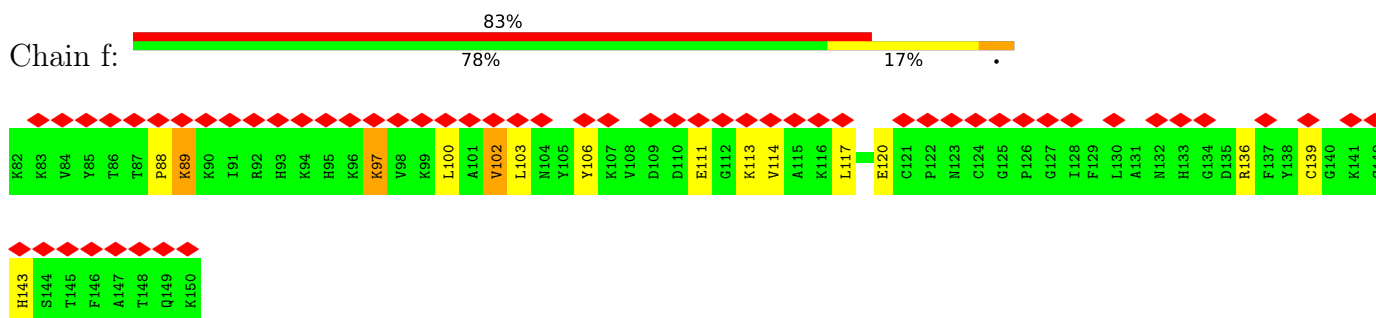
• Molecule 77: 40S ribosomal protein S29



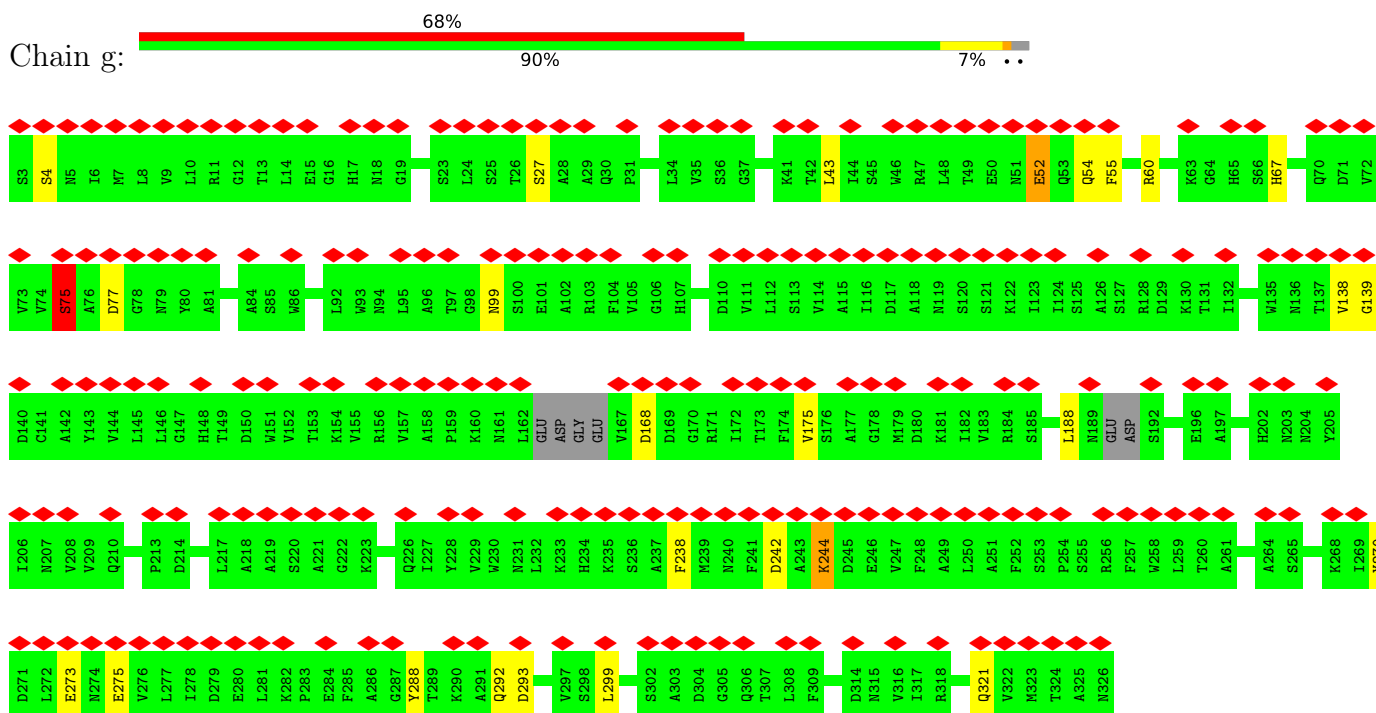
• Molecule 78: KLLA0C04809p



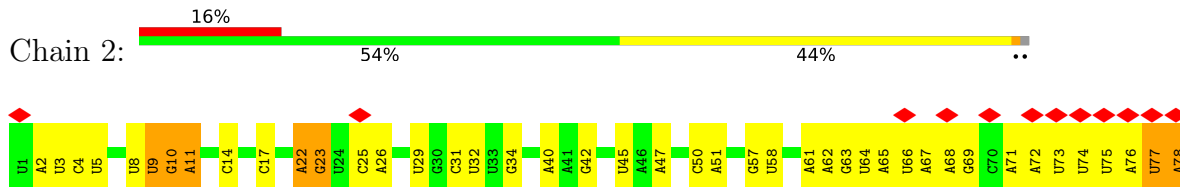
• Molecule 79: Ubiquitin-40S ribosomal protein S27a

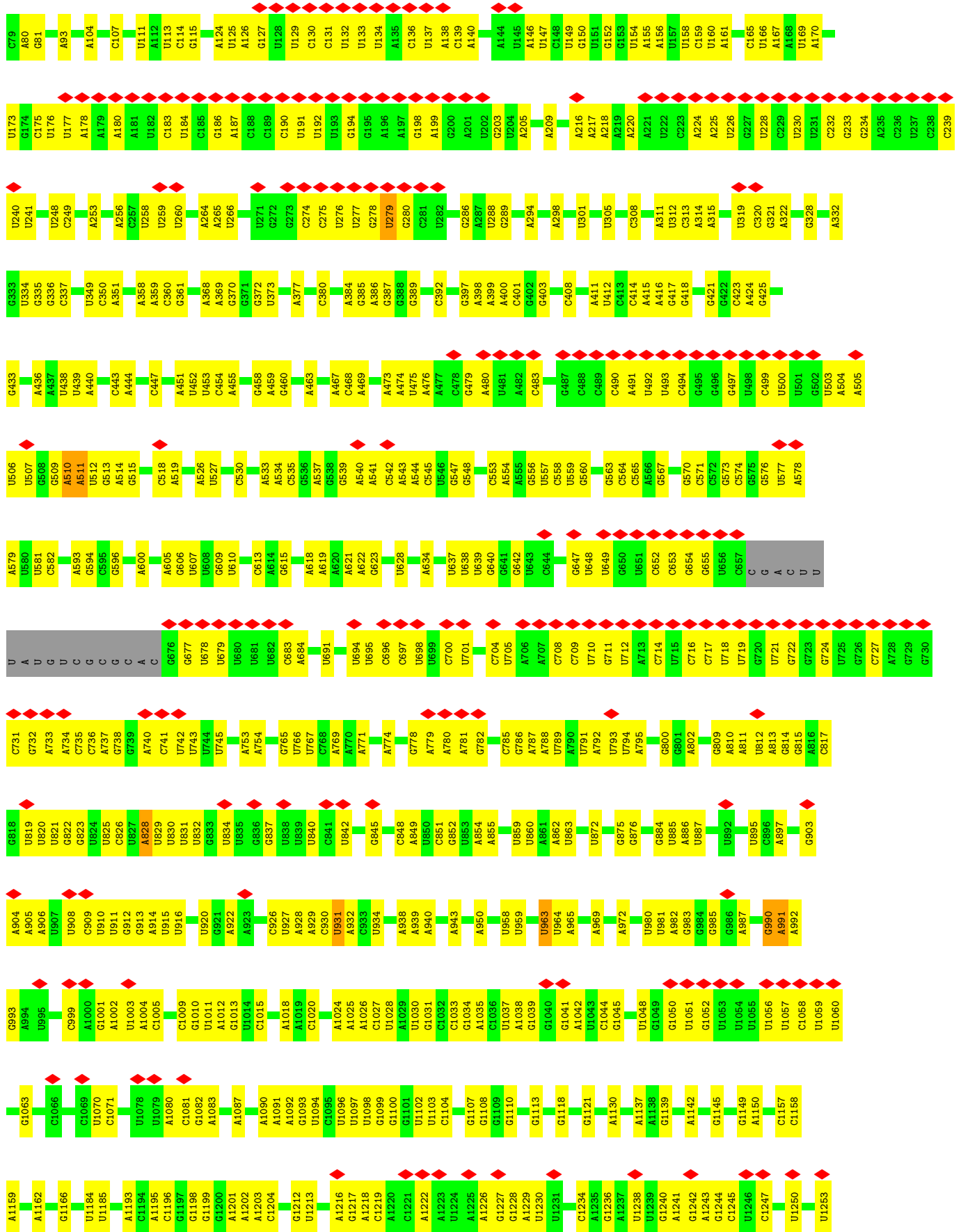


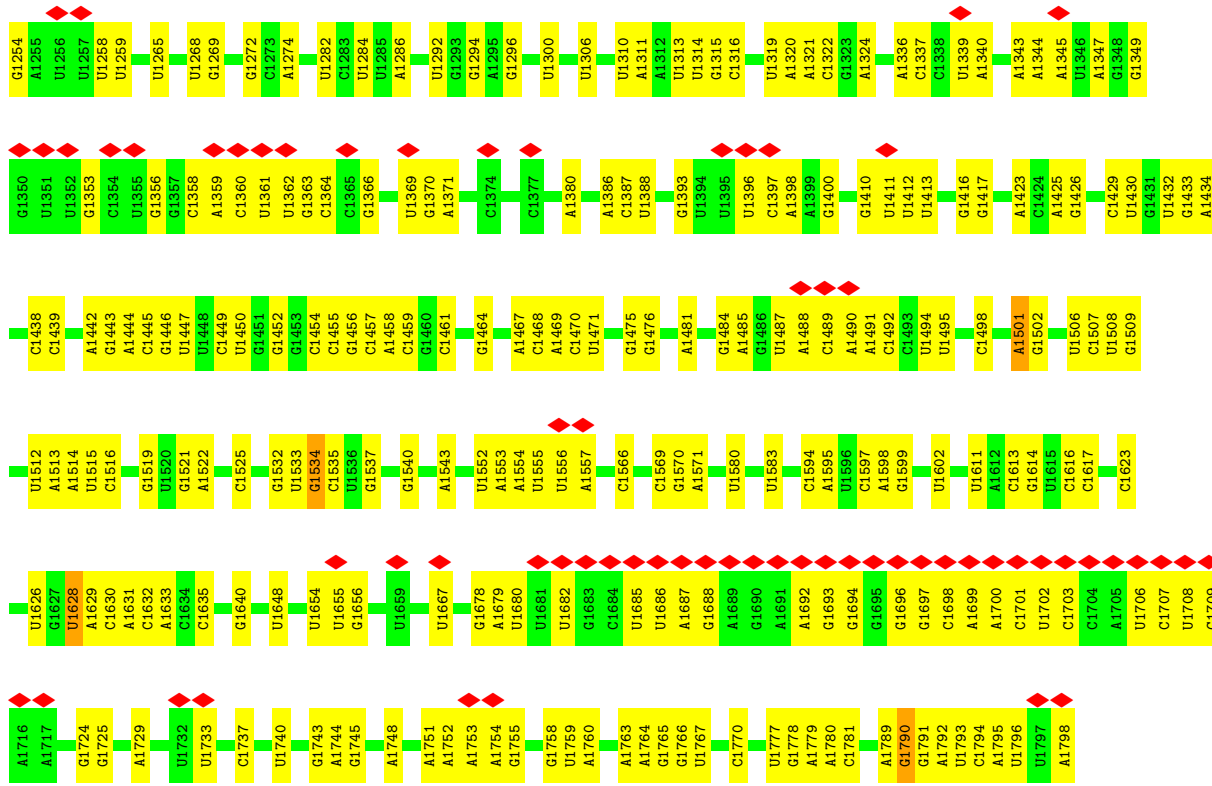
• Molecule 80: KLLA0E12277p



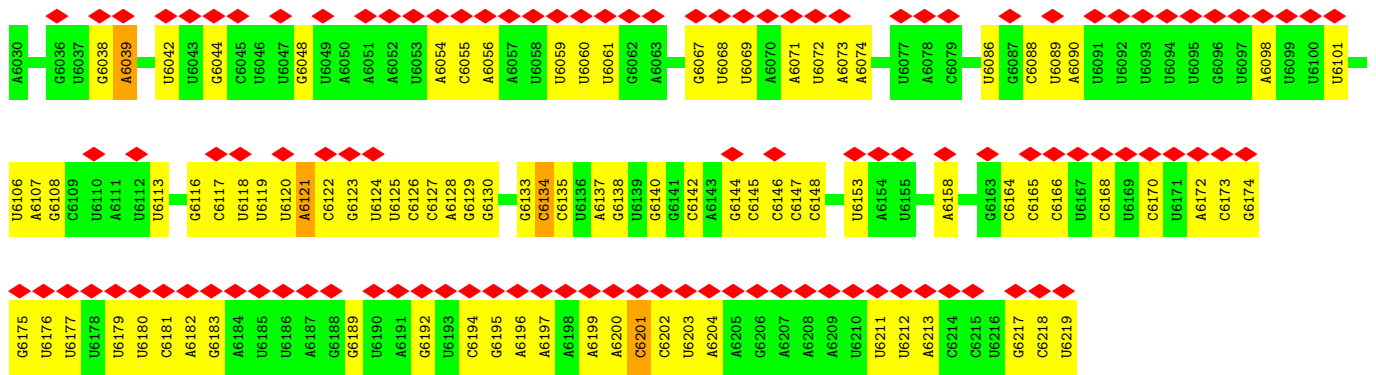
• Molecule 81: 18S ribosomal RNA



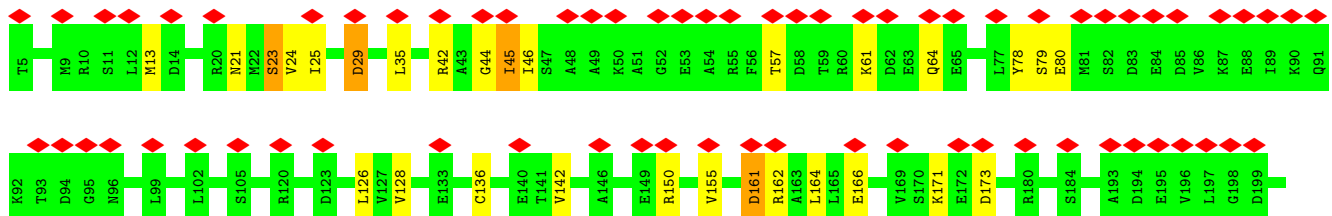
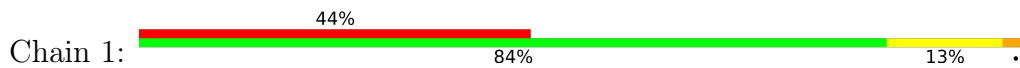


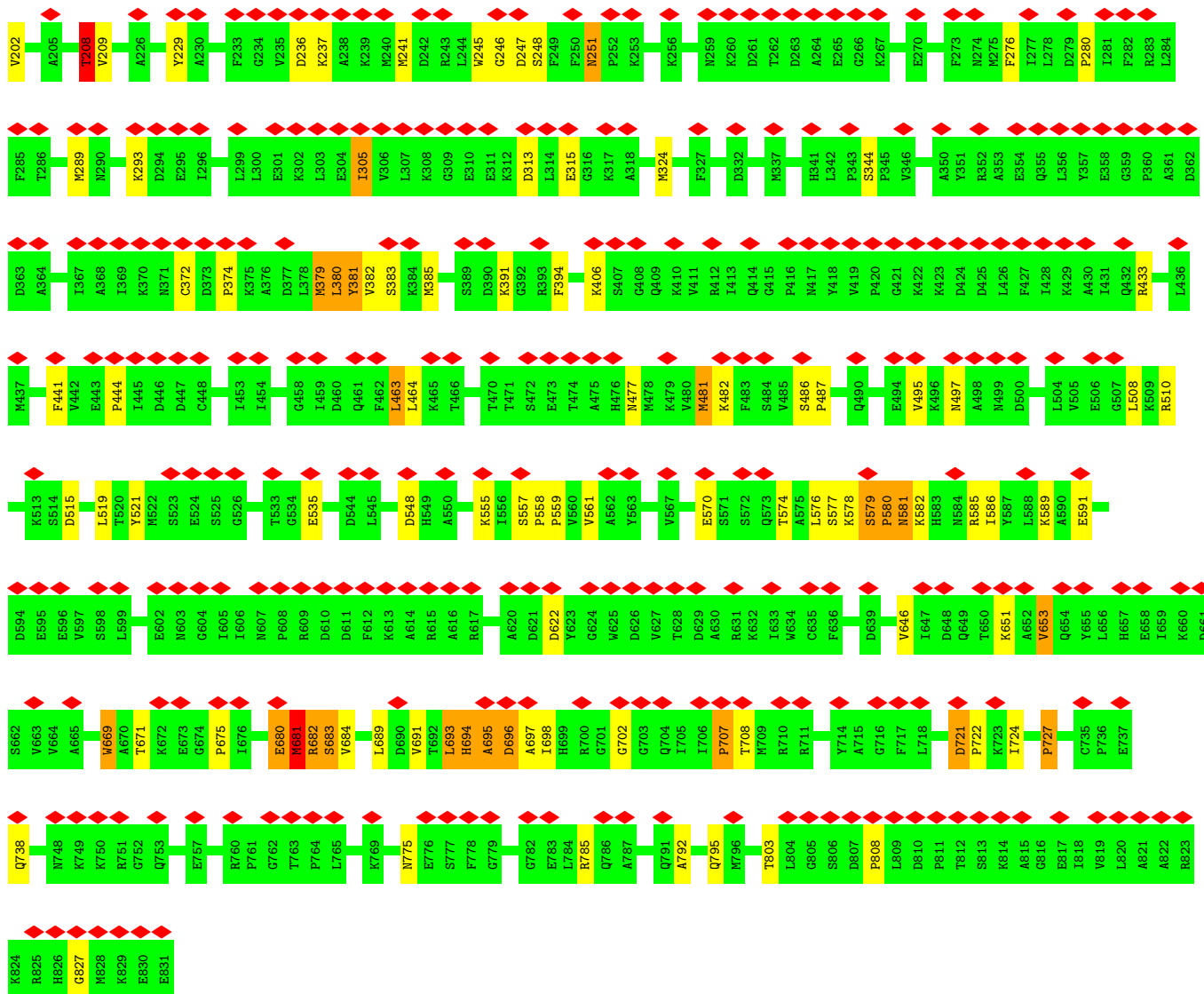


• Molecule 82: cricket paralysis virus IRES



• Molecule 83: Eft2p





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	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	0.793	Depositor
Minimum map value	-0.578	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	428.80002, 428.80002, 428.80002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	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: 6EM, MG, GCP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	5	0.51	19/78233 (0.0%)	0.81	74/121966 (0.1%)
2	7	0.38	0/2883	0.71	0/4491
3	8	0.47	0/3714	0.78	2/5781 (0.0%)
4	AA	0.62	0/1926	0.92	3/2588 (0.1%)
5	BB	0.61	0/3136	0.86	1/4225 (0.0%)
6	CC	0.54	0/2780	0.83	2/3760 (0.1%)
7	DD	0.43	0/2436	0.71	0/3292
8	EE	0.43	0/1322	0.79	2/1776 (0.1%)
9	FF	0.58	0/1810	0.80	0/2440
10	GG	0.44	0/1846	0.69	0/2486
11	HH	0.43	0/1547	0.73	0/2083
12	II	0.48	0/1725	0.74	0/2310
13	JJ	0.40	0/1370	0.71	0/1835
14	LL	0.48	0/1607	0.78	0/2156
15	MM	0.44	0/1060	0.74	0/1430
16	NN	0.69	0/1746	0.88	0/2339
17	OO	0.72	0/1602	0.79	0/2151
18	PP	0.58	0/1455	0.79	1/1952 (0.1%)
19	QQ	0.48	0/1469	0.81	1/1970 (0.1%)
20	RR	0.47	0/1539	0.78	0/2047
21	SS	0.52	0/1452	0.76	0/1956
22	TT	0.51	0/1286	0.76	0/1722
23	UU	0.38	0/824	0.59	0/1113
24	VV	0.58	0/991	0.84	0/1331
25	WW	0.51	0/528	0.74	0/703
26	XX	0.47	0/979	0.75	0/1320
27	YY	0.45	0/1003	0.78	0/1339
28	ZZ	0.46	0/1114	0.75	0/1493
29	aa	0.57	0/1186	0.83	1/1590 (0.1%)
30	bb	0.43	0/468	0.68	0/621
31	cc	0.45	0/748	0.68	0/1005
32	dd	0.48	0/885	0.72	0/1186

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	ee	0.59	0/998	0.78	0/1332
34	ff	0.64	0/855	0.83	0/1150
35	gg	0.52	0/961	0.84	0/1281
36	hh	0.43	0/970	0.71	0/1291
37	ii	0.43	0/773	0.79	0/1029
38	jj	0.73	0/690	0.93	2/913 (0.2%)
39	kk	0.47	0/626	0.82	0/835
40	ll	0.60	0/435	0.93	1/577 (0.2%)
41	mm	0.49	0/416	0.78	0/552
42	nn	0.43	0/234	0.91	0/300
43	oo	0.47	0/825	0.81	0/1086
44	pp	0.62	0/667	0.95	1/891 (0.1%)
45	qq	0.60	4/1748 (0.2%)	0.83	7/2350 (0.3%)
46	rr	0.41	0/1535	0.67	0/2077
48	A	0.40	0/1656	0.71	0/2264
49	B	0.40	0/1747	0.69	0/2353
50	C	0.45	0/1659	0.81	4/2252 (0.2%)
51	D	0.37	0/1769	0.61	0/2378
52	E	0.42	0/2122	0.75	0/2861
53	F	0.37	0/1628	0.65	2/2198 (0.1%)
54	G	0.45	2/1835 (0.1%)	0.70	0/2451
55	H	0.37	0/1507	0.66	0/2028
56	I	0.42	0/1519	0.73	0/2033
57	J	0.56	2/1495 (0.1%)	0.82	2/2001 (0.1%)
58	K	0.39	0/831	0.57	1/1123 (0.1%)
59	L	0.43	0/1276	0.76	0/1718
60	M	0.40	0/929	0.59	0/1255
61	N	0.41	0/1210	0.71	0/1628
62	O	0.42	0/953	0.75	1/1279 (0.1%)
63	P	0.50	1/1000 (0.1%)	0.71	1/1343 (0.1%)
64	Q	0.38	0/1125	0.61	0/1510
65	R	0.37	0/1042	0.70	0/1399
66	S	0.43	0/1212	0.69	1/1629 (0.1%)
67	T	0.36	0/1129	0.60	0/1520
68	U	0.35	0/857	0.60	0/1158
69	V	0.40	0/696	0.68	0/938
70	W	0.51	0/1039	0.81	0/1399
71	X	0.48	0/1145	0.83	1/1526 (0.1%)
72	Y	0.39	0/1075	0.65	0/1433
73	Z	0.39	0/567	0.63	0/762
74	a	0.48	0/810	0.92	1/1084 (0.1%)
75	b	0.36	0/627	0.68	0/847
76	c	0.36	0/496	0.69	0/666

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	d	0.38	0/457	0.61	0/607
78	e	0.36	0/450	0.65	0/599
79	f	0.43	0/562	0.65	0/751
80	g	0.36	0/2521	0.58	0/3431
81	2	0.36	6/42269 (0.0%)	0.78	20/65862 (0.0%)
82	4	0.30	0/4407	0.84	6/6849 (0.1%)
83	1	0.42	1/6540 (0.0%)	0.80	10/8853 (0.1%)
All	All	0.47	35/230565 (0.0%)	0.78	148/338109 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	5	0	6
4	AA	0	2
5	BB	0	1
6	CC	0	3
7	DD	0	1
8	EE	0	3
9	FF	0	2
14	LL	0	1
21	SS	0	1
27	YY	0	1
28	ZZ	0	1
29	aa	0	1
34	ff	0	1
35	gg	0	2
44	pp	0	3
45	qq	0	3
46	rr	0	1
48	A	0	2
49	B	0	1
50	C	0	3
51	D	0	1
52	E	0	3
53	F	0	1
58	K	0	1
59	L	0	1
62	O	0	1
63	P	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
64	Q	0	1
65	R	0	2
69	V	0	1
70	W	0	2
71	X	0	1
74	a	0	4
79	f	0	2
80	g	0	1
83	1	0	16
All	All	0	78

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2219	G	O3'-P	-16.66	1.41	1.61
57	J	170	GLY	CA-C	11.07	1.69	1.51
81	2	510	A	O3'-P	9.75	1.72	1.61
45	qq	123	LEU	N-CA	7.99	1.62	1.46
1	5	2239	A	O3'-P	-7.87	1.51	1.61
57	J	170	GLY	N-CA	7.70	1.57	1.46
81	2	511	A	O5'-C5'	7.35	1.56	1.44
1	5	2219	G	C3'-O3'	-7.15	1.32	1.42
54	G	154	ARG	CA-C	6.45	1.69	1.52
1	5	627	C	O3'-P	-6.36	1.53	1.61
45	qq	119	GLN	CA-C	6.21	1.69	1.52
1	5	2782	G	O3'-P	-6.15	1.53	1.61
1	5	29	C	O3'-P	-6.04	1.53	1.61
1	5	2479	U	O3'-P	-5.98	1.53	1.61
81	2	991	A	O3'-P	-5.90	1.54	1.61
81	2	77	U	O3'-P	5.70	1.68	1.61
1	5	918	G	O3'-P	-5.63	1.54	1.61
1	5	2377	U	O3'-P	-5.62	1.54	1.61
1	5	2691	U	O3'-P	-5.51	1.54	1.61
1	5	3015	U	O3'-P	-5.48	1.54	1.61
81	2	940	A	O3'-P	-5.46	1.54	1.61
1	5	2217	C	O3'-P	-5.45	1.54	1.61
1	5	1129	A	O3'-P	-5.44	1.54	1.61
1	5	2958	G	O3'-P	-5.39	1.54	1.61
63	P	19	GLY	N-CA	5.35	1.54	1.46
1	5	1378	A	O3'-P	-5.34	1.54	1.61
1	5	899	C	O3'-P	-5.33	1.54	1.61
45	qq	120	VAL	N-CA	5.32	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	2328	C	O3'-P	-5.29	1.54	1.61
83	1	585	ARG	N-CA	-5.22	1.35	1.46
54	G	154	ARG	N-CA	5.20	1.56	1.46
1	5	1581	A	O3'-P	-5.07	1.55	1.61
81	2	1790	G	O3'-P	-5.06	1.55	1.61
45	qq	120	VAL	CA-CB	5.06	1.65	1.54
1	5	3025	U	O3'-P	-5.06	1.55	1.61

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	1	581	ASN	N-CA-CB	18.89	144.59	110.60
1	5	2049	G	N9-C1'-C2'	-12.44	97.83	114.00
81	2	511	A	P-O5'-C5'	10.73	138.07	120.90
83	1	580	PRO	N-CA-C	10.27	138.81	112.10
81	2	23	G	N9-C1'-C2'	-10.23	100.70	114.00
45	qq	124	LEU	CA-CB-CG	9.47	137.08	115.30
82	4	6121	A	C4'-C3'-O3'	9.31	131.63	113.00
1	5	2219	G	C8-N9-C1'	-8.92	115.40	127.00
82	4	6201	C	N1-C1'-C2'	-8.87	102.24	112.00
45	qq	123	LEU	CA-CB-CG	8.84	135.62	115.30
1	5	2151	A	O5'-P-OP1	-8.52	98.03	105.70
83	1	581	ASN	N-CA-C	-8.35	88.46	111.00
81	2	931	U	C2'-C3'-O3'	-8.25	91.35	109.50
1	5	3207	G	C2'-C3'-O3'	8.02	127.15	109.50
1	5	2630	G	C2'-C3'-O3'	7.89	126.85	109.50
81	2	1628	U	C4'-C3'-O3'	7.86	128.73	113.00
1	5	596	U	C2'-C3'-O3'	7.83	126.73	109.50
1	5	2218	G	O4'-C1'-N9	7.82	114.45	108.20
1	5	2218	G	C1'-C2'-O2'	7.77	133.92	110.60
1	5	297	G	C2'-C3'-O3'	7.74	126.53	109.50
81	2	78	A	C4'-C3'-O3'	7.70	128.41	113.00
1	5	1196	A	C2'-C3'-O3'	7.44	125.86	109.50
3	8	8	C	N1-C1'-C2'	-7.42	103.84	112.00
1	5	2053	C	N1-C1'-C2'	-7.42	103.84	112.00
1	5	65	A	C2'-C3'-O3'	7.35	125.67	109.50
4	AA	174	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	5	2285	G	N9-C1'-C2'	-7.26	104.01	112.00
1	5	2239	A	C5'-C4'-O4'	7.24	117.79	109.10
1	5	2219	G	P-O3'-C3'	-7.21	111.04	119.70
1	5	3055	A	C4-N9-C1'	7.19	139.23	126.30
81	2	11	A	N9-C1'-C2'	-7.17	104.11	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	3055	A	C8-N9-C1'	-7.05	115.01	127.70
1	5	957	U	N1-C1'-C2'	6.88	122.94	114.00
1	5	1209	C	C2'-C3'-O3'	6.86	124.68	113.70
1	5	2049	G	C4'-C3'-O3'	6.78	126.56	113.00
50	C	149	TRP	CA-CB-CG	6.74	126.50	113.70
83	1	381	TYR	N-CA-C	6.60	128.82	111.00
81	2	9	U	N1-C1'-C2'	-6.59	104.75	112.00
1	5	2050	A	C4'-C3'-O3'	-6.58	95.59	109.40
1	5	2946	U	N1-C1'-C2'	6.55	122.52	114.00
81	2	78	A	C5'-C4'-C3'	6.55	126.48	116.00
83	1	380	LEU	N-CA-C	6.55	128.68	111.00
8	EE	114	ARG	N-CA-C	6.49	128.52	111.00
1	5	2062	A	N9-C1'-C2'	6.39	122.31	114.00
8	EE	13	VAL	C-N-CD	-6.39	106.54	120.60
83	1	585	ARG	CA-C-N	-6.35	103.22	117.20
45	qq	122	ARG	N-CA-C	6.30	128.02	111.00
1	5	1452	A	C2'-C3'-O3'	-6.18	95.90	109.50
71	X	7	ARG	NE-CZ-NH2	-6.17	117.22	120.30
81	2	911	U	N1-C1'-C2'	6.16	122.01	114.00
82	4	6039	A	C4'-C3'-O3'	6.16	125.33	113.00
1	5	1255	C	C2'-C3'-O3'	6.16	123.55	113.70
1	5	3257	A	C2'-C3'-O3'	6.14	123.52	113.70
1	5	2229	U	O5'-P-OP2	-6.10	100.21	105.70
1	5	2922	U	C2'-C3'-O3'	6.08	123.43	113.70
1	5	2050	A	C5'-C4'-O4'	6.08	116.39	109.10
57	J	170	GLY	N-CA-C	6.07	128.28	113.10
1	5	2219	G	O4'-C1'-N9	6.04	113.03	108.20
1	5	298	U	C2'-C3'-O3'	6.03	123.35	113.70
53	F	220	GLU	N-CA-C	6.00	127.21	111.00
81	2	1534	G	C2'-C3'-O3'	5.99	123.29	113.70
1	5	3325	U	C2'-C3'-O3'	5.95	123.21	113.70
38	jj	21	ARG	NE-CZ-NH2	-5.92	117.34	120.30
58	K	55	VAL	N-CA-C	-5.92	95.03	111.00
1	5	2481	C	C5'-C4'-O4'	5.91	116.19	109.10
82	4	6134	C	N1-C1'-C2'	-5.88	105.53	112.00
50	C	149	TRP	N-CA-CB	5.84	121.12	110.60
1	5	707	A	C2'-C3'-O3'	5.73	122.87	113.70
1	5	1452	A	N9-C1'-C2'	5.73	121.44	114.00
1	5	1531	G	C2'-C3'-O3'	5.72	122.85	113.70
1	5	1608	C	O5'-P-OP2	-5.71	100.56	105.70
29	aa	21	ARG	NE-CZ-NH2	-5.68	117.46	120.30
81	2	1501	A	C2'-C3'-O3'	5.68	122.79	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	2	22	A	N9-C1'-C2'	-5.67	105.76	112.00
1	5	2032	U	C2'-C3'-O3'	5.64	122.72	113.70
81	2	10	G	N9-C1'-C2'	-5.63	105.80	112.00
1	5	2218	G	P-O5'-C5'	-5.63	111.89	120.90
81	2	963	U	C2'-C3'-O3'	5.61	122.68	113.70
1	5	336	A	C8-N9-C1'	-5.58	117.65	127.70
1	5	336	A	N9-C1'-C2'	5.58	121.25	114.00
44	pp	47	VAL	CB-CA-C	5.57	121.99	111.40
4	AA	207	VAL	CB-CA-C	-5.57	100.81	111.40
18	PP	69	ARG	NE-CZ-NH1	5.57	123.08	120.30
53	F	165	SER	C-N-CD	-5.56	108.38	120.60
1	5	307	A	N9-C1'-C2'	5.56	121.22	114.00
1	5	282	G	C2'-C3'-O3'	5.55	122.57	113.70
45	qq	123	LEU	CB-CG-CD1	5.54	120.42	111.00
1	5	336	A	C4-N9-C1'	5.54	136.27	126.30
1	5	1337	A	O5'-P-OP2	-5.53	100.73	105.70
1	5	2238	U	C4'-C3'-O3'	5.52	124.04	113.00
81	2	828	A	C2'-C3'-O3'	5.48	122.47	113.70
1	5	2217	C	O3'-P-O5'	-5.47	93.60	104.00
83	1	579	SER	C-N-CD	5.47	139.89	128.40
82	4	6039	A	N9-C1'-C2'	-5.46	105.99	112.00
1	5	2529	C	N1-C1'-C2'	5.44	121.08	114.00
1	5	887	G	C4'-C3'-O3'	5.43	123.86	113.00
5	BB	159	ARG	NE-CZ-NH2	-5.42	117.59	120.30
50	C	174	LEU	C-N-CA	5.39	135.18	121.70
3	8	7	U	N1-C1'-C2'	-5.38	106.08	112.00
45	qq	125	GLY	N-CA-C	5.37	126.53	113.10
83	1	585	ARG	C-N-CA	5.37	135.13	121.70
1	5	2510	U	N1-C1'-C2'	5.37	120.98	114.00
6	CC	348	LYS	N-CA-C	5.37	125.50	111.00
1	5	1052	U	C2'-C3'-O3'	5.37	122.29	113.70
1	5	1155	A	C2'-C3'-O3'	5.36	122.27	113.70
1	5	96	G	O5'-P-OP2	-5.34	100.90	105.70
1	5	2217	C	P-O3'-C3'	-5.31	113.33	119.70
4	AA	204	MET	CA-CB-CG	5.31	122.33	113.30
1	5	1926	U	C4'-C3'-O3'	5.30	123.60	113.00
66	S	93	ASN	N-CA-C	5.29	125.29	111.00
1	5	1863	U	C2'-C3'-O3'	5.29	122.16	113.70
1	5	1600	C	C2'-C3'-O3'	5.28	122.15	113.70
62	O	133	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	5	364	G	C2'-C3'-O3'	5.27	122.14	113.70
1	5	2241	G	N9-C1'-C2'	5.27	120.85	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	2054	U	C4'-C3'-O3'	5.27	123.54	113.00
6	CC	202	ARG	NE-CZ-NH2	5.27	122.93	120.30
83	1	208	THR	C-N-CA	5.24	134.81	121.70
1	5	238	A	C2'-C3'-O3'	5.24	122.08	113.70
45	qq	175	ASP	CB-CG-OD2	5.23	123.01	118.30
1	5	3135	A	C2'-C3'-O3'	5.23	122.06	113.70
81	2	990	G	C4'-C3'-O3'	5.21	123.42	113.00
1	5	2341	A	C2'-C3'-O3'	5.19	122.00	113.70
1	5	2372	G	O5'-P-OP2	-5.18	101.04	105.70
1	5	1337	A	O5'-P-OP1	5.17	116.91	110.70
81	2	78	A	P-O5'-C5'	5.16	129.16	120.90
1	5	1278	G	C2'-C3'-O3'	5.16	121.95	113.70
1	5	78	U	O4'-C4'-C3'	-5.14	98.86	104.00
57	J	49	LEU	CA-CB-CG	5.13	127.10	115.30
63	P	20	VAL	N-CA-C	5.11	124.80	111.00
82	4	6121	A	C2'-C3'-O3'	-5.10	98.28	109.50
1	5	2784	G	C2'-C3'-O3'	-5.09	98.30	109.50
45	qq	119	GLN	CA-CB-CG	5.08	124.57	113.40
1	5	987	C	C2'-C3'-O3'	5.07	121.81	113.70
1	5	2239	A	P-O3'-C3'	-5.07	113.62	119.70
19	QQ	178	ARG	NE-CZ-NH1	-5.07	117.77	120.30
81	2	279	U	C2'-C3'-O3'	5.06	121.80	113.70
50	C	82	LYS	C-N-CA	5.06	134.35	121.70
1	5	2285	G	C2'-C3'-O3'	-5.06	98.37	109.50
1	5	2238	U	N1-C1'-C2'	-5.05	106.44	112.00
1	5	886	A	O5'-P-OP1	-5.04	101.17	105.70
81	2	469	A	C2'-C3'-O3'	5.04	121.76	113.70
74	a	83	ILE	CB-CA-C	-5.04	101.53	111.60
81	2	77	U	P-O3'-C3'	5.04	125.74	119.70
1	5	844	C	C4'-C3'-O3'	5.02	123.04	113.00
38	jj	11	ARG	NE-CZ-NH1	5.02	122.81	120.30
83	1	161	ASP	N-CA-C	5.01	124.54	111.00
40	ll	45	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
83	1	463	LEU	Peptide
83	1	464	LEU	Peptide
83	1	576	LEU	Peptide
83	1	577	SER	Peptide

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Mol	Chain	Res	Type	Group
83	1	669	TRP	Peptide
83	1	680	GLU	Peptide
83	1	681	MET	Peptide
83	1	682	ARG	Peptide
83	1	683	SER	Peptide
83	1	684	VAL	Peptide
83	1	693	LEU	Peptide
83	1	694	HIS	Peptide
83	1	695	ALA	Peptide
83	1	696	ASP	Peptide
83	1	697	ALA	Peptide
83	1	707	PRO	Peptide
1	5	1178	G	Sidechain
1	5	2049	G	Sidechain
1	5	2218	G	Sidechain
1	5	2219	G	Sidechain
1	5	2285	G	Sidechain
1	5	2629	G	Sidechain
48	A	164	ASN	Peptide
48	A	33	GLN	Peptide
4	AA	196	TRP	Peptide
4	AA	33	ASP	Peptide
49	B	35	PRO	Peptide
5	BB	331	THR	Peptide
50	C	111	ASP	Peptide
50	C	148	TYR	Peptide
50	C	177	ALA	Peptide
6	CC	148	ILE	Peptide
6	CC	80	GLY	Peptide
6	CC	82	THR	Peptide
51	D	176	LEU	Peptide
7	DD	3	PHE	Peptide
52	E	116	ASP	Peptide
52	E	128	LYS	Peptide
52	E	67	GLN	Peptide
8	EE	110	SER	Peptide
8	EE	112	LYS	Mainchain
8	EE	65	GLY	Peptide
53	F	165	SER	Peptide
9	FF	112	THR	Peptide
9	FF	220	PHE	Peptide
58	K	54	PHE	Peptide

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Mol	Chain	Res	Type	Group
59	L	152	GLN	Peptide
14	LL	74	GLY	Peptide
62	O	129	LYS	Peptide
63	P	15	TYR	Peptide
64	Q	40	GLN	Peptide
65	R	78	ARG	Peptide
65	R	79	GLU	Peptide
21	SS	12	ARG	Peptide
69	V	13	VAL	Peptide
70	W	56	HIS	Peptide
70	W	75	ILE	Peptide
71	X	63	GLN	Peptide
27	YY	55	GLU	Peptide
28	ZZ	88	ASP	Peptide
74	a	34	LYS	Peptide
74	a	49	ALA	Peptide
74	a	83	ILE	Peptide
74	a	9	GLY	Peptide
29	aa	112	VAL	Peptide
79	f	102	VAL	Peptide
79	f	103	LEU	Peptide
34	ff	103	TYR	Peptide
80	g	75	SER	Peptide
35	gg	26	PRO	Peptide
35	gg	8	ARG	Peptide
44	pp	37	TYR	Peptide
44	pp	55	TRP	Peptide
44	pp	56	SER	Peptide
45	qq	117	ILE	Peptide
45	qq	120	VAL	Peptide
45	qq	123	LEU	Peptide
46	rr	20	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	AA	247/249 (99%)	198 (80%)	35 (14%)	14 (6%)	1	18
5	BB	382/384 (100%)	311 (81%)	52 (14%)	19 (5%)	2	21
6	CC	357/360 (99%)	273 (76%)	57 (16%)	27 (8%)	1	12
7	DD	293/295 (99%)	254 (87%)	27 (9%)	12 (4%)	3	26
8	EE	157/170 (92%)	127 (81%)	22 (14%)	8 (5%)	2	20
9	FF	220/222 (99%)	182 (83%)	25 (11%)	13 (6%)	1	18
10	GG	231/233 (99%)	198 (86%)	25 (11%)	8 (4%)	3	30
11	HH	189/191 (99%)	168 (89%)	19 (10%)	2 (1%)	14	53
12	II	203/216 (94%)	179 (88%)	20 (10%)	4 (2%)	7	41
13	JJ	166/168 (99%)	136 (82%)	20 (12%)	10 (6%)	1	17
14	LL	195/197 (99%)	170 (87%)	17 (9%)	8 (4%)	3	26
15	MM	134/136 (98%)	124 (92%)	5 (4%)	5 (4%)	3	28
16	NN	200/202 (99%)	172 (86%)	25 (12%)	3 (2%)	10	47
17	OO	196/198 (99%)	88 (45%)	40 (20%)	68 (35%)	0	0
18	PP	178/180 (99%)	152 (85%)	19 (11%)	7 (4%)	3	27
19	QQ	182/184 (99%)	155 (85%)	23 (13%)	4 (2%)	6	39
20	RR	186/188 (99%)	155 (83%)	25 (13%)	6 (3%)	4	31
21	SS	167/169 (99%)	144 (86%)	18 (11%)	5 (3%)	4	33
22	TT	156/158 (99%)	126 (81%)	22 (14%)	8 (5%)	2	20
23	UU	98/100 (98%)	86 (88%)	12 (12%)	0	100	100
24	VV	130/132 (98%)	115 (88%)	10 (8%)	5 (4%)	3	27
25	WW	60/62 (97%)	53 (88%)	7 (12%)	0	100	100
26	XX	119/121 (98%)	107 (90%)	11 (9%)	1 (1%)	19	59
27	YY	123/125 (98%)	104 (85%)	16 (13%)	3 (2%)	6	37
28	ZZ	132/134 (98%)	107 (81%)	17 (13%)	8 (6%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	aa	145/147 (99%)	121 (83%)	17 (12%)	7 (5%)	2	22
30	bb	55/57 (96%)	48 (87%)	5 (9%)	2 (4%)	3	29
31	cc	95/97 (98%)	83 (87%)	12 (13%)	0	100	100
32	dd	104/106 (98%)	90 (86%)	9 (9%)	5 (5%)	2	22
33	ee	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	19	59
34	ff	103/105 (98%)	94 (91%)	8 (8%)	1 (1%)	15	55
35	gg	119/121 (98%)	102 (86%)	9 (8%)	8 (7%)	1	15
36	hh	114/116 (98%)	100 (88%)	11 (10%)	3 (3%)	5	35
37	ii	96/98 (98%)	75 (78%)	16 (17%)	5 (5%)	2	20
38	jj	83/85 (98%)	66 (80%)	16 (19%)	1 (1%)	13	51
39	kk	74/76 (97%)	55 (74%)	16 (22%)	3 (4%)	3	26
40	ll	47/49 (96%)	38 (81%)	7 (15%)	2 (4%)	2	24
41	mm	49/51 (96%)	41 (84%)	7 (14%)	1 (2%)	7	41
42	nn	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
43	oo	99/101 (98%)	74 (75%)	21 (21%)	4 (4%)	3	26
44	pp	85/87 (98%)	62 (73%)	14 (16%)	9 (11%)	0	7
45	qq	215/217 (99%)	166 (77%)	33 (15%)	16 (7%)	1	13
46	rr	193/195 (99%)	147 (76%)	30 (16%)	16 (8%)	1	10
48	A	204/206 (99%)	160 (78%)	31 (15%)	13 (6%)	1	17
49	B	212/214 (99%)	162 (76%)	43 (20%)	7 (3%)	4	31
50	C	215/217 (99%)	170 (79%)	34 (16%)	11 (5%)	2	20
51	D	221/223 (99%)	190 (86%)	24 (11%)	7 (3%)	4	31
52	E	258/260 (99%)	220 (85%)	26 (10%)	12 (5%)	2	22
53	F	204/206 (99%)	168 (82%)	29 (14%)	7 (3%)	3	31
54	G	224/226 (99%)	188 (84%)	28 (12%)	8 (4%)	3	29
55	H	182/184 (99%)	149 (82%)	21 (12%)	12 (7%)	1	16
56	I	184/200 (92%)	148 (80%)	29 (16%)	7 (4%)	3	27
57	J	180/182 (99%)	151 (84%)	19 (11%)	10 (6%)	2	19
58	K	94/96 (98%)	78 (83%)	12 (13%)	4 (4%)	2	24
59	L	153/155 (99%)	122 (80%)	24 (16%)	7 (5%)	2	23
60	M	120/122 (98%)	94 (78%)	22 (18%)	4 (3%)	4	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	N	148/150 (99%)	129 (87%)	17 (12%)	2 (1%)	11	48
62	O	125/127 (98%)	104 (83%)	18 (14%)	3 (2%)	6	37
63	P	121/123 (98%)	98 (81%)	16 (13%)	7 (6%)	1	18
64	Q	139/141 (99%)	120 (86%)	12 (9%)	7 (5%)	2	21
65	R	127/129 (98%)	99 (78%)	23 (18%)	5 (4%)	3	27
66	S	143/145 (99%)	117 (82%)	21 (15%)	5 (4%)	3	30
67	T	141/143 (99%)	126 (89%)	13 (9%)	2 (1%)	11	48
68	U	104/106 (98%)	92 (88%)	9 (9%)	3 (3%)	4	33
69	V	85/87 (98%)	66 (78%)	14 (16%)	5 (6%)	1	18
70	W	127/129 (98%)	104 (82%)	18 (14%)	5 (4%)	3	27
71	X	143/145 (99%)	112 (78%)	20 (14%)	11 (8%)	1	12
72	Y	132/134 (98%)	111 (84%)	13 (10%)	8 (6%)	1	17
73	Z	68/70 (97%)	57 (84%)	8 (12%)	3 (4%)	2	23
74	a	98/100 (98%)	68 (69%)	13 (13%)	17 (17%)	0	2
75	b	80/82 (98%)	61 (76%)	15 (19%)	4 (5%)	2	21
76	c	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
77	d	51/53 (96%)	40 (78%)	11 (22%)	0	100	100
78	e	53/55 (96%)	46 (87%)	4 (8%)	3 (6%)	1	18
79	f	67/69 (97%)	49 (73%)	12 (18%)	6 (9%)	1	9
80	g	312/324 (96%)	251 (80%)	50 (16%)	11 (4%)	3	30
83	1	825/827 (100%)	654 (79%)	120 (14%)	51 (6%)	1	17
All	All	12121/12322 (98%)	9932 (82%)	1590 (13%)	599 (5%)	4	21

All (599) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AA	10	LYS
4	AA	34	TYR
4	AA	92	LYS
4	AA	181	LYS
4	AA	197	PRO
4	AA	222	ALA
5	BB	4	ARG
5	BB	222	LYS
5	BB	226	PHE

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Mol	Chain	Res	Type
5	BB	255	TRP
6	CC	23	PRO
6	CC	84	ARG
6	CC	105	THR
6	CC	148	ILE
6	CC	149	PRO
6	CC	182	VAL
6	CC	292	SER
6	CC	352	SER
6	CC	353	ALA
7	DD	20	PHE
8	EE	13	VAL
8	EE	14	PRO
8	EE	66	PRO
8	EE	127	LYS
8	EE	129	ILE
9	FF	90	ASN
9	FF	139	SER
9	FF	156	GLN
9	FF	161	SER
9	FF	214	PRO
9	FF	216	LYS
9	FF	219	HIS
9	FF	230	GLU
10	GG	75	ALA
10	GG	126	PRO
10	GG	163	ILE
11	HH	3	TYR
12	II	24	ARG
12	II	145	LYS
13	JJ	8	PRO
13	JJ	64	LYS
14	LL	3	ILE
14	LL	47	ALA
16	NN	75	VAL
17	OO	20[A]	LEU
17	OO	24[A]	VAL
17	OO	32[A]	GLN
17	OO	34[A]	ILE
17	OO	35[A]	VAL
17	OO	40[A]	GLU
17	OO	42[A]	LEU

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Mol	Chain	Res	Type
17	OO	45[A]	SER
17	OO	50[A]	ARG
17	OO	51[A]	ASN
17	OO	56[A]	HIS
17	OO	64[A]	ALA
17	OO	66[A]	ASN
17	OO	67[A]	LYS
17	OO	84[A]	ALA
17	OO	86[A]	ARG
17	OO	94[A]	ALA
17	OO	95[A]	ARG
17	OO	98[A]	ALA
17	OO	99[A]	ALA
17	OO	100[A]	LEU
17	OO	111[A]	PRO
17	OO	112[A]	PRO
17	OO	121[A]	VAL
17	OO	125[A]	LEU
17	OO	130[A]	LEU
17	OO	139[A]	LEU
17	OO	140[A]	GLY
17	OO	142[A]	LEU
17	OO	144[A]	THR
17	OO	157[A]	LEU
17	OO	158[A]	GLU
17	OO	161[A]	ARG
17	OO	162[A]	LYS
17	OO	177[A]	ALA
17	OO	183[A]	SER
17	OO	189[A]	GLU
17	OO	191[A]	SER
17	OO	193[A]	LYS
19	QQ	23	ASN
20	RR	22	ILE
20	RR	135	LYS
21	SS	18	SER
21	SS	133	ALA
24	VV	44	SER
27	YY	104	VAL
28	ZZ	9	LYS
28	ZZ	87	LEU
28	ZZ	89	VAL

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Mol	Chain	Res	Type
28	ZZ	102	GLU
29	aa	34	MET
29	aa	50	PRO
29	aa	78	LEU
29	aa	93	SER
32	dd	84	ASP
34	ff	104	PRO
35	gg	7	PHE
35	gg	56	THR
35	gg	60	ARG
35	gg	75	ALA
35	gg	77	GLY
35	gg	82	ALA
37	ii	13	LYS
37	ii	29	ARG
39	kk	51	LEU
40	ll	3	ALA
43	oo	6	LYS
43	oo	61	LYS
44	pp	37	TYR
44	pp	56	SER
44	pp	63	THR
45	qq	24	LYS
45	qq	119	GLN
45	qq	120	VAL
45	qq	121	PRO
45	qq	124	LEU
45	qq	172	VAL
45	qq	213	ALA
46	rr	70	SER
46	rr	106	LYS
46	rr	156	SER
48	A	130	ALA
48	A	197	ILE
49	B	35	PRO
49	B	100	PHE
50	C	57	SER
50	C	59	GLU
50	C	83	ASP
50	C	175	ILE
51	D	164	VAL
52	E	117	GLU

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Mol	Chain	Res	Type
52	E	129	VAL
53	F	59	SER
54	G	154	ARG
55	H	32	PRO
55	H	64	VAL
55	H	74	GLN
56	I	22	ARG
56	I	52	ASN
57	J	171	ARG
58	K	81	ASN
58	K	88	PRO
59	L	3	THR
59	L	105	LYS
59	L	133	LYS
62	O	91	SER
63	P	20	VAL
63	P	29	PRO
64	Q	40	GLN
65	R	26	MET
65	R	121	VAL
66	S	92	VAL
68	U	118	ILE
69	V	30	SER
70	W	57	ARG
71	X	4	GLY
71	X	12	ALA
71	X	42	PRO
71	X	63	GLN
71	X	64	PRO
71	X	131	SER
72	Y	30	PRO
74	a	10	ARG
74	a	18	VAL
74	a	75	ILE
74	a	81	ALA
74	a	86	VAL
75	b	21	LEU
78	e	11	ALA
79	f	111	GLU
79	f	143	HIS
80	g	293	ASP
83	1	23	SER

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Mol	Chain	Res	Type
83	1	46	ILE
83	1	162	ARG
83	1	209	VAL
83	1	247	ASP
83	1	251	ASN
83	1	305	ILE
83	1	382	VAL
83	1	406	LYS
83	1	444	PRO
83	1	548	ASP
83	1	559	PRO
83	1	578	LYS
83	1	579	SER
83	1	581	ASN
83	1	591	GLU
83	1	683	SER
83	1	691	VAL
83	1	695	ALA
83	1	702	GLY
83	1	707	PRO
83	1	721	ASP
83	1	722	PRO
83	1	727	PRO
4	AA	33	ASP
4	AA	104	LEU
4	AA	144	ASN
4	AA	154	ALA
5	BB	140	ASN
5	BB	252	ILE
5	BB	269	GLN
5	BB	317	ILE
5	BB	351	LEU
5	BB	382	THR
6	CC	14	GLU
6	CC	293	THR
6	CC	311	HIS
6	CC	341	SER
6	CC	342	LYS
6	CC	343	LYS
7	DD	5	LYS
7	DD	26	GLY
8	EE	115	ALA

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Mol	Chain	Res	Type
8	EE	128	GLU
9	FF	104	ARG
10	GG	74	ILE
12	II	187	ALA
13	JJ	25	GLU
13	JJ	114	ILE
14	LL	6	ASN
14	LL	28	GLN
14	LL	190	LYS
15	MM	36	VAL
17	OO	6[A]	PRO
17	OO	15[A]	HIS
17	OO	16[A]	LEU
17	OO	59[A]	LEU
17	OO	105[A]	VAL
17	OO	123[A]	GLN
17	OO	146[A]	VAL
17	OO	159[A]	GLU
17	OO	173[A]	LYS
17	OO	174[A]	ALA
17	OO	187[A]	GLY
17	OO	188[A]	THR
17	OO	195[A]	ALA
17	OO	198[A]	GLY
18	PP	166	ALA
22	TT	12	ARG
22	TT	18	ASP
22	TT	46	GLY
22	TT	80	VAL
24	VV	21	ALA
24	VV	54	LEU
27	YY	55	GLU
28	ZZ	5	LEU
28	ZZ	59	ALA
30	bb	25	LYS
30	bb	26	THR
37	ii	30	LYS
43	oo	14	GLY
44	pp	47	VAL
44	pp	48	LYS
44	pp	60	CYS
45	qq	9	VAL

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Mol	Chain	Res	Type
45	qq	125	GLY
46	rr	38	GLN
46	rr	94	SER
46	rr	95	LEU
46	rr	126	VAL
48	A	72	ASP
48	A	97	PRO
48	A	120	LEU
50	C	65	SER
50	C	149	TRP
50	C	153	LEU
51	D	217	VAL
52	E	68	ARG
52	E	119	ALA
52	E	120	SER
52	E	186	GLY
52	E	201	HIS
52	E	205	PHE
53	F	166	PRO
53	F	206	GLY
54	G	122	GLU
54	G	156	TYR
55	H	10	SER
55	H	13	PRO
55	H	53	GLY
55	H	113	PRO
56	I	10	LYS
56	I	16	ALA
56	I	17	LYS
56	I	153	ILE
57	J	65	LYS
57	J	118	LEU
60	M	82	VAL
61	N	70	LYS
61	N	133	SER
64	Q	27	GLY
64	Q	116	LEU
64	Q	138	PHE
65	R	80	ARG
65	R	127	VAL
66	S	26	ILE
67	T	43	ASN

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Mol	Chain	Res	Type
70	W	83	ILE
72	Y	61	ARG
73	Z	97	LYS
74	a	16	GLY
74	a	85	ARG
75	b	3	LEU
79	f	88	PRO
79	f	89	LYS
80	g	77	ASP
80	g	244	LYS
83	1	45	ILE
83	1	155	VAL
83	1	241	MET
83	1	245	TRP
83	1	280	PRO
83	1	497	ASN
83	1	724	ILE
4	AA	180	LEU
4	AA	201	GLY
5	BB	5	LYS
5	BB	22	ALA
5	BB	36	ASP
5	BB	173	GLN
5	BB	174	LYS
6	CC	106	TRP
6	CC	140	HIS
6	CC	201	GLN
6	CC	268	ALA
6	CC	269	SER
6	CC	305	ALA
6	CC	320	ASN
7	DD	259	LYS
10	GG	38	ALA
13	JJ	138	VAL
13	JJ	144	CYS
13	JJ	168	ASP
15	MM	5	SER
15	MM	29	ALA
16	NN	97	SER
17	OO	13[A]	LYS
17	OO	48[A]	PHE
17	OO	63[A]	THR

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Mol	Chain	Res	Type
17	OO	114[A]	ASP
17	OO	143[A]	SER
17	OO	167[A]	GLU
18	PP	17	ALA
18	PP	161	SER
19	QQ	183	ALA
20	RR	129	GLY
21	SS	13	ARG
21	SS	24	LEU
22	TT	47	SER
27	YY	103	LYS
28	ZZ	70	PRO
29	aa	48	TYR
35	gg	57	LEU
37	ii	28	TYR
39	kk	6	ALA
39	kk	40	GLN
45	qq	71	ALA
45	qq	113	SER
45	qq	129	SER
45	qq	209	THR
46	rr	28	PHE
46	rr	68	PHE
46	rr	69	ILE
46	rr	111	ALA
46	rr	197	GLN
48	A	94	GLY
48	A	195	TRP
49	B	209	ASN
49	B	223	PHE
50	C	151	THR
51	D	44	THR
51	D	163	PRO
51	D	178	ARG
52	E	77	ARG
52	E	127	LYS
52	E	195	ILE
53	F	77	GLY
53	F	83	ARG
55	H	132	PRO
60	M	78	PRO
63	P	12	PHE

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Mol	Chain	Res	Type
64	Q	14	LYS
65	R	100	LEU
69	V	4	ASP
69	V	44	ARG
70	W	78	ARG
71	X	47	SER
72	Y	64	TYR
74	a	12	LYS
74	a	20	PRO
74	a	33	ASP
74	a	49	ALA
74	a	51	ARG
74	a	84	VAL
78	e	61	SER
79	f	97	LYS
80	g	4	SER
80	g	52	GLU
80	g	54	GLN
83	1	29	ASP
83	1	379	MET
83	1	653	VAL
4	AA	103	PRO
5	BB	227	GLU
6	CC	131	VAL
6	CC	338	LYS
6	CC	351	PRO
7	DD	21	ARG
7	DD	44	TYR
10	GG	24	PRO
10	GG	32	ASN
13	JJ	10	ARG
14	LL	4	SER
14	LL	155	GLU
15	MM	6	VAL
16	NN	81	TYR
17	OO	39[A]	ALA
17	OO	77[A]	PRO
17	OO	83[A]	LYS
17	OO	175[A]	TYR
21	SS	167	ARG
22	TT	146	ASN
24	VV	82	SER

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Mol	Chain	Res	Type
26	XX	64	GLU
29	aa	124	ILE
32	dd	15	ASN
32	dd	28	ARG
32	dd	82	GLU
33	ee	123	LYS
36	hh	84	LYS
36	hh	85	THR
37	ii	63	ASN
38	jj	20	LYS
40	ll	20	ASN
41	mm	79	GLU
44	pp	57	CYS
44	pp	61	ASN
45	qq	61	PRO
46	rr	189	VAL
48	A	26	ALA
48	A	103	THR
48	A	167	LYS
48	A	193	GLN
49	B	210	VAL
50	C	41	VAL
51	D	93	ASP
52	E	223	ASN
54	G	165	GLY
55	H	111	LYS
57	J	67	PRO
57	J	69	ARG
57	J	147	MET
59	L	30	LYS
59	L	55	ASP
62	O	18	ARG
63	P	101	VAL
64	Q	115	THR
66	S	12	GLN
67	T	50	SER
68	U	71	PRO
69	V	22	ARG
71	X	24	TRP
71	X	89	ASN
73	Z	58	ARG
74	a	8	ASN

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Mol	Chain	Res	Type
80	g	288	TYR
83	1	208	THR
83	1	246	GLY
83	1	589	LYS
83	1	675	PRO
83	1	681	MET
83	1	795	GLN
4	AA	56	ALA
5	BB	155	ALA
5	BB	383	LEU
6	CC	317	PRO
7	DD	6	ASP
7	DD	258	LYS
7	DD	276	LYS
8	EE	8	TYR
9	FF	205	SER
11	HH	110	LYS
14	LL	130	GLY
15	MM	41	GLN
17	OO	38[A]	ARG
18	PP	158	GLU
18	PP	165	VAL
19	QQ	168	THR
19	QQ	179	ARG
20	RR	53	LYS
22	TT	127	GLN
24	VV	53	SER
28	ZZ	19	ALA
29	aa	49	HIS
36	hh	86	ARG
44	pp	51	ALA
45	qq	7	SER
45	qq	25	LYS
46	rr	80	PRO
46	rr	149	ARG
48	A	28	ASN
49	B	145	LYS
50	C	226	THR
53	F	82	LYS
54	G	173	PRO
54	G	177	ARG
55	H	134	GLU

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Mol	Chain	Res	Type
56	I	40	THR
57	J	18	PRO
57	J	134	ILE
58	K	83	PRO
63	P	69	GLU
63	P	121	ILE
66	S	14	ILE
68	U	21	LYS
72	Y	36	SER
72	Y	63	GLN
73	Z	73	GLY
74	a	83	ILE
75	b	62	VAL
80	g	139	GLY
80	g	168	ASP
83	1	44	GLY
83	1	792	ALA
6	CC	78	GLY
7	DD	7	ILE
7	DD	125	VAL
13	JJ	108	GLU
17	OO	160[A]	LYS
18	PP	160	ALA
20	RR	130	ASN
22	TT	69	LYS
43	oo	95	GLY
50	C	44	THR
53	F	221	ARG
54	G	8	PRO
57	J	120	LYS
58	K	94	GLY
59	L	4	GLU
63	P	28	MET
71	X	130	VAL
72	Y	29	HIS
72	Y	51	GLU
72	Y	66	GLY
74	a	82	ARG
78	e	47	VAL
80	g	75	SER
83	1	372	CYS
83	1	374	PRO

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Mol	Chain	Res	Type
83	1	481	MET
83	1	486	SER
83	1	487	PRO
5	BB	223	GLY
7	DD	4	ILE
9	FF	175	ILE
9	FF	213	VAL
17	OO	85[A]	VAL
35	gg	59	PRO
46	rr	133	GLY
69	V	82	VAL
83	1	580	PRO
13	JJ	65	ILE
17	OO	71[A]	PRO
32	dd	66	GLY
55	H	8	ILE
59	L	7	VAL
60	M	97	ILE
66	S	76	PRO
70	W	29	PRO
71	X	53	VAL
75	b	39	GLY
83	1	558	PRO
83	1	827	GLY
12	II	93	PRO
18	PP	117	ILE
20	RR	94	VAL
48	A	158	VAL
49	B	206	PRO
51	D	130	GLY
54	G	70	PRO
60	M	48	GLY
64	Q	39	VAL
74	a	36	ILE
79	f	102	VAL
80	g	138	VAL
9	FF	188	VAL
10	GG	35	ILE
17	OO	76[A]	ALA
55	H	98	ILE
62	O	118	VAL
83	1	808	PRO

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Mol	Chain	Res	Type
57	J	162	SER
70	W	76	SER

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	AA	190/190 (100%)	174 (92%)	16 (8%)	11	42
5	BB	323/323 (100%)	272 (84%)	51 (16%)	2	17
6	CC	288/291 (99%)	253 (88%)	35 (12%)	5	26
7	DD	243/243 (100%)	215 (88%)	28 (12%)	5	29
8	EE	139/147 (95%)	128 (92%)	11 (8%)	12	44
9	FF	188/188 (100%)	167 (89%)	21 (11%)	6	30
10	GG	192/194 (99%)	175 (91%)	17 (9%)	9	40
11	HH	173/173 (100%)	155 (90%)	18 (10%)	7	33
12	II	177/185 (96%)	156 (88%)	21 (12%)	5	27
13	JJ	144/144 (100%)	130 (90%)	14 (10%)	8	36
14	LL	162/162 (100%)	149 (92%)	13 (8%)	12	43
15	MM	109/109 (100%)	93 (85%)	16 (15%)	3	20
16	NN	175/175 (100%)	156 (89%)	19 (11%)	6	32
17	OO	163/163 (100%)	136 (83%)	27 (17%)	2	15
18	PP	148/148 (100%)	132 (89%)	16 (11%)	6	32
19	QQ	150/150 (100%)	139 (93%)	11 (7%)	14	46
20	RR	152/152 (100%)	147 (97%)	5 (3%)	38	69
21	SS	154/154 (100%)	145 (94%)	9 (6%)	20	55
22	TT	135/135 (100%)	118 (87%)	17 (13%)	4	24
23	UU	90/90 (100%)	90 (100%)	0	100	100
24	VV	101/101 (100%)	90 (89%)	11 (11%)	6	32
25	WW	54/54 (100%)	52 (96%)	2 (4%)	34	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	XX	106/106 (100%)	91 (86%)	15 (14%)	3	21
27	YY	111/111 (100%)	102 (92%)	9 (8%)	11	43
28	ZZ	115/115 (100%)	106 (92%)	9 (8%)	12	44
29	aa	117/117 (100%)	104 (89%)	13 (11%)	6	31
30	bb	45/45 (100%)	44 (98%)	1 (2%)	52	77
31	cc	79/79 (100%)	72 (91%)	7 (9%)	9	40
32	dd	95/95 (100%)	88 (93%)	7 (7%)	13	46
33	ee	106/106 (100%)	100 (94%)	6 (6%)	20	55
34	ff	90/90 (100%)	84 (93%)	6 (7%)	16	50
35	gg	102/102 (100%)	100 (98%)	2 (2%)	55	79
36	hh	104/104 (100%)	100 (96%)	4 (4%)	33	66
37	ii	79/79 (100%)	70 (89%)	9 (11%)	5	29
38	jj	69/69 (100%)	61 (88%)	8 (12%)	5	29
39	kk	68/68 (100%)	63 (93%)	5 (7%)	13	46
40	ll	44/44 (100%)	41 (93%)	3 (7%)	16	50
41	mm	46/46 (100%)	42 (91%)	4 (9%)	10	41
42	nn	23/23 (100%)	19 (83%)	4 (17%)	2	12
43	oo	86/86 (100%)	76 (88%)	10 (12%)	5	29
44	pp	69/69 (100%)	58 (84%)	11 (16%)	2	16
45	qq	198/198 (100%)	181 (91%)	17 (9%)	10	41
46	rr	162/162 (100%)	147 (91%)	15 (9%)	9	38
48	A	174/174 (100%)	159 (91%)	15 (9%)	10	41
49	B	196/196 (100%)	178 (91%)	18 (9%)	9	39
50	C	176/176 (100%)	152 (86%)	24 (14%)	3	22
51	D	185/185 (100%)	165 (89%)	20 (11%)	6	32
52	E	223/223 (100%)	199 (89%)	24 (11%)	6	32
53	F	174/174 (100%)	165 (95%)	9 (5%)	23	58
54	G	192/192 (100%)	179 (93%)	13 (7%)	16	50
55	H	164/164 (100%)	152 (93%)	12 (7%)	14	46
56	I	148/158 (94%)	131 (88%)	17 (12%)	5	29
57	J	153/153 (100%)	137 (90%)	16 (10%)	7	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	K	88/88 (100%)	81 (92%)	7 (8%)	12	43
59	L	136/136 (100%)	123 (90%)	13 (10%)	8	37
60	M	97/97 (100%)	92 (95%)	5 (5%)	23	58
61	N	127/127 (100%)	112 (88%)	15 (12%)	5	28
62	O	96/96 (100%)	87 (91%)	9 (9%)	8	38
63	P	105/105 (100%)	92 (88%)	13 (12%)	4	26
64	Q	117/117 (100%)	111 (95%)	6 (5%)	24	58
65	R	117/117 (100%)	107 (92%)	10 (8%)	10	41
66	S	128/128 (100%)	112 (88%)	16 (12%)	4	25
67	T	117/117 (100%)	110 (94%)	7 (6%)	19	54
68	U	96/96 (100%)	92 (96%)	4 (4%)	30	63
69	V	73/73 (100%)	65 (89%)	8 (11%)	6	31
70	W	110/110 (100%)	94 (86%)	16 (14%)	3	20
71	X	120/120 (100%)	107 (89%)	13 (11%)	6	32
72	Y	108/108 (100%)	99 (92%)	9 (8%)	11	42
73	Z	60/60 (100%)	57 (95%)	3 (5%)	24	59
74	a	85/85 (100%)	73 (86%)	12 (14%)	3	21
75	b	72/72 (100%)	68 (94%)	4 (6%)	21	56
76	c	55/55 (100%)	52 (94%)	3 (6%)	21	57
77	d	46/46 (100%)	43 (94%)	3 (6%)	17	51
78	e	49/49 (100%)	46 (94%)	3 (6%)	18	53
79	f	58/60 (97%)	48 (83%)	10 (17%)	2	13
80	g	265/270 (98%)	246 (93%)	19 (7%)	14	47
83	1	700/702 (100%)	612 (87%)	88 (13%)	4	24
All	All	10374/10414 (100%)	9367 (90%)	1007 (10%)	12	36

All (1007) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AA	21	ARG
4	AA	32	LEU
4	AA	51	ASP
4	AA	92	LYS
4	AA	96	LEU

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Mol	Chain	Res	Type
4	AA	123	ARG
4	AA	126	LEU
4	AA	130	SER
4	AA	143	ASP
4	AA	161	ASP
4	AA	180	LEU
4	AA	190	ARG
4	AA	193	ARG
4	AA	204	MET
4	AA	241	ARG
4	AA	243	THR
5	BB	4	ARG
5	BB	7	GLU
5	BB	10	ARG
5	BB	14	LEU
5	BB	21	ARG
5	BB	45	SER
5	BB	54	SER
5	BB	56	ILE
5	BB	58	ARG
5	BB	59	ASP
5	BB	60	LEU
5	BB	80	ASP
5	BB	84	ILE
5	BB	87	VAL
5	BB	100	ARG
5	BB	101	SER
5	BB	102	LEU
5	BB	103	THR
5	BB	117	ARG
5	BB	121	ASN
5	BB	125	SER
5	BB	128	LYS
5	BB	162	VAL
5	BB	164	THR
5	BB	169	THR
5	BB	187	SER
5	BB	193	ASP
5	BB	241	LYS
5	BB	255	TRP
5	BB	262	TRP
5	BB	266	ARG

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Mol	Chain	Res	Type
5	BB	272	TYR
5	BB	274	HIS
5	BB	289	ASP
5	BB	290	ASP
5	BB	304	THR
5	BB	305	ILE
5	BB	306	THR
5	BB	323	ILE
5	BB	324	LEU
5	BB	325	LYS
5	BB	328	ILE
5	BB	331	THR
5	BB	332	ARG
5	BB	336	VAL
5	BB	339	ARG
5	BB	355	THR
5	BB	369	ARG
5	BB	370	PHE
5	BB	382	THR
5	BB	384	LYS
6	CC	19	ASP
6	CC	31	ARG
6	CC	37	SER
6	CC	41	SER
6	CC	58	HIS
6	CC	85	SER
6	CC	92	ASN
6	CC	93	MET
6	CC	95	ARG
6	CC	98	ARG
6	CC	105	THR
6	CC	107	ARG
6	CC	120	TYR
6	CC	122	THR
6	CC	134	LEU
6	CC	138	ARG
6	CC	156	LEU
6	CC	157	GLN
6	CC	175	HIS
6	CC	177	ASP
6	CC	180	LYS
6	CC	182	VAL

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Mol	Chain	Res	Type
6	CC	194	TYR
6	CC	198	ARG
6	CC	202	ARG
6	CC	206	LEU
6	CC	215	VAL
6	CC	232	SER
6	CC	235	LEU
6	CC	238	LEU
6	CC	247	PHE
6	CC	270	VAL
6	CC	346	GLN
6	CC	350	LYS
6	CC	356	LEU
7	DD	4	ILE
7	DD	22	ARG
7	DD	28	THR
7	DD	51	LEU
7	DD	54	ARG
7	DD	59	ASP
7	DD	67	SER
7	DD	70	THR
7	DD	75	LEU
7	DD	89	THR
7	DD	94	ASN
7	DD	101	THR
7	DD	103	LEU
7	DD	116	ASP
7	DD	144	VAL
7	DD	147	ASP
7	DD	152	ARG
7	DD	154	THR
7	DD	155	THR
7	DD	179	ARG
7	DD	184	ASP
7	DD	193	ASP
7	DD	195	LEU
7	DD	213	ASP
7	DD	214	ASP
7	DD	230	ASP
7	DD	278	THR
7	DD	293	LEU
8	EE	29	ARG

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Mol	Chain	Res	Type
8	EE	48	LYS
8	EE	50	VAL
8	EE	74	LEU
8	EE	76	ARG
8	EE	82	VAL
8	EE	111	ARG
8	EE	114	ARG
8	EE	126	LYS
8	EE	154	LEU
8	EE	174	LYS
9	FF	30	ARG
9	FF	53	GLU
9	FF	57	ARG
9	FF	70	SER
9	FF	71	SER
9	FF	75	SER
9	FF	81	VAL
9	FF	85	ARG
9	FF	87	LYS
9	FF	90	ASN
9	FF	110	SER
9	FF	112	THR
9	FF	140	THR
9	FF	156	GLN
9	FF	181	LEU
9	FF	218	LYS
9	FF	221	ILE
9	FF	225	SER
9	FF	226	PHE
9	FF	233	ILE
9	FF	236	LEU
10	GG	28	SER
10	GG	62	LYS
10	GG	70	VAL
10	GG	123	GLU
10	GG	130	VAL
10	GG	135	LEU
10	GG	144	ASN
10	GG	154	ASN
10	GG	155	ASP
10	GG	165	LEU
10	GG	168	LEU

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Mol	Chain	Res	Type
10	GG	184	ARG
10	GG	196	VAL
10	GG	220	ASN
10	GG	222	LEU
10	GG	231	HIS
10	GG	240	LYS
11	HH	5	GLN
11	HH	11	ASP
11	HH	41	ILE
11	HH	42	ASP
11	HH	69	ARG
11	HH	80	THR
11	HH	83	THR
11	HH	91	ARG
11	HH	118	LEU
11	HH	120	ASP
11	HH	143	GLU
11	HH	157	ASN
11	HH	168	ARG
11	HH	170	LYS
11	HH	172	ILE
11	HH	173	ARG
11	HH	186	LEU
11	HH	189	GLU
12	II	7	ARG
12	II	24	ARG
12	II	30	LYS
12	II	33	ILE
12	II	40	LYS
12	II	52	LEU
12	II	57	LEU
12	II	88	ARG
12	II	90	ARG
12	II	91	VAL
12	II	115	MET
12	II	140	THR
12	II	142	ASP
12	II	144	ASN
12	II	154	ARG
12	II	163	GLN
12	II	165	ILE
12	II	169	LYS

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Mol	Chain	Res	Type
12	II	193	ASP
12	II	200	LEU
12	II	203	LYS
13	JJ	12	LEU
13	JJ	17	LEU
13	JJ	30	LEU
13	JJ	39	GLN
13	JJ	44	THR
13	JJ	56	THR
13	JJ	80	LEU
13	JJ	92	ARG
13	JJ	99	THR
13	JJ	106	ILE
13	JJ	112	LEU
13	JJ	130	VAL
13	JJ	137	ARG
13	JJ	154	THR
14	LL	5	LYS
14	LL	24	VAL
14	LL	31	LYS
14	LL	42	LYS
14	LL	49	ARG
14	LL	54	LEU
14	LL	55	ARG
14	LL	67	ARG
14	LL	69	VAL
14	LL	110	ASP
14	LL	120	GLN
14	LL	124	ILE
14	LL	194	GLU
15	MM	2	SER
15	MM	5	SER
15	MM	8	LYS
15	MM	20	VAL
15	MM	21	VAL
15	MM	22	LEU
15	MM	34	THR
15	MM	53	VAL
15	MM	63	VAL
15	MM	64	VAL
15	MM	69	THR
15	MM	74	ARG

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Mol	Chain	Res	Type
15	MM	77	LYS
15	MM	106	ARG
15	MM	121	LEU
15	MM	125	LYS
16	NN	10	LEU
16	NN	19	LEU
16	NN	22	LEU
16	NN	38	ARG
16	NN	41	ARG
16	NN	62	TYR
16	NN	80	THR
16	NN	83	LYS
16	NN	97	SER
16	NN	98	LEU
16	NN	109	ARG
16	NN	126	THR
16	NN	131	GLU
16	NN	133	ILE
16	NN	134	LEU
16	NN	136	ASP
16	NN	151	ILE
16	NN	183	THR
16	NN	196	THR
17	OO	5[A]	GLU
17	OO	20[A]	LEU
17	OO	23[A]	THR
17	OO	32[A]	GLN
17	OO	33[A]	LYS
17	OO	34[A]	ILE
17	OO	38[A]	ARG
17	OO	42[A]	LEU
17	OO	43[A]	ASN
17	OO	47[A]	GLU
17	OO	60[A]	ARG
17	OO	69[A]	ARG
17	OO	78[A]	SER
17	OO	81[A]	PHE
17	OO	82[A]	TYR
17	OO	107[A]	GLU
17	OO	114[A]	ASP
17	OO	116[A]	LYS
17	OO	117[A]	LYS

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Mol	Chain	Res	Type
17	OO	118[A]	ARG
17	OO	119[A]	VAL
17	OO	125[A]	LEU
17	OO	127[A]	VAL
17	OO	130[A]	LEU
17	OO	150[A]	TYR
17	OO	152[A]	ASP
17	OO	168[A]	TYR
18	PP	24	VAL
18	PP	26	TYR
18	PP	52	LEU
18	PP	55	GLN
18	PP	118	GLN
18	PP	119	VAL
18	PP	120	ASN
18	PP	142	SER
18	PP	144	SER
18	PP	145	HIS
18	PP	153	LYS
18	PP	161	SER
18	PP	164	LYS
18	PP	168	LEU
18	PP	171	ARG
18	PP	173	ARG
19	QQ	17	THR
19	QQ	32	LEU
19	QQ	41	ASP
19	QQ	49	LEU
19	QQ	95	GLU
19	QQ	105	ARG
19	QQ	135	GLN
19	QQ	144	ARG
19	QQ	148	GLU
19	QQ	165	ILE
19	QQ	168	THR
20	RR	60	ARG
20	RR	91	SER
20	RR	99	LEU
20	RR	119	LEU
20	RR	128	LYS
21	SS	40	ARG
21	SS	45	LEU

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Mol	Chain	Res	Type
21	SS	52	LYS
21	SS	97	VAL
21	SS	117	ARG
21	SS	122	HIS
21	SS	137	ARG
21	SS	171	PHE
21	SS	172	TYR
22	TT	18	ASP
22	TT	41	ASP
22	TT	55	LYS
22	TT	72	VAL
22	TT	75	ILE
22	TT	78	LYS
22	TT	79	MET
22	TT	83	ARG
22	TT	88	ARG
22	TT	93	VAL
22	TT	97	LYS
22	TT	126	VAL
22	TT	127	GLN
22	TT	128	LEU
22	TT	139	ARG
22	TT	148	PRO
22	TT	157	GLU
24	VV	11	PHE
24	VV	33	ASN
24	VV	47	ASN
24	VV	48	ARG
24	VV	56	ASP
24	VV	63	LYS
24	VV	64	LYS
24	VV	83	LYS
24	VV	98	ASN
24	VV	102	ILE
24	VV	131	SER
25	WW	42	GLN
25	WW	58	HIS
26	XX	26	VAL
26	XX	27	ARG
26	XX	31	SER
26	XX	36	LYS
26	XX	45	LYS

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Mol	Chain	Res	Type
26	XX	56	ARG
26	XX	63	ILE
26	XX	68	THR
26	XX	73	MET
26	XX	82	LEU
26	XX	115	ARG
26	XX	133	LEU
26	XX	135	ILE
26	XX	137	ASN
26	XX	142	ILE
27	YY	9	SER
27	YY	50	ILE
27	YY	54	ASP
27	YY	55	GLU
27	YY	74	TYR
27	YY	95	VAL
27	YY	104	VAL
27	YY	112	ASP
27	YY	126	LEU
28	ZZ	34	LYS
28	ZZ	46	ILE
28	ZZ	51	LEU
28	ZZ	56	ARG
28	ZZ	57	GLN
28	ZZ	72	ILE
28	ZZ	89	VAL
28	ZZ	109	GLU
28	ZZ	121	ARG
29	aa	4	ARG
29	aa	5	LEU
29	aa	16	SER
29	aa	27	LYS
29	aa	43	THR
29	aa	44	ASN
29	aa	60	TYR
29	aa	65	GLN
29	aa	76	ASP
29	aa	115	LYS
29	aa	120	ASP
29	aa	128	ARG
29	aa	130	VAL
30	bb	32	LEU

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Mol	Chain	Res	Type
31	cc	16	LEU
31	cc	41	LEU
31	cc	54	SER
31	cc	61	MET
31	cc	66	LYS
31	cc	83	LYS
31	cc	93	LEU
32	dd	5	LYS
32	dd	8	VAL
32	dd	52	ASP
32	dd	55	LEU
32	dd	64	ILE
32	dd	76	SER
32	dd	105	HIS
33	ee	6	HIS
33	ee	19	ARG
33	ee	23	ASP
33	ee	33	ARG
33	ee	50	ILE
33	ee	75	LEU
34	ff	17	GLN
34	ff	20	LYS
34	ff	33	GLU
34	ff	77	ASN
34	ff	81	VAL
34	ff	105	SER
35	gg	60	ARG
35	gg	62	TYR
36	hh	69	LEU
36	hh	81	ARG
36	hh	85	THR
36	hh	102	GLU
37	ii	18	ASN
37	ii	34	SER
37	ii	57	LEU
37	ii	58	ILE
37	ii	62	ARG
37	ii	75	LYS
37	ii	76	ARG
37	ii	84	LYS
37	ii	99	ARG
38	jj	5	THR

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Mol	Chain	Res	Type
38	jj	7	SER
38	jj	15	SER
38	jj	17	THR
38	jj	24	ARG
38	jj	45	ARG
38	jj	59	THR
38	jj	75	LYS
39	kk	8	ILE
39	kk	32	ASN
39	kk	51	LEU
39	kk	53	THR
39	kk	73	PHE
40	ll	6	SER
40	ll	21	ARG
40	ll	29	LEU
41	mm	85	LEU
41	mm	97	ARG
41	mm	106	ARG
41	mm	113	ARG
42	nn	2	ARG
42	nn	6	ARG
42	nn	13	LEU
42	nn	16	LYS
43	oo	12	CYS
43	oo	29	LYS
43	oo	45	ARG
43	oo	47	GLN
43	oo	48	SER
43	oo	61	LYS
43	oo	78	LYS
43	oo	83	LEU
43	oo	85	LEU
43	oo	93	LEU
44	pp	10	ILE
44	pp	11	THR
44	pp	20	SER
44	pp	40	SER
44	pp	46	CYS
44	pp	49	ARG
44	pp	58	SER
44	pp	60	CYS
44	pp	71	LEU

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Mol	Chain	Res	Type
44	pp	81	SER
44	pp	84	ARG
45	qq	3	LYS
45	qq	8	HIS
45	qq	34	LEU
45	qq	49	PHE
45	qq	67	ILE
45	qq	97	LYS
45	qq	102	LYS
45	qq	105	LYS
45	qq	107	TYR
45	qq	122	ARG
45	qq	177	ASP
45	qq	179	LEU
45	qq	191	VAL
45	qq	198	TRP
45	qq	199	GLN
45	qq	207	LYS
45	qq	214	TYR
46	rr	20	TYR
46	rr	35	VAL
46	rr	37	SER
46	rr	39	GLN
46	rr	48	ARG
46	rr	62	ARG
46	rr	90	PHE
46	rr	91	THR
46	rr	120	ASP
46	rr	122	TRP
46	rr	134	LYS
46	rr	135	THR
46	rr	149	ARG
46	rr	187	LEU
46	rr	195	ASN
48	A	9	LEU
48	A	34	GLU
48	A	56	LYS
48	A	79	ARG
48	A	109	ASN
48	A	134	LYS
48	A	135	GLU
48	A	146	LEU

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Mol	Chain	Res	Type
48	A	150	ASP
48	A	173	ILE
48	A	177	LEU
48	A	195	TRP
48	A	197	ILE
48	A	198	MET
48	A	205	ARG
49	B	47	LEU
49	B	48	VAL
49	B	70	LEU
49	B	81	PHE
49	B	84	VAL
49	B	89	ASP
49	B	96	LEU
49	B	99	ASN
49	B	100	PHE
49	B	118	GLN
49	B	119	THR
49	B	120	LEU
49	B	127	VAL
49	B	145	LYS
49	B	179	SER
49	B	181	LEU
49	B	191	GLU
49	B	208	GLN
50	C	49	LEU
50	C	51	LYS
50	C	71	PHE
50	C	82	LYS
50	C	86	MET
50	C	88	ILE
50	C	89	LYS
50	C	94	GLN
50	C	99	GLN
50	C	100	ARG
50	C	111	ASP
50	C	122	THR
50	C	142	ILE
50	C	145	ARG
50	C	146	ARG
50	C	149	TRP
50	C	166	LYS

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Mol	Chain	Res	Type
50	C	169	SER
50	C	174	LEU
50	C	186	SER
50	C	212	LEU
50	C	225	ASN
50	C	234	LEU
50	C	235	TRP
51	D	5	ILE
51	D	7	LYS
51	D	11	LEU
51	D	51	ARG
51	D	65	ARG
51	D	113	LEU
51	D	122	VAL
51	D	134	CYS
51	D	135	GLU
51	D	139	SER
51	D	141	LYS
51	D	143	ARG
51	D	157	LEU
51	D	158	ILE
51	D	162	GLN
51	D	173	ARG
51	D	177	LEU
51	D	178	ARG
51	D	179	GLN
51	D	222	VAL
52	E	6	LYS
52	E	9	LEU
52	E	18	TRP
52	E	37	LYS
52	E	38	LEU
52	E	42	LEU
52	E	51	ARG
52	E	68	ARG
52	E	77	ARG
52	E	79	ASP
52	E	123	LEU
52	E	127	LYS
52	E	133	LYS
52	E	139	VAL
52	E	143	ASP

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Mol	Chain	Res	Type
52	E	159	THR
52	E	163	ASP
52	E	176	ASP
52	E	187	ARG
52	E	206	ASP
52	E	208	VAL
52	E	225	VAL
52	E	245	LYS
52	E	247	THR
53	F	101	MET
53	F	114	ARG
53	F	121	GLU
53	F	158	ARG
53	F	186	PHE
53	F	188	ASN
53	F	192	ILE
53	F	196	LEU
53	F	220	GLU
54	G	52	ILE
54	G	75	LEU
54	G	81	HIS
54	G	92	ARG
54	G	95	LYS
54	G	96	SER
54	G	141	ILE
54	G	152	ASP
54	G	159	ARG
54	G	164	LYS
54	G	178	LEU
54	G	182	GLN
54	G	215	ARG
55	H	11	GLN
55	H	16	LEU
55	H	47	ARG
55	H	80	GLU
55	H	81	LEU
55	H	110	GLN
55	H	114	ARG
55	H	126	LEU
55	H	139	ARG
55	H	168	SER
55	H	174	ASN

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Mol	Chain	Res	Type
55	H	180	GLN
56	I	8	ARG
56	I	10	LYS
56	I	24	LYS
56	I	25	ARG
56	I	29	LEU
56	I	62	THR
56	I	72	VAL
56	I	75	LYS
56	I	77	ARG
56	I	86	SER
56	I	92	ARG
56	I	101	ILE
56	I	138	LYS
56	I	140	THR
56	I	144	TRP
56	I	161	PHE
56	I	170	ILE
57	J	28	LEU
57	J	30	LEU
57	J	37	LYS
57	J	49	LEU
57	J	69	ARG
57	J	83	ILE
57	J	86	LEU
57	J	89	ASP
57	J	93	LEU
57	J	94	ASP
57	J	126	ARG
57	J	132	ARG
57	J	145	SER
57	J	149	ARG
57	J	175	LYS
57	J	176	ARG
58	K	20	VAL
58	K	40	LEU
58	K	54	PHE
58	K	55	VAL
58	K	59	PHE
58	K	76	LEU
58	K	86	ILE
59	L	8	GLN

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Mol	Chain	Res	Type
59	L	55	ASP
59	L	67	ARG
59	L	77	SER
59	L	80	MET
59	L	83	THR
59	L	84	ILE
59	L	87	ARG
59	L	90	TYR
59	L	105	LYS
59	L	125	VAL
59	L	136	ARG
59	L	153	PHE
60	M	55	LEU
60	M	67	LEU
60	M	91	TRP
60	M	104	ARG
60	M	105	LYS
61	N	3	ARG
61	N	12	SER
61	N	17	PRO
61	N	25	TRP
61	N	49	GLN
61	N	64	LYS
61	N	72	LEU
61	N	88	LEU
61	N	89	TYR
61	N	115	LEU
61	N	119	GLU
61	N	121	ARG
61	N	124	ARG
61	N	139	TRP
61	N	142	GLU
62	O	37	GLU
62	O	51	ASP
62	O	58	TYR
62	O	67	VAL
62	O	71	CYS
62	O	86	THR
62	O	110	LEU
62	O	114	ARG
62	O	124	ASP
63	P	17	TYR

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Mol	Chain	Res	Type
63	P	18	LYS
63	P	21	ASP
63	P	32	ASP
63	P	40	ARG
63	P	43	ARG
63	P	52	LYS
63	P	57	MET
63	P	79	HIS
63	P	81	ARG
63	P	84	ILE
63	P	89	MET
63	P	127	ARG
64	Q	19	VAL
64	Q	53	LEU
64	Q	121	SER
64	Q	125	GLU
64	Q	128	LYS
64	Q	142	TYR
65	R	5	ARG
65	R	6	THR
65	R	16	LEU
65	R	47	ARG
65	R	56	HIS
65	R	66	VAL
65	R	88	VAL
65	R	127	VAL
65	R	128	ARG
65	R	130	ARG
66	S	16	ARG
66	S	36	ARG
66	S	41	ARG
66	S	49	LYS
66	S	73	MET
66	S	74	GLN
66	S	84	TRP
66	S	93	ASN
66	S	96	LYS
66	S	100	SER
66	S	105	LEU
66	S	126	ARG
66	S	131	LEU
66	S	136	GLN

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Mol	Chain	Res	Type
66	S	137	HIS
66	S	144	ARG
67	T	7	ARG
67	T	57	ARG
67	T	60	SER
67	T	63	ARG
67	T	68	ARG
67	T	85	ASN
67	T	86	ARG
68	U	52	LYS
68	U	85	ARG
68	U	86	ILE
68	U	94	GLU
69	V	12	TYR
69	V	17	CYS
69	V	28	ASP
69	V	33	GLN
69	V	38	GLN
69	V	56	SER
69	V	60	ARG
69	V	67	ASP
70	W	2	THR
70	W	15	ASN
70	W	23	ARG
70	W	24	GLN
70	W	25	VAL
70	W	26	LEU
70	W	28	ARG
70	W	40	VAL
70	W	51	GLU
70	W	61	ILE
70	W	66	ASN
70	W	70	ASN
70	W	83	ILE
70	W	107	SER
70	W	111	MET
70	W	130	TYR
71	X	9	LEU
71	X	19	ARG
71	X	23	ARG
71	X	63	GLN
71	X	70	LYS

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Mol	Chain	Res	Type
71	X	71	CYS
71	X	84	THR
71	X	98	GLU
71	X	99	ASN
71	X	102	VAL
71	X	107	PHE
71	X	109	ARG
71	X	130	VAL
72	Y	3	ASP
72	Y	6	THR
72	Y	27	VAL
72	Y	31	ASN
72	Y	46	GLU
72	Y	98	GLU
72	Y	110	GLN
72	Y	116	LYS
72	Y	121	THR
73	Z	68	ARG
73	Z	77	ARG
73	Z	97	LYS
74	a	5	ARG
74	a	7	SER
74	a	8	ASN
74	a	18	VAL
74	a	23	CYS
74	a	28	ARG
74	a	32	LYS
74	a	39	MET
74	a	50	ILE
74	a	64	LEU
74	a	75	ILE
74	a	76	SER
75	b	7	LEU
75	b	9	HIS
75	b	21	LEU
75	b	67	THR
76	c	16	LEU
76	c	32	PHE
76	c	56	LEU
77	d	21	CYS
77	d	40	ARG
77	d	49	ASP

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Mol	Chain	Res	Type
78	e	17	GLN
78	e	22	GLU
78	e	33	ARG
79	f	89	LYS
79	f	97	LYS
79	f	100	LEU
79	f	106	TYR
79	f	113	LYS
79	f	114	VAL
79	f	117	LEU
79	f	120	GLU
79	f	136	ARG
79	f	139	CYS
80	g	27	SER
80	g	43	LEU
80	g	52	GLU
80	g	55	PHE
80	g	60	ARG
80	g	67	HIS
80	g	75	SER
80	g	99	ASN
80	g	175	VAL
80	g	188	LEU
80	g	238	PHE
80	g	242	ASP
80	g	244	LYS
80	g	270	TYR
80	g	273	GLU
80	g	275	GLU
80	g	292	GLN
80	g	299	LEU
80	g	321	GLN
83	1	13	MET
83	1	21	ASN
83	1	23	SER
83	1	24	VAL
83	1	25	ILE
83	1	29	ASP
83	1	35	LEU
83	1	42	ARG
83	1	45	ILE
83	1	57	THR

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Mol	Chain	Res	Type
83	1	61	LYS
83	1	64	GLN
83	1	78	TYR
83	1	79	SER
83	1	80	GLU
83	1	126	LEU
83	1	128	VAL
83	1	136	CYS
83	1	142	VAL
83	1	150	ARG
83	1	161	ASP
83	1	164	LEU
83	1	166	GLU
83	1	171	LYS
83	1	173	ASP
83	1	202	VAL
83	1	208	THR
83	1	229	TYR
83	1	236	ASP
83	1	237	LYS
83	1	248	SER
83	1	251	ASN
83	1	276	PHE
83	1	289	MET
83	1	293	LYS
83	1	305	ILE
83	1	313	ASP
83	1	315	GLU
83	1	324	MET
83	1	344	SER
83	1	379	MET
83	1	380	LEU
83	1	381	TYR
83	1	383	SER
83	1	385	MET
83	1	391	LYS
83	1	394	PHE
83	1	433	ARG
83	1	441	PHE
83	1	463	LEU
83	1	477	ASN
83	1	481	MET

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Mol	Chain	Res	Type
83	1	482	LYS
83	1	495	VAL
83	1	508	LEU
83	1	510	ARG
83	1	515	ASP
83	1	519	LEU
83	1	521	TYR
83	1	535	GLU
83	1	555	LYS
83	1	557	SER
83	1	561	VAL
83	1	570	GLU
83	1	574	THR
83	1	582	LYS
83	1	586	ILE
83	1	622	ASP
83	1	646	VAL
83	1	651	LYS
83	1	653	VAL
83	1	669	TRP
83	1	671	THR
83	1	680	GLU
83	1	681	MET
83	1	682	ARG
83	1	689	LEU
83	1	693	LEU
83	1	694	HIS
83	1	696	ASP
83	1	698	ILE
83	1	708	THR
83	1	721	ASP
83	1	727	PRO
83	1	738	GLN
83	1	775	ASN
83	1	785	ARG
83	1	803	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
4	AA	97	ASN
4	AA	132	ASN

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Mol	Chain	Res	Type
4	AA	187	HIS
4	AA	209	HIS
4	AA	211	HIS
4	AA	233	GLN
5	BB	173	GLN
5	BB	177	HIS
5	BB	274	HIS
5	BB	313	HIS
5	BB	371	GLN
6	CC	36	HIS
6	CC	48	GLN
6	CC	157	GLN
6	CC	307	GLN
7	DD	13	HIS
7	DD	39	GLN
8	EE	171	HIS
9	FF	90	ASN
9	FF	241	ASN
10	GG	137	HIS
10	GG	144	ASN
10	GG	220	ASN
11	HH	5	GLN
11	HH	50	ASN
12	II	14	ASN
12	II	144	ASN
14	LL	114	GLN
17	OO	91[A]	HIS
18	PP	42	GLN
19	QQ	73	GLN
19	QQ	166	GLN
20	RR	130	ASN
21	SS	88	HIS
22	TT	49	HIS
22	TT	54	HIS
22	TT	146	ASN
24	VV	98	ASN
24	VV	132	ASN
26	XX	137	ASN
28	ZZ	79	HIS
29	aa	41	HIS
29	aa	44	ASN
30	bb	12	GLN

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Mol	Chain	Res	Type
32	dd	57	GLN
33	ee	35	GLN
35	gg	52	GLN
37	ii	19	GLN
38	jj	47	HIS
38	jj	69	HIS
39	kk	32	ASN
45	qq	12	HIS
45	qq	94	ASN
45	qq	199	GLN
46	rr	39	GLN
46	rr	191	GLN
46	rr	195	ASN
48	A	109	ASN
49	B	178	ASN
50	C	115	HIS
50	C	152	ASN
51	D	179	GLN
52	E	67	GLN
53	F	81	ASN
53	F	172	GLN
53	F	202	ASN
54	G	176	GLN
54	G	190	GLN
57	J	48	GLN
59	L	14	GLN
59	L	37	ASN
61	N	49	GLN
62	O	29	HIS
63	P	79	HIS
64	Q	83	GLN
66	S	89	GLN
66	S	137	HIS
67	T	25	GLN
67	T	85	ASN
69	V	33	GLN
70	W	64	GLN
71	X	18	HIS
71	X	22	ASN
71	X	79	ASN
71	X	99	ASN
72	Y	29	HIS

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Mol	Chain	Res	Type
72	Y	31	ASN
73	Z	95	HIS
75	b	49	HIS
80	g	321	GLN
83	1	30	HIS
83	1	101	ASN
83	1	432	GLN
83	1	583	HIS
83	1	584	ASN
83	1	644	ASN
83	1	699	HIS
83	1	704	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3265/3270 (99%)	984 (30%)	198 (6%)
2	7	120/121 (99%)	22 (18%)	4 (3%)
3	8	156/157 (99%)	40 (25%)	6 (3%)
81	2	1778/1798 (98%)	790 (44%)	127 (7%)
82	4	184/190 (96%)	90 (48%)	24 (13%)
All	All	5503/5536 (99%)	1926 (34%)	359 (6%)

All (1926) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	6	A
1	5	15	C
1	5	18	G
1	5	21	G
1	5	22	G
1	5	26	A
1	5	40	A
1	5	43	A
1	5	44	U
1	5	45	A
1	5	48	A
1	5	49	A
1	5	57	A
1	5	59	G
1	5	60	A

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Mol	Chain	Res	Type
1	5	65	A
1	5	66	A
1	5	68	C
1	5	73	C
1	5	75	G
1	5	76	G
1	5	85	A
1	5	87	U
1	5	92	G
1	5	96	G
1	5	99	A
1	5	109	A
1	5	110	G
1	5	111	C
1	5	113	C
1	5	115	A
1	5	117	U
1	5	120	G
1	5	121	A
1	5	122	A
1	5	128	G
1	5	133	U
1	5	134	U
1	5	136	G
1	5	143	G
1	5	146	U
1	5	150	A
1	5	156	A
1	5	157	A
1	5	161	G
1	5	165	A
1	5	166	C
1	5	167	U
1	5	168	U
1	5	169	U
1	5	170	G
1	5	171	U
1	5	174	C
1	5	177	G
1	5	182	U
1	5	187	A
1	5	190	U

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Mol	Chain	Res	Type
1	5	191	U
1	5	198	A
1	5	200	C
1	5	210	U
1	5	211	A
1	5	213	A
1	5	218	G
1	5	219	A
1	5	220	G
1	5	221	A
1	5	224	C
1	5	234	G
1	5	239	U
1	5	240	C
1	5	241	C
1	5	244	G
1	5	248	U
1	5	249	U
1	5	250	U
1	5	251	G
1	5	252	U
1	5	253	A
1	5	254	A
1	5	266	C
1	5	269	G
1	5	282	G
1	5	283	G
1	5	284	A
1	5	285	A
1	5	286	U
1	5	295	A
1	5	298	U
1	5	299	G
1	5	305	U
1	5	306	A
1	5	307	A
1	5	315	C
1	5	319	A
1	5	323	A
1	5	329	U
1	5	336	A
1	5	338	A

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Mol	Chain	Res	Type
1	5	339	C
1	5	343	U
1	5	349	A
1	5	350	C
1	5	368	G
1	5	370	U
1	5	374	A
1	5	376	G
1	5	378	A
1	5	385	A
1	5	395	A
1	5	398	A
1	5	399	A
1	5	401	U
1	5	403	C
1	5	404	G
1	5	407	A
1	5	420	G
1	5	421	G
1	5	422	A
1	5	429	U
1	5	436	A
1	5	437	G
1	5	438	A
1	5	439	C
1	5	440	A
1	5	441	U
1	5	443	G
1	5	478	U
1	5	486	U
1	5	487	U
1	5	491	U
1	5	492	A
1	5	494	A
1	5	503	A
1	5	506	G
1	5	507	U
1	5	512	C
1	5	514	G
1	5	518	C
1	5	519	G
1	5	520	G

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Mol	Chain	Res	Type
1	5	521	U
1	5	525	G
1	5	528	U
1	5	529	U
1	5	530	A
1	5	531	U
1	5	532	A
1	5	533	G
1	5	537	G
1	5	542	A
1	5	543	A
1	5	545	A
1	5	551	A
1	5	552	G
1	5	565	A
1	5	567	U
1	5	573	U
1	5	575	U
1	5	577	G
1	5	580	A
1	5	581	A
1	5	582	G
1	5	584	A
1	5	589	G
1	5	590	G
1	5	594	A
1	5	595	A
1	5	596	U
1	5	597	G
1	5	598	G
1	5	609	C
1	5	615	U
1	5	620	A
1	5	622	A
1	5	633	A
1	5	640	C
1	5	644	U
1	5	650	A
1	5	654	U
1	5	660	U
1	5	664	A
1	5	670	G

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Mol	Chain	Res	Type
1	5	671	U
1	5	672	A
1	5	678	A
1	5	681	G
1	5	683	A
1	5	685	G
1	5	688	A
1	5	694	G
1	5	698	A
1	5	699	G
1	5	708	A
1	5	709	G
1	5	721	G
1	5	724	C
1	5	729	C
1	5	736	C
1	5	737	U
1	5	738	U
1	5	741	G
1	5	742	A
1	5	745	G
1	5	747	U
1	5	748	U
1	5	751	A
1	5	752	G
1	5	755	A
1	5	756	G
1	5	757	A
1	5	758	G
1	5	770	G
1	5	772	A
1	5	777	A
1	5	778	A
1	5	779	A
1	5	788	A
1	5	794	C
1	5	797	G
1	5	801	A
1	5	805	U
1	5	808	A
1	5	817	A
1	5	832	C

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Mol	Chain	Res	Type
1	5	842	U
1	5	845	U
1	5	850	U
1	5	861	C
1	5	867	A
1	5	868	U
1	5	878	G
1	5	879	G
1	5	885	A
1	5	886	A
1	5	887	G
1	5	888	A
1	5	890	U
1	5	891	A
1	5	892	A
1	5	894	C
1	5	908	G
1	5	915	C
1	5	924	G
1	5	930	C
1	5	931	U
1	5	932	C
1	5	933	A
1	5	941	A
1	5	945	G
1	5	949	G
1	5	950	U
1	5	951	A
1	5	952	U
1	5	953	C
1	5	955	G
1	5	962	G
1	5	965	G
1	5	972	G
1	5	973	A
1	5	974	A
1	5	981	G
1	5	986	A
1	5	987	C
1	5	988	C
1	5	989	G
1	5	990	G

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Mol	Chain	Res	Type
1	5	992	G
1	5	994	U
1	5	995	G
1	5	996	A
1	5	997	A
1	5	999	U
1	5	1000	G
1	5	1003	C
1	5	1005	U
1	5	1006	G
1	5	1018	A
1	5	1020	C
1	5	1025	A
1	5	1034	G
1	5	1035	A
1	5	1036	A
1	5	1043	G
1	5	1052	U
1	5	1053	U
1	5	1056	A
1	5	1058	G
1	5	1064	A
1	5	1065	U
1	5	1066	U
1	5	1067	U
1	5	1069	A
1	5	1074	A
1	5	1075	G
1	5	1078	C
1	5	1087	G
1	5	1088	G
1	5	1102	G
1	5	1115	U
1	5	1116	G
1	5	1122	U
1	5	1123	G
1	5	1124	A
1	5	1129	A
1	5	1130	A
1	5	1145	G
1	5	1146	C
1	5	1149	G

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Mol	Chain	Res	Type
1	5	1151	A
1	5	1152	U
1	5	1153	A
1	5	1156	C
1	5	1162	U
1	5	1163	C
1	5	1164	A
1	5	1167	C
1	5	1168	A
1	5	1172	C
1	5	1177	G
1	5	1179	U
1	5	1180	G
1	5	1191	U
1	5	1192	A
1	5	1193	G
1	5	1194	A
1	5	1195	C
1	5	1196	A
1	5	1197	G
1	5	1198	C
1	5	1203	C
1	5	1206	U
1	5	1207	G
1	5	1208	G
1	5	1210	C
1	5	1212	U
1	5	1213	G
1	5	1216	A
1	5	1217	G
1	5	1218	U
1	5	1223	A
1	5	1225	C
1	5	1229	U
1	5	1230	A
1	5	1234	A
1	5	1235	G
1	5	1236	U
1	5	1237	G
1	5	1248	C
1	5	1254	C
1	5	1256	G

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Mol	Chain	Res	Type
1	5	1257	A
1	5	1258	A
1	5	1263	C
1	5	1266	G
1	5	1272	A
1	5	1274	A
1	5	1276	U
1	5	1278	G
1	5	1279	A
1	5	1280	U
1	5	1281	G
1	5	1284	G
1	5	1289	A
1	5	1296	U
1	5	1301	A
1	5	1302	U
1	5	1319	U
1	5	1320	A
1	5	1321	A
1	5	1322	U
1	5	1323	A
1	5	1324	U
1	5	1326	A
1	5	1327	U
1	5	1328	G
1	5	1351	G
1	5	1356	C
1	5	1357	A
1	5	1370	A
1	5	1371	G
1	5	1390	A
1	5	1398	U
1	5	1401	U
1	5	1402	G
1	5	1405	G
1	5	1408	C
1	5	1409	U
1	5	1414	G
1	5	1417	A
1	5	1421	G
1	5	1422	C
1	5	1424	A

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Mol	Chain	Res	Type
1	5	1425	A
1	5	1426	U
1	5	1427	A
1	5	1431	A
1	5	1436	A
1	5	1446	A
1	5	1448	A
1	5	1452	A
1	5	1453	A
1	5	1455	U
1	5	1458	G
1	5	1466	U
1	5	1468	C
1	5	1471	G
1	5	1479	C
1	5	1496	G
1	5	1498	C
1	5	1499	G
1	5	1504	U
1	5	1507	G
1	5	1510	A
1	5	1513	G
1	5	1525	U
1	5	1526	U
1	5	1527	C
1	5	1528	A
1	5	1530	A
1	5	1531	G
1	5	1532	G
1	5	1533	C
1	5	1534	C
1	5	1536	A
1	5	1537	A
1	5	1539	U
1	5	1540	U
1	5	1542	C
1	5	1544	A
1	5	1545	G
1	5	1546	G
1	5	1547	C
1	5	1549	A
1	5	1550	C

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Mol	Chain	Res	Type
1	5	1551	C
1	5	1552	A
1	5	1555	G
1	5	1558	A
1	5	1559	G
1	5	1565	C
1	5	1576	U
1	5	1577	C
1	5	1584	C
1	5	1589	U
1	5	1597	C
1	5	1598	U
1	5	1599	U
1	5	1600	C
1	5	1601	A
1	5	1602	C
1	5	1608	C
1	5	1611	A
1	5	1612	A
1	5	1613	C
1	5	1614	U
1	5	1615	G
1	5	1624	G
1	5	1625	A
1	5	1627	G
1	5	1642	G
1	5	1644	G
1	5	1646	G
1	5	1652	A
1	5	1656	U
1	5	1657	U
1	5	1658	U
1	5	1671	U
1	5	1673	A
1	5	1684	A
1	5	1685	U
1	5	1686	U
1	5	1693	U
1	5	1694	C
1	5	1700	A
1	5	1710	A
1	5	1719	A

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Mol	Chain	Res	Type
1	5	1720	G
1	5	1725	C
1	5	1729	C
1	5	1731	U
1	5	1733	G
1	5	1734	U
1	5	1735	G
1	5	1739	G
1	5	1744	G
1	5	1747	G
1	5	1748	C
1	5	1749	G
1	5	1755	G
1	5	1763	U
1	5	1766	A
1	5	1777	G
1	5	1780	G
1	5	1781	G
1	5	1782	A
1	5	1783	A
1	5	1785	A
1	5	1786	G
1	5	1787	U
1	5	1789	U
1	5	1790	U
1	5	1792	A
1	5	1807	G
1	5	1808	A
1	5	1809	U
1	5	1810	A
1	5	1811	A
1	5	1815	C
1	5	1816	A
1	5	1818	C
1	5	1819	A
1	5	1823	C
1	5	1824	U
1	5	1828	A
1	5	1835	C
1	5	1836	A
1	5	1837	G
1	5	1840	U

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Mol	Chain	Res	Type
1	5	1845	U
1	5	1849	U
1	5	1850	A
1	5	1855	A
1	5	1859	U
1	5	1860	A
1	5	1862	A
1	5	1864	A
1	5	1865	A
1	5	1866	G
1	5	1870	A
1	5	1875	G
1	5	1878	A
1	5	1896	G
1	5	1917	G
1	5	1922	G
1	5	1923	G
1	5	1924	C
1	5	1925	G
1	5	1926	U
1	5	1928	A
1	5	1929	G
1	5	1941	G
1	5	1943	C
1	5	2025	G
1	5	2027	C
1	5	2032	U
1	5	2033	U
1	5	2036	U
1	5	2038	G
1	5	2041	C
1	5	2042	U
1	5	2046	G
1	5	2049	G
1	5	2050	A
1	5	2051	U
1	5	2052	G
1	5	2053	C
1	5	2054	U
1	5	2055	G
1	5	2057	A
1	5	2059	U

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Mol	Chain	Res	Type
1	5	2061	A
1	5	2062	A
1	5	2063	C
1	5	2064	G
1	5	2065	A
1	5	2069	A
1	5	2070	C
1	5	2071	U
1	5	2073	A
1	5	2080	G
1	5	2081	U
1	5	2082	A
1	5	2083	C
1	5	2087	C
1	5	2090	G
1	5	2091	G
1	5	2095	A
1	5	2100	A
1	5	2107	A
1	5	2108	A
1	5	2113	A
1	5	2114	A
1	5	2126	G
1	5	2127	A
1	5	2138	G
1	5	2139	U
1	5	2140	G
1	5	2155	U
1	5	2161	C
1	5	2165	C
1	5	2166	C
1	5	2169	U
1	5	2170	G
1	5	2173	C
1	5	2174	U
1	5	2175	G
1	5	2182	A
1	5	2191	A
1	5	2194	U
1	5	2198	A
1	5	2201	A
1	5	2213	A

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Mol	Chain	Res	Type
1	5	2217	C
1	5	2218	G
1	5	2219	G
1	5	2220	G
1	5	2221	A
1	5	2222	G
1	5	2223	U
1	5	2225	A
1	5	2226	C
1	5	2227	U
1	5	2228	A
1	5	2229	U
1	5	2230	G
1	5	2233	U
1	5	2235	U
1	5	2236	C
1	5	2237	U
1	5	2238	U
1	5	2239	A
1	5	2241	G
1	5	2242	G
1	5	2243	U
1	5	2245	G
1	5	2250	A
1	5	2251	U
1	5	2252	G
1	5	2257	G
1	5	2262	C
1	5	2263	U
1	5	2267	U
1	5	2275	C
1	5	2276	G
1	5	2277	C
1	5	2278	A
1	5	2279	U
1	5	2282	A
1	5	2284	G
1	5	2285	G
1	5	2288	U
1	5	2300	C
1	5	2301	A
1	5	2303	U

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Mol	Chain	Res	Type
1	5	2304	G
1	5	2305	U
1	5	2316	U
1	5	2336	A
1	5	2341	A
1	5	2342	A
1	5	2343	C
1	5	2344	G
1	5	2346	G
1	5	2347	C
1	5	2352	C
1	5	2354	G
1	5	2357	U
1	5	2358	C
1	5	2362	G
1	5	2366	A
1	5	2367	A
1	5	2369	G
1	5	2370	A
1	5	2371	A
1	5	2372	G
1	5	2373	A
1	5	2374	C
1	5	2380	U
1	5	2381	G
1	5	2387	G
1	5	2388	A
1	5	2390	U
1	5	2404	G
1	5	2407	A
1	5	2408	A
1	5	2412	A
1	5	2413	C
1	5	2414	A
1	5	2415	U
1	5	2416	A
1	5	2417	G
1	5	2418	A
1	5	2421	G
1	5	2422	U
1	5	2423	G
1	5	2427	C

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Mol	Chain	Res	Type
1	5	2428	A
1	5	2429	U
1	5	2430	A
1	5	2431	A
1	5	2432	G
1	5	2434	G
1	5	2438	G
1	5	2446	G
1	5	2451	U
1	5	2456	U
1	5	2457	A
1	5	2460	A
1	5	2461	C
1	5	2468	U
1	5	2469	A
1	5	2470	U
1	5	2471	A
1	5	2472	G
1	5	2473	U
1	5	2474	U
1	5	2475	U
1	5	2476	C
1	5	2479	U
1	5	2480	A
1	5	2481	C
1	5	2482	U
1	5	2483	U
1	5	2484	A
1	5	2491	U
1	5	2492	A
1	5	2493	A
1	5	2494	G
1	5	2495	C
1	5	2499	G
1	5	2500	C
1	5	2501	U
1	5	2502	G
1	5	2503	G
1	5	2506	U
1	5	2507	U
1	5	2508	C
1	5	2509	A

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Mol	Chain	Res	Type
1	5	2510	U
1	5	2511	U
1	5	2512	U
1	5	2517	C
1	5	2520	U
1	5	2521	C
1	5	2524	G
1	5	2526	A
1	5	2529	C
1	5	2530	A
1	5	2531	A
1	5	2537	U
1	5	2538	A
1	5	2540	A
1	5	2541	C
1	5	2542	G
1	5	2543	G
1	5	2547	G
1	5	2549	U
1	5	2553	G
1	5	2557	G
1	5	2561	A
1	5	2562	C
1	5	2568	C
1	5	2574	G
1	5	2575	G
1	5	2582	G
1	5	2587	G
1	5	2596	A
1	5	2604	A
1	5	2606	C
1	5	2609	U
1	5	2617	A
1	5	2620	U
1	5	2624	A
1	5	2625	A
1	5	2626	G
1	5	2630	G
1	5	2631	A
1	5	2635	A
1	5	2642	A
1	5	2646	A

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Mol	Chain	Res	Type
1	5	2647	A
1	5	2649	U
1	5	2657	A
1	5	2658	G
1	5	2659	A
1	5	2662	A
1	5	2664	A
1	5	2672	A
1	5	2682	G
1	5	2687	U
1	5	2688	G
1	5	2696	G
1	5	2697	U
1	5	2708	A
1	5	2715	A
1	5	2717	G
1	5	2720	U
1	5	2721	G
1	5	2722	G
1	5	2723	C
1	5	2726	A
1	5	2730	A
1	5	2739	G
1	5	2740	U
1	5	2741	C
1	5	2745	G
1	5	2746	G
1	5	2747	A
1	5	2764	G
1	5	2767	A
1	5	2768	G
1	5	2769	A
1	5	2770	A
1	5	2771	A
1	5	2778	C
1	5	2782	G
1	5	2784	G
1	5	2785	A
1	5	2786	U
1	5	2807	G
1	5	2811	U
1	5	2813	A

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Mol	Chain	Res	Type
1	5	2815	A
1	5	2818	G
1	5	2821	A
1	5	2824	G
1	5	2828	U
1	5	2829	U
1	5	2839	G
1	5	2840	A
1	5	2841	U
1	5	2843	U
1	5	2845	G
1	5	2848	U
1	5	2855	A
1	5	2857	C
1	5	2860	A
1	5	2864	A
1	5	2866	G
1	5	2867	C
1	5	2869	G
1	5	2872	U
1	5	2878	A
1	5	2880	G
1	5	2882	G
1	5	2886	G
1	5	2890	G
1	5	2891	U
1	5	2895	C
1	5	2903	U
1	5	2904	A
1	5	2906	G
1	5	2910	C
1	5	2915	G
1	5	2922	U
1	5	2923	U
1	5	2925	G
1	5	2936	G
1	5	2939	A
1	5	2940	G
1	5	2947	U
1	5	2948	U
1	5	2951	C
1	5	2955	A

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Mol	Chain	Res	Type
1	5	2958	G
1	5	2964	U
1	5	2965	G
1	5	2980	A
1	5	2989	A
1	5	2991	U
1	5	2996	G
1	5	2998	G
1	5	3008	A
1	5	3017	A
1	5	3023	U
1	5	3024	U
1	5	3025	U
1	5	3026	U
1	5	3027	G
1	5	3040	C
1	5	3041	A
1	5	3042	G
1	5	3046	U
1	5	3047	U
1	5	3048	G
1	5	3054	A
1	5	3055	A
1	5	3059	A
1	5	3060	C
1	5	3062	A
1	5	3069	G
1	5	3072	U
1	5	3077	G
1	5	3083	C
1	5	3090	A
1	5	3093	U
1	5	3098	A
1	5	3099	U
1	5	3110	A
1	5	3113	C
1	5	3119	U
1	5	3121	U
1	5	3122	C
1	5	3123	U
1	5	3124	U
1	5	3125	U

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Mol	Chain	Res	Type
1	5	3126	G
1	5	3133	A
1	5	3136	A
1	5	3138	A
1	5	3139	U
1	5	3140	A
1	5	3141	G
1	5	3142	A
1	5	3143	A
1	5	3144	G
1	5	3147	U
1	5	3149	A
1	5	3152	A
1	5	3155	A
1	5	3161	C
1	5	3163	U
1	5	3164	U
1	5	3165	U
1	5	3175	U
1	5	3176	G
1	5	3185	C
1	5	3186	A
1	5	3187	G
1	5	3188	G
1	5	3195	A
1	5	3197	G
1	5	3203	C
1	5	3206	A
1	5	3207	G
1	5	3208	C
1	5	3210	G
1	5	3211	A
1	5	3212	A
1	5	3213	A
1	5	3214	G
1	5	3215	G
1	5	3217	U
1	5	3220	G
1	5	3221	G
1	5	3227	U
1	5	3231	G
1	5	3233	C

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Mol	Chain	Res	Type
1	5	3236	A
1	5	3238	U
1	5	3241	A
1	5	3243	U
1	5	3244	G
1	5	3245	U
1	5	3246	C
1	5	3247	A
1	5	3249	U
1	5	3250	U
1	5	3253	C
1	5	3254	G
1	5	3257	A
1	5	3258	G
1	5	3262	A
1	5	3263	A
1	5	3272	U
1	5	3273	A
1	5	3275	A
1	5	3281	U
1	5	3284	A
1	5	3285	U
1	5	3286	G
1	5	3287	U
1	5	3291	A
1	5	3299	U
1	5	3303	A
1	5	3309	U
1	5	3310	A
1	5	3313	G
1	5	3316	G
1	5	3319	U
1	5	3322	U
1	5	3324	G
1	5	3326	U
1	5	3336	U
1	5	3337	G
1	5	3346	C
1	5	3350	C
1	5	3351	G
1	5	3354	G
1	5	3357	U

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Mol	Chain	Res	Type
1	5	3358	G
1	5	3360	U
1	5	3364	U
2	7	6	C
2	7	13	A
2	7	22	A
2	7	38	U
2	7	41	G
2	7	50	U
2	7	51	A
2	7	52	G
2	7	54	U
2	7	65	G
2	7	73	C
2	7	74	C
2	7	76	A
2	7	77	G
2	7	91	G
2	7	93	C
2	7	99	G
2	7	101	G
2	7	102	A
2	7	104	A
2	7	112	G
2	7	121	U
3	8	2	A
3	8	7	U
3	8	8	C
3	8	13	A
3	8	21	C
3	8	23	U
3	8	25	G
3	8	34	U
3	8	35	C
3	8	38	U
3	8	47	C
3	8	48	A
3	8	51	G
3	8	59	A
3	8	62	U
3	8	63	G
3	8	79	A

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Mol	Chain	Res	Type
3	8	81	U
3	8	84	C
3	8	86	U
3	8	87	G
3	8	90	U
3	8	91	C
3	8	95	A
3	8	97	A
3	8	100	U
3	8	104	A
3	8	105	A
3	8	106	C
3	8	108	C
3	8	111	A
3	8	113	U
3	8	116	G
3	8	125	U
3	8	126	A
3	8	127	U
3	8	129	C
3	8	144	G
3	8	156	U
3	8	157	U
81	2	2	A
81	2	3	U
81	2	4	C
81	2	5	U
81	2	8	U
81	2	9	U
81	2	10	G
81	2	11	A
81	2	14	C
81	2	17	C
81	2	22	A
81	2	23	G
81	2	25	C
81	2	26	A
81	2	29	U
81	2	31	C
81	2	32	U
81	2	34	G
81	2	40	A

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Mol	Chain	Res	Type
81	2	42	G
81	2	45	U
81	2	47	A
81	2	50	C
81	2	51	A
81	2	57	G
81	2	58	U
81	2	61	A
81	2	62	A
81	2	63	G
81	2	64	U
81	2	65	A
81	2	67	A
81	2	68	A
81	2	69	G
81	2	71	A
81	2	72	A
81	2	73	U
81	2	74	U
81	2	75	U
81	2	76	A
81	2	77	U
81	2	78	A
81	2	80	A
81	2	81	G
81	2	93	A
81	2	104	A
81	2	107	C
81	2	111	U
81	2	113	U
81	2	114	C
81	2	115	G
81	2	124	A
81	2	125	U
81	2	126	A
81	2	127	G
81	2	129	U
81	2	130	C
81	2	131	C
81	2	132	U
81	2	133	U
81	2	134	U

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Mol	Chain	Res	Type
81	2	136	C
81	2	137	U
81	2	138	A
81	2	139	C
81	2	140	A
81	2	146	A
81	2	147	U
81	2	149	U
81	2	150	G
81	2	152	G
81	2	154	U
81	2	155	A
81	2	156	A
81	2	158	U
81	2	159	C
81	2	160	U
81	2	161	A
81	2	165	C
81	2	166	U
81	2	167	A
81	2	169	U
81	2	170	A
81	2	173	U
81	2	175	C
81	2	176	U
81	2	177	U
81	2	178	A
81	2	180	A
81	2	183	C
81	2	184	U
81	2	186	G
81	2	187	A
81	2	190	C
81	2	191	U
81	2	192	U
81	2	194	G
81	2	198	G
81	2	199	A
81	2	203	G
81	2	205	A
81	2	209	A
81	2	217	A

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Mol	Chain	Res	Type
81	2	218	A
81	2	220	A
81	2	224	A
81	2	225	A
81	2	226	U
81	2	228	U
81	2	230	U
81	2	232	C
81	2	233	G
81	2	234	G
81	2	239	C
81	2	240	U
81	2	241	U
81	2	249	C
81	2	253	A
81	2	256	A
81	2	259	U
81	2	260	U
81	2	264	A
81	2	265	A
81	2	266	U
81	2	274	C
81	2	275	C
81	2	276	U
81	2	277	U
81	2	278	G
81	2	279	U
81	2	280	G
81	2	286	G
81	2	288	U
81	2	289	G
81	2	294	A
81	2	298	A
81	2	301	U
81	2	305	U
81	2	308	C
81	2	311	A
81	2	312	U
81	2	313	C
81	2	314	A
81	2	315	A
81	2	319	U

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Mol	Chain	Res	Type
81	2	320	C
81	2	321	G
81	2	322	A
81	2	328	G
81	2	332	A
81	2	334	U
81	2	335	G
81	2	336	G
81	2	337	C
81	2	349	U
81	2	350	C
81	2	351	A
81	2	358	A
81	2	359	A
81	2	360	C
81	2	361	G
81	2	368	A
81	2	369	A
81	2	370	G
81	2	372	G
81	2	373	U
81	2	377	A
81	2	380	C
81	2	384	A
81	2	385	G
81	2	386	A
81	2	387	G
81	2	389	G
81	2	392	C
81	2	397	G
81	2	399	A
81	2	400	A
81	2	401	C
81	2	403	G
81	2	408	C
81	2	411	A
81	2	412	U
81	2	414	C
81	2	415	A
81	2	416	A
81	2	417	G
81	2	418	G

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Mol	Chain	Res	Type
81	2	421	G
81	2	423	C
81	2	424	A
81	2	425	G
81	2	433	G
81	2	436	A
81	2	438	U
81	2	439	U
81	2	440	A
81	2	443	C
81	2	444	A
81	2	447	C
81	2	452	U
81	2	453	U
81	2	454	C
81	2	455	A
81	2	458	G
81	2	459	A
81	2	460	G
81	2	463	A
81	2	467	A
81	2	468	C
81	2	474	A
81	2	475	U
81	2	476	A
81	2	479	G
81	2	480	A
81	2	483	C
81	2	490	C
81	2	491	A
81	2	492	U
81	2	493	U
81	2	494	C
81	2	497	G
81	2	499	C
81	2	500	U
81	2	503	U
81	2	504	A
81	2	505	A
81	2	506	U
81	2	507	U
81	2	509	G

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Mol	Chain	Res	Type
81	2	510	A
81	2	511	A
81	2	512	U
81	2	513	G
81	2	514	A
81	2	515	G
81	2	518	C
81	2	519	A
81	2	526	A
81	2	527	U
81	2	530	C
81	2	533	A
81	2	534	A
81	2	535	C
81	2	537	A
81	2	539	G
81	2	540	A
81	2	541	A
81	2	542	C
81	2	543	A
81	2	544	A
81	2	545	C
81	2	547	G
81	2	548	G
81	2	553	C
81	2	554	A
81	2	556	G
81	2	557	U
81	2	558	C
81	2	559	U
81	2	560	G
81	2	563	G
81	2	565	C
81	2	567	G
81	2	570	G
81	2	571	C
81	2	573	G
81	2	574	C
81	2	576	G
81	2	577	U
81	2	578	A
81	2	579	A

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Mol	Chain	Res	Type
81	2	581	U
81	2	582	C
81	2	593	A
81	2	594	G
81	2	596	G
81	2	600	A
81	2	605	A
81	2	606	G
81	2	607	U
81	2	609	G
81	2	610	U
81	2	613	C
81	2	615	G
81	2	618	A
81	2	619	A
81	2	622	A
81	2	623	G
81	2	634	A
81	2	637	U
81	2	638	U
81	2	639	U
81	2	640	G
81	2	642	G
81	2	647	G
81	2	648	U
81	2	649	U
81	2	652	C
81	2	653	C
81	2	654	G
81	2	655	G
81	2	677	G
81	2	678	U
81	2	679	U
81	2	683	C
81	2	684	A
81	2	691	U
81	2	694	U
81	2	695	U
81	2	696	C
81	2	697	C
81	2	698	U
81	2	701	U

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Mol	Chain	Res	Type
81	2	704	C
81	2	705	U
81	2	708	C
81	2	709	C
81	2	710	U
81	2	711	G
81	2	712	U
81	2	714	C
81	2	716	C
81	2	717	C
81	2	718	U
81	2	719	U
81	2	722	G
81	2	724	G
81	2	727	C
81	2	731	C
81	2	732	G
81	2	733	A
81	2	734	A
81	2	735	C
81	2	736	C
81	2	737	A
81	2	738	G
81	2	740	A
81	2	741	C
81	2	742	U
81	2	743	U
81	2	745	U
81	2	753	A
81	2	754	A
81	2	765	G
81	2	766	U
81	2	767	U
81	2	769	A
81	2	771	A
81	2	774	A
81	2	778	G
81	2	779	A
81	2	780	A
81	2	781	A
81	2	782	G
81	2	785	C

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Mol	Chain	Res	Type
81	2	786	G
81	2	787	A
81	2	788	A
81	2	789	U
81	2	791	U
81	2	792	A
81	2	793	U
81	2	794	U
81	2	795	A
81	2	800	G
81	2	802	A
81	2	809	G
81	2	810	A
81	2	811	A
81	2	812	U
81	2	813	A
81	2	814	G
81	2	815	G
81	2	817	C
81	2	819	U
81	2	820	U
81	2	821	U
81	2	822	G
81	2	823	G
81	2	825	U
81	2	826	C
81	2	828	A
81	2	829	U
81	2	830	U
81	2	831	U
81	2	832	U
81	2	834	U
81	2	837	G
81	2	840	U
81	2	842	U
81	2	845	G
81	2	848	C
81	2	849	A
81	2	851	C
81	2	852	G
81	2	855	A
81	2	859	U

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Mol	Chain	Res	Type
81	2	860	U
81	2	862	A
81	2	863	U
81	2	872	U
81	2	875	G
81	2	876	G
81	2	884	G
81	2	885	U
81	2	886	A
81	2	887	U
81	2	895	U
81	2	897	A
81	2	903	G
81	2	904	A
81	2	905	A
81	2	906	A
81	2	908	U
81	2	909	C
81	2	910	U
81	2	912	G
81	2	913	G
81	2	914	A
81	2	915	U
81	2	916	U
81	2	920	U
81	2	922	A
81	2	926	C
81	2	927	U
81	2	928	A
81	2	929	A
81	2	930	C
81	2	931	U
81	2	932	A
81	2	934	U
81	2	938	A
81	2	939	A
81	2	943	A
81	2	950	A
81	2	958	U
81	2	959	U
81	2	964	U
81	2	965	A

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Mol	Chain	Res	Type
81	2	969	A
81	2	972	A
81	2	980	U
81	2	981	U
81	2	982	A
81	2	983	G
81	2	985	G
81	2	987	A
81	2	990	G
81	2	991	A
81	2	992	A
81	2	993	G
81	2	999	C
81	2	1001	G
81	2	1002	A
81	2	1003	U
81	2	1004	A
81	2	1005	C
81	2	1009	C
81	2	1010	G
81	2	1011	U
81	2	1012	A
81	2	1013	G
81	2	1015	C
81	2	1018	A
81	2	1020	C
81	2	1024	A
81	2	1025	A
81	2	1026	A
81	2	1027	C
81	2	1028	U
81	2	1030	U
81	2	1031	G
81	2	1033	C
81	2	1035	A
81	2	1037	U
81	2	1038	A
81	2	1039	G
81	2	1041	G
81	2	1042	A
81	2	1044	C
81	2	1045	G

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Mol	Chain	Res	Type
81	2	1048	U
81	2	1050	G
81	2	1051	U
81	2	1052	G
81	2	1056	U
81	2	1057	U
81	2	1058	C
81	2	1059	U
81	2	1060	U
81	2	1063	G
81	2	1070	U
81	2	1071	C
81	2	1080	A
81	2	1081	C
81	2	1082	G
81	2	1083	A
81	2	1087	A
81	2	1090	A
81	2	1091	A
81	2	1092	A
81	2	1093	G
81	2	1094	U
81	2	1096	U
81	2	1097	U
81	2	1098	U
81	2	1099	G
81	2	1100	G
81	2	1102	U
81	2	1103	U
81	2	1104	C
81	2	1107	G
81	2	1108	G
81	2	1110	G
81	2	1113	G
81	2	1118	G
81	2	1121	G
81	2	1130	A
81	2	1137	A
81	2	1139	G
81	2	1142	A
81	2	1145	G
81	2	1149	G

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Mol	Chain	Res	Type
81	2	1150	A
81	2	1157	C
81	2	1158	C
81	2	1159	A
81	2	1162	A
81	2	1166	G
81	2	1184	U
81	2	1185	U
81	2	1193	A
81	2	1195	A
81	2	1196	C
81	2	1198	G
81	2	1199	G
81	2	1201	A
81	2	1202	A
81	2	1203	A
81	2	1204	C
81	2	1212	G
81	2	1213	U
81	2	1216	A
81	2	1217	G
81	2	1218	A
81	2	1219	C
81	2	1222	A
81	2	1226	A
81	2	1227	G
81	2	1228	G
81	2	1229	A
81	2	1230	U
81	2	1234	C
81	2	1236	G
81	2	1238	U
81	2	1240	G
81	2	1241	A
81	2	1242	G
81	2	1243	A
81	2	1244	G
81	2	1245	C
81	2	1247	C
81	2	1250	U
81	2	1253	U
81	2	1254	G

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Mol	Chain	Res	Type
81	2	1258	U
81	2	1259	U
81	2	1265	U
81	2	1268	U
81	2	1269	G
81	2	1272	G
81	2	1274	A
81	2	1282	U
81	2	1284	U
81	2	1292	U
81	2	1294	G
81	2	1296	G
81	2	1300	U
81	2	1306	U
81	2	1310	U
81	2	1311	A
81	2	1313	U
81	2	1314	U
81	2	1315	G
81	2	1316	C
81	2	1319	U
81	2	1320	A
81	2	1321	A
81	2	1322	C
81	2	1324	A
81	2	1336	A
81	2	1337	C
81	2	1339	U
81	2	1340	A
81	2	1343	A
81	2	1344	A
81	2	1345	A
81	2	1347	A
81	2	1349	G
81	2	1353	G
81	2	1356	G
81	2	1358	C
81	2	1359	A
81	2	1360	C
81	2	1361	U
81	2	1362	U
81	2	1363	G

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Mol	Chain	Res	Type
81	2	1364	C
81	2	1366	G
81	2	1369	U
81	2	1370	G
81	2	1371	A
81	2	1380	A
81	2	1386	A
81	2	1387	C
81	2	1388	U
81	2	1393	G
81	2	1396	U
81	2	1397	C
81	2	1398	A
81	2	1400	G
81	2	1410	G
81	2	1411	U
81	2	1412	U
81	2	1413	U
81	2	1416	G
81	2	1417	G
81	2	1423	A
81	2	1425	A
81	2	1426	G
81	2	1429	C
81	2	1430	U
81	2	1432	U
81	2	1433	G
81	2	1434	A
81	2	1438	C
81	2	1439	C
81	2	1442	A
81	2	1443	G
81	2	1444	A
81	2	1445	C
81	2	1446	G
81	2	1447	U
81	2	1449	C
81	2	1450	U
81	2	1452	G
81	2	1454	C
81	2	1455	C
81	2	1456	G

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Mol	Chain	Res	Type
81	2	1457	C
81	2	1458	A
81	2	1459	C
81	2	1461	C
81	2	1464	G
81	2	1467	A
81	2	1468	C
81	2	1469	A
81	2	1470	C
81	2	1471	U
81	2	1475	G
81	2	1476	G
81	2	1481	A
81	2	1484	G
81	2	1485	A
81	2	1487	U
81	2	1488	A
81	2	1489	C
81	2	1490	A
81	2	1491	A
81	2	1492	C
81	2	1494	U
81	2	1495	U
81	2	1498	C
81	2	1502	G
81	2	1506	U
81	2	1507	C
81	2	1508	U
81	2	1509	G
81	2	1512	U
81	2	1513	A
81	2	1514	A
81	2	1515	U
81	2	1516	C
81	2	1519	G
81	2	1521	G
81	2	1522	A
81	2	1525	C
81	2	1532	G
81	2	1533	U
81	2	1534	G
81	2	1535	C

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Mol	Chain	Res	Type
81	2	1537	G
81	2	1540	G
81	2	1543	A
81	2	1552	U
81	2	1553	A
81	2	1554	A
81	2	1555	U
81	2	1556	U
81	2	1557	A
81	2	1566	C
81	2	1569	C
81	2	1570	G
81	2	1571	A
81	2	1580	U
81	2	1583	U
81	2	1594	C
81	2	1595	A
81	2	1597	C
81	2	1598	A
81	2	1599	G
81	2	1602	U
81	2	1611	U
81	2	1614	G
81	2	1616	C
81	2	1617	C
81	2	1623	C
81	2	1626	U
81	2	1629	A
81	2	1630	C
81	2	1632	C
81	2	1633	A
81	2	1635	C
81	2	1640	G
81	2	1648	U
81	2	1654	U
81	2	1655	U
81	2	1656	G
81	2	1667	U
81	2	1678	G
81	2	1679	A
81	2	1680	U
81	2	1682	U

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Mol	Chain	Res	Type
81	2	1685	U
81	2	1686	U
81	2	1687	A
81	2	1688	G
81	2	1692	A
81	2	1693	G
81	2	1694	G
81	2	1696	G
81	2	1697	G
81	2	1698	C
81	2	1699	A
81	2	1700	A
81	2	1701	C
81	2	1702	U
81	2	1703	C
81	2	1706	U
81	2	1707	C
81	2	1708	U
81	2	1709	C
81	2	1710	A
81	2	1711	G
81	2	1712	A
81	2	1725	G
81	2	1729	A
81	2	1733	U
81	2	1737	C
81	2	1740	U
81	2	1743	G
81	2	1744	A
81	2	1745	G
81	2	1748	A
81	2	1751	A
81	2	1752	A
81	2	1753	A
81	2	1754	A
81	2	1755	G
81	2	1758	G
81	2	1759	U
81	2	1760	A
81	2	1763	A
81	2	1764	A
81	2	1766	G

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Mol	Chain	Res	Type
81	2	1767	U
81	2	1770	C
81	2	1777	U
81	2	1778	G
81	2	1779	A
81	2	1780	A
81	2	1781	C
81	2	1789	A
81	2	1790	G
81	2	1791	G
81	2	1792	A
81	2	1793	U
81	2	1794	C
81	2	1796	U
81	2	1798	A
82	4	6038	G
82	4	6039	A
82	4	6042	U
82	4	6044	G
82	4	6048	G
82	4	6054	A
82	4	6055	C
82	4	6056	A
82	4	6059	U
82	4	6060	U
82	4	6061	U
82	4	6067	G
82	4	6068	U
82	4	6069	U
82	4	6071	A
82	4	6072	U
82	4	6073	A
82	4	6074	A
82	4	6086	U
82	4	6088	C
82	4	6089	U
82	4	6090	A
82	4	6098	A
82	4	6101	U
82	4	6106	U
82	4	6107	A
82	4	6108	G

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Mol	Chain	Res	Type
82	4	6113	U
82	4	6116	G
82	4	6117	C
82	4	6118	U
82	4	6119	U
82	4	6120	U
82	4	6121	A
82	4	6122	C
82	4	6123	G
82	4	6124	U
82	4	6125	U
82	4	6126	C
82	4	6127	C
82	4	6128	A
82	4	6129	G
82	4	6130	G
82	4	6133	G
82	4	6134	C
82	4	6135	C
82	4	6137	A
82	4	6138	G
82	4	6140	G
82	4	6142	C
82	4	6144	G
82	4	6145	C
82	4	6146	C
82	4	6147	C
82	4	6148	C
82	4	6153	U
82	4	6158	A
82	4	6164	C
82	4	6165	C
82	4	6166	C
82	4	6168	C
82	4	6170	C
82	4	6172	A
82	4	6173	C
82	4	6175	G
82	4	6176	U
82	4	6177	U
82	4	6179	U
82	4	6180	U

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Mol	Chain	Res	Type
82	4	6181	C
82	4	6182	A
82	4	6183	G
82	4	6189	G
82	4	6192	G
82	4	6194	C
82	4	6195	G
82	4	6196	A
82	4	6197	A
82	4	6199	A
82	4	6200	A
82	4	6201	C
82	4	6202	C
82	4	6203	U
82	4	6204	A
82	4	6211	U
82	4	6212	U
82	4	6213	A
82	4	6217	G
82	4	6218	C
82	4	6219	U

All (359) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	43	A
1	5	65	A
1	5	66	A
1	5	99	A
1	5	112	U
1	5	119	U
1	5	121	A
1	5	156	A
1	5	166	C
1	5	210	U
1	5	217	U
1	5	238	A
1	5	282	G
1	5	283	G
1	5	297	G
1	5	298	U
1	5	420	G

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Mol	Chain	Res	Type
1	5	436	A
1	5	489	G
1	5	518	C
1	5	529	U
1	5	555	G
1	5	561	G
1	5	562	A
1	5	580	A
1	5	593	U
1	5	596	U
1	5	598	G
1	5	609	C
1	5	707	A
1	5	735	U
1	5	736	C
1	5	737	U
1	5	741	G
1	5	757	A
1	5	787	A
1	5	844	C
1	5	859	A
1	5	860	U
1	5	867	A
1	5	887	G
1	5	908	G
1	5	950	U
1	5	952	U
1	5	964	G
1	5	985	U
1	5	987	C
1	5	998	A
1	5	1004	U
1	5	1035	A
1	5	1052	U
1	5	1065	U
1	5	1068	G
1	5	1115	U
1	5	1155	A
1	5	1167	C
1	5	1179	U
1	5	1193	G
1	5	1196	A

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Mol	Chain	Res	Type
1	5	1209	C
1	5	1212	U
1	5	1233	G
1	5	1255	C
1	5	1257	A
1	5	1278	G
1	5	1300	U
1	5	1316	G
1	5	1323	A
1	5	1326	A
1	5	1390	A
1	5	1403	C
1	5	1421	G
1	5	1452	A
1	5	1496	G
1	5	1525	U
1	5	1531	G
1	5	1539	U
1	5	1549	A
1	5	1558	A
1	5	1575	U
1	5	1576	U
1	5	1598	U
1	5	1600	C
1	5	1610	U
1	5	1685	U
1	5	1693	U
1	5	1719	A
1	5	1747	G
1	5	1777	G
1	5	1785	A
1	5	1788	U
1	5	1815	C
1	5	1816	A
1	5	1827	A
1	5	1848	A
1	5	1922	G
1	5	1924	C
1	5	1925	G
1	5	2032	U
1	5	2040	U
1	5	2041	C

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Mol	Chain	Res	Type
1	5	2050	A
1	5	2051	U
1	5	2052	G
1	5	2058	A
1	5	2062	A
1	5	2070	C
1	5	2079	G
1	5	2081	U
1	5	2107	A
1	5	2113	A
1	5	2166	C
1	5	2173	C
1	5	2218	G
1	5	2219	G
1	5	2228	A
1	5	2235	U
1	5	2236	C
1	5	2237	U
1	5	2238	U
1	5	2249	A
1	5	2250	A
1	5	2252	G
1	5	2274	G
1	5	2276	G
1	5	2278	A
1	5	2284	G
1	5	2285	G
1	5	2341	A
1	5	2343	C
1	5	2346	G
1	5	2369	G
1	5	2416	A
1	5	2417	G
1	5	2422	U
1	5	2429	U
1	5	2437	A
1	5	2455	A
1	5	2456	U
1	5	2468	U
1	5	2469	A
1	5	2481	C
1	5	2482	U

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Mol	Chain	Res	Type
1	5	2491	U
1	5	2507	U
1	5	2518	G
1	5	2529	C
1	5	2530	A
1	5	2539	U
1	5	2540	A
1	5	2553	G
1	5	2561	A
1	5	2586	G
1	5	2630	G
1	5	2645	G
1	5	2648	A
1	5	2657	A
1	5	2696	G
1	5	2722	G
1	5	2739	G
1	5	2740	U
1	5	2745	G
1	5	2769	A
1	5	2785	A
1	5	2786	U
1	5	2840	A
1	5	2854	U
1	5	2866	G
1	5	2890	G
1	5	2918	G
1	5	2922	U
1	5	2939	A
1	5	3023	U
1	5	3024	U
1	5	3046	U
1	5	3061	C
1	5	3122	C
1	5	3125	U
1	5	3135	A
1	5	3140	A
1	5	3163	U
1	5	3164	U
1	5	3186	A
1	5	3196	C
1	5	3207	G

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Mol	Chain	Res	Type
1	5	3214	G
1	5	3220	G
1	5	3237	U
1	5	3242	A
1	5	3245	U
1	5	3248	U
1	5	3257	A
1	5	3261	U
1	5	3284	A
1	5	3285	U
1	5	3308	G
1	5	3309	U
1	5	3325	U
2	7	13	A
2	7	49	G
2	7	76	A
2	7	111	U
3	8	7	U
3	8	8	C
3	8	34	U
3	8	79	A
3	8	81	U
3	8	126	A
81	2	2	A
81	2	3	U
81	2	8	U
81	2	10	G
81	2	11	A
81	2	45	U
81	2	66	U
81	2	72	A
81	2	73	U
81	2	114	C
81	2	129	U
81	2	130	C
81	2	131	C
81	2	133	U
81	2	177	U
81	2	186	G
81	2	209	A
81	2	216	A
81	2	217	A

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Mol	Chain	Res	Type
81	2	239	C
81	2	248	U
81	2	258	U
81	2	265	A
81	2	277	U
81	2	279	U
81	2	314	A
81	2	321	G
81	2	336	G
81	2	368	A
81	2	398	A
81	2	399	A
81	2	415	A
81	2	439	U
81	2	451	A
81	2	452	U
81	2	454	C
81	2	473	A
81	2	497	G
81	2	509	G
81	2	542	C
81	2	556	G
81	2	557	U
81	2	563	G
81	2	564	C
81	2	570	G
81	2	576	G
81	2	577	U
81	2	605	A
81	2	621	A
81	2	628	U
81	2	638	U
81	2	695	U
81	2	700	C
81	2	704	C
81	2	708	C
81	2	710	U
81	2	719	U
81	2	721	U
81	2	740	A
81	2	766	U
81	2	779	A

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Mol	Chain	Res	Type
81	2	792	A
81	2	794	U
81	2	809	G
81	2	811	A
81	2	826	C
81	2	828	A
81	2	854	A
81	2	884	G
81	2	885	U
81	2	886	A
81	2	909	C
81	2	912	G
81	2	913	G
81	2	927	U
81	2	929	A
81	2	930	C
81	2	931	U
81	2	963	U
81	2	990	G
81	2	1002	A
81	2	1003	U
81	2	1010	G
81	2	1027	C
81	2	1033	C
81	2	1034	G
81	2	1044	C
81	2	1056	U
81	2	1060	U
81	2	1080	A
81	2	1090	A
81	2	1098	U
81	2	1107	G
81	2	1157	C
81	2	1195	A
81	2	1243	A
81	2	1286	A
81	2	1292	U
81	2	1320	A
81	2	1343	A
81	2	1386	A
81	2	1412	U
81	2	1442	A

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Mol	Chain	Res	Type
81	2	1455	C
81	2	1470	C
81	2	1491	A
81	2	1501	A
81	2	1515	U
81	2	1532	G
81	2	1534	G
81	2	1556	U
81	2	1580	U
81	2	1598	A
81	2	1613	C
81	2	1628	U
81	2	1631	A
81	2	1632	C
81	2	1654	U
81	2	1655	U
81	2	1678	G
81	2	1724	G
81	2	1752	A
81	2	1759	U
81	2	1763	A
81	2	1765	G
81	2	1792	A
81	2	1795	A
82	4	6038	G
82	4	6106	U
82	4	6119	U
82	4	6120	U
82	4	6122	C
82	4	6124	U
82	4	6127	C
82	4	6133	G
82	4	6134	C
82	4	6137	A
82	4	6144	G
82	4	6165	C
82	4	6172	A
82	4	6174	G
82	4	6177	U
82	4	6181	C
82	4	6194	C
82	4	6195	G

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Mol	Chain	Res	Type
82	4	6196	A
82	4	6200	A
82	4	6201	C
82	4	6203	U
82	4	6211	U
82	4	6218	C

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 88 ligands modelled in this entry, 86 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
86	GCP	1	902	84	27,34,34	1.84	6 (22%)	34,54,54	2.10	9 (26%)
87	6EM	1	903	83	7,9,9	1.03	1 (14%)	9,13,13	2.69	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	GCP	1	902	84	-	1/15/38/38	0/3/3/3
87	6EM	1	903	83	-	5/12/12/12	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	902	GCP	PG-O1G	5.77	1.62	1.50
86	1	902	GCP	C5-C6	4.10	1.48	1.41
86	1	902	GCP	PG-O3G	-3.23	1.47	1.54
86	1	902	GCP	PG-O2G	3.02	1.61	1.54
86	1	902	GCP	C5-C4	2.28	1.47	1.40
87	1	903	6EM	C3-C5	-2.11	1.50	1.53
86	1	902	GCP	PB-O2B	2.01	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
87	1	903	6EM	C3-C5-N7	5.32	122.06	115.28
86	1	902	GCP	C2-N3-C4	4.80	120.84	115.36
86	1	902	GCP	C4-C5-C6	-4.53	116.47	120.80
86	1	902	GCP	C2-N1-C6	4.30	122.76	115.93
86	1	902	GCP	PB-O3A-PA	-4.01	119.83	132.56
86	1	902	GCP	C5-C6-N1	-3.92	118.07	123.43
87	1	903	6EM	C9-N4-C3	3.86	120.13	110.51
86	1	902	GCP	N3-C2-N1	-3.78	122.19	127.22
87	1	903	6EM	O6-C5-C3	-3.71	115.79	120.49
86	1	902	GCP	C4-C5-N7	-2.78	106.51	109.40
86	1	902	GCP	O2G-PG-C3B	2.66	112.85	106.40
86	1	902	GCP	C3'-C2'-C1'	2.54	104.81	100.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

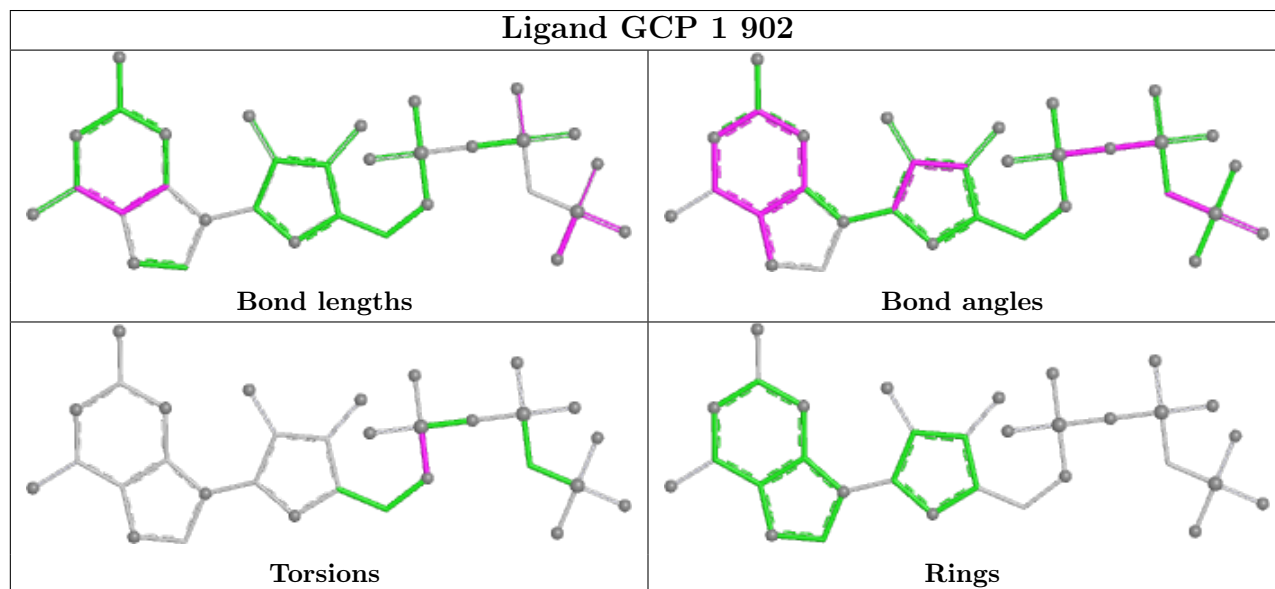
Mol	Chain	Res	Type	Atoms
86	1	902	GCP	C5'-O5'-PA-O1A
87	1	903	6EM	C1-C2-C3-C5
87	1	903	6EM	C1-C2-C3-N4
87	1	903	6EM	C2-C3-N4-C9
87	1	903	6EM	C2-C3-N4-C10
87	1	903	6EM	N4-C3-C5-N7

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	5	2
47	KK	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	443:G	O3'	466:G	P	31.65
1	5	1948:C	O3'	2019:G	P	17.88
1	KK	23:UNK	C	28:UNK	N	3.41

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	KK	52:UNK	C	54:UNK	N	3.29

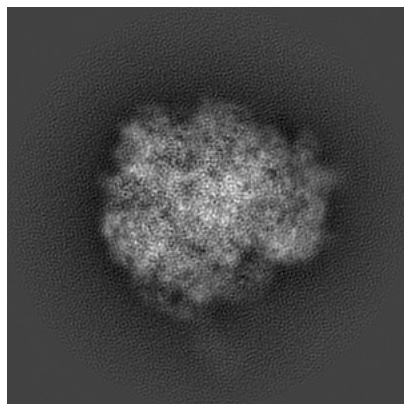
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8123. These allow visual inspection of the internal detail of the map and identification of artifacts.

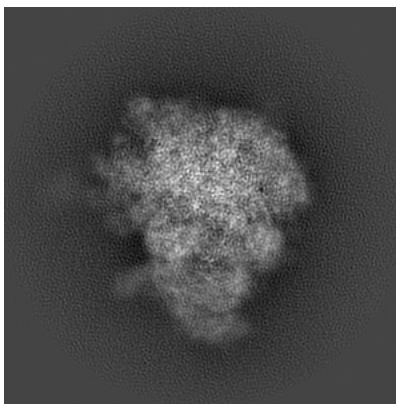
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

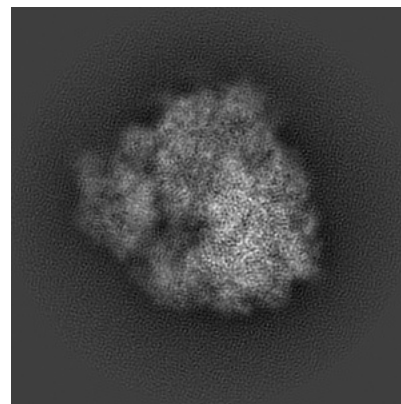
6.1.1 Primary map



X

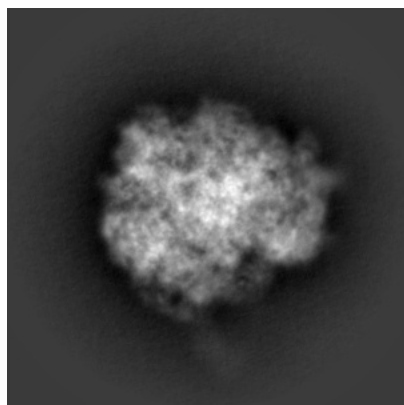


Y

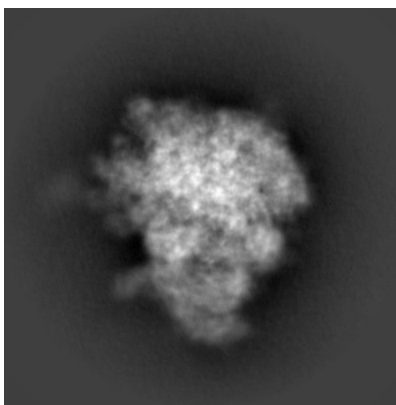


Z

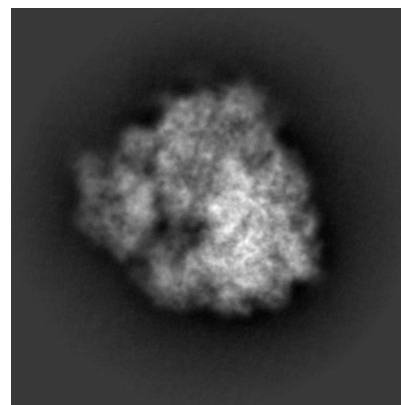
6.1.2 Raw map



X



Y

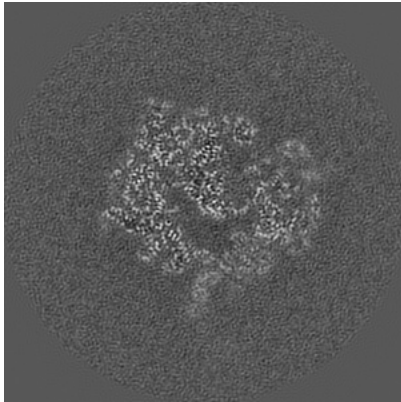


Z

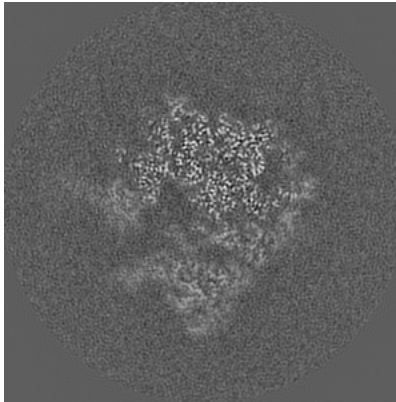
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

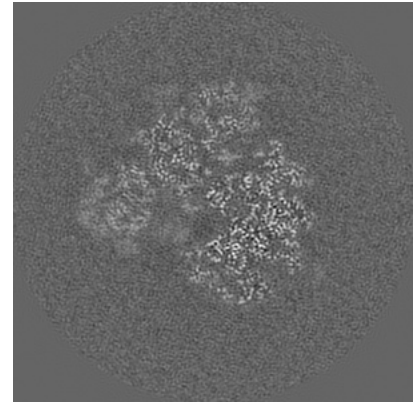
6.2.1 Primary map



X Index: 160

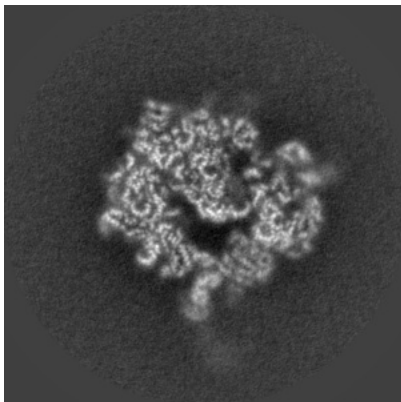


Y Index: 160

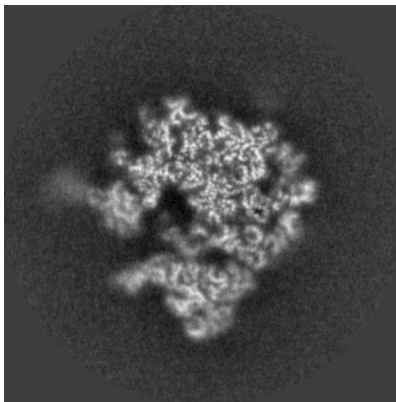


Z Index: 160

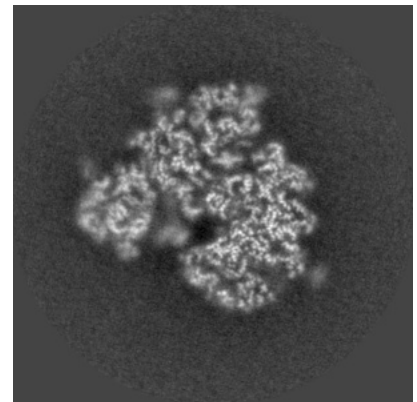
6.2.2 Raw map



X Index: 160



Y Index: 160

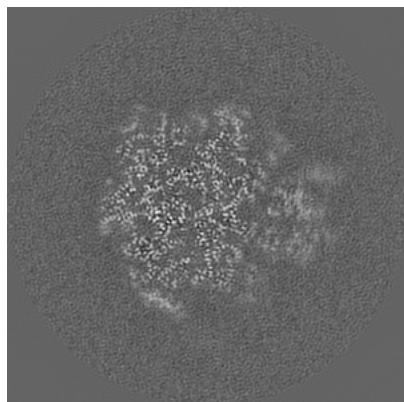


Z Index: 160

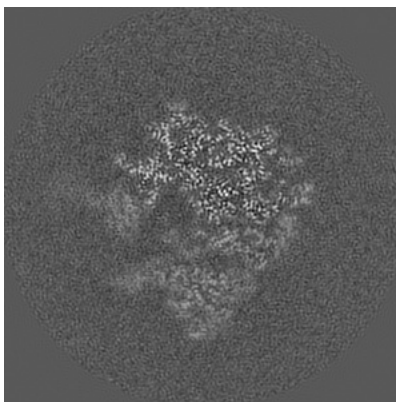
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

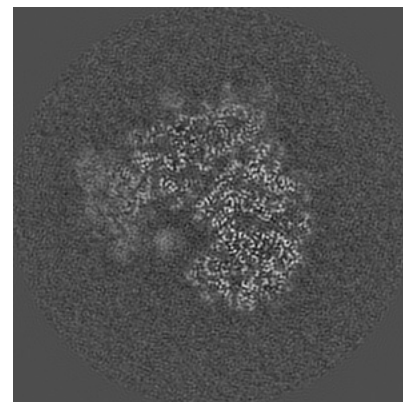
6.3.1 Primary map



X Index: 186

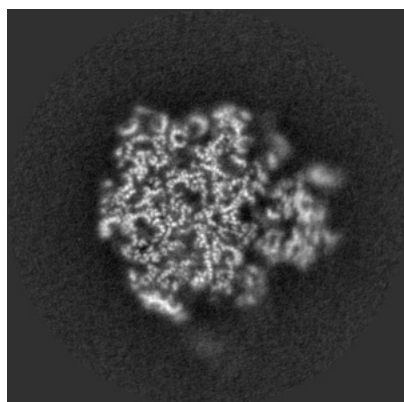


Y Index: 161

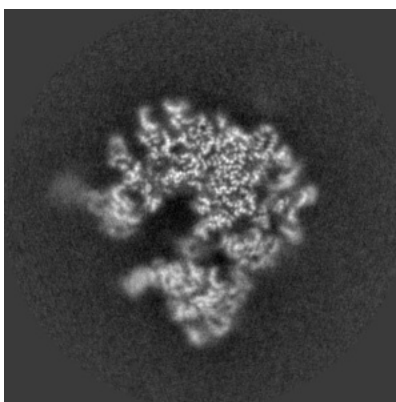


Z Index: 170

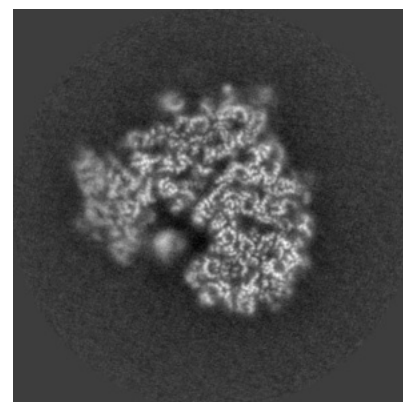
6.3.2 Raw map



X Index: 186



Y Index: 156

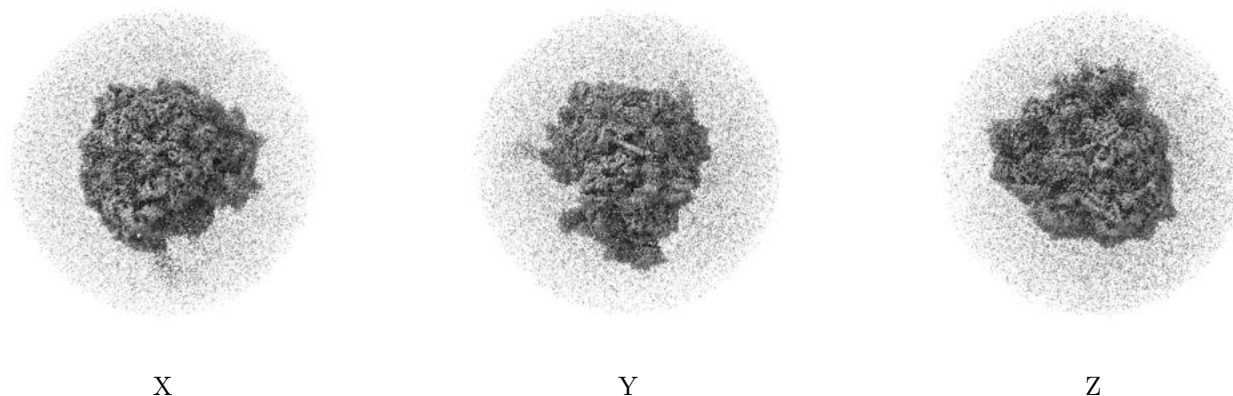


Z Index: 170

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

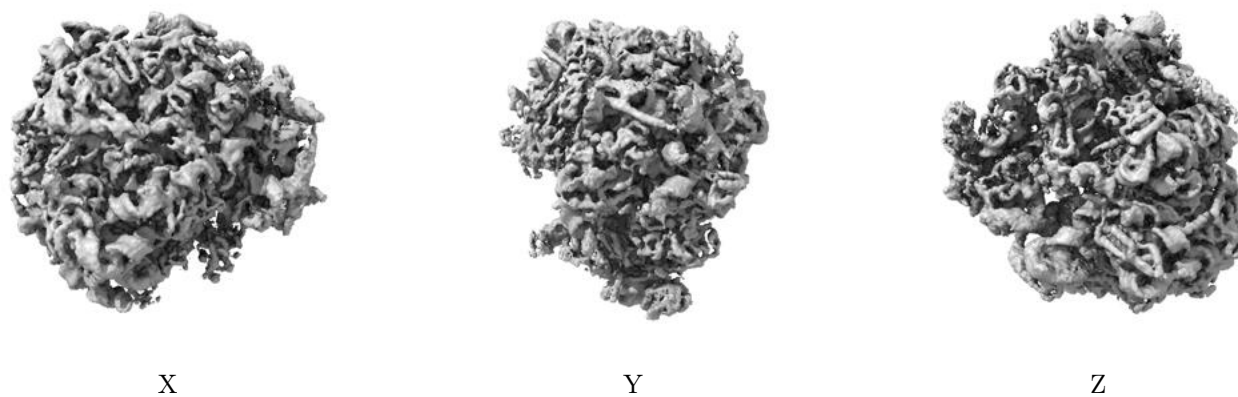
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

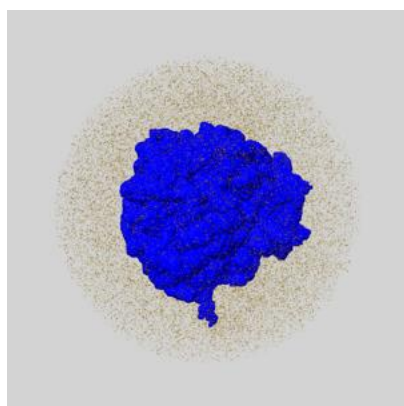
6.5 Mask visualisation [i](#)

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

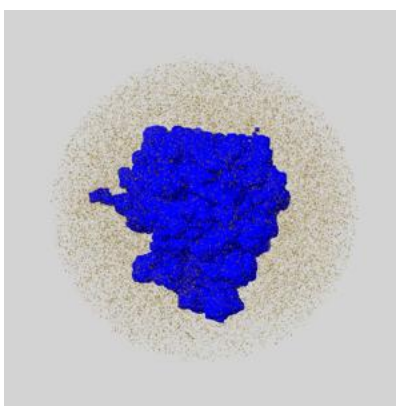
A mask typically either:

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

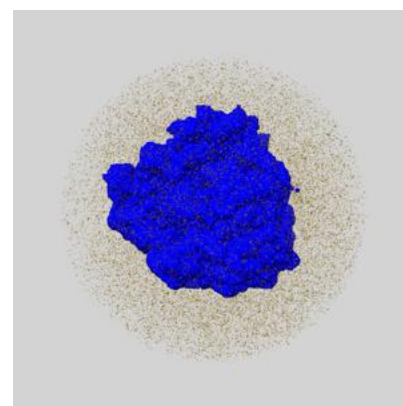
6.5.1 emd_8123_msk_1.map [i](#)



X



Y

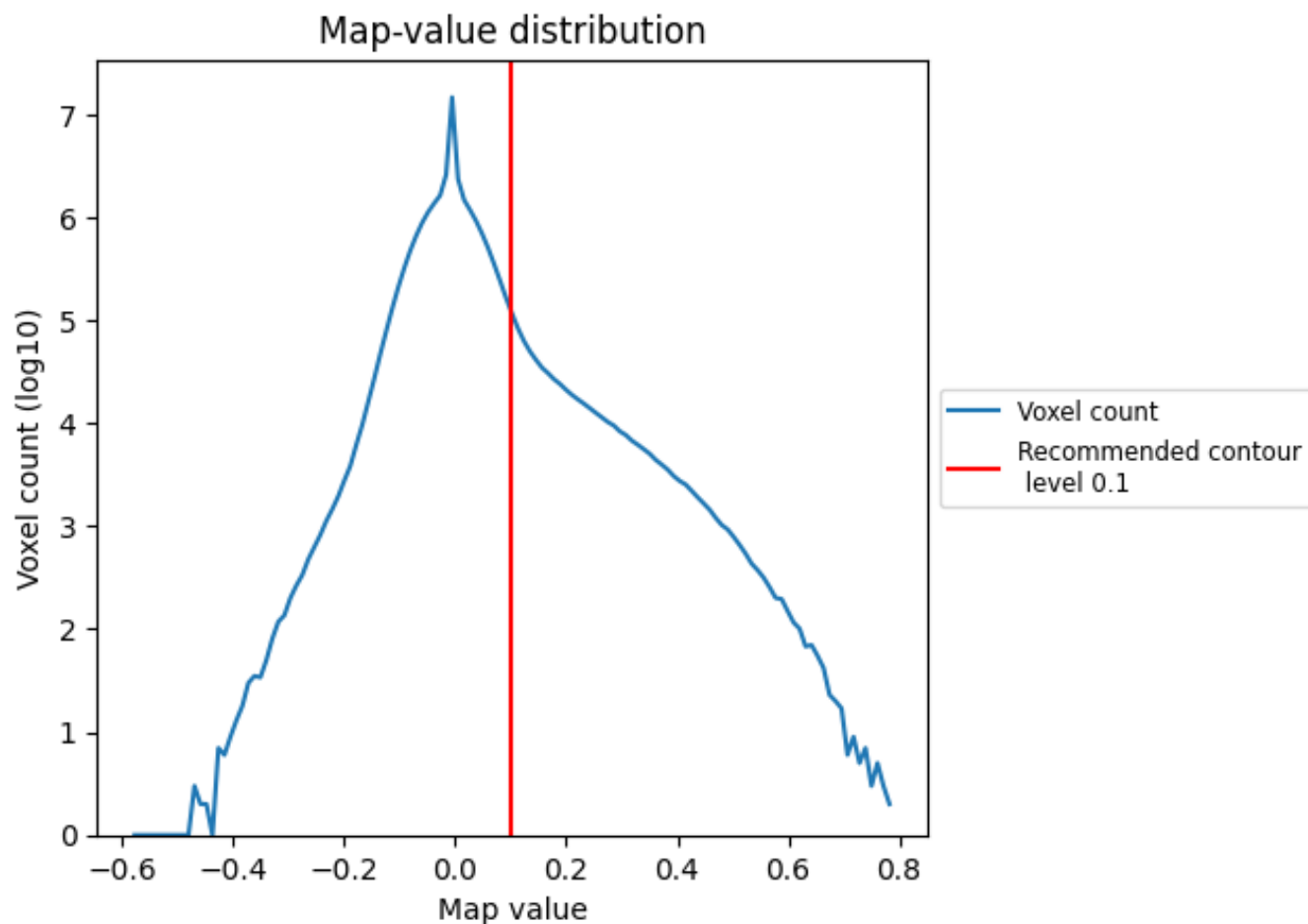


Z

7 Map analysis [i](#)

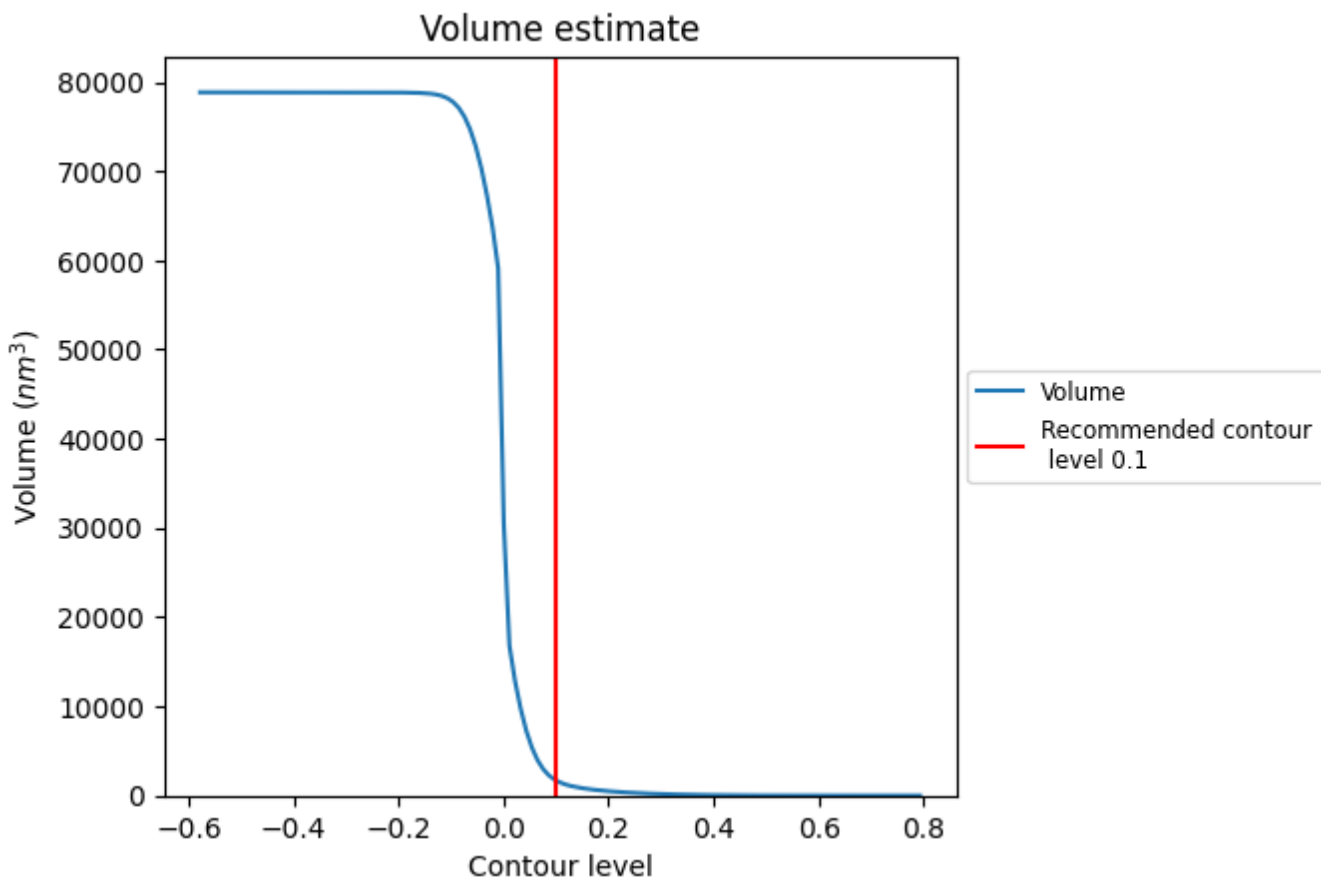
This section contains the results of statistical analysis of the map.

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.

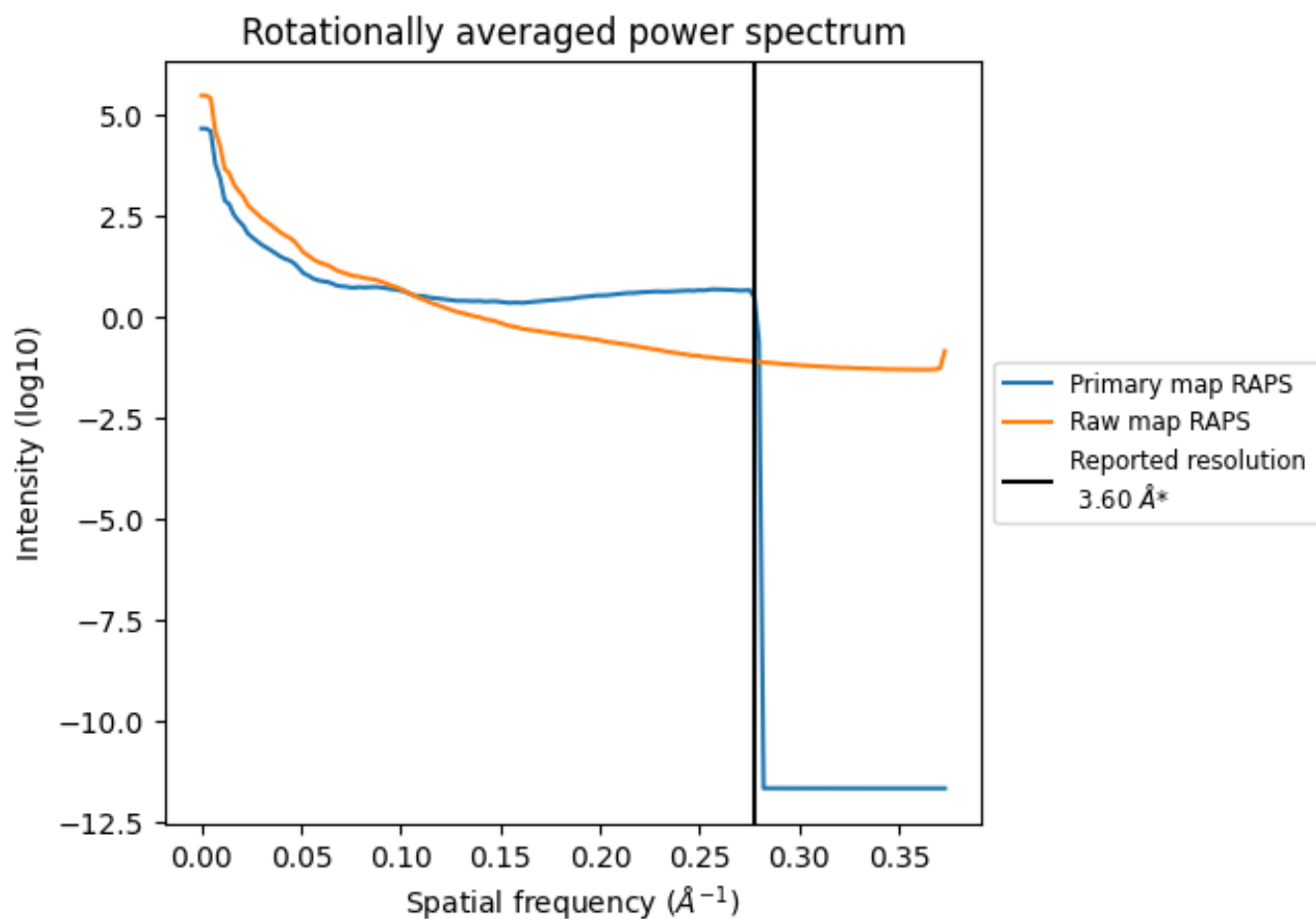
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1706 nm³; this corresponds to an approximate mass of 1541 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

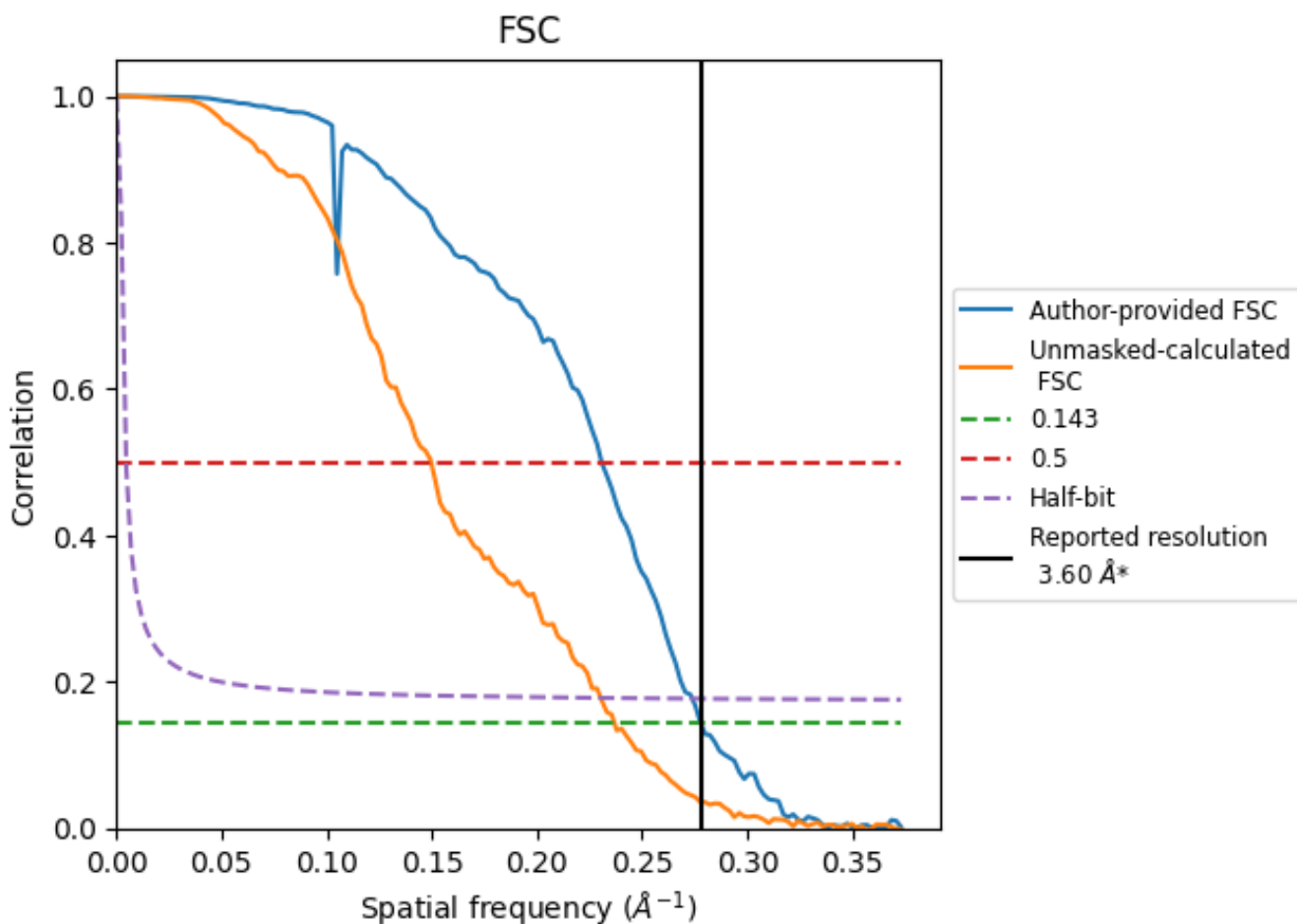


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

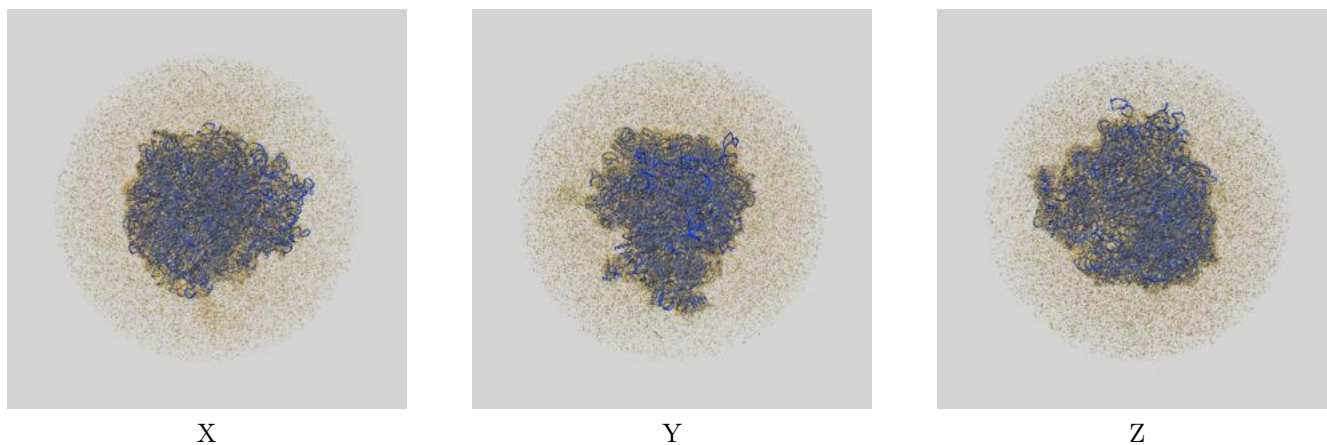
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.33	3.65
Unmasked-calculated*	4.22	6.69	4.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.22 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

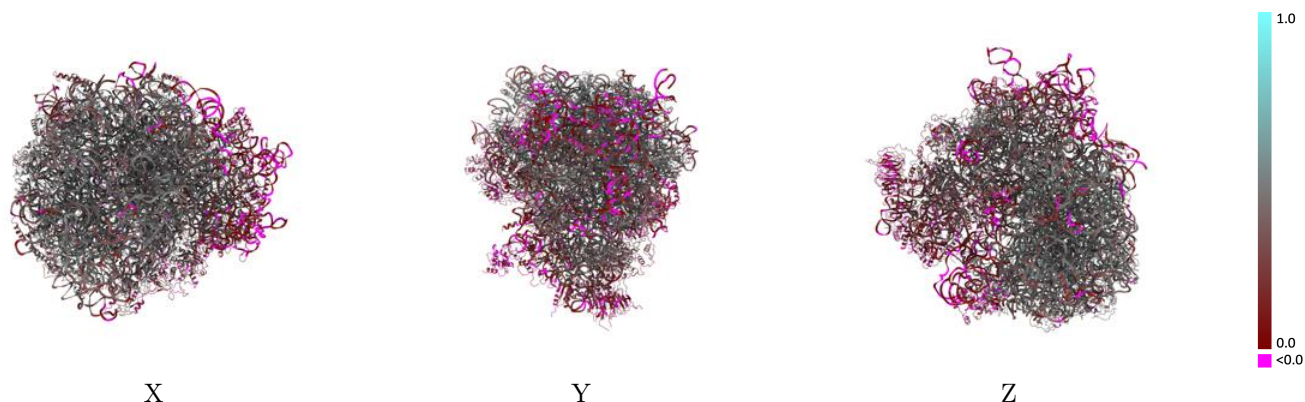
This section contains information regarding the fit between EMDB map EMD-8123 and PDB model 5IT7. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



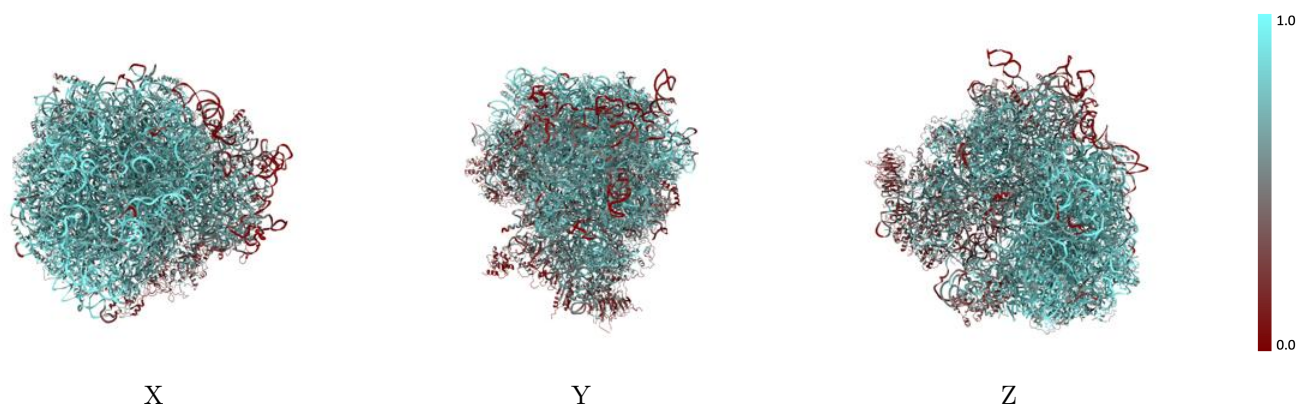
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



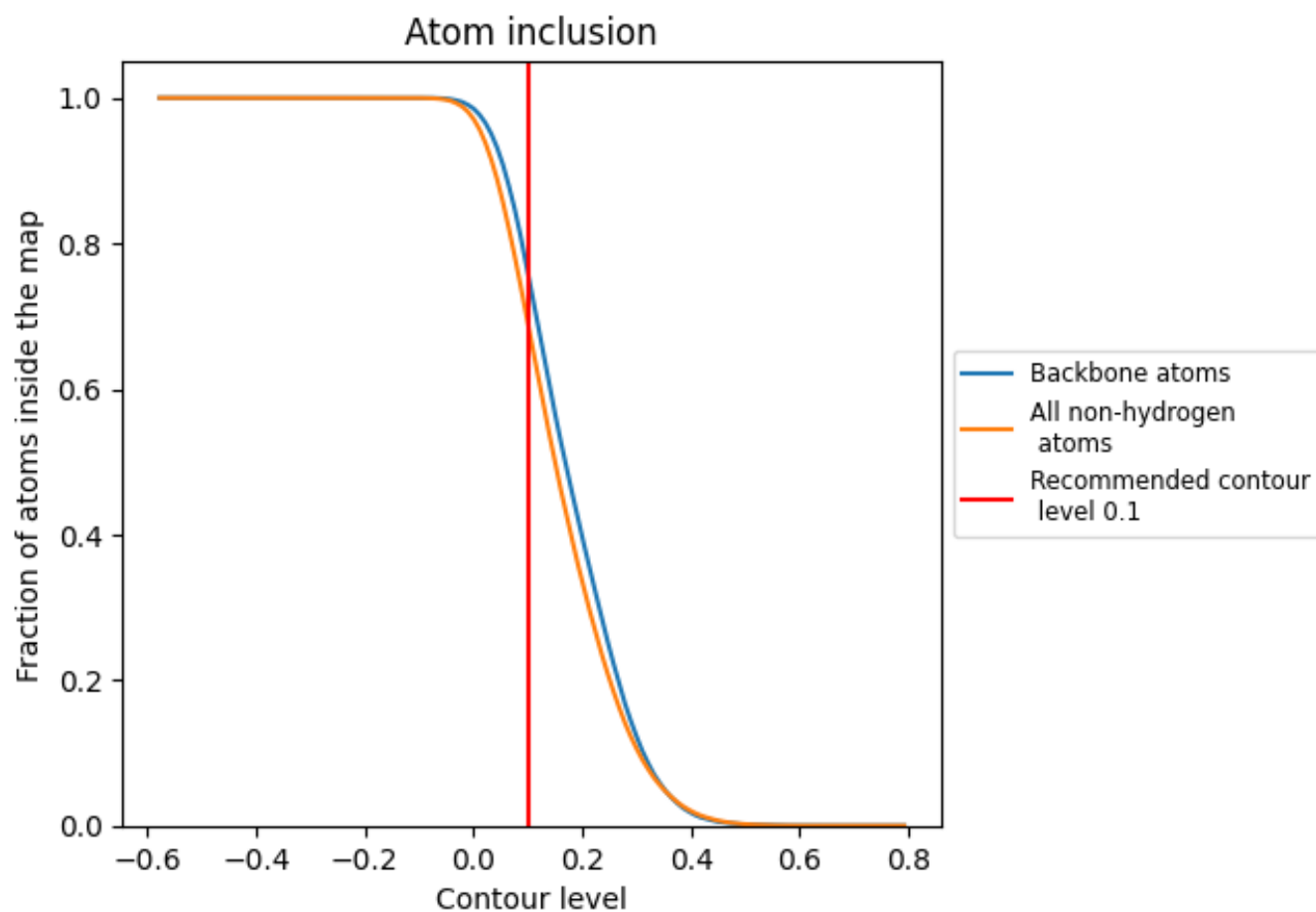
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6910	 0.3580
1	 0.4515	 0.2850
2	 0.6799	 0.2900
4	 0.3605	 0.0710
5	 0.8269	 0.4120
7	 0.8965	 0.4420
8	 0.8689	 0.4390
A	 0.6402	 0.3480
AA	 0.7467	 0.4820
B	 0.5234	 0.2830
BB	 0.7563	 0.4680
C	 0.6908	 0.4200
CC	 0.7429	 0.4550
D	 0.4115	 0.2220
DD	 0.7005	 0.3970
E	 0.6264	 0.3710
EE	 0.6994	 0.4020
F	 0.3473	 0.1690
FF	 0.7721	 0.4590
G	 0.4093	 0.1840
GG	 0.7031	 0.4140
H	 0.5612	 0.3020
HH	 0.7039	 0.4410
I	 0.5320	 0.2880
II	 0.7337	 0.4630
J	 0.6511	 0.3720
JJ	 0.6437	 0.3630
K	 0.3530	 0.1400
KK	 0.2490	 0.1270
L	 0.5778	 0.3540
LL	 0.7184	 0.4290
M	 0.1126	 0.0080
MM	 0.7500	 0.4410
N	 0.6222	 0.3860
NN	 0.7887	 0.4960

















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Chain	Atom inclusion	Q-score
O	0.6037	0.3550
OO	0.8109	0.4960
P	0.3274	0.1460
PP	0.7392	0.4480
Q	0.4315	0.2100
QQ	0.7647	0.4760
R	0.4387	0.2190
RR	0.6779	0.4030
S	0.2845	0.1310
SS	0.7618	0.4760
T	0.4333	0.2070
TT	0.7545	0.4660
U	0.3337	0.1720
UU	0.6302	0.3760
V	0.6432	0.3730
VV	0.7075	0.4670
W	0.7480	0.4740
WW	0.7359	0.4570
X	0.6536	0.4420
XX	0.7179	0.4540
Y	0.5467	0.2820
YY	0.7322	0.4410
Z	0.3720	0.1310
ZZ	0.7238	0.4020
a	0.6304	0.3740
aa	0.7684	0.4700
b	0.5410	0.3040
bb	0.7242	0.4260
c	0.3629	0.1930
cc	0.6841	0.4300
d	0.5293	0.2700
dd	0.7239	0.4480
e	0.4872	0.3020
ee	0.7518	0.4740
f	0.1719	0.0470
ff	0.7790	0.5020
g	0.2982	0.1230
gg	0.6757	0.4270
hh	0.7320	0.4360
ii	0.6865	0.3910
jj	0.8246	0.5040
kk	0.6112	0.3480

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Chain	Atom inclusion	Q-score
ll	 0.7789	 0.4820
mm	 0.7204	 0.4660
nn	 0.4528	 0.3530
oo	 0.6926	 0.4360
pp	 0.7071	 0.4600
qq	 0.2447	 0.0580
rr	 0.2681	 0.2120