



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:20 PM UTC

PDB ID : 6UZ7 / pdb_00006uz7
EMDB ID : EMD-20952
Title : K.lactis 80S ribosome with p/PE tRNA and eIF5B
Authors : Fernandez, I.S.; Huang, B.Y.
Deposited on : 2019-11-14
Resolution : 3.60 Å(reported)
Based on initial model : 3U5B

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:

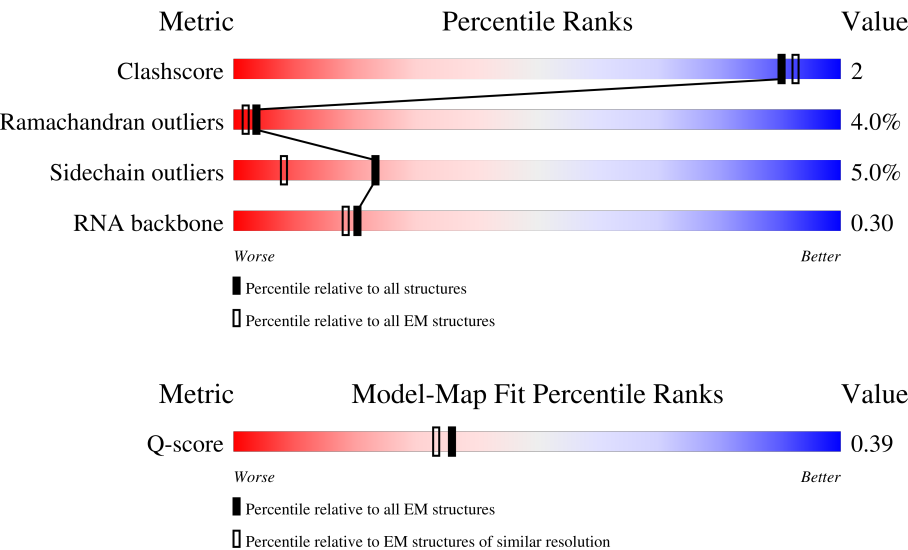
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	3364	13% 66% 29% • •
2	7	121	• 75% 23% •
3	8	2825	• • 94%

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Mol	Chain	Length	Quality of chain
4	AA	254	
5	AB	387	
6	AC	363	
7	AD	297	
8	AE	175	
9	AF	241	
10	AG	255	
11	AH	191	
12	AI	220	
13	AJ	174	
14	AL	199	
15	AM	138	
16	AN	204	
17	AO	199	
18	AP	184	
19	AQ	186	
20	AR	189	
21	AS	172	
22	AT	160	
23	AU	122	
24	AV	137	
25	AW	155	
26	AX	142	
27	AY	127	
28	AZ	136	

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Mol	Chain	Length	Quality of chain
29	Ba	149	
30	Bb	62	
31	Bc	105	
32	Bd	114	
33	Be	130	
34	Bf	107	
35	Bg	125	
36	Bh	120	
37	Bi	100	
38	Bj	88	
39	Bk	78	
40	Bl	51	
41	Bm	128	
42	Bn	23	
43	Bo	106	
44	Bp	92	
45	Bq	217	
46	Br	311	
47	AK	147	
48	A	254	
49	B	255	
50	C	259	
51	D	237	
52	E	261	
53	F	227	

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Mol	Chain	Length	Quality of chain
54	G	236	88% 89% 7% .
55	H	190	68% 86% 11% .
56	I	201	77% 82% 11% 6%
57	J	188	50% 85% 11% . .
58	K	106	91% 79% 10% . 9%
59	L	156	51% 84% 8% . 7%
60	M	134	91% 83% 7% . 9%
61	N	151	56% 90% 9% .
62	O	137	72% 85% 8% 7%
63	P	142	82% 66% 16% . 16%
64	Q	143	97% 94% . .
65	R	136	81% 81% 9% . 10%
66	S	146	93% 80% 14% 5%
67	T	144	99% 93% 6% .
68	U	117	88% 80% 9% . 9%
69	V	87	51% 87% 13%
70	W	130	12% 85% 15% .
71	X	145	42% 86% 12% . .
72	Y	135	79% 85% 11% . .
73	Z	108	65% 63% . 35%
74	a	119	47% 70% 13% . 16%
75	b	82	70% 94% 6%
76	c	67	94% 90% . 6%
77	d	56	86% 88% 7% 5%
78	e	63	67% 83% 5% 13%

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Mol	Chain	Length	Quality of chain
79	f	150	29%25%71% ••
80	g	326	97%89%8% •
81	2	1798	45%54%42% ••
82	1	967	52%49%11%38% ••
83	3	76	92%47%49% •

2 Entry composition

There are 85 unique types of molecules in this entry. The entry contains 211187 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3269	Total	C	N	O	P	0	0
			69874	31213	12576	22816	3269		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1923	A	C	conflict	GB 1241923359
5	2021	U	C	conflict	GB 1241923359
5	2051	U	C	conflict	GB 1241923359

- Molecule 2 is a RNA chain called RNA (121-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	157	Total	C	N	O	P	0	0
			3326	1488	573	1108	157		

- Molecule 4 is a protein called KLLA0D16027p.

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

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

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

- Molecule 6 is a protein called KLLA0B07139p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	360	Total	C	N	O	S	0	0
			2743	1725	522	493	3		

- Molecule 7 is a protein called KLLA0D06941p.

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

- Molecule 8 is a protein called KLLA0B04686p.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AE	164	Total	C	N	O	0	0
			1321	847	247	227		

- Molecule 9 is a protein called KLLA0D03410p.

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

- Molecule 10 is a protein called KLLA0E00573p.

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

- Molecule 11 is a protein called KLLA0F04499p.

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

- Molecule 12 is a protein called KLLA0D05643p.

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

- Molecule 13 is a protein called KLLA0F08261p.

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

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

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

- Molecule 15 is a protein called KLLA0B13409p.

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

- Molecule 16 is a protein called Ribosomal protein L15.

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

- Molecule 17 is a protein called KLLA0F04675p.

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

- Molecule 18 is a protein called KLLA0A06336p.

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

- Molecule 19 is a protein called KLLA0A07227p.

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

- Molecule 20 is a protein called KLLA0E12453p.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AS	169	Total	C	N	O	S	0	0
			1422	916	265	238	3		

- Molecule 22 is a protein called KLLA0E23651p.

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

- Molecule 23 is a protein called KLLA0D05181p.

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

- Molecule 24 is a protein called KLLA0E06997p.

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

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

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

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

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

- Molecule 27 is a protein called KLLA0B05742p.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	AY	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	AZ	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	Ba	147	Total	C	N	O	S	0	0
			1156	740	225	189	2		

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

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	Bc	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	Bd	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	Be	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	Bf	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	Bg	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	Bh	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	Bi	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	Bj	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	Bk	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	Bl	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	Bm	51	Total	C	N	O	S	0	0
			410	254	85	66	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bn	23	Total	C	N	O	S	0	0
			218	133	60	24	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bo	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	Bp	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	Bq	217	Total	C	N	O	S	0	0
			1716	1097	297	313	9		

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

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

- Molecule 47 is a protein called GDPCP.

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

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

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

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

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

- Molecule 50 is a protein called KLLA0F09812p.

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

- Molecule 51 is a protein called KLLA0D08305p.

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

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

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

- Molecule 53 is a protein called KLLA0D10659p.

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

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

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

- Molecule 55 is a protein called 40S ribosomal protein S7.

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

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

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

- Molecule 57 is a protein called KLLA0E23673p.

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

- Molecule 58 is a protein called KLLA0B08173p.

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

- Molecule 59 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	L	145	Total	C	N	O	S	0	0
			1168	745	222	198	3		

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

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

- Molecule 61 is a protein called KLLA0F18040p.

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

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

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

- Molecule 63 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	P	119	Total	C	N	O	S	0	0
			950	611	170	164	5		

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

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

- Molecule 65 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	R	123	Total	C	N	O	S	0	0
			983	614	181	185	3		

- Molecule 66 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	S	138	Total	C	N	O	S	0	0
			1138	707	231	198	2		

- 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	143	Total	C	N	O	S	0	0
			1110	704	214	189	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 40S ribosomal protein S25.

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 40S ribosomal protein S26.

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 40S ribosomal protein S30.

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	44	Total	C	N	O	S	0	0
			337	213	65	55	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
81	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

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 a protein called KLLA0F23265p.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	1	600	Total	C	N	O	S	0	0
			4702	2981	808	890	23		

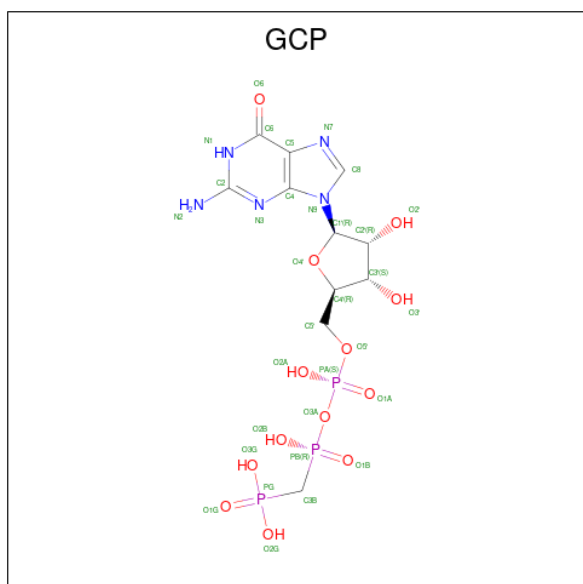
- Molecule 83 is a RNA chain called RNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
83	3	76	Total	C	N	O	P	0	0
			1623	725	295	528	75		

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	Bj	1	Total	Zn	0
			1	1	
84	Bm	1	Total	Zn	0
			1	1	
84	Bo	1	Total	Zn	0
			1	1	
84	a	1	Total	Zn	0
			1	1	
84	b	1	Total	Zn	0
			1	1	
84	f	1	Total	Zn	0
			1	1	

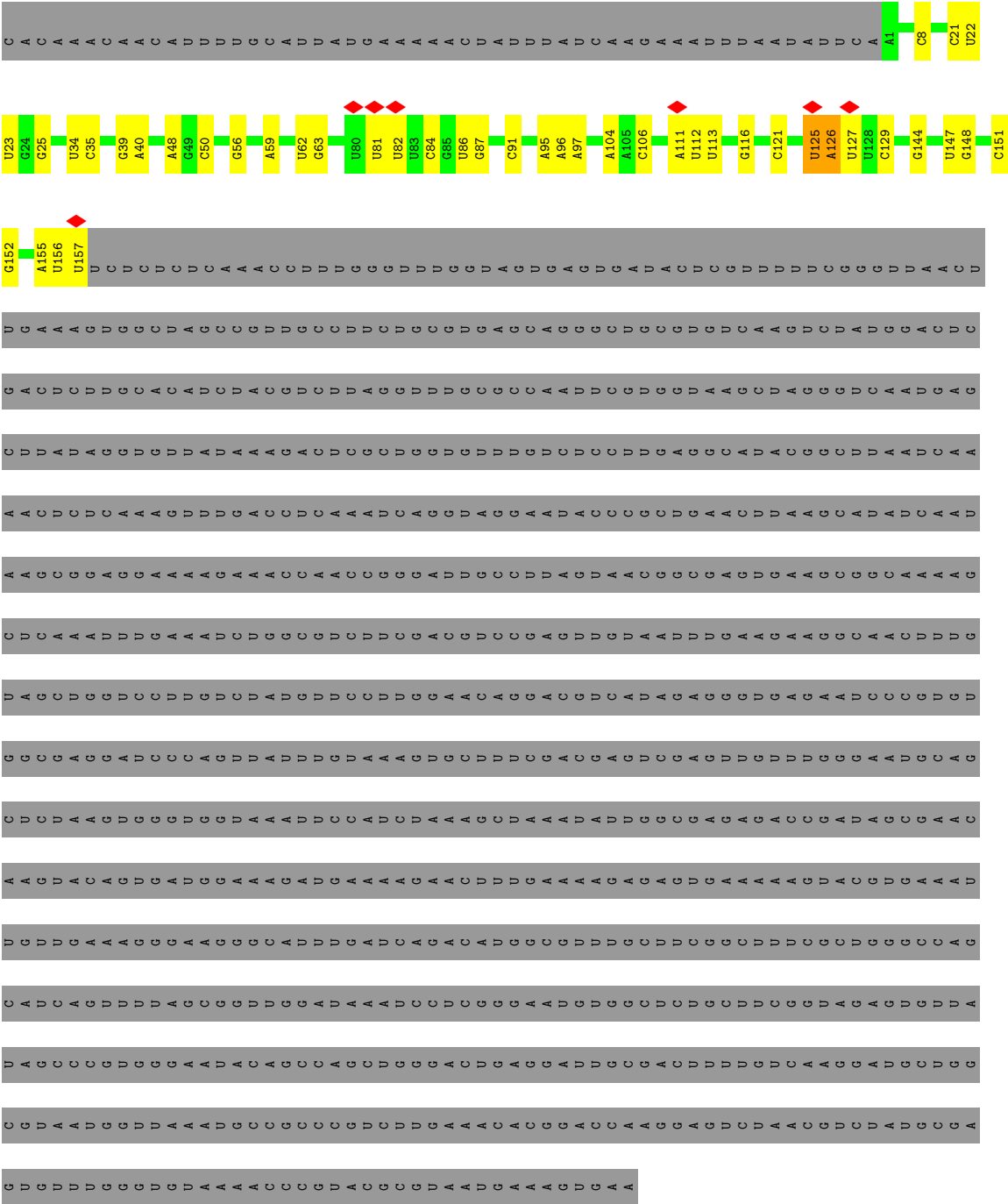
- Molecule 85 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



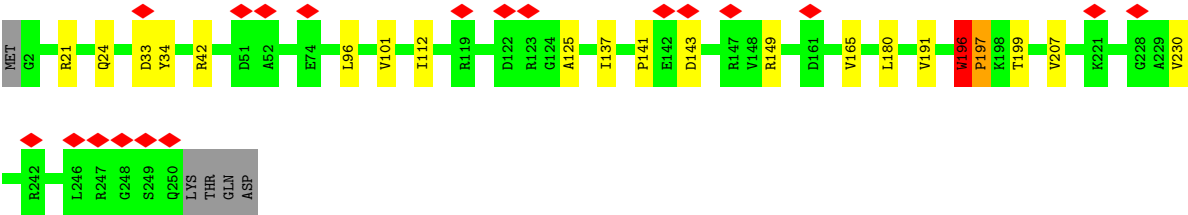
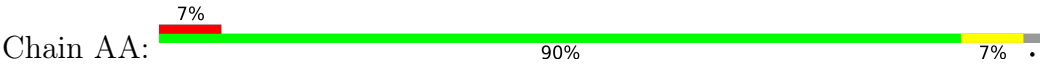
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
85	1	1	32	11	5	13	3	0

WORLDWIDE
PDB
PROTEIN DATA BANK

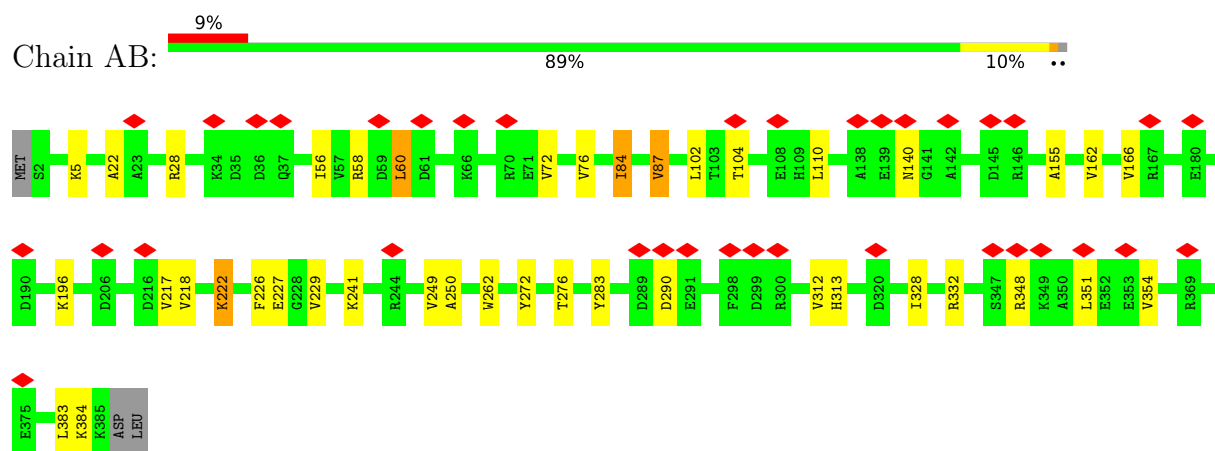
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U A A C C G A A C G A A A C A C U G G G A A G G C A A A U U C U G G U G C C A A G C C G G U A A U U C C A A G
U A G C G G U A U A U U A A A G U G U G U G C C A A G U U A A A G C U C G U A A C U U G G G U C U G U G U
C C G G U C C G A C U U A U G U U C G G C G C A A C U U G G U U C A A C C G G A U C C U U C U G G C U A A C C U G
U A C U C C U U G U G G U G C C A A A C C A A G G A C U U U A C U U U A A A A A A A A A A A G A G U U G U C A A A
G C A G G C G A A A G C U C G C A A U A A A U U A A G C A A U G G A A U A A A A A A A A A A A A A A A A A A
U G U U G G U U U C C U A A G A C C A U U C G U U A A U G A A U U U A A G G A C G G U C C G G G G A A U C C A G U U A U C A A
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A U U G C G A U A A A C G A A C C G A A C C U U A A C C U A
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U G A U G C C C U U A A G A C G G U U C C G G A A C C G G A A C C A A G G A A G G A A A A A A A A A A A A
C C U U G G C C G A A G G U C C U G G G A A A C C U U U G G A
U A A U U U G C C U U C A A G G A
A C G U C C C U C C U U C C U U U C C A A C A A C C G G C C C G U A A C C U A G G A A A A A A A A A A A A A A
C C U C A A G G U U A A G A
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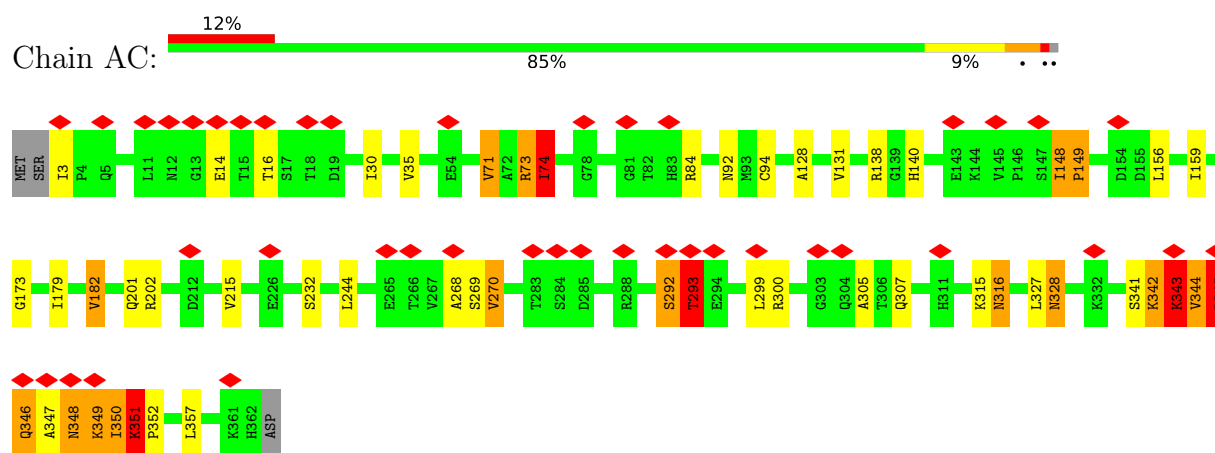
● Molecule 4: KLLA0D16027p



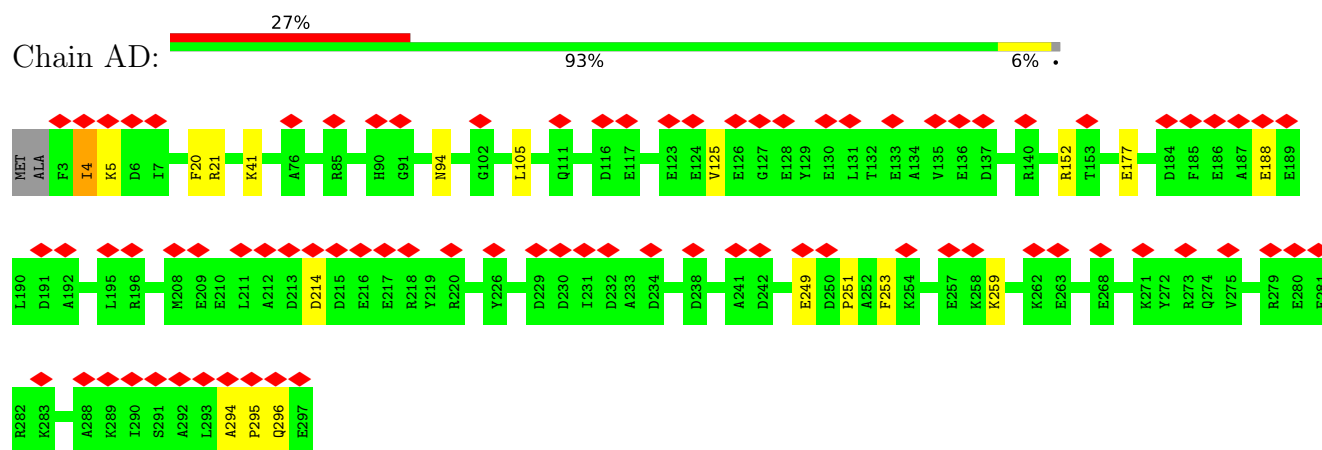
- Molecule 5: 60S ribosomal protein L3



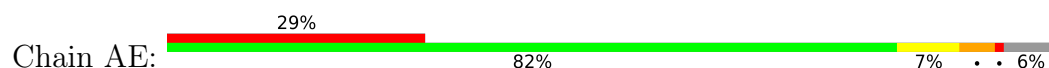
- Molecule 6: KLLA0B07139p

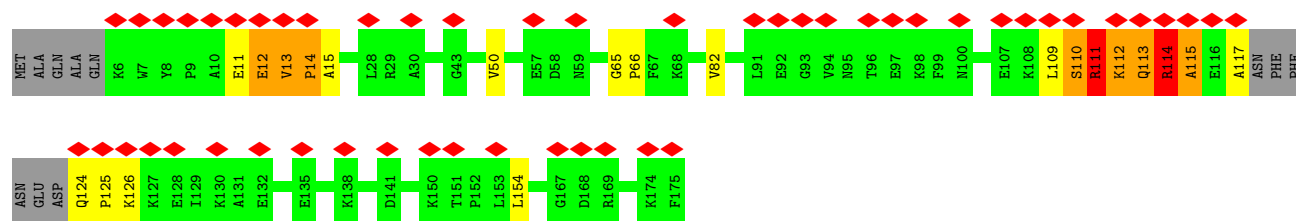


- Molecule 7: KLLA0D06941p

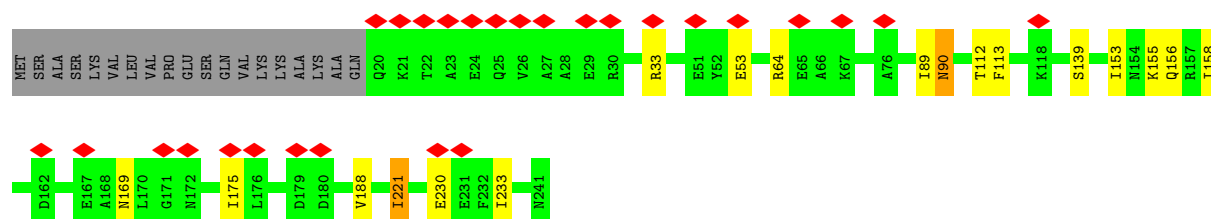
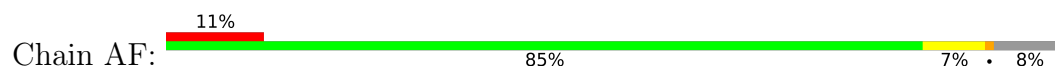


- Molecule 8: KLLA0B04686p

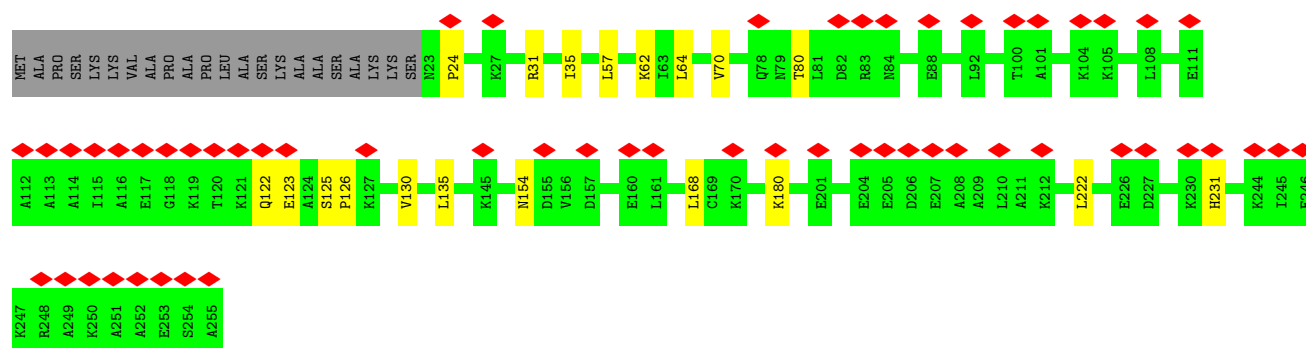
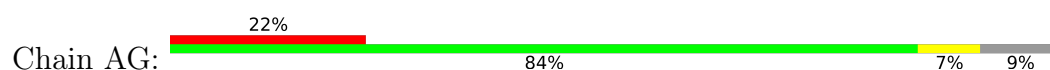




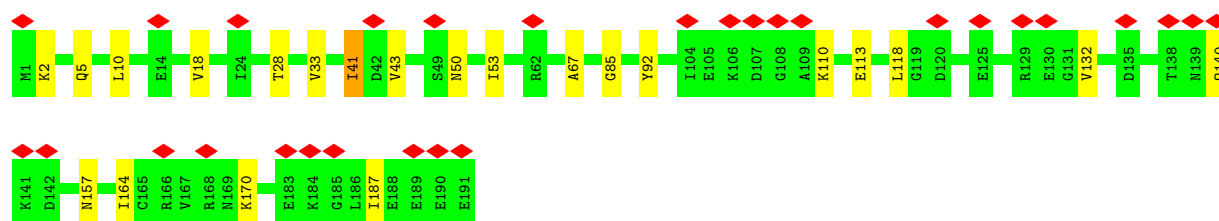
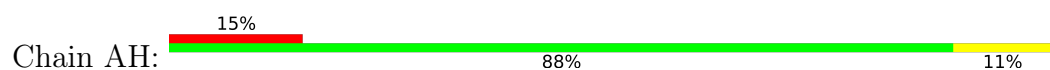
• Molecule 9: KLLA0D03410p



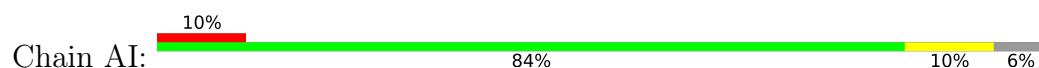
• Molecule 10: KLLA0E00573p

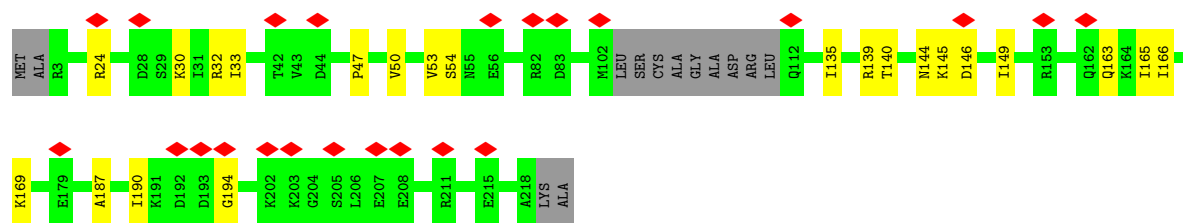


• Molecule 11: KLLA0F04499p

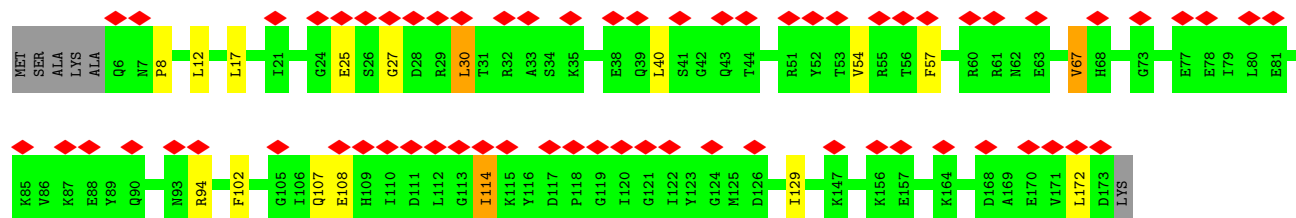
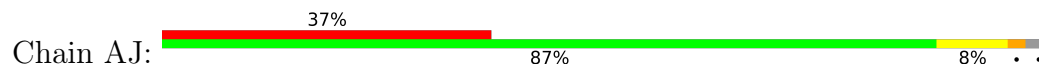


• Molecule 12: KLLA0D05643p

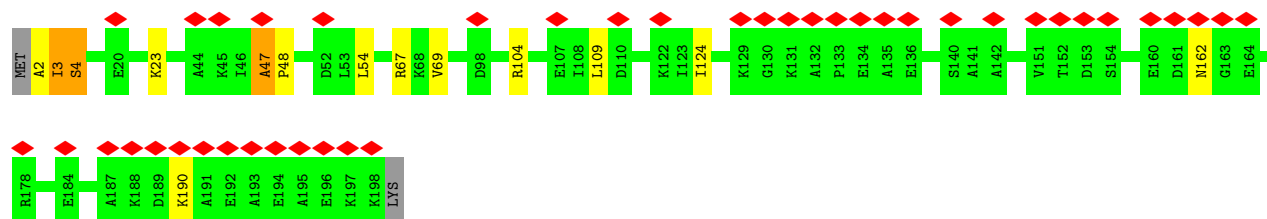
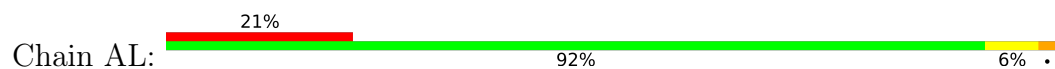




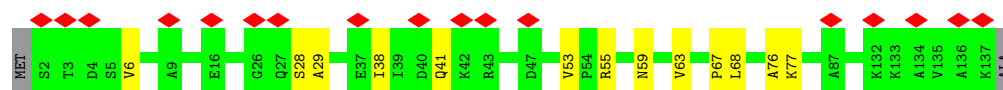
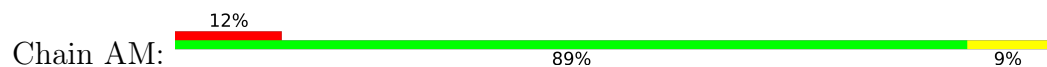
• Molecule 13: KLLA0F08261p



• Molecule 14: 60S ribosomal protein L13



• Molecule 15: KLLA0B13409p

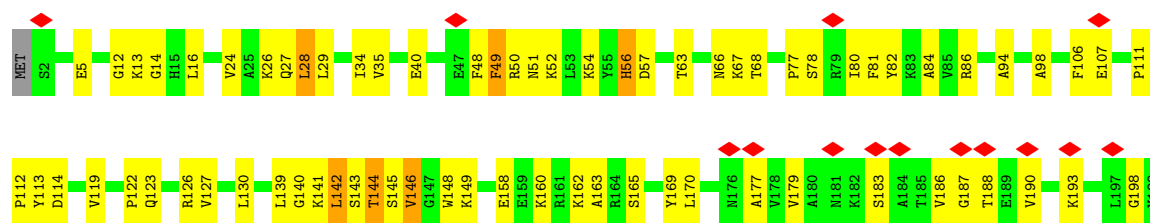


• Molecule 16: Ribosomal protein L15

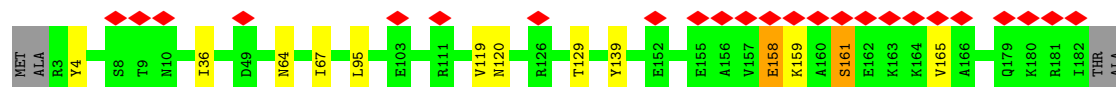
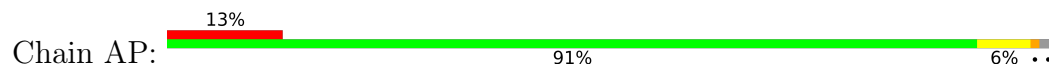


• Molecule 17: KLLA0F04675p





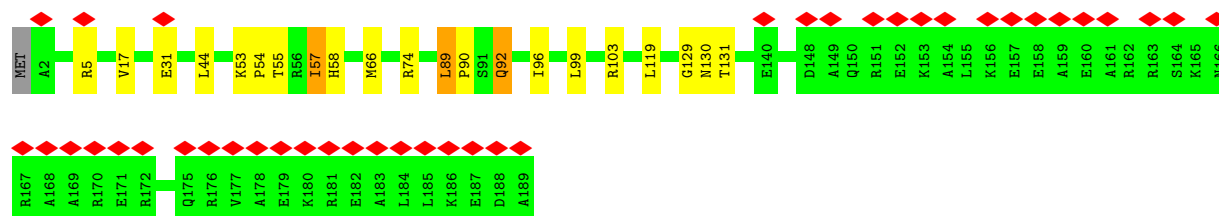
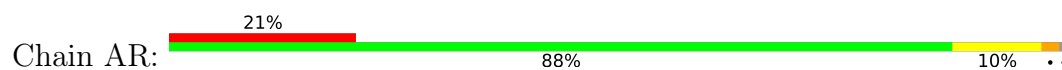
• Molecule 18: KLLA0A06336p



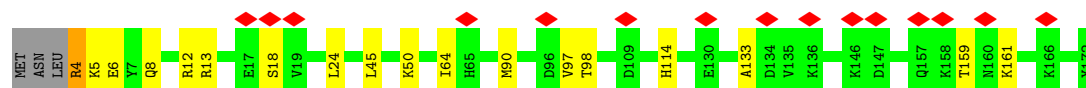
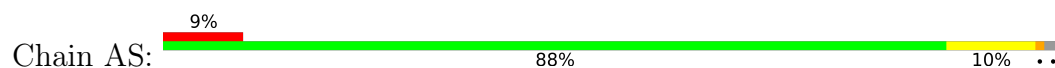
• Molecule 19: KLLA0A07227p



• Molecule 20: KLLA0E12453p



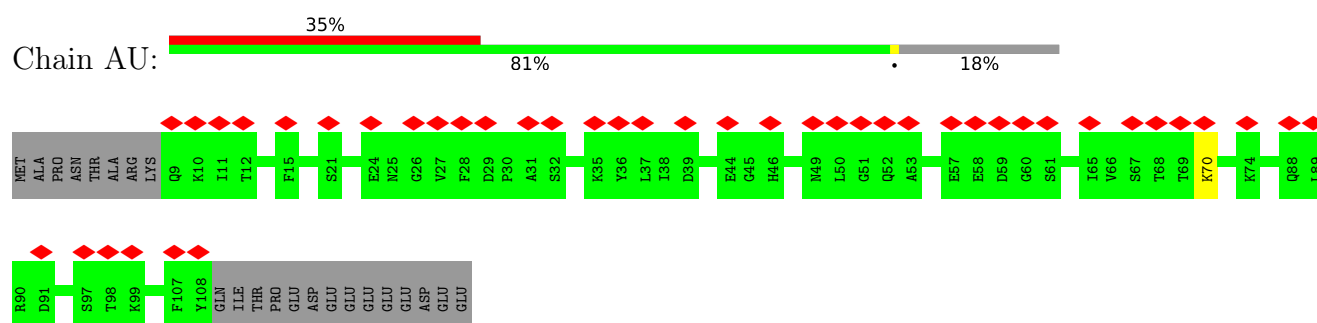
• Molecule 21: 60S ribosomal protein L20



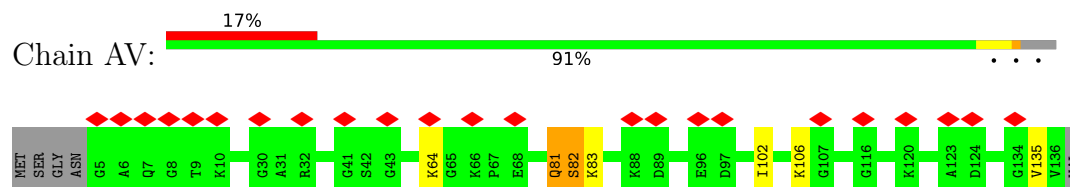
• Molecule 22: KLLA0E23651p



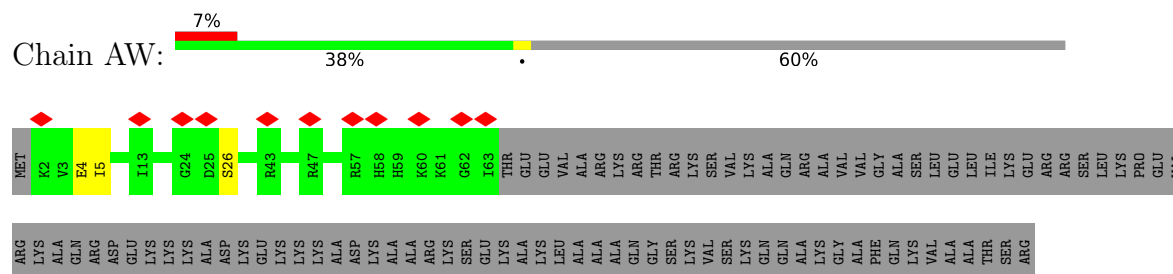
• Molecule 23: KLLA0D05181p



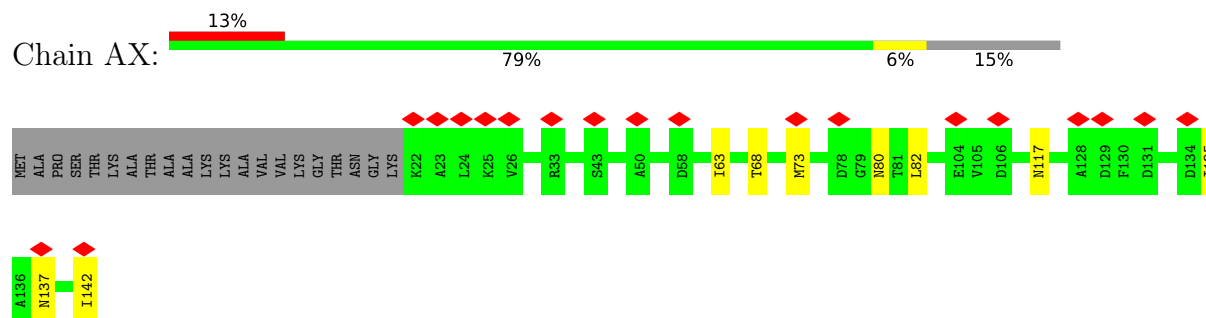
• Molecule 24: KLLA0E06997p



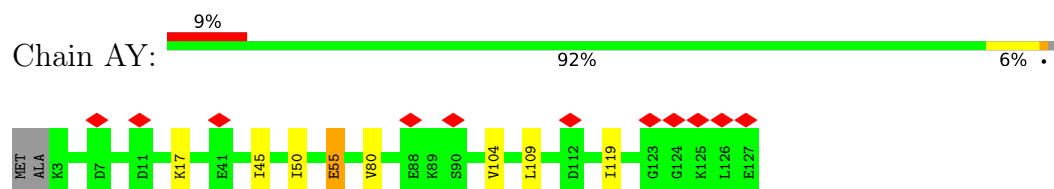
• Molecule 25: 60S ribosomal protein L24



• Molecule 26: 60S ribosomal protein L25

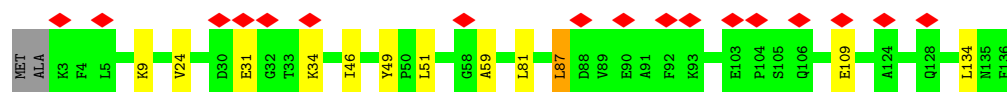


• Molecule 27: KLLA0B05742p

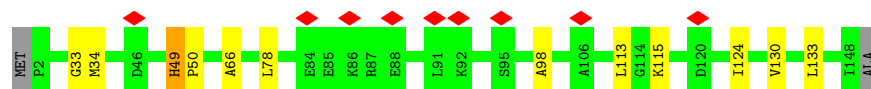


• Molecule 28: KLLA0E03455p

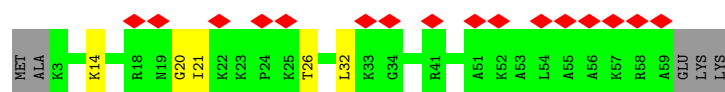
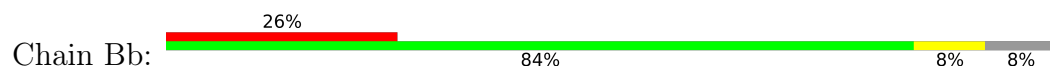




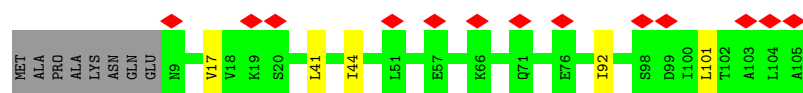
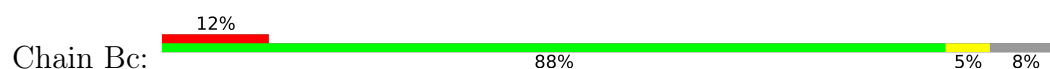
- Molecule 29: RPL28



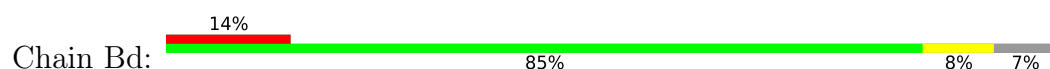
- Molecule 30: 60S ribosomal protein L29



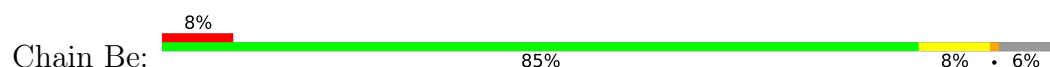
- Molecule 31: 60S ribosomal protein L30



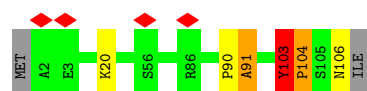
- Molecule 32: KLLA0B02937p



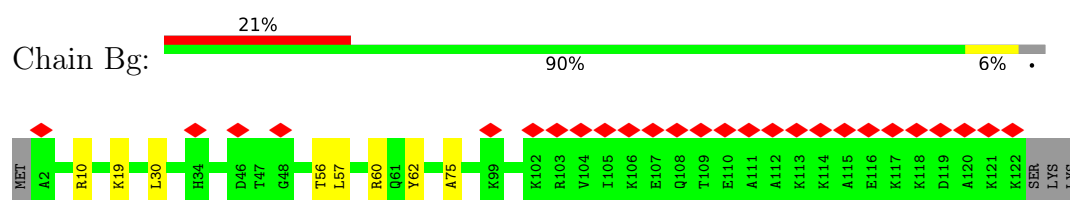
- Molecule 33: KLLA0E06843p



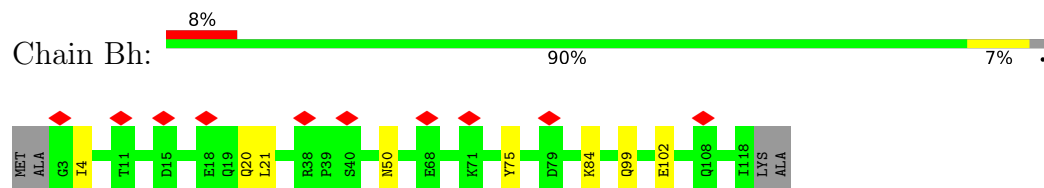
- Molecule 34: KLLA0D07405p



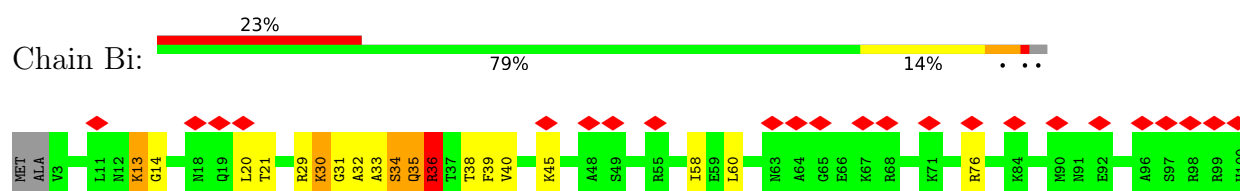
- Molecule 35: KLLA0C08371p



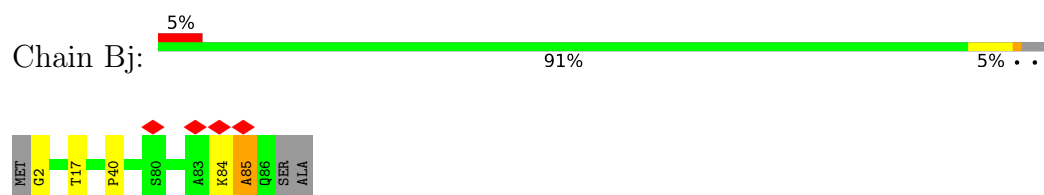
- Molecule 36: KLLA0F05247p



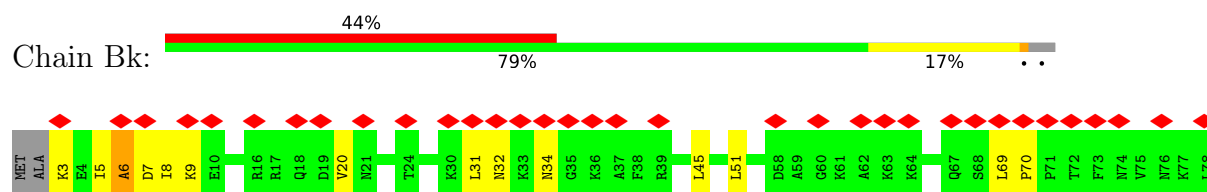
- Molecule 37: 60S ribosomal protein L36



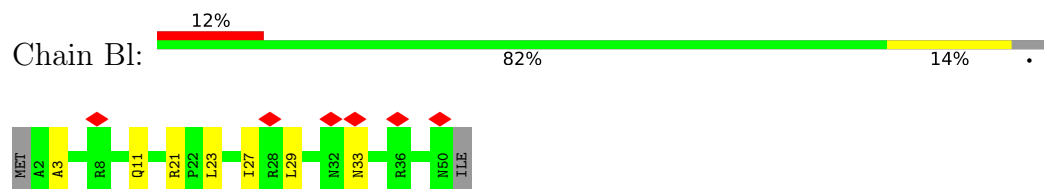
- Molecule 38: Ribosomal protein L37



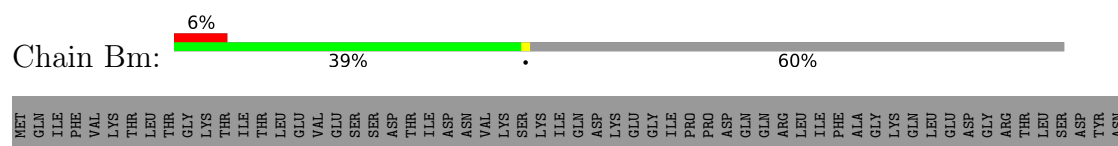
- Molecule 39: KLLA0C18216p

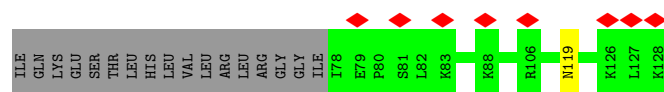


- Molecule 40: 60S ribosomal protein L39

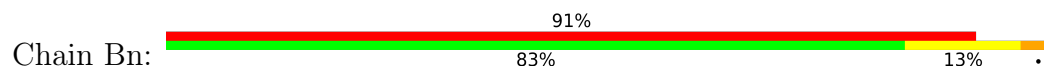


- Molecule 41: Ubiquitin fusion protein

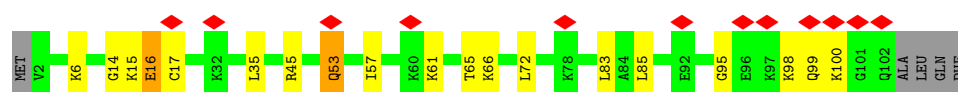
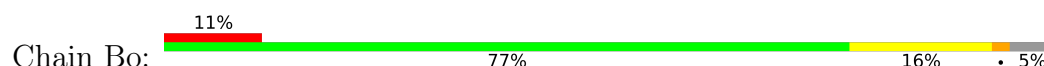




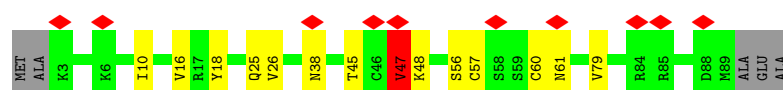
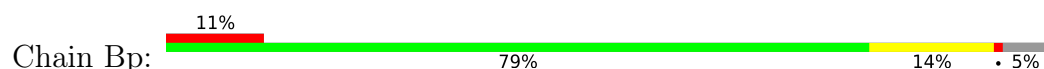
- Molecule 42: 60S ribosomal protein L41



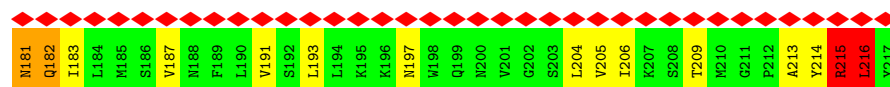
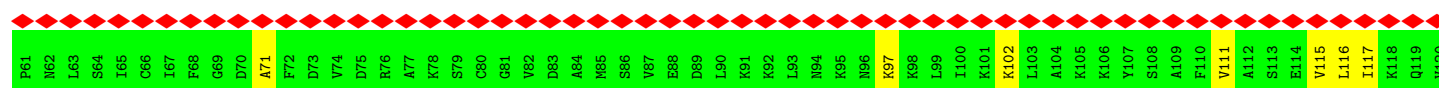
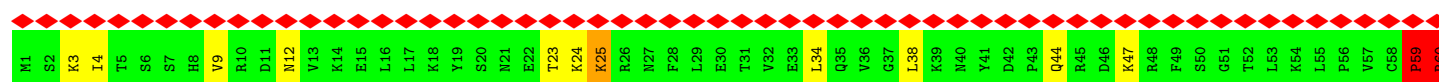
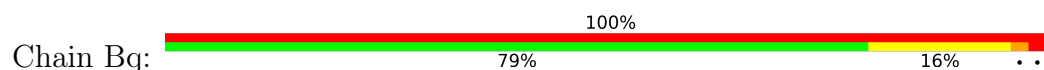
- Molecule 43: 60S ribosomal protein L44



- Molecule 44: KLLA0E05941p

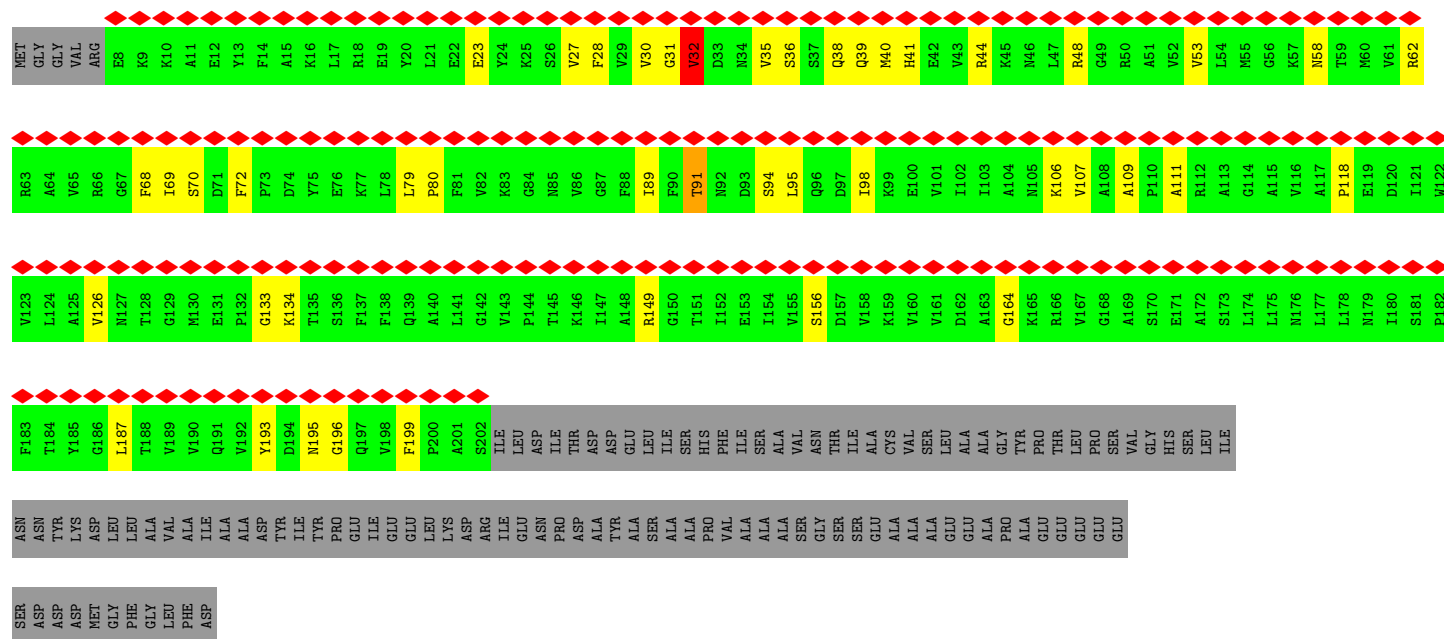


- Molecule 45: Ribosomal protein

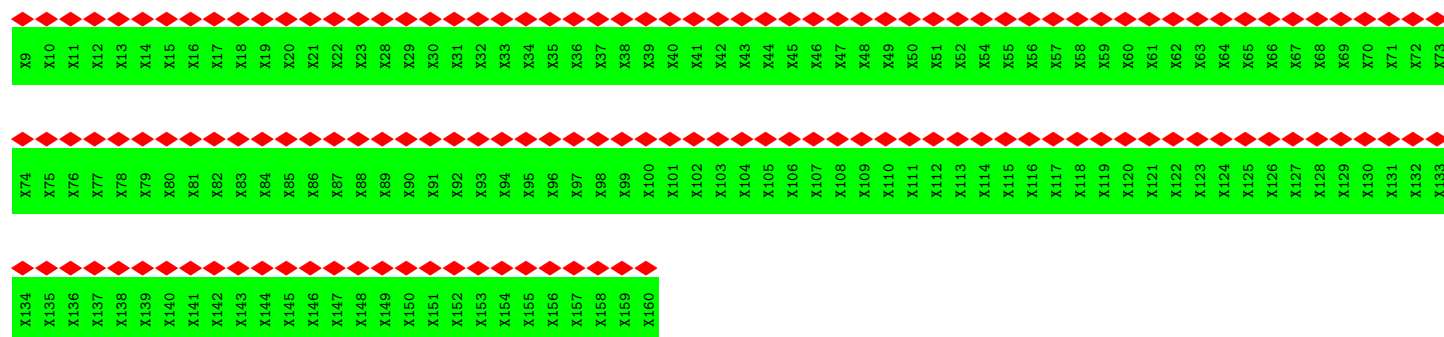


- Molecule 46: 60S acidic ribosomal protein P0

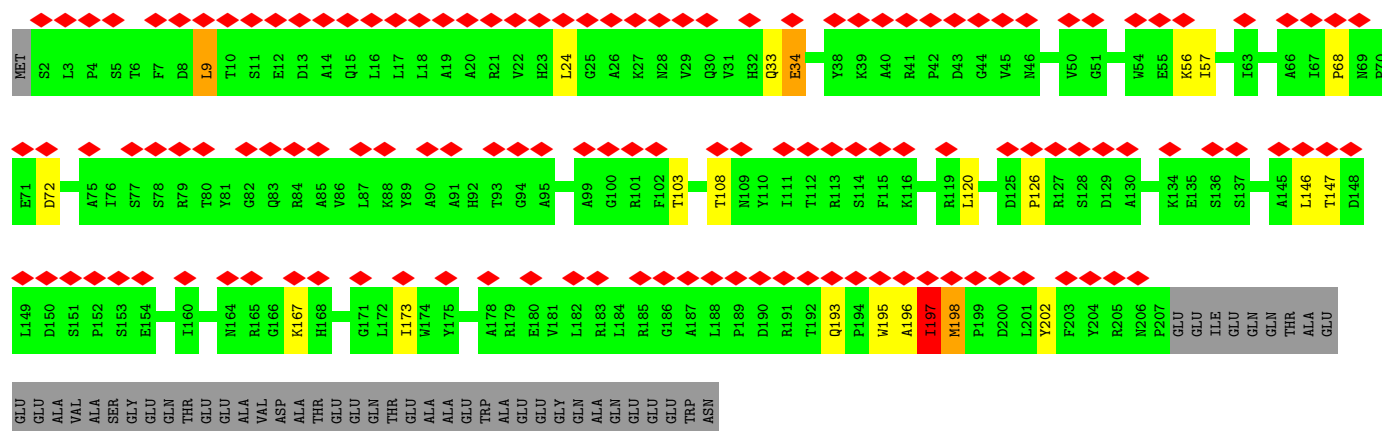
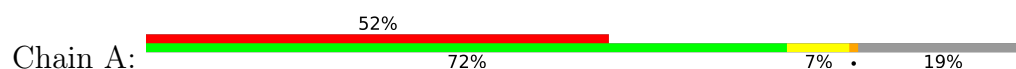




• Molecule 47: GDCPC

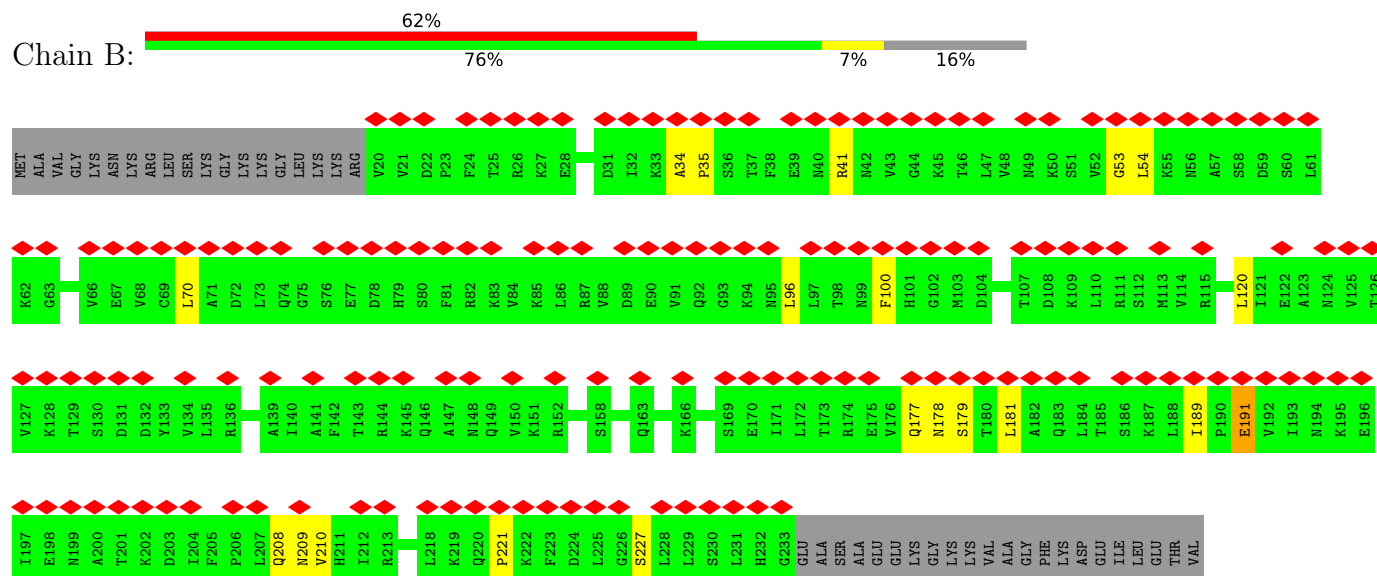


• Molecule 48: 40S ribosomal protein S0



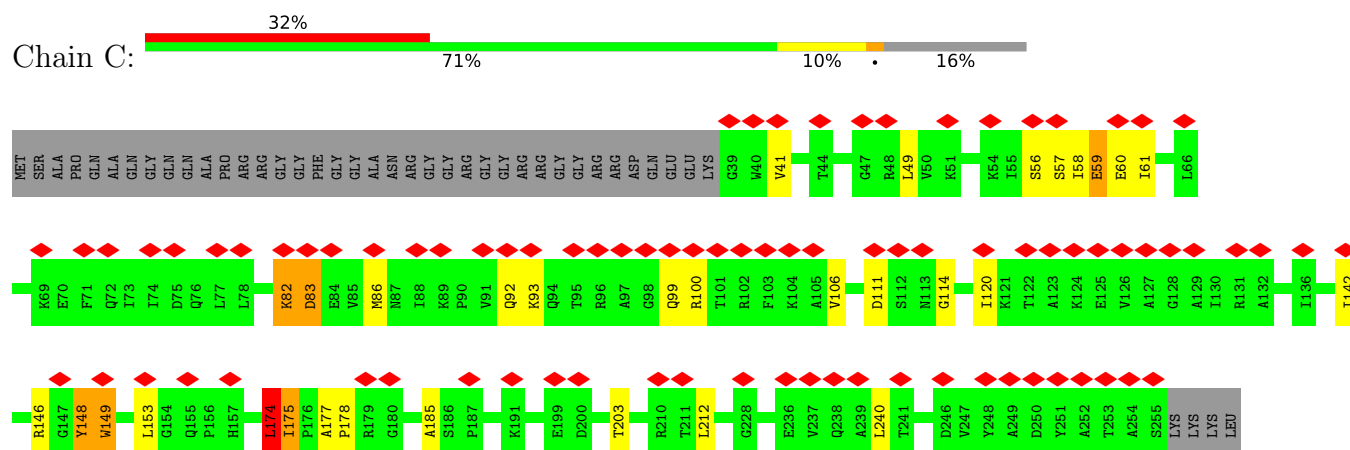
• Molecule 49: 40S ribosomal protein S1

Chain B:



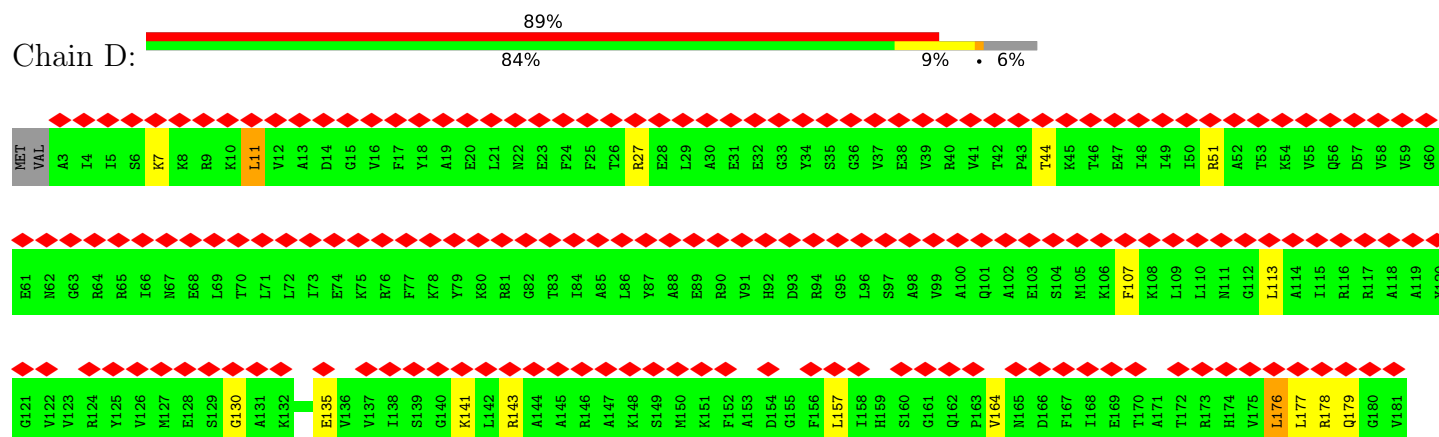
• Molecule 50: KLLA0F09812p

Chain C:



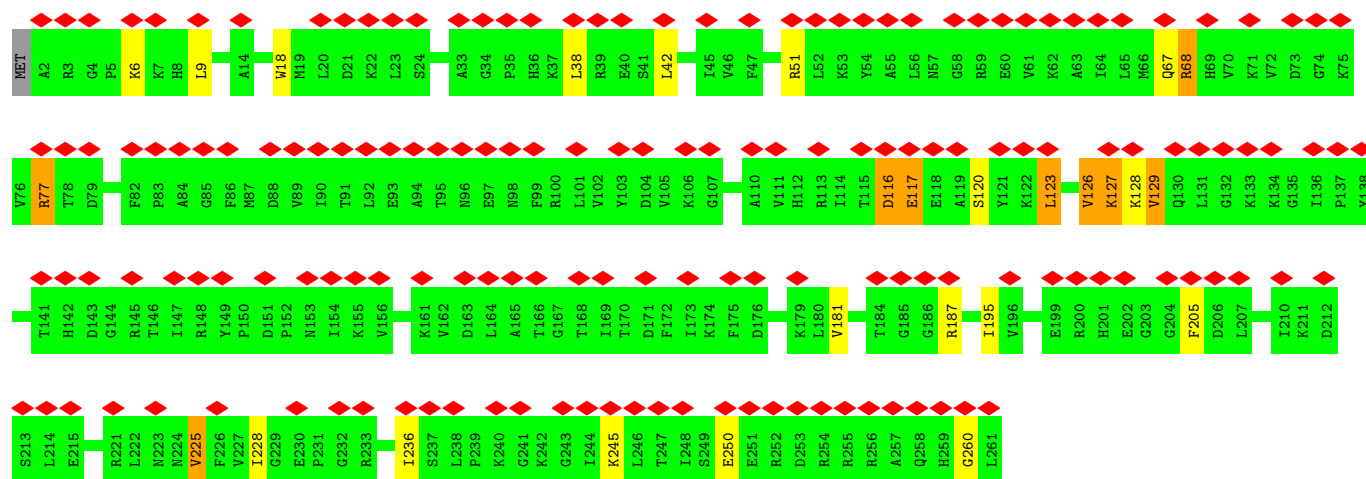
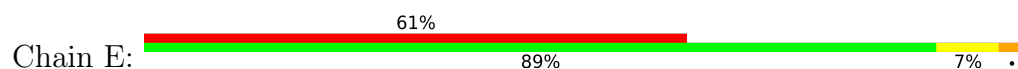
• Molecule 51: KLLA0D08305p

Chain D:

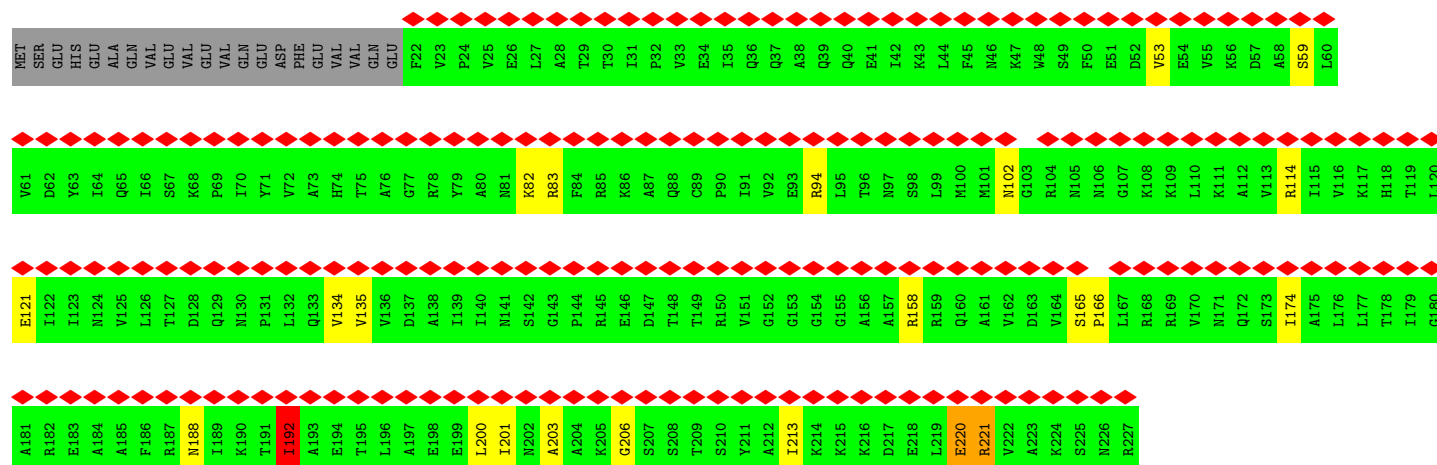
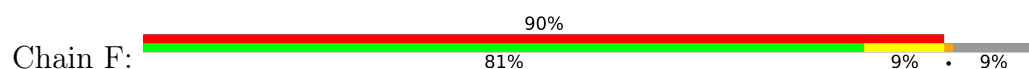




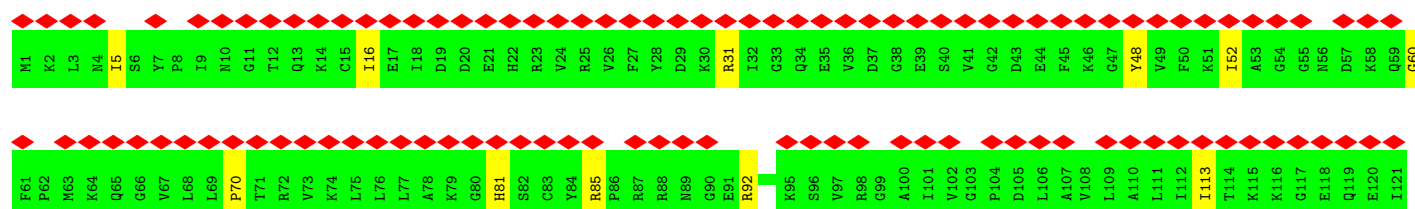
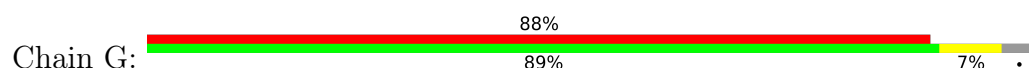
• Molecule 52: 40S ribosomal protein S4

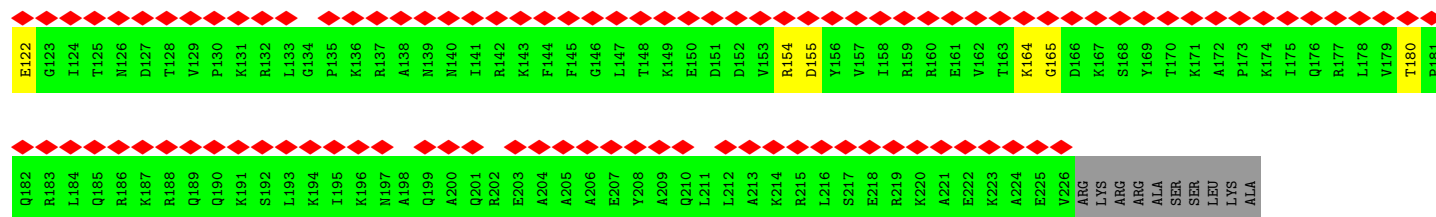


• Molecule 53: KLLA0D10659p

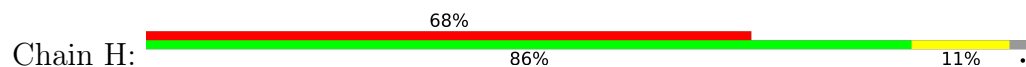


• Molecule 54: 40S ribosomal protein S6





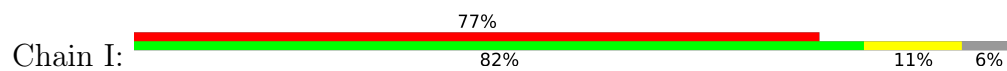
• Molecule 55: 40S ribosomal protein S7



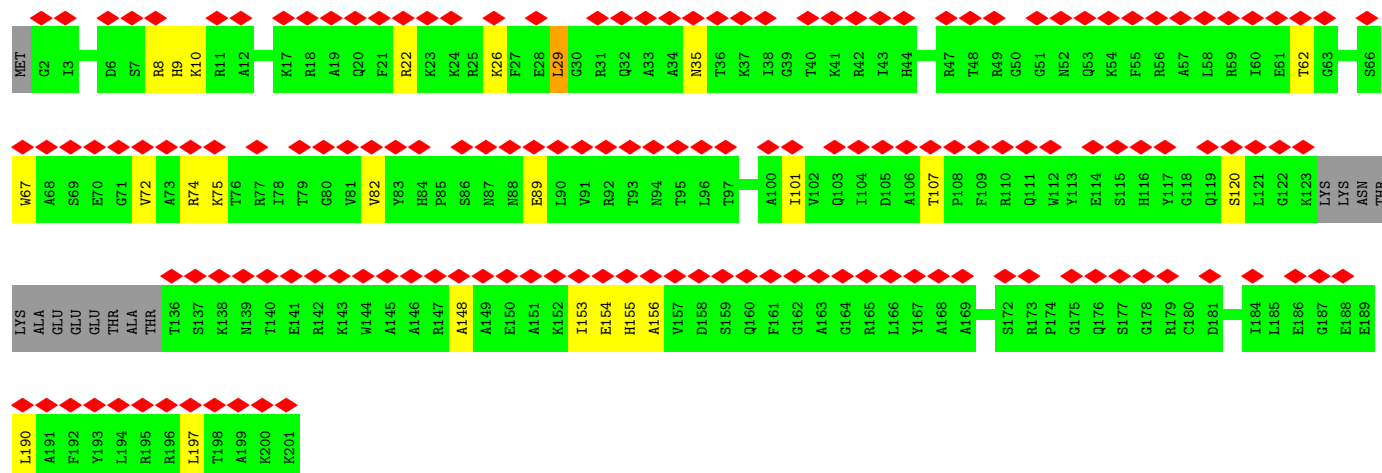
Chain H:



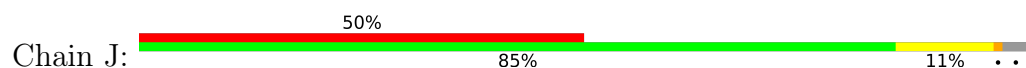
• Molecule 56: 40S ribosomal protein S8



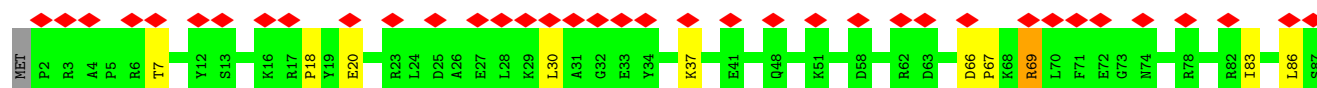
Chain I:

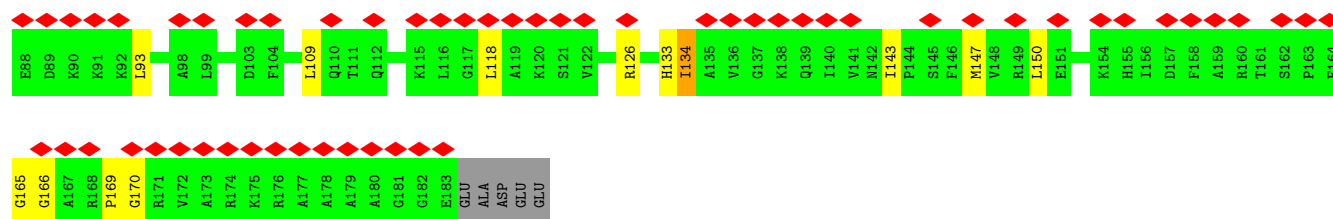


• Molecule 57: KLLA0E23673p

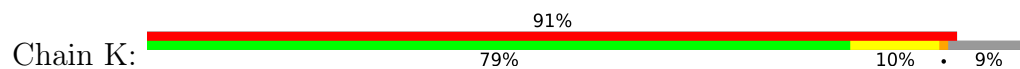


Chain J:

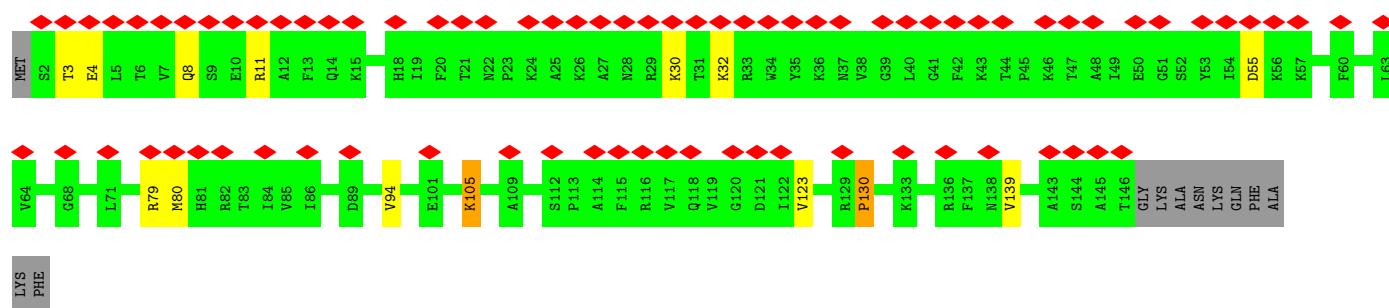
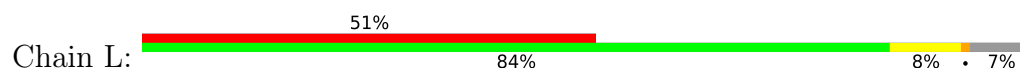




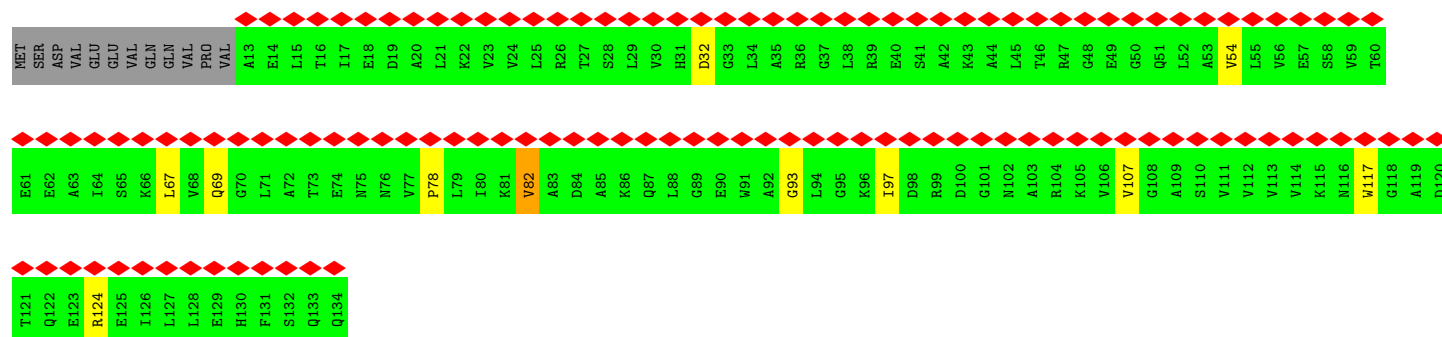
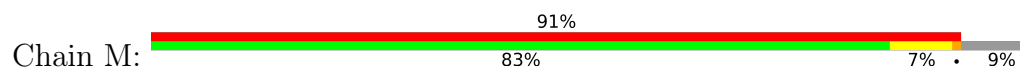
• Molecule 58: KLLA0B08173p



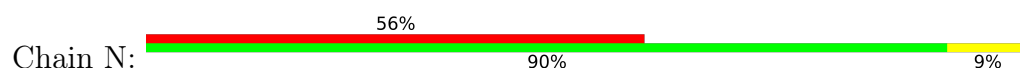
• Molecule 59: KLLA0A10483p

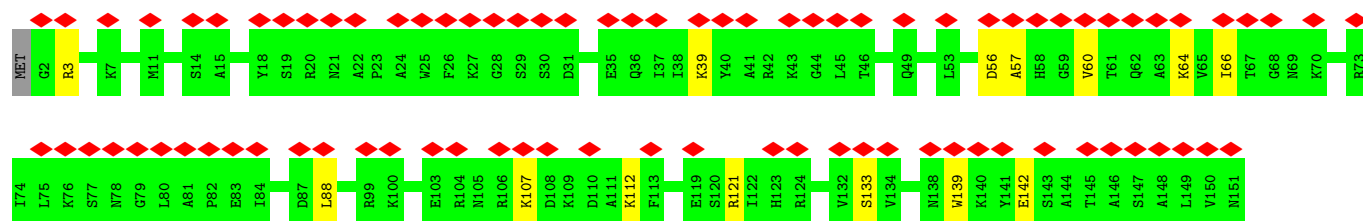


• Molecule 60: 40S ribosomal protein S12

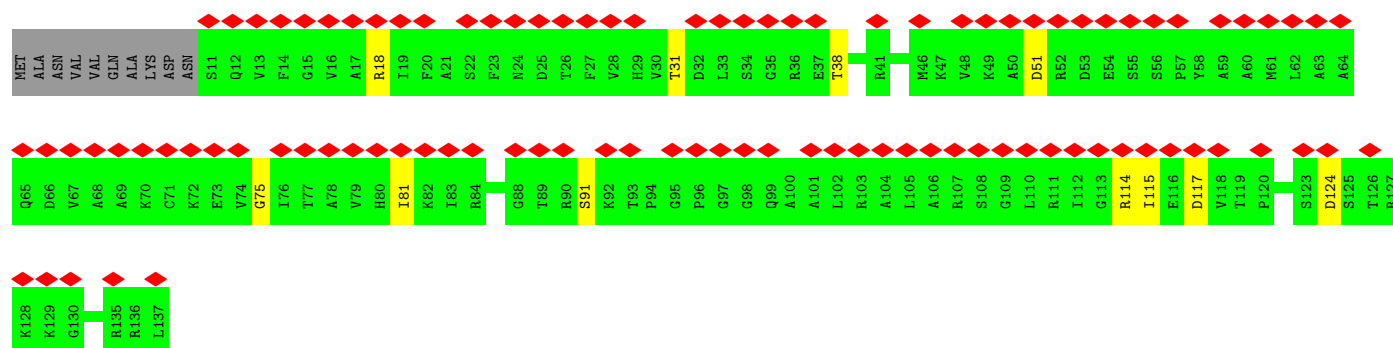
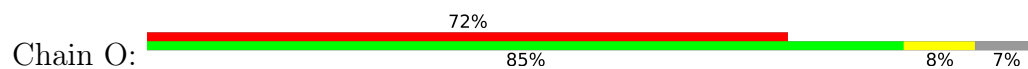


• Molecule 61: KLLA0F18040p

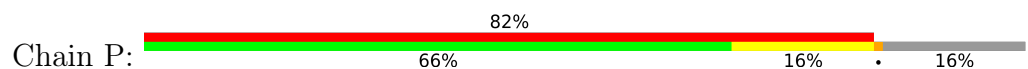




• Molecule 62: 40S ribosomal protein S14

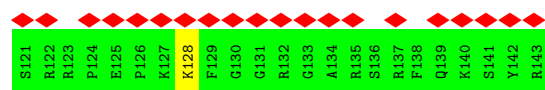


• Molecule 63: KLLA0F07843p

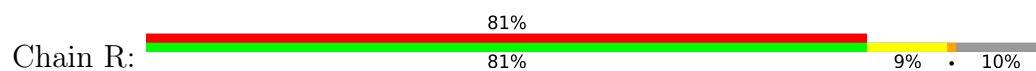


• Molecule 64: 40S ribosomal protein S16

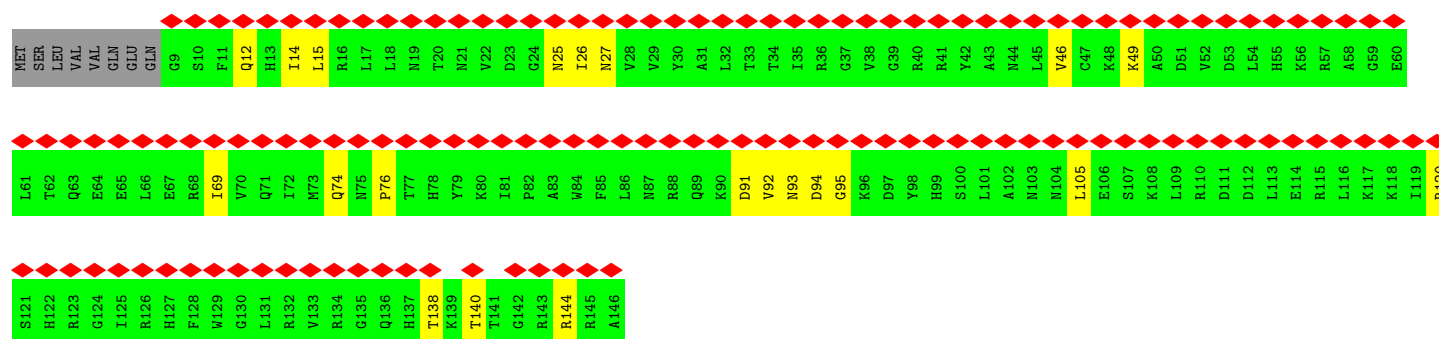
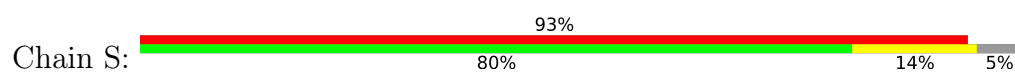




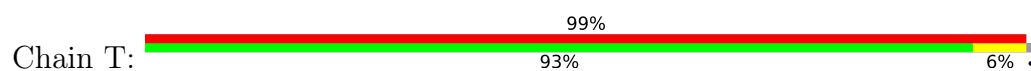
• Molecule 65: KLLA0B01474p



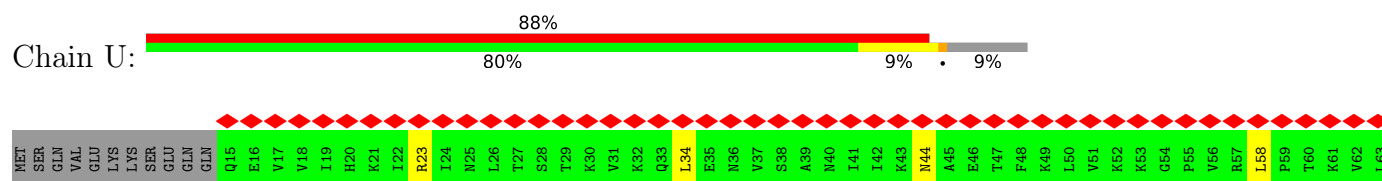
• Molecule 66: KLLA0B01562p



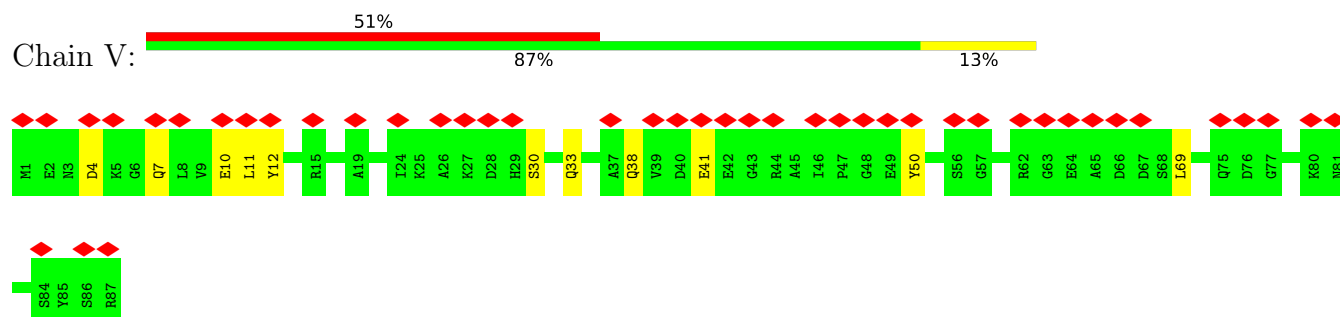
• Molecule 67: KLLA0A07194p



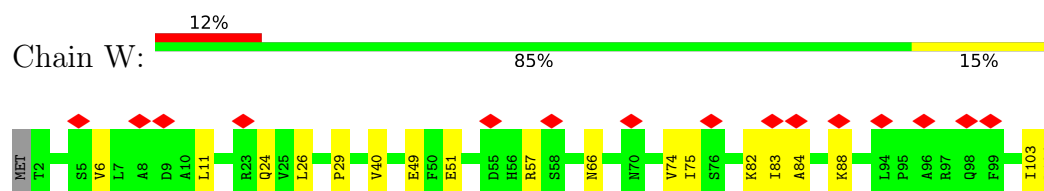
• Molecule 68: KLLA0F25542p



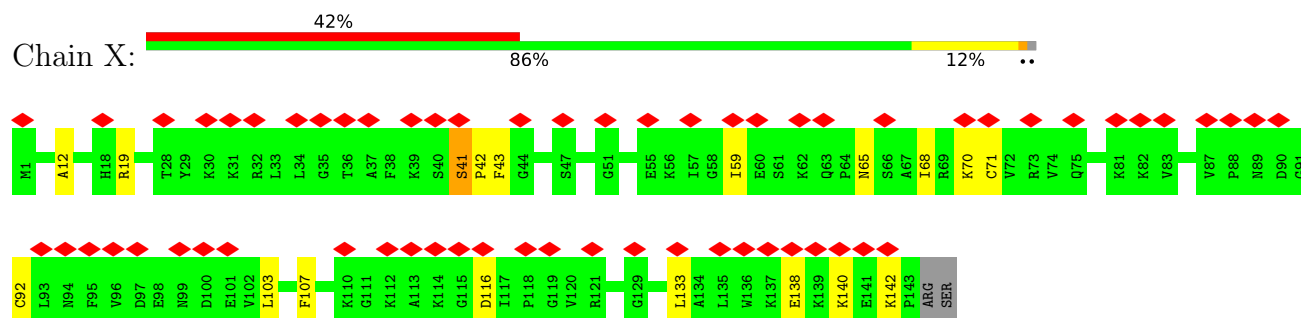
• Molecule 69: 40S ribosomal protein S21



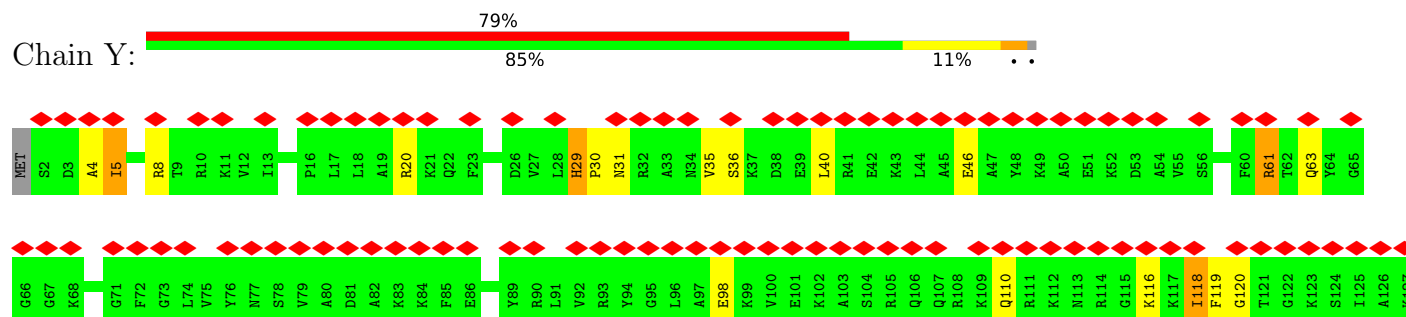
• Molecule 70: 40S ribosomal protein S22

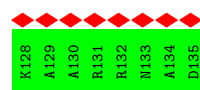


• Molecule 71: RPS23

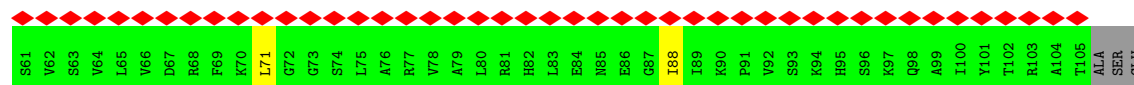


• Molecule 72: 40S ribosomal protein S24

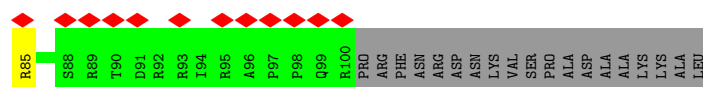
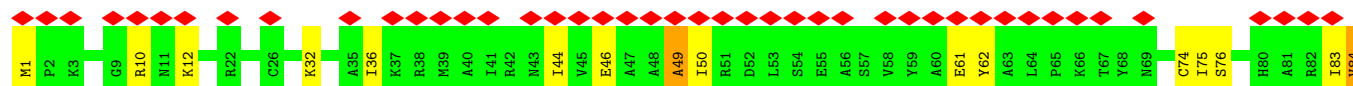




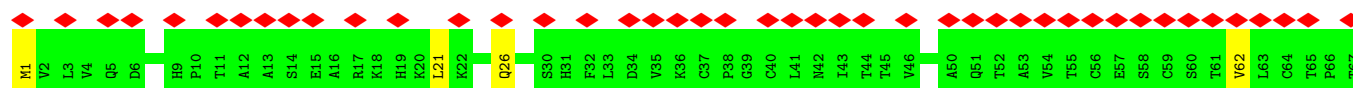
• Molecule 73: 40S ribosomal protein S25



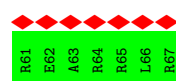
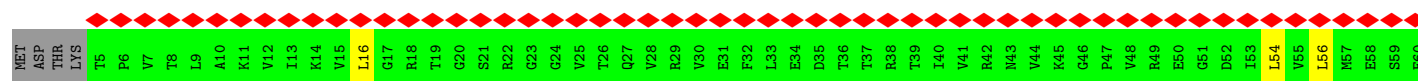
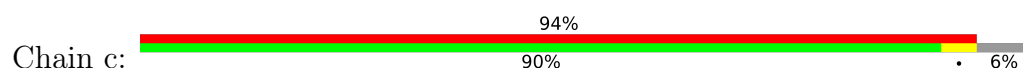
• Molecule 74: 40S ribosomal protein S26



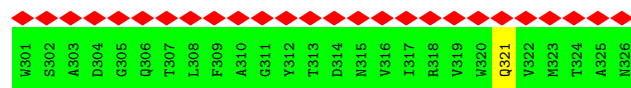
• Molecule 75: 40S ribosomal protein S27



• Molecule 76: 40S ribosomal protein S28



• Molecule 77: 40S ribosomal protein S29



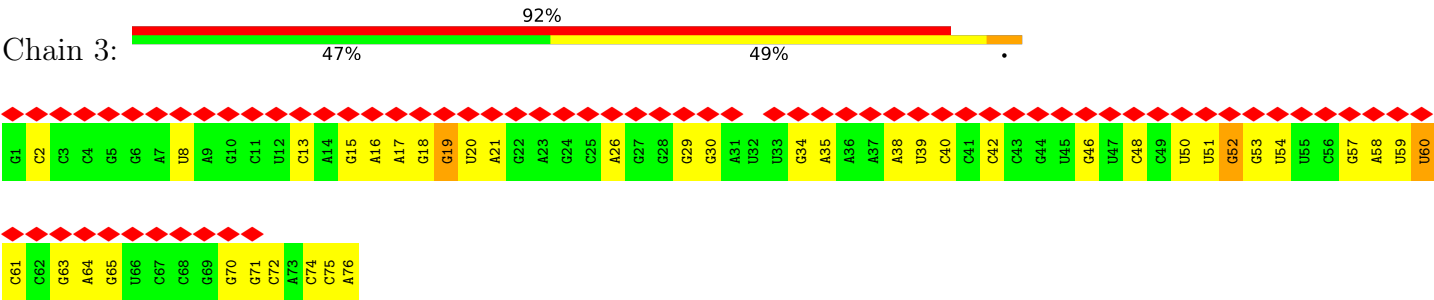
• Molecule 81: 18S ribosomal RNA







● Molecule 83: RNA (76-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.588	Depositor
Minimum map value	-0.380	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.11	Depositor
Map size ($\text{\AA}$)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/78206	0.68	63/121916 (0.1%)
2	7	0.37	0/2883	0.63	0/4491
3	8	0.37	0/3714	0.65	2/5781 (0.0%)
4	AA	0.55	0/1926	0.71	0/2588
5	AB	0.55	0/3136	0.71	0/4225
6	AC	0.70	1/2792 (0.0%)	0.91	3/3777 (0.1%)
7	AD	0.55	0/2436	0.74	0/3292
8	AE	0.62	0/1343	0.81	2/1804 (0.1%)
9	AF	0.59	0/1810	0.80	0/2440
10	AG	0.58	0/1846	0.84	2/2486 (0.1%)
11	AH	0.55	0/1547	0.72	0/2083
12	AI	0.54	0/1725	0.69	0/2310
13	AJ	0.58	0/1370	0.79	1/1835 (0.1%)
14	AL	0.58	0/1607	0.81	0/2156
15	AM	0.58	0/1060	0.83	0/1430
16	AN	0.56	0/1746	0.76	0/2339
17	AO	0.27	0/1602	0.63	0/2151
18	AP	0.57	0/1455	0.81	0/1952
19	AQ	0.56	0/1469	0.79	0/1970
20	AR	0.62	0/1539	0.85	0/2047
21	AS	0.55	0/1458	0.74	0/1964
22	AT	0.55	0/1286	0.70	0/1722
23	AU	0.55	0/824	0.72	0/1113
24	AV	0.59	1/991 (0.1%)	0.73	0/1331
25	AW	0.55	0/528	0.68	0/703
26	AX	0.54	0/979	0.72	0/1320
27	AY	0.59	0/1003	0.74	0/1339
28	AZ	0.58	0/1114	0.80	0/1493
29	Ba	0.56	0/1186	0.82	2/1590 (0.1%)
30	Bb	0.54	0/468	0.76	0/621
31	Bc	0.57	0/748	0.74	0/1005
32	Bd	0.53	0/885	0.67	0/1186

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Be	0.56	0/998	0.71	0/1332
34	Bf	0.55	0/855	0.71	0/1150
35	Bg	0.57	0/961	0.76	0/1281
36	Bh	0.58	0/970	0.81	0/1291
37	Bi	0.63	0/773	0.85	0/1029
38	Bj	0.58	0/690	0.77	0/913
39	Bk	0.67	1/626 (0.2%)	0.96	0/835
40	Bl	0.59	0/435	0.75	0/577
41	Bm	0.58	0/416	0.74	0/552
42	Bn	0.59	0/219	0.82	0/281
43	Bo	0.56	0/825	0.81	2/1086 (0.2%)
44	Bp	0.63	0/667	0.91	0/891
45	Bq	0.63	1/1742 (0.1%)	0.93	2/2342 (0.1%)
46	Br	0.63	0/1535	0.86	1/2077 (0.0%)
48	A	0.60	0/1656	0.79	0/2264
49	B	0.59	1/1747 (0.1%)	0.74	0/2353
50	C	0.60	0/1659	0.84	4/2252 (0.2%)
51	D	0.58	0/1769	0.78	0/2378
52	E	0.58	0/2122	0.81	6/2861 (0.2%)
53	F	0.59	0/1628	0.86	3/2198 (0.1%)
54	G	0.56	0/1835	0.74	0/2451
55	H	0.58	0/1507	0.76	0/2028
56	I	0.59	0/1519	0.77	0/2033
57	J	0.60	0/1495	0.82	0/2001
58	K	0.57	0/831	0.82	2/1123 (0.2%)
59	L	0.61	0/1194	0.75	0/1611
60	M	0.60	0/929	0.79	0/1255
61	N	0.57	0/1210	0.83	0/1628
62	O	0.58	0/953	0.81	0/1279
63	P	0.66	0/969	0.89	5/1302 (0.4%)
64	Q	0.59	0/1125	0.78	0/1510
65	R	0.57	0/994	0.83	0/1335
66	S	0.65	0/1157	0.82	0/1554
67	T	0.57	0/1129	0.80	0/1520
68	U	0.59	0/857	0.71	0/1158
69	V	0.54	0/696	0.73	0/938
70	W	0.56	0/1039	0.77	0/1399
71	X	0.59	0/1128	0.79	2/1504 (0.1%)
72	Y	0.60	0/1075	0.84	2/1433 (0.1%)
73	Z	0.59	0/567	0.74	0/762
74	a	0.64	0/810	0.84	0/1084
75	b	0.53	0/627	0.74	0/847
76	c	0.57	0/496	0.68	0/666

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	d	0.53	0/457	0.65	0/607
78	e	0.55	0/450	0.71	0/599
79	f	0.56	0/344	0.70	0/458
80	g	0.56	0/2521	0.70	2/3431 (0.1%)
81	2	0.38	0/42269	0.70	31/65862 (0.0%)
82	1	0.61	0/4776	0.88	5/6459 (0.1%)
83	3	0.38	0/1815	0.72	1/2829 (0.0%)
All	All	0.47	5/225749 (0.0%)	0.73	143/331069 (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	2	0
4	AA	0	1
6	AC	0	7
8	AE	0	8
29	Ba	0	1
34	Bf	0	1
37	Bi	0	4
39	Bk	0	1
45	Bq	0	6
65	R	0	1
72	Y	0	2
74	a	0	1
82	1	0	6
All	All	2	39

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AC	74	ILE	C-N	16.36	1.50	1.33
45	Bq	60	ARG	C-N	7.05	1.50	1.33
24	AV	81	GLN	CA-C	5.46	1.55	1.52
49	B	189	ILE	CA-CB	5.45	1.57	1.54
39	Bk	70	PRO	CA-C	5.23	1.54	1.51

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	Bq	60	ARG	CA-C-N	15.53	139.25	119.84
45	Bq	60	ARG	C-N-CA	15.53	139.25	119.84
6	AC	74	ILE	CA-C-N	14.22	137.72	120.23
6	AC	74	ILE	C-N-CA	14.22	137.72	120.23
1	5	1191	U	N1-C1'-C2'	10.60	127.90	112.00
81	2	1534	G	C2'-C3'-O3'	9.46	123.69	109.50
10	AG	125	SER	CA-C-N	8.80	130.84	119.84
10	AG	125	SER	C-N-CA	8.80	130.84	119.84
1	5	297	G	C2'-C3'-O3'	8.56	122.33	109.50
1	5	2422	U	C4'-C3'-O3'	8.49	122.13	109.40
1	5	1194	A	C2'-C3'-O3'	8.30	121.94	109.50
81	2	72	A	C4'-C3'-O3'	8.19	121.69	109.40
3	8	125	U	C2'-C3'-O3'	8.03	121.55	109.50
52	E	116	ASP	N-CA-C	7.96	120.73	111.02
81	2	542	C	C4'-C3'-O3'	7.96	121.34	109.40
1	5	2939	A	C4'-C3'-O3'	7.90	121.25	109.40
1	5	2922	U	C2'-C3'-O3'	7.76	121.14	109.50
1	5	2506	U	C5'-C4'-C3'	7.72	127.58	116.00
1	5	2032	U	C2'-C3'-O3'	7.70	121.04	109.50
81	2	700	C	C2'-C3'-O3'	7.66	120.99	109.50
1	5	1278	G	C2'-C3'-O3'	7.66	120.98	109.50
1	5	2455	A	C2'-C3'-O3'	7.55	120.83	109.50
1	5	1323	A	C2'-C3'-O3'	7.49	120.74	109.50
83	3	19	G	C4'-C3'-O3'	7.42	120.52	109.40
1	5	2217	C	C4'-C3'-O3'	7.38	124.06	113.00
1	5	2530	A	C4'-C3'-O3'	7.34	120.42	109.40
1	5	1035	A	C2'-C3'-O3'	7.31	120.46	109.50
81	2	1243	A	C2'-C3'-O3'	7.26	120.40	109.50
71	X	41	SER	CA-C-N	7.25	128.90	119.84
71	X	41	SER	C-N-CA	7.25	128.90	119.84
1	5	2061	A	C4'-C3'-O3'	7.24	120.26	109.40
52	E	116	ASP	CA-C-N	7.24	134.72	121.70
52	E	116	ASP	C-N-CA	7.24	134.72	121.70
81	2	1714	C	C4'-C3'-O3'	7.21	120.21	109.40
81	2	828	A	C2'-C3'-O3'	7.18	120.27	109.50
29	Ba	49	HIS	CA-C-N	7.11	128.72	119.84
29	Ba	49	HIS	C-N-CA	7.11	128.72	119.84
81	2	1598	A	C4'-C3'-O3'	7.11	120.06	109.40
1	5	298	U	C2'-C3'-O3'	7.08	120.12	109.50
1	5	987	C	C2'-C3'-O3'	7.07	120.10	109.50
1	5	1785	A	C2'-C3'-O3'	7.05	120.08	109.50
1	5	2469	A	C2'-C3'-O3'	7.03	120.05	109.50
63	P	18	LYS	N-CA-C	6.99	119.08	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	998	A	C4'-C3'-O3'	6.95	119.83	109.40
58	K	87	PHE	CA-C-N	6.94	128.52	119.84
58	K	87	PHE	C-N-CA	6.94	128.52	119.84
53	F	220	GLU	CA-C-N	6.94	134.19	121.70
53	F	220	GLU	C-N-CA	6.94	134.19	121.70
1	5	518	C	C4'-C3'-O3'	6.90	119.75	109.40
1	5	735	U	C2'-C3'-O3'	6.84	119.75	109.50
1	5	2946	U	C4'-C3'-O3'	6.83	119.65	109.40
81	2	279	U	C2'-C3'-O3'	6.82	119.74	109.50
1	5	1611	A	C2'-C3'-O3'	6.58	119.37	109.50
1	5	1612	A	C2'-C3'-O3'	6.56	119.33	109.50
81	2	1765	G	C2'-C3'-O3'	6.43	119.15	109.50
82	1	596	GLU	CA-C-N	6.40	133.22	121.70
82	1	596	GLU	C-N-CA	6.40	133.22	121.70
81	2	65	A	C4'-C3'-O3'	6.39	118.99	109.40
1	5	3257	A	C2'-C3'-O3'	6.35	123.22	113.70
1	5	887	G	C4'-C3'-O3'	6.30	122.45	113.00
50	C	174	LEU	CA-C-N	6.28	133.00	121.70
50	C	174	LEU	C-N-CA	6.28	133.00	121.70
81	2	695	U	C4'-C3'-O3'	6.20	118.70	109.40
81	2	277	U	C2'-C3'-O3'	6.19	118.78	109.50
6	AC	344	VAL	CA-C-O	-6.06	113.20	120.78
1	5	692	U	C2'-C3'-O3'	6.04	118.57	109.50
1	5	887	G	C2'-C3'-O3'	-5.98	104.73	113.70
81	2	452	U	N1-C1'-C2'	5.94	120.91	112.00
1	5	930	C	C2'-C3'-O3'	-5.92	104.82	113.70
81	2	721	U	C2'-C3'-O3'	5.91	118.36	109.50
1	5	121	A	C2'-C3'-O3'	5.83	118.25	109.50
1	5	3237	U	C4'-C3'-O3'	5.82	118.12	109.40
81	2	708	C	C4'-C3'-O3'	5.81	118.12	109.40
81	2	73	U	C2'-C3'-O3'	5.78	118.17	109.50
81	2	1195	A	C2'-C3'-O3'	5.76	118.13	109.50
1	5	2529	C	N1-C1'-C2'	5.73	120.60	112.00
1	5	3046	U	C2'-C3'-O3'	5.73	118.09	109.50
53	F	192	ILE	N-CA-C	5.72	121.23	109.34
1	5	166	C	C4'-C3'-O3'	5.71	117.97	109.40
1	5	3196	C	C2'-C3'-O3'	5.71	118.07	109.50
80	g	75	SER	CA-C-N	5.68	131.92	121.70
80	g	75	SER	C-N-CA	5.68	131.92	121.70
1	5	1685	U	C2'-C3'-O3'	5.66	117.99	109.50
81	2	1491	A	C3'-C2'-O2'	5.64	119.16	110.70
8	AE	65	GLY	CA-C-N	5.61	126.85	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AE	65	GLY	C-N-CA	5.61	126.85	119.84
63	P	28	MET	CA-C-N	5.57	126.80	119.84
63	P	28	MET	C-N-CA	5.57	126.80	119.84
52	E	126	VAL	CA-C-N	5.55	131.69	121.70
52	E	126	VAL	C-N-CA	5.55	131.69	121.70
81	2	177	U	C2'-C3'-O3'	5.55	117.82	109.50
50	C	148	TYR	CA-C-N	5.54	131.66	121.70
50	C	148	TYR	C-N-CA	5.54	131.66	121.70
1	5	1300	U	C4'-C3'-O3'	5.53	117.69	109.40
82	1	954	TRP	CA-C-N	5.53	131.65	121.70
82	1	954	TRP	C-N-CA	5.53	131.65	121.70
13	AJ	27	GLY	N-CA-C	5.51	116.74	111.67
81	2	903	G	C2'-C3'-O3'	5.51	121.97	113.70
43	Bo	16	GLU	CA-C-N	5.51	131.61	121.70
43	Bo	16	GLU	C-N-CA	5.51	131.61	121.70
46	Br	40	MET	N-CA-C	-5.50	105.61	112.93
1	5	1212	U	C2'-C3'-O3'	5.47	117.71	109.50
81	2	1613	C	C4'-C3'-O3'	5.42	117.54	109.40
1	5	3252	G	C2'-C3'-O3'	5.41	117.62	109.50
81	2	1080	A	C4'-C3'-O3'	5.41	117.51	109.40
1	5	2506	U	C5'-C4'-O4'	5.40	117.90	109.80
81	2	829	U	C2'-C3'-O3'	5.39	117.58	109.50
1	5	2456	U	C2'-C3'-O3'	5.39	117.58	109.50
81	2	909	C	C3'-C2'-O2'	5.37	118.76	110.70
1	5	2437	A	C4'-C3'-O3'	5.35	117.43	109.40
1	5	2041	C	C2'-C3'-O3'	5.34	121.72	113.70
1	5	2041	C	C3'-C2'-O2'	5.33	118.70	110.70
1	5	1326	A	C2'-C3'-O3'	5.33	117.50	109.50
1	5	3285	U	C2'-C3'-O3'	5.33	117.49	109.50
81	2	66	U	C2'-C3'-O3'	5.32	117.48	109.50
1	5	2474	U	C4'-C3'-O3'	5.30	117.36	109.40
1	5	1600	C	N1-C1'-C2'	5.29	119.94	112.00
82	1	454	ARG	N-CA-C	5.29	119.04	112.58
1	5	3325	U	C3'-C2'-O2'	5.29	118.63	110.70
3	8	126	A	C4'-C3'-O3'	5.28	117.32	109.40
1	5	2909	A	C2'-C3'-O3'	5.28	117.42	109.50
1	5	1255	C	C3'-C2'-O2'	5.25	118.58	110.70
1	5	1539	U	C4'-C3'-O3'	5.25	120.87	113.00
1	5	3308	G	C4'-C3'-O3'	5.22	117.22	109.40
81	2	1343	A	C3'-C2'-O2'	5.19	118.48	110.70
1	5	2341	A	C4'-C3'-O3'	5.18	117.17	109.40
63	P	37	ALA	N-CA-C	5.16	112.66	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
81	2	564	C	C4'-C3'-O3'	5.14	117.11	109.40
1	5	3349	U	C4'-C3'-O3'	5.13	117.10	109.40
1	5	3257	A	C3'-C2'-O2'	5.12	118.38	110.70
63	P	16	SER	N-CA-C	5.11	114.58	107.73
1	5	3285	U	C4'-C3'-O3'	5.08	117.03	109.40
81	2	912	G	C2'-C3'-O3'	5.08	121.32	113.70
1	5	3089	U	C4'-C3'-O3'	5.08	117.02	109.40
1	5	2081	U	C2'-C3'-O3'	5.07	117.11	109.50
1	5	3349	U	C2'-C3'-O3'	5.06	117.09	109.50
1	5	3162	U	C2'-C3'-O3'	5.05	117.08	109.50
72	Y	29	HIS	CA-C-N	5.05	126.16	119.84
72	Y	29	HIS	C-N-CA	5.05	126.16	119.84
81	2	1628	U	C4'-C3'-O3'	5.05	120.57	113.00
1	5	2645	G	C4'-C3'-O3'	5.04	116.96	109.40
81	2	217	A	C3'-C2'-O2'	5.03	118.24	110.70
52	E	116	ASP	CA-C-O	-5.00	115.57	121.07

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	5	1191	U	C1'
1	5	2506	U	C4'

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
82	1	442	THR	Peptide
82	1	443	PRO	Peptide
82	1	446	GLU	Peptide
82	1	799	ASP	Peptide
82	1	801	ILE	Peptide
82	1	802	TYR	Peptide
4	AA	196	TRP	Peptide
6	AC	343	LYS	Peptide
6	AC	345	ASP	Peptide
6	AC	346	GLN	Peptide
6	AC	347	ALA	Peptide
6	AC	349	LYS	Peptide
6	AC	351	LYS	Peptide
6	AC	73	ARG	Peptide
8	AE	110	SER	Peptide
8	AE	111	ARG	Peptide

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Mol	Chain	Res	Type	Group
8	AE	113	GLN	Peptide
8	AE	114	ARG	Peptide
8	AE	12	GLU	Peptide
8	AE	13	VAL	Peptide
8	AE	14	PRO	Peptide
8	AE	15	ALA	Peptide
29	Ba	49	HIS	Peptide
34	Bf	103	TYR	Peptide
37	Bi	32	ALA	Peptide
37	Bi	33	ALA	Peptide
37	Bi	34	SER	Peptide
37	Bi	35	GLN	Peptide
39	Bk	5	ILE	Peptide
45	Bq	179	LEU	Peptide
45	Bq	180	VAL	Peptide
45	Bq	214	TYR	Peptide
45	Bq	215	ARG	Peptide
45	Bq	216	LEU	Peptide
45	Bq	59	PRO	Peptide
65	R	78	ARG	Peptide
72	Y	120	GLY	Peptide
72	Y	29	HIS	Peptide
74	a	49	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	69874	0	35111	122	0
2	7	2579	0	1304	3	0
3	8	3326	0	1680	0	0
4	AA	1892	0	1954	8	0
5	AB	3064	0	3140	13	0
6	AC	2743	0	2865	25	0
7	AD	2384	0	2337	1	0
8	AE	1321	0	1412	34	0
9	AF	1774	0	1832	4	0
10	AG	1817	0	1927	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AH	1528	0	1596	7	0
12	AI	1690	0	1729	3	0
13	AJ	1349	0	1382	3	0
14	AL	1581	0	1661	4	0
15	AM	1045	0	1126	2	0
16	AN	1709	0	1763	1	0
17	AO	1571	0	1669	3	0
18	AP	1432	0	1465	4	0
19	AQ	1444	0	1541	2	0
20	AR	1522	0	1622	14	0
21	AS	1422	0	1466	9	0
22	AT	1262	0	1309	1	0
23	AU	807	0	821	0	0
24	AV	976	0	1021	2	0
25	AW	515	0	532	1	0
26	AX	964	0	1031	1	0
27	AY	992	0	1070	1	0
28	AZ	1089	0	1150	3	0
29	Ba	1156	0	1206	0	0
30	Bb	458	0	486	0	0
31	Bc	740	0	792	1	0
32	Bd	869	0	920	1	0
33	Be	980	0	1048	2	0
34	Bf	837	0	861	2	0
35	Bg	951	0	1036	0	0
36	Bh	961	0	1062	1	0
37	Bi	766	0	840	13	0
38	Bj	675	0	678	2	0
39	Bk	619	0	675	6	0
40	Bl	428	0	464	0	0
41	Bm	410	0	447	0	0
42	Bn	218	0	266	3	0
43	Bo	814	0	875	3	0
44	Bp	660	0	690	4	0
45	Bq	1716	0	1819	65	0
46	Br	1508	0	1542	10	0
47	AK	735	0	178	0	0
48	A	1616	0	1636	6	0
49	B	1722	0	1795	2	0
50	C	1629	0	1710	11	0
51	D	1744	0	1826	4	0
52	E	2078	0	2157	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	F	1609	0	1679	7	0
54	G	1812	0	1911	3	0
55	H	1483	0	1579	2	0
56	I	1493	0	1515	5	0
57	J	1471	0	1554	4	0
58	K	809	0	810	1	0
59	L	1168	0	1227	3	0
60	M	922	0	953	2	0
61	N	1187	0	1251	2	0
62	O	942	0	979	4	0
63	P	950	0	1001	10	0
64	Q	1105	0	1170	1	0
65	R	983	0	1033	3	0
66	S	1138	0	1161	5	0
67	T	1110	0	1124	1	0
68	U	845	0	913	5	0
69	V	687	0	682	0	0
70	W	1021	0	1056	5	0
71	X	1110	0	1192	4	0
72	Y	1061	0	1111	10	0
73	Z	558	0	585	0	0
74	a	798	0	854	6	0
75	b	617	0	643	0	0
76	c	494	0	534	1	0
77	d	446	0	436	0	0
78	e	443	0	481	0	0
79	f	337	0	333	1	0
80	g	2466	0	2406	5	0
81	2	37797	0	19016	93	0
82	1	4702	0	4822	62	0
83	3	1623	0	823	12	0
84	Bj	1	0	0	0	0
84	Bm	1	0	0	0	0
84	Bo	1	0	0	0	0
84	a	1	0	0	0	0
84	b	1	0	0	0	0
84	f	1	0	0	0	0
85	1	32	0	14	0	0
All	All	211187	0	157373	618	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (618) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AE:113:GLN:HA	8:AE:117:ALA:CB	1.12	1.54
81:2:214:A:C6	81:2:241:U:C4	1.95	1.54
1:5:2502:G:N2	1:5:2516:A:C4	1.77	1.51
8:AE:113:GLN:CA	8:AE:117:ALA:HB3	1.33	1.51
81:2:214:A:C2	81:2:241:U:O4	1.63	1.50
45:Bq:205:VAL:HA	45:Bq:216:LEU:CD2	1.47	1.44
45:Bq:169:VAL:O	45:Bq:179:LEU:CD1	1.65	1.42
45:Bq:204:LEU:O	45:Bq:216:LEU:CB	1.69	1.37
81:2:214:A:C6	81:2:241:U:C5	2.11	1.37
45:Bq:205:VAL:HA	45:Bq:216:LEU:CG	1.57	1.35
37:Bi:34:SER:OG	37:Bi:38:THR:HG23	1.17	1.34
81:2:214:A:C5	81:2:241:U:C4	2.15	1.33
81:2:214:A:C5	81:2:241:U:N3	1.98	1.32
45:Bq:204:LEU:O	45:Bq:216:LEU:HB3	1.19	1.31
8:AE:13:VAL:HG22	8:AE:14:PRO:CD	1.63	1.28
1:5:3073:U:C4	1:5:3097:A:N7	2.00	1.27
45:Bq:180:VAL:O	45:Bq:183:ILE:HB	1.34	1.26
1:5:2187:G:C6	1:5:2197:A:N1	1.95	1.23
45:Bq:169:VAL:O	45:Bq:179:LEU:HD11	1.24	1.21
81:2:214:A:C4	81:2:241:U:N3	2.09	1.20
8:AE:13:VAL:CG2	8:AE:14:PRO:HD3	1.72	1.19
45:Bq:148:VAL:HG22	45:Bq:152:LYS:HE3	1.22	1.18
81:2:214:A:N1	81:2:241:U:O4	1.76	1.17
81:2:214:A:N6	81:2:241:U:C5	2.11	1.17
1:5:2880:G:C2	1:5:3098:A:C8	2.33	1.16
1:5:2880:G:N1	1:5:3098:A:N7	1.93	1.16
45:Bq:205:VAL:CA	45:Bq:216:LEU:HD23	1.77	1.13
45:Bq:169:VAL:O	45:Bq:179:LEU:HD12	1.46	1.13
81:2:321:G:C6	81:2:336:G:O6	2.03	1.12
37:Bi:34:SER:OG	37:Bi:38:THR:CG2	1.97	1.12
82:1:400:ALA:HB2	82:1:799:ASP:O	1.48	1.11
1:5:2187:G:C5	1:5:2197:A:N1	2.16	1.11
81:2:214:A:N7	81:2:241:U:C2	2.20	1.10
45:Bq:205:VAL:HA	45:Bq:216:LEU:HD23	1.21	1.10
45:Bq:205:VAL:HA	45:Bq:216:LEU:HG	1.33	1.10
81:2:214:A:N1	81:2:241:U:C4	2.15	1.09
20:AR:53:LYS:HG2	20:AR:54:PRO:HD2	1.11	1.08
45:Bq:180:VAL:HG12	45:Bq:183:ILE:HD12	1.16	1.06
45:Bq:205:VAL:CG1	45:Bq:216:LEU:HB2	1.84	1.06
45:Bq:204:LEU:O	45:Bq:216:LEU:CG	2.03	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:Bq:180:VAL:HG12	45:Bq:183:ILE:CD1	1.85	1.05
45:Bq:205:VAL:CA	45:Bq:216:LEU:CD2	2.34	1.04
1:5:2502:G:C2	1:5:2516:A:C4	2.46	1.03
45:Bq:205:VAL:HG12	45:Bq:216:LEU:HB2	1.06	1.03
45:Bq:180:VAL:O	45:Bq:183:ILE:CB	2.05	1.03
81:2:214:A:C8	81:2:241:U:C2	2.47	1.02
1:5:3073:U:O4	1:5:3097:A:C8	2.12	1.02
81:2:214:A:C2	81:2:241:U:C4	2.47	1.02
20:AR:53:LYS:HG2	20:AR:54:PRO:CD	1.91	1.00
8:AE:113:GLN:CA	8:AE:117:ALA:CB	2.09	0.99
45:Bq:180:VAL:CG1	45:Bq:183:ILE:HD12	1.91	0.99
1:5:2880:G:C6	1:5:3098:A:N7	2.28	0.99
82:1:383:LYS:HD2	82:1:442:THR:HG23	1.43	0.98
81:2:214:A:C5	81:2:241:U:C2	2.52	0.98
1:5:2502:G:N2	1:5:2516:A:N3	2.11	0.97
45:Bq:205:VAL:CB	45:Bq:216:LEU:HD23	1.95	0.97
81:2:214:A:C4	81:2:241:U:C4	2.49	0.96
81:2:321:G:N1	81:2:336:G:C6	2.33	0.96
1:5:3073:U:O4	1:5:3097:A:N7	1.99	0.96
8:AE:113:GLN:HA	8:AE:117:ALA:HB1	1.47	0.96
83:3:51:U:N3	83:3:64:A:N1	2.13	0.95
1:5:2880:G:N1	1:5:3098:A:C8	2.33	0.95
1:5:2502:G:N2	1:5:2516:A:N9	1.99	0.95
1:5:564:G:O2'	8:AE:14:PRO:O	1.86	0.94
37:Bi:36:ARG:HH11	37:Bi:36:ARG:HG2	1.33	0.94
72:Y:119:PHE:HE1	81:2:86:A:C5'	1.82	0.93
45:Bq:204:LEU:O	45:Bq:216:LEU:HG	1.70	0.92
45:Bq:205:VAL:CA	45:Bq:216:LEU:HG	2.00	0.92
45:Bq:204:LEU:C	45:Bq:216:LEU:HG	1.95	0.92
1:5:2502:G:C2	1:5:2516:A:C5	2.59	0.91
45:Bq:180:VAL:O	45:Bq:183:ILE:N	2.04	0.90
45:Bq:205:VAL:HG12	45:Bq:216:LEU:CB	1.98	0.90
45:Bq:205:VAL:CA	45:Bq:216:LEU:CG	2.47	0.89
82:1:400:ALA:CB	82:1:799:ASP:O	2.20	0.89
20:AR:53:LYS:CG	20:AR:54:PRO:HD2	2.02	0.89
45:Bq:148:VAL:CG2	45:Bq:152:LYS:HE3	2.04	0.88
1:5:2187:G:C4	1:5:2197:A:N1	2.37	0.88
21:AS:159:THR:HG23	21:AS:161:LYS:O	1.76	0.85
45:Bq:180:VAL:O	45:Bq:183:ILE:CA	2.24	0.85
45:Bq:205:VAL:HB	45:Bq:216:LEU:HD23	1.58	0.85
1:5:2502:G:H22	1:5:2516:A:C1'	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AE:113:GLN:HA	8:AE:117:ALA:CA	2.04	0.84
81:2:214:A:C8	81:2:241:U:O2	2.31	0.83
37:Bi:34:SER:HG	37:Bi:38:THR:HG23	1.42	0.82
82:1:799:ASP:N	82:1:799:ASP:OD1	2.11	0.82
81:2:321:G:N1	81:2:336:G:O6	2.09	0.81
1:5:2187:G:C6	1:5:2197:A:C6	2.69	0.80
72:Y:119:PHE:HE1	81:2:86:A:H5''	1.45	0.79
1:5:2194:U:H6	1:5:2194:U:C5'	1.95	0.79
1:5:2257:G:C2	1:5:2258:U:N3	2.51	0.79
83:3:50:U:O2	83:3:65:G:N2	2.16	0.79
81:2:1114:U:H2'	81:2:1114:U:O2	1.82	0.78
6:AC:74:ILE:HD11	6:AC:94:CYS:SG	2.24	0.78
45:Bq:180:VAL:C	45:Bq:183:ILE:H	1.90	0.78
1:5:2880:G:N2	1:5:3098:A:C8	2.52	0.78
60:M:54:VAL:HG13	60:M:82:VAL:HG21	1.65	0.77
1:5:2501:U:H5''	1:5:2501:U:H6	1.49	0.77
45:Bq:148:VAL:HG22	45:Bq:152:LYS:CE	2.10	0.77
82:1:801:ILE:HA	82:1:804:LEU:HD23	1.67	0.77
81:2:214:A:N6	81:2:241:U:C6	2.52	0.77
81:2:1358:C:H2'	81:2:1359:A:H8	1.50	0.75
81:2:115:G:N2	81:2:333:G:N2	2.35	0.75
72:Y:119:PHE:HE1	81:2:86:A:H5'	1.50	0.75
83:3:50:U:C2	83:3:65:G:N2	2.55	0.75
8:AE:113:GLN:C	8:AE:117:ALA:HB3	2.12	0.74
74:a:49:ALA:HB3	74:a:50:ILE:HA	1.69	0.74
20:AR:89:LEU:HD12	20:AR:89:LEU:C	2.13	0.73
80:g:75:SER:HB3	80:g:76:ALA:HB3	1.69	0.73
81:2:214:A:N3	81:2:241:U:O4	2.21	0.73
1:5:1162:U:O2	17:AO:49:PHE:CE1	2.41	0.73
81:2:644:C:O2	81:2:690:A:C2	2.41	0.73
72:Y:119:PHE:CE1	81:2:86:A:C5'	2.71	0.73
72:Y:119:PHE:CE1	81:2:86:A:H5'	2.23	0.72
45:Bq:180:VAL:HA	45:Bq:183:ILE:HD12	1.71	0.71
1:5:2880:G:C6	1:5:3098:A:C5	2.78	0.71
45:Bq:59:PRO:HD2	45:Bq:152:LYS:O	1.89	0.71
6:AC:350:ILE:N	6:AC:350:ILE:HD12	2.05	0.71
82:1:596:GLU:HA	82:1:597:ALA:CB	2.21	0.71
20:AR:92:GLN:O	20:AR:96:ILE:HD12	1.92	0.69
1:5:2502:G:N1	1:5:2516:A:C5	2.59	0.69
54:G:5:ILE:HD12	54:G:16:ILE:HD13	1.73	0.69
45:Bq:180:VAL:C	45:Bq:183:ILE:HB	2.17	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:E:67:GLN:HA	52:E:68:ARG:HB2	1.73	0.69
1:5:3073:U:N3	1:5:3097:A:C5	2.61	0.68
72:Y:35:VAL:HG21	72:Y:40:LEU:HD11	1.75	0.68
8:AE:13:VAL:HG22	8:AE:14:PRO:HD3	0.79	0.68
8:AE:13:VAL:CG2	8:AE:14:PRO:CD	2.51	0.68
45:Bq:180:VAL:HA	45:Bq:183:ILE:CG1	2.24	0.68
1:5:591:C:OP2	8:AE:111:ARG:NH1	2.25	0.68
6:AC:156:LEU:HD12	6:AC:159:ILE:HD12	1.76	0.68
1:5:3073:U:N3	1:5:3097:A:N7	2.42	0.67
45:Bq:59:PRO:HD2	45:Bq:153:SER:HA	1.76	0.67
81:2:321:G:C2	81:2:336:G:C6	2.82	0.67
1:5:2257:G:N2	1:5:2258:U:O2	2.27	0.67
82:1:445:HIS:NE2	82:1:802:TYR:OH	2.27	0.66
83:3:52:G:N1	83:3:63:G:N2	2.42	0.66
6:AC:342:LYS:O	6:AC:344:VAL:N	2.29	0.66
8:AE:113:GLN:HE21	8:AE:114:ARG:HB2	1.61	0.66
1:5:3073:U:C2	1:5:3097:A:N6	2.64	0.66
6:AC:349:LYS:HB3	6:AC:351:LYS:HB2	1.78	0.66
46:Br:91:THR:HG23	46:Br:98:ILE:HD13	1.77	0.66
81:2:1359:A:N3	81:2:1359:A:H2'	2.10	0.66
45:Bq:148:VAL:O	45:Bq:152:LYS:HG3	1.95	0.66
82:1:774:LEU:HG	82:1:804:LEU:HD12	1.77	0.66
48:A:57:ILE:HD11	48:A:173:ILE:HD11	1.79	0.65
8:AE:114:ARG:HG3	8:AE:115:ALA:HA	1.79	0.64
1:5:1160:C:N3	1:5:1286:U:O2	2.31	0.64
1:5:2257:G:C2	1:5:2258:U:C2	2.86	0.64
45:Bq:180:VAL:HA	45:Bq:183:ILE:CD1	2.27	0.64
82:1:599:ILE:HD13	82:1:614:VAL:HG12	1.80	0.64
1:5:1319:U:H4'	1:5:1320:A:H5'	1.80	0.63
21:AS:6:GLU:O	21:AS:6:GLU:HG3	1.98	0.63
45:Bq:191:VAL:HG22	45:Bq:197:ASN:HB3	1.81	0.63
37:Bi:36:ARG:HG2	37:Bi:36:ARG:NH1	2.08	0.63
63:P:122:THR:HG21	81:2:1452:G:H4'	1.79	0.63
42:Bn:6:ARG:CZ	81:2:1114:U:H5'	2.28	0.63
1:5:2880:G:N2	1:5:3098:A:H8	1.94	0.63
45:Bq:59:PRO:CD	45:Bq:153:SER:HA	2.28	0.63
2:7:97:A:H4'	9:AF:221:ILE:HD11	1.80	0.63
1:5:2194:U:H6	1:5:2194:U:H5''	1.65	0.62
13:AJ:30:LEU:HD21	13:AJ:67:VAL:HG13	1.80	0.62
80:g:75:SER:CB	80:g:76:ALA:HB3	2.29	0.62
8:AE:13:VAL:HG13	8:AE:14:PRO:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:321:G:O6	81:2:336:G:O6	2.18	0.62
1:5:2502:G:O6	1:5:2515:C:N3	2.32	0.61
43:Bo:53:GLN:HG2	43:Bo:57:ILE:HD11	1.82	0.61
1:5:2502:G:N2	1:5:2516:A:C1'	2.57	0.61
50:C:174:LEU:HA	50:C:175:ILE:HB	1.82	0.61
1:5:518:C:H2'	1:5:518:C:O2	2.00	0.61
1:5:1321:A:O5'	1:5:1321:A:H8	1.84	0.60
6:AC:350:ILE:HD12	6:AC:350:ILE:H	1.65	0.60
37:Bi:36:ARG:HH11	37:Bi:36:ARG:CG	2.12	0.60
45:Bq:205:VAL:N	45:Bq:216:LEU:HG	2.15	0.60
1:5:2257:G:N1	1:5:2258:U:N3	2.50	0.60
82:1:596:GLU:HA	82:1:597:ALA:HB3	1.82	0.60
45:Bq:180:VAL:CB	45:Bq:183:ILE:HD12	2.31	0.59
1:5:2257:G:C6	1:5:2258:U:O4	2.55	0.59
81:2:1114:U:O2	81:2:1115:A:C8	2.54	0.59
20:AR:57:ILE:HG22	20:AR:57:ILE:O	2.02	0.59
8:AE:109:LEU:O	8:AE:111:ARG:HA	2.02	0.59
81:2:115:G:H21	81:2:333:G:N2	2.00	0.59
1:5:927:U:H6	1:5:927:U:O5'	1.86	0.59
1:5:1162:U:O2	17:AO:49:PHE:CZ	2.55	0.59
1:5:2217:C:H4'	1:5:2218:G:OP2	2.03	0.59
8:AE:114:ARG:N	8:AE:117:ALA:N	2.51	0.58
11:AH:41:ILE:HD11	11:AH:67:ALA:HB1	1.84	0.58
50:C:82:LYS:HA	50:C:83:ASP:HB2	1.86	0.58
81:2:645:U:H1'	81:2:689:G:N2	2.19	0.58
1:5:1600:C:H2'	1:5:1600:C:O2	2.03	0.58
6:AC:343:LYS:HB3	6:AC:344:VAL:HA	1.85	0.58
52:E:116:ASP:HB2	52:E:117:GLU:HB2	1.86	0.58
82:1:417:ILE:HG21	82:1:578:LEU:HD11	1.85	0.58
82:1:446:GLU:HG2	82:1:447:SER:HA	1.85	0.58
1:5:2529:C:H2'	1:5:2529:C:O2	2.04	0.58
6:AC:3:ILE:HG22	6:AC:3:ILE:O	2.03	0.57
45:Bq:180:VAL:CA	45:Bq:183:ILE:HD12	2.34	0.57
1:5:2503:G:H3'	1:5:2503:G:H8	1.69	0.57
14:AL:47:ALA:HB3	14:AL:48:PRO:HD3	1.85	0.57
1:5:2422:U:H4'	1:5:2423:G:OP1	2.05	0.57
1:5:3073:U:C2	1:5:3097:A:C6	2.93	0.57
32:Bd:32:ALA:HB1	32:Bd:59:ILE:HD11	1.86	0.57
82:1:804:LEU:O	82:1:804:LEU:HG	2.05	0.56
82:1:442:THR:HG22	82:1:444:GLY:H	1.70	0.56
81:2:240:U:H2'	81:2:240:U:O2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:1:801:ILE:HD13	82:1:801:ILE:O	2.06	0.56
37:Bi:34:SER:HB3	37:Bi:35:GLN:HA	1.88	0.56
81:2:214:A:C6	81:2:241:U:C6	2.84	0.56
81:2:1114:U:O2	81:2:1114:U:C2'	2.54	0.56
1:5:2502:G:H3'	1:5:2503:G:H5''	1.88	0.56
57:J:83:ILE:HD11	57:J:147:MET:HE3	1.88	0.55
6:AC:351:LYS:HD2	6:AC:351:LYS:O	2.07	0.55
82:1:802:TYR:N	82:1:802:TYR:CD2	2.73	0.55
72:Y:118:ILE:HD13	72:Y:118:ILE:O	2.06	0.55
45:Bq:115:VAL:HG23	45:Bq:116:LEU:HD22	1.89	0.55
81:2:1454:C:O2	81:2:1454:C:O4'	2.24	0.55
28:AZ:24:VAL:HG11	28:AZ:87:LEU:HD23	1.88	0.55
50:C:106:VAL:HG22	50:C:120:ILE:HD12	1.89	0.55
82:1:960:LEU:HD23	82:1:963:VAL:HG11	1.89	0.55
83:3:51:U:N3	83:3:64:A:C2	2.68	0.55
2:7:73:C:O2	2:7:73:C:O4'	2.25	0.54
43:Bo:72:LEU:HD11	43:Bo:83:LEU:HD12	1.88	0.54
45:Bq:23:THR:O	45:Bq:25:LYS:N	2.41	0.54
21:AS:159:THR:CG2	21:AS:161:LYS:O	2.53	0.54
62:O:117:ASP:HB2	74:a:44:ILE:HD11	1.89	0.54
81:2:25:C:O2	81:2:25:C:O4'	2.24	0.54
1:5:1407:U:C4	6:AC:71:VAL:O	2.61	0.54
1:5:2503:G:H3'	1:5:2503:G:C8	2.42	0.54
6:AC:348:ASN:OD1	6:AC:348:ASN:N	2.41	0.54
1:5:2500:C:H3'	1:5:2501:U:H5''	1.90	0.54
13:AJ:102:PHE:CE2	13:AJ:129:ILE:HD13	2.42	0.54
1:5:2502:G:N1	1:5:2516:A:N7	2.56	0.53
1:5:2196:C:H3'	1:5:2196:C:H6	1.73	0.53
82:1:445:HIS:C	82:1:445:HIS:CD2	2.85	0.53
82:1:954:TRP:HA	82:1:955:MET:HB2	1.90	0.53
81:2:214:A:C8	81:2:241:U:N3	2.70	0.53
82:1:446:GLU:CB	82:1:475:GLN:NE2	2.72	0.53
81:2:158:U:H2'	81:2:158:U:O2	2.07	0.53
27:AY:45:ILE:HD11	27:AY:119:ILE:HG23	1.91	0.53
8:AE:114:ARG:NH1	8:AE:114:ARG:HG2	2.23	0.53
82:1:463:ILE:HD11	82:1:577:LEU:HD21	1.91	0.53
1:5:885:A:C8	4:AA:199:THR:HG21	2.44	0.52
56:I:10:LYS:HE2	81:2:338:C:OP1	2.09	0.52
81:2:214:A:N9	81:2:241:U:N3	2.56	0.52
82:1:945:PHE:HA	82:1:946:ARG:C	2.35	0.52
8:AE:113:GLN:HE21	8:AE:114:ARG:HD3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
81:2:1015:C:O4'	81:2:1015:C:O2	2.26	0.52
81:2:646:G:C5	81:2:688:G:C2	2.98	0.52
83:3:52:G:H1	83:3:63:G:N2	2.07	0.52
63:P:57:MET:HE3	63:P:89:MET:HE2	1.92	0.52
46:Br:53:VAL:HG22	46:Br:89:ILE:HG23	1.91	0.52
11:AH:28:THR:HG22	11:AH:33:VAL:HG12	1.92	0.52
67:T:2:PRO:HB2	81:2:1359:A:O2'	2.09	0.52
21:AS:6:GLU:HG3	21:AS:64:ILE:HB	1.92	0.52
1:5:1407:U:C5	6:AC:71:VAL:O	2.63	0.52
1:5:2510:U:O2	1:5:2510:U:C2'	2.58	0.52
1:5:2413:C:O2	1:5:2413:C:C2'	2.57	0.51
1:5:1840:U:O2'	20:AR:58:HIS:HD2	1.93	0.51
8:AE:113:GLN:HA	8:AE:117:ALA:HB3	0.52	0.51
45:Bq:215:ARG:O	45:Bq:215:ARG:HG2	2.10	0.51
48:A:24:LEU:HD21	65:R:106:THR:HG21	1.92	0.51
51:D:176:LEU:HB2	51:D:177:LEU:HA	1.92	0.51
81:2:214:A:C5	81:2:241:U:C5	2.75	0.51
81:2:1765:G:O2'	81:2:1766:G:OP2	2.27	0.51
82:1:446:GLU:HB2	82:1:475:GLN:NE2	2.26	0.51
82:1:461:ILE:HD12	82:1:580:LEU:HD11	1.93	0.51
82:1:864:ALA:HB2	82:1:928:LEU:HD22	1.93	0.51
1:5:117:U:O2	1:5:117:U:C2'	2.58	0.51
31:Bc:17:VAL:HG11	31:Bc:92:ILE:HD12	1.92	0.51
46:Br:44:ARG:HG3	46:Br:53:VAL:HG21	1.92	0.51
70:W:82:LYS:O	70:W:84:ALA:N	2.43	0.51
33:Be:122:ALA:HA	33:Be:124:ALA:N	2.25	0.51
81:2:338:C:H2'	81:2:338:C:O2	2.11	0.51
83:3:51:U:O2	83:3:64:A:H2	1.94	0.51
1:5:135:C:C2'	1:5:135:C:O2	2.59	0.51
1:5:2180:U:O2	1:5:2180:U:O4'	2.29	0.51
6:AC:35:VAL:HG21	6:AC:244:LEU:HD21	1.93	0.51
6:AC:350:ILE:H	6:AC:350:ILE:CD1	2.22	0.51
45:Bq:12:ASN:HD21	45:Bq:216:LEU:HD21	1.76	0.51
68:U:34:LEU:HD11	68:U:89:ARG:HG3	1.93	0.51
21:AS:8:GLN:HB2	21:AS:64:ILE:HD11	1.91	0.51
82:1:484:ARG:HA	82:1:485:ASP:C	2.36	0.51
82:1:774:LEU:HB3	82:1:804:LEU:CD1	2.41	0.51
82:1:776:PHE:HE2	82:1:801:ILE:HB	1.75	0.51
1:5:518:C:O2	1:5:518:C:C2'	2.58	0.50
1:5:776:G:H5'	6:AC:74:ILE:N	2.25	0.50
57:J:7:THR:HG21	81:2:758:U:H5''	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:X:41:SER:O	71:X:43:PHE:N	2.44	0.50
1:5:3245:U:O2	1:5:3245:U:O4'	2.30	0.50
20:AR:53:LYS:CG	20:AR:54:PRO:CD	2.76	0.50
70:W:11:LEU:HD12	70:W:74:VAL:CG2	2.41	0.50
71:X:59:ILE:HD12	71:X:71:CYS:SG	2.52	0.50
81:2:214:A:N3	81:2:241:U:C4	2.74	0.50
81:2:1714:C:H4'	81:2:1715:G:OP1	2.11	0.50
1:5:2529:C:O2	1:5:2529:C:C2'	2.59	0.50
1:5:3073:U:C4	1:5:3097:A:C5	2.89	0.50
8:AE:114:ARG:CG	8:AE:114:ARG:HH11	2.24	0.50
68:U:23:ARG:HB2	68:U:117:ILE:HD12	1.94	0.50
82:1:774:LEU:CG	82:1:804:LEU:HD12	2.41	0.50
45:Bq:180:VAL:HA	45:Bq:183:ILE:HG13	1.91	0.50
46:Br:27:VAL:HG12	46:Br:193:TYR:HB2	1.94	0.50
6:AC:350:ILE:N	6:AC:350:ILE:CD1	2.73	0.50
45:Bq:60:ARG:HB2	45:Bq:152:LYS:HB3	1.93	0.50
70:W:40:VAL:HG11	70:W:103:ILE:HD12	1.93	0.50
44:Bp:47:VAL:HG13	44:Bp:48:LYS:HA	1.93	0.50
45:Bq:204:LEU:O	45:Bq:216:LEU:HB2	1.93	0.50
83:3:50:U:O2	83:3:65:G:C2	2.64	0.50
1:5:887:G:C6	4:AA:207:VAL:HG21	2.47	0.50
39:Bk:8:ILE:HG12	39:Bk:9:LYS:HA	1.94	0.50
57:J:7:THR:HG21	81:2:758:U:C5'	2.41	0.50
28:AZ:46:ILE:HD11	28:AZ:49:TYR:CE1	2.47	0.50
1:5:264:G:OP1	37:Bi:34:SER:O	2.29	0.49
1:5:987:C:O2	1:5:987:C:C2'	2.60	0.49
37:Bi:36:ARG:O	37:Bi:39:PHE:N	2.45	0.49
1:5:2384:C:H5'	4:AA:207:VAL:HG22	1.94	0.49
45:Bq:169:VAL:C	45:Bq:179:LEU:HD12	2.31	0.49
48:A:33:GLN:N	48:A:34:GLU:HB2	2.27	0.49
81:2:829:U:O2	81:2:829:U:C2'	2.59	0.49
82:1:443:PRO:O	82:1:451:LEU:CD1	2.60	0.49
55:H:122:HIS:CE1	55:H:177:THR:HG22	2.47	0.49
5:AB:229:VAL:HG11	5:AB:249:VAL:HG23	1.93	0.49
53:F:135:VAL:HG22	53:F:200:LEU:HD13	1.94	0.49
82:1:454:ARG:N	82:1:455:GLY:HA2	2.27	0.49
21:AS:4:ARG:HA	21:AS:4:ARG:HD3	1.58	0.49
37:Bi:20:LEU:HB3	37:Bi:21:THR:HB	1.95	0.49
62:O:81:ILE:HB	62:O:115:ILE:HG22	1.95	0.49
74:a:84:VAL:O	81:2:1795:A:N6	2.45	0.49
1:5:2804:C:O2	1:5:2804:C:O4'	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:AC:351:LYS:HE3	9:AF:64:ARG:HB3	1.94	0.49
20:AR:92:GLN:O	20:AR:92:GLN:HG3	2.13	0.49
8:AE:114:ARG:HA	8:AE:117:ALA:N	2.28	0.48
8:AE:13:VAL:HG13	8:AE:14:PRO:CD	2.42	0.48
82:1:443:PRO:O	82:1:451:LEU:HD12	2.14	0.48
83:3:52:G:H5''	83:3:52:G:H8	1.77	0.48
51:D:176:LEU:CB	51:D:177:LEU:HA	2.43	0.48
81:2:1456:G:H2'	81:2:1456:G:N3	2.27	0.48
1:5:2194:U:C5'	1:5:2194:U:C6	2.86	0.48
72:Y:119:PHE:CE1	81:2:86:A:H5''	2.35	0.48
59:L:130:PRO:O	81:2:335:G:H5'	2.14	0.48
72:Y:119:PHE:CD1	72:Y:119:PHE:C	2.92	0.48
50:C:174:LEU:HA	50:C:175:ILE:CB	2.44	0.48
18:AP:158:GLU:HA	18:AP:159:LYS:HB2	1.94	0.48
21:AS:90:MET:HE1	21:AS:114:HIS:CE1	2.49	0.48
50:C:58:ILE:O	50:C:60:GLU:N	2.46	0.48
81:2:1558:U:O2	81:2:1558:U:O4'	2.30	0.48
12:AI:53:VAL:HG21	12:AI:166:ILE:HD12	1.96	0.48
39:Bk:8:ILE:CG1	39:Bk:9:LYS:HA	2.43	0.48
53:F:114:ARG:HD2	64:Q:43:ILE:HD12	1.96	0.48
6:AC:292:SER:O	6:AC:293:THR:HG23	2.13	0.48
1:5:2257:G:N2	1:5:2258:U:C2	2.83	0.47
1:5:3073:U:N1	1:5:3097:A:N6	2.62	0.47
8:AE:113:GLN:HG2	8:AE:114:ARG:HB2	1.96	0.47
46:Br:31:GLY:HA2	46:Br:32:VAL:HB	1.96	0.47
82:1:823:PHE:CG	82:1:823:PHE:O	2.67	0.47
81:2:452:U:O2	81:2:452:U:H2'	2.12	0.47
26:AX:68:THR:HA	26:AX:73:MET:HE1	1.95	0.47
45:Bq:136:THR:HG23	45:Bq:138:VAL:HG23	1.95	0.47
59:L:3:THR:HB	59:L:4:GLU:HA	1.96	0.47
70:W:11:LEU:HD12	70:W:74:VAL:HG22	1.96	0.47
1:5:2503:G:C8	1:5:2503:G:C3'	2.98	0.47
81:2:1292:U:O2	81:2:1292:U:O4'	2.31	0.47
50:C:177:ALA:HB1	50:C:178:PRO:HD2	1.97	0.47
1:5:2413:C:O2	1:5:2413:C:O2'	2.31	0.47
51:D:11:LEU:HD22	68:U:84:MET:HE1	1.96	0.47
74:a:74:CYS:O	74:a:76:SER:N	2.48	0.47
82:1:839:ILE:HD12	82:1:846:ILE:HG22	1.96	0.47
1:5:2194:U:H5''	1:5:2194:U:C6	2.48	0.47
20:AR:58:HIS:ND1	20:AR:58:HIS:C	2.73	0.47
50:C:58:ILE:HG23	50:C:61:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:1:727:LEU:HD12	82:1:730:LEU:HD23	1.96	0.47
82:1:803:HIS:O	82:1:806:ASP:N	2.48	0.47
1:5:3036:U:OP1	20:AR:58:HIS:HA	2.15	0.47
82:1:468:ILE:HA	82:1:533:ILE:HD11	1.96	0.47
81:2:911:U:H2'	81:2:911:U:O2	2.15	0.47
11:AH:18:VAL:HG21	11:AH:53:ILE:HD11	1.97	0.47
46:Br:195:ASN:HB3	46:Br:196:GLY:HA3	1.97	0.46
82:1:834:ASN:CG	82:1:852:ILE:HD11	2.40	0.46
82:1:940:LEU:HD13	82:1:941:LYS:N	2.30	0.46
1:5:1841:C:H5'	20:AR:58:HIS:HB2	1.96	0.46
68:U:44:ASN:HD21	68:U:106:ILE:HD11	1.81	0.46
82:1:400:ALA:HB1	82:1:800:ILE:HG12	1.97	0.46
82:1:443:PRO:O	82:1:451:LEU:HG	2.16	0.46
57:J:133:HIS:HB2	57:J:134:ILE:HD12	1.96	0.46
82:1:730:LEU:HD21	82:1:747:VAL:CG1	2.45	0.46
1:5:2506:U:OP2	49:B:227:SER:N	2.49	0.46
1:5:2915:G:N3	5:AB:250:ALA:HB1	2.31	0.46
8:AE:114:ARG:HB2	8:AE:117:ALA:O	2.15	0.46
8:AE:114:ARG:HG2	8:AE:114:ARG:HH11	1.80	0.46
81:2:829:U:O2	81:2:829:U:H2'	2.15	0.46
4:AA:180:LEU:HD11	44:Bp:26:VAL:HG21	1.96	0.46
46:Br:36:SER:N	46:Br:107:VAL:HG11	2.30	0.46
81:2:506:U:O2	81:2:506:U:O4'	2.33	0.46
81:2:1716:A:H2'	81:2:1717:A:C8	2.49	0.46
1:5:1161:A:H3'	1:5:1161:A:N3	2.30	0.46
1:5:1207:G:N2	1:5:1215:A:OP1	2.49	0.46
1:5:2510:U:O2	1:5:2510:U:H2'	2.15	0.46
1:5:3125:U:H3'	1:5:3126:G:C5'	2.46	0.46
5:AB:217:VAL:HG11	5:AB:328:ILE:HG23	1.98	0.46
8:AE:13:VAL:CB	8:AE:14:PRO:CD	2.94	0.46
13:AJ:54:VAL:HG11	13:AJ:57:PHE:CD2	2.50	0.46
52:E:128:LYS:HA	52:E:129:VAL:HB	1.98	0.46
81:2:214:A:N1	81:2:241:U:C5	2.65	0.46
1:5:1194:A:O2'	1:5:1195:C:OP2	2.28	0.46
39:Bk:20:VAL:HG11	39:Bk:45:LEU:HD22	1.98	0.46
45:Bq:117:ILE:HG22	45:Bq:117:ILE:O	2.15	0.46
50:C:82:LYS:HA	50:C:83:ASP:CB	2.45	0.46
70:W:6:VAL:HG13	70:W:29:PRO:HB2	1.98	0.46
14:AL:3:ILE:HG23	14:AL:4:SER:OG	2.15	0.46
56:I:26:LYS:O	56:I:29:LEU:HD12	2.15	0.46
82:1:492:VAL:CG1	82:1:559:ILE:HD13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:3073:U:C4	1:5:3097:A:C8	2.76	0.45
15:AM:55:ARG:NH2	15:AM:76:ALA:O	2.50	0.45
1:5:1452:A:H2'	1:5:1452:A:N3	2.32	0.45
63:P:18:LYS:HA	66:S:91:ASP:C	2.40	0.45
81:2:333:G:H2'	81:2:334:U:H6	1.81	0.45
1:5:1321:A:C5	1:5:1322:U:H1'	2.51	0.45
11:AH:164:ILE:HG22	11:AH:164:ILE:O	2.15	0.45
53:F:203:ALA:HA	53:F:213:ILE:HD11	1.97	0.45
81:2:333:G:H2'	81:2:334:U:C6	2.51	0.45
1:5:2502:G:H2'	1:5:2503:G:C5	2.51	0.45
5:AB:87:VAL:HG21	5:AB:110:LEU:HD23	1.99	0.45
5:AB:218:VAL:HG13	5:AB:276:THR:HG22	1.99	0.45
53:F:220:GLU:HB3	53:F:221:ARG:HB2	1.97	0.45
83:3:60:U:H2'	83:3:60:U:O2	2.17	0.45
4:AA:137:ILE:HD11	4:AA:149:ARG:HB2	1.97	0.45
45:Bq:34:LEU:HD22	45:Bq:204:LEU:HD22	1.98	0.45
83:3:50:U:C2	83:3:65:G:C2	3.04	0.45
1:5:995:G:N2	1:5:997:A:OP2	2.49	0.45
1:5:2194:U:C6	1:5:2194:U:C4'	2.99	0.45
2:7:78:U:H2'	2:7:79:A:H5'	1.98	0.45
81:2:452:U:O2	81:2:452:U:C2'	2.64	0.45
82:1:390:ILE:HG22	82:1:570:VAL:HG13	1.99	0.45
1:5:2414:A:H2'	1:5:2414:A:N3	2.32	0.45
34:Bf:103:TYR:HB2	34:Bf:104:PRO:CD	2.46	0.45
45:Bq:204:LEU:C	45:Bq:216:LEU:CB	2.73	0.45
59:L:123:VAL:HG13	59:L:139:VAL:HG13	1.98	0.45
1:5:327:A:OP1	14:AL:23:LYS:NZ	2.49	0.45
72:Y:4:ALA:C	72:Y:5:ILE:HD12	2.42	0.45
81:2:646:G:C5	81:2:688:G:N1	2.85	0.45
10:AG:70:VAL:HG12	16:AN:21:PHE:CZ	2.51	0.45
81:2:279:U:O2'	81:2:280:G:OP2	2.29	0.45
1:5:2255:U:OP1	1:5:2255:U:C6	2.69	0.44
62:O:31:THR:HG22	62:O:38:THR:HG22	1.99	0.44
82:1:405:GLN:HB3	82:1:448:PHE:CE1	2.53	0.44
12:AI:146:ASP:HA	12:AI:149:ILE:HG22	1.99	0.44
19:AQ:120:GLU:HB3	19:AQ:122:ILE:HD13	1.99	0.44
45:Bq:59:PRO:HD2	45:Bq:153:SER:CA	2.45	0.44
65:R:20:TYR:CE2	65:R:38:ILE:HD13	2.52	0.44
82:1:562:THR:HG21	82:1:573:LEU:HD23	1.98	0.44
82:1:827:ALA:HB2	82:1:939:THR:HG21	2.00	0.44
66:S:46:VAL:HG11	66:S:69:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:U:58:LEU:HD12	68:U:88:LYS:HG2	2.00	0.44
1:5:2196:C:C3'	1:5:2196:C:C6	3.01	0.44
4:AA:112:ILE:HD13	44:Bp:79:VAL:HG22	1.99	0.44
45:Bq:187:VAL:O	45:Bq:191:VAL:HG23	2.18	0.44
81:2:336:G:H4'	81:2:336:G:OP2	2.18	0.44
81:2:1712:A:H2'	81:2:1713:G:O4'	2.18	0.44
1:5:1162:U:C2	17:AO:49:PHE:CE1	3.05	0.44
1:5:1733:G:H3'	1:5:1734:U:H5''	1.99	0.44
8:AE:114:ARG:NH1	8:AE:114:ARG:CG	2.81	0.44
45:Bq:111:VAL:HG13	45:Bq:138:VAL:HG21	1.99	0.44
82:1:803:HIS:C	82:1:805:PHE:N	2.75	0.44
1:5:1717:G:H5'	39:Bk:3:LYS:HD2	2.00	0.44
81:2:1598:A:H2'	81:2:1598:A:N3	2.32	0.44
1:5:1161:A:N3	1:5:1161:A:C2'	2.80	0.43
55:H:49:ILE:HG21	55:H:172:VAL:HG22	2.00	0.43
56:I:101:ILE:HD12	56:I:101:ILE:N	2.33	0.43
81:2:1396:U:H3'	81:2:1397:C:C5'	2.48	0.43
5:AB:84:ILE:HG23	5:AB:162:VAL:HG13	2.00	0.43
71:X:65:ASN:ND2	71:X:116:ASP:OD2	2.50	0.43
82:1:821:ALA:HB1	82:1:822:GLU:HA	2.00	0.43
1:5:1194:A:C4	1:5:1195:C:C5	3.06	0.43
45:Bq:12:ASN:CG	45:Bq:206:ILE:HD12	2.43	0.43
45:Bq:115:VAL:CG2	45:Bq:116:LEU:HD22	2.47	0.43
5:AB:218:VAL:HG22	5:AB:276:THR:HG22	2.01	0.43
6:AC:351:LYS:HB3	6:AC:351:LYS:HE2	1.50	0.43
38:Bj:84:LYS:O	38:Bj:85:ALA:HB2	2.18	0.43
62:O:117:ASP:CB	74:a:44:ILE:HD11	2.47	0.43
42:Bn:4:LYS:NZ	81:2:1775:G:N7	2.67	0.43
43:Bo:98:LYS:HB3	43:Bo:99:GLN:HA	2.00	0.43
53:F:134:VAL:HG11	53:F:201:ILE:HD12	2.00	0.43
1:5:2501:U:H5''	1:5:2501:U:C6	2.40	0.43
1:5:2502:G:N2	1:5:2516:A:H1'	2.31	0.43
52:E:126:VAL:HA	52:E:127:LYS:CB	2.48	0.43
81:2:1038:A:O2'	81:2:1039:G:O5'	2.34	0.43
6:AC:344:VAL:HG13	6:AC:345:ASP:CG	2.44	0.43
21:AS:97:VAL:HG13	21:AS:98:THR:HG23	2.01	0.43
1:5:1161:A:N3	1:5:1161:A:H2'	2.34	0.43
7:AD:294:ALA:HB3	7:AD:295:PRO:HD3	2.01	0.43
48:A:126:PRO:CG	48:A:147:THR:HG22	2.48	0.43
58:K:3:ILE:HG23	58:K:41:PHE:CD2	2.54	0.43
63:P:19:GLY:HA3	66:S:94:ASP:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AG:80:THR:HG21	10:AG:180:LYS:HE3	2.00	0.43
82:1:380:ASP:O	82:1:381:THR:C	2.62	0.43
6:AC:327:LEU:O	6:AC:328:ASN:C	2.62	0.42
8:AE:11:GLU:OE2	33:Be:90:LYS:HB2	2.18	0.42
8:AE:112:LYS:O	8:AE:117:ALA:HB1	2.19	0.42
8:AE:124:GLN:N	8:AE:125:PRO:CD	2.82	0.42
1:5:2107:A:HO2'	38:Bj:2:GLY:N	2.17	0.42
39:Bk:3:LYS:HD3	39:Bk:51:LEU:HG	2.02	0.42
53:F:94:ARG:HB3	53:F:174:ILE:HD13	2.02	0.42
1:5:2502:G:N1	1:5:2516:A:C8	2.87	0.42
5:AB:58:ARG:HD3	5:AB:354:VAL:HG13	2.01	0.42
24:AV:135:VAL:HG11	25:AW:26:SER:HB3	2.02	0.42
37:Bi:36:ARG:NH1	37:Bi:36:ARG:CG	2.73	0.42
39:Bk:6:ALA:HB3	39:Bk:7:ASP:HA	2.00	0.42
53:F:165:SER:HB3	76:c:54:LEU:HD23	2.01	0.42
63:P:21:ASP:O	66:S:93:ASN:ND2	2.52	0.42
80:g:6:ILE:HD11	80:g:258:TRP:CZ2	2.54	0.42
82:1:674:ALA:HB3	82:1:677:LEU:HD21	2.01	0.42
1:5:591:C:P	8:AE:111:ARG:NH1	2.93	0.42
46:Br:195:ASN:HB3	46:Br:196:GLY:CA	2.49	0.42
48:A:197:ILE:HG23	48:A:198:MET:N	2.34	0.42
63:P:57:MET:HE3	63:P:89:MET:CE	2.49	0.42
81:2:1513:A:O2'	81:2:1516:C:N4	2.52	0.42
1:5:1525:U:O2	1:5:1525:U:C2'	2.68	0.42
1:5:2061:A:N3	1:5:2061:A:H2'	2.34	0.42
9:AF:153:ILE:HG23	9:AF:169:ASN:HD21	1.84	0.42
81:2:646:G:O6	81:2:688:G:C6	2.72	0.42
82:1:596:GLU:HA	82:1:597:ALA:HB2	1.99	0.42
83:3:60:U:O2	83:3:60:U:C2'	2.66	0.42
5:AB:60:LEU:HD12	5:AB:72:VAL:HG21	2.01	0.42
8:AE:114:ARG:CA	8:AE:117:ALA:N	2.83	0.42
28:AZ:46:ILE:HD11	28:AZ:49:TYR:CD1	2.54	0.42
81:2:1712:A:C2	81:2:1713:G:C5	3.07	0.42
15:AM:67:PRO:C	15:AM:68:LEU:HD12	2.44	0.42
20:AR:99:LEU:HD11	20:AR:103:ARG:NH1	2.33	0.42
44:Bp:38:ASN:HA	44:Bp:45:THR:HG22	2.02	0.42
46:Br:30:VAL:CG1	46:Br:89:ILE:HD12	2.50	0.42
48:A:196:ALA:HA	48:A:197:ILE:HG22	2.00	0.42
50:C:148:TYR:HA	50:C:149:TRP:CB	2.49	0.42
56:I:154:GLU:O	56:I:156:ALA:N	2.53	0.42
63:P:18:LYS:O	66:S:95:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:1322:U:C3'	1:5:1322:U:C6	3.02	0.42
12:AI:54:SER:HB2	12:AI:135:ILE:HD11	2.00	0.42
18:AP:64:ASN:HA	18:AP:67:ILE:HD12	2.01	0.42
42:Bn:6:ARG:NH1	81:2:1114:U:C4'	2.83	0.42
52:E:67:GLN:CA	52:E:68:ARG:HB2	2.46	0.42
82:1:801:ILE:HD13	82:1:801:ILE:C	2.45	0.42
1:5:2255:U:O2	1:5:2255:U:O2'	2.22	0.42
4:AA:101:VAL:HG22	4:AA:165:VAL:HG22	2.02	0.42
5:AB:222:LYS:O	5:AB:272:TYR:N	2.51	0.42
56:I:82:VAL:HG12	56:I:197:LEU:HD21	2.02	0.42
61:N:60:VAL:HG13	61:N:66:ILE:HD12	2.02	0.42
80:g:92:LEU:HD11	80:g:137:THR:HG23	2.01	0.42
1:5:2505:A:N3	1:5:2505:A:H2'	2.34	0.42
5:AB:283:TYR:CD1	5:AB:354:VAL:HG11	2.55	0.42
36:Bh:4:ILE:HD12	36:Bh:50:ASN:HB3	2.01	0.42
1:5:135:C:O2	1:5:135:C:O2'	2.38	0.41
1:5:2257:G:C6	1:5:2258:U:C4	3.07	0.41
11:AH:85:GLY:HA3	11:AH:187:ILE:HD12	2.01	0.41
14:AL:2:ALA:O	14:AL:3:ILE:HG22	2.20	0.41
45:Bq:9:VAL:HG22	45:Bq:180:VAL:HG11	2.01	0.41
54:G:48:TYR:HB3	54:G:113:ILE:HD11	2.01	0.41
54:G:48:TYR:CD1	54:G:113:ILE:HD11	2.55	0.41
1:5:2529:C:O2'	10:AG:31:ARG:NH1	2.53	0.41
5:AB:383:LEU:HA	5:AB:384:LYS:HA	1.90	0.41
24:AV:81:GLN:O	24:AV:82:SER:CB	2.68	0.41
51:D:186:VAL:HG12	51:D:188:ILE:CD1	2.50	0.41
82:1:963:VAL:HG12	82:1:964:PHE:CD1	2.55	0.41
18:AP:129:THR:HG23	18:AP:139:TYR:HB2	2.02	0.41
22:AT:65:TYR:CD1	22:AT:75:ILE:HG23	2.54	0.41
45:Bq:59:PRO:HD3	45:Bq:153:SER:HA	2.00	0.41
45:Bq:205:VAL:HA	45:Bq:216:LEU:CB	2.39	0.41
46:Br:79:LEU:N	46:Br:80:PRO:CD	2.83	0.41
1:5:1322:U:C6	1:5:1322:U:H3'	2.55	0.41
11:AH:41:ILE:HD12	11:AH:43:VAL:HG13	2.01	0.41
18:AP:36:ILE:CD1	18:AP:95:LEU:HD11	2.50	0.41
34:Bf:90:PRO:O	34:Bf:91:ALA:HB3	2.20	0.41
37:Bi:36:ARG:NH1	37:Bi:40:VAL:HG21	2.36	0.41
71:X:68:ILE:HD12	71:X:68:ILE:N	2.36	0.41
82:1:800:ILE:HG13	82:1:803:HIS:CD2	2.56	0.41
82:1:803:HIS:O	82:1:805:PHE:N	2.54	0.41
82:1:803:HIS:C	82:1:805:PHE:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:1:954:TRP:HA	82:1:955:MET:CB	2.50	0.41
6:AC:148:ILE:HB	6:AC:149:PRO:CD	2.51	0.41
19:AQ:157:PRO:HA	19:AQ:158:HIS:HA	1.86	0.41
20:AR:89:LEU:HD12	20:AR:90:PRO:N	2.35	0.41
37:Bi:29:ARG:O	37:Bi:31:GLY:N	2.52	0.41
52:E:123:LEU:HD13	52:E:236:ILE:HD11	2.01	0.41
52:E:181:VAL:CG2	52:E:225:VAL:HG22	2.51	0.41
65:R:78:ARG:CB	65:R:79:GLU:HA	2.50	0.41
81:2:238:C:H3'	81:2:238:C:C6	2.56	0.41
21:AS:6:GLU:O	21:AS:6:GLU:CG	2.66	0.41
45:Bq:179:LEU:N	45:Bq:180:VAL:HG22	2.35	0.41
81:2:542:C:O2	81:2:542:C:O4'	2.39	0.41
4:AA:196:TRP:HB3	4:AA:197:PRO:CD	2.50	0.41
49:B:34:ALA:HB3	49:B:41:ARG:HA	2.03	0.41
63:P:89:MET:SD	63:P:89:MET:N	2.94	0.41
74:a:49:ALA:CB	74:a:50:ILE:HA	2.44	0.41
82:1:560:VAL:HG11	82:1:573:LEU:HD22	2.03	0.41
5:AB:312:VAL:HG12	5:AB:313:HIS:CD2	2.56	0.41
8:AE:114:ARG:HG3	8:AE:115:ALA:CA	2.48	0.41
61:N:56:ASP:OD1	61:N:57:ALA:N	2.54	0.41
1:5:3285:U:O2	1:5:3285:U:O4'	2.35	0.41
63:P:98:ASN:HB3	63:P:122:THR:HG22	2.02	0.41
80:g:188:LEU:HD13	80:g:189:ASN:N	2.36	0.41
81:2:238:C:C6	81:2:238:C:C3'	3.03	0.41
81:2:737:A:O2'	81:2:738:G:O5'	2.37	0.41
82:1:526:PHE:CE2	82:1:530:LEU:HD12	2.56	0.41
82:1:953:ASP:HB3	82:1:954:TRP:CG	2.56	0.41
6:AC:30:ILE:HD11	6:AC:128:ALA:HB2	2.03	0.41
6:AC:315:LYS:O	6:AC:316:ASN:CB	2.69	0.41
81:2:897:A:N6	81:2:911:U:H1'	2.36	0.41
82:1:868:ASP:OD1	82:1:868:ASP:N	2.54	0.41
1:5:2501:U:H2'	1:5:2502:G:H4'	2.03	0.40
63:P:34:VAL:HG21	63:P:45:PHE:CG	2.56	0.40
79:f:142:CYS:O	79:f:144:SER:N	2.54	0.40
50:C:177:ALA:HB1	50:C:178:PRO:CD	2.50	0.40
1:5:2502:G:C2	1:5:2516:A:C6	3.08	0.40
81:2:646:G:C6	81:2:688:G:C6	3.09	0.40
81:2:911:U:H4'	81:2:912:G:O3'	2.20	0.40
1:5:2254:C:H6	1:5:2254:C:O5'	2.03	0.40
6:AC:74:ILE:O	6:AC:74:ILE:CG2	2.70	0.40
9:AF:153:ILE:HB	9:AF:158:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AH:41:ILE:HD11	11:AH:67:ALA:CB	2.49	0.40
50:C:185:ALA:HB2	50:C:203:THR:HG21	2.03	0.40
60:M:107:VAL:HG21	81:2:1226:A:OP1	2.21	0.40
81:2:214:A:N7	81:2:241:U:N1	2.64	0.40

There are no symmetry-related clashes.

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	247/254 (97%)	216 (87%)	24 (10%)	7 (3%)	4	26
5	AB	382/387 (99%)	321 (84%)	51 (13%)	10 (3%)	4	27
6	AC	358/363 (99%)	279 (78%)	54 (15%)	25 (7%)	1	10
7	AD	293/297 (99%)	266 (91%)	15 (5%)	12 (4%)	2	19
8	AE	159/175 (91%)	138 (87%)	16 (10%)	5 (3%)	3	25
9	AF	220/241 (91%)	196 (89%)	17 (8%)	7 (3%)	3	24
10	AG	231/255 (91%)	213 (92%)	14 (6%)	4 (2%)	7	35
11	AH	189/191 (99%)	162 (86%)	24 (13%)	3 (2%)	7	36
12	AI	203/220 (92%)	181 (89%)	16 (8%)	6 (3%)	3	25
13	AJ	166/174 (95%)	147 (89%)	12 (7%)	7 (4%)	2	19
14	AL	195/199 (98%)	172 (88%)	19 (10%)	4 (2%)	5	31
15	AM	134/138 (97%)	116 (87%)	14 (10%)	4 (3%)	3	25
16	AN	200/204 (98%)	189 (94%)	11 (6%)	0	100	100
17	AO	196/199 (98%)	94 (48%)	38 (19%)	64 (33%)	0	0
18	AP	178/184 (97%)	156 (88%)	17 (10%)	5 (3%)	4	26
19	AQ	182/186 (98%)	163 (90%)	18 (10%)	1 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AR	186/189 (98%)	171 (92%)	12 (6%)	3 (2%)	7	36
21	AS	167/172 (97%)	152 (91%)	10 (6%)	5 (3%)	3	25
22	AT	156/160 (98%)	138 (88%)	16 (10%)	2 (1%)	9	39
23	AU	98/122 (80%)	89 (91%)	9 (9%)	0	100	100
24	AV	130/137 (95%)	118 (91%)	10 (8%)	2 (2%)	8	37
25	AW	60/155 (39%)	57 (95%)	3 (5%)	0	100	100
26	AX	119/142 (84%)	110 (92%)	9 (8%)	0	100	100
27	AY	123/127 (97%)	107 (87%)	14 (11%)	2 (2%)	7	36
28	AZ	132/136 (97%)	111 (84%)	17 (13%)	4 (3%)	3	25
29	Ba	145/149 (97%)	120 (83%)	19 (13%)	6 (4%)	2	19
30	Bb	55/62 (89%)	47 (86%)	6 (11%)	2 (4%)	2	22
31	Bc	95/105 (90%)	88 (93%)	7 (7%)	0	100	100
32	Bd	104/114 (91%)	94 (90%)	6 (6%)	4 (4%)	2	21
33	Be	120/130 (92%)	111 (92%)	6 (5%)	3 (2%)	4	28
34	Bf	103/107 (96%)	94 (91%)	6 (6%)	3 (3%)	3	26
35	Bg	119/125 (95%)	105 (88%)	9 (8%)	5 (4%)	2	19
36	Bh	114/120 (95%)	106 (93%)	5 (4%)	3 (3%)	4	27
37	Bi	96/100 (96%)	81 (84%)	10 (10%)	5 (5%)	1	15
38	Bj	83/88 (94%)	75 (90%)	6 (7%)	2 (2%)	4	29
39	Bk	74/78 (95%)	61 (82%)	11 (15%)	2 (3%)	4	27
40	Bl	47/51 (92%)	41 (87%)	4 (8%)	2 (4%)	2	18
41	Bm	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
42	Bn	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
43	Bo	99/106 (93%)	76 (77%)	15 (15%)	8 (8%)	1	8
44	Bp	85/92 (92%)	71 (84%)	8 (9%)	6 (7%)	1	10
45	Bq	215/217 (99%)	171 (80%)	29 (14%)	15 (7%)	1	10
46	Br	193/311 (62%)	140 (72%)	33 (17%)	20 (10%)	0	5
48	A	204/254 (80%)	174 (85%)	21 (10%)	9 (4%)	2	18
49	B	212/255 (83%)	181 (85%)	22 (10%)	9 (4%)	2	19
50	C	215/259 (83%)	178 (83%)	29 (14%)	8 (4%)	2	21
51	D	221/237 (93%)	193 (87%)	19 (9%)	9 (4%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	E	258/261 (99%)	225 (87%)	22 (8%)	11 (4%)	2	18
53	F	204/227 (90%)	166 (81%)	29 (14%)	9 (4%)	2	18
54	G	224/236 (95%)	196 (88%)	22 (10%)	6 (3%)	4	27
55	H	182/190 (96%)	155 (85%)	18 (10%)	9 (5%)	1	16
56	I	184/201 (92%)	158 (86%)	19 (10%)	7 (4%)	2	21
57	J	180/188 (96%)	146 (81%)	25 (14%)	9 (5%)	1	16
58	K	94/106 (89%)	81 (86%)	9 (10%)	4 (4%)	2	18
59	L	143/156 (92%)	127 (89%)	12 (8%)	4 (3%)	4	26
60	M	120/134 (90%)	99 (82%)	15 (12%)	6 (5%)	1	16
61	N	148/151 (98%)	137 (93%)	10 (7%)	1 (1%)	18	51
62	O	125/137 (91%)	106 (85%)	13 (10%)	6 (5%)	2	16
63	P	117/142 (82%)	90 (77%)	18 (15%)	9 (8%)	1	9
64	Q	139/143 (97%)	121 (87%)	14 (10%)	4 (3%)	3	26
65	R	121/136 (89%)	96 (79%)	22 (18%)	3 (2%)	4	28
66	S	136/146 (93%)	112 (82%)	17 (12%)	7 (5%)	1	15
67	T	141/144 (98%)	123 (87%)	14 (10%)	4 (3%)	4	26
68	U	104/117 (89%)	89 (86%)	13 (12%)	2 (2%)	6	33
69	V	85/87 (98%)	70 (82%)	11 (13%)	4 (5%)	2	17
70	W	127/130 (98%)	106 (84%)	19 (15%)	2 (2%)	7	36
71	X	141/145 (97%)	116 (82%)	21 (15%)	4 (3%)	4	26
72	Y	132/135 (98%)	112 (85%)	15 (11%)	5 (4%)	2	21
73	Z	68/108 (63%)	60 (88%)	6 (9%)	2 (3%)	3	26
74	a	98/119 (82%)	78 (80%)	12 (12%)	8 (8%)	0	8
75	b	80/82 (98%)	67 (84%)	10 (12%)	3 (4%)	2	21
76	c	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
77	d	51/56 (91%)	42 (82%)	8 (16%)	1 (2%)	6	32
78	e	53/63 (84%)	50 (94%)	2 (4%)	1 (2%)	6	33
79	f	40/150 (27%)	28 (70%)	8 (20%)	4 (10%)	0	5
80	g	312/326 (96%)	250 (80%)	52 (17%)	10 (3%)	3	24
82	1	598/967 (62%)	465 (78%)	103 (17%)	30 (5%)	1	16
All	All	11839/13368 (89%)	10064 (85%)	1297 (11%)	478 (4%)	4	20

All (478) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AA	34	TYR
4	AA	196	TRP
4	AA	197	PRO
5	AB	5	LYS
5	AB	351	LEU
6	AC	74	ILE
6	AC	148	ILE
6	AC	149	PRO
6	AC	182	VAL
6	AC	270	VAL
6	AC	300	ARG
6	AC	316	ASN
6	AC	342	LYS
6	AC	352	PRO
7	AD	4	ILE
10	AG	126	PRO
13	AJ	25	GLU
13	AJ	114	ILE
14	AL	3	ILE
14	AL	4	SER
14	AL	47	ALA
17	AO	13	LYS
17	AO	16	LEU
17	AO	29	LEU
17	AO	35	VAL
17	AO	48	PHE
17	AO	50	ARG
17	AO	56	HIS
17	AO	57	ASP
17	AO	67	LYS
17	AO	68	THR
17	AO	78	SER
17	AO	86	ARG
17	AO	94	ALA
17	AO	112	PRO
17	AO	114	ASP
17	AO	122	PRO
17	AO	123	GLN
17	AO	126	ARG
17	AO	127	VAL
17	AO	130	LEU
17	AO	139	LEU

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Mol	Chain	Res	Type
17	AO	141	LYS
17	AO	146	VAL
17	AO	158	GLU
17	AO	160	LYS
17	AO	162	LYS
17	AO	169	TYR
17	AO	170	LEU
17	AO	179	VAL
17	AO	183	SER
17	AO	186	VAL
17	AO	187	GLY
17	AO	188	THR
17	AO	190	VAL
17	AO	193	LYS
21	AS	18	SER
27	AY	55	GLU
28	AZ	51	LEU
28	AZ	59	ALA
29	Ba	50	PRO
29	Ba	78	LEU
34	Bf	104	PRO
37	Bi	30	LYS
39	Bk	6	ALA
39	Bk	32	ASN
40	Bl	33	ASN
43	Bo	66	LYS
45	Bq	24	LYS
45	Bq	59	PRO
45	Bq	181	ASN
46	Br	41	HIS
46	Br	70	SER
48	A	197	ILE
49	B	35	PRO
49	B	191	GLU
50	C	59	GLU
51	D	176	LEU
52	E	117	GLU
53	F	192	ILE
53	F	221	ARG
54	G	122	GLU
54	G	154	ARG
55	H	64	VAL

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Mol	Chain	Res	Type
56	I	22	ARG
56	I	35	ASN
56	I	148	ALA
56	I	155	HIS
58	K	88	PRO
59	L	105	LYS
62	O	91	SER
63	P	20	VAL
63	P	29	PRO
64	Q	40	GLN
66	S	92	VAL
69	V	10	GLU
70	W	83	ILE
71	X	12	ALA
71	X	42	PRO
71	X	138	GLU
72	Y	30	PRO
74	a	10	ARG
74	a	75	ILE
79	f	143	HIS
80	g	52	GLU
82	1	442	THR
82	1	461	ILE
82	1	597	ALA
82	1	653	ARG
82	1	868	ASP
82	1	876	THR
82	1	911	PRO
82	1	941	LYS
4	AA	33	ASP
5	AB	226	PHE
6	AC	16	THR
6	AC	268	ALA
6	AC	292	SER
6	AC	293	THR
6	AC	305	ALA
6	AC	341	SER
6	AC	343	LYS
7	AD	5	LYS
7	AD	20	PHE
7	AD	21	ARG
7	AD	188	GLU

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Mol	Chain	Res	Type
7	AD	296	GLN
8	AE	114	ARG
9	AF	90	ASN
9	AF	139	SER
9	AF	156	GLN
12	AI	145	LYS
12	AI	187	ALA
15	AM	6	VAL
17	AO	12	GLY
17	AO	34	ILE
17	AO	40	GLU
17	AO	49	PHE
17	AO	51	ASN
17	AO	66	ASN
17	AO	81	PHE
17	AO	84	ALA
17	AO	98	ALA
17	AO	113	TYR
17	AO	140	GLY
17	AO	144	THR
17	AO	145	SER
17	AO	148	TRP
17	AO	163	ALA
17	AO	165	SER
17	AO	177	ALA
17	AO	198	GLY
18	AP	165	VAL
21	AS	133	ALA
24	AV	82	SER
24	AV	106	LYS
27	AY	109	LEU
28	AZ	87	LEU
29	Ba	124	ILE
33	Be	124	ALA
35	Bg	60	ARG
35	Bg	75	ALA
37	Bi	14	GLY
37	Bi	36	ARG
38	Bj	85	ALA
43	Bo	6	LYS
44	Bp	56	SER
44	Bp	60	CYS

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Mol	Chain	Res	Type
44	Bp	61	ASN
46	Br	69	ILE
46	Br	95	LEU
46	Br	126	VAL
49	B	177	GLN
50	C	57	SER
51	D	217	VAL
52	E	68	ARG
52	E	120	SER
52	E	127	LYS
52	E	195	ILE
53	F	59	SER
53	F	206	GLY
55	H	53	GLY
56	I	62	THR
56	I	153	ILE
59	L	55	ASP
60	M	78	PRO
62	O	18	ARG
63	P	101	VAL
63	P	121	ILE
66	S	26	ILE
67	T	39	THR
69	V	30	SER
73	Z	71	LEU
74	a	84	VAL
74	a	85	ARG
75	b	21	LEU
80	g	77	ASP
80	g	201	GLY
82	1	382	GLY
82	1	431	THR
82	1	445	HIS
82	1	457	SER
82	1	487	LYS
82	1	793	ILE
82	1	800	ILE
82	1	801	ILE
5	AB	140	ASN
6	AC	84	ARG
6	AC	140	HIS
6	AC	173	GLY

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Mol	Chain	Res	Type
6	AC	232	SER
6	AC	269	SER
7	AD	214	ASP
7	AD	253	PHE
8	AE	66	PRO
8	AE	112	LYS
8	AE	115	ALA
9	AF	230	GLU
12	AI	24	ARG
13	AJ	8	PRO
14	AL	190	LYS
15	AM	28	SER
15	AM	29	ALA
15	AM	41	GLN
17	AO	24	VAL
17	AO	27	GLN
17	AO	54	LYS
17	AO	77	PRO
17	AO	111	PRO
17	AO	143	SER
18	AP	161	SER
19	AQ	175	ALA
20	AR	131	THR
28	AZ	9	LYS
32	Bd	83	GLU
32	Bd	84	ASP
35	Bg	10	ARG
35	Bg	56	THR
35	Bg	57	LEU
40	Bl	3	ALA
43	Bo	14	GLY
43	Bo	65	THR
45	Bq	71	ALA
45	Bq	129	SER
45	Bq	209	THR
46	Br	23	GLU
46	Br	38	GLN
46	Br	58	ASN
46	Br	111	ALA
48	A	72	ASP
49	B	181	LEU
49	B	209	ASN

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Mol	Chain	Res	Type
50	C	111	ASP
50	C	153	LEU
50	C	175	ILE
51	D	220	PRO
52	E	205	PHE
54	G	70	PRO
54	G	165	GLY
55	H	98	ILE
57	J	18	PRO
57	J	67	PRO
57	J	118	LEU
58	K	54	PHE
58	K	83	PRO
59	L	30	LYS
60	M	82	VAL
62	O	51	ASP
62	O	114	ARG
63	P	125	PRO
64	Q	116	LEU
65	R	26	MET
65	R	72	LYS
65	R	100	LEU
66	S	140	THR
67	T	119	LYS
69	V	4	ASP
70	W	57	ARG
72	Y	61	ARG
74	a	61	GLU
79	f	144	SER
80	g	244	LYS
80	g	256	ARG
82	1	443	PRO
82	1	451	LEU
82	1	695	GLU
82	1	720	VAL
4	AA	143	ASP
6	AC	131	VAL
6	AC	345	ASP
7	AD	249	GLU
8	AE	110	SER
11	AH	50	ASN
12	AI	47	PRO

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Mol	Chain	Res	Type
12	AI	144	ASN
13	AJ	108	GLU
17	AO	28	LEU
17	AO	52	LYS
17	AO	142	LEU
18	AP	4	TYR
18	AP	158	GLU
20	AR	130	ASN
21	AS	13	ARG
21	AS	24	LEU
22	AT	125	ALA
29	Ba	66	ALA
29	Ba	98	ALA
32	Bd	82	GLU
34	Bf	91	ALA
37	Bi	13	LYS
43	Bo	53	GLN
44	Bp	47	VAL
45	Bq	25	LYS
45	Bq	128	LEU
45	Bq	182	GLN
45	Bq	213	ALA
46	Br	68	PHE
46	Br	106	LYS
46	Br	149	ARG
46	Br	156	SER
48	A	9	LEU
48	A	167	LYS
48	A	193	GLN
48	A	202	TYR
51	D	196	THR
52	E	77	ARG
53	F	82	LYS
53	F	83	ARG
53	F	166	PRO
54	G	155	ASP
55	H	32	PRO
55	H	110	GLN
56	I	120	SER
57	J	69	ARG
57	J	169	PRO
60	M	117	TRP

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Mol	Chain	Res	Type
62	O	75	GLY
62	O	124	ASP
63	P	52	LYS
66	S	12	GLN
67	T	50	SER
67	T	53	TRP
72	Y	63	GLN
75	b	75	GLU
80	g	4	SER
80	g	41	LYS
80	g	75	SER
80	g	139	GLY
82	1	467	ASP
82	1	519	GLU
82	1	590	LYS
82	1	804	LEU
82	1	963	VAL
4	AA	125	ALA
5	AB	22	ALA
5	AB	28	ARG
5	AB	155	ALA
5	AB	348	ARG
6	AC	14	GLU
7	AD	259	LYS
9	AF	113	PHE
10	AG	24	PRO
10	AG	122	GLN
11	AH	110	LYS
13	AJ	94	ARG
17	AO	14	GLY
17	AO	63	THR
21	AS	12	ARG
22	AT	122	GLN
29	Ba	33	GLY
33	Be	12	LYS
33	Be	123	LYS
36	Bh	75	TYR
36	Bh	99	GLN
43	Bo	15	LYS
43	Bo	17	CYS
44	Bp	57	CYS
45	Bq	216	LEU

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Mol	Chain	Res	Type
46	Br	28	PHE
48	A	103	THR
48	A	195	TRP
49	B	179	SER
50	C	41	VAL
50	C	56	SER
51	D	44	THR
51	D	143	ARG
51	D	164	VAL
52	E	245	LYS
55	H	13	PRO
55	H	160	GLN
60	M	32	ASP
64	Q	27	GLY
66	S	14	ILE
66	S	76	PRO
66	S	144	ARG
69	V	7	GLN
71	X	70	LYS
72	Y	36	SER
74	a	62	TYR
75	b	62	VAL
79	f	127	GLY
80	g	293	ASP
82	1	413	PRO
4	AA	141	PRO
5	AB	227	GLU
7	AD	125	VAL
11	AH	2	LYS
13	AJ	12	LEU
13	AJ	172	LEU
30	Bb	20	GLY
30	Bb	21	ILE
34	Bf	103	TYR
36	Bh	84	LYS
37	Bi	45	LYS
44	Bp	18	TYR
46	Br	94	SER
48	A	68	PRO
49	B	53	GLY
49	B	210	VAL
51	D	221	SER

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Mol	Chain	Res	Type
52	E	260	GLY
53	F	102	ASN
55	H	146	GLY
57	J	134	ILE
61	N	133	SER
63	P	23	GLU
63	P	69	GLU
63	P	120	SER
64	Q	115	THR
68	U	72	ASN
73	Z	88	ILE
78	e	47	VAL
79	f	102	VAL
82	1	372	ILE
10	AG	35	ILE
12	AI	194	GLY
57	J	165	GLY
57	J	166	GLY
60	M	93	GLY
60	M	97	ILE
74	a	36	ILE
43	Bo	95	GLY
45	Bq	4	ILE
45	Bq	60	ARG
46	Br	32	VAL
46	Br	118	PRO
51	D	130	GLY
54	G	60	GLY
55	H	132	PRO
5	AB	87	VAL
6	AC	328	ASN
7	AD	251	PRO
20	AR	129	GLY
45	Bq	180	VAL
46	Br	109	ALA
46	Br	133	GLY
52	E	129	VAL
53	F	53	VAL
68	U	86	ILE
9	AF	175	ILE
9	AF	188	VAL
18	AP	119	VAL

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Mol	Chain	Res	Type
32	Bd	66	GLY
45	Bq	169	VAL
46	Br	164	GLY
50	C	114	GLY
52	E	228	ILE
57	J	170	GLY
58	K	94	GLY
59	L	130	PRO
74	a	83	ILE
82	1	414	ILE
49	B	221	PRO
72	Y	5	ILE
77	d	25	GLY
38	Bj	40	PRO
82	1	648	PRO
82	1	962	PRO

5.3.2 Protein sidechains ⓘ

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	190/195 (97%)	184 (97%)	6 (3%)	34	58
5	AB	323/326 (99%)	310 (96%)	13 (4%)	28	54
6	AC	291/294 (99%)	271 (93%)	20 (7%)	14	41
7	AD	243/244 (100%)	237 (98%)	6 (2%)	42	63
8	AE	141/150 (94%)	134 (95%)	7 (5%)	22	49
9	AF	188/204 (92%)	180 (96%)	8 (4%)	26	52
10	AG	192/209 (92%)	182 (95%)	10 (5%)	21	48
11	AH	173/173 (100%)	163 (94%)	10 (6%)	18	46
12	AI	177/187 (95%)	167 (94%)	10 (6%)	19	47
13	AJ	144/148 (97%)	138 (96%)	6 (4%)	26	53
14	AL	162/164 (99%)	155 (96%)	7 (4%)	26	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AM	109/110 (99%)	104 (95%)	5 (5%)	24	51
16	AN	175/177 (99%)	171 (98%)	4 (2%)	44	64
17	AO	163/164 (99%)	150 (92%)	13 (8%)	11	37
18	AP	148/150 (99%)	146 (99%)	2 (1%)	59	71
19	AQ	150/151 (99%)	146 (97%)	4 (3%)	39	61
20	AR	152/153 (99%)	141 (93%)	11 (7%)	13	40
21	AS	154/157 (98%)	150 (97%)	4 (3%)	40	62
22	AT	135/137 (98%)	129 (96%)	6 (4%)	25	52
23	AU	90/110 (82%)	89 (99%)	1 (1%)	65	74
24	AV	101/105 (96%)	98 (97%)	3 (3%)	36	59
25	AW	54/127 (42%)	52 (96%)	2 (4%)	30	56
26	AX	106/120 (88%)	99 (93%)	7 (7%)	15	43
27	AY	111/112 (99%)	106 (96%)	5 (4%)	24	51
28	AZ	115/116 (99%)	110 (96%)	5 (4%)	26	52
29	Ba	117/118 (99%)	112 (96%)	5 (4%)	26	52
30	Bb	45/49 (92%)	42 (93%)	3 (7%)	15	42
31	Bc	79/85 (93%)	76 (96%)	3 (4%)	29	55
32	Bd	95/100 (95%)	92 (97%)	3 (3%)	34	58
33	Be	106/110 (96%)	100 (94%)	6 (6%)	18	46
34	Bf	90/92 (98%)	87 (97%)	3 (3%)	33	58
35	Bg	102/106 (96%)	99 (97%)	3 (3%)	37	60
36	Bh	104/106 (98%)	101 (97%)	3 (3%)	37	60
37	Bi	79/80 (99%)	73 (92%)	6 (8%)	12	39
38	Bj	69/71 (97%)	68 (99%)	1 (1%)	59	71
39	Bk	68/69 (99%)	65 (96%)	3 (4%)	25	52
40	Bl	44/46 (96%)	39 (89%)	5 (11%)	5	26
41	Bm	46/116 (40%)	45 (98%)	1 (2%)	45	65
42	Bn	21/21 (100%)	18 (86%)	3 (14%)	3	19
43	Bo	86/90 (96%)	80 (93%)	6 (7%)	14	41
44	Bp	69/71 (97%)	65 (94%)	4 (6%)	18	46
45	Bq	198/198 (100%)	185 (93%)	13 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	Br	162/251 (64%)	152 (94%)	10 (6%)	16	44
48	A	174/211 (82%)	166 (95%)	8 (5%)	24	51
49	B	196/228 (86%)	188 (96%)	8 (4%)	27	53
50	C	176/203 (87%)	161 (92%)	15 (8%)	10	35
51	D	185/196 (94%)	173 (94%)	12 (6%)	15	43
52	E	223/224 (100%)	212 (95%)	11 (5%)	22	49
53	F	174/194 (90%)	170 (98%)	4 (2%)	44	64
54	G	192/200 (96%)	185 (96%)	7 (4%)	31	56
55	H	164/170 (96%)	157 (96%)	7 (4%)	26	52
56	I	148/159 (93%)	138 (93%)	10 (7%)	14	42
57	J	153/158 (97%)	142 (93%)	11 (7%)	13	40
58	K	88/96 (92%)	82 (93%)	6 (7%)	14	42
59	L	129/137 (94%)	122 (95%)	7 (5%)	20	47
60	M	97/109 (89%)	94 (97%)	3 (3%)	35	59
61	N	127/128 (99%)	118 (93%)	9 (7%)	13	40
62	O	96/104 (92%)	96 (100%)	0	100	100
63	P	103/119 (87%)	98 (95%)	5 (5%)	22	49
64	Q	117/119 (98%)	116 (99%)	1 (1%)	70	76
65	R	112/124 (90%)	107 (96%)	5 (4%)	24	51
66	S	121/129 (94%)	113 (93%)	8 (7%)	15	43
67	T	117/118 (99%)	113 (97%)	4 (3%)	32	57
68	U	96/107 (90%)	94 (98%)	2 (2%)	47	65
69	V	73/73 (100%)	66 (90%)	7 (10%)	8	32
70	W	110/111 (99%)	101 (92%)	9 (8%)	10	36
71	X	118/120 (98%)	111 (94%)	7 (6%)	18	45
72	Y	108/109 (99%)	99 (92%)	9 (8%)	10	35
73	Z	60/88 (68%)	60 (100%)	0	100	100
74	a	85/100 (85%)	81 (95%)	4 (5%)	23	50
75	b	72/72 (100%)	70 (97%)	2 (3%)	38	60
76	c	55/59 (93%)	53 (96%)	2 (4%)	31	56
77	d	46/48 (96%)	43 (94%)	3 (6%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	e	49/55 (89%)	47 (96%)	2 (4%)	27	53
79	f	35/133 (26%)	34 (97%)	1 (3%)	37	60
80	g	265/272 (97%)	254 (96%)	11 (4%)	26	53
82	1	522/836 (62%)	468 (90%)	54 (10%)	7	30
All	All	10153/11271 (90%)	9643 (95%)	510 (5%)	23	49

All (510) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	AA	21	ARG
4	AA	24	GLN
4	AA	42	ARG
4	AA	96	LEU
4	AA	191	VAL
4	AA	230	VAL
5	AB	56	ILE
5	AB	60	LEU
5	AB	76	VAL
5	AB	84	ILE
5	AB	102	LEU
5	AB	104	THR
5	AB	166	VAL
5	AB	196	LYS
5	AB	222	LYS
5	AB	241	LYS
5	AB	262	TRP
5	AB	290	ASP
5	AB	332	ARG
6	AC	71	VAL
6	AC	73	ARG
6	AC	74	ILE
6	AC	92	ASN
6	AC	138	ARG
6	AC	179	ILE
6	AC	182	VAL
6	AC	201	GLN
6	AC	202	ARG
6	AC	215	VAL
6	AC	270	VAL
6	AC	293	THR
6	AC	299	LEU

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Mol	Chain	Res	Type
6	AC	307	GLN
6	AC	343	LYS
6	AC	346	GLN
6	AC	348	ASN
6	AC	350	ILE
6	AC	351	LYS
6	AC	357	LEU
7	AD	4	ILE
7	AD	41	LYS
7	AD	94	ASN
7	AD	105	LEU
7	AD	152	ARG
7	AD	177	GLU
8	AE	12	GLU
8	AE	50	VAL
8	AE	82	VAL
8	AE	111	ARG
8	AE	114	ARG
8	AE	126	LYS
8	AE	154	LEU
9	AF	33	ARG
9	AF	53	GLU
9	AF	89	ILE
9	AF	90	ASN
9	AF	112	THR
9	AF	155	LYS
9	AF	221	ILE
9	AF	233	ILE
10	AG	57	LEU
10	AG	62	LYS
10	AG	64	LEU
10	AG	123	GLU
10	AG	130	VAL
10	AG	135	LEU
10	AG	154	ASN
10	AG	168	LEU
10	AG	222	LEU
10	AG	231	HIS
11	AH	5	GLN
11	AH	10	LEU
11	AH	41	ILE
11	AH	92	TYR

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Mol	Chain	Res	Type
11	AH	113	GLU
11	AH	118	LEU
11	AH	132	VAL
11	AH	140	GLN
11	AH	157	ASN
11	AH	170	LYS
12	AI	30	LYS
12	AI	32	ARG
12	AI	33	ILE
12	AI	50	VAL
12	AI	139	ARG
12	AI	140	THR
12	AI	163	GLN
12	AI	165	ILE
12	AI	169	LYS
12	AI	190	ILE
13	AJ	17	LEU
13	AJ	30	LEU
13	AJ	40	LEU
13	AJ	67	VAL
13	AJ	107	GLN
13	AJ	114	ILE
14	AL	54	LEU
14	AL	67	ARG
14	AL	69	VAL
14	AL	104	ARG
14	AL	109	LEU
14	AL	124	ILE
14	AL	162	ASN
15	AM	38	ILE
15	AM	53	VAL
15	AM	59	ASN
15	AM	63	VAL
15	AM	77	LYS
16	AN	19	LEU
16	AN	38	ARG
16	AN	133	ILE
16	AN	151	ILE
17	AO	5	GLU
17	AO	26	LYS
17	AO	28	LEU
17	AO	56	HIS

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Mol	Chain	Res	Type
17	AO	80	ILE
17	AO	82	TYR
17	AO	106	PHE
17	AO	107	GLU
17	AO	119	VAL
17	AO	142	LEU
17	AO	144	THR
17	AO	146	VAL
17	AO	149	LYS
18	AP	120	ASN
18	AP	161	SER
19	AQ	111	LYS
19	AQ	135	GLN
19	AQ	168	THR
19	AQ	178	ARG
20	AR	5	ARG
20	AR	17	VAL
20	AR	31	GLU
20	AR	44	LEU
20	AR	55	THR
20	AR	57	ILE
20	AR	66	MET
20	AR	74	ARG
20	AR	89	LEU
20	AR	92	GLN
20	AR	119	LEU
21	AS	4	ARG
21	AS	5	LYS
21	AS	45	LEU
21	AS	50	LYS
22	AT	18	ASP
22	AT	75	ILE
22	AT	104	GLU
22	AT	131	GLN
22	AT	139	ARG
22	AT	143	THR
23	AU	70	LYS
24	AV	64	LYS
24	AV	83	LYS
24	AV	102	ILE
25	AW	4	GLU
25	AW	5	ILE

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Mol	Chain	Res	Type
26	AX	63	ILE
26	AX	80	ASN
26	AX	82	LEU
26	AX	117	ASN
26	AX	135	ILE
26	AX	137	ASN
26	AX	142	ILE
27	AY	17	LYS
27	AY	50	ILE
27	AY	55	GLU
27	AY	80	VAL
27	AY	104	VAL
28	AZ	31	GLU
28	AZ	34	LYS
28	AZ	81	LEU
28	AZ	109	GLU
28	AZ	134	LEU
29	Ba	34	MET
29	Ba	113	LEU
29	Ba	115	LYS
29	Ba	130	VAL
29	Ba	133	LEU
30	Bb	14	LYS
30	Bb	26	THR
30	Bb	32	LEU
31	Bc	41	LEU
31	Bc	44	ILE
31	Bc	101	LEU
32	Bd	6	ASP
32	Bd	13	THR
32	Bd	55	LEU
33	Be	19	ARG
33	Be	27	ARG
33	Be	33	ARG
33	Be	54	THR
33	Be	75	LEU
33	Be	82	LEU
34	Bf	20	LYS
34	Bf	103	TYR
34	Bf	106	ASN
35	Bg	19	LYS
35	Bg	30	LEU

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Mol	Chain	Res	Type
35	Bg	62	TYR
36	Bh	20	GLN
36	Bh	21	LEU
36	Bh	102	GLU
37	Bi	13	LYS
37	Bi	30	LYS
37	Bi	36	ARG
37	Bi	58	ILE
37	Bi	60	LEU
37	Bi	76	ARG
38	Bj	17	THR
39	Bk	31	LEU
39	Bk	34	ASN
39	Bk	69	LEU
40	Bl	11	GLN
40	Bl	21	ARG
40	Bl	23	LEU
40	Bl	27	ILE
40	Bl	29	LEU
41	Bm	119	ASN
42	Bn	6	ARG
42	Bn	9	ARG
42	Bn	13	LEU
43	Bo	16	GLU
43	Bo	35	LEU
43	Bo	45	ARG
43	Bo	61	LYS
43	Bo	85	LEU
43	Bo	100	LYS
44	Bp	10	ILE
44	Bp	16	VAL
44	Bp	25	GLN
44	Bp	47	VAL
45	Bq	3	LYS
45	Bq	38	LEU
45	Bq	44	GLN
45	Bq	47	LYS
45	Bq	60	ARG
45	Bq	97	LYS
45	Bq	102	LYS
45	Bq	180	VAL
45	Bq	181	ASN

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Mol	Chain	Res	Type
45	Bq	182	GLN
45	Bq	193	LEU
45	Bq	215	ARG
45	Bq	216	LEU
46	Br	32	VAL
46	Br	35	VAL
46	Br	39	GLN
46	Br	48	ARG
46	Br	62	ARG
46	Br	72	PHE
46	Br	91	THR
46	Br	134	LYS
46	Br	187	LEU
46	Br	199	PHE
48	A	9	LEU
48	A	34	GLU
48	A	56	LYS
48	A	108	THR
48	A	120	LEU
48	A	146	LEU
48	A	197	ILE
48	A	198	MET
49	B	54	LEU
49	B	70	LEU
49	B	96	LEU
49	B	100	PHE
49	B	120	LEU
49	B	178	ASN
49	B	191	GLU
49	B	208	GLN
50	C	49	LEU
50	C	59	GLU
50	C	82	LYS
50	C	83	ASP
50	C	86	MET
50	C	92	GLN
50	C	93	LYS
50	C	99	GLN
50	C	100	ARG
50	C	142	ILE
50	C	146	ARG
50	C	149	TRP

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Mol	Chain	Res	Type
50	C	174	LEU
50	C	212	LEU
50	C	240	LEU
51	D	7	LYS
51	D	11	LEU
51	D	27	ARG
51	D	51	ARG
51	D	107	PHE
51	D	113	LEU
51	D	135	GLU
51	D	141	LYS
51	D	157	LEU
51	D	178	ARG
51	D	179	GLN
51	D	185	LYS
52	E	6	LYS
52	E	9	LEU
52	E	18	TRP
52	E	38	LEU
52	E	42	LEU
52	E	51	ARG
52	E	77	ARG
52	E	123	LEU
52	E	187	ARG
52	E	225	VAL
52	E	250	GLU
53	F	121	GLU
53	F	158	ARG
53	F	188	ASN
53	F	192	ILE
54	G	31	ARG
54	G	52	ILE
54	G	81	HIS
54	G	85	ARG
54	G	92	ARG
54	G	164	LYS
54	G	180	THR
55	H	11	GLN
55	H	16	LEU
55	H	19	GLN
55	H	80	GLU
55	H	99	LEU

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Mol	Chain	Res	Type
55	H	174	ASN
55	H	180	GLN
56	I	8	ARG
56	I	9	HIS
56	I	29	LEU
56	I	67	TRP
56	I	72	VAL
56	I	74	ARG
56	I	75	LYS
56	I	89	GLU
56	I	107	THR
56	I	190	LEU
57	J	20	GLU
57	J	30	LEU
57	J	37	LYS
57	J	66	ASP
57	J	69	ARG
57	J	86	LEU
57	J	93	LEU
57	J	109	LEU
57	J	126	ARG
57	J	143	ILE
57	J	150	LEU
58	K	21	LEU
58	K	40	LEU
58	K	54	PHE
58	K	76	LEU
58	K	80	LEU
58	K	86	ILE
59	L	8	GLN
59	L	11	ARG
59	L	32	LYS
59	L	79	ARG
59	L	80	MET
59	L	94	VAL
59	L	105	LYS
60	M	67	LEU
60	M	69	GLN
60	M	124	ARG
61	N	3	ARG
61	N	39	LYS
61	N	64	LYS

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Mol	Chain	Res	Type
61	N	88	LEU
61	N	107	LYS
61	N	112	LYS
61	N	121	ARG
61	N	139	TRP
61	N	142	GLU
63	P	8	ARG
63	P	15	TYR
63	P	17	TYR
63	P	57	MET
63	P	79	HIS
64	Q	128	LYS
65	R	11	ARG
65	R	16	LEU
65	R	46	LEU
65	R	88	VAL
65	R	91	LEU
66	S	15	LEU
66	S	25	ASN
66	S	27	ASN
66	S	49	LYS
66	S	74	GLN
66	S	105	LEU
66	S	120	ARG
66	S	138	THR
67	T	45	LEU
67	T	63	ARG
67	T	79	LEU
67	T	124	ILE
68	U	84	MET
68	U	115	GLU
69	V	11	LEU
69	V	12	TYR
69	V	33	GLN
69	V	38	GLN
69	V	41	GLU
69	V	50	TYR
69	V	69	LEU
70	W	24	GLN
70	W	26	LEU
70	W	49	GLU
70	W	51	GLU

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Mol	Chain	Res	Type
70	W	66	ASN
70	W	75	ILE
70	W	88	LYS
70	W	104	LEU
70	W	125	ILE
71	X	19	ARG
71	X	92	CYS
71	X	103	LEU
71	X	107	PHE
71	X	133	LEU
71	X	140	LYS
71	X	142	LYS
72	Y	8	ARG
72	Y	20	ARG
72	Y	31	ASN
72	Y	46	GLU
72	Y	61	ARG
72	Y	98	GLU
72	Y	110	GLN
72	Y	116	LYS
72	Y	118	ILE
74	a	1	MET
74	a	12	LYS
74	a	32	LYS
74	a	46	GLU
75	b	1	MET
75	b	26	GLN
76	c	16	LEU
76	c	56	LEU
77	d	10	HIS
77	d	30	LEU
77	d	40	ARG
78	e	22	GLU
78	e	26	LYS
79	f	103	LEU
80	g	43	LEU
80	g	65	HIS
80	g	67	HIS
80	g	74	VAL
80	g	156	ARG
80	g	175	VAL
80	g	202	HIS

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Mol	Chain	Res	Type
80	g	210	GLN
80	g	244	LYS
80	g	292	GLN
80	g	321	GLN
82	1	412	PHE
82	1	419	GLN
82	1	442	THR
82	1	447	SER
82	1	450	ASN
82	1	451	LEU
82	1	456	SER
82	1	470	HIS
82	1	484	ARG
82	1	486	ARG
82	1	487	LYS
82	1	530	LEU
82	1	540	GLN
82	1	546	LEU
82	1	547	TYR
82	1	555	LYS
82	1	573	LEU
82	1	620	TYR
82	1	627	ILE
82	1	645	THR
82	1	649	LEU
82	1	652	LEU
82	1	653	ARG
82	1	660	HIS
82	1	668	LEU
82	1	675	ASN
82	1	689	VAL
82	1	706	LEU
82	1	709	LEU
82	1	754	LYS
82	1	770	LEU
82	1	778	VAL
82	1	782	LYS
82	1	786	GLN
82	1	791	GLN
82	1	793	ILE
82	1	799	ASP
82	1	800	ILE

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Mol	Chain	Res	Type
82	1	801	ILE
82	1	802	TYR
82	1	804	LEU
82	1	812	GLN
82	1	815	LEU
82	1	822	GLU
82	1	857	LYS
82	1	866	LYS
82	1	868	ASP
82	1	874	ARG
82	1	878	LEU
82	1	882	VAL
82	1	894	GLU
82	1	896	LYS
82	1	899	GLN
82	1	954	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
4	AA	7	ASN
4	AA	83	HIS
4	AA	86	GLN
4	AA	140	ASN
4	AA	233	GLN
5	AB	13	HIS
5	AB	68	HIS
5	AB	143	GLN
5	AB	173	GLN
5	AB	231	HIS
5	AB	243	HIS
5	AB	319	ASN
6	AC	5	GLN
6	AC	116	ASN
6	AC	140	HIS
6	AC	296	GLN
6	AC	346	GLN
7	AD	90	HIS
7	AD	264	GLN
8	AE	26	GLN
8	AE	70	ASN
8	AE	78	ASN

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Mol	Chain	Res	Type
8	AE	95	ASN
8	AE	113	GLN
8	AE	166	ASN
9	AF	90	ASN
9	AF	106	ASN
9	AF	107	GLN
9	AF	228	ASN
10	AG	37	GLN
10	AG	60	GLN
10	AG	220	ASN
11	AH	5	GLN
11	AH	50	ASN
11	AH	64	HIS
11	AH	140	GLN
11	AH	169	ASN
12	AI	12	GLN
12	AI	14	ASN
12	AI	23	ASN
12	AI	59	GLN
12	AI	92	HIS
12	AI	95	HIS
12	AI	123	HIS
13	AJ	20	ASN
13	AJ	43	GLN
13	AJ	150	ASN
15	AM	59	ASN
15	AM	62	GLN
16	AN	57	GLN
16	AN	90	ASN
16	AN	139	HIS
16	AN	184	GLN
17	AO	32	GLN
17	AO	51	ASN
17	AO	91	HIS
17	AO	123	GLN
18	AP	40	ASN
18	AP	125	GLN
18	AP	133	HIS
19	AQ	9	GLN
19	AQ	58	ASN
19	AQ	73	GLN
20	AR	3	ASN

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Mol	Chain	Res	Type
20	AR	7	GLN
20	AR	39	ASN
20	AR	58	HIS
20	AR	175	GLN
21	AS	49	HIS
22	AT	5	HIS
22	AT	22	HIS
22	AT	77	ASN
22	AT	95	HIS
22	AT	127	GLN
22	AT	131	GLN
23	AU	101	ASN
24	AV	81	GLN
24	AV	98	ASN
24	AV	132	ASN
25	AW	42	GLN
26	AX	55	ASN
26	AX	137	ASN
27	AY	81	GLN
27	AY	100	HIS
28	AZ	36	HIS
28	AZ	40	HIS
28	AZ	57	GLN
29	Ba	74	ASN
32	Bd	105	HIS
33	Be	13	HIS
33	Be	88	HIS
33	Be	98	HIS
34	Bf	106	ASN
35	Bg	11	ASN
36	Bh	50	ASN
36	Bh	113	GLN
38	Bj	13	ASN
38	Bj	47	HIS
40	Bl	4	GLN
40	Bl	32	ASN
40	Bl	43	ASN
41	Bm	117	HIS
41	Bm	119	ASN
43	Bo	102	GLN
45	Bq	27	ASN
45	Bq	35	GLN

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Mol	Chain	Res	Type
45	Bq	140	HIS
46	Br	34	ASN
46	Br	39	GLN
48	A	46	ASN
48	A	49	ASN
48	A	109	ASN
48	A	163	ASN
49	B	92	GLN
49	B	95	ASN
49	B	118	GLN
49	B	146	GLN
49	B	178	ASN
49	B	183	GLN
50	C	92	GLN
50	C	214	ASN
50	C	225	ASN
51	D	195	ASN
52	E	67	GLN
52	E	188	ASN
53	F	81	ASN
53	F	105	ASN
53	F	160	GLN
53	F	202	ASN
54	G	56	ASN
54	G	119	GLN
54	G	182	GLN
54	G	201	GLN
55	H	147	ASN
55	H	170	GLN
55	H	174	ASN
56	I	35	ASN
56	I	53	GLN
56	I	119	GLN
56	I	160	GLN
58	K	17	GLN
58	K	29	GLN
59	L	14	GLN
59	L	16	GLN
60	M	51	GLN
61	N	151	ASN
62	O	12	GLN
64	Q	32	ASN

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Mol	Chain	Res	Type
64	Q	139	GLN
65	R	48	ASN
65	R	95	HIS
65	R	101	ASN
66	S	13	HIS
66	S	122	HIS
67	T	17	ASN
67	T	70	GLN
67	T	91	HIS
69	V	21	ASN
69	V	33	GLN
69	V	38	GLN
70	W	66	ASN
70	W	113	HIS
71	X	22	ASN
71	X	48	HIS
72	Y	29	HIS
72	Y	31	ASN
72	Y	110	GLN
74	a	8	ASN
75	b	5	GLN
75	b	26	GLN
75	b	31	HIS
75	b	42	ASN
75	b	49	HIS
78	e	57	ASN
79	f	95	HIS
79	f	132	ASN
80	g	5	ASN
80	g	32	ASN
80	g	70	GLN
80	g	119	ASN
80	g	226	GLN
80	g	295	HIS
80	g	315	ASN
80	g	321	GLN
80	g	326	ASN
82	1	460	ASN
82	1	475	GLN
82	1	495	ASN
82	1	540	GLN
82	1	786	GLN

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Mol	Chain	Res	Type
82	1	791	GLN
82	1	803	HIS
82	1	812	GLN
82	1	899	GLN
82	1	948	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3260/3364 (96%)	988 (30%)	153 (4%)
2	7	120/121 (99%)	27 (22%)	2 (1%)
3	8	156/2825 (5%)	41 (26%)	5 (3%)
81	2	1778/1798 (98%)	775 (43%)	94 (5%)
83	3	75/76 (98%)	35 (46%)	6 (8%)
All	All	5389/8184 (65%)	1866 (34%)	260 (4%)

All (1866) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	9	U
1	5	20	A
1	5	22	G
1	5	40	A
1	5	43	A
1	5	45	A
1	5	48	A
1	5	49	A
1	5	51	A
1	5	57	A
1	5	59	G
1	5	60	A
1	5	65	A
1	5	66	A
1	5	67	A
1	5	92	G
1	5	96	G
1	5	109	A
1	5	110	G
1	5	117	U
1	5	118	U
1	5	121	A

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Mol	Chain	Res	Type
1	5	122	A
1	5	125	C
1	5	127	G
1	5	133	U
1	5	134	U
1	5	135	C
1	5	136	G
1	5	141	C
1	5	142	C
1	5	143	G
1	5	146	U
1	5	148	G
1	5	150	A
1	5	156	A
1	5	157	A
1	5	161	G
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
1	5	191	U
1	5	192	C
1	5	194	U
1	5	199	A
1	5	200	C
1	5	205	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	231	G
1	5	239	U
1	5	240	C

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Mol	Chain	Res	Type
1	5	241	C
1	5	247	A
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	283	G
1	5	284	A
1	5	285	A
1	5	286	U
1	5	294	U
1	5	295	A
1	5	297	G
1	5	298	U
1	5	299	G
1	5	305	U
1	5	314	U
1	5	315	C
1	5	316	U
1	5	317	A
1	5	323	A
1	5	326	U
1	5	329	U
1	5	336	A
1	5	339	C
1	5	340	C
1	5	348	A
1	5	350	C
1	5	352	A
1	5	356	C
1	5	374	A
1	5	375	A
1	5	376	G
1	5	379	C
1	5	385	A
1	5	390	G
1	5	391	A

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Mol	Chain	Res	Type
1	5	397	A
1	5	398	A
1	5	399	A
1	5	401	U
1	5	402	A
1	5	403	C
1	5	404	G
1	5	406	G
1	5	407	A
1	5	411	U
1	5	421	G
1	5	422	A
1	5	423	A
1	5	425	G
1	5	429	U
1	5	433	A
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	492	A
1	5	496	C
1	5	503	A
1	5	506	G
1	5	512	C
1	5	514	G
1	5	516	U
1	5	518	C
1	5	519	G
1	5	520	G
1	5	523	G
1	5	524	A
1	5	530	A
1	5	532	A
1	5	533	G
1	5	537	G
1	5	542	A
1	5	543	A
1	5	551	A
1	5	552	G

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Mol	Chain	Res	Type
1	5	554	U
1	5	561	G
1	5	562	A
1	5	565	A
1	5	570	G
1	5	573	U
1	5	577	G
1	5	582	G
1	5	584	A
1	5	594	A
1	5	595	A
1	5	597	G
1	5	605	G
1	5	609	C
1	5	615	U
1	5	620	A
1	5	622	A
1	5	623	C
1	5	633	A
1	5	634	G
1	5	635	U
1	5	639	A
1	5	640	C
1	5	648	C
1	5	649	G
1	5	650	A
1	5	651	G
1	5	654	U
1	5	660	U
1	5	664	A
1	5	671	U
1	5	672	A
1	5	678	A
1	5	681	G
1	5	682	A
1	5	683	A
1	5	685	G
1	5	688	A
1	5	691	G
1	5	692	U
1	5	693	A
1	5	694	G

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Mol	Chain	Res	Type
1	5	695	G
1	5	698	A
1	5	708	A
1	5	709	G
1	5	710	G
1	5	731	G
1	5	732	A
1	5	736	C
1	5	738	U
1	5	745	G
1	5	747	U
1	5	748	U
1	5	752	G
1	5	756	G
1	5	757	A
1	5	758	G
1	5	770	G
1	5	771	G
1	5	772	A
1	5	777	A
1	5	779	A
1	5	785	U
1	5	788	A
1	5	798	A
1	5	801	A
1	5	808	A
1	5	813	G
1	5	818	A
1	5	819	A
1	5	820	C
1	5	832	C
1	5	835	G
1	5	840	G
1	5	845	U
1	5	850	U
1	5	860	U
1	5	861	C
1	5	866	A
1	5	867	A
1	5	868	U
1	5	870	U
1	5	878	G

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Mol	Chain	Res	Type
1	5	879	G
1	5	885	A
1	5	887	G
1	5	888	A
1	5	894	C
1	5	896	A
1	5	900	A
1	5	908	G
1	5	912	G
1	5	915	C
1	5	916	C
1	5	924	G
1	5	930	C
1	5	931	U
1	5	938	A
1	5	949	G
1	5	950	U
1	5	952	U
1	5	953	C
1	5	955	G
1	5	964	G
1	5	965	G
1	5	973	A
1	5	974	A
1	5	981	G
1	5	985	U
1	5	986	A
1	5	987	C
1	5	988	C
1	5	989	G
1	5	990	G
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	1004	U
1	5	1005	U
1	5	1006	G
1	5	1008	C

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Mol	Chain	Res	Type
1	5	1011	A
1	5	1018	A
1	5	1020	C
1	5	1028	A
1	5	1034	G
1	5	1035	A
1	5	1036	A
1	5	1039	C
1	5	1042	U
1	5	1051	A
1	5	1053	U
1	5	1054	G
1	5	1064	A
1	5	1065	U
1	5	1066	U
1	5	1067	U
1	5	1068	G
1	5	1069	A
1	5	1074	A
1	5	1088	G
1	5	1093	U
1	5	1101	A
1	5	1102	G
1	5	1109	U
1	5	1122	U
1	5	1123	G
1	5	1124	A
1	5	1130	A
1	5	1132	G
1	5	1137	G
1	5	1145	G
1	5	1149	G
1	5	1151	A
1	5	1152	U
1	5	1153	A
1	5	1160	C
1	5	1167	C
1	5	1172	C
1	5	1178	G
1	5	1180	G
1	5	1183	A
1	5	1191	U

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Mol	Chain	Res	Type
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	1199	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	1220	G
1	5	1222	A
1	5	1224	U
1	5	1225	C
1	5	1226	C
1	5	1229	U
1	5	1233	G
1	5	1234	A
1	5	1235	G
1	5	1236	U
1	5	1237	G
1	5	1244	A
1	5	1248	C
1	5	1250	C
1	5	1254	C
1	5	1255	C
1	5	1256	G
1	5	1257	A
1	5	1258	A
1	5	1265	A
1	5	1268	C
1	5	1278	G
1	5	1279	A
1	5	1280	U

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Mol	Chain	Res	Type
1	5	1283	C
1	5	1284	G
1	5	1287	C
1	5	1297	A
1	5	1301	A
1	5	1302	U
1	5	1316	G
1	5	1318	U
1	5	1319	U
1	5	1320	A
1	5	1322	U
1	5	1323	A
1	5	1324	U
1	5	1325	G
1	5	1327	U
1	5	1328	G
1	5	1334	A
1	5	1348	G
1	5	1354	G
1	5	1356	C
1	5	1357	A
1	5	1360	G
1	5	1361	A
1	5	1362	C
1	5	1370	A
1	5	1383	G
1	5	1389	A
1	5	1390	A
1	5	1401	U
1	5	1402	G
1	5	1405	G
1	5	1408	C
1	5	1412	G
1	5	1421	G
1	5	1425	A
1	5	1431	A
1	5	1444	G
1	5	1447	G
1	5	1448	A
1	5	1451	G
1	5	1452	A
1	5	1453	A

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Mol	Chain	Res	Type
1	5	1454	G
1	5	1455	U
1	5	1456	G
1	5	1461	A
1	5	1463	G
1	5	1471	G
1	5	1475	A
1	5	1479	C
1	5	1482	U
1	5	1494	U
1	5	1497	U
1	5	1498	C
1	5	1502	C
1	5	1504	U
1	5	1507	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	1535	U
1	5	1536	A
1	5	1537	A
1	5	1539	U
1	5	1540	U
1	5	1544	A
1	5	1546	G
1	5	1547	C
1	5	1549	A
1	5	1550	C
1	5	1551	C
1	5	1552	A
1	5	1554	C
1	5	1555	G
1	5	1558	A
1	5	1562	A
1	5	1564	U
1	5	1568	G

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Mol	Chain	Res	Type
1	5	1576	U
1	5	1577	C
1	5	1581	A
1	5	1584	C
1	5	1588	A
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	1612	A
1	5	1613	C
1	5	1614	U
1	5	1615	G
1	5	1626	C
1	5	1627	G
1	5	1644	G
1	5	1647	G
1	5	1652	A
1	5	1656	U
1	5	1657	U
1	5	1658	U
1	5	1662	C
1	5	1663	U
1	5	1672	U
1	5	1682	G
1	5	1684	A
1	5	1685	U
1	5	1686	U
1	5	1687	G
1	5	1693	U
1	5	1712	G
1	5	1719	A
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

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Mol	Chain	Res	Type
1	5	1739	G
1	5	1749	G
1	5	1760	C
1	5	1761	C
1	5	1766	A
1	5	1767	A
1	5	1777	G
1	5	1781	G
1	5	1782	A
1	5	1783	A
1	5	1784	U
1	5	1785	A
1	5	1786	G
1	5	1787	U
1	5	1788	U
1	5	1789	U
1	5	1790	U
1	5	1792	A
1	5	1807	G
1	5	1809	U
1	5	1810	A
1	5	1811	A
1	5	1814	G
1	5	1815	C
1	5	1817	G
1	5	1818	C
1	5	1835	C
1	5	1837	G
1	5	1840	U
1	5	1843	A
1	5	1847	G
1	5	1848	A
1	5	1849	U
1	5	1854	U
1	5	1855	A
1	5	1861	G
1	5	1862	A
1	5	1864	A
1	5	1874	G
1	5	1875	G
1	5	1878	A
1	5	1879	A

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Mol	Chain	Res	Type
1	5	1884	A
1	5	1895	C
1	5	1898	G
1	5	1919	U
1	5	1922	G
1	5	1923	A
1	5	1925	G
1	5	1926	U
1	5	1927	G
1	5	1928	A
1	5	1929	G
1	5	1939	C
1	5	1943	C
1	5	1947	G
1	5	2020	U
1	5	2022	G
1	5	2025	G
1	5	2027	C
1	5	2029	G
1	5	2030	C
1	5	2033	U
1	5	2034	G
1	5	2036	U
1	5	2039	G
1	5	2041	C
1	5	2042	U
1	5	2045	U
1	5	2051	U
1	5	2054	U
1	5	2058	A
1	5	2059	U
1	5	2060	U
1	5	2061	A
1	5	2062	A
1	5	2063	C
1	5	2064	G
1	5	2066	U
1	5	2067	C
1	5	2069	A
1	5	2070	C
1	5	2071	U
1	5	2080	G

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Mol	Chain	Res	Type
1	5	2081	U
1	5	2082	A
1	5	2083	C
1	5	2089	A
1	5	2090	G
1	5	2091	G
1	5	2097	C
1	5	2100	A
1	5	2107	A
1	5	2108	A
1	5	2111	A
1	5	2125	C
1	5	2127	A
1	5	2129	G
1	5	2133	A
1	5	2137	A
1	5	2143	G
1	5	2145	U
1	5	2149	G
1	5	2154	G
1	5	2161	C
1	5	2162	U
1	5	2163	G
1	5	2167	A
1	5	2174	U
1	5	2175	G
1	5	2177	A
1	5	2180	U
1	5	2182	A
1	5	2185	G
1	5	2192	A
1	5	2193	A
1	5	2194	U
1	5	2196	C
1	5	2198	A
1	5	2201	A
1	5	2202	A
1	5	2217	C
1	5	2218	G
1	5	2221	A
1	5	2222	G
1	5	2225	A

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Mol	Chain	Res	Type
1	5	2226	C
1	5	2227	U
1	5	2228	A
1	5	2229	U
1	5	2230	G
1	5	2231	A
1	5	2232	C
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	2248	A
1	5	2250	A
1	5	2251	U
1	5	2252	G
1	5	2255	U
1	5	2256	C
1	5	2257	G
1	5	2267	U
1	5	2274	G
1	5	2275	C
1	5	2276	G
1	5	2279	U
1	5	2282	A
1	5	2284	G
1	5	2285	G
1	5	2290	A
1	5	2300	C
1	5	2301	A
1	5	2303	U
1	5	2304	G
1	5	2305	U
1	5	2326	A
1	5	2342	A
1	5	2343	C
1	5	2344	G
1	5	2346	G
1	5	2347	C

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Mol	Chain	Res	Type
1	5	2352	C
1	5	2354	G
1	5	2357	U
1	5	2360	G
1	5	2362	G
1	5	2364	G
1	5	2366	A
1	5	2369	G
1	5	2370	A
1	5	2371	A
1	5	2372	G
1	5	2373	A
1	5	2379	U
1	5	2380	U
1	5	2381	G
1	5	2382	A
1	5	2387	G
1	5	2388	A
1	5	2397	U
1	5	2404	G
1	5	2408	A
1	5	2409	G
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	2419	G
1	5	2420	G
1	5	2421	G
1	5	2422	U
1	5	2423	G
1	5	2426	G
1	5	2427	C
1	5	2428	A
1	5	2429	U
1	5	2438	G
1	5	2442	C
1	5	2446	G
1	5	2451	U

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Mol	Chain	Res	Type
1	5	2452	G
1	5	2456	U
1	5	2457	A
1	5	2459	C
1	5	2460	A
1	5	2463	A
1	5	2466	U
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	2477	U
1	5	2478	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	2498	A
1	5	2499	G
1	5	2500	C
1	5	2501	U
1	5	2502	G
1	5	2503	G
1	5	2505	A
1	5	2506	U
1	5	2507	U
1	5	2508	C
1	5	2509	A
1	5	2510	U
1	5	2511	U
1	5	2512	U
1	5	2513	U
1	5	2514	C
1	5	2521	C

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Mol	Chain	Res	Type
1	5	2522	U
1	5	2523	A
1	5	2524	G
1	5	2529	C
1	5	2530	A
1	5	2531	A
1	5	2532	A
1	5	2535	C
1	5	2536	C
1	5	2537	U
1	5	2540	A
1	5	2541	C
1	5	2542	G
1	5	2549	U
1	5	2553	G
1	5	2557	G
1	5	2562	C
1	5	2563	A
1	5	2568	C
1	5	2571	G
1	5	2574	G
1	5	2575	G
1	5	2582	G
1	5	2595	C
1	5	2596	A
1	5	2597	U
1	5	2607	G
1	5	2616	G
1	5	2620	U
1	5	2621	C
1	5	2623	U
1	5	2624	A
1	5	2625	A
1	5	2631	A
1	5	2633	U
1	5	2635	A
1	5	2636	U
1	5	2642	A
1	5	2645	G
1	5	2646	A
1	5	2647	A
1	5	2649	U

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Mol	Chain	Res	Type
1	5	2657	A
1	5	2658	G
1	5	2659	A
1	5	2662	A
1	5	2664	A
1	5	2667	G
1	5	2671	A
1	5	2672	A
1	5	2673	A
1	5	2676	C
1	5	2678	C
1	5	2682	G
1	5	2687	U
1	5	2691	U
1	5	2696	G
1	5	2697	U
1	5	2707	A
1	5	2708	A
1	5	2715	A
1	5	2720	U
1	5	2721	G
1	5	2730	A
1	5	2740	U
1	5	2744	C
1	5	2745	G
1	5	2746	G
1	5	2750	U
1	5	2758	A
1	5	2764	G
1	5	2767	A
1	5	2768	G
1	5	2769	A
1	5	2771	A
1	5	2772	A
1	5	2778	C
1	5	2782	G
1	5	2785	A
1	5	2789	C
1	5	2790	U
1	5	2812	C
1	5	2813	A
1	5	2815	A

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Mol	Chain	Res	Type
1	5	2817	C
1	5	2824	G
1	5	2829	U
1	5	2839	G
1	5	2843	U
1	5	2845	G
1	5	2855	A
1	5	2866	G
1	5	2867	C
1	5	2869	G
1	5	2871	A
1	5	2872	U
1	5	2879	A
1	5	2880	G
1	5	2884	U
1	5	2891	U
1	5	2903	U
1	5	2904	A
1	5	2910	C
1	5	2911	G
1	5	2915	G
1	5	2922	U
1	5	2923	U
1	5	2925	G
1	5	2934	G
1	5	2940	G
1	5	2946	U
1	5	2947	U
1	5	2948	U
1	5	2949	U
1	5	2950	A
1	5	2951	C
1	5	2964	U
1	5	2965	G
1	5	2967	U
1	5	2969	U
1	5	2979	A
1	5	2980	A
1	5	2985	A
1	5	2996	G
1	5	3006	U
1	5	3007	C

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Mol	Chain	Res	Type
1	5	3024	U
1	5	3025	U
1	5	3027	G
1	5	3030	G
1	5	3040	C
1	5	3041	A
1	5	3046	U
1	5	3047	U
1	5	3053	G
1	5	3054	A
1	5	3060	C
1	5	3063	U
1	5	3067	C
1	5	3070	G
1	5	3077	G
1	5	3078	C
1	5	3084	G
1	5	3085	C
1	5	3090	A
1	5	3092	G
1	5	3095	A
1	5	3097	A
1	5	3099	U
1	5	3107	A
1	5	3110	A
1	5	3121	U
1	5	3123	U
1	5	3124	U
1	5	3125	U
1	5	3126	G
1	5	3127	C
1	5	3133	A
1	5	3134	C
1	5	3136	A
1	5	3140	A
1	5	3141	G
1	5	3142	A
1	5	3144	G
1	5	3147	U
1	5	3148	A
1	5	3149	A
1	5	3150	G

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Mol	Chain	Res	Type
1	5	3155	A
1	5	3162	U
1	5	3163	U
1	5	3164	U
1	5	3165	U
1	5	3166	U
1	5	3170	G
1	5	3174	C
1	5	3175	U
1	5	3176	G
1	5	3177	A
1	5	3180	C
1	5	3181	A
1	5	3182	U
1	5	3184	G
1	5	3185	C
1	5	3186	A
1	5	3187	G
1	5	3191	G
1	5	3192	G
1	5	3197	G
1	5	3199	U
1	5	3202	U
1	5	3204	U
1	5	3205	U
1	5	3206	A
1	5	3207	G
1	5	3208	C
1	5	3212	A
1	5	3213	A
1	5	3215	G
1	5	3216	C
1	5	3217	U
1	5	3220	G
1	5	3221	G
1	5	3227	U
1	5	3228	G
1	5	3231	G
1	5	3236	A
1	5	3237	U
1	5	3238	U
1	5	3243	U

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Mol	Chain	Res	Type
1	5	3245	U
1	5	3247	A
1	5	3250	U
1	5	3252	G
1	5	3253	C
1	5	3254	G
1	5	3256	A
1	5	3258	G
1	5	3260	A
1	5	3262	A
1	5	3265	U
1	5	3272	U
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	3294	G
1	5	3303	A
1	5	3304	A
1	5	3309	U
1	5	3310	A
1	5	3313	G
1	5	3316	G
1	5	3318	C
1	5	3319	U
1	5	3322	U
1	5	3323	U
1	5	3324	G
1	5	3325	U
1	5	3326	U
1	5	3330	A
1	5	3337	G
1	5	3346	C
1	5	3350	C
1	5	3351	G
1	5	3357	U
1	5	3358	G
1	5	3361	U
1	5	3362	U
1	5	3364	U

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Mol	Chain	Res	Type
2	7	7	G
2	7	13	A
2	7	18	C
2	7	22	A
2	7	27	A
2	7	31	U
2	7	41	G
2	7	54	U
2	7	61	G
2	7	64	A
2	7	65	G
2	7	73	C
2	7	74	C
2	7	76	A
2	7	79	A
2	7	91	G
2	7	92	A
2	7	93	C
2	7	94	C
2	7	101	G
2	7	102	A
2	7	104	A
2	7	110	G
2	7	112	G
2	7	113	C
2	7	118	A
2	7	119	U
3	8	8	C
3	8	21	C
3	8	23	U
3	8	25	G
3	8	34	U
3	8	35	C
3	8	39	G
3	8	40	A
3	8	48	A
3	8	50	C
3	8	56	G
3	8	59	A
3	8	62	U
3	8	63	G
3	8	81	U

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Mol	Chain	Res	Type
3	8	82	U
3	8	84	C
3	8	86	U
3	8	87	G
3	8	91	C
3	8	95	A
3	8	96	A
3	8	97	A
3	8	104	A
3	8	106	C
3	8	111	A
3	8	112	U
3	8	113	U
3	8	116	G
3	8	121	C
3	8	126	A
3	8	127	U
3	8	129	C
3	8	144	G
3	8	147	U
3	8	148	G
3	8	151	C
3	8	152	G
3	8	155	A
3	8	156	U
3	8	157	U
81	2	2	A
81	2	3	U
81	2	4	C
81	2	9	U
81	2	11	A
81	2	17	C
81	2	18	C
81	2	24	U
81	2	25	C
81	2	26	A
81	2	31	C
81	2	34	G
81	2	36	C
81	2	39	A
81	2	40	A
81	2	42	G

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Mol	Chain	Res	Type
81	2	47	A
81	2	48	G
81	2	51	A
81	2	54	C
81	2	56	U
81	2	57	G
81	2	59	C
81	2	60	U
81	2	61	A
81	2	62	A
81	2	63	G
81	2	64	U
81	2	65	A
81	2	66	U
81	2	67	A
81	2	68	A
81	2	69	G
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	93	A
81	2	95	G
81	2	104	A
81	2	110	U
81	2	111	U
81	2	114	C
81	2	115	G
81	2	116	U
81	2	118	U
81	2	124	A
81	2	125	U
81	2	126	A
81	2	127	G
81	2	128	U
81	2	129	U
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	141	U
81	2	146	A
81	2	148	C
81	2	149	U
81	2	152	G
81	2	156	A
81	2	158	U
81	2	159	C
81	2	160	U
81	2	161	A
81	2	167	A
81	2	173	U
81	2	175	C
81	2	176	U
81	2	177	U
81	2	178	A
81	2	179	A
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	193	U
81	2	194	G
81	2	196	A
81	2	199	A
81	2	203	G
81	2	208	U
81	2	209	A
81	2	216	A
81	2	217	A
81	2	218	A
81	2	219	A
81	2	220	A
81	2	227	G
81	2	228	U

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Mol	Chain	Res	Type
81	2	230	U
81	2	232	C
81	2	233	G
81	2	234	G
81	2	235	A
81	2	238	C
81	2	239	C
81	2	240	U
81	2	244	U
81	2	247	U
81	2	249	C
81	2	256	A
81	2	257	C
81	2	258	U
81	2	259	U
81	2	261	U
81	2	263	G
81	2	264	A
81	2	265	A
81	2	266	U
81	2	267	C
81	2	268	G
81	2	269	C
81	2	270	A
81	2	271	U
81	2	272	G
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	281	C
81	2	286	G
81	2	288	U
81	2	298	A
81	2	301	U
81	2	308	C
81	2	309	C
81	2	311	A
81	2	312	U

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Mol	Chain	Res	Type
81	2	313	C
81	2	315	A
81	2	318	U
81	2	319	U
81	2	320	C
81	2	321	G
81	2	324	G
81	2	328	G
81	2	332	A
81	2	336	G
81	2	339	U
81	2	344	U
81	2	346	G
81	2	359	A
81	2	360	C
81	2	362	G
81	2	369	A
81	2	371	G
81	2	377	A
81	2	383	G
81	2	384	A
81	2	386	A
81	2	392	C
81	2	395	G
81	2	397	G
81	2	399	A
81	2	400	A
81	2	401	C
81	2	403	G
81	2	404	C
81	2	412	U
81	2	415	A
81	2	416	A
81	2	417	G
81	2	418	G
81	2	421	G
81	2	423	C
81	2	425	G
81	2	427	A
81	2	430	C
81	2	432	C
81	2	433	G

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Mol	Chain	Res	Type
81	2	438	U
81	2	439	U
81	2	443	C
81	2	447	C
81	2	452	U
81	2	453	U
81	2	454	C
81	2	461	G
81	2	467	A
81	2	468	C
81	2	473	A
81	2	474	A
81	2	475	U
81	2	476	A
81	2	479	G
81	2	484	A
81	2	487	G
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	498	U
81	2	499	C
81	2	500	U
81	2	502	G
81	2	504	A
81	2	505	A
81	2	506	U
81	2	507	U
81	2	509	G
81	2	510	A
81	2	511	A
81	2	514	A
81	2	515	G
81	2	518	C
81	2	526	A
81	2	533	A
81	2	537	A
81	2	538	G
81	2	539	G

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Mol	Chain	Res	Type
81	2	540	A
81	2	541	A
81	2	542	C
81	2	543	A
81	2	544	A
81	2	547	G
81	2	554	A
81	2	556	G
81	2	557	U
81	2	558	C
81	2	559	U
81	2	561	G
81	2	563	G
81	2	565	C
81	2	570	G
81	2	571	C
81	2	573	G
81	2	575	G
81	2	576	G
81	2	577	U
81	2	578	A
81	2	579	A
81	2	585	G
81	2	593	A
81	2	594	G
81	2	596	G
81	2	607	U
81	2	609	G
81	2	610	U
81	2	618	A
81	2	619	A
81	2	622	A
81	2	623	G
81	2	625	U
81	2	634	A
81	2	638	U
81	2	639	U
81	2	640	G
81	2	643	U
81	2	644	C
81	2	647	G
81	2	648	U

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Mol	Chain	Res	Type
81	2	649	U
81	2	650	G
81	2	652	C
81	2	653	C
81	2	654	G
81	2	655	G
81	2	677	G
81	2	679	U
81	2	681	U
81	2	684	A
81	2	686	C
81	2	690	A
81	2	691	U
81	2	693	U
81	2	695	U
81	2	696	C
81	2	697	C
81	2	698	U
81	2	701	U
81	2	704	C
81	2	705	U
81	2	708	C
81	2	709	C
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	721	U
81	2	722	G
81	2	723	G
81	2	724	G
81	2	725	U
81	2	727	C
81	2	729	G
81	2	730	G
81	2	731	C
81	2	732	G
81	2	733	A
81	2	734	A
81	2	736	C

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Mol	Chain	Res	Type
81	2	738	G
81	2	740	A
81	2	741	C
81	2	742	U
81	2	743	U
81	2	750	U
81	2	753	A
81	2	754	A
81	2	756	A
81	2	757	A
81	2	765	G
81	2	766	U
81	2	767	U
81	2	768	C
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	786	G
81	2	787	A
81	2	788	A
81	2	790	A
81	2	791	U
81	2	793	U
81	2	794	U
81	2	795	A
81	2	798	A
81	2	800	G
81	2	802	A
81	2	803	A
81	2	810	A
81	2	811	A
81	2	812	U
81	2	813	A
81	2	815	G
81	2	817	C
81	2	819	U
81	2	820	U

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Mol	Chain	Res	Type
81	2	821	U
81	2	822	G
81	2	823	G
81	2	825	U
81	2	828	A
81	2	829	U
81	2	830	U
81	2	831	U
81	2	832	U
81	2	833	G
81	2	834	U
81	2	837	G
81	2	838	U
81	2	842	U
81	2	843	A
81	2	844	G
81	2	845	G
81	2	846	A
81	2	848	C
81	2	849	A
81	2	850	U
81	2	851	C
81	2	852	G
81	2	854	A
81	2	855	A
81	2	862	A
81	2	863	U
81	2	864	A
81	2	875	G
81	2	876	G
81	2	886	A
81	2	887	U
81	2	888	U
81	2	894	G
81	2	895	U
81	2	897	A
81	2	900	G
81	2	903	G
81	2	904	A
81	2	905	A
81	2	906	A
81	2	907	U

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Mol	Chain	Res	Type
81	2	908	U
81	2	909	C
81	2	910	U
81	2	911	U
81	2	912	G
81	2	913	G
81	2	914	A
81	2	915	U
81	2	920	U
81	2	927	U
81	2	930	C
81	2	932	A
81	2	934	U
81	2	941	G
81	2	942	C
81	2	944	U
81	2	948	C
81	2	950	A
81	2	951	A
81	2	958	U
81	2	959	U
81	2	963	U
81	2	965	A
81	2	969	A
81	2	981	U
81	2	983	G
81	2	984	G
81	2	991	A
81	2	992	A
81	2	994	A
81	2	996	G
81	2	1003	U
81	2	1004	A
81	2	1005	C
81	2	1006	C
81	2	1011	U
81	2	1015	C
81	2	1016	U
81	2	1019	A
81	2	1020	C
81	2	1025	A
81	2	1026	A

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Mol	Chain	Res	Type
81	2	1027	C
81	2	1029	A
81	2	1030	U
81	2	1031	G
81	2	1038	A
81	2	1039	G
81	2	1041	G
81	2	1044	C
81	2	1048	U
81	2	1049	G
81	2	1050	G
81	2	1051	U
81	2	1052	G
81	2	1054	U
81	2	1057	U
81	2	1058	C
81	2	1060	U
81	2	1066	C
81	2	1075	A
81	2	1079	U
81	2	1080	A
81	2	1081	C
81	2	1082	G
81	2	1087	A
81	2	1091	A
81	2	1096	U
81	2	1097	U
81	2	1099	G
81	2	1107	G
81	2	1108	G
81	2	1110	G
81	2	1112	A
81	2	1113	G
81	2	1114	U
81	2	1123	A
81	2	1125	G
81	2	1130	A
81	2	1134	U
81	2	1137	A
81	2	1138	A
81	2	1139	G
81	2	1142	A

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Mol	Chain	Res	Type
81	2	1149	G
81	2	1150	A
81	2	1154	G
81	2	1157	C
81	2	1158	C
81	2	1161	C
81	2	1163	G
81	2	1164	G
81	2	1166	G
81	2	1169	G
81	2	1172	C
81	2	1173	C
81	2	1175	G
81	2	1184	U
81	2	1185	U
81	2	1186	U
81	2	1189	C
81	2	1190	U
81	2	1191	C
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	1206	C
81	2	1208	C
81	2	1209	C
81	2	1210	A
81	2	1212	G
81	2	1215	C
81	2	1216	A
81	2	1217	G
81	2	1218	A
81	2	1222	A
81	2	1223	A
81	2	1225	A
81	2	1227	G
81	2	1228	G
81	2	1229	A

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Mol	Chain	Res	Type
81	2	1232	G
81	2	1234	C
81	2	1236	G
81	2	1237	A
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	1254	G
81	2	1255	A
81	2	1258	U
81	2	1259	U
81	2	1260	G
81	2	1261	U
81	2	1268	U
81	2	1269	G
81	2	1271	U
81	2	1272	G
81	2	1277	G
81	2	1282	U
81	2	1284	U
81	2	1286	A
81	2	1289	U
81	2	1292	U
81	2	1293	G
81	2	1306	U
81	2	1311	A
81	2	1313	U
81	2	1314	U
81	2	1320	A
81	2	1321	A
81	2	1322	C
81	2	1323	G
81	2	1330	A
81	2	1336	A
81	2	1339	U
81	2	1340	A
81	2	1342	U

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Mol	Chain	Res	Type
81	2	1344	A
81	2	1345	A
81	2	1347	A
81	2	1348	G
81	2	1349	G
81	2	1351	U
81	2	1352	U
81	2	1353	G
81	2	1355	U
81	2	1356	G
81	2	1359	A
81	2	1360	C
81	2	1361	U
81	2	1362	U
81	2	1363	G
81	2	1364	C
81	2	1365	C
81	2	1366	G
81	2	1367	G
81	2	1369	U
81	2	1370	G
81	2	1373	U
81	2	1374	C
81	2	1375	U
81	2	1378	U
81	2	1384	G
81	2	1388	U
81	2	1389	A
81	2	1390	U
81	2	1395	U
81	2	1396	U
81	2	1397	C
81	2	1398	A
81	2	1400	G
81	2	1402	C
81	2	1403	G
81	2	1406	G
81	2	1410	G
81	2	1411	U
81	2	1412	U
81	2	1413	U
81	2	1419	A

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Mol	Chain	Res	Type
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	1441	U
81	2	1443	G
81	2	1444	A
81	2	1447	U
81	2	1448	U
81	2	1449	C
81	2	1451	G
81	2	1453	G
81	2	1454	C
81	2	1455	C
81	2	1456	G
81	2	1457	C
81	2	1458	A
81	2	1459	C
81	2	1463	C
81	2	1469	A
81	2	1471	U
81	2	1474	C
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	1502	G
81	2	1503	A
81	2	1504	G
81	2	1506	U

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Mol	Chain	Res	Type
81	2	1507	C
81	2	1508	U
81	2	1509	G
81	2	1512	U
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	1528	C
81	2	1532	G
81	2	1533	U
81	2	1534	G
81	2	1535	C
81	2	1536	U
81	2	1538	G
81	2	1540	G
81	2	1543	A
81	2	1546	G
81	2	1551	G
81	2	1553	A
81	2	1555	U
81	2	1556	U
81	2	1557	A
81	2	1566	C
81	2	1567	A
81	2	1569	C
81	2	1580	U
81	2	1581	A
81	2	1583	U
81	2	1588	G
81	2	1590	A
81	2	1595	A
81	2	1598	A
81	2	1599	G
81	2	1600	C
81	2	1604	C
81	2	1606	U
81	2	1608	G
81	2	1611	U
81	2	1612	A

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Mol	Chain	Res	Type
81	2	1614	G
81	2	1615	U
81	2	1616	C
81	2	1619	U
81	2	1620	G
81	2	1621	C
81	2	1622	C
81	2	1626	U
81	2	1629	A
81	2	1633	A
81	2	1636	G
81	2	1637	C
81	2	1638	C
81	2	1640	G
81	2	1643	G
81	2	1644	C
81	2	1647	G
81	2	1649	A
81	2	1655	U
81	2	1656	G
81	2	1660	G
81	2	1668	G
81	2	1672	C
81	2	1674	U
81	2	1679	A
81	2	1682	U
81	2	1685	U
81	2	1686	U
81	2	1687	A
81	2	1688	G
81	2	1689	A
81	2	1692	A
81	2	1693	G
81	2	1694	G
81	2	1695	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

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Mol	Chain	Res	Type
81	2	1703	C
81	2	1705	A
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	1713	G
81	2	1714	C
81	2	1715	G
81	2	1716	A
81	2	1721	U
81	2	1729	A
81	2	1736	U
81	2	1738	A
81	2	1746	G
81	2	1748	A
81	2	1751	A
81	2	1752	A
81	2	1753	A
81	2	1754	A
81	2	1758	G
81	2	1760	A
81	2	1763	A
81	2	1764	A
81	2	1766	G
81	2	1767	U
81	2	1768	U
81	2	1776	G
81	2	1778	G
81	2	1780	A
81	2	1781	C
81	2	1784	G
81	2	1786	G
81	2	1789	A
81	2	1790	G
81	2	1791	G
81	2	1792	A
81	2	1793	U
81	2	1794	C

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Mol	Chain	Res	Type
81	2	1795	A
81	2	1796	U
81	2	1798	A
83	3	2	C
83	3	8	U
83	3	13	C
83	3	15	G
83	3	16	A
83	3	17	A
83	3	18	G
83	3	19	G
83	3	20	U
83	3	21	A
83	3	26	A
83	3	29	G
83	3	30	G
83	3	34	G
83	3	35	A
83	3	38	A
83	3	39	U
83	3	40	C
83	3	42	C
83	3	46	G
83	3	48	C
83	3	52	G
83	3	53	G
83	3	54	U
83	3	57	G
83	3	58	A
83	3	59	U
83	3	60	U
83	3	61	C
83	3	70	G
83	3	71	G
83	3	72	C
83	3	74	C
83	3	75	C
83	3	76	A

All (260) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	5	65	A
1	5	121	A
1	5	148	G
1	5	166	C
1	5	240	C
1	5	248	U
1	5	249	U
1	5	283	G
1	5	297	G
1	5	298	U
1	5	397	A
1	5	401	U
1	5	406	G
1	5	489	G
1	5	517	U
1	5	518	C
1	5	561	G
1	5	567	U
1	5	580	A
1	5	593	U
1	5	634	G
1	5	691	G
1	5	692	U
1	5	707	A
1	5	731	G
1	5	735	U
1	5	756	G
1	5	867	A
1	5	887	G
1	5	932	C
1	5	949	G
1	5	951	A
1	5	964	G
1	5	985	U
1	5	987	C
1	5	998	A
1	5	1035	A
1	5	1066	U
1	5	1068	G
1	5	1123	G
1	5	1131	C

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Mol	Chain	Res	Type
1	5	1152	U
1	5	1167	C
1	5	1179	U
1	5	1191	U
1	5	1193	G
1	5	1194	A
1	5	1212	U
1	5	1234	A
1	5	1255	C
1	5	1278	G
1	5	1300	U
1	5	1319	U
1	5	1323	A
1	5	1326	A
1	5	1451	G
1	5	1453	A
1	5	1526	U
1	5	1531	G
1	5	1539	U
1	5	1551	C
1	5	1576	U
1	5	1600	C
1	5	1611	A
1	5	1612	A
1	5	1626	C
1	5	1664	U
1	5	1685	U
1	5	1720	G
1	5	1762	C
1	5	1785	A
1	5	1790	U
1	5	1809	U
1	5	1810	A
1	5	1815	C
1	5	1894	U
1	5	2032	U
1	5	2040	U
1	5	2041	C
1	5	2059	U
1	5	2061	A
1	5	2081	U
1	5	2107	A

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Mol	Chain	Res	Type
1	5	2113	A
1	5	2173	C
1	5	2217	C
1	5	2225	A
1	5	2228	A
1	5	2230	G
1	5	2231	A
1	5	2237	U
1	5	2250	A
1	5	2251	U
1	5	2274	G
1	5	2341	A
1	5	2343	C
1	5	2416	A
1	5	2422	U
1	5	2437	A
1	5	2455	A
1	5	2456	U
1	5	2468	U
1	5	2469	A
1	5	2472	G
1	5	2474	U
1	5	2477	U
1	5	2483	U
1	5	2506	U
1	5	2507	U
1	5	2511	U
1	5	2512	U
1	5	2522	U
1	5	2529	C
1	5	2530	A
1	5	2538	A
1	5	2539	U
1	5	2540	A
1	5	2553	G
1	5	2561	A
1	5	2595	C
1	5	2603	A
1	5	2644	A
1	5	2645	G
1	5	2672	A
1	5	2696	G

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Mol	Chain	Res	Type
1	5	2745	G
1	5	2879	A
1	5	2909	A
1	5	2918	G
1	5	2922	U
1	5	2939	A
1	5	2946	U
1	5	2947	U
1	5	3024	U
1	5	3046	U
1	5	3061	C
1	5	3084	G
1	5	3122	C
1	5	3162	U
1	5	3174	C
1	5	3176	G
1	5	3184	G
1	5	3186	A
1	5	3196	C
1	5	3237	U
1	5	3242	A
1	5	3252	G
1	5	3257	A
1	5	3285	U
1	5	3308	G
1	5	3309	U
1	5	3325	U
1	5	3349	U
2	7	13	A
2	7	111	U
3	8	22	U
3	8	39	G
3	8	112	U
3	8	125	U
3	8	126	A
81	2	3	U
81	2	61	A
81	2	65	A
81	2	66	U
81	2	72	A
81	2	73	U
81	2	130	C

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Mol	Chain	Res	Type
81	2	131	C
81	2	177	U
81	2	216	A
81	2	217	A
81	2	258	U
81	2	263	G
81	2	271	U
81	2	277	U
81	2	278	G
81	2	279	U
81	2	452	U
81	2	497	G
81	2	537	A
81	2	542	C
81	2	556	G
81	2	564	C
81	2	570	G
81	2	605	A
81	2	621	A
81	2	694	U
81	2	695	U
81	2	697	C
81	2	700	C
81	2	708	C
81	2	721	U
81	2	740	A
81	2	742	U
81	2	765	G
81	2	794	U
81	2	810	A
81	2	818	G
81	2	828	A
81	2	854	A
81	2	903	G
81	2	909	C
81	2	911	U
81	2	912	G
81	2	943	A
81	2	958	U
81	2	1056	U
81	2	1060	U
81	2	1080	A

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Mol	Chain	Res	Type
81	2	1107	G
81	2	1157	C
81	2	1185	U
81	2	1189	C
81	2	1192	A
81	2	1195	A
81	2	1216	A
81	2	1228	G
81	2	1241	A
81	2	1243	A
81	2	1343	A
81	2	1369	U
81	2	1374	C
81	2	1389	A
81	2	1397	C
81	2	1410	G
81	2	1412	U
81	2	1429	C
81	2	1444	A
81	2	1447	U
81	2	1455	C
81	2	1456	G
81	2	1491	A
81	2	1514	A
81	2	1520	U
81	2	1532	G
81	2	1534	G
81	2	1535	C
81	2	1554	A
81	2	1580	U
81	2	1598	A
81	2	1613	C
81	2	1628	U
81	2	1643	G
81	2	1655	U
81	2	1678	G
81	2	1686	U
81	2	1713	G
81	2	1714	C
81	2	1752	A
81	2	1753	A
81	2	1765	G

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Mol	Chain	Res	Type
81	2	1767	U
81	2	1791	G
81	2	1792	A
83	3	16	A
83	3	19	G
83	3	34	G
83	3	58	A
83	3	71	G
83	3	74	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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
85	GCP	1	1001	-	32,34,34	1.49	7 (21%)	49,54,54	1.82	10 (20%)

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
85	GCP	1	1001	-	-	7/19/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	1	1001	GCP	C5-C4	3.31	1.47	1.38
85	1	1001	GCP	PB-O3A	2.99	1.61	1.58
85	1	1001	GCP	PG-O2G	2.90	1.61	1.55
85	1	1001	GCP	PG-O3G	2.85	1.61	1.55
85	1	1001	GCP	C5-N7	-2.14	1.34	1.39
85	1	1001	GCP	C6-N1	-2.12	1.34	1.38
85	1	1001	GCP	PB-O2B	2.06	1.61	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	1	1001	GCP	C5-C4-N3	-6.12	118.65	128.39
85	1	1001	GCP	C2-N3-C4	5.18	121.23	112.30
85	1	1001	GCP	N9-C4-N3	4.62	135.19	125.95
85	1	1001	GCP	C6-C5-N7	3.36	136.41	130.29
85	1	1001	GCP	PB-O3A-PA	-3.00	122.58	132.37
85	1	1001	GCP	C4-C5-N7	-2.57	106.60	110.67
85	1	1001	GCP	O6-C6-C5	-2.21	120.70	126.53
85	1	1001	GCP	C5-C6-N1	2.06	118.49	113.25
85	1	1001	GCP	O3G-PG-C3B	2.05	111.37	106.40
85	1	1001	GCP	C3'-C2'-C1'	2.05	105.33	101.46

There are no chirality outliers.

All (7) torsion outliers are listed below:

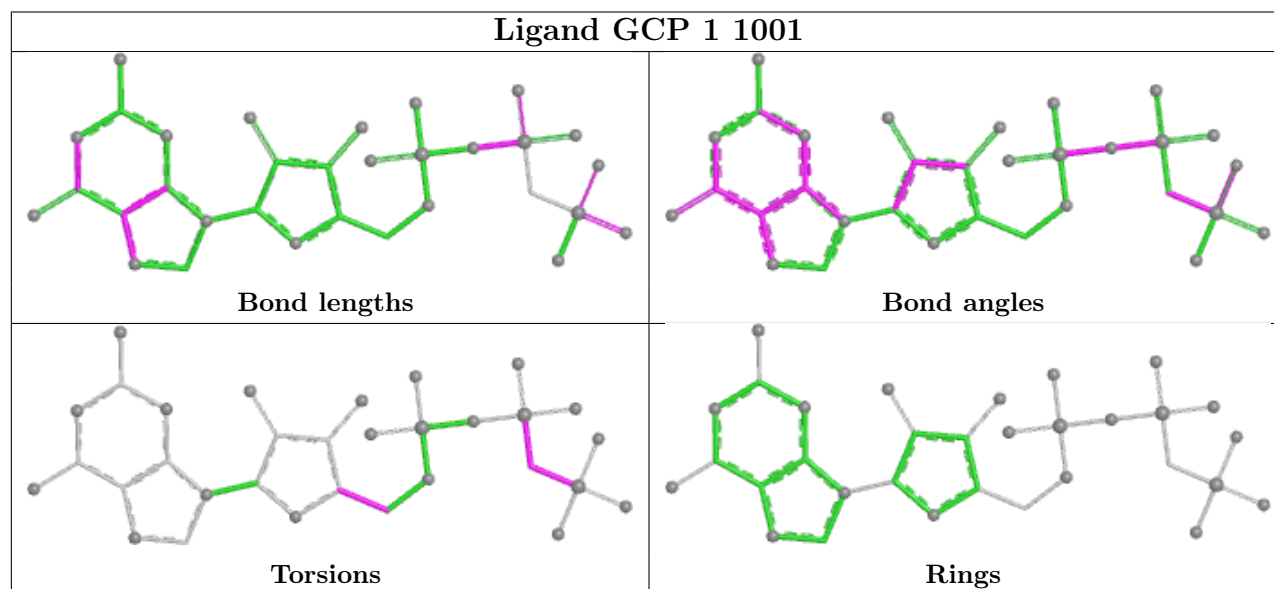
Mol	Chain	Res	Type	Atoms
85	1	1001	GCP	PB-C3B-PG-O1G
85	1	1001	GCP	PB-C3B-PG-O2G
85	1	1001	GCP	PB-C3B-PG-O3G
85	1	1001	GCP	PG-C3B-PB-O3A
85	1	1001	GCP	PG-C3B-PB-O2B
85	1	1001	GCP	PG-C3B-PB-O1B
85	1	1001	GCP	O4'-C4'-C5'-O5'

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	AK	2
8	AE	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AE	116:GLU	C	117:ALA	N	6.39
1	5	2049:G	O3'	2050:A	P	6.33
1	AK	52:UNK	C	54:UNK	N	5.65

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AK	23:UNK	C	28:UNK	N	3.69
1	5	2196:C	O3'	2197:A	P	3.40

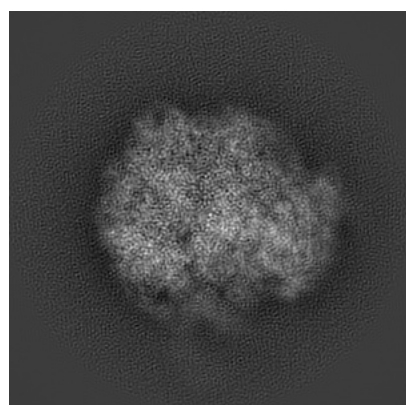
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20952. These allow visual inspection of the internal detail of the map and identification of artifacts.

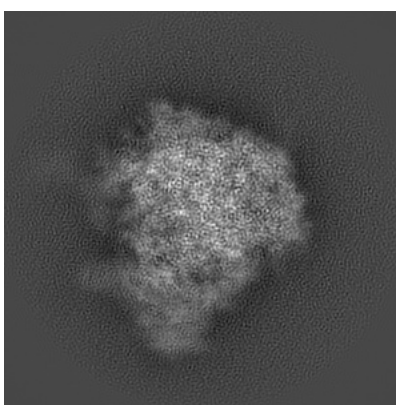
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

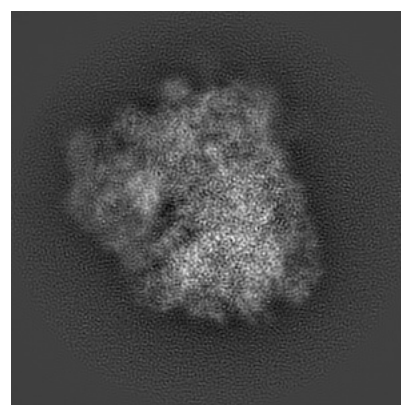
6.1.1 Primary map



X



Y

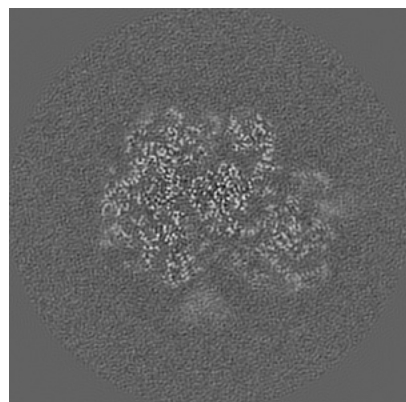


Z

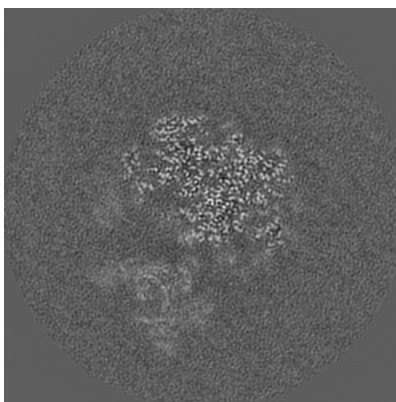
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

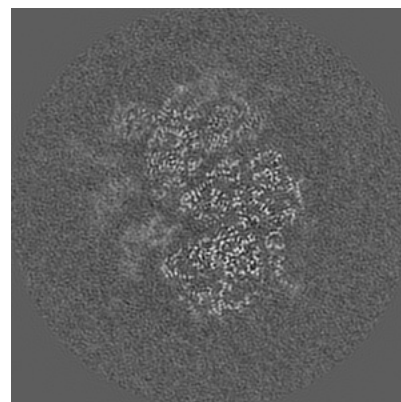
6.2.1 Primary map



X Index: 200



Y Index: 200

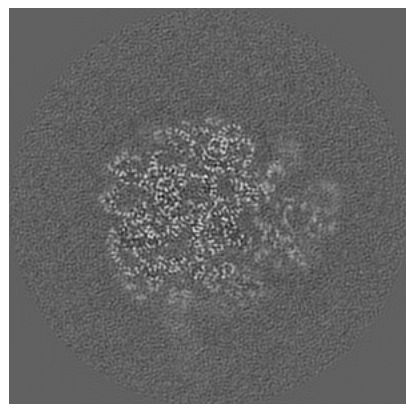


Z Index: 200

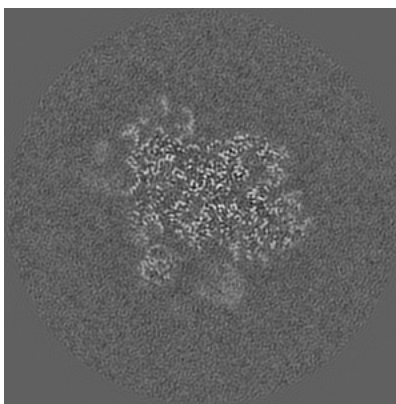
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

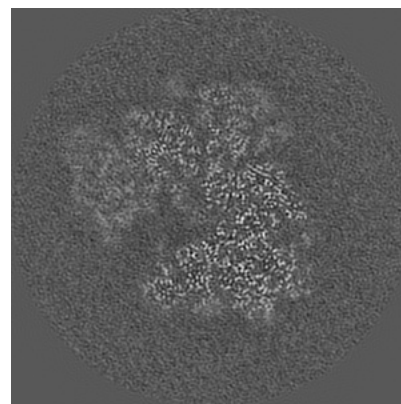
6.3.1 Primary map



X Index: 230



Y Index: 158

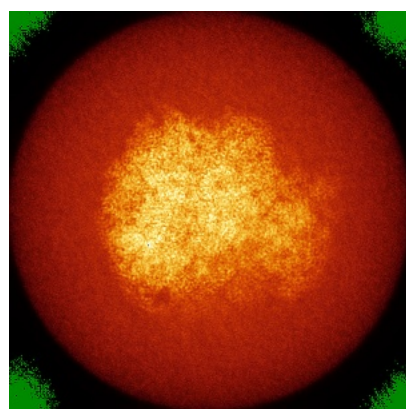


Z Index: 176

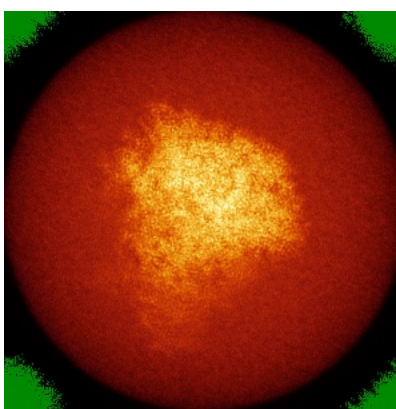
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

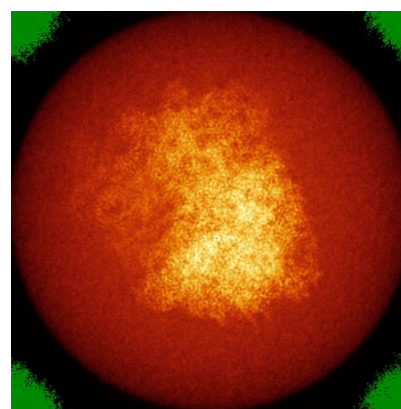
6.4.1 Primary map



X



Y

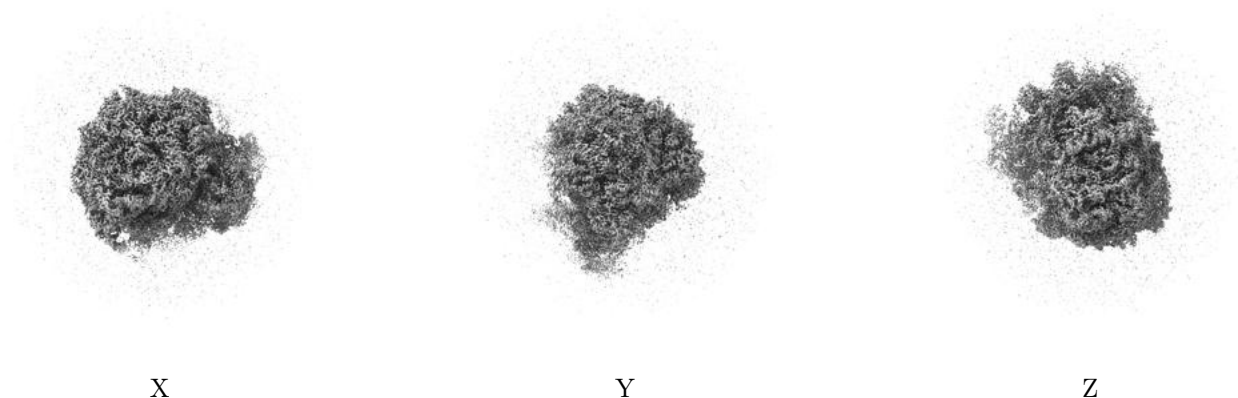


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

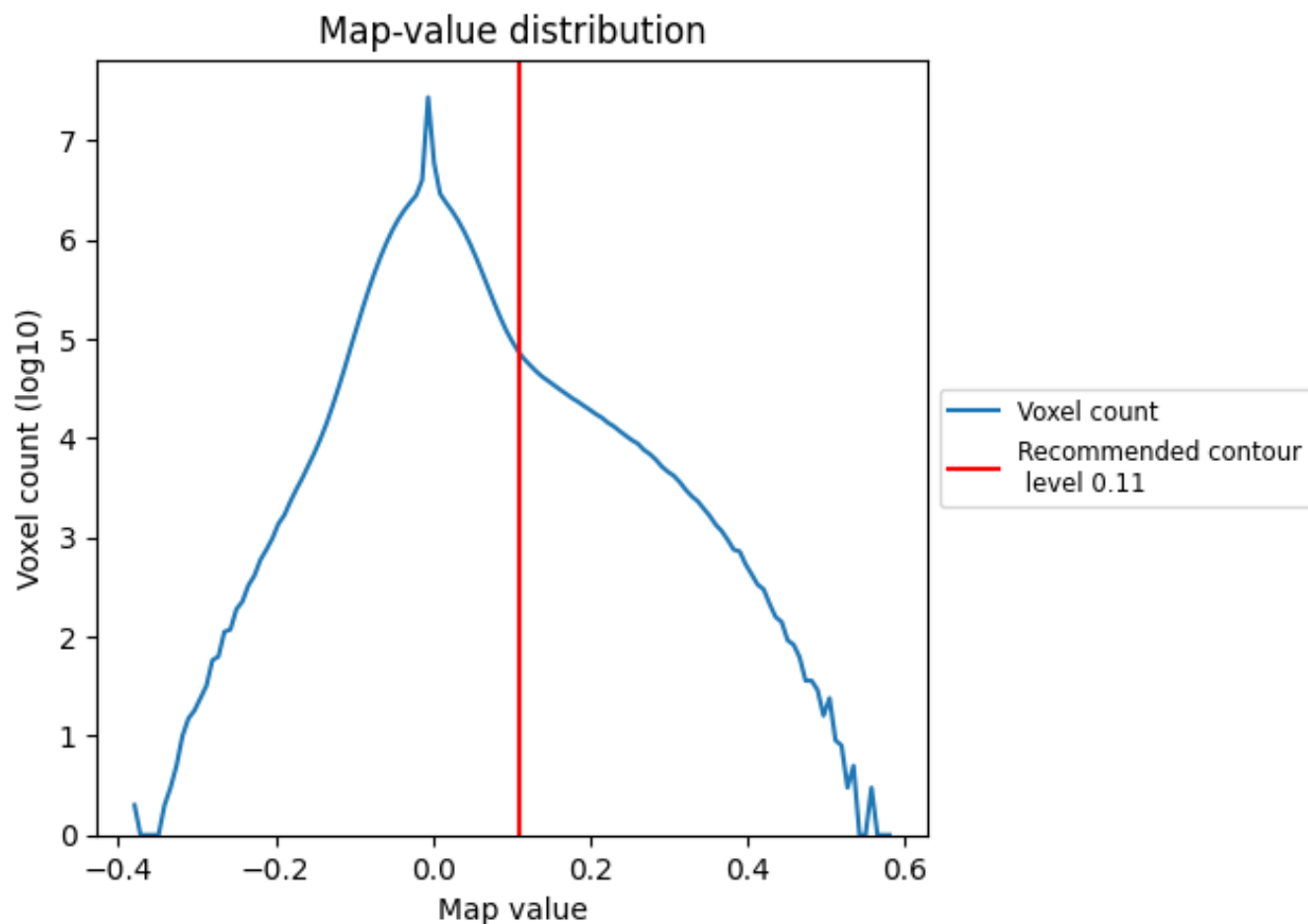
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

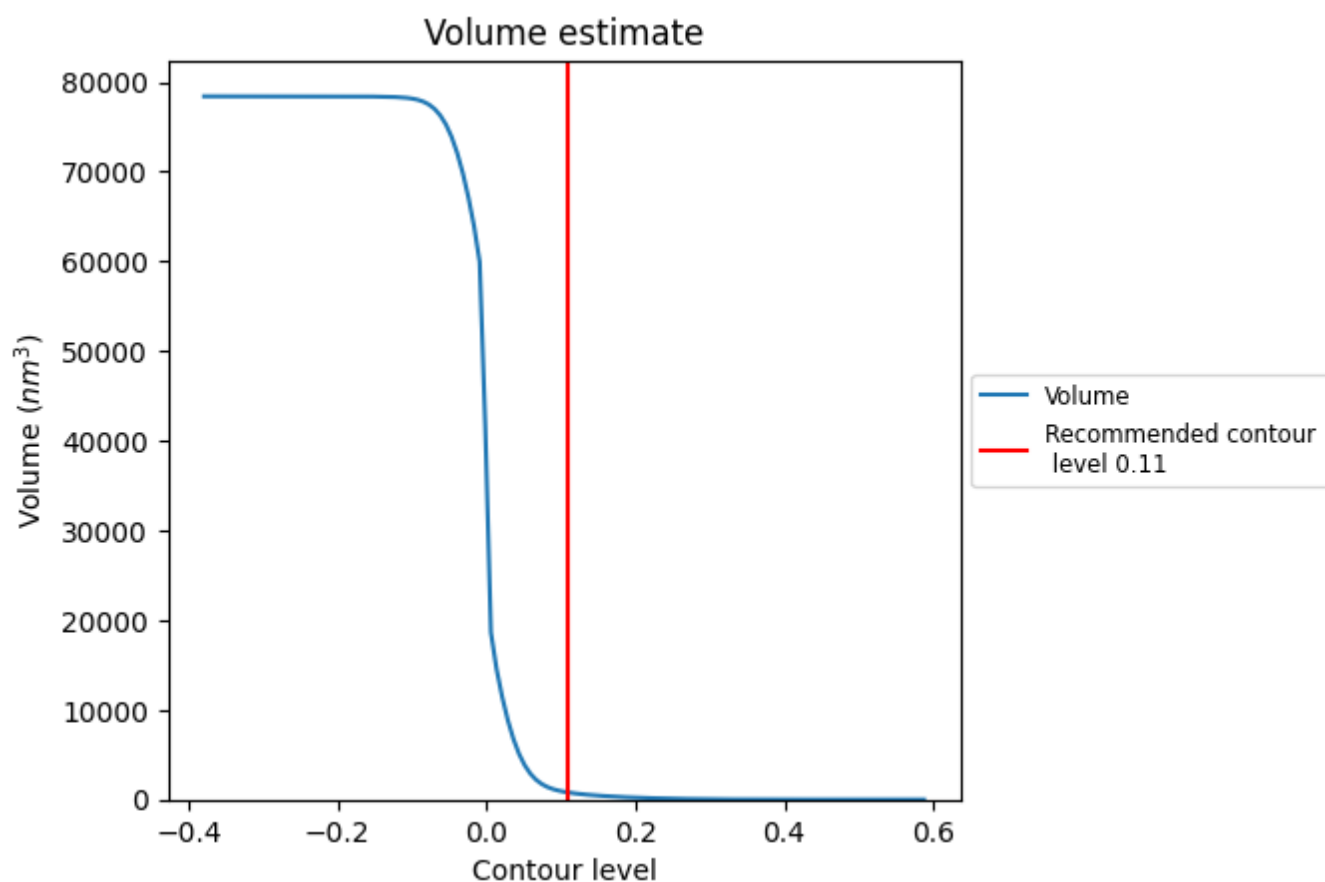
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

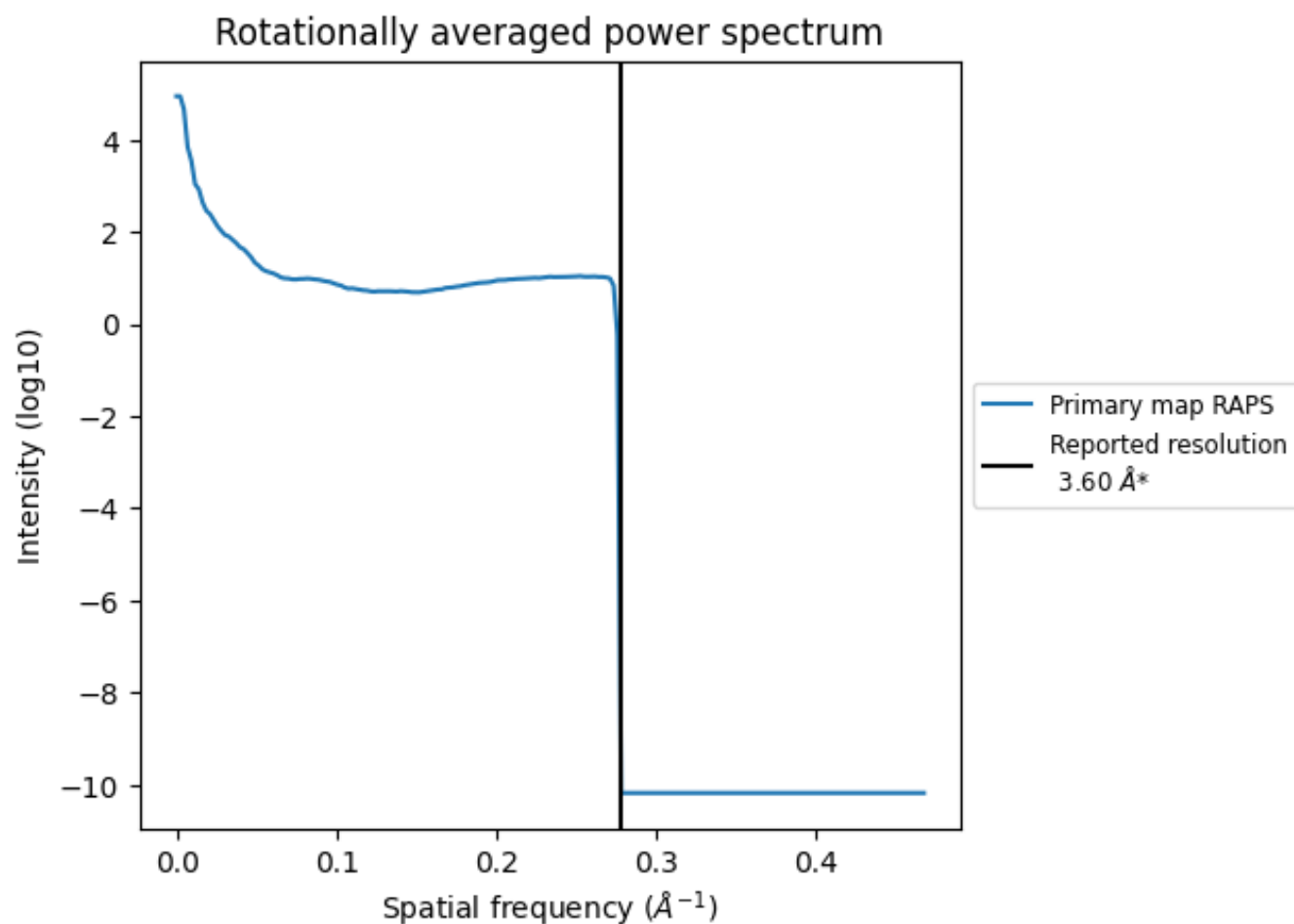
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 787 nm³; this corresponds to an approximate mass of 711 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 ⓘ



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

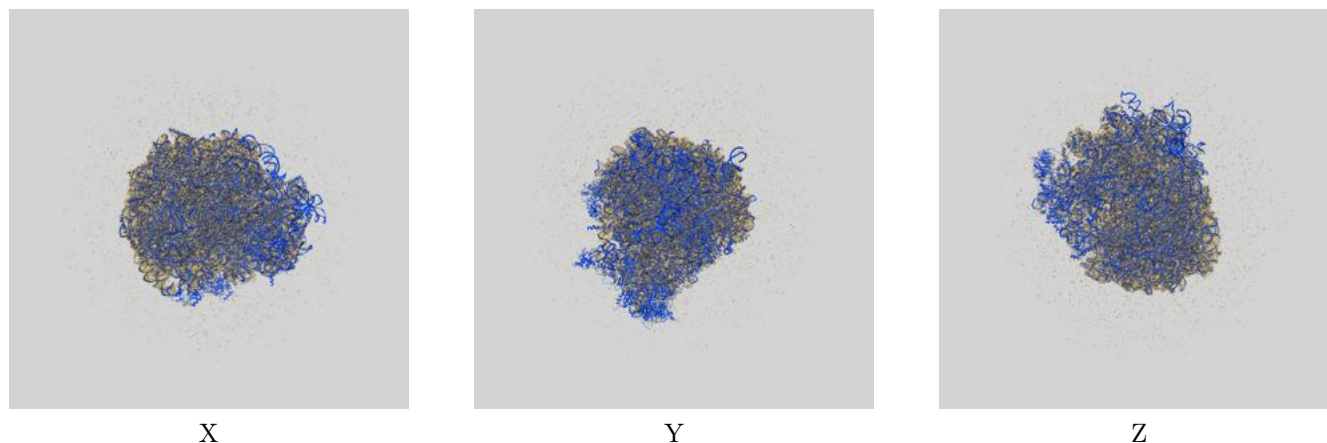
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

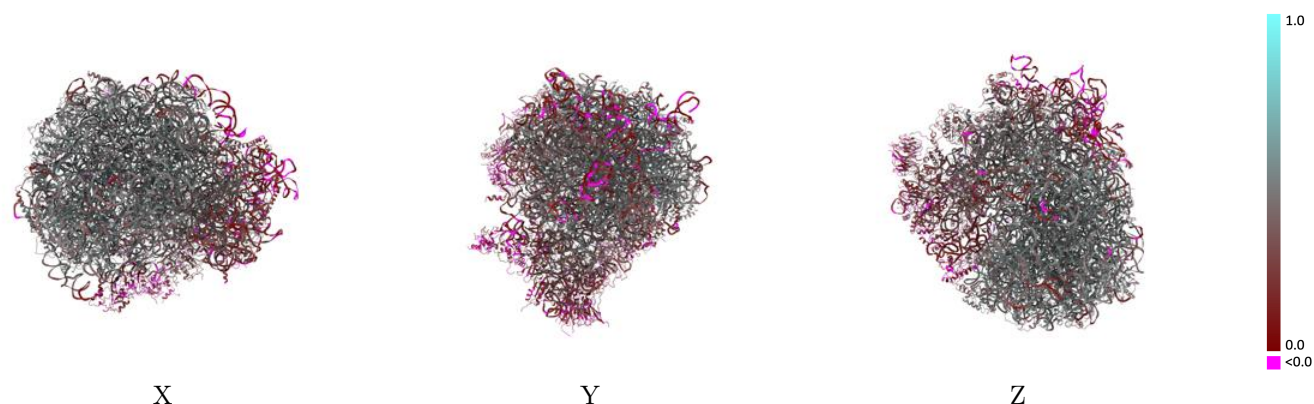
This section contains information regarding the fit between EMDB map EMD-20952 and PDB model 6UZ7. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



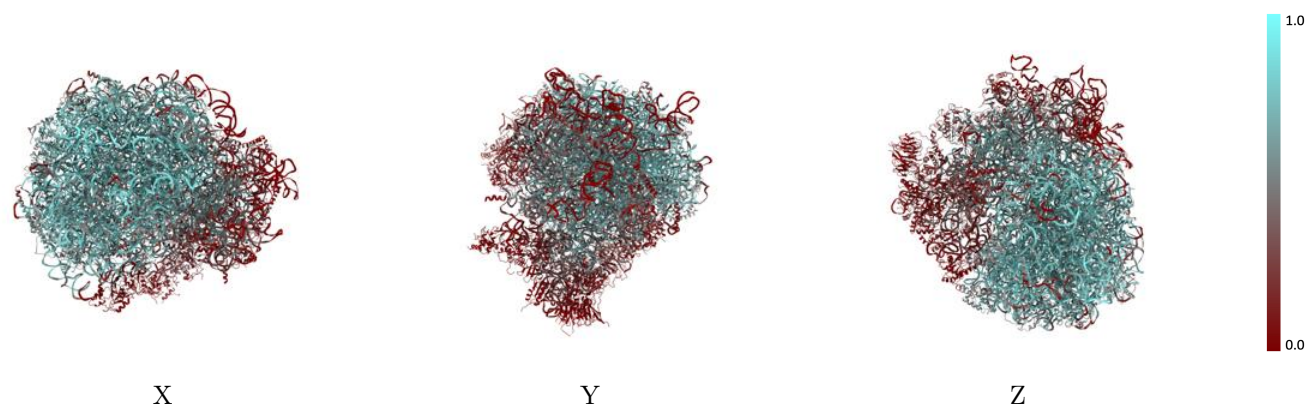
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



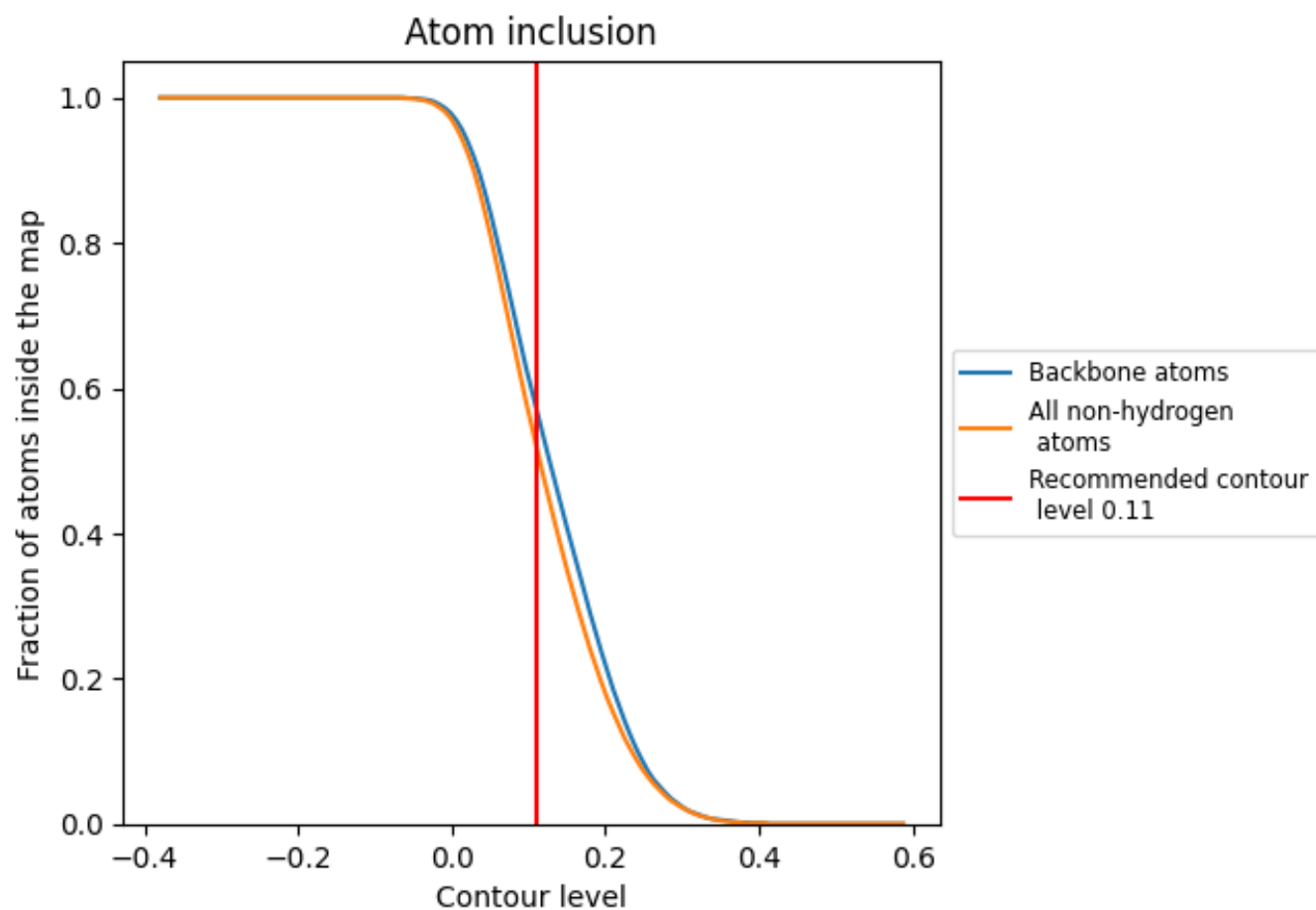
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 52% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5200	 0.3900
1	 0.2170	 0.3570
2	 0.4230	 0.3290
3	 0.2380	 0.2170
5	 0.7020	 0.4420
7	 0.7830	 0.4790
8	 0.7630	 0.4730
A	 0.3340	 0.3440
AA	 0.6580	 0.4920
AB	 0.6710	 0.4920
AC	 0.6330	 0.4730
AD	 0.5450	 0.4330
AE	 0.5100	 0.4230
AF	 0.6550	 0.4730
AG	 0.5510	 0.4400
AH	 0.5830	 0.4690
AI	 0.6300	 0.4810
AJ	 0.4720	 0.4050
AK	 0.0080	 0.0410
AL	 0.5730	 0.4520
AM	 0.5940	 0.4720
AN	 0.7240	 0.5110
AO	 0.6910	 0.5000
AP	 0.6410	 0.4700
AQ	 0.6470	 0.4950
AR	 0.5540	 0.4380
AS	 0.6530	 0.4920
AT	 0.6200	 0.4710
AU	 0.4240	 0.4050
AV	 0.6040	 0.4940
AW	 0.6190	 0.4790
AX	 0.5980	 0.4580
AY	 0.6180	 0.4580
AZ	 0.6010	 0.4430
B	 0.2850	 0.3630



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Chain	Atom inclusion	Q-score
Ba	 0.7030	 0.5000
Bb	 0.5630	 0.4500
Bc	 0.5810	 0.4590
Bd	 0.6290	 0.4830
Be	 0.6170	 0.4760
Bf	 0.7070	 0.5080
Bg	 0.5670	 0.4440
Bh	 0.6150	 0.4740
Bi	 0.5270	 0.4310
Bj	 0.7320	 0.5150
Bk	 0.4300	 0.3690
Bl	 0.6340	 0.4810
Bm	 0.5820	 0.4800
Bn	 0.1730	 0.2430
Bo	 0.5890	 0.4680
Bp	 0.6170	 0.4680
Bq	 0.0250	 0.0860
Br	 0.0150	 0.1060
C	 0.4500	 0.4040
D	 0.1030	 0.2240
E	 0.3540	 0.3740
F	 0.0390	 0.1680
G	 0.1440	 0.2400
H	 0.2770	 0.3410
I	 0.2180	 0.2820
J	 0.3910	 0.3650
K	 0.0530	 0.1820
L	 0.3920	 0.3760
M	 0.0050	 0.0710
N	 0.3870	 0.3750
O	 0.2760	 0.3630
P	 0.0710	 0.1780
Q	 0.0690	 0.2130
R	 0.1370	 0.2480
S	 0.0610	 0.1430
T	 0.0690	 0.2050
U	 0.0750	 0.2000
V	 0.4320	 0.4250
W	 0.5880	 0.4640
X	 0.4470	 0.4300
Y	 0.2230	 0.3260
Z	 0.0050	 0.0990

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Chain	Atom inclusion	Q-score
a	 0.3660	 0.3450
b	 0.2920	 0.3310
c	 0.0440	 0.2110
d	 0.1920	 0.3010
e	 0.2210	 0.2980
f	 0.0090	 0.1220
g	 0.0270	 0.1600