



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:26 AM UTC

PDB ID : 8P60 / pdb_00008p60
EMDB ID : EMD-17457
Title : Spraguea lophii ribosome dimer
Authors : Gil Diez, P.; McLaren, M.; Isupov, M.N.; Daum, B.; Connors, R.; Williams, B.
Deposited on : 2023-05-24
Resolution : 14.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

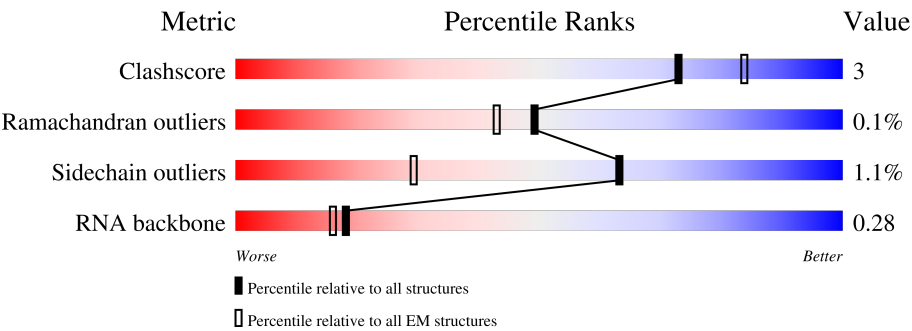
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : 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 14.30 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.



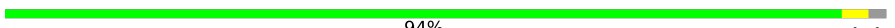
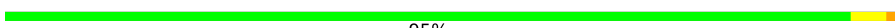
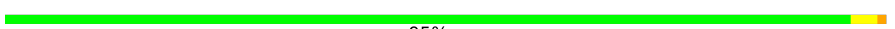
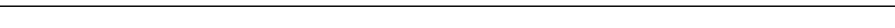
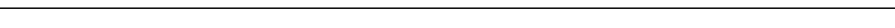
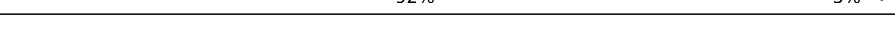
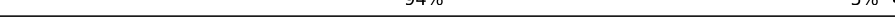
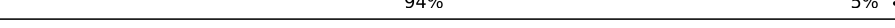
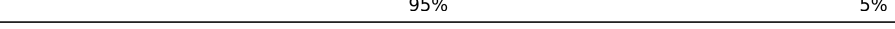
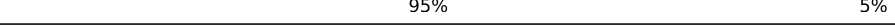
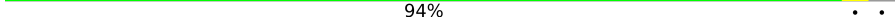
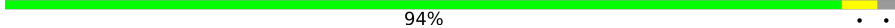
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	K50	2618	60% 30% • 5%
1	L50	2618	60% 30% • 5%
2	K70	119	59% 37% • •
2	L70	119	60% 36% • •
3	KA0	246	96% •
3	LA0	246	96% •
4	KAA	147	93% 7%

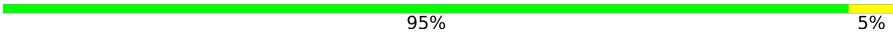
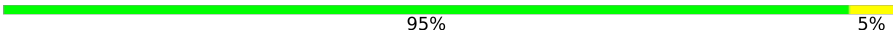
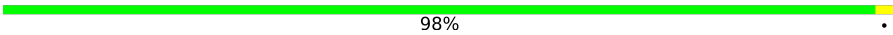
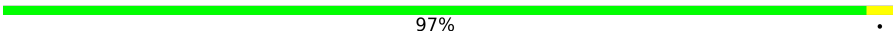
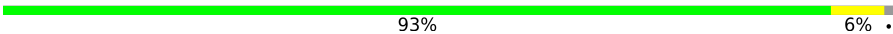
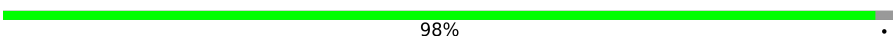
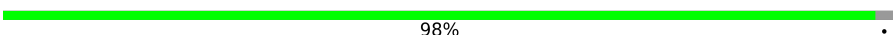
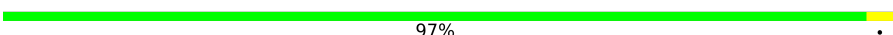
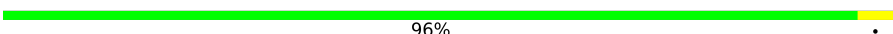
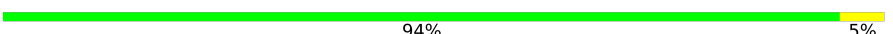
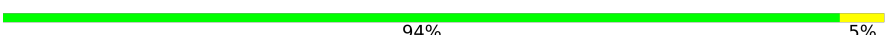
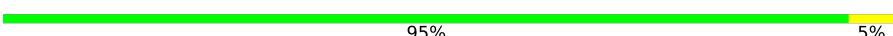
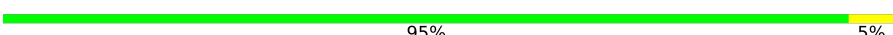
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Mol	Chain	Length	Quality of chain
4	LAA	147	 93% 7%
5	KB0	392	 94% ..
5	LB0	392	 94% ..
6	KC0	328	 95% ..
6	LC0	328	 95% ..
7	KCC	110	 88% .. 10%
7	LCC	110	 88% .. 10%
8	KD0	291	 93% ..
8	LD0	291	 92% ..
9	KDD	110	 98% ..
9	LDD	110	 99% ..
10	KE0	171	 89% 6% ..
10	LE0	171	 89% 6% ..
11	KEE	139	 92% 5% ..
11	LEE	139	 92% 5% ..
12	KF0	235	 94% 5% ..
12	LF0	235	 94% 5% ..
13	KFF	111	 95% 5%
13	LFF	111	 95% 5%
14	KG0	206	 93% ..
14	LG0	206	 94% ..
15	KGG	106	 92% 5% ..
15	LGG	106	 92% 6% ..
16	KH0	187	 94% ..
16	LH0	187	 94% ..

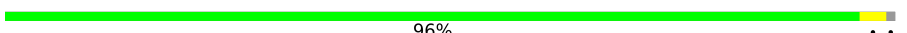
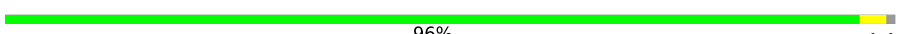
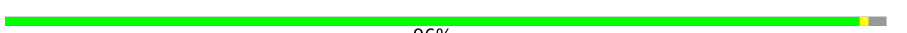
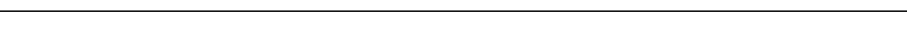
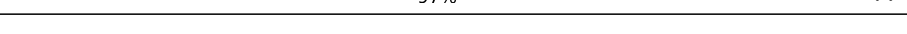
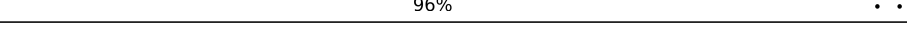
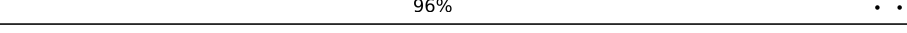
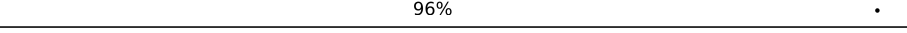
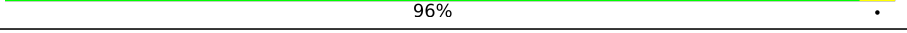
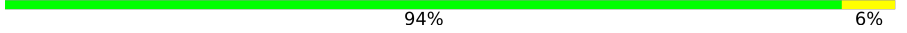
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Mol	Chain	Length	Quality of chain
17	KHH	119	 95% 5%
17	LHH	119	 95% 5%
18	KI0	218	 98% .
18	LI0	218	 97% .
19	KII	98	 92% 7% .
19	LII	98	 93% 6% .
20	KJ0	171	 91% 6% .
20	LJ0	171	 91% 6% .
21	KJJ	92	 90% 7% .
21	LJJ	92	 90% 7% .
22	KL0	165	 92% 7% ..
22	LL0	165	 91% 8% ..
23	KLL	52	 98% .
23	LLL	52	 98% .
24	KM0	115	 97% .
24	LM0	115	 96% .
25	KMM	127	 41% 59%
25	LMM	127	 41% 59%
26	KN0	204	 94% 5%
26	LN0	204	 94% 5%
27	KO0	198	 95% 5%
27	LO0	198	 95% 5%
28	KOO	104	 93% . .
28	LOO	104	 92% . .
29	KP0	167	 87% . . 8%

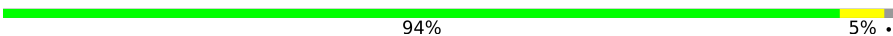
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Mol	Chain	Length	Quality of chain
29	LP0	167	 89% .. 8%
30	KPP	89	 92% ...
30	LPP	89	 92% ...
31	KQ0	183	 96% ..
31	LQ0	183	 96% ..
32	KR0	168	 96% ..
32	LR0	168	 97% ..
33	KS0	171	 96% ..
33	LS0	171	 96% ..
34	KT0	158	 91% 8% ..
34	LT0	158	 91% 8% ..
35	KU0	113	 86% 12% .
35	LU0	113	 86% 12% .
36	KV0	142	 97% ..
36	LV0	142	 97% ..
37	KW0	131	 66% 10% .. 22%
37	LW0	131	 66% 10% .. 22%
38	KX0	113	 96% ..
38	LX0	113	 96% ..
39	KY0	131	 96% .
39	LY0	131	 96% .
40	KZ0	153	 75% 23% .
40	LZ0	153	 75% 23% .
41	MD1	151	 94% 6%
41	MD2	151	 94% 6%

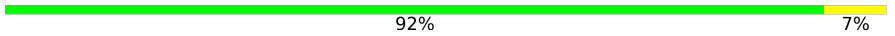
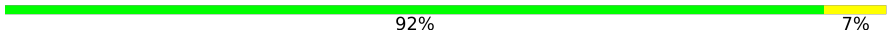
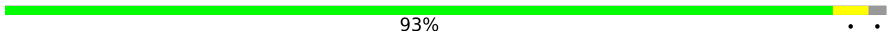
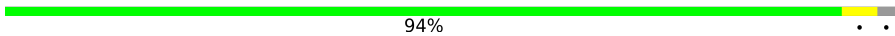
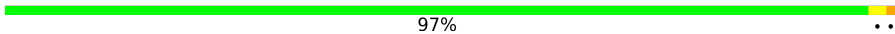
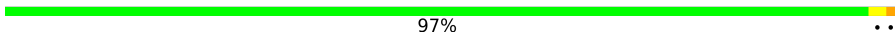
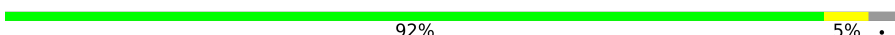
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Mol	Chain	Length	Quality of chain
42	R60	1368	
42	S60	1368	
43	RA0	233	
43	SA0	233	
44	RAA	102	
44	SAA	102	
45	RB0	230	
45	SB0	230	
46	RBB	82	
46	SBB	82	
47	RC0	248	
47	SC0	248	
48	RCC	65	
48	SCC	65	
49	RD0	242	
49	SD0	242	
50	RDD	65	
50	SDD	65	
51	RE0	280	
51	SE0	280	
52	REE	60	
52	SEE	60	
53	RF0	195	
53	SF0	195	
54	RFF	150	

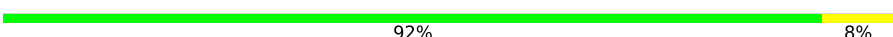
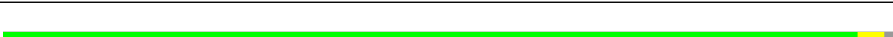
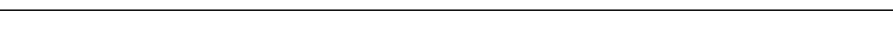
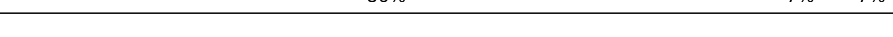
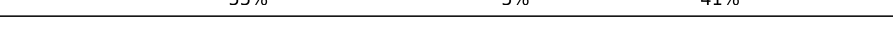
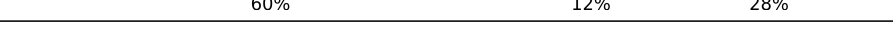
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Mol	Chain	Length	Quality of chain
54	SFF	150	
55	RG0	230	
55	SG0	230	
56	RGG	326	
56	SGG	326	
57	RH0	164	
57	SH0	164	
58	RI0	173	
58	SI0	173	
59	RJ0	184	
59	SJ0	184	
60	RK0	107	
60	SK0	107	
61	RL0	155	
61	SL0	155	
62	RM0	130	
62	SM0	130	
63	RN0	143	
63	SN0	143	
64	RO0	135	
64	SO0	135	
65	RQ0	143	
65	SQ0	143	
66	RR0	120	
66	SR0	120	

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Mol	Chain	Length	Quality of chain
67	RS0	160	
67	SS0	160	
68	RT0	143	
68	ST0	143	
69	RU0	119	
69	SU0	119	
70	RV0	67	
70	SV0	67	
71	RW0	128	
71	SW0	128	
72	RX0	141	
72	SX0	141	
73	RY0	146	
73	SY0	146	
74	RZ0	128	
74	SZ0	128	
75	RP0	163	
75	SP0	163	

2 Entry composition [i](#)

There are 76 unique types of molecules in this entry. The entry contains 343629 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 RNA 28S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L50	2499	Total	C	N	O	P	0	0
			53655	23950	9876	17330	2499		
1	K50	2499	Total	C	N	O	P	0	0
			53655	23950	9876	17330	2499		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L70	119	Total	C	N	O	P	0	0
			2542	1136	459	828	119		
2	K70	119	Total	C	N	O	P	0	0
			2542	1136	459	828	119		

- Molecule 3 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LA0	245	Total	C	N	O	S	0	0
			1889	1189	361	334	5		
3	KA0	245	Total	C	N	O	S	0	0
			1889	1189	361	334	5		

- Molecule 4 is a protein called Ribosomal protein L18e/L15P.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LAA	147	Total	C	N	O	S	0	0
			1167	738	229	194	6		
4	KAA	147	Total	C	N	O	S	0	0
			1167	738	229	194	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB0	383	Total	C	N	O	S	0	0
			3039	1926	559	543	11		
5	KB0	383	Total	C	N	O	S	0	0
			3039	1926	559	543	11		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC0	327	Total	C	N	O	S	0	0
			2604	1629	478	485	12		
6	KC0	327	Total	C	N	O	S	0	0
			2604	1629	478	485	12		

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LCC	99	Total	C	N	O	S	0	0
			781	504	126	148	3		
7	KCC	99	Total	C	N	O	S	0	0
			781	504	126	148	3		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LD0	281	Total	C	N	O	S	0	0
			2298	1451	410	426	11		
8	KD0	281	Total	C	N	O	S	0	0
			2298	1451	410	426	11		

- Molecule 9 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LDD	109	Total	C	N	O	S	0	0
			895	575	163	154	3		
9	KDD	109	Total	C	N	O	S	0	0
			895	575	163	154	3		

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE0	165	Total	C	N	O	S	0	0
			1371	879	227	262	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	KE0	165	Total	C	N	O	S	0	0
			1371	879	227	262	3		

- Molecule 11 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LEE	135	Total	C	N	O	S	0	0
			1090	697	205	182	6		
11	KEE	135	Total	C	N	O	S	0	0
			1090	697	205	182	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LF0	231	Total	C	N	O	S	0	0
			1933	1234	342	350	7		
12	KF0	231	Total	C	N	O	S	0	0
			1933	1234	342	350	7		

- Molecule 13 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LFF	111	Total	C	N	O	S	0	0
			893	567	159	162	5		
13	KFF	111	Total	C	N	O	S	0	0
			893	567	159	162	5		

- Molecule 14 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG0	199	Total	C	N	O	S	0	0
			1590	1015	275	290	10		
14	KG0	199	Total	C	N	O	S	0	0
			1590	1015	275	290	10		

- Molecule 15 is a protein called Ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LGG	104	Total	C	N	O	S	0	0
			819	504	169	139	7		
15	KGG	104	Total	C	N	O	S	0	0
			819	504	169	139	7		

- Molecule 16 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LH0	183	Total	C	N	O	S	0	0
			1477	951	252	266	8		
16	KH0	183	Total	C	N	O	S	0	0
			1477	951	252	266	8		

- Molecule 17 is a protein called Ribosomal L29 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LHH	119	Total	C	N	O	S	0	0
			992	626	188	175	3		
17	KHH	119	Total	C	N	O	S	0	0
			992	626	188	175	3		

- Molecule 18 is a protein called S60 ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LI0	217	Total	C	N	O	S	0	0
			1750	1096	333	308	13		
18	KI0	217	Total	C	N	O	S	0	0
			1750	1096	333	308	13		

- Molecule 19 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LII	97	Total	C	N	O	S	0	0
			784	496	146	136	6		
19	KII	97	Total	C	N	O	S	0	0
			784	496	146	136	6		

- Molecule 20 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LJ0	167	Total	C	N	O	S	0	0
			1332	847	242	236	7		
20	KJ0	167	Total	C	N	O	S	0	0
			1332	847	242	236	7		

- Molecule 21 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LJJ	89	Total	C	N	O	S	0	0
			701	427	146	118	10		
21	KJJ	89	Total	C	N	O	S	0	0
			701	427	146	118	10		

- Molecule 22 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LL0	164	Total	C	N	O	S	0	0
			1353	857	252	232	12		
22	KL0	164	Total	C	N	O	S	0	0
			1353	857	252	232	12		

- Molecule 23 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LLL	51	Total	C	N	O	S	0	0
			427	272	87	65	3		
23	KLL	51	Total	C	N	O	S	0	0
			427	272	87	65	3		

- Molecule 24 is a protein called Transposase.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LM0	115	Total	C	N	O	S	0	0
			927	588	151	183	5		
24	KM0	115	Total	C	N	O	S	0	0
			927	588	151	183	5		

- Molecule 25 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LMM	52	Total	C	N	O	S	0	0
			427	264	89	70	4		
25	KMM	52	Total	C	N	O	S	0	0
			427	264	89	70	4		

- Molecule 26 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LN0	203	Total	C	N	O	S	0	0
			1688	1055	346	276	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	KN0	203	Total	C	N	O	S	0	0
			1688	1055	346	276	11		

- Molecule 27 is a protein called Ribosomal protein L13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LO0	198	Total	C	N	O	S	0	0
			1598	1018	286	280	14		
27	KO0	198	Total	C	N	O	S	0	0
			1598	1018	286	280	14		

- Molecule 28 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LOO	100	Total	C	N	O	S	0	0
			801	504	163	130	4		
28	KOO	100	Total	C	N	O	S	0	0
			801	504	163	130	4		

- Molecule 29 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LP0	154	Total	C	N	O	S	0	0
			1238	794	225	213	6		
29	KP0	154	Total	C	N	O	S	0	0
			1238	794	225	213	6		

- Molecule 30 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LPP	87	Total	C	N	O	S	0	0
			684	427	131	116	10		
30	KPP	87	Total	C	N	O	S	0	0
			684	427	131	116	10		

- Molecule 31 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LQ0	182	Total	C	N	O	S	0	0
			1491	950	270	266	5		
31	KQ0	182	Total	C	N	O	S	0	0
			1491	950	270	266	5		

- Molecule 32 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LR0	164	Total	C	N	O	S	0	0
			1336	832	261	236	7		
32	KR0	164	Total	C	N	O	S	0	0
			1336	832	261	236	7		

- Molecule 33 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LS0	170	Total	C	N	O	S	0	0
			1400	898	241	256	5		
33	KS0	170	Total	C	N	O	S	0	0
			1400	898	241	256	5		

- Molecule 34 is a protein called 60s ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LT0	156	Total	C	N	O	S	0	0
			1270	808	233	224	5		
34	KT0	156	Total	C	N	O	S	0	0
			1270	808	233	224	5		

- Molecule 35 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LU0	100	Total	C	N	O	S	0	0
			810	526	135	147	2		
35	KU0	100	Total	C	N	O	S	0	0
			810	526	135	147	2		

- Molecule 36 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LV0	141	Total	C	N	O	S	0	0
			1057	663	200	189	5		
36	KV0	141	Total	C	N	O	S	0	0
			1057	663	200	189	5		

- Molecule 37 is a protein called Ribosomal protein L24E.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LW0	102	Total	C	N	O	S	0	0
			832	539	143	147	3		
37	KW0	102	Total	C	N	O	S	0	0
			832	539	143	147	3		

- Molecule 38 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LX0	112	Total	C	N	O	S	0	0
			874	562	156	155	1		
38	KX0	112	Total	C	N	O	S	0	0
			874	562	156	155	1		

- Molecule 39 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LY0	131	Total	C	N	O	S	0	0
			1048	658	197	186	7		
39	KY0	131	Total	C	N	O	S	0	0
			1048	658	197	186	7		

- Molecule 40 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LZ0	118	Total	C	N	O	S	0	0
			963	618	172	169	4		
40	KZ0	118	Total	C	N	O	S	0	0
			963	618	172	169	4		

- Molecule 41 is a protein called DNL-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	MD1	151	Total	C	N	O	S	0	0
			1229	776	201	241	11		
41	MD2	151	Total	C	N	O	S	0	0
			1229	776	201	241	11		

- Molecule 42 is a RNA chain called RNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	S60	1354	Total	C	N	O	P	0	0
			29181	13024	5463	9340	1354		

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Mol	Chain	Residues	Atoms					AltConf	Trace
42	R60	1354	Total	C	N	O	P	0	0
			29181	13024	5463	9340	1354		

- Molecule 43 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SA0	220	Total	C	N	O	S	0	0
			1725	1091	292	328	14		
43	RA0	220	Total	C	N	O	S	0	0
			1725	1091	292	328	14		

- Molecule 44 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SAA	101	Total	C	N	O	S	0	0
			827	513	163	145	6		
44	RAA	101	Total	C	N	O	S	0	0
			827	513	163	145	6		

- Molecule 45 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	SB0	204	Total	C	N	O	S	0	0
			1609	1018	286	298	7		
45	RB0	204	Total	C	N	O	S	0	0
			1609	1018	286	298	7		

- Molecule 46 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	SBB	81	Total	C	N	O	S	0	0
			627	394	108	116	9		
46	RBB	81	Total	C	N	O	S	0	0
			627	394	108	116	9		

- Molecule 47 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	SC0	226	Total	C	N	O	S	0	0
			1727	1099	300	321	7		
47	RC0	226	Total	C	N	O	S	0	0
			1727	1099	300	321	7		

- Molecule 48 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	SCC	62	Total	C	N	O	S	0	0
			476	295	86	91	4		
48	RCC	62	Total	C	N	O	S	0	0
			476	295	86	91	4		

- Molecule 49 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	SD0	216	Total	C	N	O	S	0	0
			1700	1085	300	307	8		
49	RD0	216	Total	C	N	O	S	0	0
			1700	1085	300	307	8		

- Molecule 50 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	SDD	65	Total	C	N	O	S	0	0
			550	345	102	96	7		
50	RDD	65	Total	C	N	O	S	0	0
			550	345	102	96	7		

- Molecule 51 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	SE0	260	Total	C	N	O	S	0	0
			2044	1297	361	379	7		
51	RE0	260	Total	C	N	O	S	0	0
			2044	1297	361	379	7		

- Molecule 52 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	SEE	56	Total	C	N	O	0	0
			447	284	89	74		
52	REE	56	Total	C	N	O	0	0
			447	284	89	74		

- Molecule 53 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SF0	192	Total	C	N	O	S	0	0
			1509	953	275	275	6		
53	RF0	192	Total	C	N	O	S	0	0
			1509	953	275	275	6		

- Molecule 54 is a protein called Ubiquitin/40s ribosomal protein S27a fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	SFF	58	Total	C	N	O	S	0	0
			422	261	77	79	5		
54	RFF	58	Total	C	N	O	S	0	0
			417	259	74	79	5		

- Molecule 55 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	SG0	229	Total	C	N	O	S	0	0
			1836	1179	325	328	4		
55	RG0	229	Total	C	N	O	S	0	0
			1836	1179	325	328	4		

- Molecule 56 is a protein called Guanine nucleotide binding protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	SGG	319	Total	C	N	O	S	0	0
			2478	1558	411	494	15		
56	RGG	319	Total	C	N	O	S	0	0
			2478	1558	411	494	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	SH0	163	Total	C	N	O	S	0	0
			1335	855	219	255	6		
57	RH0	163	Total	C	N	O	S	0	0
			1335	855	219	255	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	SI0	167	Total	C	N	O	S	0	0
			1347	834	266	240	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
58	RI0	167	Total	C	N	O	S	0	0
			1347	834	266	240	7		

- Molecule 59 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SJ0	168	Total	C	N	O	S	0	0
			1379	880	252	243	4		
59	RJ0	168	Total	C	N	O	S	0	0
			1379	880	252	243	4		

- Molecule 60 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	SK0	88	Total	C	N	O	S	0	0
			737	472	127	135	3		
60	RK0	88	Total	C	N	O	S	0	0
			737	472	127	135	3		

- Molecule 61 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	SL0	150	Total	C	N	O	S	0	0
			1229	790	217	216	6		
61	RL0	150	Total	C	N	O	S	0	0
			1229	790	217	216	6		

- Molecule 62 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	SM0	113	Total	C	N	O	S	0	0
			876	553	156	162	5		
62	RM0	113	Total	C	N	O	S	0	0
			876	553	156	162	5		

- Molecule 63 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	SN0	142	Total	C	N	O	S	0	0
			1130	728	196	202	4		
63	RN0	142	Total	C	N	O	S	0	0
			1130	728	196	202	4		

- Molecule 64 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	SO0	129	Total	C	N	O	S	0	0
			983	606	191	183	3		
64	RO0	129	Total	C	N	O	S	0	0
			983	606	191	183	3		

- Molecule 65 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	SQ0	142	Total	C	N	O	S	0	0
			1143	726	204	207	6		
65	RQ0	142	Total	C	N	O	S	0	0
			1143	726	204	207	6		

- Molecule 66 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	SR0	119	Total	C	N	O	S	0	0
			974	613	172	186	3		
66	RR0	119	Total	C	N	O	S	0	0
			974	613	172	186	3		

- Molecule 67 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	SS0	144	Total	C	N	O	S	0	0
			1150	720	220	207	3		
67	RS0	144	Total	C	N	O	S	0	0
			1150	720	220	207	3		

- Molecule 68 is a protein called 40S Ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	ST0	142	Total	C	N	O	S	0	0
			1161	741	208	211	1		
68	RT0	142	Total	C	N	O	S	0	0
			1161	741	208	211	1		

- Molecule 69 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SU0	100	Total	C	N	O	S	0	0
			809	515	144	143	7		
69	RU0	100	Total	C	N	O	S	0	0
			809	515	144	143	7		

- Molecule 70 is a protein called Ribosomal protein S21E.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SV0	65	Total	C	N	O	S	0	0
			521	319	96	101	5		
70	RV0	65	Total	C	N	O	S	0	0
			521	319	96	101	5		

- Molecule 71 is a protein called 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	SW0	128	Total	C	N	O	S	0	0
			1022	639	195	180	8		
71	RW0	128	Total	C	N	O	S	0	0
			1022	639	195	180	8		

- Molecule 72 is a protein called Ribosomal protein S12/S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	SX0	140	Total	C	N	O	S	0	0
			1098	692	216	186	4		
72	RX0	140	Total	C	N	O	S	0	0
			1098	692	216	186	4		

- Molecule 73 is a protein called 40s ribosomal protein s24.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	SY0	136	Total	C	N	O	S	0	0
			1118	693	215	204	6		
73	RY0	136	Total	C	N	O	S	0	0
			1118	693	215	204	6		

- Molecule 74 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	SZ0	76	Total	C	N	O	S	0	0
			633	403	116	113	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
74	RZ0	76	Total	C	N	O	S	0	0
			633	403	116	113	1		

- Molecule 75 is a protein called Ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	SP0	117	Total	C	N	O	S	0	0
			950	598	172	173	7		
75	RP0	117	Total	C	N	O	S	0	0
			950	598	172	173	7		

- Molecule 76 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
76	LGG	1	Total	Zn	0
			1	1	
76	LJJ	1	Total	Zn	0
			1	1	
76	LMM	1	Total	Zn	0
			1	1	
76	LOO	1	Total	Zn	0
			1	1	
76	LPP	1	Total	Zn	0
			1	1	
76	SAA	1	Total	Zn	0
			1	1	
76	SBB	1	Total	Zn	0
			1	1	
76	SDD	1	Total	Zn	0
			1	1	
76	SFF	1	Total	Zn	0
			1	1	
76	KGG	1	Total	Zn	0
			1	1	
76	KJJ	1	Total	Zn	0
			1	1	
76	KMM	1	Total	Zn	0
			1	1	
76	KOO	1	Total	Zn	0
			1	1	
76	KPP	1	Total	Zn	0
			1	1	

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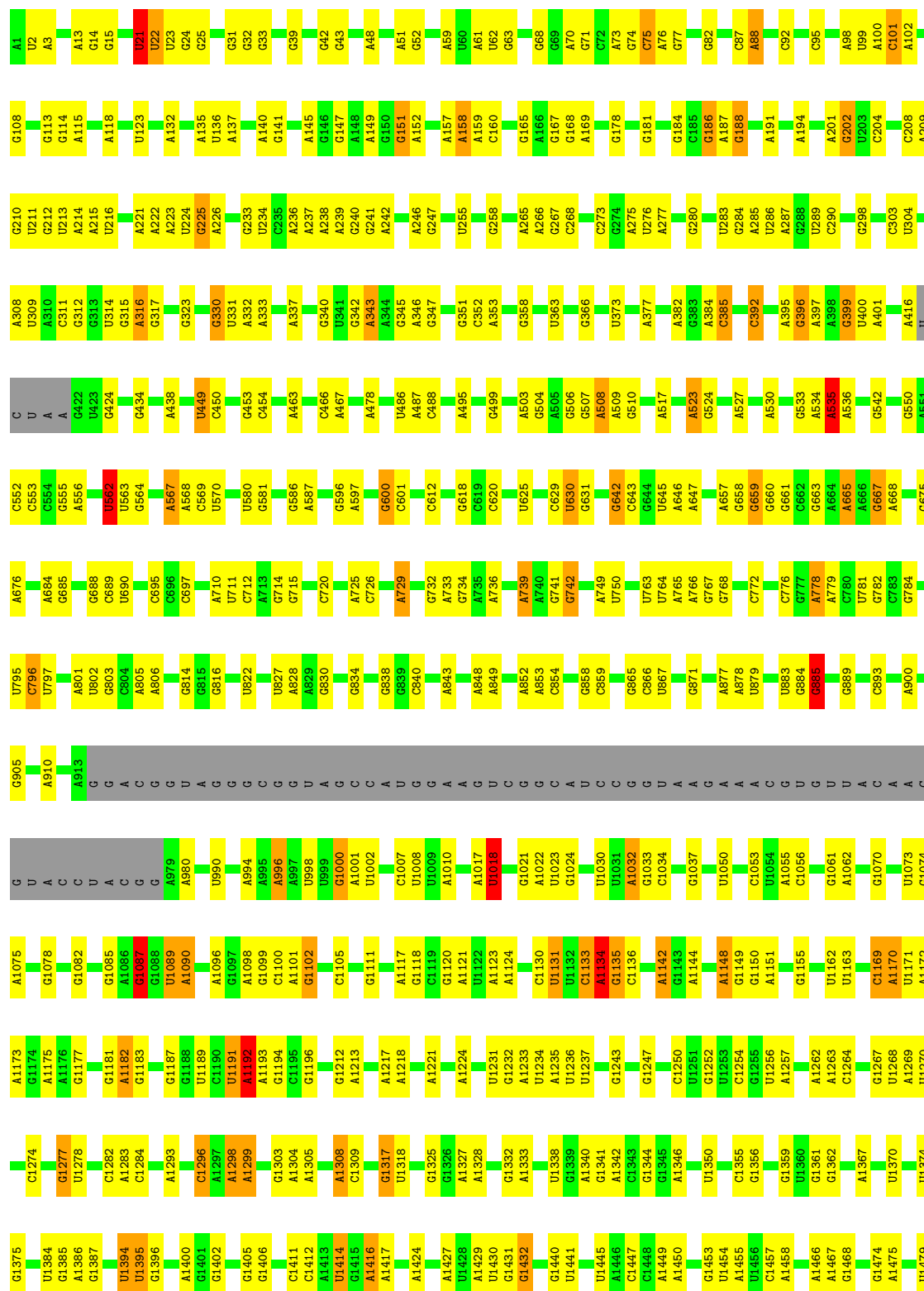
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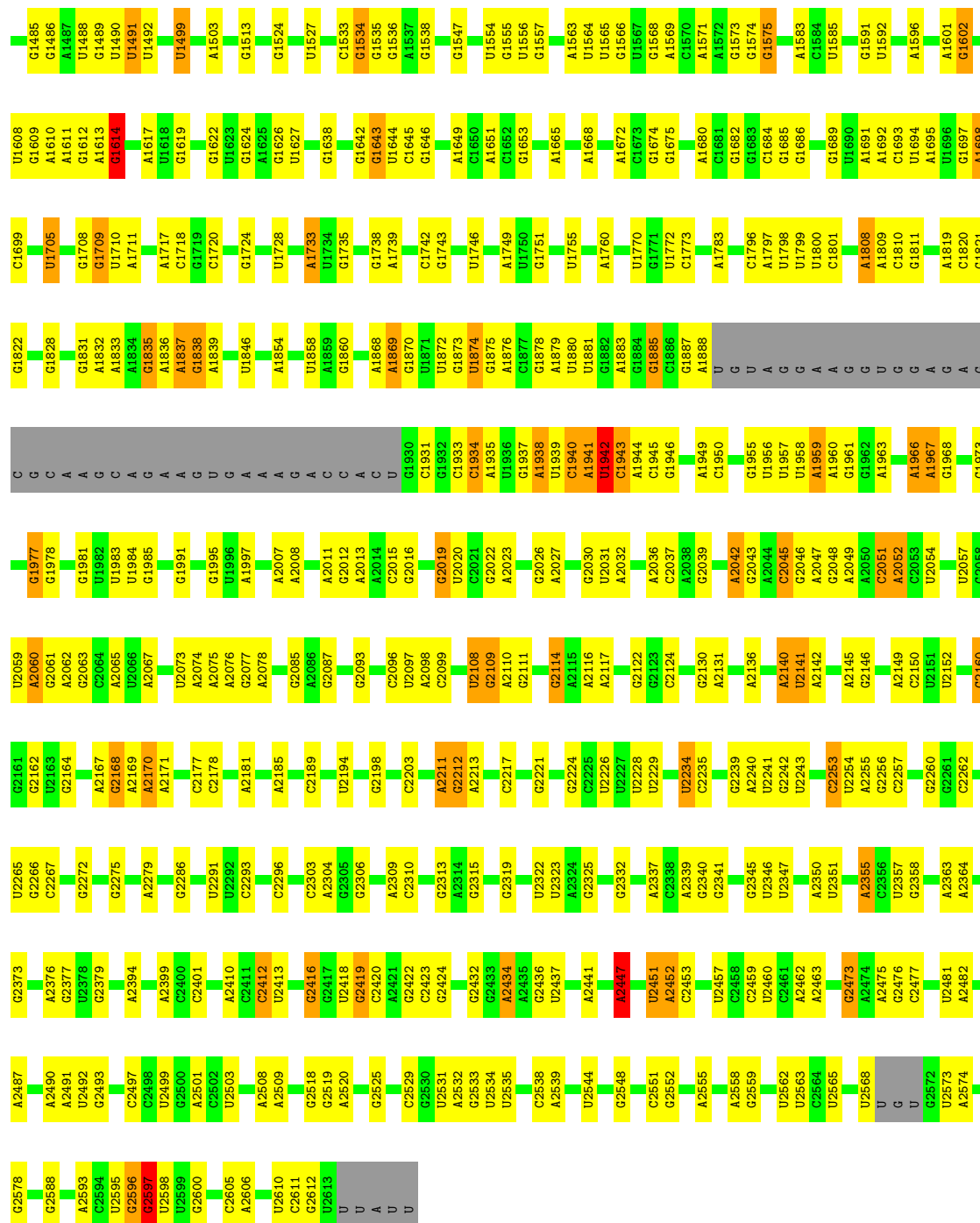
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76	RAA	1	Total 1	Zn 1	0
76	RBB	1	Total 1	Zn 1	0
76	RDD	1	Total 1	Zn 1	0
76	RFF	1	Total 1	Zn 1	0

G2578	A2487	G2373	U2265	G2161	U2059	G1977	C	G1822	A1698	U1608	U1479	U1374	U1270	A1172
G2588	A2490	A2376	G2266	G2162	A2060	G1978	G	G1828	C1699	G1609	G1486	G1375	G1274	A1173
A2593	A2491	G2377	G2267	U2163	G2061	G1979	A	G1831	U1705	A1610	U1384	U1174	C1274	A1175
G2594	U2492	U2378	G2272	G2164	G2062	G1981	A	G1832	G1708	A1611	U1488	U1385	U1277	G1176
U2595	G2493	G2379	G2275	G2165	G2063	U1982	G	A1833	G1709	G1612	G1386	G1177	U1278	G1177
G2596	C2497	A2394	G2279	A2169	A2065	U1983	C	A1834	U1710	A1613	G1489	G1387	C1282	G1151
G2597	U2499	U2399	A2279	A2170	A2066	U1985	G	G1835	A1711	G1614	U1490	U1394	A1283	A1182
U2598	A2501	A2401	G2286	A2171	A2067	G1991	A	A1836	A1717	A1617	U1491	U1395	C1284	G1183
G2600	G2502	C2401	G2291	C2177	U2073	G1995	A	A1837	G1718	G1618	U1492	G1396	A1293	G1187
C2605	U2503	C2410	U2292	C2178	A2075	U1996	G	G1838	G1719	G1619	U1499	A1400	A1296	G1188
A2606	A2508	C2411	G2293	A2181	A2076	U1997	U	A1839	C1720	G1622	C1296	G1401	C1296	U1189
U2610	A2509	U2413	G2296	A2185	A2077	G1999	A	U1846	G1724	U1623	A1297	G1402	A1297	U1191
C2611	G2518	G2416	C2303	C2189	G2085	A2007	A	A1854	U1728	G1625	A1299	G1405	A1299	A1193
U2612	G2519	G2417	A2304	U2194	A2086	A2008	C	A1858	A1733	G1638	G1303	C1411	A1304	G1194
U2613	A2520	U2418	G2305	G2198	G2087	A2011	C	A1859	U1734	G1642	A1305	G1412	A1305	G1196
U	G2525	G2419	G2306	G2199	G2089	A2012	A	G1860	G1735	G1643	G1308	A1413	A1308	G1212
A	G2525	C2420	G2309	G2203	C2096	A2013	C	A1868	G1738	U1644	A1309	U1414	A1309	A1213
U	G2529	A2421	C2310	C2203	U2097	G2015	U	A1869	G1739	G1645	G1317	U1415	G1317	A1217
G2530	U2531	G2422	G2313	A2211	A2098	G2016	C1930	U1871	C1742	G1646	U1318	A1417	U1318	A1218
A2532	G2532	A2314	A2314	G2212	C2099	U2020	G1932	U1872	G1743	G1649	A1322	A1424	A1322	A1221
G2533	G2533	G2432	G2315	A2213	A2098	G2022	C1933	G1873	G1743	G1650	G1325	A1427	G1325	A1224
U2534	U2534	G2433	G2319	C2217	A2110	A2023	C1934	U1874	U1746	G1651	G1326	U1428	G1326	U1231
U2535	G2535	A2434	G2322	G2221	A2116	G2026	U1936	G1875	A1749	G1652	A1327	U1429	A1327	G1232
G2538	G2538	A2435	U2322	G2224	A2117	A2027	G1937	G1878	U1750	G1653	G1328	U1430	A1328	A1233
A2539	A2539	U2437	U2323	G2225	A2116	G2030	A1938	U1879	G1751	G1654	G1332	G1431	U1332	U1234
U2544	U2544	A2441	G2325	U2226	A2117	G2031	C1940	U1881	U1755	A1665	A1333	G1432	U1236	U1237
G2548	G2548	A2447	G2332	U2227	A2117	A2032	U1942	G1882	A1760	A1668	U1338	A1440	U1247	G1243
C2551	C2551	U2451	A2337	U2228	G2122	A2036	C1943	G1883	U1770	A1672	G1339	U1445	A1340	G1243
G2552	G2552	A2452	G2338	G2123	C2124	C2037	C1944	G1884	G1771	C1673	A1341	A1446	G1341	U1235
A2555	A2555	C2453	A2339	C2124	G2124	G2038	G1946	G1886	U1772	G1674	A1342	G1447	U1236	U1236
G2558	A2558	U2457	G2340	G2130	G2130	G2039	A1949	G1887	U1783	G1675	U1355	U1448	U1237	G1247
G2559	G2559	C2458	G2341	A2131	A2131	A2042	C1950	A1888	A1783	A1680	A1346	A1449	A1346	C1250
U2562	U2562	U2460	G2345	A2136	A2136	G2043	G1955	U	C1796	C1681	U1350	A1450	U1350	U1251
U2563	U2563	C2461	U2347	A2140	A2140	A2044	U1956	A	A1797	G1682	U1352	G1453	U1352	G1252
G2564	G2564	A2463	A2350	U2141	U2141	G2046	U1957	G	U1798	C1683	G1355	U1454	U1355	U1253
U2565	U2565	A2463	U2351	A2142	A2142	A2047	U1958	A	U1799	G1685	G1356	A1455	G1356	G1254
U2568	U2568	G2473	G2355	A2145	A2145	G2048	A1959	A	U1800	G1686	U1357	U1456	U1357	U1255
U	U	A2474	A2356	G2146	G2146	A2049	A1960	G	C1801	G1689	G1359	A1457	U1359	U1256
G	G	A2475	G2356	A2146	A2146	A2050	G1961	G	A1808	U1690	U1360	A1458	U1360	A1257
U	U	C2476	U2357	A2149	A2149	C2051	A1962	U	A1809	G1691	A1262	A1466	A1262	A1262
G2572	G2572	C2477	G2358	U2151	U2151	C2052	A1963	G	C1810	U1592	A1263	A1467	G1362	C1264
U2573	U2573	U2481	A2363	U2152	U2152	U2054	A1965	A	G1811	U1596	A1367	G1468	A1367	G1267
A2574	A2574	A2482	A2364	G2261	G2261	U2057	A1967	G	A1819	U1695	U1370	G1474	U1370	U1268
				G2262	G2262	G2058	G1973	G	G1821	G1697		A1475		A1269

● Molecule 1: RNA 28S

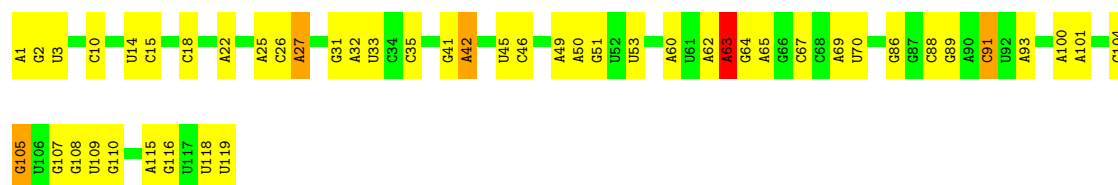
Chain K50:  60% 30% 5%





• Molecule 2: RNA 5S

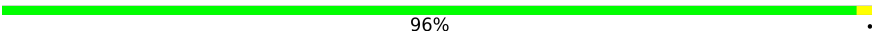
Chain L70: 60% 36%



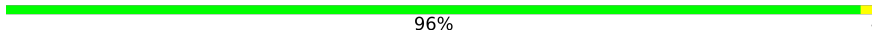
● Molecule 2: RNA 5S

Chain K70:  59% 37% ..

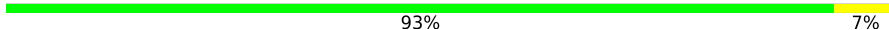
● Molecule 3: 60S ribosomal protein L8

Chain LA0:  96% .

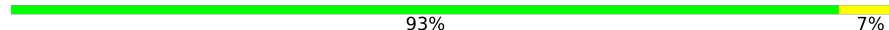
● Molecule 3: 60S ribosomal protein L8

Chain KA0:  96% .

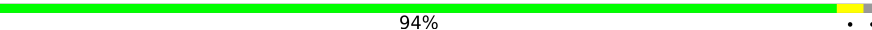
● Molecule 4: Ribosomal protein L18e/L15P

Chain LAA:  93% 7% .

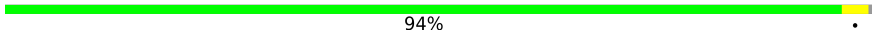
● Molecule 4: Ribosomal protein L18e/L15P

Chain KAA:  93% 7% .

● Molecule 5: 60S ribosomal protein L3

Chain LB0:  94% ..

● Molecule 5: 60S ribosomal protein L3

Chain KB0:  94% ..



- Molecule 6: 60S ribosomal protein L4

Chain LC0: 95%



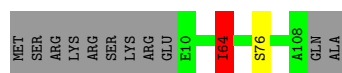
- Molecule 6: 60S ribosomal protein L4

Chain KC0: 95%



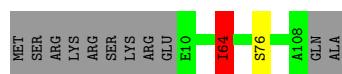
- Molecule 7: 60S ribosomal protein L3

Chain LCC: 88% 10%



- Molecule 7: 60S ribosomal protein L3

Chain KCC: 88% 10%



- Molecule 8: 60S ribosomal protein L5

Chain LD0: 92%



- Molecule 8: 60S ribosomal protein L5

Chain KD0: 93%



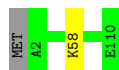
- Molecule 9: 60S ribosomal protein L31

Chain LDD: 99%



- Molecule 9: 60S ribosomal protein L31

Chain KDD: 98% ..



- Molecule 10: 60S ribosomal protein L6

Chain LE0: 89% 6% ..



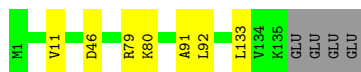
- Molecule 10: 60S ribosomal protein L6

Chain KE0: 89% 6% ..



- Molecule 11: 60S ribosomal protein L32

Chain LEE: 92% 5% .



- Molecule 11: 60S ribosomal protein L32

Chain KEE: 92% 5% .



- Molecule 12: 60S ribosomal protein L7

Chain LF0: 94% 5% .



- Molecule 12: 60S ribosomal protein L7

Chain KF0: 94% 5% .



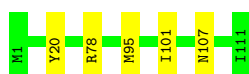
- Molecule 13: 60S ribosomal protein L35a

Chain LFF: 95% 5%



- Molecule 13: 60S ribosomal protein L35a

Chain KFF: 95% 5%



- Molecule 14: 60S ribosomal protein L8

Chain LG0: 94% . .



- Molecule 14: 60S ribosomal protein L8

Chain KG0: 93% . .



- Molecule 15: Ribosomal protein L34

Chain LGG: 92% 6% ..



- Molecule 15: Ribosomal protein L34

Chain KGG: 92% 5% ..



- Molecule 16: 60S ribosomal protein L9

Chain LH0: 94% . .



- Molecule 16: 60S ribosomal protein L9

Chain KH0: 94%



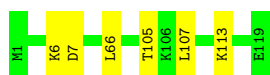
- Molecule 17: Ribosomal L29 protein

Chain LHH: 95%



- Molecule 17: Ribosomal L29 protein

Chain KHH: 95%



- Molecule 18: S60 ribosomal protein L10

Chain LI0: 97%



- Molecule 18: S60 ribosomal protein L10

Chain KI0: 98%



- Molecule 19: 60S ribosomal protein L36

Chain LII: 93%



- Molecule 19: 60S ribosomal protein L36

Chain KII: 92%



- Molecule 20: 60S ribosomal protein L11

Chain LJ0: 91% 6% .



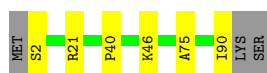
- Molecule 20: 60S ribosomal protein L11

Chain KJ0: 91% 6% .



- Molecule 21: 60S ribosomal protein L37

Chain LJJ: 90% 7% .



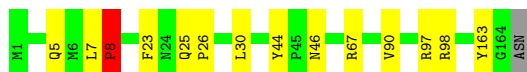
- Molecule 21: 60S ribosomal protein L37

Chain KJJ: 90% 7% .



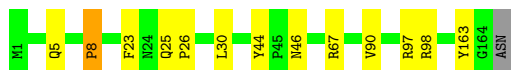
- Molecule 22: 60S ribosomal protein L13

Chain LL0: 91% 8% ..



- Molecule 22: 60S ribosomal protein L13

Chain KL0: 92% 7% ..



- Molecule 23: 60S ribosomal protein L39

Chain LLL: 98% .



- Molecule 23: 60S ribosomal protein L39

Chain KLL: 98%



- Molecule 24: Transposase

Chain LM0: 96%



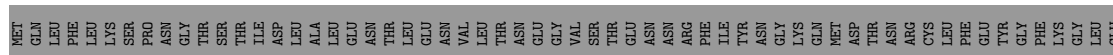
- Molecule 24: Transposase

Chain KM0: 97%



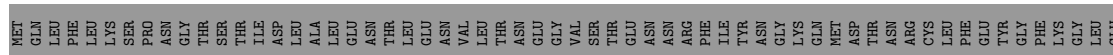
- Molecule 25: Ubiquitin

Chain LMM: 41% 59%



- Molecule 25: Ubiquitin

Chain KMM: 41% 59%

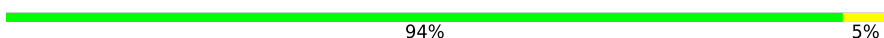


- Molecule 26: Ribosomal protein L15

Chain LN0: 94% 5%

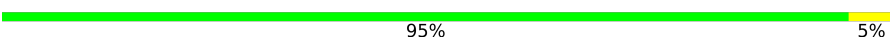


- Molecule 26: Ribosomal protein L15

Chain KN0:  94% 5%

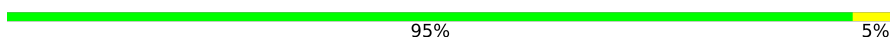


- Molecule 27: Ribosomal protein L13A

Chain LO0:  95% 5%

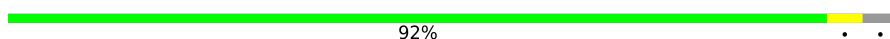


- Molecule 27: Ribosomal protein L13A

Chain KO0:  95% 5%

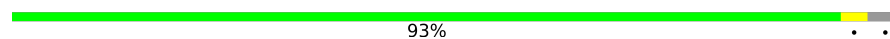


- Molecule 28: 60S ribosomal protein L44

Chain LOO:  92% . .



- Molecule 28: 60S ribosomal protein L44

Chain KOO:  93% . .



- Molecule 29: 60S ribosomal protein L17

Chain LP0:  89% . . 8%



- Molecule 29: 60S ribosomal protein L17

Chain KP0:  87% . . 8%



- Molecule 30: 60S ribosomal protein L37a

Chain LPP:  92% ..

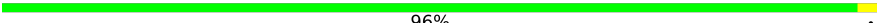


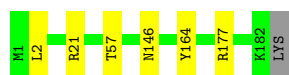
- Molecule 30: 60S ribosomal protein L37a

Chain KPP:  92% ..

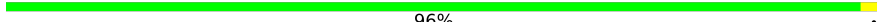


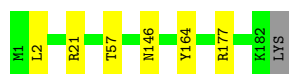
- Molecule 31: 60S ribosomal protein L18

Chain LQ0:  96% ..

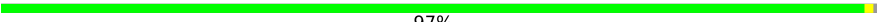


- Molecule 31: 60S ribosomal protein L18

Chain KQ0:  96% ..

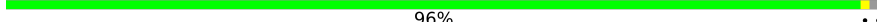


- Molecule 32: 60S ribosomal protein L19

Chain LR0:  97% ..

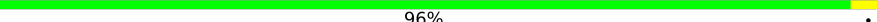


- Molecule 32: 60S ribosomal protein L19

Chain KR0:  96% ..

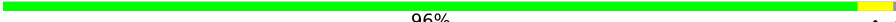


- Molecule 33: 60S ribosomal protein L20

Chain LS0:  96% ..



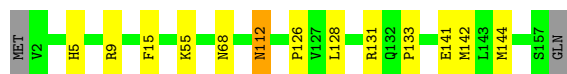
- Molecule 33: 60S ribosomal protein L20

Chain KS0:  96% ..



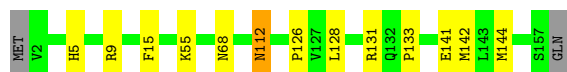
- Molecule 34: 60s ribosomal protein L21

Chain LT0:  91% 8% ..



- Molecule 34: 60s ribosomal protein L21

Chain KT0:  91% 8% ..



- Molecule 35: 60S ribosomal protein L22

Chain LU0:  86% . 12%

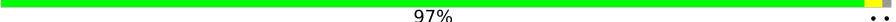


- Molecule 35: 60S ribosomal protein L22

Chain KU0:  86% . 12%

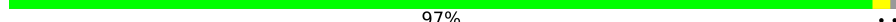


- Molecule 36: Ribosomal protein L23

Chain LV0:  97% ..



- Molecule 36: Ribosomal protein L23

Chain KV0:  97% ..



- Molecule 37: Ribosomal protein L24E

Chain LW0:  66% 10% 22%

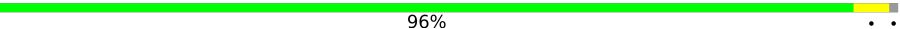


- Molecule 37: Ribosomal protein L24E

Chain KW0:  66% 10% 22%

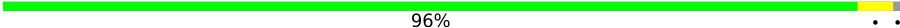


- Molecule 38: 60S ribosomal protein L23a

Chain LX0:  96%



- Molecule 38: 60S ribosomal protein L23a

Chain KX0:  96%



- Molecule 39: 60S ribosomal protein L26

Chain LY0:  96%



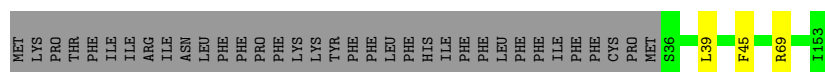
- Molecule 39: 60S ribosomal protein L26

Chain KY0:  96%



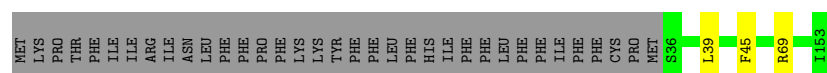
- Molecule 40: 60S ribosomal protein L27

Chain LZ0:  75% 23%



- Molecule 40: 60S ribosomal protein L27

Chain KZ0:  75% 23%

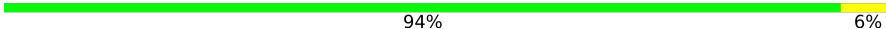


- Molecule 41: DNL-type domain-containing protein

Chain MD1:  94% 6%



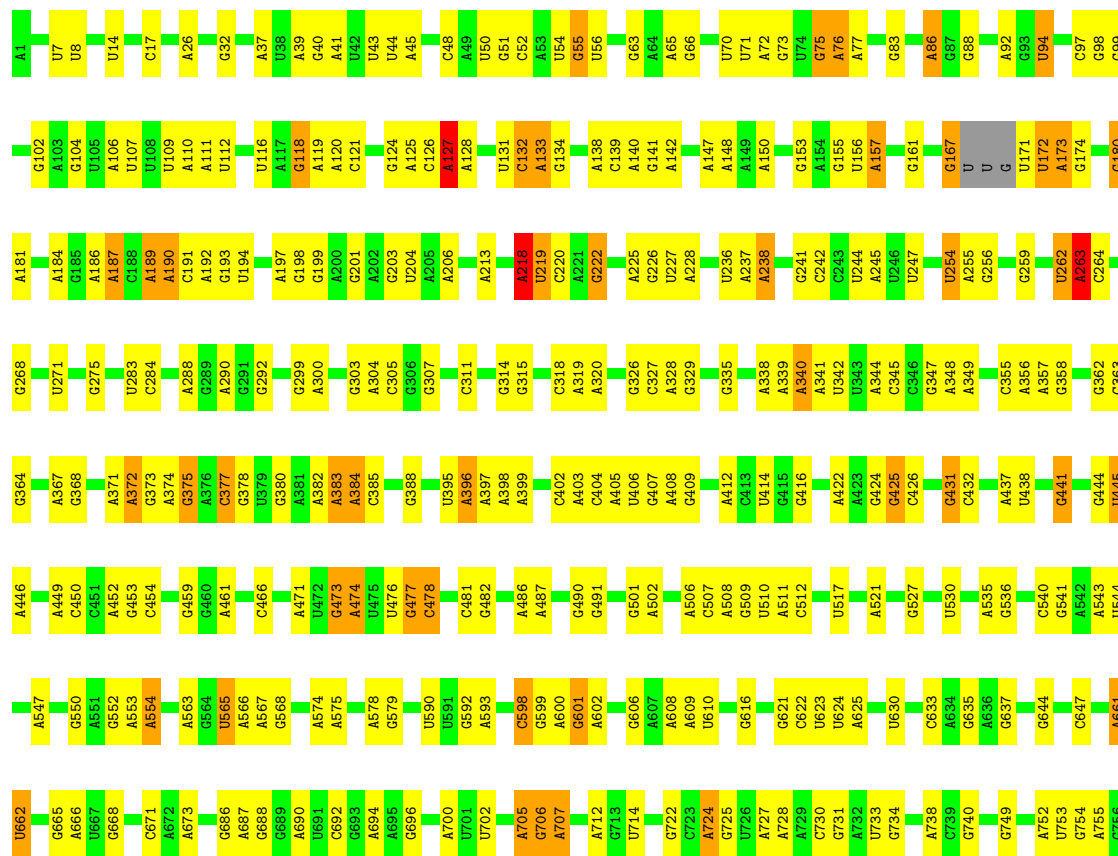
- Molecule 41: DNL-type domain-containing protein

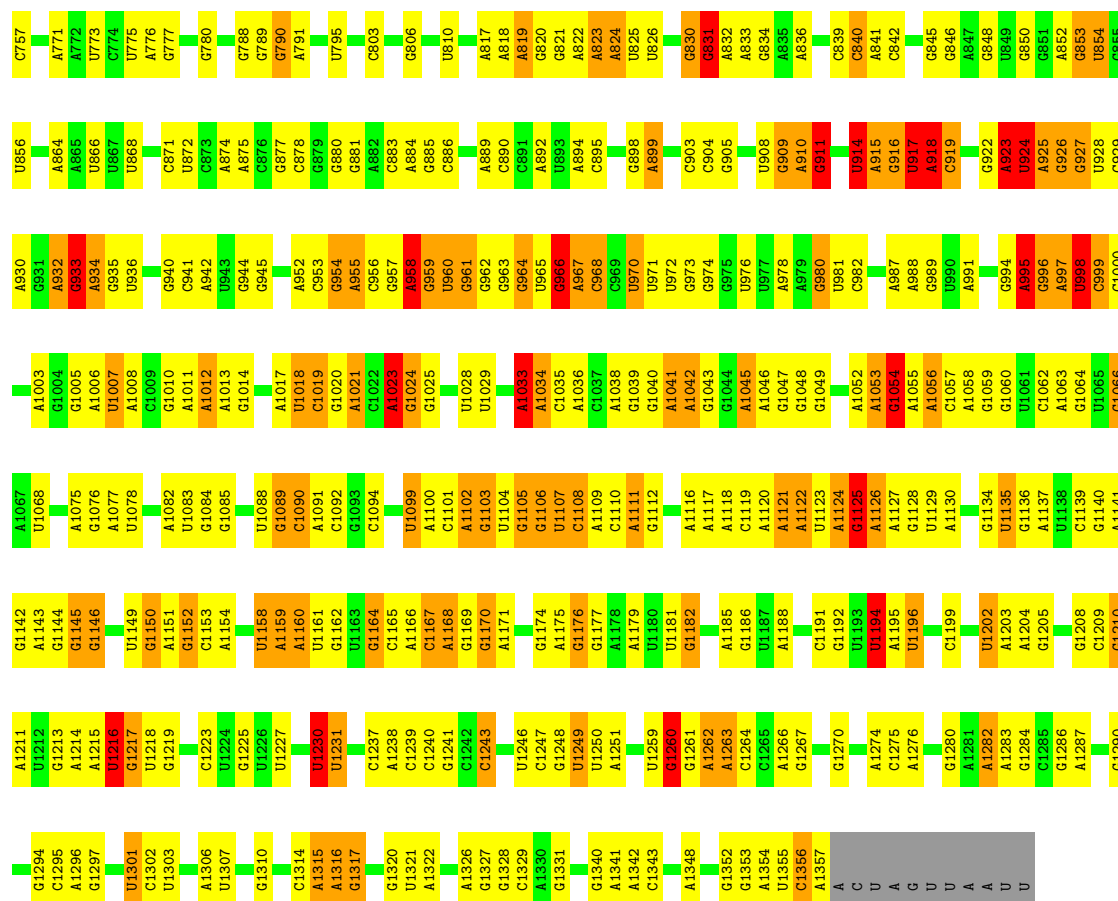
Chain MD2:  94% 6%



- Molecule 42: RNA 16S

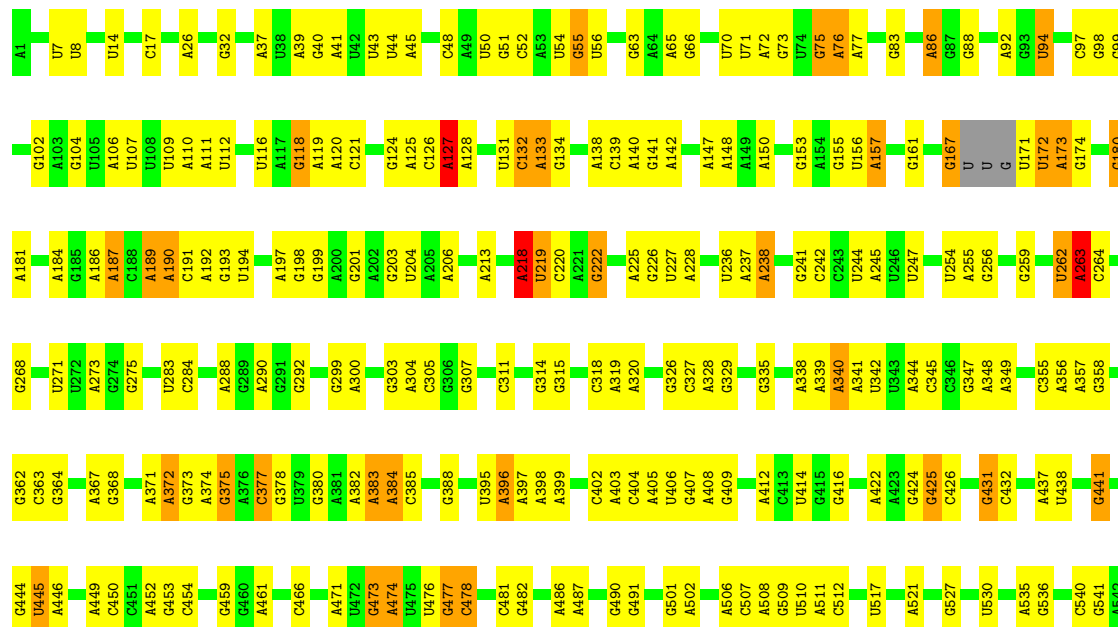
Chain S60:  49% 38% 10%

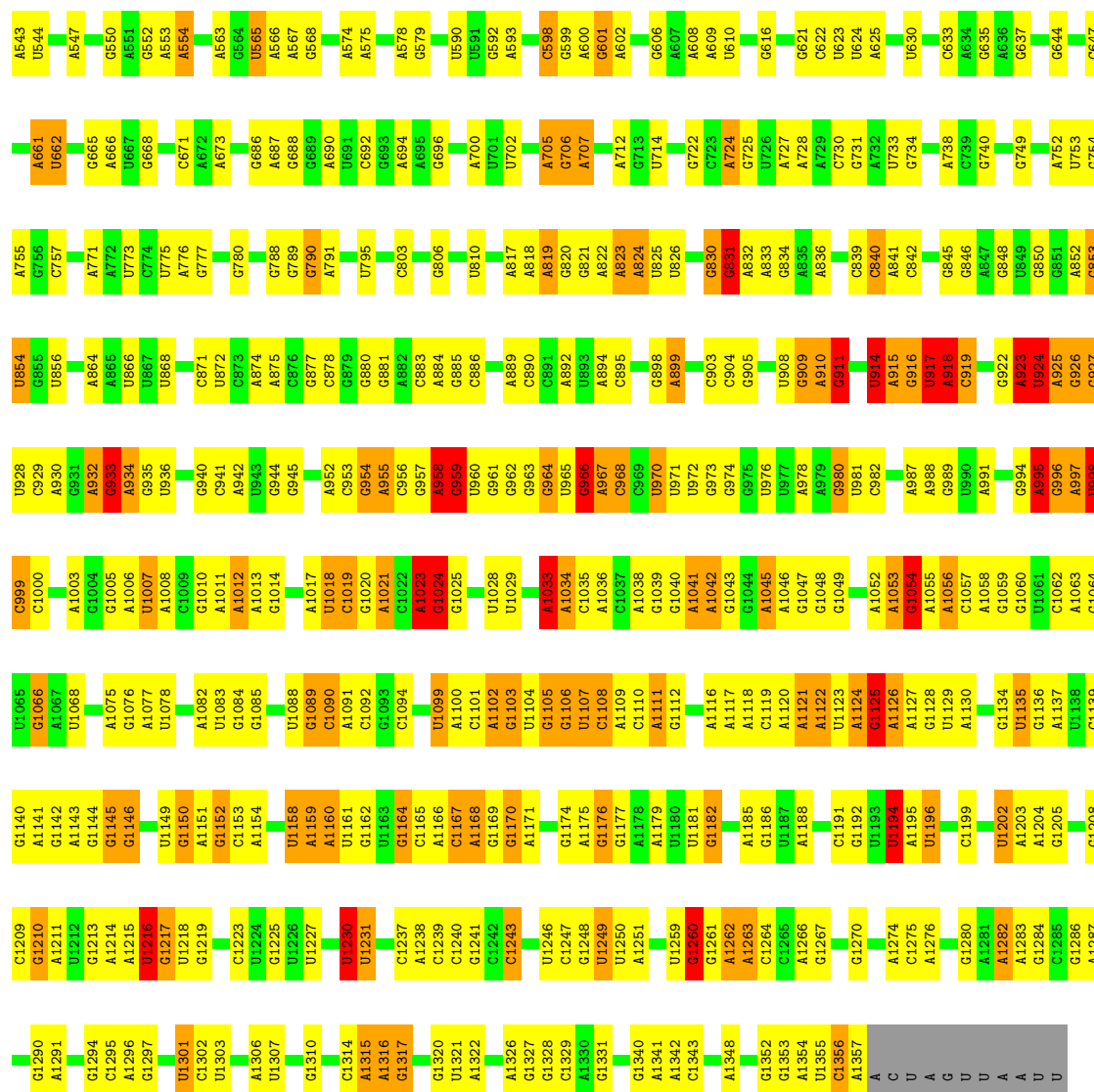




• Molecule 42: RNA 16S

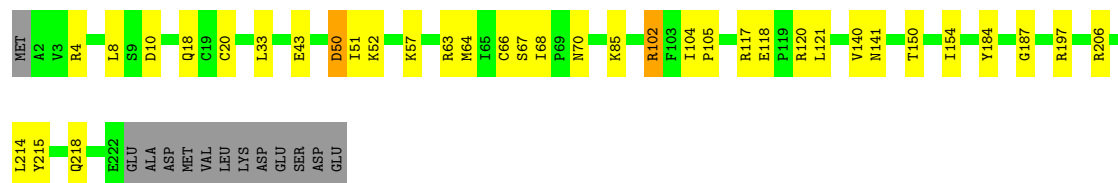
Chain R60: 49% 38% 9% ..





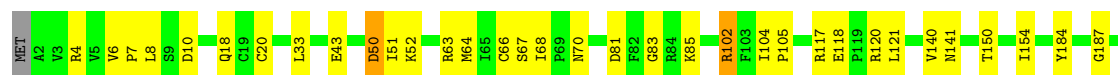
• Molecule 43: 40S ribosomal protein S0

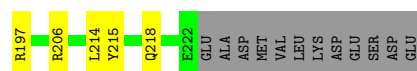
Chain SA0: 79% 15% 6%



• Molecule 43: 40S ribosomal protein S0

Chain RA0: 78% 16% 6%





- Molecule 44: 40S ribosomal protein S26

Chain SAA: 92% 7%



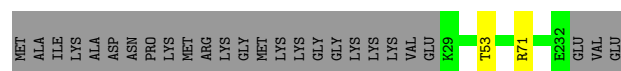
- Molecule 44: 40S ribosomal protein S26

Chain RAA: 92% 7%



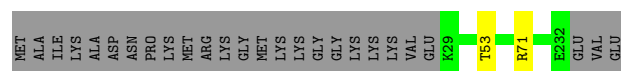
- Molecule 45: 40S ribosomal protein S1

Chain SB0: 88% 11%



- Molecule 45: 40S ribosomal protein S1

Chain RB0: 88% 11%



- Molecule 46: 40S ribosomal protein S27

Chain SBB: 94% 5%



- Molecule 46: 40S ribosomal protein S27

Chain RBB: 93% 6%



- Molecule 47: 40S ribosomal protein S2

Chain SC0: 81% 10% 9%



-
- ```

graph LR
 P231[P231] --> I232[I232]
 I232 --> L233[L233]
 L233 --> I240[I240]
 I240 --> E243[E243]
 E243 --> R248[R248]

```

- |     |
|-----|
| MET |
| S2  |
| I41 |
| M42 |
| G43 |
| P44 |
| I45 |
| L50 |
| D55 |
| C56 |
| E57 |
| R58 |
| E59 |
| H60 |
| R61 |
| R62 |
| G63 |
| ARG |
| PHE |

- |     |
|-----|
| MET |
| S2  |
| I41 |
| M42 |
| G43 |
| P44 |
| I45 |
| L50 |
| D55 |
| C56 |
| E57 |
| R58 |
| E59 |
| H60 |
| R61 |
| R62 |
| G63 |
| ARG |
| PHE |

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|
| MET | GLN | ASN | GLN | LYS | LEU | ILE | PHE | PHE | PRO | GLN | LEU | ILE | PHE | PHE | ASN | PHE | GLN | ILE | PHE | PHE | THR | LEU | W25 | A30 | I33 | K34 | R35 | R36 | H68 | Q94 | K101 | I184 | Q188 | P169 | I207 | K211 | W215 | M230 | I234 | L237 | P238 | I239 | K240 | GLU | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |            |            |            |            |            |            |            |            |            |             |             |             |             |             |             |             |             |             |             |             |             |             |            |            |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|------------|------------|
| NET | GLN | ASN | GLN | LYS | SER | ILE | PHE | PRO | GLN | LEU | ILE | PHE | PHE | ASN | ILE | PHE | GLN | ILE | PHE | PHE | THR | LEU | <b>K25</b> | <b>K26</b> | <b>A30</b> | <b>K33</b> | <b>K34</b> | <b>K35</b> | <b>K36</b> | <b>H68</b> | <b>Q94</b> | <b>K101</b> | <b>I184</b> | <b>Q188</b> | <b>P169</b> | <b>I207</b> | <b>K211</b> | <b>K215</b> | <b>M230</b> | <b>I234</b> | <b>L237</b> | <b>P238</b> | <b>I239</b> | <b>K240</b> | <b>GLU</b> | <b>GLI</b> |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|------------|------------|

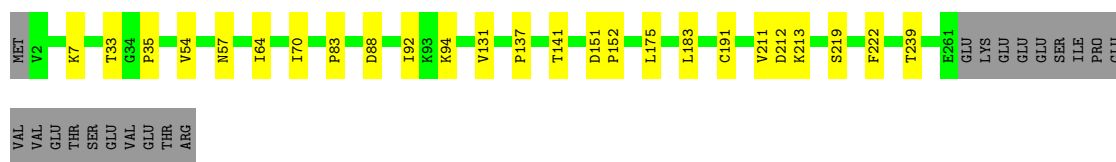
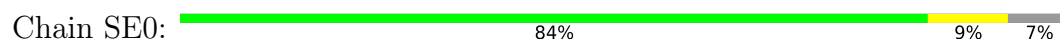
- 



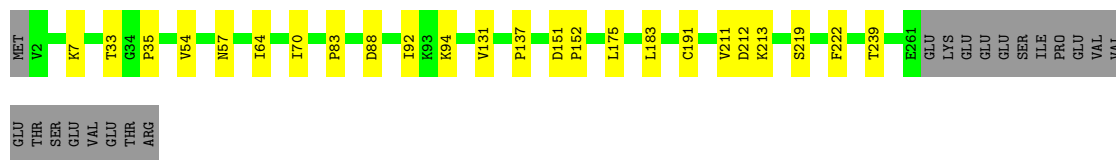
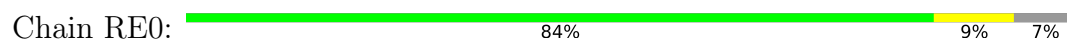
- Molecule 50: 40S ribosomal protein S29



- Molecule 51: 40S ribosomal protein S4



- Molecule 51: 40S ribosomal protein S4



- Molecule 52: 40S ribosomal protein S30



- Molecule 52: 40S ribosomal protein S30



- Molecule 53: 40S ribosomal protein S5



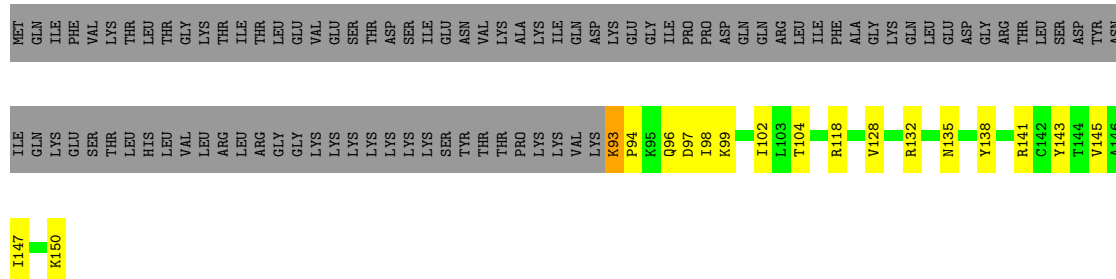
- Molecule 53: 40S ribosomal protein S5

Chain RF0:  86% 12% ..



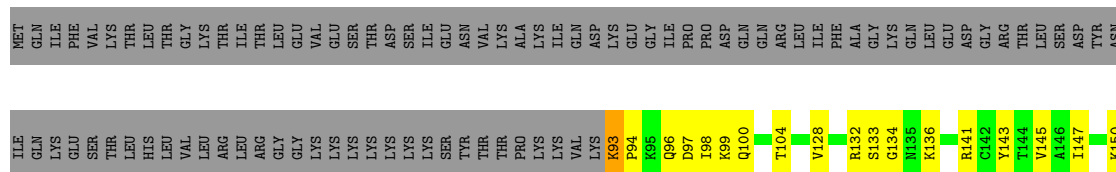
- Molecule 54: Ubiquitin/40s ribosomal protein S27a fusion

Chain SFF:  27% 11% . 61%

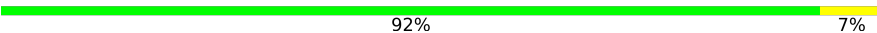


- Molecule 54: Ubiquitin/40s ribosomal protein S27a fusion

Chain RFF:  27% 11% . 61%

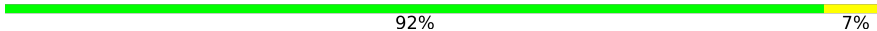


- Molecule 55: 40S ribosomal protein S6

Chain SG0:  92% 7%



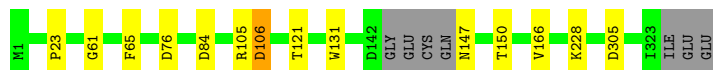
- Molecule 55: 40S ribosomal protein S6

Chain RG0:  92% 7%

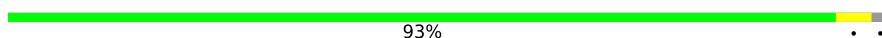


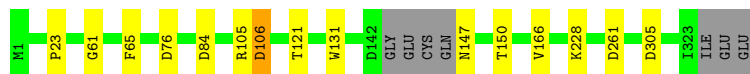
- Molecule 56: Guanine nucleotide binding protein beta subunit

Chain SGG:  94% . .

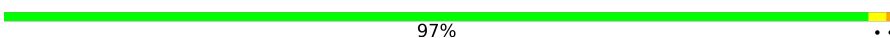


- Molecule 56: Guanine nucleotide binding protein beta subunit

Chain RGG:  93% . .

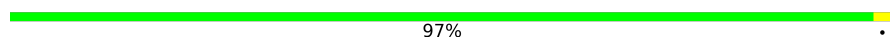


- Molecule 57: 40S ribosomal protein S7

Chain SH0:  97% . . .



- Molecule 57: 40S ribosomal protein S7

Chain RH0:  97% . . .



- Molecule 58: 40S ribosomal protein S8

Chain SI0:  91% 5% .



- Molecule 58: 40S ribosomal protein S8

Chain RI0:  92% 5% .



- Molecule 59: 40S ribosomal protein S9

Chain SJ0:  86% 5% 9%



- Molecule 59: 40S ribosomal protein S9

Chain RJ0:  86% 5% 9%



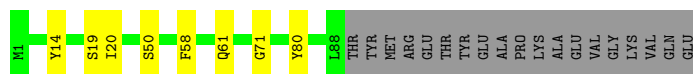
- Molecule 60: 40S ribosomal protein S10

Chain SK0:  75% 7% 18%



- Molecule 60: 40S ribosomal protein S10

Chain RK0:  75% 7% 18%



- Molecule 61: 40S ribosomal protein S11

Chain SL0:  92% 5% .



- Molecule 61: 40S ribosomal protein S11

Chain RL0:  92% 5% .



- Molecule 62: 40S ribosomal protein S12

Chain SM0:  82% 5% 13%



- Molecule 62: 40S ribosomal protein S12

Chain RM0:  82% 5% 13%



- Molecule 63: 40S ribosomal protein S13

Chain SN0:  90% 9% .



- Molecule 63: 40S ribosomal protein S13

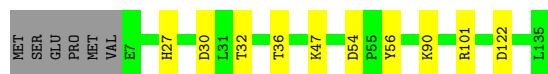


Chain RN0:  90% 9% .



- Molecule 64: 40S ribosomal protein S14

Chain SO0:  88% 7% .



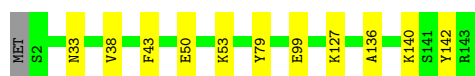
- Molecule 64: 40S ribosomal protein S14

Chain RO0:  88% 7% .



- Molecule 65: 40S ribosomal protein S16

Chain SQ0:  92% 8% .



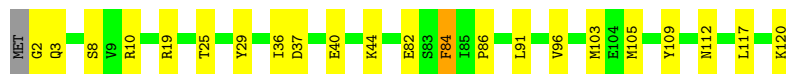
- Molecule 65: 40S ribosomal protein S16

Chain RQ0:  92% 8% .



- Molecule 66: 40S ribosomal protein S17

Chain SR0:  81% 18% ..

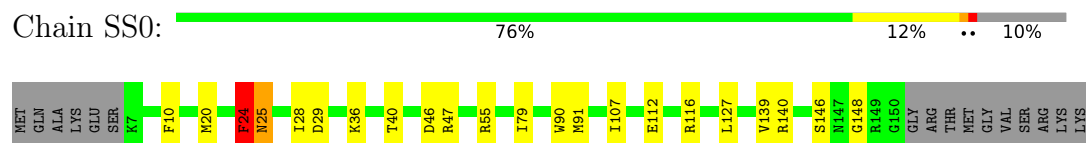


- Molecule 66: 40S ribosomal protein S17

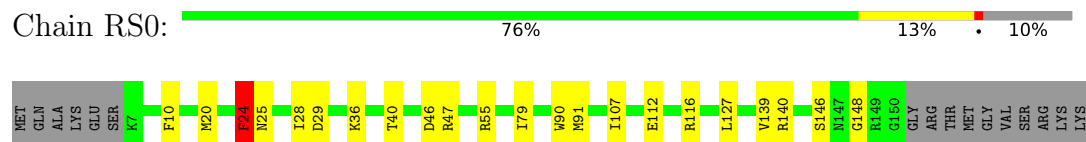
Chain RR0:  80% 18% ..



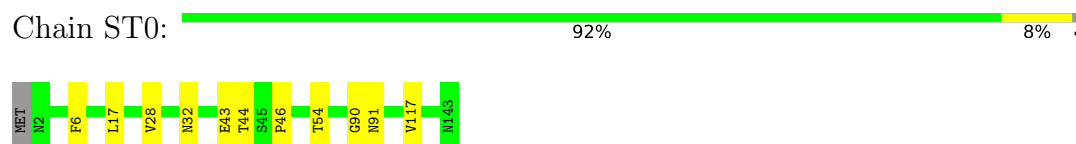
- Molecule 67: 40S ribosomal protein S18



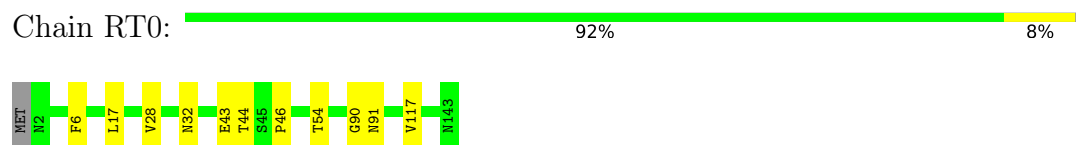
- Molecule 67: 40S ribosomal protein S18



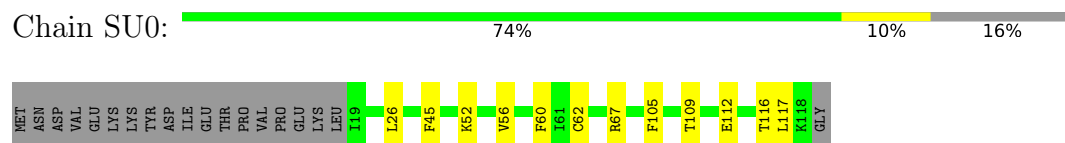
- Molecule 68: 40S Ribosomal protein S19



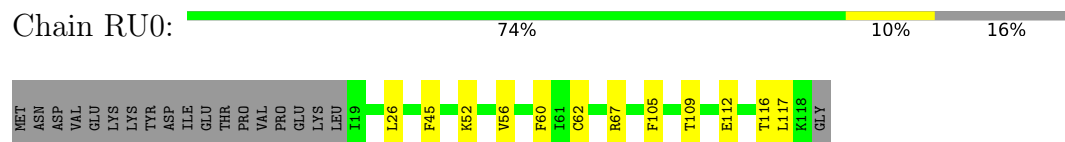
- Molecule 68: 40S Ribosomal protein S19



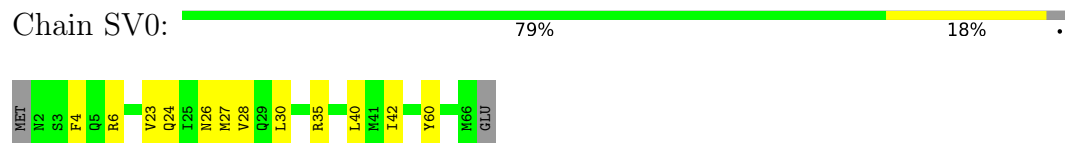
- Molecule 69: 40S ribosomal protein S20



- Molecule 69: 40S ribosomal protein S20



- Molecule 70: Ribosomal protein S21E



- Molecule 70: Ribosomal protein S21E

Chain RV0:  81% 16% .



- Molecule 71: 40S ribosomal protein S15A

Chain SW0:  91% 9%

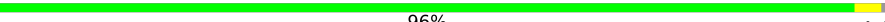


- Molecule 71: 40S ribosomal protein S15A

Chain RW0:  91% 9%

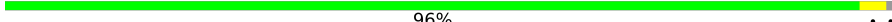


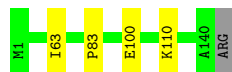
- Molecule 72: Ribosomal protein S12/S23

Chain SX0:  96% . .



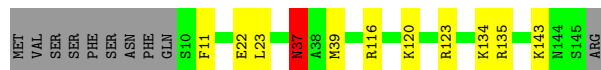
- Molecule 72: Ribosomal protein S12/S23

Chain RX0:  96% . .



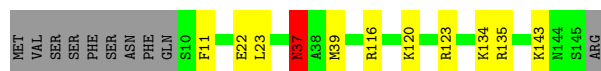
- Molecule 73: 40s ribosomal protein s24

Chain SY0:  86% 7% . 7%



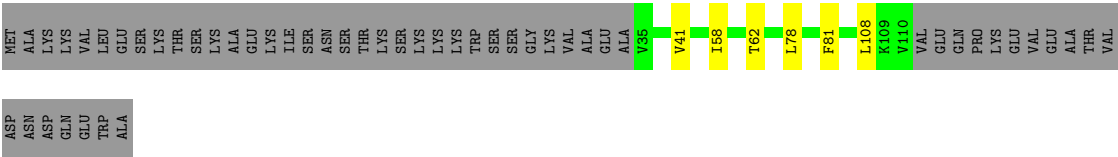
- Molecule 73: 40s ribosomal protein s24

Chain RY0:  86% 7% . 7%



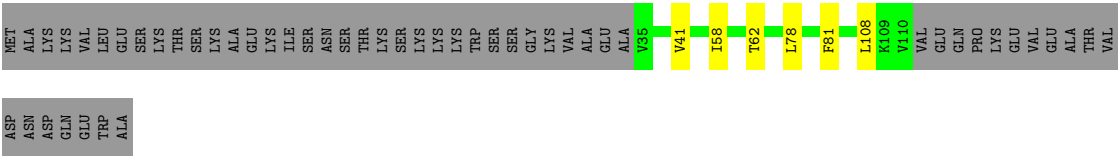
- Molecule 74: 40S ribosomal protein S25

Chain SZ0:  55% 5% 41%



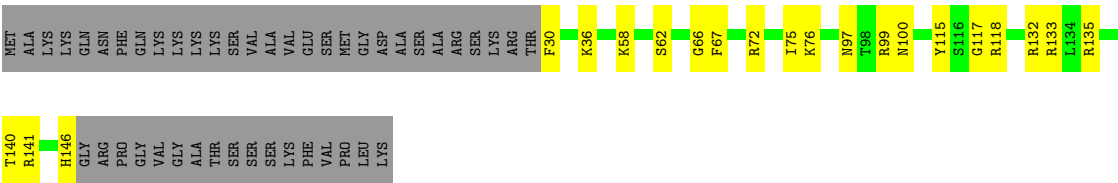
• Molecule 74: 40S ribosomal protein S25

Chain RZ0:  55% 5% 41%



• Molecule 75: Ribosomal protein S19

Chain SP0:  59% 13% 28%



• Molecule 75: Ribosomal protein S19

Chain RP0:  60% 12% 28%



## 4 Experimental information

| Property                             | Value                                                    | Source    |
|--------------------------------------|----------------------------------------------------------|-----------|
| EM reconstruction method             | SUBTOMOGRAM AVERAGING                                    | Depositor |
| Imposed symmetry                     | POINT, C2                                                | Depositor |
| Number of subtomograms used          | 1344                                                     | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                                        | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION                  | Depositor |
| Microscope                           | FEI TITAN KRIOS                                          | Depositor |
| Voltage (kV)                         | 300                                                      | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 120, 120                                                 | Depositor |
| Minimum defocus (nm)                 | 2500                                                     | Depositor |
| Maximum defocus (nm)                 | 6000                                                     | Depositor |
| Magnification                        | Not provided                                             |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k), GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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   | K50   | 0.70         | 0/60107     | 1.07        | 182/93753 (0.2%) |
| 1   | L50   | 0.70         | 0/60107     | 1.07        | 181/93753 (0.2%) |
| 2   | K70   | 0.71         | 0/2844      | 1.02        | 8/4429 (0.2%)    |
| 2   | L70   | 0.71         | 0/2844      | 1.02        | 8/4429 (0.2%)    |
| 3   | KA0   | 0.54         | 0/1926      | 1.05        | 0/2590           |
| 3   | LA0   | 0.54         | 0/1926      | 1.05        | 0/2590           |
| 4   | KAA   | 0.55         | 0/1191      | 0.94        | 0/1586           |
| 4   | LAA   | 0.55         | 0/1191      | 0.94        | 0/1586           |
| 5   | KB0   | 0.52         | 0/3092      | 0.99        | 2/4144 (0.0%)    |
| 5   | LB0   | 0.52         | 0/3092      | 0.99        | 2/4144 (0.0%)    |
| 6   | KC0   | 0.51         | 0/2646      | 1.07        | 3/3555 (0.1%)    |
| 6   | LC0   | 0.51         | 0/2646      | 1.07        | 3/3555 (0.1%)    |
| 7   | KCC   | 0.49         | 0/794       | 1.01        | 0/1067           |
| 7   | LCC   | 0.49         | 0/794       | 1.01        | 0/1067           |
| 8   | KD0   | 0.44         | 0/2328      | 1.05        | 3/3098 (0.1%)    |
| 8   | LD0   | 0.44         | 0/2328      | 1.05        | 3/3098 (0.1%)    |
| 9   | KDD   | 0.49         | 0/913       | 0.97        | 0/1223           |
| 9   | LDD   | 0.49         | 0/913       | 0.97        | 0/1223           |
| 10  | KE0   | 0.46         | 0/1394      | 1.02        | 3/1875 (0.2%)    |
| 10  | LE0   | 0.46         | 0/1394      | 1.03        | 3/1875 (0.2%)    |
| 11  | KEE   | 0.49         | 0/1108      | 1.05        | 1/1477 (0.1%)    |
| 11  | LEE   | 0.49         | 0/1108      | 1.05        | 1/1477 (0.1%)    |
| 12  | KF0   | 0.48         | 0/1963      | 0.99        | 2/2618 (0.1%)    |
| 12  | LF0   | 0.48         | 0/1963      | 1.00        | 2/2618 (0.1%)    |
| 13  | KFF   | 0.54         | 0/906       | 1.03        | 0/1207           |
| 13  | LFF   | 0.53         | 0/906       | 1.02        | 0/1207           |
| 14  | KG0   | 0.47         | 0/1612      | 1.06        | 0/2163           |
| 14  | LG0   | 0.47         | 0/1612      | 1.06        | 0/2163           |
| 15  | KGG   | 0.49         | 0/825       | 1.12        | 2/1090 (0.2%)    |
| 15  | LGG   | 0.49         | 0/825       | 1.13        | 2/1090 (0.2%)    |
| 16  | KH0   | 0.48         | 0/1503      | 0.95        | 0/2018           |
| 16  | LH0   | 0.48         | 0/1503      | 0.95        | 0/2018           |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 17  | KHH   | 0.44         | 0/999   | 1.03        | 0/1324        |
| 17  | LHH   | 0.44         | 0/999   | 1.03        | 0/1324        |
| 18  | KI0   | 0.51         | 0/1781  | 0.99        | 1/2382 (0.0%) |
| 18  | LI0   | 0.51         | 0/1781  | 0.99        | 1/2382 (0.0%) |
| 19  | KII   | 0.47         | 0/790   | 1.00        | 0/1041        |
| 19  | LII   | 0.47         | 0/790   | 1.00        | 0/1041        |
| 20  | KJ0   | 0.47         | 0/1350  | 1.02        | 1/1797 (0.1%) |
| 20  | LJ0   | 0.47         | 0/1350  | 1.02        | 1/1797 (0.1%) |
| 21  | KJJ   | 0.53         | 0/710   | 1.14        | 1/932 (0.1%)  |
| 21  | LJJ   | 0.53         | 0/710   | 1.14        | 1/932 (0.1%)  |
| 22  | KL0   | 0.48         | 0/1374  | 1.12        | 2/1827 (0.1%) |
| 22  | LL0   | 0.49         | 0/1374  | 1.12        | 2/1827 (0.1%) |
| 23  | KLL   | 0.51         | 0/435   | 1.02        | 0/576         |
| 23  | LLL   | 0.51         | 0/435   | 1.02        | 0/576         |
| 24  | KM0   | 0.50         | 0/935   | 1.04        | 0/1251        |
| 24  | LM0   | 0.50         | 0/935   | 1.03        | 0/1251        |
| 25  | KMM   | 0.52         | 0/431   | 1.04        | 0/568         |
| 25  | LMM   | 0.52         | 0/431   | 1.04        | 0/568         |
| 26  | KN0   | 0.53         | 0/1722  | 1.03        | 3/2297 (0.1%) |
| 26  | LN0   | 0.53         | 0/1722  | 1.03        | 3/2297 (0.1%) |
| 27  | KO0   | 0.50         | 0/1626  | 1.03        | 2/2168 (0.1%) |
| 27  | LO0   | 0.50         | 0/1626  | 1.03        | 2/2168 (0.1%) |
| 28  | KOO   | 0.54         | 0/811   | 1.00        | 0/1071        |
| 28  | LOO   | 0.54         | 0/811   | 1.01        | 0/1071        |
| 29  | KP0   | 0.54         | 0/1262  | 1.11        | 0/1689        |
| 29  | LP0   | 0.54         | 0/1262  | 1.11        | 0/1689        |
| 30  | KPP   | 0.53         | 0/693   | 1.12        | 2/918 (0.2%)  |
| 30  | LPP   | 0.53         | 0/693   | 1.12        | 2/918 (0.2%)  |
| 31  | KQ0   | 0.47         | 0/1512  | 0.99        | 0/2014        |
| 31  | LQ0   | 0.47         | 0/1512  | 0.99        | 0/2014        |
| 32  | KR0   | 0.50         | 0/1352  | 1.04        | 0/1790        |
| 32  | LR0   | 0.49         | 0/1352  | 1.04        | 0/1790        |
| 33  | KS0   | 0.49         | 0/1422  | 0.99        | 1/1898 (0.1%) |
| 33  | LS0   | 0.49         | 0/1422  | 0.99        | 1/1898 (0.1%) |
| 34  | KT0   | 0.50         | 0/1294  | 0.98        | 1/1736 (0.1%) |
| 34  | LT0   | 0.50         | 0/1294  | 0.98        | 1/1736 (0.1%) |
| 35  | KU0   | 0.47         | 0/826   | 0.99        | 0/1104        |
| 35  | LU0   | 0.47         | 0/826   | 0.99        | 0/1104        |
| 36  | KV0   | 0.55         | 0/1068  | 1.03        | 1/1429 (0.1%) |
| 36  | LV0   | 0.55         | 0/1068  | 1.03        | 1/1429 (0.1%) |
| 37  | KW0   | 0.64         | 0/849   | 1.14        | 2/1129 (0.2%) |
| 37  | LW0   | 0.64         | 0/849   | 1.15        | 2/1129 (0.2%) |
| 38  | KX0   | 0.48         | 0/883   | 1.03        | 0/1175        |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 38  | LX0   | 0.48         | 0/883          | 1.03        | 0/1175           |
| 39  | KY0   | 0.49         | 0/1058         | 1.08        | 1/1399 (0.1%)    |
| 39  | LY0   | 0.49         | 0/1058         | 1.08        | 1/1399 (0.1%)    |
| 40  | KZ0   | 0.48         | 0/976          | 1.09        | 2/1302 (0.2%)    |
| 40  | LZ0   | 0.48         | 0/976          | 1.09        | 2/1302 (0.2%)    |
| 41  | MD1   | 0.66         | 0/1249         | 1.06        | 1/1677 (0.1%)    |
| 41  | MD2   | 0.66         | 0/1249         | 1.06        | 1/1677 (0.1%)    |
| 42  | R60   | 0.99         | 6/32725 (0.0%) | 1.11        | 127/51066 (0.2%) |
| 42  | S60   | 0.99         | 6/32725 (0.0%) | 1.11        | 125/51066 (0.2%) |
| 43  | RA0   | 0.59         | 1/1751 (0.1%)  | 1.01        | 1/2358 (0.0%)    |
| 43  | SA0   | 0.59         | 1/1751 (0.1%)  | 1.01        | 1/2358 (0.0%)    |
| 44  | RAA   | 0.57         | 0/839          | 1.06        | 0/1120           |
| 44  | SAA   | 0.57         | 0/839          | 1.06        | 0/1120           |
| 45  | RB0   | 0.50         | 0/1623         | 1.01        | 0/2169           |
| 45  | SB0   | 0.50         | 0/1623         | 1.01        | 0/2169           |
| 46  | RBB   | 0.57         | 0/634          | 0.99        | 0/844            |
| 46  | SBB   | 0.57         | 0/634          | 0.99        | 0/844            |
| 47  | RC0   | 0.51         | 0/1751         | 1.05        | 2/2359 (0.1%)    |
| 47  | SC0   | 0.51         | 0/1751         | 1.05        | 2/2359 (0.1%)    |
| 48  | RCC   | 0.54         | 0/480          | 0.97        | 2/644 (0.3%)     |
| 48  | SCC   | 0.53         | 0/480          | 0.97        | 2/644 (0.3%)     |
| 49  | RD0   | 0.50         | 0/1721         | 1.04        | 0/2304           |
| 49  | SD0   | 0.51         | 0/1721         | 1.04        | 0/2304           |
| 50  | RDD   | 0.51         | 0/559          | 1.00        | 1/742 (0.1%)     |
| 50  | SDD   | 0.51         | 0/559          | 1.00        | 1/742 (0.1%)     |
| 51  | RE0   | 0.54         | 0/2080         | 1.07        | 5/2804 (0.2%)    |
| 51  | SE0   | 0.54         | 0/2080         | 1.07        | 7/2804 (0.2%)    |
| 52  | REE   | 0.56         | 0/453          | 1.10        | 1/596 (0.2%)     |
| 52  | SEE   | 0.57         | 0/453          | 1.10        | 1/596 (0.2%)     |
| 53  | RF0   | 0.50         | 0/1527         | 1.09        | 2/2045 (0.1%)    |
| 53  | SF0   | 0.50         | 0/1527         | 1.09        | 2/2045 (0.1%)    |
| 54  | RFF   | 0.62         | 0/422          | 1.00        | 0/568            |
| 54  | SFF   | 0.62         | 0/427          | 1.00        | 0/573            |
| 55  | RG0   | 0.49         | 0/1864         | 1.05        | 1/2485 (0.0%)    |
| 55  | SG0   | 0.48         | 0/1864         | 1.05        | 1/2485 (0.0%)    |
| 56  | RGG   | 0.58         | 0/2517         | 1.05        | 4/3397 (0.1%)    |
| 56  | SGG   | 0.58         | 0/2517         | 1.05        | 3/3397 (0.1%)    |
| 57  | RH0   | 0.45         | 0/1356         | 1.02        | 1/1820 (0.1%)    |
| 57  | SH0   | 0.45         | 0/1356         | 1.02        | 1/1820 (0.1%)    |
| 58  | RI0   | 0.54         | 0/1369         | 1.02        | 1/1825 (0.1%)    |
| 58  | SI0   | 0.54         | 0/1369         | 1.02        | 1/1825 (0.1%)    |
| 59  | RJ0   | 0.51         | 0/1403         | 1.05        | 0/1880           |
| 59  | SJ0   | 0.51         | 0/1403         | 1.05        | 0/1880           |



| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 60  | RK0   | 0.49         | 0/750            | 1.08        | 0/1009            |
| 60  | SK0   | 0.49         | 0/750            | 1.08        | 0/1009            |
| 61  | RL0   | 0.55         | 0/1252           | 0.99        | 1/1672 (0.1%)     |
| 61  | SL0   | 0.55         | 0/1252           | 0.99        | 1/1672 (0.1%)     |
| 62  | RM0   | 0.56         | 0/881            | 1.15        | 1/1182 (0.1%)     |
| 62  | SM0   | 0.56         | 0/881            | 1.15        | 1/1182 (0.1%)     |
| 63  | RN0   | 0.58         | 0/1154           | 1.15        | 2/1557 (0.1%)     |
| 63  | SN0   | 0.57         | 0/1154           | 1.15        | 2/1557 (0.1%)     |
| 64  | RO0   | 0.54         | 0/993            | 1.09        | 1/1326 (0.1%)     |
| 64  | SO0   | 0.55         | 0/993            | 1.09        | 1/1326 (0.1%)     |
| 65  | RQ0   | 0.57         | 0/1163           | 1.05        | 2/1556 (0.1%)     |
| 65  | SQ0   | 0.57         | 0/1163           | 1.05        | 2/1556 (0.1%)     |
| 66  | RR0   | 0.73         | 0/985            | 1.29        | 1/1315 (0.1%)     |
| 66  | SR0   | 0.73         | 0/985            | 1.29        | 0/1315            |
| 67  | RS0   | 0.57         | 0/1165           | 1.12        | 0/1566            |
| 67  | SS0   | 0.57         | 0/1165           | 1.12        | 1/1566 (0.1%)     |
| 68  | RT0   | 0.55         | 0/1181           | 1.14        | 1/1585 (0.1%)     |
| 68  | ST0   | 0.55         | 0/1181           | 1.14        | 1/1585 (0.1%)     |
| 69  | RU0   | 0.56         | 0/824            | 1.09        | 4/1110 (0.4%)     |
| 69  | SU0   | 0.56         | 0/824            | 1.09        | 4/1110 (0.4%)     |
| 70  | RV0   | 0.50         | 0/525            | 0.96        | 0/700             |
| 70  | SV0   | 0.49         | 0/525            | 0.96        | 0/700             |
| 71  | RW0   | 0.51         | 0/1037           | 1.00        | 0/1389            |
| 71  | SW0   | 0.51         | 0/1037           | 1.00        | 0/1389            |
| 72  | RX0   | 0.55         | 0/1113           | 1.05        | 1/1486 (0.1%)     |
| 72  | SX0   | 0.55         | 0/1113           | 1.05        | 1/1486 (0.1%)     |
| 73  | RY0   | 0.49         | 0/1131           | 1.10        | 1/1503 (0.1%)     |
| 73  | SY0   | 0.49         | 0/1131           | 1.11        | 1/1503 (0.1%)     |
| 74  | RZ0   | 0.57         | 0/640            | 1.09        | 0/855             |
| 74  | SZ0   | 0.56         | 0/640            | 1.09        | 0/855             |
| 75  | RP0   | 0.53         | 0/964            | 1.08        | 0/1289            |
| 75  | SP0   | 0.54         | 0/964            | 1.08        | 0/1289            |
| All | All   | 0.69         | 14/366789 (0.0%) | 1.07        | 778/533031 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 6   | KC0   | 0                   | 1                   |
| 6   | LC0   | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 13  | KFF   | 0                   | 1                   |
| 13  | LFF   | 0                   | 1                   |
| 15  | KGG   | 0                   | 1                   |
| 15  | LGG   | 0                   | 1                   |
| All | All   | 0                   | 6                   |

All (14) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 43  | RA0   | 20   | CYS  | C-N     | 14.56 | 1.53        | 1.34     |
| 43  | SA0   | 20   | CYS  | C-N     | 14.50 | 1.53        | 1.34     |
| 42  | S60   | 934  | A    | P-O5'   | 6.94  | 1.70        | 1.59     |
| 42  | R60   | 934  | A    | P-O5'   | 6.92  | 1.70        | 1.59     |
| 42  | R60   | 934  | A    | O5'-C5' | 6.66  | 1.52        | 1.42     |
| 42  | S60   | 934  | A    | O5'-C5' | 6.65  | 1.52        | 1.42     |
| 42  | R60   | 853  | G    | O5'-C5' | 5.29  | 1.50        | 1.42     |
| 42  | S60   | 853  | G    | O5'-C5' | 5.26  | 1.50        | 1.42     |
| 42  | S60   | 1054 | G    | O5'-C5' | 5.14  | 1.50        | 1.42     |
| 42  | R60   | 1054 | G    | O5'-C5' | 5.13  | 1.50        | 1.42     |
| 42  | R60   | 1213 | G    | O5'-C5' | 5.09  | 1.50        | 1.42     |
| 42  | S60   | 1213 | G    | O5'-C5' | 5.07  | 1.50        | 1.42     |
| 42  | S60   | 1170 | G    | O5'-C5' | 5.03  | 1.50        | 1.42     |
| 42  | R60   | 1170 | G    | O5'-C5' | 5.01  | 1.50        | 1.42     |

All (778) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | L50   | 1148 | A    | C4'-C3'-O3' | 14.10  | 130.55      | 109.40   |
| 1   | K50   | 1148 | A    | C4'-C3'-O3' | 14.08  | 130.52      | 109.40   |
| 1   | K50   | 330  | G    | C2'-C3'-O3' | 12.46  | 132.40      | 113.70   |
| 1   | L50   | 523  | A    | C1'-C2'-O2' | -12.45 | 93.13       | 111.80   |
| 1   | L50   | 330  | G    | C2'-C3'-O3' | 12.44  | 132.36      | 113.70   |
| 1   | K50   | 523  | A    | C1'-C2'-O2' | -12.40 | 93.20       | 111.80   |
| 42  | S60   | 473  | G    | C2'-C3'-O3' | 11.45  | 126.67      | 109.50   |
| 42  | R60   | 473  | G    | C2'-C3'-O3' | 11.44  | 126.66      | 109.50   |
| 1   | K50   | 1808 | A    | C4'-C3'-O3' | 11.37  | 126.45      | 109.40   |
| 1   | L50   | 1808 | A    | C4'-C3'-O3' | 11.36  | 126.44      | 109.40   |
| 1   | K50   | 1000 | G    | C1'-C2'-O2' | -11.20 | 95.01       | 111.80   |
| 1   | L50   | 1000 | G    | C1'-C2'-O2' | -11.17 | 95.04       | 111.80   |
| 1   | L50   | 1018 | U    | C1'-C2'-O2' | -10.96 | 95.37       | 111.80   |
| 1   | K50   | 1018 | U    | C1'-C2'-O2' | -10.90 | 95.45       | 111.80   |
| 1   | L50   | 1395 | U    | C2'-C3'-O3' | 10.48  | 129.42      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 1   | K50   | 1395 | U    | C2'-C3'-O3' | 10.43  | 129.34      | 113.70   |
| 1   | L50   | 1733 | A    | C4'-C3'-O3' | -10.35 | 97.47       | 113.00   |
| 1   | K50   | 1733 | A    | C4'-C3'-O3' | -10.33 | 97.51       | 113.00   |
| 1   | L50   | 1959 | A    | C2'-C3'-O3' | 10.15  | 128.93      | 113.70   |
| 1   | K50   | 1959 | A    | C2'-C3'-O3' | 10.13  | 128.89      | 113.70   |
| 42  | S60   | 180  | G    | C4'-C3'-O3' | 10.12  | 128.18      | 113.00   |
| 42  | R60   | 180  | G    | C4'-C3'-O3' | 10.09  | 128.14      | 113.00   |
| 42  | S60   | 933  | G    | O3'-P-O5'   | 10.03  | 119.04      | 104.00   |
| 42  | R60   | 933  | G    | O3'-P-O5'   | 10.02  | 119.03      | 104.00   |
| 42  | R60   | 565  | U    | C2'-C3'-O3' | 10.00  | 124.50      | 109.50   |
| 1   | L50   | 2452 | A    | C4'-C3'-O3' | 10.00  | 124.40      | 109.40   |
| 42  | S60   | 565  | U    | C2'-C3'-O3' | 9.99   | 124.49      | 109.50   |
| 1   | K50   | 1614 | G    | C1'-C2'-O2' | -9.98  | 96.83       | 111.80   |
| 1   | K50   | 2452 | A    | C4'-C3'-O3' | 9.98   | 124.36      | 109.40   |
| 42  | S60   | 910  | A    | P-O3'-C3'   | -9.69  | 105.67      | 120.20   |
| 42  | R60   | 910  | A    | P-O3'-C3'   | -9.66  | 105.71      | 120.20   |
| 42  | S60   | 933  | G    | C4'-C3'-O3' | 9.49   | 127.23      | 113.00   |
| 42  | R60   | 933  | G    | C4'-C3'-O3' | 9.48   | 127.22      | 113.00   |
| 42  | S60   | 1034 | A    | P-O3'-C3'   | -9.36  | 106.16      | 120.20   |
| 42  | R60   | 1034 | A    | P-O3'-C3'   | -9.33  | 106.20      | 120.20   |
| 42  | R60   | 904  | C    | P-O3'-C3'   | -9.04  | 106.64      | 120.20   |
| 1   | L50   | 1192 | A    | C4'-C3'-O3' | -9.04  | 99.45       | 113.00   |
| 42  | S60   | 904  | C    | P-O3'-C3'   | -9.04  | 106.65      | 120.20   |
| 1   | K50   | 1192 | A    | C4'-C3'-O3' | -9.03  | 99.46       | 113.00   |
| 1   | K50   | 2597 | G    | C2'-C3'-O3' | 8.95   | 127.12      | 113.70   |
| 1   | K50   | 827  | U    | C2'-C3'-O3' | -8.94  | 100.29      | 113.70   |
| 1   | L50   | 2597 | G    | C2'-C3'-O3' | 8.94   | 127.11      | 113.70   |
| 1   | L50   | 827  | U    | C2'-C3'-O3' | -8.93  | 100.31      | 113.70   |
| 1   | L50   | 1416 | A    | C4'-C3'-O3' | -8.87  | 99.70       | 113.00   |
| 1   | K50   | 95   | C    | C2'-C3'-O3' | -8.86  | 100.41      | 113.70   |
| 1   | L50   | 95   | C    | C2'-C3'-O3' | -8.84  | 100.44      | 113.70   |
| 1   | K50   | 1416 | A    | C4'-C3'-O3' | -8.84  | 99.74       | 113.00   |
| 42  | R60   | 262  | U    | C2'-C3'-O3' | 8.81   | 126.91      | 113.70   |
| 1   | K50   | 1277 | G    | C2'-C3'-O3' | 8.80   | 126.91      | 113.70   |
| 1   | L50   | 1277 | G    | C2'-C3'-O3' | 8.78   | 126.88      | 113.70   |
| 42  | S60   | 262  | U    | C2'-C3'-O3' | 8.76   | 126.84      | 113.70   |
| 42  | R60   | 917  | U    | P-O3'-C3'   | -8.62  | 107.26      | 120.20   |
| 42  | S60   | 917  | U    | P-O3'-C3'   | -8.58  | 107.33      | 120.20   |
| 1   | K50   | 1192 | A    | C2'-C3'-O3' | 8.53   | 126.50      | 113.70   |
| 1   | L50   | 1192 | A    | C2'-C3'-O3' | 8.53   | 126.49      | 113.70   |
| 42  | S60   | 1108 | C    | P-O3'-C3'   | -8.52  | 107.42      | 120.20   |
| 42  | R60   | 127  | A    | C2'-C3'-O3' | 8.51   | 126.46      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42  | S60   | 127  | A    | C2'-C3'-O3' | 8.50  | 126.45      | 113.70   |
| 1   | L50   | 600  | G    | O4'-C1'-C2' | -8.49 | 99.11       | 107.60   |
| 1   | K50   | 600  | G    | O4'-C1'-C2' | -8.49 | 99.11       | 107.60   |
| 1   | K50   | 600  | G    | C1'-C2'-O2' | 8.48  | 121.12      | 108.40   |
| 42  | R60   | 996  | G    | P-O3'-C3'   | -8.48 | 107.49      | 120.20   |
| 1   | L50   | 600  | G    | C1'-C2'-O2' | 8.47  | 121.11      | 108.40   |
| 42  | R60   | 1108 | C    | P-O3'-C3'   | -8.47 | 107.49      | 120.20   |
| 42  | S60   | 996  | G    | P-O3'-C3'   | -8.47 | 107.50      | 120.20   |
| 42  | S60   | 383  | A    | C2'-C3'-O3' | 8.44  | 126.36      | 113.70   |
| 42  | R60   | 383  | A    | C2'-C3'-O3' | 8.41  | 126.31      | 113.70   |
| 1   | K50   | 1277 | G    | C4'-C3'-O3' | 8.33  | 125.50      | 113.00   |
| 42  | R60   | 1033 | A    | P-O3'-C3'   | -8.33 | 107.71      | 120.20   |
| 42  | S60   | 1033 | A    | P-O3'-C3'   | -8.32 | 107.72      | 120.20   |
| 1   | L50   | 1277 | G    | C4'-C3'-O3' | 8.32  | 125.48      | 113.00   |
| 42  | S60   | 1261 | G    | P-O3'-C3'   | -8.29 | 107.76      | 120.20   |
| 42  | R60   | 1261 | G    | P-O3'-C3'   | -8.26 | 107.81      | 120.20   |
| 42  | S60   | 958  | A    | P-O3'-C3'   | -8.19 | 107.91      | 120.20   |
| 42  | S60   | 965  | U    | P-O3'-C3'   | -8.18 | 107.92      | 120.20   |
| 42  | R60   | 958  | A    | P-O3'-C3'   | -8.18 | 107.93      | 120.20   |
| 1   | L50   | 1966 | A    | C2'-C3'-O3' | 8.18  | 125.96      | 113.70   |
| 42  | R60   | 965  | U    | P-O3'-C3'   | -8.17 | 107.95      | 120.20   |
| 1   | K50   | 1966 | A    | C2'-C3'-O3' | 8.15  | 125.92      | 113.70   |
| 1   | L50   | 395  | A    | C4'-C3'-O3' | -8.09 | 97.27       | 109.40   |
| 1   | K50   | 395  | A    | C4'-C3'-O3' | -8.09 | 97.27       | 109.40   |
| 2   | L70   | 63   | A    | C4'-C3'-O3' | 8.06  | 121.49      | 109.40   |
| 2   | K70   | 63   | A    | C4'-C3'-O3' | 8.04  | 121.47      | 109.40   |
| 42  | S60   | 262  | U    | C4'-C3'-O3' | 8.02  | 125.03      | 113.00   |
| 42  | R60   | 262  | U    | C4'-C3'-O3' | 8.02  | 125.03      | 113.00   |
| 42  | S60   | 598  | C    | C2'-C3'-O3' | 7.99  | 125.68      | 113.70   |
| 1   | K50   | 1967 | A    | C2'-C3'-O3' | 7.96  | 125.64      | 113.70   |
| 1   | K50   | 1491 | U    | C4'-C3'-O3' | 7.96  | 121.33      | 109.40   |
| 42  | R60   | 598  | C    | C2'-C3'-O3' | 7.95  | 125.63      | 113.70   |
| 42  | R60   | 964  | G    | P-O3'-C3'   | -7.95 | 108.27      | 120.20   |
| 42  | S60   | 964  | G    | P-O3'-C3'   | -7.93 | 108.30      | 120.20   |
| 42  | R60   | 565  | U    | C4'-C3'-O3' | 7.93  | 121.30      | 109.40   |
| 1   | L50   | 1967 | A    | C2'-C3'-O3' | 7.92  | 125.58      | 113.70   |
| 1   | L50   | 1491 | U    | C4'-C3'-O3' | 7.92  | 121.28      | 109.40   |
| 42  | S60   | 565  | U    | C4'-C3'-O3' | 7.90  | 121.26      | 109.40   |
| 42  | R60   | 956  | C    | P-O3'-C3'   | -7.85 | 108.43      | 120.20   |
| 42  | S60   | 956  | C    | P-O3'-C3'   | -7.82 | 108.47      | 120.20   |
| 1   | K50   | 778  | A    | C2'-C3'-O3' | -7.78 | 102.03      | 113.70   |
| 42  | S60   | 845  | G    | P-O3'-C3'   | -7.77 | 108.54      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42  | R60   | 845  | G    | P-O3'-C3'   | -7.77 | 108.55      | 120.20   |
| 1   | L50   | 778  | A    | C2'-C3'-O3' | -7.75 | 102.07      | 113.70   |
| 1   | L50   | 1614 | G    | C1'-C2'-O2' | -7.75 | 96.78       | 108.40   |
| 1   | L50   | 1394 | U    | C2'-C3'-O3' | 7.72  | 125.28      | 113.70   |
| 68  | RT0   | 117  | VAL  | CA-CB-CG1   | 7.70  | 123.49      | 110.40   |
| 1   | K50   | 1394 | U    | C2'-C3'-O3' | 7.69  | 125.24      | 113.70   |
| 68  | ST0   | 117  | VAL  | CA-CB-CG1   | 7.68  | 123.45      | 110.40   |
| 42  | S60   | 995  | A    | P-O3'-C3'   | -7.57 | 108.84      | 120.20   |
| 42  | R60   | 995  | A    | P-O3'-C3'   | -7.57 | 108.84      | 120.20   |
| 1   | K50   | 1838 | G    | O4'-C1'-C2' | -7.55 | 98.25       | 105.80   |
| 42  | R60   | 1260 | G    | P-O3'-C3'   | -7.55 | 108.88      | 120.20   |
| 42  | S60   | 1260 | G    | P-O3'-C3'   | -7.54 | 108.89      | 120.20   |
| 42  | S60   | 998  | U    | P-O3'-C3'   | -7.52 | 108.92      | 120.20   |
| 1   | L50   | 1838 | G    | O4'-C1'-C2' | -7.52 | 98.28       | 105.80   |
| 1   | K50   | 21   | U    | C2'-C3'-O3' | 7.51  | 124.97      | 113.70   |
| 42  | R60   | 923  | A    | P-O3'-C3'   | -7.51 | 108.94      | 120.20   |
| 1   | L50   | 21   | U    | C2'-C3'-O3' | 7.50  | 124.95      | 113.70   |
| 73  | SY0   | 37   | ASN  | CB-CA-C     | 7.49  | 125.33      | 110.42   |
| 42  | S60   | 923  | A    | P-O3'-C3'   | -7.49 | 108.97      | 120.20   |
| 42  | R60   | 998  | U    | P-O3'-C3'   | -7.49 | 108.97      | 120.20   |
| 73  | RY0   | 37   | ASN  | CB-CA-C     | 7.46  | 125.27      | 110.42   |
| 42  | S60   | 994  | G    | C4'-C3'-C2' | -7.39 | 95.21       | 102.60   |
| 42  | R60   | 824  | A    | P-O3'-C3'   | -7.38 | 109.12      | 120.20   |
| 42  | R60   | 994  | G    | C4'-C3'-C2' | -7.38 | 95.22       | 102.60   |
| 42  | S60   | 824  | A    | P-O3'-C3'   | -7.37 | 109.14      | 120.20   |
| 1   | L50   | 1585 | U    | P-O3'-C3'   | -7.35 | 109.18      | 120.20   |
| 1   | K50   | 399  | G    | C2'-C3'-O3' | 7.34  | 120.51      | 109.50   |
| 1   | L50   | 399  | G    | C2'-C3'-O3' | 7.32  | 120.48      | 109.50   |
| 1   | K50   | 1585 | U    | P-O3'-C3'   | -7.31 | 109.24      | 120.20   |
| 42  | R60   | 961  | G    | P-O3'-C3'   | -7.30 | 109.25      | 120.20   |
| 2   | K70   | 45   | U    | C2'-C3'-O3' | -7.29 | 102.76      | 113.70   |
| 42  | S60   | 961  | G    | P-O3'-C3'   | -7.29 | 109.27      | 120.20   |
| 5   | KB0   | 335  | LYS  | CB-CA-C     | 7.28  | 117.04      | 109.83   |
| 5   | LB0   | 335  | LYS  | CB-CA-C     | 7.28  | 117.04      | 109.83   |
| 42  | R60   | 724  | A    | C2'-C3'-O3' | -7.27 | 102.79      | 113.70   |
| 1   | K50   | 1709 | G    | C3'-C2'-O2' | -7.27 | 103.70      | 114.60   |
| 1   | L50   | 1709 | G    | C3'-C2'-O2' | -7.26 | 103.70      | 114.60   |
| 42  | S60   | 724  | A    | C2'-C3'-O3' | -7.26 | 102.81      | 113.70   |
| 2   | L70   | 45   | U    | C2'-C3'-O3' | -7.26 | 102.82      | 113.70   |
| 1   | K50   | 562  | U    | P-O5'-C5'   | -7.25 | 110.03      | 120.90   |
| 1   | L50   | 562  | U    | P-O5'-C5'   | -7.23 | 110.05      | 120.90   |
| 1   | L50   | 535  | A    | P-O3'-C3'   | 7.23  | 131.04      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42  | S60   | 1170 | G    | C1'-O4'-C4' | -7.21 | 102.69      | 109.90   |
| 1   | K50   | 535  | A    | P-O3'-C3'   | 7.21  | 131.01      | 120.20   |
| 42  | R60   | 1170 | G    | C1'-O4'-C4' | -7.20 | 102.70      | 109.90   |
| 1   | K50   | 1837 | A    | C2'-C3'-O3' | 7.16  | 120.24      | 109.50   |
| 26  | LN0   | 116  | PHE  | CA-CB-CG    | 7.15  | 120.95      | 113.80   |
| 1   | L50   | 1837 | A    | C2'-C3'-O3' | 7.13  | 120.19      | 109.50   |
| 1   | K50   | 1134 | A    | C2'-C3'-O3' | 7.13  | 124.39      | 113.70   |
| 26  | KN0   | 116  | PHE  | CA-CB-CG    | 7.11  | 120.91      | 113.80   |
| 1   | L50   | 1134 | A    | C2'-C3'-O3' | 7.08  | 124.31      | 113.70   |
| 1   | L50   | 395  | A    | C2'-C3'-O3' | 7.05  | 120.07      | 109.50   |
| 1   | K50   | 395  | A    | C2'-C3'-O3' | 7.02  | 120.03      | 109.50   |
| 1   | K50   | 283  | U    | C4'-C3'-O3' | -7.01 | 102.48      | 113.00   |
| 1   | L50   | 283  | U    | C4'-C3'-O3' | -7.00 | 102.50      | 113.00   |
| 1   | K50   | 1831 | G    | C2'-C3'-O3' | -6.98 | 103.23      | 113.70   |
| 1   | L50   | 1831 | G    | C2'-C3'-O3' | -6.98 | 103.24      | 113.70   |
| 1   | K50   | 1705 | U    | C4'-C3'-O3' | 6.96  | 119.84      | 109.40   |
| 1   | K50   | 642  | G    | C2'-C3'-O3' | -6.96 | 103.27      | 113.70   |
| 1   | K50   | 2418 | U    | C4'-C3'-O3' | -6.96 | 102.56      | 113.00   |
| 1   | L50   | 2418 | U    | C4'-C3'-O3' | -6.95 | 102.57      | 113.00   |
| 42  | S60   | 997  | A    | P-O3'-C3'   | -6.95 | 109.77      | 120.20   |
| 1   | L50   | 642  | G    | C2'-C3'-O3' | -6.95 | 103.28      | 113.70   |
| 42  | S60   | 831  | G    | P-O3'-C3'   | -6.94 | 109.79      | 120.20   |
| 56  | SGG   | 166  | VAL  | CA-CB-CG1   | 6.93  | 122.19      | 110.40   |
| 42  | R60   | 831  | G    | P-O3'-C3'   | -6.93 | 109.80      | 120.20   |
| 1   | L50   | 1705 | U    | C4'-C3'-O3' | 6.93  | 119.80      | 109.40   |
| 42  | R60   | 997  | A    | P-O3'-C3'   | -6.93 | 109.81      | 120.20   |
| 56  | RGG   | 166  | VAL  | CA-CB-CG1   | 6.92  | 122.17      | 110.40   |
| 42  | R60   | 1048 | G    | C4'-C3'-C2' | -6.91 | 95.69       | 102.60   |
| 42  | S60   | 1048 | G    | C4'-C3'-C2' | -6.91 | 95.69       | 102.60   |
| 42  | R60   | 109  | U    | C2'-C3'-O3' | -6.89 | 103.36      | 113.70   |
| 42  | S60   | 1107 | U    | P-O3'-C3'   | -6.88 | 109.89      | 120.20   |
| 42  | S60   | 109  | U    | C2'-C3'-O3' | -6.86 | 103.41      | 113.70   |
| 42  | R60   | 1107 | U    | P-O3'-C3'   | -6.85 | 109.92      | 120.20   |
| 37  | LW0   | 27   | ASP  | CB-CA-C     | 6.85  | 120.39      | 110.04   |
| 37  | KW0   | 27   | ASP  | CB-CA-C     | 6.83  | 120.35      | 110.04   |
| 42  | R60   | 1150 | G    | P-O3'-C3'   | -6.81 | 109.99      | 120.20   |
| 50  | RDD   | 39   | VAL  | CA-CB-CG1   | 6.81  | 121.97      | 110.40   |
| 42  | S60   | 1150 | G    | P-O3'-C3'   | -6.80 | 109.99      | 120.20   |
| 53  | SF0   | 17   | PRO  | N-CA-C      | 6.80  | 122.83      | 113.65   |
| 50  | SDD   | 39   | VAL  | CA-CB-CG1   | 6.79  | 121.94      | 110.40   |
| 1   | K50   | 2357 | U    | C2'-C3'-O3' | -6.77 | 103.54      | 113.70   |
| 1   | L50   | 2357 | U    | C2'-C3'-O3' | -6.76 | 103.56      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42  | S60   | 1167 | C    | P-O3'-C3'   | -6.76 | 110.06      | 120.20   |
| 1   | L50   | 1942 | U    | C2'-C3'-O3' | 6.75  | 119.63      | 109.50   |
| 42  | R60   | 1135 | U    | C3'-C2'-C1' | -6.75 | 94.55       | 101.30   |
| 53  | RF0   | 17   | PRO  | N-CA-C      | 6.75  | 122.77      | 113.65   |
| 1   | L50   | 14   | G    | C4'-C3'-O3' | -6.75 | 102.88      | 113.00   |
| 42  | S60   | 1168 | A    | P-O3'-C3'   | -6.74 | 110.09      | 120.20   |
| 42  | S60   | 1135 | U    | C3'-C2'-C1' | -6.73 | 94.57       | 101.30   |
| 1   | L50   | 535  | A    | C4'-C3'-O3' | 6.73  | 119.50      | 109.40   |
| 42  | R60   | 1167 | C    | P-O3'-C3'   | -6.73 | 110.10      | 120.20   |
| 1   | K50   | 14   | G    | C4'-C3'-O3' | -6.73 | 102.91      | 113.00   |
| 1   | K50   | 535  | A    | C4'-C3'-O3' | 6.72  | 119.49      | 109.40   |
| 1   | K50   | 1942 | U    | C2'-C3'-O3' | 6.72  | 119.59      | 109.50   |
| 42  | R60   | 1168 | A    | P-O3'-C3'   | -6.72 | 110.11      | 120.20   |
| 42  | R60   | 1174 | G    | C3'-C2'-C1' | 6.67  | 107.97      | 101.30   |
| 42  | R60   | 1231 | U    | P-O3'-C3'   | -6.67 | 110.20      | 120.20   |
| 42  | S60   | 1231 | U    | P-O3'-C3'   | -6.66 | 110.22      | 120.20   |
| 1   | K50   | 1709 | G    | C1'-C2'-O2' | -6.64 | 101.83      | 111.80   |
| 42  | S60   | 1174 | G    | C3'-C2'-C1' | 6.63  | 107.93      | 101.30   |
| 42  | S60   | 1176 | G    | O4'-C4'-C3' | 6.62  | 110.62      | 104.00   |
| 42  | S60   | 1125 | G    | C3'-C2'-C1' | -6.61 | 94.69       | 101.30   |
| 1   | K50   | 1000 | G    | C3'-C2'-O2' | -6.60 | 104.70      | 114.60   |
| 42  | R60   | 1125 | G    | C3'-C2'-C1' | -6.60 | 94.70       | 101.30   |
| 57  | SH0   | 107  | PHE  | CA-CB-CG    | -6.60 | 107.20      | 113.80   |
| 1   | L50   | 1709 | G    | C1'-C2'-O2' | -6.60 | 101.91      | 111.80   |
| 1   | L50   | 1000 | G    | C3'-C2'-O2' | -6.58 | 104.73      | 114.60   |
| 57  | RH0   | 107  | PHE  | CA-CB-CG    | -6.57 | 107.23      | 113.80   |
| 42  | R60   | 1176 | G    | O4'-C4'-C3' | 6.55  | 110.55      | 104.00   |
| 52  | REE   | 49   | VAL  | CA-CB-CG1   | 6.54  | 121.51      | 110.40   |
| 1   | L50   | 663  | G    | C2'-C3'-O3' | -6.53 | 103.90      | 113.70   |
| 1   | K50   | 2531 | U    | C4'-C3'-O3' | -6.53 | 103.20      | 113.00   |
| 42  | R60   | 1038 | A    | C4'-C3'-C2' | -6.53 | 96.07       | 102.60   |
| 42  | R60   | 1023 | A    | P-O3'-C3'   | -6.53 | 110.41      | 120.20   |
| 42  | S60   | 1038 | A    | C4'-C3'-C2' | -6.53 | 96.07       | 102.60   |
| 1   | L50   | 2531 | U    | C4'-C3'-O3' | -6.52 | 103.23      | 113.00   |
| 42  | S60   | 1023 | A    | P-O3'-C3'   | -6.51 | 110.43      | 120.20   |
| 52  | SEE   | 49   | VAL  | CA-CB-CG1   | 6.50  | 121.45      | 110.40   |
| 1   | K50   | 663  | G    | C2'-C3'-O3' | -6.50 | 103.95      | 113.70   |
| 1   | L50   | 2265 | U    | C2'-C3'-O3' | -6.49 | 103.97      | 113.70   |
| 47  | SC0   | 129  | ARG  | CB-CA-C     | -6.49 | 98.21       | 108.91   |
| 1   | L50   | 562  | U    | C5'-C4'-C3' | -6.48 | 106.28      | 116.00   |
| 47  | RC0   | 129  | ARG  | CB-CA-C     | -6.48 | 98.22       | 108.91   |
| 42  | R60   | 1135 | U    | C4'-C3'-O3' | 6.48  | 122.72      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42  | S60   | 1135 | U    | C4'-C3'-O3' | 6.47  | 122.71      | 113.00   |
| 1   | K50   | 2265 | U    | C2'-C3'-O3' | -6.46 | 104.00      | 113.70   |
| 1   | L50   | 1709 | G    | C2'-C3'-O3' | -6.45 | 99.83       | 109.50   |
| 1   | K50   | 562  | U    | C5'-C4'-C3' | -6.45 | 106.33      | 116.00   |
| 1   | K50   | 1709 | G    | C2'-C3'-O3' | -6.44 | 99.84       | 109.50   |
| 1   | L50   | 2451 | U    | C2'-C3'-O3' | -6.42 | 104.07      | 113.70   |
| 42  | S60   | 1021 | A    | C4'-C3'-O3' | -6.42 | 99.77       | 109.40   |
| 42  | R60   | 1021 | A    | C4'-C3'-O3' | -6.42 | 99.78       | 109.40   |
| 1   | K50   | 1942 | U    | C1'-C2'-O2' | -6.41 | 102.19      | 111.80   |
| 2   | K70   | 91   | C    | C2'-C3'-O3' | -6.41 | 104.09      | 113.70   |
| 1   | L50   | 1942 | U    | C1'-C2'-O2' | -6.41 | 102.19      | 111.80   |
| 1   | K50   | 2451 | U    | C2'-C3'-O3' | -6.41 | 104.09      | 113.70   |
| 1   | K50   | 1709 | G    | C1'-O4'-C4' | -6.40 | 103.30      | 109.70   |
| 42  | R60   | 1202 | U    | C4'-C3'-O3' | -6.40 | 103.40      | 113.00   |
| 1   | K50   | 629  | C    | C4'-C3'-O3' | -6.40 | 103.40      | 113.00   |
| 40  | LZ0   | 69   | ARG  | CB-CG-CD    | 6.40  | 126.01      | 111.30   |
| 42  | R60   | 1043 | G    | P-O3'-C3'   | -6.39 | 110.61      | 120.20   |
| 2   | L70   | 91   | C    | C2'-C3'-O3' | -6.38 | 104.13      | 113.70   |
| 1   | L50   | 629  | C    | C4'-C3'-O3' | -6.38 | 103.43      | 113.00   |
| 42  | S60   | 1043 | G    | P-O3'-C3'   | -6.38 | 110.64      | 120.20   |
| 42  | S60   | 1202 | U    | C4'-C3'-O3' | -6.37 | 103.44      | 113.00   |
| 42  | R60   | 1041 | A    | P-O3'-C3'   | -6.37 | 110.64      | 120.20   |
| 40  | KZ0   | 69   | ARG  | CB-CG-CD    | 6.37  | 125.95      | 111.30   |
| 42  | S60   | 1041 | A    | P-O3'-C3'   | -6.37 | 110.65      | 120.20   |
| 69  | RU0   | 45   | PHE  | CA-CB-CG    | 6.36  | 120.16      | 113.80   |
| 1   | L50   | 2114 | G    | C4'-C3'-C2' | -6.35 | 96.25       | 102.60   |
| 72  | SX0   | 83   | PRO  | N-CA-C      | 6.35  | 122.55      | 113.47   |
| 1   | K50   | 2114 | G    | C4'-C3'-C2' | -6.35 | 96.25       | 102.60   |
| 1   | L50   | 1709 | G    | C1'-O4'-C4' | -6.34 | 103.36      | 109.70   |
| 1   | K50   | 1445 | U    | C4'-C3'-O3' | 6.34  | 118.91      | 109.40   |
| 42  | S60   | 1356 | C    | O5'-P-OP1   | -6.33 | 89.00       | 108.00   |
| 42  | R60   | 1356 | C    | O5'-P-OP1   | -6.33 | 89.00       | 108.00   |
| 42  | S60   | 1216 | U    | P-O3'-C3'   | -6.33 | 110.71      | 120.20   |
| 42  | R60   | 1216 | U    | P-O3'-C3'   | -6.32 | 110.72      | 120.20   |
| 6   | LC0   | 223  | ASP  | CA-CB-CG    | 6.32  | 118.92      | 112.60   |
| 72  | RX0   | 83   | PRO  | N-CA-C      | 6.31  | 122.50      | 113.47   |
| 69  | SU0   | 45   | PHE  | CA-CB-CG    | 6.31  | 120.11      | 113.80   |
| 1   | L50   | 1445 | U    | C4'-C3'-O3' | 6.30  | 118.85      | 109.40   |
| 1   | L50   | 1102 | G    | O4'-C1'-C2' | -6.28 | 99.52       | 105.80   |
| 6   | KC0   | 223  | ASP  | CA-CB-CG    | 6.28  | 118.88      | 112.60   |
| 1   | K50   | 1000 | G    | C1'-O4'-C4' | -6.27 | 103.43      | 109.70   |
| 1   | K50   | 1102 | G    | O4'-C1'-C2' | -6.27 | 99.53       | 105.80   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | L50   | 1000 | G    | C1'-O4'-C4' | -6.25 | 103.45      | 109.70   |
| 42  | R60   | 914  | U    | C4'-C3'-O3' | 6.25  | 118.78      | 109.40   |
| 8   | LD0   | 78   | ASP  | CA-CB-CG    | 6.23  | 118.83      | 112.60   |
| 42  | S60   | 914  | U    | C4'-C3'-O3' | 6.22  | 118.74      | 109.40   |
| 69  | RU0   | 105  | PHE  | CA-CB-CG    | 6.22  | 120.02      | 113.80   |
| 69  | SU0   | 105  | PHE  | CA-CB-CG    | 6.21  | 120.01      | 113.80   |
| 42  | S60   | 944  | G    | P-O3'-C3'   | -6.21 | 110.89      | 120.20   |
| 42  | R60   | 944  | G    | P-O3'-C3'   | -6.21 | 110.89      | 120.20   |
| 8   | KD0   | 78   | ASP  | CA-CB-CG    | 6.20  | 118.80      | 112.60   |
| 64  | RO0   | 54   | ASP  | CA-CB-CG    | 6.20  | 118.80      | 112.60   |
| 1   | L50   | 225  | G    | C2'-C3'-O3' | 6.19  | 122.98      | 113.70   |
| 42  | S60   | 960  | U    | P-O3'-C3'   | -6.18 | 110.93      | 120.20   |
| 64  | SO0   | 54   | ASP  | CA-CB-CG    | 6.17  | 118.77      | 112.60   |
| 42  | R60   | 960  | U    | P-O3'-C3'   | -6.15 | 110.97      | 120.20   |
| 12  | LF0   | 193  | PHE  | CA-CB-CG    | 6.15  | 119.95      | 113.80   |
| 1   | K50   | 225  | G    | C2'-C3'-O3' | 6.14  | 122.92      | 113.70   |
| 1   | K50   | 1835 | G    | P-O5'-C5'   | -6.14 | 111.69      | 120.90   |
| 12  | KF0   | 193  | PHE  | CA-CB-CG    | 6.14  | 119.94      | 113.80   |
| 42  | S60   | 966  | G    | P-O3'-C3'   | -6.13 | 111.00      | 120.20   |
| 42  | R60   | 966  | G    | P-O3'-C3'   | -6.13 | 111.00      | 120.20   |
| 1   | L50   | 1835 | G    | P-O5'-C5'   | -6.13 | 111.71      | 120.90   |
| 42  | R60   | 1103 | G    | O4'-C1'-C2' | -6.13 | 99.67       | 105.80   |
| 42  | S60   | 1103 | G    | O4'-C1'-C2' | -6.12 | 99.68       | 105.80   |
| 1   | K50   | 645  | U    | C4'-C3'-O3' | 6.11  | 118.56      | 109.40   |
| 1   | L50   | 645  | U    | C4'-C3'-O3' | 6.10  | 118.55      | 109.40   |
| 1   | L50   | 729  | A    | C1'-C2'-O2' | -6.09 | 99.27       | 108.40   |
| 6   | KC0   | 57   | ARG  | CG-CD-NE    | -6.09 | 98.61       | 112.00   |
| 6   | LC0   | 57   | ARG  | CG-CD-NE    | -6.09 | 98.61       | 112.00   |
| 1   | K50   | 115  | A    | C2'-C3'-O3' | -6.09 | 104.57      | 113.70   |
| 26  | KN0   | 131  | GLU  | CB-CG-CD    | 6.08  | 122.94      | 112.60   |
| 1   | L50   | 115  | A    | C2'-C3'-O3' | -6.07 | 104.59      | 113.70   |
| 26  | LN0   | 131  | GLU  | CB-CG-CD    | 6.07  | 122.91      | 112.60   |
| 1   | K50   | 1534 | G    | C2'-C3'-O3' | -6.06 | 104.61      | 113.70   |
| 42  | R60   | 1230 | U    | P-O3'-C3'   | -6.06 | 111.11      | 120.20   |
| 42  | S60   | 1230 | U    | P-O3'-C3'   | -6.05 | 111.12      | 120.20   |
| 1   | L50   | 1534 | G    | C2'-C3'-O3' | -6.05 | 104.62      | 113.70   |
| 1   | K50   | 729  | A    | C1'-C2'-O2' | -6.05 | 99.32       | 108.40   |
| 1   | L50   | 1098 | A    | C4'-C3'-O3' | -6.05 | 103.93      | 113.00   |
| 1   | K50   | 1098 | A    | C4'-C3'-O3' | -6.03 | 103.95      | 113.00   |
| 42  | S60   | 118  | G    | C4'-C3'-O3' | 6.03  | 118.44      | 109.40   |
| 6   | LC0   | 87   | ALA  | N-CA-C      | 6.02  | 118.73      | 108.67   |
| 1   | K50   | 665  | A    | C4'-C3'-O3' | 6.02  | 118.43      | 109.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | L50   | 665  | A    | C4'-C3'-O3' | 6.01  | 118.42      | 109.40   |
| 6   | KC0   | 87   | ALA  | N-CA-C      | 6.01  | 118.71      | 108.67   |
| 42  | R60   | 1125 | G    | C2'-C3'-O3' | 6.01  | 122.71      | 113.70   |
| 42  | S60   | 1125 | G    | C2'-C3'-O3' | 6.00  | 122.70      | 113.70   |
| 1   | L50   | 1212 | G    | C4'-C3'-O3' | -6.00 | 104.00      | 113.00   |
| 47  | RC0   | 221  | VAL  | CA-CB-CG1   | 6.00  | 120.60      | 110.40   |
| 47  | SC0   | 221  | VAL  | CA-CB-CG1   | 6.00  | 120.59      | 110.40   |
| 51  | RE0   | 151  | ASP  | CA-CB-CG    | 5.99  | 118.59      | 112.60   |
| 22  | KL0   | 67   | ARG  | CG-CD-NE    | 5.99  | 125.18      | 112.00   |
| 22  | LL0   | 67   | ARG  | CG-CD-NE    | 5.98  | 125.16      | 112.00   |
| 42  | R60   | 118  | G    | C4'-C3'-O3' | 5.98  | 118.37      | 109.40   |
| 1   | K50   | 2499 | U    | C2'-C3'-O3' | -5.98 | 104.73      | 113.70   |
| 1   | L50   | 725  | A    | O3'-P-O5'   | -5.97 | 95.04       | 104.00   |
| 1   | L50   | 2499 | U    | C2'-C3'-O3' | -5.97 | 104.74      | 113.70   |
| 1   | L50   | 342  | G    | C2'-C3'-O3' | -5.97 | 104.75      | 113.70   |
| 51  | SE0   | 151  | ASP  | CA-CB-CG    | 5.97  | 118.57      | 112.60   |
| 55  | RG0   | 56   | ASP  | CA-CB-CG    | 5.97  | 118.57      | 112.60   |
| 1   | K50   | 1212 | G    | C4'-C3'-O3' | -5.97 | 104.05      | 113.00   |
| 42  | R60   | 830  | G    | P-O3'-C3'   | -5.96 | 111.25      | 120.20   |
| 1   | K50   | 61   | A    | C4'-C3'-O3' | -5.96 | 104.06      | 113.00   |
| 1   | K50   | 725  | A    | O3'-P-O5'   | -5.96 | 95.06       | 104.00   |
| 37  | LW0   | 27   | ASP  | CA-CB-CG    | 5.96  | 118.56      | 112.60   |
| 42  | S60   | 830  | G    | P-O3'-C3'   | -5.96 | 111.27      | 120.20   |
| 1   | L50   | 2419 | G    | C2'-C3'-O3' | 5.95  | 118.43      | 109.50   |
| 1   | K50   | 342  | G    | C2'-C3'-O3' | -5.95 | 104.77      | 113.70   |
| 42  | R60   | 477  | G    | C2'-C3'-O3' | -5.94 | 104.79      | 113.70   |
| 1   | L50   | 667  | G    | C4'-C3'-O3' | 5.94  | 121.91      | 113.00   |
| 1   | L50   | 1414 | U    | C2'-C3'-O3' | 5.94  | 118.41      | 109.50   |
| 1   | L50   | 61   | A    | C4'-C3'-O3' | -5.93 | 104.10      | 113.00   |
| 42  | S60   | 477  | G    | C2'-C3'-O3' | -5.93 | 104.80      | 113.70   |
| 42  | S60   | 1186 | G    | C3'-C2'-C1' | -5.93 | 95.56       | 101.50   |
| 1   | K50   | 1819 | A    | C2'-C3'-O3' | -5.93 | 104.81      | 113.70   |
| 42  | R60   | 1186 | G    | C3'-C2'-C1' | -5.93 | 95.57       | 101.50   |
| 42  | R60   | 1194 | U    | C4'-C3'-O3' | -5.93 | 104.11      | 113.00   |
| 1   | K50   | 1414 | U    | C2'-C3'-O3' | 5.92  | 118.39      | 109.50   |
| 1   | K50   | 2419 | G    | C2'-C3'-O3' | 5.92  | 118.38      | 109.50   |
| 37  | KW0   | 27   | ASP  | CA-CB-CG    | 5.92  | 118.52      | 112.60   |
| 55  | SG0   | 56   | ASP  | CA-CB-CG    | 5.91  | 118.51      | 112.60   |
| 42  | S60   | 1194 | U    | C4'-C3'-O3' | -5.91 | 104.14      | 113.00   |
| 1   | K50   | 667  | G    | C4'-C3'-O3' | 5.91  | 121.86      | 113.00   |
| 1   | L50   | 1819 | A    | C2'-C3'-O3' | -5.90 | 104.86      | 113.70   |
| 5   | KB0   | 336  | ARG  | CG-CD-NE    | 5.89  | 124.95      | 112.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 10  | KE0   | 22   | ASP  | CA-C-N      | 5.88  | 123.94      | 120.24   |
| 10  | KE0   | 22   | ASP  | C-N-CA      | 5.88  | 123.94      | 120.24   |
| 5   | LB0   | 336  | ARG  | CG-CD-NE    | 5.87  | 124.92      | 112.00   |
| 1   | L50   | 805  | A    | C2'-C3'-O3' | -5.87 | 104.89      | 113.70   |
| 42  | R60   | 1286 | G    | C4'-C3'-O3' | -5.87 | 104.20      | 113.00   |
| 42  | S60   | 1286 | G    | C4'-C3'-O3' | -5.86 | 104.21      | 113.00   |
| 42  | S60   | 894  | A    | P-O3'-C3'   | -5.85 | 111.42      | 120.20   |
| 1   | K50   | 805  | A    | C2'-C3'-O3' | -5.85 | 104.92      | 113.70   |
| 42  | R60   | 894  | A    | P-O3'-C3'   | -5.85 | 111.43      | 120.20   |
| 1   | L50   | 742  | G    | C4'-C3'-O3' | -5.85 | 100.63      | 109.40   |
| 1   | L50   | 552  | C    | C2'-C3'-O3' | -5.84 | 104.93      | 113.70   |
| 10  | LE0   | 22   | ASP  | CA-C-N      | 5.84  | 123.92      | 120.24   |
| 10  | LE0   | 22   | ASP  | C-N-CA      | 5.84  | 123.92      | 120.24   |
| 1   | K50   | 552  | C    | C2'-C3'-O3' | -5.84 | 104.93      | 113.70   |
| 1   | L50   | 805  | A    | O3'-P-O5'   | -5.84 | 95.24       | 104.00   |
| 26  | LN0   | 123  | GLN  | CB-CA-C     | -5.83 | 97.91       | 110.45   |
| 1   | K50   | 805  | A    | O3'-P-O5'   | -5.83 | 95.25       | 104.00   |
| 62  | SM0   | 91   | PHE  | CA-CB-CG    | 5.83  | 119.63      | 113.80   |
| 1   | K50   | 742  | G    | C4'-C3'-O3' | -5.82 | 100.67      | 109.40   |
| 26  | KN0   | 123  | GLN  | CB-CA-C     | -5.82 | 97.95       | 110.45   |
| 42  | S60   | 1134 | G    | P-O3'-C3'   | -5.81 | 111.48      | 120.20   |
| 42  | R60   | 955  | A    | C4'-C3'-C2' | -5.81 | 96.79       | 102.60   |
| 42  | S60   | 563  | A    | C2'-C3'-O3' | -5.81 | 104.99      | 113.70   |
| 42  | R60   | 563  | A    | C2'-C3'-O3' | -5.81 | 104.99      | 113.70   |
| 42  | R60   | 1134 | G    | P-O3'-C3'   | -5.80 | 111.49      | 120.20   |
| 1   | K50   | 280  | G    | C4'-C3'-C2' | -5.80 | 96.80       | 102.60   |
| 1   | K50   | 1074 | G    | C2'-C3'-O3' | 5.80  | 122.39      | 113.70   |
| 1   | L50   | 1967 | A    | C4'-C3'-O3' | 5.79  | 121.69      | 113.00   |
| 1   | L50   | 1262 | A    | C4'-C3'-O3' | -5.79 | 104.32      | 113.00   |
| 1   | L50   | 1074 | G    | C2'-C3'-O3' | 5.78  | 122.37      | 113.70   |
| 22  | KL0   | 8    | PRO  | N-CA-C      | 5.78  | 124.38      | 112.47   |
| 62  | RM0   | 91   | PHE  | CA-CB-CG    | 5.77  | 119.57      | 113.80   |
| 1   | K50   | 1262 | A    | C4'-C3'-O3' | -5.77 | 104.35      | 113.00   |
| 22  | LL0   | 8    | PRO  | N-CA-C      | 5.77  | 124.35      | 112.47   |
| 1   | L50   | 280  | G    | C4'-C3'-C2' | -5.76 | 96.84       | 102.60   |
| 1   | K50   | 1967 | A    | C4'-C3'-O3' | 5.76  | 121.64      | 113.00   |
| 42  | R60   | 918  | A    | P-O3'-C3'   | -5.76 | 111.56      | 120.20   |
| 69  | SU0   | 67   | ARG  | CG-CD-NE    | 5.75  | 124.64      | 112.00   |
| 42  | S60   | 918  | A    | P-O3'-C3'   | -5.74 | 111.59      | 120.20   |
| 69  | RU0   | 67   | ARG  | CG-CD-NE    | 5.74  | 124.62      | 112.00   |
| 42  | S60   | 222  | G    | C4'-C3'-C2' | -5.73 | 96.87       | 102.60   |
| 42  | R60   | 819  | A    | P-O3'-C3'   | 5.73  | 128.79      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | L50   | 147  | G    | P-O3'-C3'   | -5.73 | 111.61      | 120.20   |
| 15  | LGG   | 24   | ARG  | CG-CD-NE    | -5.73 | 99.40       | 112.00   |
| 42  | S60   | 963  | G    | P-O3'-C3'   | -5.73 | 111.61      | 120.20   |
| 1   | K50   | 1303 | G    | C4'-C3'-C2' | -5.72 | 96.88       | 102.60   |
| 1   | K50   | 2074 | A    | C2'-C3'-O3' | -5.72 | 105.11      | 113.70   |
| 15  | KGG   | 24   | ARG  | CG-CD-NE    | -5.72 | 99.41       | 112.00   |
| 42  | S60   | 955  | A    | C4'-C3'-C2' | -5.72 | 96.88       | 102.60   |
| 42  | R60   | 963  | G    | P-O3'-C3'   | -5.71 | 111.63      | 120.20   |
| 42  | S60   | 262  | U    | O4'-C4'-C3' | -5.71 | 98.29       | 104.00   |
| 42  | S60   | 819  | A    | P-O3'-C3'   | 5.71  | 128.76      | 120.20   |
| 1   | L50   | 1303 | G    | C4'-C3'-C2' | -5.70 | 96.90       | 102.60   |
| 1   | L50   | 2373 | G    | C4'-C3'-C2' | -5.70 | 96.90       | 102.60   |
| 42  | R60   | 222  | G    | C4'-C3'-C2' | -5.69 | 96.91       | 102.60   |
| 42  | S60   | 960  | U    | C4'-C3'-C2' | -5.69 | 96.91       | 102.60   |
| 1   | L50   | 2074 | A    | C2'-C3'-O3' | -5.68 | 105.17      | 113.70   |
| 1   | L50   | 586  | G    | C4'-C3'-O3' | 5.68  | 117.92      | 109.40   |
| 1   | K50   | 147  | G    | P-O3'-C3'   | -5.68 | 111.68      | 120.20   |
| 1   | K50   | 1627 | U    | C2'-C3'-O3' | -5.68 | 105.18      | 113.70   |
| 1   | L50   | 1627 | U    | C2'-C3'-O3' | -5.68 | 105.18      | 113.70   |
| 42  | R60   | 262  | U    | O4'-C4'-C3' | -5.68 | 98.32       | 104.00   |
| 1   | K50   | 2373 | G    | C4'-C3'-C2' | -5.68 | 96.92       | 102.60   |
| 42  | S60   | 111  | A    | C2'-C3'-O3' | -5.67 | 105.19      | 113.70   |
| 1   | K50   | 1400 | A    | C2'-C3'-O3' | 5.67  | 118.01      | 109.50   |
| 42  | R60   | 960  | U    | C4'-C3'-C2' | -5.67 | 96.93       | 102.60   |
| 1   | L50   | 1277 | G    | C4'-C3'-C2' | -5.67 | 96.93       | 102.60   |
| 1   | K50   | 659  | G    | C2'-C3'-O3' | 5.67  | 118.00      | 109.50   |
| 18  | KI0   | 173  | PHE  | CA-CB-CG    | 5.67  | 119.47      | 113.80   |
| 18  | LI0   | 173  | PHE  | CA-CB-CG    | 5.66  | 119.46      | 113.80   |
| 27  | LO0   | 45   | PRO  | CB-CA-C     | -5.66 | 103.98      | 111.23   |
| 1   | K50   | 586  | G    | C4'-C3'-O3' | 5.66  | 117.89      | 109.40   |
| 1   | K50   | 1317 | G    | P-O3'-C3'   | -5.66 | 111.71      | 120.20   |
| 1   | L50   | 1981 | G    | C4'-C3'-O3' | -5.66 | 104.51      | 113.00   |
| 1   | K50   | 1981 | G    | C4'-C3'-O3' | -5.66 | 104.51      | 113.00   |
| 1   | L50   | 1317 | G    | P-O3'-C3'   | -5.66 | 111.71      | 120.20   |
| 1   | K50   | 1277 | G    | C4'-C3'-C2' | -5.66 | 96.94       | 102.60   |
| 1   | K50   | 1192 | A    | N9-C1'-C2'  | 5.65  | 120.48      | 112.00   |
| 42  | R60   | 111  | A    | C2'-C3'-O3' | -5.65 | 105.22      | 113.70   |
| 1   | L50   | 659  | G    | C2'-C3'-O3' | 5.65  | 117.97      | 109.50   |
| 21  | KJJ   | 21   | ARG  | NE-CZ-NH2   | 5.65  | 124.28      | 119.20   |
| 1   | K50   | 884  | G    | C4'-C3'-O3' | -5.65 | 104.53      | 113.00   |
| 51  | RE0   | 212  | ASP  | CA-CB-CG    | 5.64  | 118.24      | 112.60   |
| 1   | L50   | 1400 | A    | C2'-C3'-O3' | 5.64  | 117.96      | 109.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 12  | KF0   | 89   | ARG  | CB-CG-CD    | 5.64  | 124.27      | 111.30   |
| 1   | L50   | 1192 | A    | N9-C1'-C2'  | 5.63  | 120.45      | 112.00   |
| 27  | KO0   | 45   | PRO  | CB-CA-C     | -5.62 | 104.03      | 111.23   |
| 1   | L50   | 567  | A    | C2'-C3'-O3' | 5.62  | 117.93      | 109.50   |
| 1   | K50   | 1614 | G    | C3'-C2'-O2' | -5.62 | 106.18      | 114.60   |
| 1   | K50   | 725  | A    | C2'-C3'-O3' | -5.61 | 105.28      | 113.70   |
| 12  | LF0   | 89   | ARG  | CB-CG-CD    | 5.61  | 124.20      | 111.30   |
| 42  | S60   | 1102 | A    | C2'-C3'-O3' | -5.61 | 105.29      | 113.70   |
| 1   | L50   | 884  | G    | C4'-C3'-O3' | -5.61 | 104.59      | 113.00   |
| 1   | K50   | 567  | A    | C2'-C3'-O3' | 5.60  | 117.91      | 109.50   |
| 21  | LJJ   | 21   | ARG  | NE-CZ-NH2   | 5.60  | 124.24      | 119.20   |
| 42  | S60   | 340  | A    | C4'-C3'-O3' | -5.59 | 104.61      | 113.00   |
| 42  | R60   | 1102 | A    | C2'-C3'-O3' | -5.59 | 105.32      | 113.70   |
| 42  | S60   | 933  | G    | C2'-C3'-O3' | -5.58 | 105.33      | 113.70   |
| 1   | K50   | 1499 | U    | C2'-C3'-O3' | 5.58  | 122.07      | 113.70   |
| 42  | S60   | 854  | U    | P-O3'-C3'   | -5.58 | 111.83      | 120.20   |
| 42  | S60   | 1005 | G    | C4'-C3'-C2' | -5.58 | 97.02       | 102.60   |
| 42  | R60   | 213  | A    | P-O3'-C3'   | -5.58 | 111.84      | 120.20   |
| 1   | L50   | 725  | A    | C2'-C3'-O3' | -5.57 | 105.34      | 113.70   |
| 1   | L50   | 1499 | U    | C2'-C3'-O3' | 5.57  | 122.06      | 113.70   |
| 42  | R60   | 1153 | C    | P-O3'-C3'   | -5.57 | 111.84      | 120.20   |
| 51  | SE0   | 212  | ASP  | CA-CB-CG    | 5.57  | 118.17      | 112.60   |
| 1   | K50   | 2447 | A    | P-O5'-C5'   | -5.57 | 112.54      | 120.90   |
| 42  | R60   | 933  | G    | C2'-C3'-O3' | -5.57 | 105.34      | 113.70   |
| 53  | RF0   | 17   | PRO  | CB-CA-C     | -5.57 | 103.52      | 112.21   |
| 1   | L50   | 2447 | A    | P-O5'-C5'   | -5.56 | 112.56      | 120.90   |
| 42  | R60   | 340  | A    | C4'-C3'-O3' | -5.56 | 104.66      | 113.00   |
| 42  | S60   | 213  | A    | P-O3'-C3'   | -5.56 | 111.86      | 120.20   |
| 1   | L50   | 2012 | G    | O3'-P-O5'   | -5.55 | 95.67       | 104.00   |
| 27  | LO0   | 65   | PRO  | CB-CA-C     | -5.55 | 103.96      | 111.85   |
| 1   | K50   | 2168 | G    | C2'-C3'-O3' | -5.55 | 105.37      | 113.70   |
| 42  | R60   | 842  | C    | C4'-C3'-O3' | -5.55 | 104.67      | 113.00   |
| 1   | L50   | 1684 | C    | C2'-C3'-O3' | -5.55 | 105.37      | 113.70   |
| 42  | S60   | 1153 | C    | P-O3'-C3'   | -5.55 | 111.88      | 120.20   |
| 27  | KO0   | 65   | PRO  | CB-CA-C     | -5.55 | 103.97      | 111.85   |
| 1   | L50   | 1783 | A    | P-O3'-C3'   | -5.54 | 111.89      | 120.20   |
| 53  | SF0   | 17   | PRO  | CB-CA-C     | -5.54 | 103.56      | 112.21   |
| 1   | K50   | 1684 | C    | C2'-C3'-O3' | -5.54 | 105.39      | 113.70   |
| 1   | K50   | 1783 | A    | P-O3'-C3'   | -5.54 | 111.89      | 120.20   |
| 42  | R60   | 854  | U    | P-O3'-C3'   | -5.54 | 111.89      | 120.20   |
| 1   | L50   | 385  | C    | C2'-C3'-O3' | -5.54 | 105.39      | 113.70   |
| 1   | L50   | 814  | G    | C4'-C3'-O3' | -5.54 | 104.69      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | K50   | 385  | C    | C2'-C3'-O3' | -5.54 | 105.39      | 113.70   |
| 1   | K50   | 2012 | G    | O3'-P-O5'   | -5.54 | 95.69       | 104.00   |
| 42  | S60   | 842  | C    | C4'-C3'-O3' | -5.54 | 104.69      | 113.00   |
| 42  | S60   | 1215 | A    | C3'-C2'-O2' | 5.54  | 119.00      | 110.70   |
| 42  | R60   | 1005 | G    | C4'-C3'-C2' | -5.53 | 97.07       | 102.60   |
| 1   | L50   | 2168 | G    | C2'-C3'-O3' | -5.53 | 105.41      | 113.70   |
| 1   | K50   | 814  | G    | C4'-C3'-O3' | -5.53 | 104.71      | 113.00   |
| 42  | R60   | 1215 | A    | C3'-C2'-O2' | 5.52  | 118.98      | 110.70   |
| 63  | RN0   | 5    | TYR  | CB-CA-C     | 5.52  | 118.82      | 109.55   |
| 11  | KEE   | 46   | ASP  | CA-CB-CG    | 5.51  | 118.11      | 112.60   |
| 1   | L50   | 151  | G    | C4'-C3'-O3' | 5.51  | 117.66      | 109.40   |
| 42  | R60   | 1243 | C    | C4'-C3'-O3' | -5.51 | 104.74      | 113.00   |
| 63  | SN0   | 5    | TYR  | CB-CA-C     | 5.50  | 118.78      | 109.55   |
| 39  | LY0   | 53   | ASP  | CB-CA-C     | 5.49  | 120.69      | 109.76   |
| 42  | S60   | 1243 | C    | C4'-C3'-O3' | -5.49 | 104.77      | 113.00   |
| 2   | L70   | 46   | C    | P-O3'-C3'   | -5.48 | 111.97      | 120.20   |
| 1   | K50   | 151  | G    | C4'-C3'-O3' | 5.48  | 117.62      | 109.40   |
| 15  | KGG   | 58   | ARG  | CB-CA-C     | 5.48  | 117.33      | 109.11   |
| 39  | KY0   | 53   | ASP  | CB-CA-C     | 5.48  | 120.67      | 109.76   |
| 2   | K70   | 86   | G    | C4'-C3'-C2' | -5.47 | 97.12       | 102.60   |
| 48  | SCC   | 60   | HIS  | CA-C-N      | 5.47  | 128.37      | 120.38   |
| 48  | SCC   | 60   | HIS  | C-N-CA      | 5.47  | 128.37      | 120.38   |
| 58  | RI0   | 166  | PHE  | CA-CB-CG    | 5.47  | 119.27      | 113.80   |
| 20  | KJ0   | 115  | PRO  | N-CA-C      | 5.47  | 120.95      | 113.84   |
| 2   | L70   | 86   | G    | C4'-C3'-C2' | -5.46 | 97.14       | 102.60   |
| 42  | R60   | 903  | C    | P-O3'-C3'   | -5.46 | 112.01      | 120.20   |
| 11  | LEE   | 46   | ASP  | CA-CB-CG    | 5.45  | 118.05      | 112.60   |
| 42  | S60   | 903  | C    | P-O3'-C3'   | -5.45 | 112.02      | 120.20   |
| 58  | SI0   | 166  | PHE  | CA-CB-CG    | 5.45  | 119.25      | 113.80   |
| 20  | LJ0   | 115  | PRO  | N-CA-C      | 5.44  | 120.91      | 113.84   |
| 15  | LGG   | 58   | ARG  | CB-CA-C     | 5.44  | 117.27      | 109.11   |
| 48  | RCC   | 60   | HIS  | CA-C-N      | 5.44  | 128.32      | 120.38   |
| 48  | RCC   | 60   | HIS  | C-N-CA      | 5.44  | 128.32      | 120.38   |
| 2   | K70   | 46   | C    | P-O3'-C3'   | -5.44 | 112.05      | 120.20   |
| 42  | R60   | 911  | G    | C2'-C3'-O3' | -5.43 | 105.55      | 113.70   |
| 42  | S60   | 911  | G    | C2'-C3'-O3' | -5.43 | 105.55      | 113.70   |
| 1   | L50   | 1984 | U    | C4'-C3'-O3' | -5.43 | 104.86      | 113.00   |
| 42  | S60   | 263  | A    | C5'-C4'-C3' | -5.43 | 107.86      | 116.00   |
| 43  | SA0   | 50   | ASP  | CA-CB-CG    | 5.42  | 118.02      | 112.60   |
| 1   | L50   | 2203 | C    | C2'-C3'-O3' | -5.42 | 105.58      | 113.70   |
| 1   | K50   | 2203 | C    | C2'-C3'-O3' | -5.42 | 105.58      | 113.70   |
| 69  | RU0   | 56   | VAL  | CA-CB-CG1   | 5.42  | 119.61      | 110.40   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 2   | K70   | 31   | G    | C4'-C3'-O3' | -5.42 | 104.88      | 113.00   |
| 1   | K50   | 141  | G    | O4'-C1'-C2' | -5.41 | 100.39      | 105.80   |
| 1   | K50   | 1984 | U    | C4'-C3'-O3' | -5.41 | 104.88      | 113.00   |
| 42  | R60   | 263  | A    | C5'-C4'-C3' | -5.41 | 107.88      | 116.00   |
| 43  | RA0   | 50   | ASP  | CA-CB-CG    | 5.41  | 118.01      | 112.60   |
| 2   | L70   | 31   | G    | C4'-C3'-O3' | -5.41 | 104.88      | 113.00   |
| 30  | LPP   | 8    | VAL  | CA-CB-CG1   | 5.41  | 119.60      | 110.40   |
| 42  | S60   | 109  | U    | O3'-P-O5'   | -5.41 | 95.88       | 104.00   |
| 42  | S60   | 803  | C    | C2'-C3'-O3' | -5.41 | 105.58      | 113.70   |
| 65  | RQ0   | 38   | VAL  | CA-CB-CG1   | 5.41  | 119.59      | 110.40   |
| 1   | L50   | 141  | G    | O4'-C1'-C2' | -5.40 | 100.40      | 105.80   |
| 42  | R60   | 109  | U    | O3'-P-O5'   | -5.40 | 95.90       | 104.00   |
| 1   | L50   | 1007 | C    | C2'-C3'-O3' | -5.40 | 105.60      | 113.70   |
| 1   | K50   | 392  | C    | C2'-C3'-O3' | -5.40 | 105.60      | 113.70   |
| 30  | KPP   | 8    | VAL  | CA-CB-CG1   | 5.40  | 119.58      | 110.40   |
| 1   | K50   | 1983 | U    | C2'-C3'-O3' | -5.39 | 105.61      | 113.70   |
| 42  | R60   | 1356 | C    | O4'-C4'-C3' | -5.39 | 100.71      | 106.10   |
| 42  | R60   | 803  | C    | C2'-C3'-O3' | -5.39 | 105.62      | 113.70   |
| 1   | L50   | 392  | C    | C2'-C3'-O3' | -5.39 | 105.62      | 113.70   |
| 65  | SQ0   | 38   | VAL  | CA-CB-CG1   | 5.39  | 119.56      | 110.40   |
| 42  | R60   | 1164 | G    | C2'-C3'-O3' | -5.39 | 105.62      | 113.70   |
| 42  | S60   | 1164 | G    | C2'-C3'-O3' | -5.38 | 105.63      | 113.70   |
| 1   | L50   | 42   | G    | C4'-C3'-C2' | -5.38 | 97.22       | 102.60   |
| 69  | SU0   | 56   | VAL  | CA-CB-CG1   | 5.38  | 119.54      | 110.40   |
| 42  | R60   | 1041 | A    | C2'-C3'-O3' | -5.38 | 105.63      | 113.70   |
| 1   | L50   | 449  | U    | C4'-C3'-O3' | -5.38 | 104.93      | 113.00   |
| 1   | K50   | 1733 | A    | N9-C1'-C2'  | 5.38  | 120.06      | 112.00   |
| 1   | L50   | 2194 | U    | C2'-C3'-O3' | -5.37 | 105.64      | 113.70   |
| 1   | K50   | 1007 | C    | C2'-C3'-O3' | -5.37 | 105.64      | 113.70   |
| 1   | L50   | 1983 | U    | C2'-C3'-O3' | -5.37 | 105.64      | 113.70   |
| 30  | LPP   | 49   | ARG  | CG-CD-NE    | 5.37  | 123.81      | 112.00   |
| 1   | K50   | 1414 | U    | P-O5'-C5'   | -5.37 | 112.85      | 120.90   |
| 1   | L50   | 1733 | A    | N9-C1'-C2'  | 5.36  | 120.05      | 112.00   |
| 1   | K50   | 75   | C    | C2'-C3'-O3' | 5.36  | 121.74      | 113.70   |
| 1   | K50   | 449  | U    | C4'-C3'-O3' | -5.36 | 104.96      | 113.00   |
| 42  | S60   | 1356 | C    | O4'-C4'-C3' | -5.36 | 100.74      | 106.10   |
| 1   | K50   | 42   | G    | C4'-C3'-C2' | -5.36 | 97.25       | 102.60   |
| 1   | L50   | 75   | C    | C2'-C3'-O3' | 5.35  | 121.73      | 113.70   |
| 1   | K50   | 342  | G    | P-O3'-C3'   | -5.35 | 112.17      | 120.20   |
| 1   | L50   | 1414 | U    | P-O5'-C5'   | -5.35 | 112.87      | 120.90   |
| 30  | KPP   | 49   | ARG  | CG-CD-NE    | 5.35  | 123.77      | 112.00   |
| 1   | L50   | 342  | G    | P-O3'-C3'   | -5.35 | 112.18      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | K50   | 1942 | U    | C3'-C2'-O2' | 5.35  | 122.62      | 114.60   |
| 65  | RQ0   | 38   | VAL  | CB-CA-C     | 5.35  | 115.66      | 110.63   |
| 1   | L50   | 734  | G    | C4'-C3'-O3' | -5.34 | 104.98      | 113.00   |
| 1   | L50   | 1942 | U    | C3'-C2'-O2' | 5.34  | 122.61      | 114.60   |
| 1   | K50   | 2194 | U    | C2'-C3'-O3' | -5.34 | 105.69      | 113.70   |
| 42  | R60   | 822  | A    | C3'-C2'-O2' | 5.34  | 118.71      | 110.70   |
| 65  | SQ0   | 38   | VAL  | CB-CA-C     | 5.33  | 115.64      | 110.63   |
| 1   | K50   | 1298 | A    | C5'-C4'-C3' | -5.33 | 108.00      | 116.00   |
| 42  | S60   | 1041 | A    | C2'-C3'-O3' | -5.33 | 105.71      | 113.70   |
| 1   | K50   | 1234 | U    | N1-C1'-C2'  | 5.33  | 119.99      | 112.00   |
| 1   | L50   | 630  | U    | C4'-C3'-O3' | 5.33  | 117.39      | 109.40   |
| 1   | K50   | 535  | A    | C1'-C2'-O2' | -5.32 | 103.82      | 111.80   |
| 2   | L70   | 42   | A    | C2'-C3'-O3' | -5.32 | 105.72      | 113.70   |
| 1   | K50   | 92   | C    | C2'-C3'-O3' | -5.32 | 105.72      | 113.70   |
| 1   | K50   | 734  | G    | C4'-C3'-O3' | -5.32 | 105.02      | 113.00   |
| 42  | S60   | 822  | A    | C3'-C2'-O2' | 5.31  | 118.67      | 110.70   |
| 1   | L50   | 535  | A    | C1'-C2'-O2' | -5.31 | 103.83      | 111.80   |
| 2   | K70   | 42   | A    | C2'-C3'-O3' | -5.31 | 105.74      | 113.70   |
| 1   | L50   | 1234 | U    | N1-C1'-C2'  | 5.31  | 119.96      | 112.00   |
| 51  | RE0   | 88   | ASP  | CA-CB-CG    | 5.31  | 117.91      | 112.60   |
| 1   | L50   | 2422 | G    | C2'-C3'-O3' | 5.31  | 121.66      | 113.70   |
| 1   | L50   | 337  | A    | C5'-C4'-C3' | -5.30 | 108.05      | 116.00   |
| 1   | L50   | 1298 | A    | C5'-C4'-C3' | -5.30 | 108.05      | 116.00   |
| 1   | L50   | 92   | C    | C2'-C3'-O3' | -5.30 | 105.75      | 113.70   |
| 42  | S60   | 1145 | G    | C4'-C3'-O3' | -5.30 | 105.05      | 113.00   |
| 61  | SL0   | 76   | PRO  | N-CA-C      | 5.30  | 120.73      | 113.84   |
| 1   | L50   | 1432 | G    | C2'-C3'-O3' | -5.30 | 105.75      | 113.70   |
| 1   | K50   | 337  | A    | C5'-C4'-C3' | -5.30 | 108.05      | 116.00   |
| 8   | LD0   | 121  | LEU  | CA-C-N      | 5.29  | 127.63      | 120.38   |
| 8   | LD0   | 121  | LEU  | C-N-CA      | 5.29  | 127.63      | 120.38   |
| 51  | SE0   | 239  | THR  | CA-C-N      | 5.29  | 127.63      | 120.38   |
| 51  | SE0   | 239  | THR  | C-N-CA      | 5.29  | 127.63      | 120.38   |
| 1   | K50   | 1432 | G    | C2'-C3'-O3' | -5.29 | 105.76      | 113.70   |
| 51  | RE0   | 239  | THR  | CA-C-N      | 5.29  | 127.63      | 120.38   |
| 51  | RE0   | 239  | THR  | C-N-CA      | 5.29  | 127.63      | 120.38   |
| 42  | S60   | 692  | C    | C2'-C3'-O3' | -5.29 | 105.77      | 113.70   |
| 8   | KD0   | 121  | LEU  | CA-C-N      | 5.29  | 127.62      | 120.38   |
| 8   | KD0   | 121  | LEU  | C-N-CA      | 5.29  | 127.62      | 120.38   |
| 42  | S60   | 201  | G    | P-O3'-C3'   | -5.28 | 112.27      | 120.20   |
| 1   | K50   | 2355 | A    | C4'-C3'-O3' | -5.28 | 105.08      | 113.00   |
| 42  | R60   | 601  | G    | C4'-C3'-C2' | -5.28 | 97.32       | 102.60   |
| 61  | RL0   | 76   | PRO  | N-CA-C      | 5.28  | 120.71      | 113.84   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | K50   | 2422 | G    | C2'-C3'-O3' | 5.28  | 121.62      | 113.70   |
| 42  | S60   | 601  | G    | C4'-C3'-C2' | -5.28 | 97.32       | 102.60   |
| 51  | SE0   | 88   | ASP  | CA-CB-CG    | 5.27  | 117.87      | 112.60   |
| 1   | K50   | 630  | U    | C4'-C3'-O3' | 5.27  | 117.31      | 109.40   |
| 1   | L50   | 2332 | G    | C4'-C3'-C2' | -5.27 | 97.33       | 102.60   |
| 1   | L50   | 2355 | A    | C4'-C3'-O3' | -5.27 | 105.09      | 113.00   |
| 56  | SGG   | 106  | ASP  | CA-CB-CG    | 5.27  | 117.87      | 112.60   |
| 1   | L50   | 1293 | A    | C5'-C4'-C3' | -5.26 | 108.10      | 116.00   |
| 42  | R60   | 850  | G    | C4'-C3'-C2' | -5.26 | 97.34       | 102.60   |
| 56  | RGG   | 106  | ASP  | CA-CB-CG    | 5.26  | 117.86      | 112.60   |
| 1   | L50   | 1608 | U    | C4'-C3'-O3' | -5.26 | 105.11      | 113.00   |
| 1   | K50   | 739  | A    | C5'-C4'-C3' | -5.26 | 108.11      | 116.00   |
| 1   | K50   | 1293 | A    | C5'-C4'-C3' | -5.26 | 108.11      | 116.00   |
| 1   | L50   | 1608 | U    | C2'-C3'-O3' | -5.26 | 105.81      | 113.70   |
| 1   | K50   | 323  | G    | C4'-C3'-C2' | -5.26 | 97.34       | 102.60   |
| 1   | K50   | 1608 | U    | C2'-C3'-O3' | -5.26 | 105.81      | 113.70   |
| 1   | K50   | 2332 | G    | C4'-C3'-C2' | -5.26 | 97.34       | 102.60   |
| 42  | R60   | 1106 | G    | C4'-C3'-O3' | -5.26 | 105.11      | 113.00   |
| 1   | L50   | 739  | A    | C5'-C4'-C3' | -5.26 | 108.11      | 116.00   |
| 42  | R60   | 1145 | G    | C4'-C3'-O3' | -5.26 | 105.11      | 113.00   |
| 1   | K50   | 1796 | C    | C4'-C3'-O3' | -5.25 | 105.12      | 113.00   |
| 42  | R60   | 275  | G    | C4'-C3'-C2' | -5.25 | 97.35       | 102.60   |
| 1   | L50   | 2457 | U    | C2'-C3'-O3' | -5.25 | 105.82      | 113.70   |
| 1   | L50   | 1182 | A    | P-O3'-C3'   | 5.25  | 128.07      | 120.20   |
| 42  | S60   | 275  | G    | C4'-C3'-C2' | -5.25 | 97.35       | 102.60   |
| 1   | K50   | 1608 | U    | C4'-C3'-O3' | -5.25 | 105.13      | 113.00   |
| 1   | L50   | 323  | G    | C4'-C3'-C2' | -5.25 | 97.36       | 102.60   |
| 42  | R60   | 692  | C    | C2'-C3'-O3' | -5.24 | 105.84      | 113.70   |
| 42  | R60   | 1012 | A    | C4'-C3'-C2' | -5.24 | 97.36       | 102.60   |
| 42  | S60   | 1106 | G    | C4'-C3'-O3' | -5.24 | 105.14      | 113.00   |
| 1   | L50   | 1796 | C    | C4'-C3'-O3' | -5.24 | 105.14      | 113.00   |
| 1   | K50   | 2457 | U    | C2'-C3'-O3' | -5.24 | 105.85      | 113.70   |
| 42  | S60   | 850  | G    | C4'-C3'-C2' | -5.23 | 97.37       | 102.60   |
| 42  | S60   | 1012 | A    | C4'-C3'-C2' | -5.23 | 97.37       | 102.60   |
| 42  | R60   | 201  | G    | P-O3'-C3'   | -5.23 | 112.36      | 120.20   |
| 63  | SN0   | 86   | GLU  | CB-CG-CD    | 5.23  | 121.49      | 112.60   |
| 42  | R60   | 773  | U    | C2'-C3'-O3' | -5.23 | 105.86      | 113.70   |
| 42  | S60   | 1111 | A    | C4'-C3'-O3' | -5.22 | 105.17      | 113.00   |
| 42  | R60   | 1111 | A    | C4'-C3'-O3' | -5.22 | 105.18      | 113.00   |
| 1   | K50   | 208  | C    | C2'-C3'-O3' | 5.21  | 117.32      | 109.50   |
| 1   | L50   | 208  | C    | C2'-C3'-O3' | 5.21  | 117.31      | 109.50   |
| 42  | S60   | 425  | G    | C2'-C3'-O3' | -5.21 | 101.69      | 109.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 63  | RN0   | 86   | GLU  | CB-CG-CD    | 5.21  | 121.45      | 112.60   |
| 1   | L50   | 1263 | A    | C3'-C2'-O2' | 5.21  | 118.51      | 110.70   |
| 1   | L50   | 1602 | G    | C4'-C3'-C2' | -5.21 | 97.39       | 102.60   |
| 42  | S60   | 773  | U    | C2'-C3'-O3' | -5.20 | 105.89      | 113.70   |
| 1   | K50   | 596  | G    | C4'-C3'-C2' | -5.20 | 97.40       | 102.60   |
| 42  | R60   | 1125 | G    | C3'-C2'-O2' | 5.20  | 118.50      | 110.70   |
| 1   | K50   | 1182 | A    | P-O3'-C3'   | 5.20  | 128.00      | 120.20   |
| 42  | R60   | 425  | G    | C2'-C3'-O3' | -5.20 | 101.70      | 109.50   |
| 42  | S60   | 441  | G    | C4'-C3'-C2' | -5.20 | 97.40       | 102.60   |
| 33  | KS0   | 87   | ASP  | CA-CB-CG    | 5.19  | 117.79      | 112.60   |
| 1   | L50   | 1575 | G    | C4'-C3'-C2' | -5.18 | 97.42       | 102.60   |
| 42  | R60   | 1021 | A    | O4'-C4'-C3' | -5.18 | 100.92      | 106.10   |
| 33  | LS0   | 87   | ASP  | CA-CB-CG    | 5.18  | 117.78      | 112.60   |
| 56  | SGG   | 23   | PRO  | N-CA-C      | 5.18  | 118.47      | 111.22   |
| 1   | K50   | 1575 | G    | C4'-C3'-C2' | -5.17 | 97.42       | 102.60   |
| 1   | K50   | 1263 | A    | C3'-C2'-O2' | 5.17  | 118.45      | 110.70   |
| 1   | K50   | 2315 | G    | C4'-C3'-C2' | -5.17 | 97.43       | 102.60   |
| 42  | S60   | 1218 | U    | C4'-C3'-O3' | -5.17 | 105.25      | 113.00   |
| 1   | K50   | 1602 | G    | C4'-C3'-C2' | -5.17 | 97.43       | 102.60   |
| 42  | S60   | 895  | C    | P-O3'-C3'   | -5.17 | 112.45      | 120.20   |
| 42  | R60   | 441  | G    | C4'-C3'-C2' | -5.17 | 97.44       | 102.60   |
| 1   | K50   | 690  | U    | C4'-C3'-C2' | -5.16 | 97.44       | 102.60   |
| 42  | S60   | 1125 | G    | C3'-C2'-O2' | 5.16  | 118.44      | 110.70   |
| 42  | S60   | 1021 | A    | O4'-C4'-C3' | -5.16 | 100.94      | 106.10   |
| 1   | K50   | 33   | G    | C2'-C3'-O3' | -5.16 | 105.96      | 113.70   |
| 42  | R60   | 1218 | U    | C4'-C3'-O3' | -5.16 | 105.26      | 113.00   |
| 1   | L50   | 2315 | G    | C4'-C3'-C2' | -5.16 | 97.44       | 102.60   |
| 10  | LE0   | 91   | ASP  | CA-CB-CG    | 5.15  | 117.75      | 112.60   |
| 1   | L50   | 33   | G    | C2'-C3'-O3' | -5.15 | 105.97      | 113.70   |
| 1   | L50   | 596  | G    | C4'-C3'-C2' | -5.15 | 97.45       | 102.60   |
| 1   | L50   | 690  | U    | C4'-C3'-C2' | -5.15 | 97.45       | 102.60   |
| 42  | R60   | 1053 | A    | C3'-C2'-O2' | 5.15  | 118.42      | 110.70   |
| 1   | K50   | 1073 | U    | C2'-C3'-O3' | -5.15 | 105.98      | 113.70   |
| 10  | KE0   | 91   | ASP  | CA-CB-CG    | 5.15  | 117.75      | 112.60   |
| 41  | MD2   | 101  | GLN  | OE1-CD-NE2  | -5.15 | 117.45      | 122.60   |
| 42  | R60   | 895  | C    | P-O3'-C3'   | -5.15 | 112.48      | 120.20   |
| 42  | S60   | 263  | A    | C4'-C3'-O3' | -5.14 | 105.28      | 113.00   |
| 1   | K50   | 739  | A    | C2'-C3'-O3' | 5.14  | 121.41      | 113.70   |
| 1   | L50   | 1073 | U    | C2'-C3'-O3' | -5.14 | 106.00      | 113.70   |
| 1   | K50   | 2412 | C    | P-O5'-C5'   | -5.13 | 113.20      | 120.90   |
| 42  | R60   | 238  | A    | C4'-C3'-O3' | -5.13 | 105.30      | 113.00   |
| 1   | L50   | 149  | A    | C4'-C3'-O3' | -5.13 | 105.30      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 42  | R60   | 459  | G    | C4'-C3'-C2' | -5.13 | 97.47       | 102.60   |
| 1   | L50   | 1503 | A    | C4'-C3'-O3' | -5.13 | 105.31      | 113.00   |
| 1   | L50   | 2412 | C    | P-O5'-C5'   | -5.13 | 113.21      | 120.90   |
| 42  | R60   | 263  | A    | C4'-C3'-O3' | -5.13 | 105.31      | 113.00   |
| 36  | KV0   | 61   | ASP  | CA-CB-CG    | 5.12  | 117.72      | 112.60   |
| 42  | S60   | 459  | G    | C4'-C3'-C2' | -5.12 | 97.48       | 102.60   |
| 56  | RGG   | 23   | PRO  | N-CA-C      | 5.12  | 118.39      | 111.22   |
| 1   | L50   | 739  | A    | C2'-C3'-O3' | 5.12  | 121.38      | 113.70   |
| 1   | K50   | 1503 | A    | C4'-C3'-O3' | -5.12 | 105.33      | 113.00   |
| 42  | S60   | 1053 | A    | C3'-C2'-O2' | 5.11  | 118.36      | 110.70   |
| 1   | K50   | 1187 | G    | C2'-C3'-O3' | -5.11 | 106.04      | 113.70   |
| 42  | S60   | 238  | A    | C4'-C3'-O3' | -5.11 | 105.34      | 113.00   |
| 1   | K50   | 149  | A    | C4'-C3'-O3' | -5.11 | 105.34      | 113.00   |
| 1   | L50   | 797  | U    | C5'-C4'-C3' | -5.10 | 108.35      | 116.00   |
| 1   | K50   | 996  | A    | C1'-C2'-O2' | -5.10 | 104.15      | 111.80   |
| 1   | L50   | 1187 | G    | C2'-C3'-O3' | -5.10 | 106.05      | 113.70   |
| 1   | K50   | 2341 | G    | C4'-C3'-C2' | -5.09 | 97.51       | 102.60   |
| 1   | L50   | 996  | A    | C1'-C2'-O2' | -5.09 | 104.17      | 111.80   |
| 1   | L50   | 1622 | G    | C4'-C3'-C2' | -5.09 | 97.51       | 102.60   |
| 36  | LV0   | 61   | ASP  | CA-CB-CG    | 5.09  | 117.69      | 112.60   |
| 1   | K50   | 797  | U    | C5'-C4'-C3' | -5.08 | 108.37      | 116.00   |
| 34  | LT0   | 15   | PHE  | CA-CB-CG    | 5.08  | 118.88      | 113.80   |
| 1   | K50   | 994  | A    | C2'-C3'-O3' | 5.07  | 117.11      | 109.50   |
| 1   | L50   | 2341 | G    | C4'-C3'-C2' | -5.07 | 97.53       | 102.60   |
| 42  | R60   | 885  | G    | C4'-C3'-C2' | -5.07 | 97.53       | 102.60   |
| 41  | MD1   | 101  | GLN  | OE1-CD-NE2  | -5.07 | 117.53      | 122.60   |
| 1   | L50   | 994  | A    | C2'-C3'-O3' | 5.07  | 117.10      | 109.50   |
| 1   | K50   | 2234 | U    | C2'-C3'-O3' | 5.06  | 117.09      | 109.50   |
| 1   | L50   | 2350 | A    | C2'-C3'-O3' | -5.06 | 106.11      | 113.70   |
| 67  | SS0   | 25   | ASN  | N-CA-C      | -5.06 | 105.76      | 112.24   |
| 1   | L50   | 1087 | G    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 42  | S60   | 218  | A    | C2'-C3'-O3' | 5.06  | 117.09      | 109.50   |
| 1   | K50   | 1087 | G    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 1   | K50   | 1622 | G    | C4'-C3'-C2' | -5.06 | 97.54       | 102.60   |
| 1   | K50   | 2253 | C    | C2'-C3'-O3' | -5.06 | 106.11      | 113.70   |
| 1   | L50   | 1101 | A    | C4'-C3'-O3' | -5.06 | 101.81      | 109.40   |
| 1   | K50   | 2350 | A    | C2'-C3'-O3' | -5.05 | 106.12      | 113.70   |
| 1   | L50   | 697  | C    | C2'-C3'-O3' | -5.05 | 106.12      | 113.70   |
| 1   | L50   | 2234 | U    | C2'-C3'-O3' | 5.05  | 117.08      | 109.50   |
| 42  | S60   | 924  | U    | P-O3'-C3'   | -5.05 | 112.62      | 120.20   |
| 42  | R60   | 263  | A    | P-O5'-C5'   | -5.05 | 113.32      | 120.90   |
| 42  | R60   | 924  | U    | P-O3'-C3'   | -5.05 | 112.62      | 120.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | L50   | 2346 | U    | C4'-C3'-O3' | -5.05 | 101.83      | 109.40   |
| 42  | S60   | 885  | G    | C4'-C3'-C2' | -5.05 | 97.55       | 102.60   |
| 1   | K50   | 697  | C    | C2'-C3'-O3' | -5.05 | 106.13      | 113.70   |
| 1   | K50   | 1101 | A    | C4'-C3'-O3' | -5.05 | 101.83      | 109.40   |
| 1   | L50   | 1338 | U    | C2'-C3'-O3' | -5.05 | 106.13      | 113.70   |
| 42  | S60   | 263  | A    | P-O5'-C5'   | -5.05 | 113.33      | 120.90   |
| 1   | K50   | 1835 | G    | C3'-C2'-C1' | 5.04  | 106.34      | 101.30   |
| 2   | K70   | 31   | G    | P-O3'-C3'   | -5.04 | 112.63      | 120.20   |
| 42  | S60   | 889  | A    | C2'-C3'-O3' | -5.04 | 106.14      | 113.70   |
| 1   | K50   | 2346 | U    | C4'-C3'-O3' | -5.04 | 101.83      | 109.40   |
| 42  | R60   | 218  | A    | C2'-C3'-O3' | 5.04  | 117.06      | 109.50   |
| 42  | S60   | 1101 | C    | C4'-C3'-O3' | -5.04 | 105.44      | 113.00   |
| 2   | L70   | 31   | G    | P-O3'-C3'   | -5.04 | 112.64      | 120.20   |
| 1   | L50   | 885  | G    | C5'-C4'-C3' | -5.04 | 108.45      | 116.00   |
| 1   | K50   | 2019 | G    | C4'-C3'-C2' | -5.04 | 97.56       | 102.60   |
| 1   | L50   | 2019 | G    | C4'-C3'-C2' | -5.03 | 97.57       | 102.60   |
| 40  | LZ0   | 45   | PHE  | CA-CB-CG    | 5.03  | 118.83      | 113.80   |
| 1   | L50   | 1835 | G    | C3'-C2'-C1' | 5.03  | 106.33      | 101.30   |
| 1   | K50   | 1162 | U    | C1'-C2'-O2' | -5.03 | 100.85      | 108.40   |
| 1   | K50   | 1977 | G    | C2'-C3'-O3' | 5.03  | 117.05      | 109.50   |
| 1   | K50   | 2242 | G    | C2'-C3'-O3' | -5.03 | 106.15      | 113.70   |
| 34  | KT0   | 15   | PHE  | CA-CB-CG    | 5.03  | 118.83      | 113.80   |
| 42  | R60   | 1101 | C    | C4'-C3'-O3' | -5.03 | 105.46      | 113.00   |
| 1   | L50   | 1417 | A    | C4'-C3'-O3' | -5.03 | 105.46      | 113.00   |
| 1   | L50   | 2181 | A    | C4'-C3'-O3' | -5.03 | 105.46      | 113.00   |
| 42  | R60   | 889  | A    | C2'-C3'-O3' | -5.03 | 106.16      | 113.70   |
| 56  | RGG   | 261  | ASP  | CA-CB-CG    | 5.03  | 117.63      | 112.60   |
| 51  | SE0   | 141  | THR  | CA-C-N      | 5.03  | 127.27      | 120.38   |
| 51  | SE0   | 141  | THR  | C-N-CA      | 5.03  | 127.27      | 120.38   |
| 66  | RR0   | 47   | ARG  | NE-CZ-NH2   | 5.02  | 123.72      | 119.20   |
| 1   | L50   | 1162 | U    | C1'-C2'-O2' | -5.02 | 100.87      | 108.40   |
| 1   | K50   | 140  | A    | O3'-P-O5'   | -5.02 | 96.47       | 104.00   |
| 1   | K50   | 1417 | A    | C4'-C3'-O3' | -5.02 | 105.47      | 113.00   |
| 1   | K50   | 1942 | U    | O4'-C4'-C3' | -5.02 | 101.08      | 106.10   |
| 1   | K50   | 1338 | U    | C2'-C3'-O3' | -5.02 | 106.18      | 113.70   |
| 1   | L50   | 140  | A    | O3'-P-O5'   | -5.01 | 96.48       | 104.00   |
| 1   | L50   | 1977 | G    | C2'-C3'-O3' | 5.01  | 117.02      | 109.50   |
| 40  | KZ0   | 45   | PHE  | CA-CB-CG    | 5.01  | 118.81      | 113.80   |
| 1   | L50   | 2253 | C    | C2'-C3'-O3' | -5.01 | 106.18      | 113.70   |
| 42  | S60   | 254  | U    | C2'-C3'-O3' | 5.00  | 117.00      | 109.50   |
| 42  | R60   | 1024 | G    | P-O3'-C3'   | -5.00 | 112.70      | 120.20   |
| 42  | R60   | 1291 | A    | C4'-C3'-O3' | -5.00 | 105.50      | 113.00   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | L50   | 698  | U    | C4'-C3'-O3' | -5.00 | 105.50      | 113.00   |
| 1   | L50   | 2108 | U    | C4'-C3'-O3' | -5.00 | 105.50      | 113.00   |
| 1   | L50   | 2242 | G    | C2'-C3'-O3' | -5.00 | 106.20      | 113.70   |
| 1   | K50   | 885  | G    | C5'-C4'-C3' | -5.00 | 108.50      | 116.00   |
| 1   | K50   | 1773 | C    | C3'-C2'-O2' | 5.00  | 118.20      | 110.70   |
| 1   | K50   | 2181 | A    | C4'-C3'-O3' | -5.00 | 105.50      | 113.00   |
| 42  | R60   | 959  | G    | P-O3'-C3'   | -5.00 | 112.70      | 120.20   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 6   | KC0   | 87  | ALA  | Peptide |
| 13  | KFF   | 101 | ILE  | Peptide |
| 15  | KGG   | 77  | GLY  | Peptide |
| 6   | LC0   | 87  | ALA  | Peptide |
| 13  | LFF   | 101 | ILE  | Peptide |
| 15  | LGG   | 77  | GLY  | 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   | K50   | 53655 | 0        | 26955    | 123     | 0            |
| 1   | L50   | 53655 | 0        | 26955    | 123     | 0            |
| 2   | K70   | 2542  | 0        | 1282     | 9       | 0            |
| 2   | L70   | 2542  | 0        | 1282     | 8       | 0            |
| 3   | KA0   | 1889  | 0        | 1985     | 12      | 0            |
| 3   | LA0   | 1889  | 0        | 1985     | 12      | 0            |
| 4   | KAA   | 1167  | 0        | 1214     | 7       | 0            |
| 4   | LAA   | 1167  | 0        | 1214     | 6       | 0            |
| 5   | KB0   | 3039  | 0        | 3183     | 5       | 0            |
| 5   | LB0   | 3039  | 0        | 3183     | 6       | 0            |
| 6   | KC0   | 2604  | 0        | 2638     | 12      | 0            |
| 6   | LC0   | 2604  | 0        | 2638     | 11      | 0            |
| 7   | KCC   | 781   | 0        | 803      | 2       | 0            |
| 7   | LCC   | 781   | 0        | 803      | 2       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 8   | KD0   | 2298  | 0        | 2384     | 7       | 0            |
| 8   | LD0   | 2298  | 0        | 2384     | 8       | 0            |
| 9   | KDD   | 895   | 0        | 948      | 1       | 0            |
| 9   | LDD   | 895   | 0        | 948      | 0       | 0            |
| 10  | KE0   | 1371  | 0        | 1389     | 15      | 0            |
| 10  | LE0   | 1371  | 0        | 1389     | 14      | 0            |
| 11  | KEE   | 1090  | 0        | 1173     | 11      | 0            |
| 11  | LEE   | 1090  | 0        | 1173     | 11      | 0            |
| 12  | KF0   | 1933  | 0        | 2011     | 12      | 0            |
| 12  | LF0   | 1933  | 0        | 2011     | 12      | 0            |
| 13  | KFF   | 893   | 0        | 945      | 3       | 0            |
| 13  | LFF   | 893   | 0        | 945      | 3       | 0            |
| 14  | KG0   | 1590  | 0        | 1709     | 6       | 0            |
| 14  | LG0   | 1590  | 0        | 1709     | 5       | 0            |
| 15  | KGG   | 819   | 0        | 882      | 2       | 0            |
| 15  | LGG   | 819   | 0        | 882      | 3       | 0            |
| 16  | KH0   | 1477  | 0        | 1528     | 3       | 0            |
| 16  | LH0   | 1477  | 0        | 1528     | 3       | 0            |
| 17  | KHH   | 992   | 0        | 1097     | 5       | 0            |
| 17  | LHH   | 992   | 0        | 1097     | 5       | 0            |
| 18  | KI0   | 1750  | 0        | 1797     | 2       | 0            |
| 18  | LI0   | 1750  | 0        | 1797     | 3       | 0            |
| 19  | KII   | 784   | 0        | 874      | 5       | 0            |
| 19  | LII   | 784   | 0        | 874      | 4       | 0            |
| 20  | KJ0   | 1332  | 0        | 1411     | 12      | 0            |
| 20  | LJ0   | 1332  | 0        | 1411     | 12      | 0            |
| 21  | KJJ   | 701   | 0        | 753      | 4       | 0            |
| 21  | LJJ   | 701   | 0        | 753      | 4       | 0            |
| 22  | KL0   | 1353  | 0        | 1433     | 4       | 0            |
| 22  | LL0   | 1353  | 0        | 1433     | 5       | 0            |
| 23  | KLL   | 427   | 0        | 468      | 0       | 0            |
| 23  | LLL   | 427   | 0        | 468      | 0       | 0            |
| 24  | KM0   | 927   | 0        | 961      | 4       | 0            |
| 24  | LM0   | 927   | 0        | 961      | 5       | 0            |
| 25  | KMM   | 427   | 0        | 461      | 0       | 0            |
| 25  | LMM   | 427   | 0        | 461      | 0       | 0            |
| 26  | KN0   | 1688  | 0        | 1752     | 6       | 0            |
| 26  | LN0   | 1688  | 0        | 1752     | 6       | 0            |
| 27  | KO0   | 1598  | 0        | 1681     | 5       | 0            |
| 27  | LO0   | 1598  | 0        | 1681     | 5       | 0            |
| 28  | KOO   | 801   | 0        | 886      | 3       | 0            |
| 28  | LOO   | 801   | 0        | 886      | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 29  | KP0   | 1238  | 0        | 1304     | 4       | 0            |
| 29  | LP0   | 1238  | 0        | 1304     | 3       | 0            |
| 30  | KPP   | 684   | 0        | 720      | 2       | 0            |
| 30  | LPP   | 684   | 0        | 720      | 2       | 0            |
| 31  | KQ0   | 1491  | 0        | 1587     | 6       | 0            |
| 31  | LQ0   | 1491  | 0        | 1587     | 7       | 0            |
| 32  | KR0   | 1336  | 0        | 1430     | 1       | 0            |
| 32  | LR0   | 1336  | 0        | 1430     | 0       | 0            |
| 33  | KS0   | 1400  | 0        | 1450     | 1       | 0            |
| 33  | LS0   | 1400  | 0        | 1450     | 1       | 0            |
| 34  | KT0   | 1270  | 0        | 1321     | 18      | 0            |
| 34  | LT0   | 1270  | 0        | 1321     | 18      | 0            |
| 35  | KU0   | 810   | 0        | 834      | 1       | 0            |
| 35  | LU0   | 810   | 0        | 834      | 1       | 0            |
| 36  | KV0   | 1057  | 0        | 1139     | 1       | 0            |
| 36  | LV0   | 1057  | 0        | 1139     | 1       | 0            |
| 37  | KW0   | 832   | 0        | 873      | 47      | 0            |
| 37  | LW0   | 832   | 0        | 873      | 47      | 0            |
| 38  | KX0   | 874   | 0        | 956      | 5       | 0            |
| 38  | LX0   | 874   | 0        | 956      | 5       | 0            |
| 39  | KY0   | 1048  | 0        | 1135     | 2       | 0            |
| 39  | LY0   | 1048  | 0        | 1135     | 2       | 0            |
| 40  | KZ0   | 963   | 0        | 1022     | 2       | 0            |
| 40  | LZ0   | 963   | 0        | 1022     | 2       | 0            |
| 41  | MD1   | 1229  | 0        | 1216     | 10      | 0            |
| 41  | MD2   | 1229  | 0        | 1216     | 9       | 0            |
| 42  | R60   | 29181 | 0        | 14605    | 320     | 0            |
| 42  | S60   | 29181 | 0        | 14604    | 323     | 0            |
| 43  | RA0   | 1725  | 0        | 1750     | 144     | 0            |
| 43  | SA0   | 1725  | 0        | 1750     | 140     | 0            |
| 44  | RAA   | 827   | 0        | 859      | 17      | 0            |
| 44  | SAA   | 827   | 0        | 859      | 17      | 0            |
| 45  | RB0   | 1609  | 0        | 1728     | 6       | 0            |
| 45  | SB0   | 1609  | 0        | 1728     | 6       | 0            |
| 46  | RBB   | 627   | 0        | 651      | 4       | 0            |
| 46  | SBB   | 627   | 0        | 651      | 3       | 0            |
| 47  | RC0   | 1727  | 0        | 1802     | 97      | 0            |
| 47  | SC0   | 1727  | 0        | 1802     | 95      | 0            |
| 48  | RCC   | 476   | 0        | 488      | 17      | 0            |
| 48  | SCC   | 476   | 0        | 488      | 17      | 0            |
| 49  | RD0   | 1700  | 0        | 1815     | 32      | 0            |
| 49  | SD0   | 1700  | 0        | 1815     | 32      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 50  | RDD   | 550   | 0        | 542      | 28      | 0            |
| 50  | SDD   | 550   | 0        | 542      | 30      | 0            |
| 51  | RE0   | 2044  | 0        | 2116     | 26      | 0            |
| 51  | SE0   | 2044  | 0        | 2116     | 26      | 0            |
| 52  | REE   | 447   | 0        | 483      | 1       | 0            |
| 52  | SEE   | 447   | 0        | 483      | 1       | 0            |
| 53  | RF0   | 1509  | 0        | 1604     | 39      | 0            |
| 53  | SF0   | 1509  | 0        | 1604     | 40      | 0            |
| 54  | RFF   | 417   | 0        | 402      | 42      | 0            |
| 54  | SFF   | 422   | 0        | 412      | 44      | 0            |
| 55  | RG0   | 1836  | 0        | 1972     | 41      | 0            |
| 55  | SG0   | 1836  | 0        | 1972     | 40      | 0            |
| 56  | RGG   | 2478  | 0        | 2458     | 24      | 0            |
| 56  | SGG   | 2478  | 0        | 2458     | 24      | 0            |
| 57  | RH0   | 1335  | 0        | 1356     | 2       | 0            |
| 57  | SH0   | 1335  | 0        | 1356     | 2       | 0            |
| 58  | RI0   | 1347  | 0        | 1379     | 9       | 0            |
| 58  | SI0   | 1347  | 0        | 1379     | 10      | 0            |
| 59  | RJ0   | 1379  | 0        | 1436     | 17      | 0            |
| 59  | SJ0   | 1379  | 0        | 1436     | 16      | 0            |
| 60  | RK0   | 737   | 0        | 746      | 16      | 0            |
| 60  | SK0   | 737   | 0        | 746      | 16      | 0            |
| 61  | RL0   | 1229  | 0        | 1302     | 5       | 0            |
| 61  | SL0   | 1229  | 0        | 1302     | 5       | 0            |
| 62  | RM0   | 876   | 0        | 937      | 6       | 0            |
| 62  | SM0   | 876   | 0        | 937      | 5       | 0            |
| 63  | RN0   | 1130  | 0        | 1189     | 11      | 0            |
| 63  | SN0   | 1130  | 0        | 1189     | 11      | 0            |
| 64  | RO0   | 983   | 0        | 1028     | 14      | 0            |
| 64  | SO0   | 983   | 0        | 1028     | 14      | 0            |
| 65  | RQ0   | 1143  | 0        | 1171     | 20      | 0            |
| 65  | SQ0   | 1143  | 0        | 1171     | 20      | 0            |
| 66  | RR0   | 974   | 0        | 1003     | 101     | 0            |
| 66  | SR0   | 974   | 0        | 1003     | 101     | 0            |
| 67  | RS0   | 1150  | 0        | 1207     | 35      | 0            |
| 67  | SS0   | 1150  | 0        | 1207     | 36      | 0            |
| 68  | RT0   | 1161  | 0        | 1219     | 10      | 0            |
| 68  | ST0   | 1161  | 0        | 1219     | 10      | 0            |
| 69  | RU0   | 809   | 0        | 838      | 14      | 0            |
| 69  | SU0   | 809   | 0        | 838      | 14      | 0            |
| 70  | RV0   | 521   | 0        | 525      | 73      | 0            |
| 70  | SV0   | 521   | 0        | 525      | 73      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 71  | RW0   | 1022   | 0        | 1052     | 20      | 0            |
| 71  | SW0   | 1022   | 0        | 1052     | 19      | 0            |
| 72  | RX0   | 1098   | 0        | 1183     | 3       | 0            |
| 72  | SX0   | 1098   | 0        | 1183     | 3       | 0            |
| 73  | RY0   | 1118   | 0        | 1166     | 14      | 0            |
| 73  | SY0   | 1118   | 0        | 1166     | 11      | 0            |
| 74  | RZ0   | 633    | 0        | 678      | 14      | 0            |
| 74  | SZ0   | 633    | 0        | 678      | 13      | 0            |
| 75  | RP0   | 950    | 0        | 984      | 56      | 0            |
| 75  | SP0   | 950    | 0        | 984      | 59      | 0            |
| 76  | KGG   | 1      | 0        | 0        | 0       | 0            |
| 76  | KJJ   | 1      | 0        | 0        | 0       | 0            |
| 76  | KMM   | 1      | 0        | 0        | 0       | 0            |
| 76  | KOO   | 1      | 0        | 0        | 0       | 0            |
| 76  | KPP   | 1      | 0        | 0        | 0       | 0            |
| 76  | LGG   | 1      | 0        | 0        | 0       | 0            |
| 76  | LJJ   | 1      | 0        | 0        | 0       | 0            |
| 76  | LMM   | 1      | 0        | 0        | 0       | 0            |
| 76  | LOO   | 1      | 0        | 0        | 0       | 0            |
| 76  | LPP   | 1      | 0        | 0        | 0       | 0            |
| 76  | RAA   | 1      | 0        | 0        | 0       | 0            |
| 76  | RBB   | 1      | 0        | 0        | 0       | 0            |
| 76  | RDD   | 1      | 0        | 0        | 0       | 0            |
| 76  | RFF   | 1      | 0        | 0        | 0       | 0            |
| 76  | SAA   | 1      | 0        | 0        | 0       | 0            |
| 76  | SBB   | 1      | 0        | 0        | 0       | 0            |
| 76  | SDD   | 1      | 0        | 0        | 0       | 0            |
| 76  | SFF   | 1      | 0        | 0        | 0       | 0            |
| All | All   | 343629 | 0        | 266537   | 2024    | 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 3.

All (2024) 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) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:SA0:70:ASN:HB2 | 47:SC0:240:ILE:CD1 | 1.35                     | 1.54              |
| 43:RA0:70:ASN:HB2 | 47:RC0:240:ILE:CD1 | 1.35                     | 1.49              |
| 47:SC0:51:SER:HB2 | 70:SV0:6:ARG:NH2   | 1.30                     | 1.45              |
| 49:SD0:238:PRO:C  | 66:SR0:19:ARG:HH12 | 1.27                     | 1.42              |
| 47:RC0:51:SER:HB2 | 70:RV0:6:ARG:NH2   | 1.30                     | 1.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 49:RD0:238:PRO:C    | 66:RR0:19:ARG:HH12  | 1.27                     | 1.39              |
| 20:KJ0:82:LYS:HB3   | 75:RP0:30:PHE:CE2   | 1.62                     | 1.35              |
| 43:SA0:70:ASN:HB2   | 47:SC0:240:ILE:CG1  | 1.56                     | 1.34              |
| 43:RA0:70:ASN:HB2   | 47:RC0:240:ILE:CG1  | 1.56                     | 1.34              |
| 43:RA0:70:ASN:CB    | 47:RC0:240:ILE:HD11 | 1.59                     | 1.33              |
| 20:LJ0:82:LYS:HB3   | 75:SP0:30:PHE:CE2   | 1.62                     | 1.32              |
| 43:SA0:141:ASN:O    | 70:SV0:23:VAL:HG23  | 1.21                     | 1.31              |
| 43:SA0:70:ASN:CB    | 47:SC0:240:ILE:HD11 | 1.59                     | 1.30              |
| 43:RA0:141:ASN:O    | 70:RV0:23:VAL:HG23  | 1.21                     | 1.29              |
| 3:LA0:241:ARG:NH1   | 42:S60:592:G:H4'    | 1.51                     | 1.25              |
| 49:SD0:239:ILE:N    | 66:SR0:19:ARG:HH12  | 1.35                     | 1.25              |
| 3:KA0:241:ARG:NH1   | 42:R60:592:G:H4'    | 1.51                     | 1.24              |
| 49:RD0:239:ILE:N    | 66:RR0:19:ARG:HH12  | 1.35                     | 1.23              |
| 50:RDD:8:TYR:CE2    | 75:RP0:72:ARG:HD2   | 1.75                     | 1.22              |
| 49:SD0:238:PRO:C    | 66:SR0:19:ARG:NH1   | 1.98                     | 1.20              |
| 50:SDD:8:TYR:CE2    | 75:SP0:72:ARG:HD2   | 1.75                     | 1.20              |
| 49:RD0:238:PRO:C    | 66:RR0:19:ARG:NH1   | 1.98                     | 1.19              |
| 43:SA0:63:ARG:CZ    | 70:SV0:30:LEU:HG    | 1.75                     | 1.17              |
| 43:RA0:63:ARG:CZ    | 70:RV0:30:LEU:HG    | 1.75                     | 1.16              |
| 47:RC0:51:SER:CB    | 70:RV0:6:ARG:HH21   | 1.60                     | 1.15              |
| 47:SC0:51:SER:CB    | 70:SV0:6:ARG:HH21   | 1.60                     | 1.15              |
| 37:KW0:99:LYS:HA    | 37:KW0:102:LYS:HE2  | 1.30                     | 1.13              |
| 47:SC0:51:SER:CB    | 70:SV0:6:ARG:NH2    | 2.11                     | 1.13              |
| 37:LW0:99:LYS:HA    | 37:LW0:102:LYS:HE2  | 1.30                     | 1.13              |
| 47:RC0:51:SER:CB    | 70:RV0:6:ARG:NH2    | 2.11                     | 1.12              |
| 43:SA0:70:ASN:CG    | 47:SC0:240:ILE:HG12 | 1.74                     | 1.12              |
| 43:SA0:63:ARG:HG2   | 70:SV0:30:LEU:HD21  | 1.31                     | 1.11              |
| 54:SFF:104:THR:HG22 | 54:RFF:98:ILE:O     | 1.50                     | 1.11              |
| 43:SA0:141:ASN:C    | 70:SV0:23:VAL:HG23  | 1.76                     | 1.11              |
| 43:RA0:70:ASN:CG    | 47:RC0:240:ILE:HG12 | 1.73                     | 1.10              |
| 43:RA0:141:ASN:C    | 70:RV0:23:VAL:HG23  | 1.76                     | 1.09              |
| 20:LJ0:82:LYS:CB    | 75:SP0:30:PHE:HE2   | 1.65                     | 1.09              |
| 20:KJ0:82:LYS:CB    | 75:RP0:30:PHE:HE2   | 1.65                     | 1.09              |
| 54:SFF:104:THR:HG21 | 54:RFF:99:LYS:HA    | 1.35                     | 1.09              |
| 43:RA0:70:ASN:CB    | 47:RC0:240:ILE:CD1  | 2.22                     | 1.08              |
| 47:RC0:219:PRO:HB3  | 71:RW0:66:ARG:NH2   | 1.68                     | 1.08              |
| 47:SC0:219:PRO:HB3  | 71:SW0:66:ARG:NH2   | 1.68                     | 1.08              |
| 1:L50:1691:A:N6     | 42:S60:1248:G:H4'   | 1.68                     | 1.08              |
| 73:SY0:22:GLU:O     | 73:SY0:23:LEU:HG    | 1.53                     | 1.07              |
| 34:LT0:126:PRO:HB2  | 34:LT0:128:LEU:HG   | 1.34                     | 1.07              |
| 1:K50:1691:A:N6     | 42:R60:1248:G:H4'   | 1.68                     | 1.07              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 43:SA0:70:ASN:CB    | 47:SC0:240:ILE:CD1 | 2.22                     | 1.07              |
| 43:SA0:117:ARG:HH12 | 47:SC0:243:GLU:CD  | 1.64                     | 1.05              |
| 43:RA0:187:GLY:HA2  | 70:RV0:35:ARG:NH2  | 1.71                     | 1.05              |
| 1:L50:535:A:O2'     | 31:LQ0:146:ASN:HB3 | 1.55                     | 1.05              |
| 37:LW0:83:PHE:CD1   | 55:SG0:144:LYS:HG2 | 1.92                     | 1.05              |
| 43:SA0:63:ARG:O     | 70:SV0:28:VAL:HG22 | 1.55                     | 1.05              |
| 43:RA0:63:ARG:HG2   | 70:RV0:30:LEU:HD21 | 1.31                     | 1.05              |
| 43:RA0:70:ASN:CB    | 47:RC0:240:ILE:CG1 | 2.35                     | 1.05              |
| 1:K50:535:A:O2'     | 31:KQ0:146:ASN:HB3 | 1.55                     | 1.05              |
| 73:RY0:22:GLU:O     | 73:RY0:23:LEU:HG   | 1.54                     | 1.05              |
| 3:LA0:241:ARG:HH12  | 42:S60:592:G:C4'   | 1.69                     | 1.05              |
| 43:RA0:63:ARG:O     | 70:RV0:28:VAL:HG22 | 1.55                     | 1.05              |
| 50:RDD:12:LEU:HD21  | 75:RP0:67:PHE:CD2  | 1.92                     | 1.05              |
| 43:SA0:70:ASN:CB    | 47:SC0:240:ILE:CG1 | 2.35                     | 1.04              |
| 1:K50:1695:A:N1     | 42:R60:1249:U:C5'  | 2.20                     | 1.04              |
| 34:KT0:126:PRO:HB2  | 34:KT0:128:LEU:HG  | 1.34                     | 1.04              |
| 50:SDD:12:LEU:HD21  | 75:SP0:67:PHE:CD2  | 1.92                     | 1.04              |
| 3:KA0:241:ARG:HH12  | 42:R60:592:G:C4'   | 1.69                     | 1.04              |
| 43:SA0:141:ASN:O    | 70:SV0:23:VAL:CG2  | 2.05                     | 1.04              |
| 47:SC0:136:TRP:HH2  | 59:SJ0:59:ILE:CG2  | 1.71                     | 1.04              |
| 43:RA0:64:MET:HB3   | 70:RV0:27:MET:HG2  | 1.38                     | 1.03              |
| 1:L50:1695:A:N1     | 42:S60:1249:U:C5'  | 2.20                     | 1.03              |
| 37:LW0:83:PHE:CD1   | 37:LW0:84:PRO:HD2  | 1.93                     | 1.03              |
| 37:KW0:83:PHE:CD1   | 55:RG0:144:LYS:CG  | 2.41                     | 1.03              |
| 37:KW0:83:PHE:CD1   | 55:RG0:144:LYS:HG2 | 1.92                     | 1.03              |
| 43:RA0:117:ARG:HH12 | 47:RC0:243:GLU:CD  | 1.64                     | 1.03              |
| 47:RC0:136:TRP:HH2  | 59:RJ0:59:ILE:CG2  | 1.71                     | 1.03              |
| 43:RA0:141:ASN:O    | 70:RV0:23:VAL:CG2  | 2.05                     | 1.03              |
| 43:RA0:215:TYR:CD1  | 66:RR0:84:PHE:CE2  | 2.46                     | 1.03              |
| 55:RG0:140:LYS:O    | 55:RG0:144:LYS:HD3 | 1.58                     | 1.03              |
| 37:LW0:83:PHE:CD1   | 55:SG0:144:LYS:CG  | 2.41                     | 1.03              |
| 43:SA0:215:TYR:CD1  | 66:SR0:84:PHE:CE2  | 2.46                     | 1.03              |
| 55:SG0:140:LYS:O    | 55:SG0:144:LYS:HD3 | 1.58                     | 1.03              |
| 43:SA0:64:MET:HB3   | 70:SV0:27:MET:HG2  | 1.38                     | 1.02              |
| 43:SA0:187:GLY:HA2  | 70:SV0:35:ARG:NH2  | 1.71                     | 1.02              |
| 10:KE0:55:GLU:OE2   | 10:KE0:117:ARG:HG3 | 1.59                     | 1.02              |
| 43:SA0:63:ARG:CG    | 70:SV0:30:LEU:HD21 | 1.90                     | 1.02              |
| 50:SDD:12:LEU:CD1   | 75:SP0:75:ILE:HG21 | 1.90                     | 1.02              |
| 37:KW0:83:PHE:CD1   | 37:KW0:84:PRO:HD2  | 1.93                     | 1.02              |
| 50:RDD:12:LEU:CD1   | 75:RP0:75:ILE:HG21 | 1.90                     | 1.02              |
| 10:LE0:55:GLU:OE2   | 10:LE0:117:ARG:HG3 | 1.59                     | 1.01              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:L50:1695:A:N1     | 42:S60:1249:U:H5'   | 1.76                     | 1.00              |
| 1:K50:1695:A:N1     | 42:R60:1249:U:H5'   | 1.76                     | 1.00              |
| 55:SG0:147:PHE:HZ   | 55:SG0:160:LYS:HE2  | 1.22                     | 1.00              |
| 55:RG0:147:PHE:HZ   | 55:RG0:160:LYS:HE2  | 1.23                     | 1.00              |
| 43:RA0:63:ARG:CG    | 70:RV0:30:LEU:HD21  | 1.89                     | 0.99              |
| 1:K50:1695:A:C2     | 42:R60:1249:U:H5''  | 1.97                     | 0.99              |
| 1:L50:1695:A:C2     | 42:S60:1249:U:H5''  | 1.97                     | 0.99              |
| 54:SFF:145:VAL:HG11 | 54:RFF:136:LYS:CB   | 1.93                     | 0.99              |
| 49:SD0:239:ILE:N    | 66:SR0:19:ARG:NH1   | 2.05                     | 0.98              |
| 42:S60:973:G:H1     | 44:SAA:90:TRP:HZ2   | 1.09                     | 0.98              |
| 49:RD0:239:ILE:N    | 66:RR0:19:ARG:NH1   | 2.05                     | 0.97              |
| 3:LA0:241:ARG:HH12  | 42:S60:592:G:H4'    | 1.13                     | 0.97              |
| 42:R60:973:G:H1     | 44:RAA:90:TRP:HZ2   | 1.09                     | 0.97              |
| 47:RC0:230:ASN:N    | 70:RV0:24:GLN:HE22  | 1.61                     | 0.97              |
| 47:SC0:230:ASN:N    | 70:SV0:24:GLN:HE22  | 1.61                     | 0.96              |
| 37:LW0:98:ASN:ND2   | 55:SG0:147:PHE:HA   | 1.81                     | 0.96              |
| 43:RA0:215:TYR:HA   | 66:RR0:84:PHE:CD2   | 2.01                     | 0.96              |
| 37:KW0:98:ASN:ND2   | 55:RG0:147:PHE:HA   | 1.81                     | 0.96              |
| 44:SAA:47:ALA:CB    | 48:SCC:61:ARG:HE    | 1.78                     | 0.96              |
| 43:RA0:63:ARG:NE    | 70:RV0:30:LEU:HG    | 1.81                     | 0.96              |
| 43:SA0:215:TYR:HA   | 66:SR0:84:PHE:CD2   | 2.01                     | 0.95              |
| 44:RAA:47:ALA:CB    | 48:RCC:61:ARG:HE    | 1.78                     | 0.95              |
| 43:SA0:63:ARG:NE    | 70:SV0:30:LEU:HG    | 1.81                     | 0.95              |
| 56:SGG:65:PHE:CE2   | 66:SR0:29:TYR:CE2   | 2.55                     | 0.95              |
| 56:RGG:65:PHE:CE2   | 66:RR0:29:TYR:CE2   | 2.55                     | 0.95              |
| 42:S60:554:A:N3     | 71:SW0:103:THR:HG22 | 1.83                     | 0.94              |
| 20:KJ0:82:LYS:CB    | 75:RP0:30:PHE:CE2   | 2.44                     | 0.93              |
| 43:RA0:70:ASN:HB2   | 47:RC0:240:ILE:HD11 | 0.95                     | 0.93              |
| 43:RA0:184:TYR:CD1  | 70:RV0:35:ARG:NH1   | 2.36                     | 0.93              |
| 50:SDD:8:TYR:O      | 75:SP0:67:PHE:N     | 2.01                     | 0.93              |
| 20:KJ0:82:LYS:HB3   | 75:RP0:30:PHE:CD2   | 2.03                     | 0.93              |
| 1:L50:1691:A:N6     | 42:S60:1248:G:C4'   | 2.32                     | 0.93              |
| 43:SA0:51:ILE:HG13  | 66:SR0:105:MET:SD   | 2.09                     | 0.93              |
| 47:SC0:51:SER:HB2   | 70:SV0:6:ARG:HH22   | 1.15                     | 0.93              |
| 43:RA0:70:ASN:CA    | 47:RC0:240:ILE:HD11 | 1.98                     | 0.93              |
| 50:RDD:8:TYR:O      | 75:RP0:67:PHE:N     | 2.01                     | 0.93              |
| 43:SA0:70:ASN:CA    | 47:SC0:240:ILE:HD11 | 1.98                     | 0.93              |
| 43:RA0:51:ILE:HG13  | 66:RR0:105:MET:SD   | 2.09                     | 0.93              |
| 20:LJ0:82:LYS:HB3   | 75:SP0:30:PHE:CD2   | 2.03                     | 0.92              |
| 43:SA0:70:ASN:HB2   | 47:SC0:240:ILE:HD11 | 0.95                     | 0.92              |
| 1:K50:1691:A:N6     | 42:R60:1248:G:C4'   | 2.32                     | 0.92              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:R60:554:A:N3     | 71:RW0:103:THR:HG22 | 1.83                     | 0.92              |
| 43:SA0:184:TYR:CD1  | 70:SV0:35:ARG:NH1   | 2.36                     | 0.92              |
| 1:K50:1695:A:N1     | 42:R60:1249:U:H5''  | 1.85                     | 0.92              |
| 43:SA0:63:ARG:HD3   | 70:SV0:30:LEU:HD23  | 1.52                     | 0.91              |
| 10:LE0:100:ILE:HD11 | 24:LM0:102:PHE:HB2  | 1.49                     | 0.91              |
| 43:RA0:120:ARG:HE   | 47:RC0:232:ILE:HG21 | 1.35                     | 0.91              |
| 43:SA0:4:ARG:O      | 70:SV0:30:LEU:HD12  | 1.69                     | 0.91              |
| 10:KE0:100:ILE:HD11 | 24:KM0:102:PHE:HB2  | 1.49                     | 0.91              |
| 43:RA0:63:ARG:HD3   | 70:RV0:30:LEU:HD23  | 1.52                     | 0.91              |
| 37:KW0:99:LYS:CA    | 37:KW0:102:LYS:HE2  | 2.00                     | 0.91              |
| 42:R60:973:G:N1     | 44:RAA:90:TRP:CZ2   | 2.39                     | 0.91              |
| 43:SA0:51:ILE:HD12  | 66:SR0:105:MET:HG2  | 1.53                     | 0.90              |
| 43:RA0:51:ILE:HD12  | 66:RR0:105:MET:HG2  | 1.53                     | 0.90              |
| 50:RDD:8:TYR:CE2    | 75:RP0:72:ARG:CD    | 2.54                     | 0.90              |
| 47:SC0:230:ASN:HB2  | 70:SV0:24:GLN:CD    | 1.96                     | 0.90              |
| 42:S60:958:A:H3'    | 42:S60:959:G:H21    | 1.37                     | 0.90              |
| 42:R60:958:A:H3'    | 42:R60:959:G:H21    | 1.37                     | 0.90              |
| 43:SA0:120:ARG:HE   | 47:SC0:232:ILE:HG21 | 1.35                     | 0.90              |
| 47:RC0:230:ASN:HB2  | 70:RV0:24:GLN:CD    | 1.96                     | 0.90              |
| 1:L50:1695:A:N1     | 42:S60:1249:U:H5''  | 1.85                     | 0.90              |
| 43:RA0:4:ARG:O      | 70:RV0:30:LEU:HD12  | 1.69                     | 0.90              |
| 43:RA0:184:TYR:O    | 70:RV0:35:ARG:HD2   | 1.72                     | 0.90              |
| 3:KA0:241:ARG:HH12  | 42:R60:592:G:H4'    | 1.13                     | 0.90              |
| 47:RC0:136:TRP:CH2  | 59:RJ0:59:ILE:CG2   | 2.54                     | 0.90              |
| 42:S60:973:G:N1     | 44:SAA:90:TRP:CZ2   | 2.39                     | 0.89              |
| 47:SC0:136:TRP:CH2  | 59:SJ0:59:ILE:CG2   | 2.54                     | 0.89              |
| 37:LW0:99:LYS:CA    | 37:LW0:102:LYS:HE2  | 2.00                     | 0.89              |
| 50:SDD:8:TYR:CE2    | 75:SP0:72:ARG:CD    | 2.54                     | 0.89              |
| 42:S60:203:G:N3     | 51:SE0:33:THR:HG21  | 1.88                     | 0.89              |
| 47:RC0:130:PRO:HB2  | 70:RV0:4:PHE:CZ     | 2.07                     | 0.89              |
| 42:R60:203:G:N3     | 51:RE0:33:THR:HG21  | 1.88                     | 0.89              |
| 43:RA0:70:ASN:ND2   | 47:RC0:240:ILE:HG12 | 1.88                     | 0.89              |
| 50:RDD:8:TYR:CD2    | 75:RP0:72:ARG:HD2   | 2.08                     | 0.89              |
| 43:SA0:184:TYR:O    | 70:SV0:35:ARG:HD2   | 1.72                     | 0.89              |
| 47:SC0:130:PRO:HB2  | 70:SV0:4:PHE:CZ     | 2.07                     | 0.89              |
| 47:RC0:230:ASN:H    | 70:RV0:24:GLN:HE22  | 0.91                     | 0.89              |
| 43:RA0:67:SER:OG    | 70:RV0:40:LEU:CD2   | 2.21                     | 0.89              |
| 43:RA0:117:ARG:NH1  | 47:RC0:243:GLU:OE2  | 2.06                     | 0.88              |
| 47:RC0:51:SER:HB2   | 70:RV0:6:ARG:HH22   | 1.15                     | 0.88              |
| 37:LW0:99:LYS:HA    | 37:LW0:102:LYS:CE   | 2.03                     | 0.88              |
| 3:LA0:241:ARG:NH1   | 42:S60:592:G:C4'    | 2.33                     | 0.88              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 43:SA0:67:SER:OG   | 70:SV0:40:LEU:CD2   | 2.21                     | 0.88              |
| 43:SA0:117:ARG:NH1 | 47:SC0:243:GLU:OE2  | 2.06                     | 0.88              |
| 43:SA0:70:ASN:ND2  | 47:SC0:240:ILE:HG12 | 1.88                     | 0.88              |
| 43:RA0:63:ARG:HD3  | 70:RV0:30:LEU:CD2   | 2.03                     | 0.88              |
| 43:SA0:63:ARG:HD3  | 70:SV0:30:LEU:CD2   | 2.03                     | 0.88              |
| 37:KW0:99:LYS:HA   | 37:KW0:102:LYS:CE   | 2.03                     | 0.88              |
| 20:LJ0:82:LYS:CB   | 75:SP0:30:PHE:CE2   | 2.44                     | 0.87              |
| 48:SCC:58:ARG:HH12 | 64:SO0:101:ARG:HH22 | 1.19                     | 0.87              |
| 50:RDD:12:LEU:CD2  | 75:RP0:67:PHE:CD2   | 2.57                     | 0.87              |
| 50:RDD:8:TYR:CZ    | 75:RP0:72:ARG:HD2   | 2.09                     | 0.87              |
| 42:S60:973:G:N1    | 44:SAA:90:TRP:HZ2   | 1.72                     | 0.87              |
| 47:SC0:230:ASN:H   | 70:SV0:24:GLN:HE22  | 0.91                     | 0.87              |
| 47:RC0:230:ASN:H   | 70:RV0:24:GLN:NE2   | 1.73                     | 0.87              |
| 43:SA0:67:SER:OG   | 70:SV0:40:LEU:HD22  | 1.75                     | 0.87              |
| 50:SDD:8:TYR:CZ    | 75:SP0:72:ARG:HD2   | 2.09                     | 0.87              |
| 47:SC0:230:ASN:H   | 70:SV0:24:GLN:NE2   | 1.73                     | 0.86              |
| 50:SDD:12:LEU:CD2  | 75:SP0:67:PHE:CD2   | 2.57                     | 0.86              |
| 50:SDD:8:TYR:CD2   | 75:SP0:72:ARG:HD2   | 2.08                     | 0.86              |
| 43:SA0:70:ASN:CB   | 47:SC0:240:ILE:HG12 | 1.99                     | 0.86              |
| 42:R60:973:G:N1    | 44:RAA:90:TRP:HZ2   | 1.72                     | 0.86              |
| 37:LW0:26:ASP:O    | 37:LW0:27:ASP:OD1   | 1.94                     | 0.86              |
| 48:RCC:58:ARG:HH12 | 64:RO0:101:ARG:HH22 | 1.19                     | 0.85              |
| 43:RA0:70:ASN:CB   | 47:RC0:240:ILE:HG12 | 1.99                     | 0.85              |
| 42:R60:1084:G:N2   | 75:RP0:117:GLY:O    | 2.09                     | 0.85              |
| 42:R60:914:U:H3    | 42:R60:918:A:H61    | 1.23                     | 0.85              |
| 42:S60:706:G:H2'   | 42:S60:706:G:N3     | 1.92                     | 0.85              |
| 43:SA0:120:ARG:HE  | 47:SC0:232:ILE:CG2  | 1.88                     | 0.85              |
| 43:RA0:67:SER:OG   | 70:RV0:40:LEU:HD22  | 1.75                     | 0.85              |
| 43:RA0:120:ARG:HE  | 47:RC0:232:ILE:CG2  | 1.89                     | 0.85              |
| 42:S60:1084:G:N2   | 75:SP0:117:GLY:O    | 2.09                     | 0.84              |
| 20:KJ0:82:LYS:HB3  | 75:RP0:30:PHE:HE2   | 1.06                     | 0.84              |
| 37:KW0:26:ASP:O    | 37:KW0:27:ASP:OD1   | 1.94                     | 0.84              |
| 42:S60:1149:U:OP1  | 67:SS0:139:VAL:N    | 2.10                     | 0.84              |
| 42:R60:826:U:O2'   | 47:RC0:81:GLN:O     | 1.94                     | 0.84              |
| 50:SDD:12:LEU:HD11 | 75:SP0:75:ILE:HG21  | 1.59                     | 0.84              |
| 47:RC0:219:PRO:HB3 | 71:RW0:66:ARG:HH22  | 1.39                     | 0.84              |
| 42:S60:995:A:H3'   | 42:S60:996:G:H8     | 1.42                     | 0.84              |
| 42:R60:1149:U:OP1  | 67:RS0:139:VAL:N    | 2.10                     | 0.84              |
| 42:S60:826:U:O2'   | 47:SC0:81:GLN:O     | 1.94                     | 0.84              |
| 42:S60:914:U:H3    | 42:S60:918:A:H61    | 1.24                     | 0.84              |
| 42:R60:706:G:N3    | 42:R60:706:G:H2'    | 1.92                     | 0.83              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 43:RA0:51:ILE:HD11  | 66:RR0:105:MET:HE3  | 1.60                     | 0.83              |
| 42:S60:705:A:N3     | 42:S60:706:G:C6     | 2.46                     | 0.83              |
| 55:SG0:147:PHE:CZ   | 55:SG0:160:LYS:HE2  | 2.13                     | 0.83              |
| 42:R60:995:A:H3'    | 42:R60:996:G:H8     | 1.42                     | 0.83              |
| 47:SC0:219:PRO:HB3  | 71:SW0:66:ARG:HH22  | 1.39                     | 0.83              |
| 53:SF0:118:ARG:HD2  | 53:SF0:125:MET:HB3  | 1.59                     | 0.83              |
| 42:R60:705:A:N3     | 42:R60:706:G:C6     | 2.46                     | 0.83              |
| 43:SA0:215:TYR:O    | 66:SR0:84:PHE:HE2   | 1.62                     | 0.83              |
| 67:SS0:90:TRP:CZ3   | 67:SS0:91:MET:HE2   | 2.13                     | 0.83              |
| 67:RS0:90:TRP:CZ3   | 67:RS0:91:MET:HE2   | 2.14                     | 0.83              |
| 43:RA0:63:ARG:CD    | 70:RV0:30:LEU:CD2   | 2.57                     | 0.83              |
| 42:S60:923:A:H4'    | 42:S60:924:U:H2'    | 1.61                     | 0.83              |
| 41:MD2:52:LYS:HG3   | 42:R60:606:G:N2     | 1.93                     | 0.83              |
| 43:SA0:63:ARG:CD    | 70:SV0:30:LEU:CD2   | 2.57                     | 0.83              |
| 41:MD1:52:LYS:HG3   | 42:S60:606:G:N2     | 1.93                     | 0.83              |
| 43:SA0:51:ILE:HD11  | 66:SR0:105:MET:HE3  | 1.60                     | 0.83              |
| 54:SFF:147:ILE:HD11 | 54:RFF:147:ILE:HD11 | 1.59                     | 0.83              |
| 42:S60:973:G:H22    | 44:SAA:90:TRP:HH2   | 1.27                     | 0.82              |
| 42:S60:1159:A:O2'   | 75:SP0:100:ASN:ND2  | 2.11                     | 0.82              |
| 54:SFF:150:LYS:HD2  | 42:R60:915:A:O2'    | 1.77                     | 0.82              |
| 42:R60:1159:A:O2'   | 75:RP0:100:ASN:ND2  | 2.12                     | 0.82              |
| 1:K50:1728:U:HO2'   | 42:R60:1259:U:HO2'  | 1.06                     | 0.82              |
| 42:R60:923:A:H4'    | 42:R60:924:U:H2'    | 1.61                     | 0.82              |
| 50:RDD:12:LEU:HD11  | 75:RP0:75:ILE:HG21  | 1.59                     | 0.82              |
| 53:RF0:118:ARG:HD2  | 53:RF0:125:MET:HB3  | 1.59                     | 0.82              |
| 55:RG0:147:PHE:CZ   | 55:RG0:160:LYS:HE2  | 2.13                     | 0.82              |
| 49:SD0:234:ILE:HD12 | 66:SR0:8:SER:HB2    | 1.62                     | 0.81              |
| 50:RDD:8:TYR:N      | 75:RP0:67:PHE:O     | 2.13                     | 0.81              |
| 56:RGG:65:PHE:HE2   | 66:RR0:29:TYR:CE2   | 1.96                     | 0.81              |
| 50:SDD:8:TYR:N      | 75:SP0:67:PHE:O     | 2.14                     | 0.81              |
| 42:R60:173:A:C8     | 51:RE0:131:VAL:CG1  | 2.64                     | 0.81              |
| 43:RA0:215:TYR:O    | 66:RR0:84:PHE:HE2   | 1.62                     | 0.81              |
| 47:RC0:230:ASN:HB2  | 70:RV0:24:GLN:OE1   | 1.80                     | 0.81              |
| 53:RF0:39:ILE:HG21  | 65:RQ0:50:GLU:HB2   | 1.62                     | 0.81              |
| 42:S60:173:A:C8     | 51:SE0:131:VAL:CG1  | 2.64                     | 0.81              |
| 20:LJ0:82:LYS:HB3   | 75:SP0:30:PHE:HE2   | 1.06                     | 0.81              |
| 54:SFF:93:LYS:HB3   | 54:SFF:94:PRO:HD2   | 1.63                     | 0.81              |
| 42:R60:1055:A:O3'   | 47:RC0:84:ALA:HB2   | 1.81                     | 0.81              |
| 1:L50:1691:A:C6     | 42:S60:1248:G:O4'   | 2.34                     | 0.81              |
| 53:SF0:39:ILE:HG21  | 65:SQ0:50:GLU:HB2   | 1.62                     | 0.81              |
| 47:SC0:230:ASN:HB2  | 70:SV0:24:GLN:OE1   | 1.80                     | 0.81              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 53:SF0:39:ILE:CG2   | 65:SQ0:50:GLU:HB2   | 2.11                     | 0.81              |
| 53:RF0:39:ILE:CG2   | 65:RQ0:50:GLU:HB2   | 2.11                     | 0.81              |
| 56:RGG:65:PHE:CZ    | 66:RR0:29:TYR:CE2   | 2.69                     | 0.81              |
| 43:RA0:215:TYR:HA   | 66:RR0:84:PHE:CE2   | 2.16                     | 0.81              |
| 56:SGG:65:PHE:CZ    | 66:SR0:29:TYR:CE2   | 2.69                     | 0.80              |
| 43:RA0:63:ARG:HG2   | 70:RV0:30:LEU:CD2   | 2.11                     | 0.80              |
| 42:S60:1055:A:O3'   | 47:SC0:84:ALA:HB2   | 1.81                     | 0.80              |
| 43:SA0:51:ILE:CD1   | 66:SR0:105:MET:HE3  | 2.11                     | 0.80              |
| 10:KE0:23:ILE:HD11  | 11:KEE:79:ARG:HH12  | 1.45                     | 0.80              |
| 43:SA0:215:TYR:HA   | 66:SR0:84:PHE:CE2   | 2.16                     | 0.80              |
| 47:RC0:136:TRP:HH2  | 59:RJ0:59:ILE:HG21  | 1.46                     | 0.80              |
| 49:RD0:234:ILE:HD12 | 66:RR0:8:SER:HB2    | 1.62                     | 0.80              |
| 43:RA0:51:ILE:CD1   | 66:RR0:105:MET:HE3  | 2.10                     | 0.80              |
| 65:SQ0:33:ASN:ND2   | 68:ST0:6:PHE:CD2    | 2.50                     | 0.80              |
| 56:SGG:65:PHE:HE2   | 66:SR0:29:TYR:CE2   | 1.96                     | 0.80              |
| 1:K50:1691:A:C6     | 42:R60:1248:G:O4'   | 2.34                     | 0.80              |
| 34:KT0:126:PRO:HB2  | 34:KT0:128:LEU:CG   | 2.13                     | 0.79              |
| 42:R60:988:A:O2'    | 43:RA0:105:PRO:O    | 2.00                     | 0.79              |
| 10:LE0:23:ILE:HD11  | 11:LEE:79:ARG:HH12  | 1.45                     | 0.79              |
| 43:SA0:67:SER:CA    | 70:SV0:28:VAL:HG13  | 2.13                     | 0.79              |
| 47:SC0:136:TRP:HH2  | 59:SJ0:59:ILE:HG21  | 1.46                     | 0.79              |
| 47:SC0:166:LYS:HD2  | 59:SJ0:100:GLU:OE2  | 1.83                     | 0.79              |
| 49:SD0:101:LYS:NZ   | 60:SK0:14:TYR:OH    | 2.13                     | 0.79              |
| 53:RF0:96:GLY:O     | 74:RZ0:108:LEU:CD2  | 2.31                     | 0.79              |
| 54:RFF:93:LYS:HB3   | 54:RFF:94:PRO:HD2   | 1.63                     | 0.79              |
| 65:RQ0:33:ASN:ND2   | 68:RT0:6:PHE:CD2    | 2.50                     | 0.79              |
| 1:L50:796:C:H5''    | 34:LT0:131:ARG:H    | 1.48                     | 0.79              |
| 53:SF0:96:GLY:O     | 74:SZ0:108:LEU:CD2  | 2.31                     | 0.79              |
| 37:LW0:83:PHE:CG    | 37:LW0:84:PRO:HD2   | 2.18                     | 0.79              |
| 43:SA0:141:ASN:C    | 70:SV0:23:VAL:CG2   | 2.55                     | 0.79              |
| 37:LW0:83:PHE:CE1   | 55:SG0:144:LYS:HG2  | 2.17                     | 0.79              |
| 1:L50:1695:A:C2     | 42:S60:1249:U:C5'   | 2.66                     | 0.79              |
| 37:KW0:83:PHE:CD1   | 55:RG0:144:LYS:HG3  | 2.17                     | 0.79              |
| 42:S60:988:A:O2'    | 43:SA0:105:PRO:O    | 2.00                     | 0.79              |
| 37:KW0:83:PHE:CG    | 37:KW0:84:PRO:HD2   | 2.18                     | 0.79              |
| 37:LW0:83:PHE:CD1   | 55:SG0:144:LYS:HG3  | 2.17                     | 0.78              |
| 3:KA0:241:ARG:NH1   | 42:R60:592:G:C4'    | 2.33                     | 0.78              |
| 43:RA0:67:SER:CA    | 70:RV0:28:VAL:HG13  | 2.12                     | 0.78              |
| 47:RC0:166:LYS:HD2  | 59:RJ0:100:GLU:OE2  | 1.83                     | 0.78              |
| 54:SFF:99:LYS:HE2   | 54:SFF:102:ILE:HG12 | 1.63                     | 0.78              |
| 43:RA0:215:TYR:HA   | 66:RR0:84:PHE:HD2   | 1.48                     | 0.78              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 43:SA0:52:LYS:HB2  | 66:SR0:109:TYR:CZ   | 2.19                     | 0.78              |
| 50:SDD:12:LEU:CD1  | 75:SP0:75:ILE:CG2   | 2.62                     | 0.78              |
| 42:R60:973:G:H22   | 44:RAA:90:TRP:HH2   | 1.27                     | 0.78              |
| 43:RA0:63:ARG:O    | 70:RV0:28:VAL:CG2   | 2.32                     | 0.78              |
| 54:SFF:132:ARG:O   | 42:R60:918:A:H4'    | 1.84                     | 0.78              |
| 1:K50:796:C:H5''   | 34:KT0:131:ARG:H    | 1.48                     | 0.78              |
| 48:RCC:58:ARG:HH12 | 64:RO0:101:ARG:NH2  | 1.82                     | 0.78              |
| 43:SA0:215:TYR:HA  | 66:SR0:84:PHE:HD2   | 1.48                     | 0.78              |
| 55:SG0:169:VAL:CG1 | 55:SG0:176:LYS:HE2  | 2.14                     | 0.78              |
| 42:R60:1045:A:OP2  | 66:RR0:2:GLY:N      | 2.17                     | 0.78              |
| 37:KW0:83:PHE:CE1  | 55:RG0:144:LYS:HG2  | 2.17                     | 0.78              |
| 43:RA0:187:GLY:HA2 | 70:RV0:35:ARG:CZ    | 2.14                     | 0.78              |
| 43:SA0:63:ARG:O    | 70:SV0:28:VAL:CG2   | 2.32                     | 0.77              |
| 43:SA0:118:GLU:OE2 | 47:SC0:31:THR:HA    | 1.83                     | 0.77              |
| 43:SA0:206:ARG:NE  | 66:SR0:86:PRO:HG2   | 1.99                     | 0.77              |
| 3:KA0:241:ARG:CZ   | 42:R60:592:G:H4'    | 2.15                     | 0.77              |
| 42:R60:1055:A:O3'  | 47:RC0:84:ALA:CB    | 2.33                     | 0.77              |
| 53:SF0:6:THR:HG23  | 65:SQ0:53:LYS:NZ    | 2.00                     | 0.77              |
| 54:SFF:104:THR:CG2 | 54:RFF:98:ILE:O     | 2.31                     | 0.77              |
| 34:LT0:126:PRO:HB2 | 34:LT0:128:LEU:CG   | 2.13                     | 0.77              |
| 54:SFF:104:THR:CG2 | 54:RFF:99:LYS:HA    | 2.11                     | 0.77              |
| 43:RA0:52:LYS:HB2  | 66:RR0:109:TYR:CZ   | 2.19                     | 0.77              |
| 42:S60:1045:A:OP2  | 66:SR0:2:GLY:N      | 2.17                     | 0.77              |
| 42:S60:1055:A:O3'  | 47:SC0:84:ALA:CB    | 2.33                     | 0.77              |
| 43:RA0:141:ASN:C   | 70:RV0:23:VAL:CG2   | 2.55                     | 0.77              |
| 55:RG0:169:VAL:CG1 | 55:RG0:176:LYS:HE2  | 2.14                     | 0.77              |
| 43:SA0:63:ARG:HG2  | 70:SV0:30:LEU:CD2   | 2.10                     | 0.77              |
| 49:RD0:238:PRO:CA  | 66:RR0:19:ARG:HH12  | 1.98                     | 0.77              |
| 42:R60:1188:A:H5'' | 65:RQ0:136:ALA:HB2  | 1.65                     | 0.77              |
| 43:RA0:70:ASN:N    | 47:RC0:240:ILE:HD11 | 2.00                     | 0.77              |
| 43:RA0:118:GLU:OE2 | 47:RC0:31:THR:HA    | 1.84                     | 0.77              |
| 43:SA0:215:TYR:HD1 | 66:SR0:84:PHE:CD2   | 2.03                     | 0.77              |
| 49:SD0:238:PRO:CA  | 66:SR0:19:ARG:HH12  | 1.98                     | 0.77              |
| 54:SFF:97:ASP:CB   | 54:RFF:104:THR:O    | 2.32                     | 0.76              |
| 43:RA0:67:SER:HA   | 70:RV0:28:VAL:HG13  | 1.66                     | 0.76              |
| 44:RAA:47:ALA:HB1  | 48:RCC:61:ARG:HE    | 1.49                     | 0.76              |
| 50:RDD:12:LEU:CD1  | 75:RP0:75:ILE:CG2   | 2.62                     | 0.76              |
| 43:SA0:70:ASN:N    | 47:SC0:240:ILE:HD11 | 2.00                     | 0.76              |
| 37:KW0:98:ASN:ND2  | 55:RG0:147:PHE:CA   | 2.48                     | 0.76              |
| 42:R60:840:C:H4'   | 42:R60:1182:G:H5''  | 1.68                     | 0.76              |
| 43:SA0:102:ARG:H   | 43:SA0:102:ARG:HD2  | 1.49                     | 0.76              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 43:SA0:187:GLY:HA2  | 70:SV0:35:ARG:CZ    | 2.14                     | 0.76              |
| 48:SCC:58:ARG:HH12  | 64:SO0:101:ARG:NH2  | 1.82                     | 0.76              |
| 42:S60:915:A:C2     | 54:RFF:150:LYS:HG3  | 2.19                     | 0.76              |
| 42:S60:1188:A:H5''  | 65:SQ0:136:ALA:HB2  | 1.65                     | 0.76              |
| 53:SF0:40:LEU:HD23  | 65:SQ0:43:PHE:CE1   | 2.20                     | 0.76              |
| 43:RA0:206:ARG:NE   | 66:RR0:86:PRO:HG2   | 1.99                     | 0.76              |
| 53:RF0:6:THR:HG23   | 65:RQ0:53:LYS:NZ    | 2.00                     | 0.76              |
| 53:RF0:40:LEU:HD23  | 65:RQ0:43:PHE:CE1   | 2.20                     | 0.76              |
| 42:R60:173:A:H8     | 51:RE0:131:VAL:HG12 | 1.50                     | 0.76              |
| 43:RA0:52:LYS:HB2   | 66:RR0:109:TYR:CE1  | 2.21                     | 0.76              |
| 1:L50:883:U:H5''    | 24:LM0:35:ASN:HD21  | 1.51                     | 0.76              |
| 3:LA0:241:ARG:CZ    | 42:S60:592:G:H4'    | 2.15                     | 0.76              |
| 44:SAA:47:ALA:HB1   | 48:SCC:61:ARG:HE    | 1.49                     | 0.76              |
| 42:R60:982:C:H4'    | 66:RR0:10:ARG:NH1   | 2.01                     | 0.76              |
| 50:RDD:12:LEU:CD2   | 75:RP0:67:PHE:HD2   | 1.98                     | 0.76              |
| 55:RG0:170:ASN:HD21 | 55:RG0:176:LYS:HD3  | 1.50                     | 0.76              |
| 1:L50:883:U:H5''    | 24:LM0:35:ASN:ND2   | 2.01                     | 0.76              |
| 43:SA0:52:LYS:HB2   | 66:SR0:109:TYR:CE1  | 2.21                     | 0.76              |
| 43:SA0:67:SER:HA    | 70:SV0:28:VAL:HG13  | 1.66                     | 0.76              |
| 43:RA0:102:ARG:HD2  | 43:RA0:102:ARG:H    | 1.49                     | 0.76              |
| 1:K50:883:U:H5''    | 24:KM0:35:ASN:HD21  | 1.51                     | 0.75              |
| 1:L50:2497:C:H5''   | 5:LB0:280:THR:HG21  | 1.68                     | 0.75              |
| 42:S60:840:C:H4'    | 42:S60:1182:G:H5''  | 1.68                     | 0.75              |
| 37:LW0:98:ASN:HD22  | 55:SG0:147:PHE:HA   | 1.52                     | 0.75              |
| 37:LW0:98:ASN:ND2   | 55:SG0:147:PHE:CA   | 2.48                     | 0.75              |
| 54:SFF:104:THR:HG21 | 54:RFF:99:LYS:HD3   | 1.67                     | 0.75              |
| 49:RD0:101:LYS:NZ   | 60:RK0:14:TYR:OH    | 2.13                     | 0.75              |
| 42:S60:982:C:H4'    | 66:SR0:10:ARG:NH1   | 2.01                     | 0.75              |
| 55:SG0:170:ASN:HD21 | 55:SG0:176:LYS:HD3  | 1.50                     | 0.75              |
| 42:S60:173:A:H8     | 51:SE0:131:VAL:HG12 | 1.50                     | 0.75              |
| 43:RA0:215:TYR:HD1  | 66:RR0:84:PHE:CD2   | 2.03                     | 0.75              |
| 56:RGG:228:LYS:NZ   | 66:RR0:25:THR:HG22  | 2.02                     | 0.75              |
| 43:SA0:120:ARG:NE   | 47:SC0:232:ILE:HG21 | 2.02                     | 0.75              |
| 50:SDD:12:LEU:CD2   | 75:SP0:67:PHE:HD2   | 1.98                     | 0.75              |
| 1:K50:883:U:H5''    | 24:KM0:35:ASN:ND2   | 2.01                     | 0.75              |
| 41:MD2:106:TYR:CE1  | 64:RO0:47:LYS:NZ    | 2.53                     | 0.75              |
| 1:K50:2052:A:H5'    | 20:KJ0:62:ILE:HD11  | 1.69                     | 0.74              |
| 41:MD1:106:TYR:CE1  | 64:SO0:47:LYS:NZ    | 2.54                     | 0.74              |
| 1:K50:1695:A:C2     | 42:R60:1249:U:C5'   | 2.66                     | 0.74              |
| 5:KB0:336:ARG:HH11  | 5:KB0:336:ARG:HG3   | 1.51                     | 0.74              |
| 43:RA0:52:LYS:CB    | 66:RR0:109:TYR:CZ   | 2.70                     | 0.74              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 43:SA0:52:LYS:CB    | 66:SR0:109:TYR:CZ   | 2.70                     | 0.74              |
| 42:R60:173:A:C8     | 51:RE0:131:VAL:HG12 | 2.23                     | 0.74              |
| 54:SFF:145:VAL:HG21 | 54:RFF:136:LYS:N    | 2.03                     | 0.74              |
| 42:S60:173:A:C8     | 51:SE0:131:VAL:HG12 | 2.23                     | 0.74              |
| 43:SA0:215:TYR:CD1  | 66:SR0:84:PHE:CD2   | 2.76                     | 0.74              |
| 5:LB0:336:ARG:HH11  | 5:LB0:336:ARG:HG3   | 1.51                     | 0.74              |
| 42:S60:982:C:O3'    | 66:SR0:10:ARG:NH1   | 2.21                     | 0.74              |
| 43:RA0:120:ARG:NE   | 47:RC0:232:ILE:HG21 | 2.02                     | 0.74              |
| 44:SAA:51:ASP:OD2   | 48:SCC:57:GLU:O     | 2.06                     | 0.74              |
| 2:L70:27:A:OP2      | 8:LD0:62:THR:HG23   | 1.88                     | 0.73              |
| 1:K50:2497:C:H5''   | 5:KB0:280:THR:HG21  | 1.68                     | 0.73              |
| 42:R60:203:G:N3     | 51:RE0:33:THR:CG2   | 2.51                     | 0.73              |
| 37:KW0:99:LYS:CB    | 37:KW0:102:LYS:HE2  | 2.18                     | 0.73              |
| 42:S60:203:G:N3     | 51:SE0:33:THR:CG2   | 2.51                     | 0.73              |
| 43:SA0:184:TYR:CE2  | 70:SV0:35:ARG:HD3   | 2.23                     | 0.73              |
| 10:LE0:55:GLU:CD    | 10:LE0:117:ARG:HG3  | 2.13                     | 0.73              |
| 10:KE0:55:GLU:CD    | 10:KE0:117:ARG:HG3  | 2.13                     | 0.73              |
| 1:L50:1728:U:O2'    | 42:S60:1259:U:O2'   | 1.93                     | 0.73              |
| 37:LW0:99:LYS:CB    | 37:LW0:102:LYS:HE2  | 2.18                     | 0.73              |
| 67:SS0:20:MET:HG2   | 67:SS0:29:ASP:HA    | 1.71                     | 0.73              |
| 43:RA0:64:MET:CB    | 70:RV0:27:MET:HG2   | 2.17                     | 0.73              |
| 56:SGG:228:LYS:NZ   | 66:SR0:25:THR:HG22  | 2.02                     | 0.73              |
| 2:K70:27:A:OP2      | 8:KD0:62:THR:HG23   | 1.88                     | 0.73              |
| 42:R60:982:C:O3'    | 66:RR0:10:ARG:NH1   | 2.21                     | 0.73              |
| 42:R60:1315:A:H2'   | 42:R60:1316:A:H8    | 1.54                     | 0.73              |
| 49:RD0:36:ARG:NH1   | 69:RU0:112:GLU:OE2  | 2.21                     | 0.73              |
| 53:RF0:96:GLY:O     | 74:RZ0:108:LEU:HD21 | 1.88                     | 0.73              |
| 43:SA0:184:TYR:O    | 70:SV0:35:ARG:CD    | 2.36                     | 0.73              |
| 45:SB0:53:THR:HG22  | 64:SO0:30:ASP:OD2   | 1.88                     | 0.73              |
| 44:RAA:51:ASP:OD2   | 48:RCC:57:GLU:O     | 2.06                     | 0.73              |
| 1:L50:2052:A:H5'    | 20:LJ0:62:ILE:HD11  | 1.69                     | 0.73              |
| 49:SD0:36:ARG:NH1   | 69:SU0:112:GLU:OE2  | 2.21                     | 0.73              |
| 45:RB0:53:THR:HG22  | 64:RO0:30:ASP:OD2   | 1.88                     | 0.73              |
| 53:SF0:96:GLY:O     | 74:SZ0:108:LEU:HD21 | 1.88                     | 0.73              |
| 54:SFF:143:TYR:O    | 54:RFF:134:GLY:HA3  | 1.89                     | 0.73              |
| 42:S60:982:C:O2'    | 66:SR0:10:ARG:NH1   | 2.22                     | 0.72              |
| 43:RA0:184:TYR:CE2  | 70:RV0:35:ARG:HD3   | 2.24                     | 0.72              |
| 42:R60:438:U:H4'    | 72:RX0:110:LYS:HD2  | 1.72                     | 0.72              |
| 43:RA0:184:TYR:O    | 70:RV0:35:ARG:CD    | 2.36                     | 0.72              |
| 67:RS0:20:MET:HG2   | 67:RS0:29:ASP:HA    | 1.71                     | 0.72              |
| 42:S60:438:U:H4'    | 72:SX0:110:LYS:HD2  | 1.72                     | 0.72              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:995:A:H3'    | 42:S60:996:G:C8     | 2.24                     | 0.72              |
| 1:K50:1691:A:N1     | 42:R60:1248:G:O4'   | 2.23                     | 0.72              |
| 48:RCC:41:ILE:HG23  | 53:RF0:131:ASP:O    | 1.90                     | 0.72              |
| 7:LCC:64:ILE:HG22   | 40:LZ0:39:LEU:HD11  | 1.72                     | 0.71              |
| 53:SF0:95:THR:HG21  | 53:SF0:102:ILE:HG12 | 1.72                     | 0.71              |
| 43:RA0:52:LYS:HD2   | 66:RR0:109:TYR:CE1  | 2.25                     | 0.71              |
| 42:S60:1034:A:H2'   | 42:S60:1035:C:C6    | 2.26                     | 0.71              |
| 43:SA0:64:MET:CB    | 70:SV0:27:MET:HG2   | 2.17                     | 0.71              |
| 42:R60:705:A:C2     | 42:R60:706:G:O6     | 2.43                     | 0.71              |
| 42:R60:995:A:H3'    | 42:R60:996:G:C8     | 2.24                     | 0.71              |
| 43:RA0:215:TYR:CD1  | 66:RR0:84:PHE:CD2   | 2.76                     | 0.71              |
| 42:S60:854:U:OP2    | 67:SS0:148:GLY:N    | 2.24                     | 0.71              |
| 2:L70:3:U:H3        | 2:L70:116:G:H1      | 1.37                     | 0.71              |
| 42:S60:705:A:C2     | 42:S60:706:G:O6     | 2.43                     | 0.71              |
| 42:R60:854:U:OP2    | 67:RS0:148:GLY:N    | 2.24                     | 0.71              |
| 2:K70:63:A:H2'      | 18:KI0:204:GLY:O    | 1.91                     | 0.71              |
| 1:L50:1691:A:N1     | 42:S60:1248:G:O4'   | 2.23                     | 0.71              |
| 47:SC0:219:PRO:CB   | 71:SW0:66:ARG:NH2   | 2.51                     | 0.71              |
| 53:RF0:95:THR:HG21  | 53:RF0:102:ILE:HG12 | 1.72                     | 0.71              |
| 7:KCC:64:ILE:HG22   | 40:KZ0:39:LEU:HD11  | 1.72                     | 0.71              |
| 37:KW0:98:ASN:HD22  | 55:RG0:147:PHE:HA   | 1.52                     | 0.71              |
| 2:L70:63:A:H2'      | 18:LI0:204:GLY:O    | 1.91                     | 0.71              |
| 42:S60:237:A:H5'    | 58:SI0:48:VAL:CG1   | 2.21                     | 0.71              |
| 42:S60:1315:A:H2'   | 42:S60:1316:A:H8    | 1.54                     | 0.71              |
| 43:SA0:118:GLU:CD   | 47:SC0:31:THR:HG1   | 1.98                     | 0.70              |
| 43:RA0:63:ARG:CG    | 70:RV0:30:LEU:CD2   | 2.67                     | 0.70              |
| 53:RF0:40:LEU:CD2   | 65:RQ0:43:PHE:CD1   | 2.74                     | 0.70              |
| 48:SCC:41:ILE:HG23  | 53:SF0:131:ASP:O    | 1.90                     | 0.70              |
| 2:K70:3:U:H3        | 2:K70:116:G:H1      | 1.37                     | 0.70              |
| 42:R60:1034:A:H2'   | 42:R60:1035:C:C6    | 2.26                     | 0.70              |
| 43:SA0:52:LYS:HD2   | 66:SR0:109:TYR:CE1  | 2.25                     | 0.70              |
| 47:RC0:136:TRP:CH2  | 59:RJ0:59:ILE:HG21  | 2.23                     | 0.70              |
| 42:S60:1040:G:N2    | 42:S60:1042:A:H3'   | 2.06                     | 0.70              |
| 53:SF0:40:LEU:CD2   | 65:SQ0:43:PHE:CD1   | 2.73                     | 0.70              |
| 55:SG0:147:PHE:HZ   | 55:SG0:160:LYS:CE   | 2.03                     | 0.70              |
| 42:R60:982:C:O2'    | 66:RR0:10:ARG:NH1   | 2.22                     | 0.70              |
| 47:SC0:136:TRP:CH2  | 59:SJ0:59:ILE:HG21  | 2.23                     | 0.70              |
| 54:SFF:138:TYR:CB   | 54:RFF:133:SER:CB   | 2.69                     | 0.70              |
| 26:KN0:112:ASN:H    | 26:KN0:112:ASN:HD22 | 1.40                     | 0.70              |
| 43:RA0:120:ARG:HH11 | 47:RC0:232:ILE:HG21 | 1.57                     | 0.70              |
| 67:RS0:24:PHE:CZ    | 67:RS0:107:ILE:HG21 | 2.27                     | 0.70              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:666:A:OP1    | 63:SN0:132:LYS:NZ   | 2.25                     | 0.70              |
| 43:SA0:120:ARG:HH11 | 47:SC0:232:ILE:HG21 | 1.57                     | 0.70              |
| 52:SEE:5:ILE:HD12   | 72:SX0:63:ILE:HD12  | 1.74                     | 0.70              |
| 1:L50:796:C:H5''    | 34:LT0:131:ARG:N    | 2.06                     | 0.69              |
| 47:SC0:49:GLY:O     | 70:SV0:6:ARG:HB2    | 1.92                     | 0.69              |
| 42:R60:237:A:H5'    | 58:RI0:48:VAL:CG1   | 2.21                     | 0.69              |
| 47:RC0:49:GLY:O     | 70:RV0:6:ARG:HB2    | 1.92                     | 0.69              |
| 52:REE:5:ILE:HD12   | 72:RX0:63:ILE:HD12  | 1.74                     | 0.69              |
| 42:R60:237:A:H5'    | 58:RI0:48:VAL:HG13  | 1.74                     | 0.69              |
| 42:R60:1040:G:N2    | 42:R60:1042:A:H3'   | 2.06                     | 0.69              |
| 42:S60:237:A:H5'    | 58:SI0:48:VAL:HG13  | 1.74                     | 0.69              |
| 67:SS0:24:PHE:CZ    | 67:SS0:107:ILE:HG21 | 2.27                     | 0.69              |
| 1:K50:796:C:H5''    | 34:KT0:131:ARG:N    | 2.06                     | 0.69              |
| 45:SB0:53:THR:HG21  | 64:SO0:32:THR:OG1   | 1.92                     | 0.69              |
| 51:RE0:64:ILE:HD12  | 73:RY0:23:LEU:HD13  | 1.75                     | 0.69              |
| 14:LG0:119:ASP:OD1  | 14:LG0:145:THR:HA   | 1.92                     | 0.69              |
| 42:S60:1315:A:H2'   | 42:S60:1316:A:C8    | 2.28                     | 0.69              |
| 53:SF0:92:GLU:HG3   | 74:SZ0:108:LEU:HD12 | 1.73                     | 0.69              |
| 1:K50:535:A:O2'     | 31:KQ0:146:ASN:CB   | 2.39                     | 0.69              |
| 47:RC0:219:PRO:CB   | 71:RW0:66:ARG:NH2   | 2.51                     | 0.69              |
| 42:S60:915:A:H1'    | 54:RFF:150:LYS:HD2  | 1.73                     | 0.69              |
| 14:KG0:119:ASP:OD1  | 14:KG0:145:THR:HA   | 1.92                     | 0.69              |
| 42:R60:1315:A:H2'   | 42:R60:1316:A:C8    | 2.28                     | 0.69              |
| 43:RA0:67:SER:HA    | 70:RV0:28:VAL:CG1   | 2.22                     | 0.69              |
| 43:RA0:70:ASN:CG    | 47:RC0:240:ILE:CG1  | 2.58                     | 0.69              |
| 53:RF0:92:GLU:HG3   | 74:RZ0:108:LEU:HD12 | 1.73                     | 0.69              |
| 51:SE0:64:ILE:HD12  | 73:SY0:23:LEU:HD13  | 1.75                     | 0.69              |
| 42:R60:666:A:OP1    | 63:RN0:132:LYS:NZ   | 2.25                     | 0.69              |
| 42:R60:173:A:H8     | 51:RE0:131:VAL:CG1  | 2.04                     | 0.68              |
| 45:RB0:53:THR:HG21  | 64:RO0:32:THR:OG1   | 1.92                     | 0.68              |
| 26:LN0:112:ASN:HD22 | 26:LN0:112:ASN:H    | 1.40                     | 0.68              |
| 43:SA0:67:SER:HA    | 70:SV0:28:VAL:CG1   | 2.22                     | 0.68              |
| 53:SF0:6:THR:HG23   | 65:SQ0:53:LYS:HZ3   | 1.58                     | 0.68              |
| 42:R60:1035:C:H2'   | 42:R60:1036:A:C8    | 2.29                     | 0.68              |
| 42:S60:705:A:C2     | 42:S60:706:G:C6     | 2.82                     | 0.68              |
| 42:S60:1035:C:H2'   | 42:S60:1036:A:C8    | 2.29                     | 0.68              |
| 42:S60:1056:A:OP1   | 47:SC0:84:ALA:HB1   | 1.93                     | 0.68              |
| 43:RA0:67:SER:CB    | 70:RV0:28:VAL:HG13  | 2.24                     | 0.68              |
| 43:RA0:118:GLU:CD   | 47:RC0:31:THR:HG1   | 2.02                     | 0.68              |
| 36:LV0:98:LEU:HD23  | 37:LW0:21:TYR:HB2   | 1.75                     | 0.68              |
| 42:S60:915:A:N3     | 54:RFF:150:LYS:HG3  | 2.08                     | 0.68              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 56:SGG:65:PHE:HZ    | 66:SR0:29:TYR:OH   | 1.77                     | 0.68              |
| 56:RGG:65:PHE:HZ    | 66:RR0:29:TYR:OH   | 1.77                     | 0.68              |
| 42:R60:1056:A:OP1   | 47:RC0:84:ALA:HB1  | 1.93                     | 0.68              |
| 42:S60:173:A:H8     | 51:SE0:131:VAL:CG1 | 2.04                     | 0.67              |
| 49:SD0:94:GLN:HE21  | 60:SK0:19:SER:HB3  | 1.59                     | 0.67              |
| 1:L50:2109:G:H8     | 1:L50:2109:G:H5''  | 1.59                     | 0.67              |
| 42:R60:705:A:C2     | 42:R60:706:G:C6    | 2.82                     | 0.67              |
| 42:R60:1066:G:C5    | 60:RK0:58:PHE:CD1  | 2.83                     | 0.67              |
| 55:RG0:147:PHE:HZ   | 55:RG0:160:LYS:CE  | 2.03                     | 0.67              |
| 47:RC0:130:PRO:HB2  | 70:RV0:4:PHE:CE1   | 2.29                     | 0.67              |
| 36:KV0:98:LEU:HD23  | 37:KW0:21:TYR:HB2  | 1.75                     | 0.67              |
| 1:L50:535:A:O2'     | 31:LQ0:146:ASN:CB  | 2.38                     | 0.67              |
| 47:SC0:130:PRO:HB2  | 70:SV0:4:PHE:CE1   | 2.29                     | 0.67              |
| 50:SDD:12:LEU:HD23  | 75:SP0:67:PHE:HD2  | 1.59                     | 0.67              |
| 66:RR0:103:MET:CE   | 66:RR0:117:LEU:HG  | 2.25                     | 0.67              |
| 43:SA0:67:SER:CB    | 70:SV0:28:VAL:HG13 | 2.24                     | 0.67              |
| 47:SC0:166:LYS:CD   | 59:SJ0:100:GLU:OE2 | 2.43                     | 0.67              |
| 37:KW0:98:ASN:ND2   | 55:RG0:147:PHE:N   | 2.43                     | 0.67              |
| 47:RC0:166:LYS:CD   | 59:RJ0:100:GLU:OE2 | 2.43                     | 0.67              |
| 43:SA0:51:ILE:CG1   | 66:SR0:105:MET:SD  | 2.82                     | 0.66              |
| 1:K50:2045:C:H5'    | 20:KJ0:102:GLY:HA3 | 1.77                     | 0.66              |
| 42:R60:823:A:H2'    | 42:R60:824:A:C8    | 2.31                     | 0.66              |
| 1:K50:2109:G:H5''   | 1:K50:2109:G:H8    | 1.59                     | 0.66              |
| 43:RA0:51:ILE:CG1   | 66:RR0:105:MET:SD  | 2.82                     | 0.66              |
| 56:RGG:65:PHE:CZ    | 66:RR0:29:TYR:CZ   | 2.83                     | 0.66              |
| 67:RS0:90:TRP:CH2   | 67:RS0:91:MET:HE2  | 2.30                     | 0.66              |
| 20:LJ0:107:ILE:HD11 | 20:LJ0:113:TYR:HD1 | 1.60                     | 0.66              |
| 37:LW0:98:ASN:ND2   | 55:SG0:147:PHE:N   | 2.43                     | 0.66              |
| 42:S60:1066:G:C5    | 60:SK0:58:PHE:CD1  | 2.83                     | 0.66              |
| 43:RA0:70:ASN:CA    | 47:RC0:240:ILE:CD1 | 2.68                     | 0.66              |
| 49:RD0:94:GLN:HE21  | 60:RK0:19:SER:HB3  | 1.59                     | 0.66              |
| 50:RDD:12:LEU:HD23  | 75:RP0:67:PHE:HD2  | 1.59                     | 0.66              |
| 42:S60:823:A:H2'    | 42:S60:824:A:C8    | 2.31                     | 0.66              |
| 43:SA0:63:ARG:CD    | 70:SV0:30:LEU:HD21 | 2.24                     | 0.66              |
| 54:SFF:145:VAL:HG21 | 54:RFF:136:LYS:CB  | 2.25                     | 0.66              |
| 42:R60:958:A:OP1    | 47:RC0:111:ARG:NH2 | 2.28                     | 0.66              |
| 10:LE0:30:LEU:HD22  | 11:LEE:11:VAL:CG1  | 2.26                     | 0.66              |
| 42:S60:914:U:H3     | 42:S60:918:A:N6    | 1.94                     | 0.66              |
| 10:KE0:30:LEU:HD22  | 11:KEE:11:VAL:CG1  | 2.26                     | 0.66              |
| 42:R60:661:A:H4'    | 63:RN0:62:LYS:HE2  | 1.78                     | 0.66              |
| 56:SGG:65:PHE:CZ    | 66:SR0:29:TYR:CZ   | 2.83                     | 0.66              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:R60:1230:U:O2'   | 44:RAA:88:SER:HB3   | 1.96                     | 0.66              |
| 42:S60:958:A:OP1    | 47:SC0:111:ARG:NH2  | 2.28                     | 0.66              |
| 42:S60:1230:U:O2'   | 44:SAA:88:SER:HB3   | 1.96                     | 0.66              |
| 54:SFF:104:THR:CB   | 54:RFF:99:LYS:HD3   | 2.26                     | 0.66              |
| 66:SR0:103:MET:CE   | 66:SR0:117:LEU:HG   | 2.25                     | 0.66              |
| 67:RS0:139:VAL:O    | 67:RS0:139:VAL:HG12 | 1.96                     | 0.66              |
| 1:K50:1191:U:H2'    | 1:K50:1192:A:H5''   | 1.77                     | 0.65              |
| 43:SA0:70:ASN:CA    | 47:SC0:240:ILE:CD1  | 2.68                     | 0.65              |
| 56:SGG:228:LYS:HZ2  | 66:SR0:25:THR:HG22  | 1.58                     | 0.65              |
| 45:RB0:71:ARG:HD3   | 64:RO0:32:THR:HG21  | 1.78                     | 0.65              |
| 56:RGG:65:PHE:HZ    | 66:RR0:29:TYR:HH    | 1.40                     | 0.65              |
| 48:SCC:55:ASP:OD2   | 53:SF0:195:ARG:HD3  | 1.96                     | 0.65              |
| 67:SS0:90:TRP:CH2   | 67:SS0:91:MET:HE2   | 2.30                     | 0.65              |
| 48:RCC:55:ASP:OD2   | 53:RF0:195:ARG:HD3  | 1.96                     | 0.65              |
| 1:L50:1018:U:O2'    | 13:LFF:78:ARG:HD2   | 1.97                     | 0.65              |
| 1:L50:1191:U:H2'    | 1:L50:1192:A:H5''   | 1.77                     | 0.65              |
| 45:SB0:71:ARG:HD3   | 64:SO0:32:THR:HG21  | 1.78                     | 0.65              |
| 20:KJ0:107:ILE:HD11 | 20:KJ0:113:TYR:HD1  | 1.60                     | 0.65              |
| 42:R60:1066:G:C6    | 60:RK0:58:PHE:CZ    | 2.84                     | 0.65              |
| 42:S60:661:A:H4'    | 63:SN0:62:LYS:HE2   | 1.78                     | 0.65              |
| 42:S60:826:U:O2     | 47:SC0:81:GLN:HB3   | 1.96                     | 0.65              |
| 1:K50:1018:U:O2'    | 13:KFF:78:ARG:HD2   | 1.97                     | 0.65              |
| 42:R60:910:A:H62    | 42:R60:922:G:H21    | 1.44                     | 0.65              |
| 42:R60:982:C:H4'    | 66:RR0:10:ARG:HH11  | 1.62                     | 0.65              |
| 42:S60:1066:G:C6    | 60:SK0:58:PHE:CZ    | 2.84                     | 0.65              |
| 42:S60:840:C:O2'    | 42:S60:1182:G:OP1   | 2.14                     | 0.65              |
| 42:S60:892:A:N3     | 75:SP0:115:TYR:OH   | 2.29                     | 0.65              |
| 42:R60:840:C:O2'    | 42:R60:1182:G:OP1   | 2.14                     | 0.65              |
| 51:SE0:137:PRO:HG3  | 55:SG0:222:TRP:HE1  | 1.63                     | 0.64              |
| 55:SG0:169:VAL:HG11 | 55:SG0:176:LYS:HE2  | 1.79                     | 0.64              |
| 67:SS0:24:PHE:O     | 67:SS0:25:ASN:OD1   | 2.15                     | 0.64              |
| 47:RC0:136:TRP:HH2  | 59:RJ0:59:ILE:HG23  | 1.60                     | 0.64              |
| 53:RF0:6:THR:HG23   | 65:RQ0:53:LYS:HZ3   | 1.60                     | 0.64              |
| 1:K50:1691:A:C6     | 42:R60:1248:G:C4'   | 2.80                     | 0.64              |
| 1:L50:1691:A:C6     | 42:S60:1248:G:C4'   | 2.80                     | 0.64              |
| 56:SGG:65:PHE:HZ    | 66:SR0:29:TYR:HH    | 1.41                     | 0.64              |
| 42:R60:826:U:O2     | 47:RC0:81:GLN:HB3   | 1.96                     | 0.64              |
| 42:R60:1160:A:H2'   | 75:RP0:58:LYS:HD3   | 1.80                     | 0.64              |
| 67:RS0:24:PHE:O     | 67:RS0:25:ASN:OD1   | 2.15                     | 0.64              |
| 1:L50:2045:C:H5'    | 20:LJ0:102:GLY:HA3  | 1.77                     | 0.64              |
| 37:LW0:99:LYS:HA    | 37:LW0:102:LYS:CD   | 2.27                     | 0.64              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:1144:G:C2'   | 42:S60:1145:G:H5'   | 2.27                     | 0.64              |
| 49:SD0:33:ILE:HG21  | 69:SU0:26:LEU:HD21  | 1.79                     | 0.64              |
| 54:SFF:145:VAL:HG22 | 54:RFF:133:SER:O    | 1.98                     | 0.64              |
| 37:LW0:99:LYS:O     | 37:LW0:102:LYS:HG2  | 1.97                     | 0.64              |
| 42:S60:982:C:H4'    | 66:SR0:10:ARG:HH11  | 1.62                     | 0.64              |
| 1:K50:1694:U:O4     | 42:R60:1249:U:H4'   | 1.98                     | 0.64              |
| 34:KT0:5:HIS:HA     | 34:KT0:9:ARG:HD2    | 1.80                     | 0.64              |
| 37:KW0:99:LYS:HG2   | 37:KW0:102:LYS:HE2  | 1.80                     | 0.64              |
| 56:RGG:105:ARG:HH22 | 66:RR0:37:ASP:CA    | 2.11                     | 0.64              |
| 37:KW0:99:LYS:O     | 37:KW0:102:LYS:HG2  | 1.98                     | 0.64              |
| 42:R60:1144:G:C2'   | 42:R60:1145:G:H5'   | 2.27                     | 0.64              |
| 20:LJ0:107:ILE:HD11 | 20:LJ0:113:TYR:CD1  | 2.33                     | 0.64              |
| 37:LW0:99:LYS:HG2   | 37:LW0:102:LYS:NZ   | 2.13                     | 0.64              |
| 54:SFF:150:LYS:HB2  | 42:R60:915:A:H1'    | 1.80                     | 0.64              |
| 48:RCC:50:LEU:CD1   | 53:RF0:26:ILE:HD12  | 2.28                     | 0.64              |
| 49:RD0:33:ILE:HG21  | 69:RU0:26:LEU:HD21  | 1.79                     | 0.64              |
| 53:RF0:96:GLY:O     | 74:RZ0:108:LEU:HD23 | 1.97                     | 0.64              |
| 42:S60:1160:A:H2'   | 75:SP0:58:LYS:HD3   | 1.80                     | 0.63              |
| 67:SS0:24:PHE:O     | 67:SS0:25:ASN:CG    | 2.41                     | 0.63              |
| 49:RD0:94:GLN:HE21  | 60:RK0:19:SER:CB    | 2.11                     | 0.63              |
| 67:RS0:24:PHE:O     | 67:RS0:25:ASN:CG    | 2.41                     | 0.63              |
| 48:SCC:50:LEU:HD13  | 53:SF0:26:ILE:HD12  | 1.80                     | 0.63              |
| 73:SY0:116:ARG:NH2  | 73:SY0:120:LYS:HZ1  | 1.95                     | 0.63              |
| 20:KJ0:107:ILE:HD11 | 20:KJ0:113:TYR:CD1  | 2.33                     | 0.63              |
| 43:RA0:70:ASN:ND2   | 47:RC0:240:ILE:CG1  | 2.61                     | 0.63              |
| 41:MD1:52:LYS:HG3   | 42:S60:606:G:C2     | 2.32                     | 0.63              |
| 54:SFF:104:THR:CG2  | 54:RFF:99:LYS:HD3   | 2.29                     | 0.63              |
| 56:SGG:105:ARG:HH22 | 66:SR0:37:ASP:CA    | 2.11                     | 0.63              |
| 41:MD2:52:LYS:HG3   | 42:R60:606:G:C2     | 2.32                     | 0.63              |
| 49:SD0:94:GLN:HE21  | 60:SK0:19:SER:CB    | 2.11                     | 0.63              |
| 42:R60:1091:A:O4'   | 75:RP0:146:HIS:HD2  | 1.81                     | 0.63              |
| 51:RE0:137:PRO:HG3  | 55:RG0:222:TRP:HE1  | 1.63                     | 0.63              |
| 34:LT0:5:HIS:HA     | 34:LT0:9:ARG:HD2    | 1.80                     | 0.63              |
| 42:S60:1158:U:H4'   | 50:SDD:7:LYS:HE3    | 1.81                     | 0.63              |
| 54:SFF:145:VAL:CG2  | 54:RFF:133:SER:O    | 2.47                     | 0.63              |
| 66:SR0:3:GLN:HG3    | 66:SR0:3:GLN:O      | 1.99                     | 0.63              |
| 37:KW0:99:LYS:HA    | 37:KW0:102:LYS:CD   | 2.27                     | 0.63              |
| 43:RA0:206:ARG:NE   | 66:RR0:86:PRO:CG    | 2.62                     | 0.63              |
| 47:SC0:49:GLY:O     | 70:SV0:6:ARG:HD2    | 1.99                     | 0.63              |
| 42:S60:1085:G:H5''  | 75:SP0:140:THR:HG21 | 1.81                     | 0.63              |
| 53:SF0:96:GLY:O     | 74:SZ0:108:LEU:HD23 | 1.97                     | 0.63              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 37:LW0:99:LYS:HG2   | 37:LW0:102:LYS:HE2  | 1.80                     | 0.63              |
| 67:SS0:24:PHE:CE1   | 67:SS0:107:ILE:HG21 | 2.34                     | 0.63              |
| 1:L50:1694:U:O4     | 42:S60:1249:U:H4'   | 1.98                     | 0.63              |
| 42:S60:910:A:H62    | 42:S60:922:G:H21    | 1.44                     | 0.63              |
| 67:SS0:139:VAL:O    | 67:SS0:139:VAL:HG12 | 1.96                     | 0.63              |
| 42:R60:892:A:N3     | 75:RP0:115:TYR:OH   | 2.29                     | 0.63              |
| 47:RC0:49:GLY:O     | 70:RV0:6:ARG:HD2    | 1.99                     | 0.63              |
| 42:S60:1034:A:H2'   | 42:S60:1035:C:H6    | 1.63                     | 0.62              |
| 49:RD0:184:ILE:HD11 | 49:RD0:230:MET:SD   | 2.39                     | 0.62              |
| 42:S60:1091:A:O4'   | 75:SP0:146:HIS:HD2  | 1.81                     | 0.62              |
| 48:SCC:50:LEU:CD1   | 53:SF0:26:ILE:HD12  | 2.28                     | 0.62              |
| 42:S60:1105:G:C8    | 42:S60:1105:G:H5''  | 2.34                     | 0.62              |
| 43:SA0:206:ARG:NE   | 66:SR0:86:PRO:CG    | 2.62                     | 0.62              |
| 42:R60:914:U:H3     | 42:R60:918:A:N6     | 1.94                     | 0.62              |
| 56:RGG:65:PHE:HZ    | 66:RR0:29:TYR:CZ    | 2.17                     | 0.62              |
| 49:SD0:184:ILE:HD11 | 49:SD0:230:MET:SD   | 2.39                     | 0.62              |
| 54:SFF:135:ASN:HB2  | 54:RFF:145:VAL:HG23 | 1.80                     | 0.62              |
| 42:R60:1181:U:OP1   | 65:RQ0:142:TYR:HE2  | 1.82                     | 0.62              |
| 56:SGG:65:PHE:HZ    | 66:SR0:29:TYR:CZ    | 2.17                     | 0.62              |
| 37:KW0:99:LYS:HG2   | 37:KW0:102:LYS:NZ   | 2.13                     | 0.62              |
| 55:RG0:169:VAL:HG11 | 55:RG0:176:LYS:HE2  | 1.79                     | 0.62              |
| 43:RA0:52:LYS:HB3   | 66:RR0:109:TYR:CZ   | 2.35                     | 0.62              |
| 43:RA0:140:VAL:O    | 43:RA0:141:ASN:OD1  | 2.17                     | 0.62              |
| 48:RCC:50:LEU:HD13  | 53:RF0:26:ILE:HD12  | 1.79                     | 0.62              |
| 67:RS0:24:PHE:CE1   | 67:RS0:107:ILE:HG21 | 2.34                     | 0.62              |
| 42:S60:1181:U:OP1   | 65:SQ0:142:TYR:HE2  | 1.82                     | 0.62              |
| 53:SF0:40:LEU:CD2   | 65:SQ0:43:PHE:HD1   | 2.12                     | 0.62              |
| 27:LO0:1:MET:HE3    | 27:LO0:4:LYS:HD2    | 1.82                     | 0.62              |
| 66:RR0:3:GLN:HG3    | 66:RR0:3:GLN:O      | 1.99                     | 0.62              |
| 47:SC0:136:TRP:HH2  | 59:SJ0:59:ILE:HG23  | 1.60                     | 0.62              |
| 42:R60:1085:G:H5''  | 75:RP0:140:THR:HG21 | 1.81                     | 0.62              |
| 43:SA0:140:VAL:O    | 43:SA0:141:ASN:OD1  | 2.17                     | 0.62              |
| 42:R60:1158:U:O2'   | 50:RDD:7:LYS:NZ     | 2.19                     | 0.62              |
| 53:RF0:40:LEU:CD2   | 65:RQ0:43:PHE:HD1   | 2.12                     | 0.61              |
| 53:RF0:40:LEU:O     | 53:RF0:42:HIS:N     | 2.33                     | 0.61              |
| 43:SA0:51:ILE:HG13  | 66:SR0:105:MET:CE   | 2.30                     | 0.61              |
| 2:K70:26:C:OP1      | 8:KD0:62:THR:HG21   | 2.01                     | 0.61              |
| 43:SA0:215:TYR:O    | 66:SR0:84:PHE:CE2   | 2.51                     | 0.61              |
| 27:KO0:1:MET:HE3    | 27:KO0:4:LYS:HD2    | 1.82                     | 0.61              |
| 42:S60:982:C:C3'    | 66:SR0:10:ARG:NH1   | 2.63                     | 0.61              |
| 37:KW0:83:PHE:CE1   | 37:KW0:84:PRO:HD2   | 2.34                     | 0.61              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:R60:982:C:C3'    | 66:RR0:10:ARG:NH1   | 2.63                     | 0.61              |
| 37:LW0:98:ASN:HD22  | 55:SG0:146:GLY:C    | 2.08                     | 0.61              |
| 43:SA0:102:ARG:HD2  | 43:SA0:102:ARG:N    | 2.16                     | 0.61              |
| 48:SCC:58:ARG:NH1   | 64:SO0:101:ARG:NH2  | 2.49                     | 0.61              |
| 42:R60:1158:U:H4'   | 50:RDD:7:LYS:HE3    | 1.81                     | 0.61              |
| 55:RG0:169:VAL:HG12 | 55:RG0:176:LYS:HE2  | 1.82                     | 0.61              |
| 42:S60:924:U:H1'    | 42:S60:925:A:N7     | 2.16                     | 0.61              |
| 42:S60:1099:U:H1'   | 68:ST0:91:ASN:OD1   | 2.01                     | 0.61              |
| 62:SM0:67:SER:O     | 62:SM0:71:LYS:HG2   | 2.01                     | 0.61              |
| 42:R60:1034:A:H2'   | 42:R60:1035:C:H6    | 1.63                     | 0.61              |
| 43:RA0:102:ARG:HD2  | 43:RA0:102:ARG:N    | 2.16                     | 0.61              |
| 43:RA0:118:GLU:OE2  | 47:RC0:31:THR:OG1   | 2.18                     | 0.61              |
| 43:RA0:4:ARG:O      | 70:RV0:30:LEU:CD1   | 2.47                     | 0.61              |
| 42:S60:924:U:H1'    | 42:S60:925:A:C5     | 2.36                     | 0.61              |
| 42:R60:1105:G:C8    | 42:R60:1105:G:H5''  | 2.34                     | 0.61              |
| 43:RA0:63:ARG:CD    | 70:RV0:30:LEU:HD21  | 2.24                     | 0.61              |
| 42:S60:554:A:N3     | 71:SW0:103:THR:CG2  | 2.62                     | 0.61              |
| 37:KW0:98:ASN:HD22  | 55:RG0:146:GLY:C    | 2.08                     | 0.61              |
| 12:LF0:115:ASN:HD21 | 34:LT0:133:PRO:HB2  | 1.66                     | 0.60              |
| 42:S60:988:A:H4'    | 43:SA0:105:PRO:HG2  | 1.83                     | 0.60              |
| 43:RA0:51:ILE:HG13  | 66:RR0:105:MET:CE   | 2.30                     | 0.60              |
| 43:RA0:67:SER:OG    | 70:RV0:40:LEU:HD21  | 2.01                     | 0.60              |
| 43:RA0:120:ARG:NH1  | 47:RC0:232:ILE:HG21 | 2.15                     | 0.60              |
| 56:RG0:228:LYS:HZ3  | 66:RR0:25:THR:HG22  | 1.66                     | 0.60              |
| 2:L70:26:C:OP1      | 8:LD0:62:THR:HG21   | 2.01                     | 0.60              |
| 1:K50:343:A:H1'     | 19:KII:84:MET:HE3   | 1.83                     | 0.60              |
| 1:K50:2042:A:H61    | 1:K50:2054:U:H3     | 1.48                     | 0.60              |
| 42:R60:1099:U:H1'   | 68:RT0:91:ASN:OD1   | 2.01                     | 0.60              |
| 21:LJJ:90:ILE:O     | 21:LJJ:90:ILE:HG22  | 2.02                     | 0.60              |
| 43:SA0:120:ARG:NH1  | 47:SC0:232:ILE:HG21 | 2.15                     | 0.60              |
| 21:KJJ:90:ILE:O     | 21:KJJ:90:ILE:HG22  | 2.02                     | 0.60              |
| 42:R60:1166:A:O2'   | 67:RS0:90:TRP:O     | 2.19                     | 0.60              |
| 42:R60:924:U:H1'    | 42:R60:925:A:N7     | 2.16                     | 0.60              |
| 43:RA0:52:LYS:CB    | 66:RR0:109:TYR:CE1  | 2.84                     | 0.60              |
| 43:RA0:184:TYR:CE1  | 70:RV0:35:ARG:NH1   | 2.69                     | 0.60              |
| 62:RM0:67:SER:O     | 62:RM0:71:LYS:HG2   | 2.01                     | 0.60              |
| 37:LW0:83:PHE:CE1   | 37:LW0:84:PRO:HD2   | 2.34                     | 0.60              |
| 43:SA0:52:LYS:CB    | 66:SR0:109:TYR:CE1  | 2.84                     | 0.60              |
| 42:R60:924:U:H1'    | 42:R60:925:A:C5     | 2.36                     | 0.60              |
| 43:SA0:70:ASN:ND2   | 47:SC0:240:ILE:CG1  | 2.61                     | 0.60              |
| 43:SA0:184:TYR:CE1  | 70:SV0:35:ARG:NH1   | 2.69                     | 0.60              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:R60:705:A:N3     | 42:R60:706:G:O6     | 2.35                     | 0.60              |
| 43:RA0:63:ARG:NH1   | 70:RV0:30:LEU:HG    | 2.17                     | 0.60              |
| 43:SA0:70:ASN:CG    | 47:SC0:240:ILE:CG1  | 2.58                     | 0.60              |
| 1:K50:733:A:O3'     | 12:KF0:124:LYS:NZ   | 2.35                     | 0.60              |
| 62:RM0:15:LEU:HB3   | 62:RM0:122:PHE:HE2  | 1.67                     | 0.60              |
| 42:S60:1166:A:O2'   | 67:SS0:90:TRP:O     | 2.19                     | 0.60              |
| 43:SA0:117:ARG:NH1  | 47:SC0:243:GLU:CD   | 2.48                     | 0.60              |
| 42:S60:1143:A:H5'   | 67:SS0:36:LYS:HE3   | 1.84                     | 0.60              |
| 1:L50:2042:A:H61    | 1:L50:2054:U:H3     | 1.48                     | 0.60              |
| 42:S60:856:U:O4     | 67:SS0:146:SER:HB3  | 2.02                     | 0.60              |
| 42:S60:999:C:H2'    | 42:S60:1000:C:C6    | 2.37                     | 0.60              |
| 43:SA0:52:LYS:HB3   | 66:SR0:109:TYR:CZ   | 2.35                     | 0.60              |
| 55:SG0:169:VAL:HG12 | 55:SG0:176:LYS:HE2  | 1.82                     | 0.60              |
| 55:SG0:170:ASN:HD21 | 55:SG0:176:LYS:CD   | 2.15                     | 0.60              |
| 1:K50:1728:U:O2'    | 42:R60:1259:U:O2'   | 1.93                     | 0.60              |
| 42:R60:554:A:N3     | 71:RW0:103:THR:CG2  | 2.62                     | 0.60              |
| 42:R60:856:U:O4     | 67:RS0:146:SER:HB3  | 2.02                     | 0.60              |
| 43:SA0:4:ARG:O      | 70:SV0:30:LEU:CD1   | 2.47                     | 0.59              |
| 12:KF0:115:ASN:HD21 | 34:KT0:133:PRO:HB2  | 1.66                     | 0.59              |
| 37:KW0:99:LYS:HG2   | 37:KW0:102:LYS:CE   | 2.33                     | 0.59              |
| 42:R60:988:A:H4'    | 43:RA0:105:PRO:HG2  | 1.83                     | 0.59              |
| 50:RDD:34:PHE:CE1   | 60:RK0:61:GLN:NE2   | 2.70                     | 0.59              |
| 1:L50:343:A:H1'     | 19:LII:84:MET:HE3   | 1.83                     | 0.59              |
| 53:SF0:90:ILE:HG23  | 74:SZ0:58:ILE:CD1   | 2.32                     | 0.59              |
| 43:RA0:117:ARG:NH1  | 47:RC0:243:GLU:CD   | 2.48                     | 0.59              |
| 49:RD0:94:GLN:HG2   | 60:RK0:20:ILE:HG23  | 1.84                     | 0.59              |
| 42:S60:982:C:HO2'   | 66:SR0:10:ARG:HH12  | 1.51                     | 0.59              |
| 43:SA0:10:ASP:CG    | 66:SR0:112:ASN:HD21 | 2.10                     | 0.59              |
| 44:SAA:69:TYR:HE2   | 64:SO0:90:LYS:O     | 1.86                     | 0.59              |
| 42:R60:1143:A:H5'   | 67:RS0:36:LYS:HE3   | 1.84                     | 0.59              |
| 43:RA0:10:ASP:CG    | 66:RR0:112:ASN:HD21 | 2.10                     | 0.59              |
| 55:RG0:170:ASN:HD21 | 55:RG0:176:LYS:CD   | 2.15                     | 0.59              |
| 42:R60:403:A:H2'    | 42:R60:404:C:C6     | 2.37                     | 0.59              |
| 1:L50:733:A:O3'     | 12:LF0:124:LYS:NZ   | 2.35                     | 0.59              |
| 42:S60:403:A:H2'    | 42:S60:404:C:C6     | 2.37                     | 0.59              |
| 42:S60:1007:U:C4    | 56:SGG:84:ASP:OD2   | 2.56                     | 0.59              |
| 43:SA0:18:GLN:HE22  | 66:SR0:96:VAL:HB    | 1.67                     | 0.59              |
| 42:R60:945:G:OP1    | 49:RD0:211:LYS:HE3  | 2.03                     | 0.59              |
| 42:R60:1007:U:C4    | 56:RGG:84:ASP:OD2   | 2.56                     | 0.59              |
| 50:RDD:12:LEU:HD11  | 75:RP0:75:ILE:HD13  | 1.84                     | 0.59              |
| 53:RF0:90:ILE:HG23  | 74:RZ0:58:ILE:CD1   | 2.32                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:LW0:99:LYS:HG2  | 37:LW0:102:LYS:CE  | 2.33                     | 0.59              |
| 42:S60:405:A:H2'   | 42:S60:406:U:C6    | 2.38                     | 0.59              |
| 42:S60:918:A:C8    | 42:S60:919:C:C5    | 2.90                     | 0.59              |
| 50:SDD:12:LEU:HD11 | 75:SP0:75:ILE:HD13 | 1.84                     | 0.59              |
| 54:SFF:143:TYR:HB3 | 54:RFF:134:GLY:HA2 | 1.85                     | 0.59              |
| 42:R60:999:C:H2'   | 42:R60:1000:C:C6   | 2.37                     | 0.59              |
| 54:RFF:96:GLN:O    | 54:RFF:96:GLN:HG2  | 2.02                     | 0.59              |
| 42:R60:918:A:C8    | 42:R60:919:C:C5    | 2.90                     | 0.59              |
| 42:R60:1125:G:H2'  | 42:R60:1126:A:O4'  | 2.03                     | 0.59              |
| 47:RC0:148:VAL:CG2 | 71:RW0:97:PHE:HE1  | 2.15                     | 0.59              |
| 42:S60:203:G:C2    | 51:SE0:33:THR:HG21 | 2.38                     | 0.59              |
| 42:S60:705:A:N3    | 42:S60:706:G:O6    | 2.35                     | 0.59              |
| 53:SF0:40:LEU:O    | 53:SF0:42:HIS:N    | 2.33                     | 0.59              |
| 54:SFF:96:GLN:HG2  | 54:SFF:96:GLN:O    | 2.02                     | 0.59              |
| 54:SFF:132:ARG:CA  | 42:R60:918:A:O5'   | 2.51                     | 0.59              |
| 7:KCC:64:ILE:CG2   | 40:KZ0:39:LEU:HD11 | 2.33                     | 0.59              |
| 47:RC0:148:VAL:CG2 | 71:RW0:97:PHE:CE1  | 2.86                     | 0.59              |
| 10:LE0:30:LEU:CD2  | 11:LEE:11:VAL:HG13 | 2.33                     | 0.59              |
| 10:KE0:30:LEU:CD2  | 11:KEE:11:VAL:HG13 | 2.33                     | 0.59              |
| 43:RA0:63:ARG:NH1  | 70:RV0:30:LEU:H    | 2.01                     | 0.59              |
| 47:SC0:148:VAL:CG2 | 71:SW0:97:PHE:CE1  | 2.86                     | 0.59              |
| 54:SFF:118:ARG:NH1 | 54:RFF:97:ASP:CB   | 2.66                     | 0.59              |
| 37:KW0:95:ARG:HG2  | 37:KW0:99:LYS:HE3  | 1.85                     | 0.59              |
| 51:RE0:64:ILE:CD1  | 73:RY0:23:LEU:HD13 | 2.33                     | 0.59              |
| 49:SD0:94:GLN:HG2  | 60:SK0:20:ILE:HG23 | 1.84                     | 0.58              |
| 10:KE0:23:ILE:CD1  | 11:KEE:79:ARG:HH12 | 2.16                     | 0.58              |
| 12:LF0:188:LYS:HE3 | 31:LQ0:2:LEU:HD23  | 1.85                     | 0.58              |
| 42:S60:945:G:OP1   | 49:SD0:211:LYS:HE3 | 2.03                     | 0.58              |
| 43:SA0:102:ARG:H   | 43:SA0:102:ARG:CD  | 2.15                     | 0.58              |
| 12:KF0:188:LYS:HE3 | 31:KQ0:2:LEU:HD23  | 1.85                     | 0.58              |
| 42:R60:203:G:C2    | 51:RE0:33:THR:HG21 | 2.38                     | 0.58              |
| 50:SDD:34:PHE:CE1  | 60:SK0:61:GLN:NE2  | 2.70                     | 0.58              |
| 43:RA0:18:GLN:HE22 | 66:RR0:96:VAL:HB   | 1.67                     | 0.58              |
| 42:S60:1125:G:H2'  | 42:S60:1126:A:O4'  | 2.03                     | 0.58              |
| 43:SA0:118:GLU:OE2 | 47:SC0:31:THR:OG1  | 2.18                     | 0.58              |
| 44:RAA:69:TYR:HE2  | 64:RO0:90:LYS:O    | 1.86                     | 0.58              |
| 53:RF0:40:LEU:HD23 | 65:RQ0:43:PHE:CD1  | 2.38                     | 0.58              |
| 42:S60:999:C:H42   | 42:S60:1049:G:H1   | 1.52                     | 0.58              |
| 42:S60:1152:G:OP1  | 75:SP0:36:LYS:NZ   | 2.37                     | 0.58              |
| 43:SA0:63:ARG:NH1  | 70:SV0:30:LEU:H    | 2.01                     | 0.58              |
| 43:SA0:67:SER:OG   | 70:SV0:40:LEU:HD21 | 2.01                     | 0.58              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 51:SE0:64:ILE:CD1   | 73:SY0:23:LEU:HD13  | 2.33                     | 0.58              |
| 67:SS0:55:ARG:HH22  | 68:ST0:32:ASN:HD22  | 1.51                     | 0.58              |
| 48:RCC:58:ARG:NH1   | 64:RO0:101:ARG:NH2  | 2.49                     | 0.58              |
| 43:SA0:206:ARG:CZ   | 66:SR0:86:PRO:HG2   | 2.34                     | 0.58              |
| 42:R60:187:A:H62    | 42:R60:194:U:H3     | 1.51                     | 0.58              |
| 10:LE0:23:ILE:CD1   | 11:LEE:79:ARG:HH12  | 2.16                     | 0.58              |
| 37:LW0:95:ARG:HG2   | 37:LW0:99:LYS:HE3   | 1.85                     | 0.58              |
| 42:S60:1144:G:H2'   | 42:S60:1145:G:H5'   | 1.84                     | 0.58              |
| 42:R60:1144:G:H2'   | 42:R60:1145:G:H5'   | 1.84                     | 0.58              |
| 43:RA0:102:ARG:H    | 43:RA0:102:ARG:CD   | 2.15                     | 0.58              |
| 1:L50:2596:G:O2'    | 5:LB0:173:PRO:HG2   | 2.04                     | 0.58              |
| 43:SA0:51:ILE:HD12  | 66:SR0:105:MET:CG   | 2.32                     | 0.58              |
| 42:R60:405:A:H2'    | 42:R60:406:U:C6     | 2.38                     | 0.58              |
| 49:RD0:36:ARG:NH1   | 69:RU0:112:GLU:CD   | 2.62                     | 0.58              |
| 49:RD0:238:PRO:CA   | 66:RR0:19:ARG:NH1   | 2.63                     | 0.58              |
| 56:RGG:228:LYS:HZ2  | 66:RR0:25:THR:HG22  | 1.68                     | 0.58              |
| 42:R60:1023:A:P     | 66:RR0:3:GLN:CD     | 2.87                     | 0.58              |
| 42:R60:1152:G:OP1   | 75:RP0:36:LYS:NZ    | 2.37                     | 0.58              |
| 50:RDD:8:TYR:CZ     | 75:RP0:72:ARG:CD    | 2.84                     | 0.58              |
| 42:S60:1023:A:P     | 66:SR0:3:GLN:CD     | 2.87                     | 0.58              |
| 54:SFF:147:ILE:CD1  | 54:RFF:147:ILE:HD11 | 2.31                     | 0.58              |
| 37:KW0:99:LYS:CG    | 37:KW0:102:LYS:HE2  | 2.34                     | 0.58              |
| 42:R60:1107:U:H5''  | 68:RT0:43:GLU:HG2   | 1.86                     | 0.58              |
| 43:SA0:197:ARG:HB3  | 66:SR0:91:LEU:CB    | 2.34                     | 0.57              |
| 54:SFF:145:VAL:HG21 | 54:RFF:136:LYS:H    | 1.69                     | 0.57              |
| 37:LW0:83:PHE:CD1   | 37:LW0:84:PRO:CD    | 2.81                     | 0.57              |
| 42:S60:1107:U:H5''  | 68:ST0:43:GLU:HG2   | 1.86                     | 0.57              |
| 43:SA0:51:ILE:N     | 66:SR0:105:MET:SD   | 2.77                     | 0.57              |
| 53:SF0:40:LEU:HD23  | 65:SQ0:43:PHE:CD1   | 2.38                     | 0.57              |
| 34:KT0:112:ASN:C    | 34:KT0:112:ASN:HD22 | 2.11                     | 0.57              |
| 37:KW0:99:LYS:HA    | 37:KW0:102:LYS:HG2  | 1.85                     | 0.57              |
| 43:RA0:206:ARG:CZ   | 66:RR0:86:PRO:HG2   | 2.34                     | 0.57              |
| 37:LW0:99:LYS:HA    | 37:LW0:102:LYS:HG2  | 1.85                     | 0.57              |
| 47:SC0:148:VAL:CG2  | 71:SW0:97:PHE:HE1   | 2.15                     | 0.57              |
| 43:RA0:52:LYS:CD    | 66:RR0:109:TYR:CE1  | 2.87                     | 0.57              |
| 7:LCC:64:ILE:CG2    | 40:LZ0:39:LEU:HD11  | 2.33                     | 0.57              |
| 43:RA0:51:ILE:N     | 66:RR0:105:MET:SD   | 2.77                     | 0.57              |
| 43:SA0:52:LYS:CD    | 66:SR0:109:TYR:CE1  | 2.87                     | 0.57              |
| 43:SA0:120:ARG:NH1  | 47:SC0:232:ILE:HD13 | 2.19                     | 0.57              |
| 49:SD0:36:ARG:NH1   | 69:SU0:112:GLU:CD   | 2.62                     | 0.57              |
| 62:SM0:15:LEU:HB3   | 62:SM0:122:PHE:HE2  | 1.67                     | 0.57              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 37:KW0:98:ASN:HD22  | 55:RG0:147:PHE:CA   | 2.15                     | 0.57              |
| 42:R60:999:C:H42    | 42:R60:1049:G:H1    | 1.52                     | 0.57              |
| 42:R60:1091:A:O4'   | 75:RP0:146:HIS:CD2  | 2.57                     | 0.57              |
| 37:LW0:98:ASN:ND2   | 55:SG0:146:GLY:C    | 2.63                     | 0.57              |
| 43:SA0:215:TYR:CA   | 66:SR0:84:PHE:CE2   | 2.87                     | 0.57              |
| 1:K50:1691:A:C6     | 42:R60:1248:G:C1'   | 2.87                     | 0.57              |
| 43:RA0:66:CYS:HB2   | 70:RV0:28:VAL:HG21  | 1.85                     | 0.57              |
| 43:RA0:197:ARG:HB3  | 66:RR0:91:LEU:CB    | 2.34                     | 0.57              |
| 43:RA0:206:ARG:CD   | 66:RR0:86:PRO:HG2   | 2.35                     | 0.57              |
| 53:RF0:90:ILE:HG23  | 74:RZ0:58:ILE:HD13  | 1.86                     | 0.57              |
| 43:SA0:206:ARG:CD   | 66:SR0:86:PRO:HG2   | 2.35                     | 0.57              |
| 37:LW0:99:LYS:CG    | 37:LW0:102:LYS:HE2  | 2.34                     | 0.57              |
| 43:SA0:63:ARG:CG    | 70:SV0:30:LEU:CD2   | 2.67                     | 0.57              |
| 51:SE0:152:PRO:HD2  | 55:SG0:219:TYR:CE1  | 2.40                     | 0.57              |
| 1:K50:2596:G:O2'    | 5:KB0:173:PRO:HG2   | 2.04                     | 0.57              |
| 37:KW0:98:ASN:ND2   | 55:RG0:146:GLY:C    | 2.63                     | 0.57              |
| 42:R60:1160:A:H5'   | 75:RP0:133:ARG:NH2  | 2.20                     | 0.57              |
| 42:R60:1290:G:H5''  | 42:R60:1290:G:H8    | 1.70                     | 0.57              |
| 43:RA0:120:ARG:NH1  | 47:RC0:232:ILE:HD13 | 2.19                     | 0.57              |
| 43:RA0:215:TYR:CA   | 66:RR0:84:PHE:CE2   | 2.87                     | 0.57              |
| 34:LT0:112:ASN:HD22 | 34:LT0:112:ASN:C    | 2.11                     | 0.57              |
| 43:SA0:63:ARG:NH1   | 70:SV0:30:LEU:HG    | 2.17                     | 0.57              |
| 49:SD0:237:LEU:O    | 66:SR0:19:ARG:CZ    | 2.53                     | 0.57              |
| 37:LW0:99:LYS:C     | 37:LW0:102:LYS:HG2  | 2.30                     | 0.56              |
| 42:R60:923:A:H5'    | 42:R60:924:U:C4     | 2.40                     | 0.56              |
| 67:RS0:55:ARG:HH22  | 68:RT0:32:ASN:HD22  | 1.51                     | 0.56              |
| 1:L50:796:C:H5'     | 34:LT0:131:ARG:HE   | 1.70                     | 0.56              |
| 42:S60:187:A:H62    | 42:S60:194:U:H3     | 1.51                     | 0.56              |
| 42:S60:1007:U:O4    | 56:SGG:84:ASP:OD2   | 2.23                     | 0.56              |
| 43:SA0:70:ASN:HB2   | 47:SC0:240:ILE:HG13 | 1.75                     | 0.56              |
| 47:SC0:230:ASN:HB2  | 70:SV0:24:GLN:NE2   | 2.20                     | 0.56              |
| 42:R60:864:A:N7     | 75:RP0:118:ARG:NH2  | 2.53                     | 0.56              |
| 1:L50:1405:G:H2'    | 1:L50:1406:G:C8     | 2.40                     | 0.56              |
| 1:L50:1691:A:C6     | 42:S60:1248:G:C1'   | 2.87                     | 0.56              |
| 37:LW0:98:ASN:HD22  | 55:SG0:147:PHE:CA   | 2.15                     | 0.56              |
| 42:S60:864:A:N7     | 75:SP0:118:ARG:NH2  | 2.53                     | 0.56              |
| 42:S60:1230:U:H4'   | 44:SAA:88:SER:HB3   | 1.88                     | 0.56              |
| 42:S60:1290:G:H5''  | 42:S60:1290:G:H8    | 1.70                     | 0.56              |
| 43:SA0:66:CYS:HB2   | 70:SV0:28:VAL:HG21  | 1.86                     | 0.56              |
| 37:KW0:99:LYS:C     | 37:KW0:102:LYS:HG2  | 2.30                     | 0.56              |
| 20:LJ0:82:LYS:HB2   | 75:SP0:30:PHE:HE2   | 1.65                     | 0.56              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 42:S60:1066:G:C6    | 60:SK0:58:PHE:CE1  | 2.93                     | 0.56              |
| 4:KAA:70:THR:HG21   | 19:KII:6:LEU:HG    | 1.88                     | 0.56              |
| 42:R60:1230:U:H4'   | 44:RAA:88:SER:HB3  | 1.88                     | 0.56              |
| 42:S60:1089:G:O4'   | 75:SP0:141:ARG:HD3 | 2.06                     | 0.56              |
| 42:S60:1091:A:O4'   | 75:SP0:146:HIS:CD2 | 2.57                     | 0.56              |
| 53:SF0:90:ILE:HG23  | 74:SZ0:58:ILE:HD13 | 1.86                     | 0.56              |
| 2:K70:60:A:H5'      | 8:KD0:273:LYS:HG2  | 1.88                     | 0.56              |
| 42:R60:1066:G:C6    | 60:RK0:58:PHE:CE1  | 2.93                     | 0.56              |
| 42:S60:1160:A:H5'   | 75:SP0:133:ARG:NH2 | 2.20                     | 0.56              |
| 53:SF0:118:ARG:HD2  | 53:SF0:125:MET:CB  | 2.34                     | 0.56              |
| 42:S60:1108:C:H5''  | 68:ST0:44:THR:O    | 2.05                     | 0.56              |
| 42:R60:856:U:O4     | 67:RS0:146:SER:CB  | 2.54                     | 0.56              |
| 42:R60:1089:G:O4'   | 75:RP0:141:ARG:HD3 | 2.06                     | 0.56              |
| 1:K50:1405:G:H2'    | 1:K50:1406:G:C8    | 2.40                     | 0.56              |
| 47:RC0:230:ASN:HB2  | 70:RV0:24:GLN:NE2  | 2.20                     | 0.56              |
| 51:RE0:152:PRO:HD2  | 55:RG0:219:TYR:CE1 | 2.40                     | 0.56              |
| 42:S60:923:A:H5'    | 42:S60:924:U:C4    | 2.40                     | 0.56              |
| 1:K50:2198:G:H1     | 1:K50:2226:U:H3    | 1.54                     | 0.56              |
| 42:R60:852:A:H2'    | 42:R60:853:G:C8    | 2.41                     | 0.56              |
| 43:RA0:51:ILE:HD12  | 66:RR0:105:MET:CG  | 2.32                     | 0.56              |
| 42:R60:982:C:C4'    | 66:RR0:10:ARG:NH1  | 2.68                     | 0.56              |
| 42:S60:852:A:H2'    | 42:S60:853:G:C8    | 2.41                     | 0.55              |
| 42:S60:932:A:H2'    | 42:S60:933:G:C8    | 2.42                     | 0.55              |
| 42:R60:171:U:H5'    | 42:R60:172:U:H2'   | 1.88                     | 0.55              |
| 67:RS0:20:MET:HE2   | 67:RS0:29:ASP:OD1  | 2.06                     | 0.55              |
| 4:LAA:70:THR:HG21   | 19:LII:6:LEU:HG    | 1.88                     | 0.55              |
| 51:SE0:54:VAL:HG22  | 73:SY0:23:LEU:HD11 | 1.88                     | 0.55              |
| 42:R60:203:G:H21    | 51:RE0:33:THR:HG21 | 1.70                     | 0.55              |
| 42:R60:1108:C:H5''  | 68:RT0:44:THR:O    | 2.06                     | 0.55              |
| 43:RA0:63:ARG:NE    | 70:RV0:30:LEU:CG   | 2.64                     | 0.55              |
| 42:S60:203:G:H21    | 51:SE0:33:THR:HG21 | 1.70                     | 0.55              |
| 42:S60:915:A:N3     | 54:RFF:150:LYS:CG  | 2.69                     | 0.55              |
| 55:SG0:170:ASN:HD21 | 55:SG0:176:LYS:CE  | 2.19                     | 0.55              |
| 41:MD2:106:TYR:CE2  | 41:MD2:108:GLU:HA  | 2.41                     | 0.55              |
| 42:R60:1007:U:O4    | 56:RGG:84:ASP:OD2  | 2.23                     | 0.55              |
| 42:R60:1066:G:C5    | 60:RK0:58:PHE:CE1  | 2.95                     | 0.55              |
| 43:RA0:67:SER:HB2   | 70:RV0:28:VAL:HG13 | 1.88                     | 0.55              |
| 49:RD0:237:LEU:O    | 66:RR0:19:ARG:CZ   | 2.53                     | 0.55              |
| 55:RG0:170:ASN:HD21 | 55:RG0:176:LYS:CE  | 2.19                     | 0.55              |
| 42:S60:1066:G:C5    | 60:SK0:58:PHE:CE1  | 2.95                     | 0.55              |
| 37:KW0:83:PHE:CG    | 55:RG0:144:LYS:HG3 | 2.42                     | 0.55              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:982:C:C4'    | 66:SR0:10:ARG:NH1   | 2.68                     | 0.55              |
| 69:SU0:116:THR:C    | 69:SU0:117:LEU:HG   | 2.32                     | 0.55              |
| 42:R60:1084:G:O3'   | 75:RP0:99:ARG:HD3   | 2.06                     | 0.55              |
| 53:RF0:153:THR:HG21 | 53:RF0:160:LEU:HD13 | 1.88                     | 0.55              |
| 37:KW0:83:PHE:CG    | 55:RG0:144:LYS:CG   | 2.90                     | 0.55              |
| 42:R60:932:A:H2'    | 42:R60:933:G:C8     | 2.42                     | 0.55              |
| 42:R60:958:A:H3'    | 42:R60:959:G:N2     | 2.16                     | 0.55              |
| 37:LW0:83:PHE:CG    | 55:SG0:144:LYS:HG3  | 2.42                     | 0.55              |
| 42:S60:1084:G:O3'   | 75:SP0:99:ARG:HD3   | 2.06                     | 0.55              |
| 50:SDD:7:LYS:HA     | 75:SP0:67:PHE:O     | 2.07                     | 0.55              |
| 53:SF0:153:THR:HG21 | 53:SF0:160:LEU:HD13 | 1.88                     | 0.55              |
| 1:K50:796:C:H5'     | 34:KT0:131:ARG:HE   | 1.70                     | 0.55              |
| 47:RC0:229:LEU:HD12 | 70:RV0:42:ILE:HG12  | 1.89                     | 0.55              |
| 50:RDD:7:LYS:HA     | 75:RP0:67:PHE:O     | 2.07                     | 0.55              |
| 2:L70:60:A:H5'      | 8:LD0:273:LYS:HG2   | 1.88                     | 0.55              |
| 42:R60:1010:G:OP1   | 69:RU0:52:LYS:NZ    | 2.39                     | 0.55              |
| 43:RA0:68:ILE:HD12  | 43:RA0:121:LEU:HD22 | 1.89                     | 0.55              |
| 69:RU0:116:THR:C    | 69:RU0:117:LEU:HG   | 2.32                     | 0.55              |
| 1:L50:1940:C:H2'    | 1:L50:1941:A:C8     | 2.42                     | 0.55              |
| 41:MD1:106:TYR:CE2  | 41:MD1:108:GLU:HA   | 2.41                     | 0.55              |
| 42:S60:856:U:O4     | 67:SS0:146:SER:CB   | 2.54                     | 0.55              |
| 43:RA0:215:TYR:O    | 66:RR0:84:PHE:CE2   | 2.51                     | 0.55              |
| 47:SC0:130:PRO:HG2  | 70:SV0:4:PHE:CE1    | 2.42                     | 0.55              |
| 42:R60:1150:G:H2'   | 42:R60:1151:A:C8    | 2.42                     | 0.55              |
| 1:L50:275:A:N6      | 6:LC0:163:ILE:CD1   | 2.71                     | 0.54              |
| 42:S60:958:A:H3'    | 42:S60:959:G:N2     | 2.16                     | 0.54              |
| 43:SA0:68:ILE:HD12  | 43:SA0:121:LEU:HD22 | 1.89                     | 0.54              |
| 43:SA0:215:TYR:C    | 66:SR0:84:PHE:HE2   | 2.14                     | 0.54              |
| 42:R60:132:C:H3'    | 42:R60:133:A:H8     | 1.72                     | 0.54              |
| 42:R60:932:A:H3'    | 42:R60:933:G:H8     | 1.72                     | 0.54              |
| 42:R60:1160:A:OP1   | 75:RP0:133:ARG:NH1  | 2.39                     | 0.54              |
| 49:RD0:188:GLN:N    | 49:RD0:189:PRO:HD2  | 2.22                     | 0.54              |
| 53:RF0:42:HIS:ND1   | 65:RQ0:79:TYR:OH    | 2.36                     | 0.54              |
| 42:S60:1160:A:OP1   | 75:SP0:133:ARG:NH1  | 2.39                     | 0.54              |
| 42:S60:1181:U:OP1   | 65:SQ0:142:TYR:CE2  | 2.61                     | 0.54              |
| 67:SS0:20:MET:HE2   | 67:SS0:29:ASP:OD1   | 2.06                     | 0.54              |
| 43:RA0:215:TYR:C    | 66:RR0:84:PHE:HE2   | 2.14                     | 0.54              |
| 51:RE0:54:VAL:HG22  | 73:RY0:23:LEU:HD11  | 1.88                     | 0.54              |
| 42:S60:932:A:H3'    | 42:S60:933:G:H8     | 1.72                     | 0.54              |
| 33:KS0:14:ASP:CG    | 33:KS0:15:ASP:H     | 2.15                     | 0.54              |
| 42:S60:171:U:H5'    | 42:S60:172:U:H2'    | 1.88                     | 0.54              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:823:A:H2'    | 42:S60:824:A:H8     | 1.73                     | 0.54              |
| 42:S60:1158:U:O2'   | 50:SDD:7:LYS:NZ     | 2.19                     | 0.54              |
| 54:SFF:98:ILE:O     | 54:RFF:104:THR:HG22 | 2.08                     | 0.54              |
| 66:SR0:103:MET:HE1  | 66:SR0:117:LEU:HG   | 1.90                     | 0.54              |
| 10:KE0:30:LEU:HD22  | 11:KEE:11:VAL:HG13  | 1.89                     | 0.54              |
| 63:RN0:123:TYR:OH   | 63:RN0:141:PRO:HG2  | 2.07                     | 0.54              |
| 66:RR0:103:MET:HE1  | 66:RR0:117:LEU:HG   | 1.90                     | 0.54              |
| 47:SC0:229:LEU:HD12 | 70:SV0:42:ILE:HG12  | 1.89                     | 0.54              |
| 48:SCC:44:PRO:O     | 53:SF0:133:SER:CB   | 2.55                     | 0.54              |
| 1:K50:275:A:N6      | 6:KC0:163:ILE:CD1   | 2.71                     | 0.54              |
| 37:KW0:83:PHE:CG    | 55:RG0:144:LYS:HB3  | 2.43                     | 0.54              |
| 42:R60:167:G:H21    | 42:R60:173:A:H2     | 1.55                     | 0.54              |
| 42:S60:1150:G:H2'   | 42:S60:1151:A:C8    | 2.42                     | 0.54              |
| 43:SA0:63:ARG:NE    | 70:SV0:30:LEU:CG    | 2.64                     | 0.54              |
| 67:SS0:24:PHE:CZ    | 67:SS0:107:ILE:HG12 | 2.42                     | 0.54              |
| 1:L50:535:A:HO2'    | 31:LQ0:146:ASN:HB3  | 1.71                     | 0.54              |
| 42:S60:288:A:H5''   | 58:SI0:25:ARG:NH2   | 2.23                     | 0.54              |
| 56:SGG:105:ARG:HH21 | 66:SR0:36:ILE:HG22  | 1.73                     | 0.54              |
| 42:S60:982:C:C4'    | 66:SR0:10:ARG:HH11  | 2.21                     | 0.54              |
| 49:SD0:188:GLN:N    | 49:SD0:189:PRO:HD2  | 2.22                     | 0.54              |
| 49:SD0:237:LEU:HD21 | 66:SR0:40:GLU:OE2   | 2.08                     | 0.54              |
| 37:KW0:83:PHE:CD1   | 37:KW0:84:PRO:CD    | 2.81                     | 0.54              |
| 42:S60:1023:A:H5''  | 66:SR0:3:GLN:HG2    | 1.90                     | 0.54              |
| 42:S60:1208:G:OP2   | 65:SQ0:127:LYS:HE3  | 2.07                     | 0.54              |
| 50:RDD:34:PHE:CZ    | 60:RK0:61:GLN:HG2   | 2.43                     | 0.54              |
| 42:S60:1056:A:H5'   | 47:SC0:84:ALA:HA    | 1.89                     | 0.54              |
| 42:S60:1167:C:H2'   | 42:S60:1168:A:O4'   | 2.08                     | 0.54              |
| 43:SA0:67:SER:HB2   | 70:SV0:28:VAL:HG13  | 1.88                     | 0.54              |
| 43:SA0:197:ARG:CB   | 66:SR0:91:LEU:CB    | 2.86                     | 0.54              |
| 50:SDD:34:PHE:CZ    | 60:SK0:61:GLN:HG2   | 2.43                     | 0.54              |
| 42:R60:1056:A:H5'   | 47:RC0:84:ALA:HA    | 1.89                     | 0.54              |
| 42:R60:1108:C:H4'   | 68:RT0:46:PRO:HA    | 1.90                     | 0.54              |
| 54:SFF:150:LYS:NZ   | 42:R60:917:U:OP1    | 2.41                     | 0.53              |
| 42:R60:823:A:H2'    | 42:R60:824:A:H8     | 1.73                     | 0.53              |
| 67:RS0:24:PHE:CZ    | 67:RS0:107:ILE:HG12 | 2.42                     | 0.53              |
| 1:L50:2198:G:H1     | 1:L50:2226:U:H3     | 1.54                     | 0.53              |
| 37:LW0:83:PHE:CG    | 55:SG0:144:LYS:CG   | 2.90                     | 0.53              |
| 42:S60:1108:C:H4'   | 68:ST0:46:PRO:HA    | 1.90                     | 0.53              |
| 42:R60:288:A:H5''   | 58:RI0:25:ARG:NH2   | 2.23                     | 0.53              |
| 42:R60:886:C:O2'    | 50:RDD:26:THR:HB    | 2.08                     | 0.53              |
| 42:R60:1208:G:OP2   | 65:RQ0:127:LYS:HE3  | 2.07                     | 0.53              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 50:RDD:12:LEU:HD21  | 75:RP0:67:PHE:CE2  | 2.41                     | 0.53              |
| 42:S60:915:A:H2     | 54:RFF:150:LYS:HG3 | 1.73                     | 0.53              |
| 42:S60:982:C:C3'    | 66:SR0:10:ARG:HH11 | 2.22                     | 0.53              |
| 1:K50:1169:C:H1'    | 1:K50:1170:A:H8    | 1.73                     | 0.53              |
| 43:RA0:197:ARG:CB   | 66:RR0:91:LEU:CB   | 2.86                     | 0.53              |
| 48:RCC:44:PRO:O     | 53:RF0:133:SER:CB  | 2.55                     | 0.53              |
| 37:LW0:83:PHE:CG    | 55:SG0:144:LYS:HB3 | 2.43                     | 0.53              |
| 42:S60:1090:C:O2    | 75:SP0:146:HIS:CE1 | 2.62                     | 0.53              |
| 43:SA0:118:GLU:CD   | 47:SC0:31:THR:OG1  | 2.51                     | 0.53              |
| 48:SCC:43:GLY:HA3   | 53:SF0:133:SER:OG  | 2.09                     | 0.53              |
| 6:KC0:308:MET:HE2   | 12:KF0:148:SER:HB2 | 1.91                     | 0.53              |
| 12:KF0:115:ASN:ND2  | 34:KT0:133:PRO:HB2 | 2.24                     | 0.53              |
| 42:R60:982:C:C3'    | 66:RR0:10:ARG:HH11 | 2.22                     | 0.53              |
| 42:R60:982:C:C4'    | 66:RR0:10:ARG:HH11 | 2.21                     | 0.53              |
| 47:RC0:130:PRO:HG2  | 70:RV0:4:PHE:CE1   | 2.42                     | 0.53              |
| 49:RD0:237:LEU:HD21 | 66:RR0:40:GLU:OE2  | 2.08                     | 0.53              |
| 3:LA0:89:LEU:HD13   | 30:LPP:83:ILE:CD1  | 2.39                     | 0.53              |
| 24:LM0:70:ASP:O     | 24:LM0:71:ILE:HG12 | 2.09                     | 0.53              |
| 42:S60:167:G:H21    | 42:S60:173:A:H2    | 1.55                     | 0.53              |
| 1:K50:1738:G:N3     | 42:R60:1306:A:H2   | 2.06                     | 0.53              |
| 1:K50:1940:C:H2'    | 1:K50:1941:A:C8    | 2.42                     | 0.53              |
| 42:R60:1066:G:N7    | 60:RK0:58:PHE:CG   | 2.76                     | 0.53              |
| 49:RD0:94:GLN:NE2   | 60:RK0:19:SER:OG   | 2.42                     | 0.53              |
| 51:RE0:137:PRO:HG3  | 55:RG0:222:TRP:NE1 | 2.23                     | 0.53              |
| 6:LC0:308:MET:HE2   | 12:LF0:148:SER:HB2 | 1.91                     | 0.53              |
| 33:LS0:14:ASP:CG    | 33:LS0:15:ASP:H    | 2.15                     | 0.53              |
| 42:S60:132:C:H3'    | 42:S60:133:A:H8    | 1.72                     | 0.53              |
| 42:S60:932:A:H3'    | 42:S60:933:G:C8    | 2.44                     | 0.53              |
| 1:K50:1880:U:H3     | 1:K50:1938:A:H61   | 1.56                     | 0.53              |
| 42:R60:918:A:N7     | 42:R60:919:C:C4    | 2.77                     | 0.53              |
| 43:RA0:184:TYR:CZ   | 70:RV0:35:ARG:HD3  | 2.44                     | 0.53              |
| 67:RS0:28:ILE:CD1   | 67:RS0:40:THR:HB   | 2.39                     | 0.53              |
| 1:L50:401:A:N1      | 6:LC0:80:THR:HG22  | 2.24                     | 0.53              |
| 42:S60:864:A:C8     | 75:SP0:118:ARG:NH2 | 2.77                     | 0.53              |
| 42:R60:1055:A:O3'   | 47:RC0:84:ALA:HB1  | 2.07                     | 0.53              |
| 1:L50:1738:G:N3     | 42:S60:1306:A:H2   | 2.06                     | 0.53              |
| 41:MD1:42:LEU:HG    | 41:MD1:73:ILE:HD11 | 1.91                     | 0.53              |
| 42:S60:1066:G:N7    | 60:SK0:58:PHE:CG   | 2.76                     | 0.53              |
| 42:R60:1056:A:P     | 47:RC0:84:ALA:HB1  | 2.49                     | 0.53              |
| 67:RS0:139:VAL:O    | 67:RS0:139:VAL:CG1 | 2.57                     | 0.53              |
| 54:SFF:147:ILE:HD11 | 54:RFF:147:ILE:CD1 | 2.35                     | 0.53              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:K50:22:U:OP2     | 39:KY0:11:ARG:NH1   | 2.39                     | 0.53              |
| 42:R60:1181:U:OP1  | 65:RQ0:142:TYR:CE2  | 2.61                     | 0.53              |
| 43:RA0:118:GLU:CD  | 47:RC0:31:THR:OG1   | 2.51                     | 0.53              |
| 2:L70:27:A:OP2     | 8:LD0:62:THR:CG2    | 2.57                     | 0.53              |
| 12:LF0:115:ASN:ND2 | 34:LT0:133:PRO:HB2  | 2.24                     | 0.53              |
| 67:SS0:28:ILE:CD1  | 67:SS0:40:THR:HB    | 2.39                     | 0.53              |
| 42:R60:1035:C:H2'  | 42:R60:1036:A:H8    | 1.74                     | 0.53              |
| 42:R60:1167:C:H2'  | 42:R60:1168:A:O4'   | 2.08                     | 0.53              |
| 43:RA0:63:ARG:CD   | 70:RV0:30:LEU:HG    | 2.39                     | 0.53              |
| 12:LF0:70:ILE:HG13 | 34:LT0:144:MET:HE2  | 1.91                     | 0.52              |
| 48:SCC:44:PRO:O    | 53:SF0:133:SER:HB2  | 2.09                     | 0.52              |
| 10:KE0:11:ILE:HD11 | 11:KEE:92:LEU:HD23  | 1.90                     | 0.52              |
| 37:KW0:83:PHE:CD2  | 55:RG0:144:LYS:HB3  | 2.44                     | 0.52              |
| 42:R60:1090:C:O2   | 75:RP0:146:HIS:CE1  | 2.62                     | 0.52              |
| 42:R60:1181:U:H4'  | 65:RQ0:140:LYS:O    | 2.08                     | 0.52              |
| 50:SDD:8:TYR:CZ    | 75:SP0:72:ARG:CD    | 2.84                     | 0.52              |
| 51:SE0:137:PRO:HG3 | 55:SG0:222:TRP:NE1  | 2.23                     | 0.52              |
| 12:KF0:70:ILE:HG13 | 34:KT0:144:MET:HE2  | 1.91                     | 0.52              |
| 10:LE0:11:ILE:HD11 | 11:LEE:92:LEU:HD23  | 1.90                     | 0.52              |
| 37:LW0:81:ARG:HH12 | 55:SG0:148:SER:HB2  | 1.74                     | 0.52              |
| 42:S60:1056:A:P    | 47:SC0:84:ALA:HB1   | 2.49                     | 0.52              |
| 42:S60:1181:U:H4'  | 65:SQ0:140:LYS:O    | 2.08                     | 0.52              |
| 54:SFF:135:ASN:HB2 | 54:RFF:145:VAL:CG2  | 2.39                     | 0.52              |
| 63:SN0:123:TYR:OH  | 63:SN0:141:PRO:HG2  | 2.07                     | 0.52              |
| 42:R60:203:G:N2    | 51:RE0:33:THR:HG21  | 2.25                     | 0.52              |
| 1:L50:796:C:H4'    | 34:LT0:131:ARG:O    | 2.10                     | 0.52              |
| 37:LW0:83:PHE:CD2  | 55:SG0:144:LYS:HB3  | 2.44                     | 0.52              |
| 42:S60:244:U:H2'   | 42:S60:245:A:C8     | 2.44                     | 0.52              |
| 43:SA0:63:ARG:CD   | 70:SV0:30:LEU:HG    | 2.39                     | 0.52              |
| 49:SD0:94:GLN:NE2  | 60:SK0:19:SER:OG    | 2.42                     | 0.52              |
| 42:R60:244:U:H2'   | 42:R60:245:A:C8     | 2.44                     | 0.52              |
| 42:R60:932:A:H3'   | 42:R60:933:G:C8     | 2.44                     | 0.52              |
| 42:R60:1007:U:C5   | 56:RGG:84:ASP:OD2   | 2.62                     | 0.52              |
| 42:R60:1160:A:OP1  | 75:RP0:62:SER:OG    | 2.22                     | 0.52              |
| 43:RA0:120:ARG:CZ  | 47:RC0:232:ILE:HG21 | 2.39                     | 0.52              |
| 44:RAA:47:ALA:CB   | 48:RCC:61:ARG:NE    | 2.61                     | 0.52              |
| 1:L50:1169:C:H1'   | 1:L50:1170:A:H8     | 1.73                     | 0.52              |
| 47:SC0:130:PRO:HG2 | 70:SV0:4:PHE:HE1    | 1.74                     | 0.52              |
| 49:SD0:238:PRO:CA  | 66:SR0:19:ARG:NH1   | 2.63                     | 0.52              |
| 53:SF0:96:GLY:C    | 74:SZ0:108:LEU:HD21 | 2.34                     | 0.52              |
| 1:K50:796:C:H4'    | 34:KT0:131:ARG:O    | 2.10                     | 0.52              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 3:KA0:89:LEU:HD13   | 30:KPP:83:ILE:CD1   | 2.39                     | 0.52              |
| 48:RCC:43:GLY:HA3   | 53:RF0:133:SER:OG   | 2.09                     | 0.52              |
| 56:RGG:105:ARG:HH21 | 66:RR0:36:ILE:HG22  | 1.73                     | 0.52              |
| 42:S60:372:A:C4     | 59:SJ0:2:VAL:HG21   | 2.45                     | 0.52              |
| 42:S60:886:C:O2'    | 50:SDD:26:THR:HB    | 2.08                     | 0.52              |
| 43:SA0:184:TYR:CZ   | 70:SV0:35:ARG:HD3   | 2.44                     | 0.52              |
| 1:K50:401:A:N1      | 6:KC0:80:THR:HG22   | 2.24                     | 0.52              |
| 1:K50:2596:G:H5'    | 1:K50:2597:G:H5''   | 1.92                     | 0.52              |
| 37:KW0:98:ASN:CG    | 55:RG0:147:PHE:HA   | 2.35                     | 0.52              |
| 51:RE0:70:ILE:HD13  | 51:RE0:92:ILE:HG12  | 1.92                     | 0.52              |
| 53:RF0:92:GLU:HG3   | 74:RZ0:108:LEU:CD1  | 2.40                     | 0.52              |
| 55:RG0:170:ASN:ND2  | 55:RG0:176:LYS:HD3  | 2.22                     | 0.52              |
| 1:L50:22:U:OP2      | 39:LY0:11:ARG:NH1   | 2.39                     | 0.52              |
| 67:SS0:139:VAL:O    | 67:SS0:139:VAL:CG1  | 2.57                     | 0.52              |
| 12:KF0:69:LYS:HD3   | 34:KT0:141:GLU:HG2  | 1.91                     | 0.52              |
| 42:R60:1023:A:H5''  | 66:RR0:3:GLN:HG2    | 1.90                     | 0.52              |
| 53:RF0:96:GLY:C     | 74:RZ0:108:LEU:HD21 | 2.34                     | 0.52              |
| 67:RS0:24:PHE:CE1   | 67:RS0:107:ILE:CG2  | 2.92                     | 0.52              |
| 42:S60:1007:U:C5    | 56:SGG:84:ASP:OD2   | 2.62                     | 0.52              |
| 67:SS0:46:ASP:OD1   | 67:SS0:47:ARG:N     | 2.43                     | 0.52              |
| 41:MD2:42:LEU:HG    | 41:MD2:73:ILE:HD11  | 1.91                     | 0.52              |
| 42:S60:995:A:H2'    | 42:S60:996:G:O4'    | 2.10                     | 0.52              |
| 43:SA0:18:GLN:HE22  | 66:SR0:96:VAL:CB    | 2.23                     | 0.52              |
| 1:K50:290:C:O3'     | 39:KY0:33:PRO:HG3   | 2.09                     | 0.52              |
| 42:R60:372:A:C4     | 59:RJ0:2:VAL:HG21   | 2.45                     | 0.52              |
| 1:L50:1131:U:H3     | 1:L50:1135:G:H1     | 1.57                     | 0.52              |
| 37:LW0:99:LYS:HA    | 37:LW0:102:LYS:CG   | 2.40                     | 0.52              |
| 42:S60:203:G:N2     | 51:SE0:33:THR:HG21  | 2.25                     | 0.52              |
| 1:K50:1131:U:H3     | 1:K50:1135:G:H1     | 1.57                     | 0.52              |
| 43:RA0:18:GLN:HE22  | 66:RR0:96:VAL:CB    | 2.23                     | 0.52              |
| 55:RG0:176:LYS:N    | 55:RG0:176:LYS:HD2  | 2.25                     | 0.52              |
| 42:S60:918:A:N7     | 42:S60:919:C:C4     | 2.77                     | 0.51              |
| 43:SA0:120:ARG:CZ   | 47:SC0:232:ILE:HG21 | 2.39                     | 0.51              |
| 50:SDD:12:LEU:HD21  | 75:SP0:67:PHE:CE2   | 2.41                     | 0.51              |
| 50:SDD:12:LEU:HD12  | 75:SP0:75:ILE:HG21  | 1.86                     | 0.51              |
| 43:RA0:70:ASN:HB2   | 47:RC0:240:ILE:HG13 | 1.75                     | 0.51              |
| 42:S60:1010:G:OP1   | 69:SU0:52:LYS:NZ    | 2.39                     | 0.51              |
| 37:KW0:99:LYS:HA    | 37:KW0:102:LYS:CG   | 2.40                     | 0.51              |
| 64:RO0:27:HIS:CE1   | 64:RO0:36:THR:HG23  | 2.45                     | 0.51              |
| 42:S60:1055:A:O3'   | 47:SC0:84:ALA:HB1   | 2.07                     | 0.51              |
| 55:SG0:176:LYS:N    | 55:SG0:176:LYS:HD2  | 2.25                     | 0.51              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:K50:555:G:H1'     | 6:KC0:71:ARG:HH11   | 1.75                     | 0.51              |
| 42:R60:999:C:H2'    | 42:R60:1000:C:H6    | 1.76                     | 0.51              |
| 50:RDD:12:LEU:HD13  | 75:RP0:75:ILE:CG2   | 2.41                     | 0.51              |
| 1:L50:2544:U:OP1    | 5:LB0:375:THR:HG22  | 2.11                     | 0.51              |
| 56:SGG:105:ARG:HH22 | 66:SR0:37:ASP:CB    | 2.24                     | 0.51              |
| 1:K50:2544:U:OP1    | 5:KB0:375:THR:HG22  | 2.11                     | 0.51              |
| 2:K70:27:A:OP2      | 8:KD0:62:THR:CG2    | 2.57                     | 0.51              |
| 48:RCC:44:PRO:O     | 53:RF0:133:SER:HB2  | 2.09                     | 0.51              |
| 59:RJ0:100:GLU:OE1  | 59:RJ0:103:LEU:HD12 | 2.11                     | 0.51              |
| 73:RY0:22:GLU:C     | 73:RY0:23:LEU:HG    | 2.33                     | 0.51              |
| 73:RY0:116:ARG:NH2  | 73:RY0:120:LYS:HZ1  | 2.08                     | 0.51              |
| 42:S60:1066:G:N7    | 60:SK0:58:PHE:CD1   | 2.79                     | 0.51              |
| 67:SS0:24:PHE:CE1   | 67:SS0:107:ILE:CG2  | 2.92                     | 0.51              |
| 42:R60:1066:G:N7    | 60:RK0:58:PHE:CD1   | 2.79                     | 0.51              |
| 12:LF0:69:LYS:HD3   | 34:LT0:141:GLU:HG2  | 1.91                     | 0.51              |
| 47:SC0:233:LEU:HD13 | 70:SV0:26:ASN:CG    | 2.35                     | 0.51              |
| 12:KF0:70:ILE:HG12  | 34:KT0:144:MET:HG3  | 1.92                     | 0.51              |
| 42:R60:864:A:C8     | 75:RP0:118:ARG:NH2  | 2.77                     | 0.51              |
| 42:S60:1315:A:C2    | 42:S60:1316:A:N6    | 2.79                     | 0.51              |
| 53:SF0:92:GLU:HG3   | 74:SZ0:108:LEU:CD1  | 2.40                     | 0.51              |
| 1:K50:1328:A:H62    | 1:K50:1367:A:H61    | 1.59                     | 0.51              |
| 4:KAA:74:ASN:HD22   | 4:KAA:112:GLY:H     | 1.59                     | 0.51              |
| 47:RC0:130:PRO:HG2  | 70:RV0:4:PHE:HE1    | 1.74                     | 0.51              |
| 1:L50:1880:U:H3     | 1:L50:1938:A:H61    | 1.56                     | 0.51              |
| 56:SGG:65:PHE:HZ    | 66:SR0:29:TYR:CE2   | 2.27                     | 0.51              |
| 64:SO0:27:HIS:CE1   | 64:SO0:36:THR:HG23  | 2.45                     | 0.51              |
| 1:K50:535:A:HO2'    | 31:KQ0:146:ASN:HB3  | 1.71                     | 0.51              |
| 3:KA0:88:GLU:HG2    | 30:KPP:87:LYS:HE2   | 1.93                     | 0.51              |
| 10:KE0:23:ILE:HD11  | 11:KEE:79:ARG:NH1   | 2.21                     | 0.51              |
| 42:R60:995:A:H2'    | 42:R60:996:G:O4'    | 2.10                     | 0.51              |
| 49:RD0:34:LYS:HE3   | 69:RU0:60:PHE:HB3   | 1.93                     | 0.51              |
| 1:L50:396:G:N3      | 1:L50:396:G:H5''    | 2.26                     | 0.51              |
| 37:KW0:81:ARG:HH12  | 55:RG0:148:SER:HB2  | 1.73                     | 0.51              |
| 1:L50:290:C:O3'     | 39:LY0:33:PRO:HG3   | 2.09                     | 0.51              |
| 1:L50:1328:A:H62    | 1:L50:1367:A:H61    | 1.59                     | 0.51              |
| 42:S60:1124:A:H2'   | 42:S60:1125:G:C8    | 2.46                     | 0.51              |
| 42:R60:1149:U:C5    | 67:RS0:140:ARG:NH2  | 2.79                     | 0.51              |
| 47:RC0:233:LEU:HD13 | 70:RV0:26:ASN:CG    | 2.35                     | 0.51              |
| 56:RGG:105:ARG:HH22 | 66:RR0:37:ASP:CB    | 2.24                     | 0.51              |
| 1:L50:1601:A:H4'    | 3:LA0:170:LEU:O     | 2.11                     | 0.50              |
| 4:LAA:74:ASN:HD22   | 4:LAA:112:GLY:H     | 1.59                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:MD1:33:ASN:ND2  | 64:SO0:56:TYR:CE2  | 2.80                     | 0.50              |
| 51:SE0:70:ILE:HD13 | 51:SE0:92:ILE:HG12 | 1.92                     | 0.50              |
| 1:K50:1942:U:H2'   | 1:K50:1943:C:C5    | 2.46                     | 0.50              |
| 1:L50:555:G:H1'    | 6:LC0:71:ARG:HH11  | 1.75                     | 0.50              |
| 42:S60:1160:A:C2'  | 75:SP0:58:LYS:HD3  | 2.41                     | 0.50              |
| 56:SGG:65:PHE:CE2  | 66:SR0:29:TYR:CZ   | 3.00                     | 0.50              |
| 56:SGG:65:PHE:HE2  | 66:SR0:29:TYR:CD2  | 2.29                     | 0.50              |
| 67:SS0:10:PHE:HD1  | 74:SZ0:81:PHE:CD2  | 2.29                     | 0.50              |
| 1:K50:396:G:N3     | 1:K50:396:G:H5''   | 2.26                     | 0.50              |
| 42:R60:1143:A:C4   | 67:RS0:36:LYS:HB2  | 2.46                     | 0.50              |
| 53:RF0:40:LEU:HD21 | 65:RQ0:43:PHE:HD1  | 1.76                     | 0.50              |
| 67:RS0:46:ASP:OD1  | 67:RS0:47:ARG:N    | 2.43                     | 0.50              |
| 37:LW0:98:ASN:CG   | 55:SG0:147:PHE:HA  | 2.35                     | 0.50              |
| 42:S60:1149:U:C5   | 67:SS0:140:ARG:NH2 | 2.79                     | 0.50              |
| 29:KP0:30:ARG:C    | 29:KP0:30:ARG:HD3  | 2.36                     | 0.50              |
| 42:R60:926:G:H2'   | 42:R60:927:G:N7    | 2.26                     | 0.50              |
| 67:RS0:10:PHE:HD1  | 74:RZ0:81:PHE:CD2  | 2.29                     | 0.50              |
| 1:L50:1942:U:H2'   | 1:L50:1943:C:C5    | 2.46                     | 0.50              |
| 49:SD0:237:LEU:O   | 66:SR0:19:ARG:NH1  | 2.45                     | 0.50              |
| 56:SGG:228:LYS:HZ3 | 66:SR0:25:THR:HG22 | 1.76                     | 0.50              |
| 42:R60:1167:C:H4'  | 67:RS0:91:MET:O    | 2.12                     | 0.50              |
| 74:RZ0:41:VAL:HG21 | 74:RZ0:78:LEU:HD22 | 1.93                     | 0.50              |
| 1:L50:562:U:H6     | 1:L50:562:U:H5''   | 1.76                     | 0.50              |
| 1:L50:2596:G:H5'   | 1:L50:2597:G:H5''  | 1.92                     | 0.50              |
| 42:S60:917:U:H5'   | 42:S60:918:A:N3    | 2.27                     | 0.50              |
| 42:S60:1143:A:C4   | 67:SS0:36:LYS:HB2  | 2.46                     | 0.50              |
| 54:SFF:145:VAL:CG1 | 54:RFF:136:LYS:CB  | 2.80                     | 0.50              |
| 41:MD2:33:ASN:ND2  | 64:RO0:56:TYR:CE2  | 2.80                     | 0.50              |
| 53:RF0:6:THR:CG2   | 65:RQ0:53:LYS:NZ   | 2.74                     | 0.50              |
| 53:RF0:90:ILE:O    | 53:RF0:94:VAL:HG23 | 2.12                     | 0.50              |
| 1:L50:2473:G:OP1   | 16:LH0:72:LYS:HG3  | 2.12                     | 0.50              |
| 12:LF0:70:ILE:HG12 | 34:LT0:144:MET:HG3 | 1.92                     | 0.50              |
| 42:S60:966:G:H2'   | 42:S60:967:A:C8    | 2.46                     | 0.50              |
| 1:K50:562:U:H6     | 1:K50:562:U:H5''   | 1.76                     | 0.50              |
| 20:KJ0:82:LYS:HB2  | 75:RP0:30:PHE:HE2  | 1.65                     | 0.50              |
| 42:R60:966:G:H2'   | 42:R60:967:A:C8    | 2.46                     | 0.50              |
| 42:R60:1216:U:H2'  | 42:R60:1217:G:C8   | 2.47                     | 0.50              |
| 42:S60:926:G:H2'   | 42:S60:927:G:N7    | 2.26                     | 0.50              |
| 42:S60:1216:U:H2'  | 42:S60:1217:G:C8   | 2.47                     | 0.50              |
| 45:SB0:71:ARG:HB3  | 64:SO0:32:THR:HG21 | 1.93                     | 0.50              |
| 42:R60:1124:A:H2'  | 42:R60:1125:G:C8   | 2.46                     | 0.50              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:R60:1315:A:C2    | 42:R60:1316:A:N6    | 2.79                     | 0.50              |
| 29:LP0:30:ARG:C     | 29:LP0:30:ARG:HD3   | 2.36                     | 0.50              |
| 42:S60:139:C:O3'    | 55:SG0:95:LYS:NZ    | 2.45                     | 0.50              |
| 1:K50:1424:A:H5'    | 15:KGG:77:GLY:HA3   | 1.94                     | 0.50              |
| 42:R60:834:G:H5'    | 44:RAA:85:ARG:HD2   | 1.93                     | 0.50              |
| 42:R60:917:U:H5'    | 42:R60:918:A:N3     | 2.27                     | 0.50              |
| 42:R60:923:A:H5'    | 42:R60:924:U:N3     | 2.27                     | 0.50              |
| 42:R60:1160:A:C2'   | 75:RP0:58:LYS:HD3   | 2.41                     | 0.50              |
| 53:RF0:118:ARG:HD2  | 53:RF0:125:MET:CB   | 2.34                     | 0.50              |
| 42:S60:999:C:H2'    | 42:S60:1000:C:H6    | 1.76                     | 0.50              |
| 42:S60:1167:C:H4'   | 67:SS0:91:MET:O     | 2.12                     | 0.50              |
| 54:SFF:118:ARG:HH12 | 54:RFF:97:ASP:CB    | 2.24                     | 0.50              |
| 56:SGG:121:THR:HG21 | 56:SGG:131:TRP:CH2  | 2.47                     | 0.50              |
| 59:SJ0:100:GLU:OE1  | 59:SJ0:103:LEU:HD12 | 2.11                     | 0.50              |
| 45:RB0:71:ARG:HB3   | 64:RO0:32:THR:HG21  | 1.93                     | 0.50              |
| 42:S60:55:G:H5'     | 73:SY0:123:ARG:HH11 | 1.77                     | 0.49              |
| 42:S60:923:A:H5'    | 42:S60:924:U:N3     | 2.27                     | 0.49              |
| 55:SG0:170:ASN:ND2  | 55:SG0:176:LYS:HD3  | 2.22                     | 0.49              |
| 1:K50:1601:A:H4'    | 3:KA0:170:LEU:O     | 2.11                     | 0.49              |
| 53:RF0:92:GLU:CG    | 74:RZ0:108:LEU:HD12 | 2.41                     | 0.49              |
| 66:SR0:36:ILE:HD11  | 66:SR0:44:LYS:NZ    | 2.27                     | 0.49              |
| 1:K50:2051:C:C6     | 20:KJ0:56:ILE:HD11  | 2.48                     | 0.49              |
| 42:R60:55:G:H5'     | 73:RY0:123:ARG:HH11 | 1.77                     | 0.49              |
| 56:RGG:65:PHE:HE2   | 66:RR0:29:TYR:CD2   | 2.29                     | 0.49              |
| 56:RGG:121:THR:HG21 | 56:RGG:131:TRP:CH2  | 2.47                     | 0.49              |
| 3:LA0:88:GLU:HG2    | 30:LPP:87:LYS:HE2   | 1.93                     | 0.49              |
| 53:SF0:90:ILE:O     | 53:SF0:94:VAL:HG23  | 2.12                     | 0.49              |
| 56:SGG:105:ARG:HH22 | 66:SR0:37:ASP:HB2   | 1.77                     | 0.49              |
| 1:K50:1089:U:H2'    | 1:K50:1090:A:C8     | 2.47                     | 0.49              |
| 37:LW0:99:LYS:CA    | 37:LW0:102:LYS:HG2  | 2.42                     | 0.49              |
| 42:S60:1019:C:H2'   | 42:S60:1020:G:C8    | 2.47                     | 0.49              |
| 43:SA0:52:LYS:HD2   | 66:SR0:109:TYR:CD1  | 2.47                     | 0.49              |
| 49:SD0:34:LYS:HE3   | 69:SU0:60:PHE:HB3   | 1.93                     | 0.49              |
| 53:SF0:92:GLU:CG    | 74:SZ0:108:LEU:HD12 | 2.41                     | 0.49              |
| 42:R60:236:U:O2     | 58:RI0:5:ARG:NH1    | 2.46                     | 0.49              |
| 42:R60:832:A:H2'    | 42:R60:833:A:C8     | 2.47                     | 0.49              |
| 42:R60:1019:C:H2'   | 42:R60:1020:G:C8    | 2.47                     | 0.49              |
| 56:RGG:65:PHE:CE2   | 66:RR0:29:TYR:CZ    | 2.99                     | 0.49              |
| 1:L50:1089:U:H2'    | 1:L50:1090:A:C8     | 2.47                     | 0.49              |
| 53:SF0:6:THR:CG2    | 65:SQ0:53:LYS:HZ3   | 2.26                     | 0.49              |
| 42:R60:1066:G:O6    | 60:RK0:58:PHE:CE2   | 2.66                     | 0.49              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 49:RD0:237:LEU:O    | 66:RR0:19:ARG:NH1   | 2.45                     | 0.49              |
| 10:LE0:23:ILE:HD11  | 11:LEE:79:ARG:NH1   | 2.21                     | 0.49              |
| 42:S60:834:G:H5'    | 44:SAA:85:ARG:HD2   | 1.93                     | 0.49              |
| 53:SF0:40:LEU:HD21  | 65:SQ0:43:PHE:HD1   | 1.76                     | 0.49              |
| 74:SZ0:41:VAL:HG21  | 74:SZ0:78:LEU:HD22  | 1.93                     | 0.49              |
| 66:RR0:36:ILE:HD11  | 66:RR0:44:LYS:NZ    | 2.27                     | 0.49              |
| 16:LH0:7:GLU:OE2    | 16:LH0:9:LYS:HE3    | 2.13                     | 0.49              |
| 42:S60:918:A:OP1    | 54:RFF:132:ARG:CB   | 2.60                     | 0.49              |
| 42:S60:1260:G:H1    | 42:S60:1303:U:H3    | 1.61                     | 0.49              |
| 51:SE0:92:ILE:HG22  | 51:SE0:94:LYS:O     | 2.13                     | 0.49              |
| 42:R60:139:C:O3'    | 55:RG0:95:LYS:NZ    | 2.45                     | 0.49              |
| 42:R60:1165:C:H2'   | 42:R60:1166:A:C8    | 2.48                     | 0.49              |
| 43:RA0:120:ARG:HE   | 47:RC0:232:ILE:HG22 | 1.76                     | 0.49              |
| 56:RGG:105:ARG:HH22 | 66:RR0:37:ASP:HB2   | 1.77                     | 0.49              |
| 1:L50:1424:A:H5'    | 15:LGG:77:GLY:HA3   | 1.94                     | 0.49              |
| 45:SB0:53:THR:CG2   | 64:SO0:32:THR:OG1   | 2.58                     | 0.49              |
| 47:SC0:230:ASN:N    | 70:SV0:24:GLN:NE2   | 2.45                     | 0.49              |
| 42:R60:65:A:H62     | 42:R60:75:G:H21     | 1.60                     | 0.49              |
| 45:RB0:53:THR:CG2   | 64:RO0:32:THR:OG1   | 2.58                     | 0.49              |
| 1:L50:2051:C:C6     | 20:LJ0:56:ILE:HD11  | 2.48                     | 0.49              |
| 42:S60:126:C:H2'    | 42:S60:127:A:C8     | 2.48                     | 0.49              |
| 42:S60:832:A:H2'    | 42:S60:833:A:C8     | 2.47                     | 0.49              |
| 42:S60:1083:U:O2'   | 75:SP0:97:ASN:ND2   | 2.46                     | 0.49              |
| 47:SC0:216:PHE:HZ   | 71:SW0:128:TYR:HD1  | 1.59                     | 0.49              |
| 53:SF0:6:THR:HG23   | 65:SQ0:53:LYS:HZ1   | 1.77                     | 0.49              |
| 1:K50:1441:U:H4'    | 38:KX0:64:ILE:HD11  | 1.95                     | 0.49              |
| 37:KW0:99:LYS:CA    | 37:KW0:102:LYS:HG2  | 2.42                     | 0.49              |
| 1:L50:486:U:H2'     | 1:L50:487:A:C8      | 2.48                     | 0.49              |
| 42:S60:404:C:H4'    | 73:SY0:37:ASN:HA    | 1.95                     | 0.49              |
| 43:SA0:215:TYR:CD1  | 66:SR0:84:PHE:CZ    | 3.01                     | 0.49              |
| 14:LG0:17:ARG:NH1   | 26:LN0:32:GLN:HE22  | 2.10                     | 0.48              |
| 42:S60:995:A:C2'    | 42:S60:996:G:H5'    | 2.43                     | 0.48              |
| 45:RB0:71:ARG:HB3   | 64:RO0:32:THR:CG2   | 2.43                     | 0.48              |
| 47:RC0:166:LYS:CE   | 59:RJ0:100:GLU:OE2  | 2.61                     | 0.48              |
| 51:RE0:92:ILE:HG22  | 51:RE0:94:LYS:O     | 2.13                     | 0.48              |
| 1:L50:1441:U:H4'    | 38:LX0:64:ILE:HD11  | 1.94                     | 0.48              |
| 50:SDD:12:LEU:HD13  | 75:SP0:75:ILE:CG2   | 2.41                     | 0.48              |
| 53:SF0:158:LYS:HA   | 74:SZ0:62:THR:HG21  | 1.95                     | 0.48              |
| 47:RC0:229:LEU:HB2  | 70:RV0:42:ILE:HD11  | 1.94                     | 0.48              |
| 56:RGG:105:ARG:NH2  | 66:RR0:36:ILE:HG22  | 2.28                     | 0.48              |
| 1:L50:1643:G:H1     | 1:L50:1672:A:H61    | 1.61                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:S60:1066:G:O6   | 60:SK0:58:PHE:CE2  | 2.66                     | 0.48              |
| 42:S60:1262:A:H3'  | 42:S60:1263:A:H8   | 1.78                     | 0.48              |
| 44:SAA:47:ALA:CB   | 48:SCC:61:ARG:NE   | 2.61                     | 0.48              |
| 45:SB0:71:ARG:HB3  | 64:SO0:32:THR:CG2  | 2.43                     | 0.48              |
| 47:SC0:229:LEU:HB2 | 70:SV0:42:ILE:HD11 | 1.94                     | 0.48              |
| 56:SGG:105:ARG:NH2 | 66:SR0:36:ILE:HG22 | 2.28                     | 0.48              |
| 1:K50:1691:A:C2    | 42:R60:1317:G:N2   | 2.81                     | 0.48              |
| 1:K50:2447:A:H5''  | 1:K50:2447:A:H8    | 1.78                     | 0.48              |
| 42:R60:404:C:H4'   | 73:RY0:37:ASN:HA   | 1.95                     | 0.48              |
| 42:R60:1091:A:C8   | 75:RP0:146:HIS:CD2 | 3.01                     | 0.48              |
| 42:S60:1091:A:C8   | 75:SP0:146:HIS:CD2 | 3.01                     | 0.48              |
| 42:S60:1167:C:H4'  | 67:SS0:91:MET:C    | 2.38                     | 0.48              |
| 42:S60:1209:C:H2'  | 42:S60:1210:G:C8   | 2.49                     | 0.48              |
| 1:K50:1643:G:H1    | 1:K50:1672:A:H61   | 1.61                     | 0.48              |
| 37:LW0:83:PHE:CG   | 37:LW0:84:PRO:CD   | 2.92                     | 0.48              |
| 42:S60:65:A:H62    | 42:S60:75:G:H21    | 1.60                     | 0.48              |
| 42:S60:1165:C:H2'  | 42:S60:1166:A:C8   | 2.48                     | 0.48              |
| 1:K50:486:U:H2'    | 1:K50:487:A:C8     | 2.48                     | 0.48              |
| 37:KW0:83:PHE:CG   | 37:KW0:84:PRO:CD   | 2.92                     | 0.48              |
| 50:RDD:8:TYR:CE2   | 75:RP0:72:ARG:NE   | 2.82                     | 0.48              |
| 42:S60:236:U:O2    | 58:SI0:5:ARG:NH1   | 2.46                     | 0.48              |
| 14:KG0:17:ARG:NH1  | 26:KN0:32:GLN:HE22 | 2.11                     | 0.48              |
| 42:R60:126:C:H2'   | 42:R60:127:A:C8    | 2.48                     | 0.48              |
| 42:R60:1083:U:O2'  | 75:RP0:97:ASN:ND2  | 2.46                     | 0.48              |
| 42:R60:1167:C:H4'  | 67:RS0:91:MET:C    | 2.38                     | 0.48              |
| 42:R60:1209:C:H2'  | 42:R60:1210:G:C8   | 2.49                     | 0.48              |
| 1:L50:1691:A:C2    | 42:S60:1317:G:N2   | 2.81                     | 0.48              |
| 41:MD1:52:LYS:HG3  | 42:S60:606:G:H22   | 1.78                     | 0.48              |
| 43:SA0:215:TYR:CA  | 66:SR0:84:PHE:HE2  | 2.26                     | 0.48              |
| 53:SF0:6:THR:CG2   | 65:SQ0:53:LYS:NZ   | 2.74                     | 0.48              |
| 54:SFF:132:ARG:CA  | 42:R60:918:A:P     | 3.02                     | 0.48              |
| 1:K50:399:G:O6     | 6:KC0:57:ARG:NH1   | 2.46                     | 0.48              |
| 16:KH0:7:GLU:OE2   | 16:KH0:9:LYS:HE3   | 2.13                     | 0.48              |
| 42:R60:1262:A:H3'  | 42:R60:1263:A:H8   | 1.78                     | 0.48              |
| 47:RC0:216:PHE:HZ  | 71:RW0:128:TYR:HD1 | 1.59                     | 0.48              |
| 50:RDD:43:TYR:CE2  | 69:RU0:62:CYS:HB2  | 2.49                     | 0.48              |
| 1:L50:399:G:O6     | 6:LC0:57:ARG:NH1   | 2.46                     | 0.48              |
| 42:S60:237:A:C5'   | 58:SI0:48:VAL:HG13 | 2.43                     | 0.48              |
| 42:R60:377:C:OP1   | 59:RJ0:150:PRO:HD2 | 2.13                     | 0.48              |
| 43:RA0:52:LYS:HD2  | 66:RR0:109:TYR:CD1 | 2.47                     | 0.48              |
| 53:RF0:158:LYS:HA  | 74:RZ0:62:THR:HG21 | 1.95                     | 0.48              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:L50:1325:G:H22   | 1:L50:1370:U:H3     | 1.62                     | 0.48              |
| 49:SD0:239:ILE:CA  | 66:SR0:19:ARG:NH1   | 2.77                     | 0.48              |
| 42:S60:1035:C:H2'  | 42:S60:1036:A:H8    | 1.74                     | 0.48              |
| 49:SD0:68:HIS:NE2  | 69:SU0:109:THR:O    | 2.47                     | 0.48              |
| 1:K50:2109:G:H5''  | 1:K50:2109:G:C8     | 2.45                     | 0.48              |
| 1:K50:2473:G:OP1   | 16:KH0:72:LYS:HG3   | 2.12                     | 0.48              |
| 37:KW0:95:ARG:O    | 37:KW0:99:LYS:HG3   | 2.14                     | 0.48              |
| 42:R60:999:C:H2'   | 42:R60:1000:C:O4'   | 2.14                     | 0.48              |
| 43:RA0:51:ILE:CD1  | 66:RR0:105:MET:CE   | 2.89                     | 0.48              |
| 44:RAA:51:ASP:OD2  | 48:RCC:57:GLU:C     | 2.57                     | 0.48              |
| 1:L50:1609:G:N2    | 1:L50:1614:G:O2'    | 2.47                     | 0.47              |
| 1:L50:2116:A:H2'   | 1:L50:2117:A:C8     | 2.49                     | 0.47              |
| 37:LW0:95:ARG:O    | 37:LW0:99:LYS:HG3   | 2.14                     | 0.47              |
| 42:S60:125:A:H2'   | 42:S60:126:C:C6     | 2.49                     | 0.47              |
| 1:K50:2116:A:H2'   | 1:K50:2117:A:C8     | 2.49                     | 0.47              |
| 42:R60:995:A:C2'   | 42:R60:996:G:H5'    | 2.43                     | 0.47              |
| 57:RH0:121:GLY:HA3 | 71:RW0:41:LYS:HG3   | 1.96                     | 0.47              |
| 1:L50:2108:U:H6    | 1:L50:2108:U:H5''   | 1.78                     | 0.47              |
| 8:LD0:215:LYS:HE2  | 8:LD0:222:PHE:CE2   | 2.49                     | 0.47              |
| 1:K50:1325:G:H22   | 1:K50:1370:U:H3     | 1.62                     | 0.47              |
| 42:R60:1260:G:H1   | 42:R60:1303:U:H3    | 1.61                     | 0.47              |
| 10:LE0:30:LEU:HD22 | 11:LEE:11:VAL:HG13  | 1.89                     | 0.47              |
| 20:LJ0:8:ASN:HD22  | 20:LJ0:149:GLN:HE22 | 1.61                     | 0.47              |
| 42:S60:916:G:H5'   | 42:S60:916:G:H8     | 1.80                     | 0.47              |
| 42:S60:932:A:C6    | 42:S60:933:G:C6     | 3.03                     | 0.47              |
| 47:SC0:166:LYS:CE  | 59:SJ0:100:GLU:OE2  | 2.61                     | 0.47              |
| 50:SDD:43:TYR:CE2  | 69:SU0:62:CYS:HB2   | 2.49                     | 0.47              |
| 1:K50:2108:U:H6    | 1:K50:2108:U:H5''   | 1.78                     | 0.47              |
| 3:KA0:238:LYS:HD3  | 42:R60:714:U:H5'    | 1.96                     | 0.47              |
| 16:KH0:63:GLU:OE2  | 27:KO0:131:ILE:HG21 | 2.13                     | 0.47              |
| 37:KW0:83:PHE:HB2  | 55:RG0:144:LYS:HG3  | 1.97                     | 0.47              |
| 42:R60:1168:A:H3'  | 42:R60:1169:G:H8    | 1.80                     | 0.47              |
| 1:L50:2060:A:H2'   | 1:L50:2060:A:N3     | 2.29                     | 0.47              |
| 42:S60:349:A:OP1   | 51:SE0:57:ASN:ND2   | 2.48                     | 0.47              |
| 42:S60:910:A:H62   | 42:S60:922:G:N2     | 2.11                     | 0.47              |
| 42:S60:967:A:H8    | 42:S60:967:A:O5'    | 1.97                     | 0.47              |
| 42:S60:1140:G:H5'  | 42:S60:1143:A:N7    | 2.29                     | 0.47              |
| 67:SS0:112:GLU:O   | 67:SS0:116:ARG:HG2  | 2.15                     | 0.47              |
| 1:K50:1609:G:N2    | 1:K50:1614:G:O2'    | 2.47                     | 0.47              |
| 1:K50:1869:A:H5'   | 26:KN0:24:ARG:HD2   | 1.97                     | 0.47              |
| 42:R60:466:C:H4'   | 72:RX0:100:GLU:HG2  | 1.97                     | 0.47              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:R60:911:G:OP2    | 42:R60:911:G:H8     | 1.97                     | 0.47              |
| 42:R60:970:U:H6     | 42:R60:970:U:H5''   | 1.80                     | 0.47              |
| 42:R60:1140:G:H5'   | 42:R60:1143:A:N7    | 2.29                     | 0.47              |
| 43:RA0:215:TYR:CD1  | 66:RR0:84:PHE:CZ    | 3.01                     | 0.47              |
| 43:RA0:215:TYR:CA   | 66:RR0:84:PHE:HE2   | 2.26                     | 0.47              |
| 44:RAA:47:ALA:HB2   | 48:RCC:61:ARG:HE    | 1.71                     | 0.47              |
| 53:RF0:40:LEU:HD23  | 65:RQ0:43:PHE:HE1   | 1.73                     | 0.47              |
| 3:LA0:238:LYS:HD3   | 42:S60:714:U:H5'    | 1.96                     | 0.47              |
| 13:LFF:20:TYR:C     | 13:LFF:95:MET:HE2   | 2.40                     | 0.47              |
| 16:LH0:63:GLU:OE2   | 27:LO0:131:ILE:HG21 | 2.13                     | 0.47              |
| 42:S60:1151:A:C2    | 42:S60:1152:G:H1'   | 2.49                     | 0.47              |
| 54:SFF:135:ASN:OD1  | 54:RFF:143:TYR:O    | 2.32                     | 0.47              |
| 3:KA0:238:LYS:HZ2   | 42:R60:714:U:H5''   | 1.80                     | 0.47              |
| 8:KD0:215:LYS:HE2   | 8:KD0:222:PHE:CE2   | 2.49                     | 0.47              |
| 42:R60:125:A:H2'    | 42:R60:126:C:C6     | 2.49                     | 0.47              |
| 42:R60:997:A:H3'    | 42:R60:998:U:C5     | 2.50                     | 0.47              |
| 47:RC0:216:PHE:HZ   | 71:RW0:128:TYR:CD1  | 2.33                     | 0.47              |
| 53:RF0:6:THR:CG2    | 65:RQ0:53:LYS:HZ3   | 2.27                     | 0.47              |
| 1:L50:1869:A:H5'    | 26:LN0:24:ARG:HD2   | 1.96                     | 0.47              |
| 1:L50:2447:A:H8     | 1:L50:2447:A:H5''   | 1.79                     | 0.47              |
| 42:S60:958:A:OP1    | 47:SC0:111:ARG:CZ   | 2.63                     | 0.47              |
| 42:S60:1126:A:H8    | 42:S60:1164:G:H21   | 1.61                     | 0.47              |
| 1:K50:1878:G:H2'    | 1:K50:1879:A:C8     | 2.50                     | 0.47              |
| 42:R60:507:C:H2'    | 42:R60:508:A:C8     | 2.50                     | 0.47              |
| 42:R60:1208:G:C2'   | 42:R60:1209:C:H5'   | 2.44                     | 0.47              |
| 47:RC0:233:LEU:HD13 | 70:RV0:26:ASN:ND2   | 2.30                     | 0.47              |
| 63:RN0:128:TYR:HE1  | 63:RN0:132:LYS:HZ2  | 1.62                     | 0.47              |
| 67:RS0:55:ARG:HH22  | 68:RT0:32:ASN:ND2   | 2.12                     | 0.47              |
| 1:L50:2109:G:H5''   | 1:L50:2109:G:C8     | 2.45                     | 0.47              |
| 42:S60:507:C:H2'    | 42:S60:508:A:C8     | 2.50                     | 0.47              |
| 42:S60:911:G:H8     | 42:S60:911:G:OP2    | 1.97                     | 0.47              |
| 42:S60:995:A:C8     | 42:S60:996:G:C8     | 3.03                     | 0.47              |
| 42:S60:1085:G:C5'   | 75:SP0:140:THR:HG21 | 2.44                     | 0.47              |
| 47:SC0:233:LEU:HD13 | 70:SV0:26:ASN:ND2   | 2.30                     | 0.47              |
| 54:SFF:98:ILE:C     | 54:RFF:104:THR:HG22 | 2.40                     | 0.47              |
| 57:SH0:121:GLY:HA3  | 71:SW0:41:LYS:HG3   | 1.96                     | 0.47              |
| 20:KJ0:8:ASN:HD22   | 20:KJ0:149:GLN:HE22 | 1.61                     | 0.47              |
| 37:KW0:98:ASN:HD22  | 55:RG0:147:PHE:N    | 2.10                     | 0.47              |
| 42:R60:1085:G:C5'   | 75:RP0:140:THR:HG21 | 2.44                     | 0.47              |
| 42:R60:1151:A:C2    | 42:R60:1152:G:H1'   | 2.49                     | 0.47              |
| 49:RD0:68:HIS:NE2   | 69:RU0:109:THR:O    | 2.47                     | 0.47              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 50:RDD:12:LEU:HD12 | 75:RP0:75:ILE:HG21  | 1.86                     | 0.47              |
| 67:RS0:10:PHE:CD1  | 74:RZ0:81:PHE:CD2   | 3.03                     | 0.47              |
| 67:RS0:112:GLU:O   | 67:RS0:116:ARG:HG2  | 2.15                     | 0.47              |
| 37:LW0:83:PHE:HB2  | 55:SG0:144:LYS:HG3  | 1.97                     | 0.47              |
| 42:S60:705:A:C2    | 42:S60:706:G:N1     | 2.83                     | 0.47              |
| 42:S60:997:A:H3'   | 42:S60:998:U:C5     | 2.50                     | 0.47              |
| 42:S60:999:C:H2'   | 42:S60:1000:C:O4'   | 2.14                     | 0.47              |
| 42:S60:1208:G:C2'  | 42:S60:1209:C:H5'   | 2.44                     | 0.47              |
| 13:KFF:20:TYR:C    | 13:KFF:95:MET:HE2   | 2.40                     | 0.47              |
| 42:R60:237:A:C5'   | 58:RI0:48:VAL:HG13  | 2.43                     | 0.47              |
| 42:R60:967:A:H8    | 42:R60:967:A:O5'    | 1.97                     | 0.47              |
| 42:R60:1068:U:H5'  | 49:RD0:207:ILE:HD11 | 1.96                     | 0.47              |
| 47:RC0:50:HIS:O    | 70:RV0:6:ARG:NH2    | 2.48                     | 0.47              |
| 53:RF0:6:THR:HG23  | 65:RQ0:53:LYS:HZ1   | 1.75                     | 0.47              |
| 67:RS0:20:MET:CE   | 67:RS0:29:ASP:OD1   | 2.63                     | 0.47              |
| 42:S60:377:C:OP1   | 59:SJ0:150:PRO:HD2  | 2.13                     | 0.47              |
| 42:S60:1168:A:H3'  | 42:S60:1169:G:H8    | 1.80                     | 0.47              |
| 47:SC0:50:HIS:O    | 70:SV0:6:ARG:NH2    | 2.48                     | 0.47              |
| 42:R60:63:G:H2'    | 42:R60:76:A:C2      | 2.50                     | 0.47              |
| 42:R60:916:G:H5'   | 42:R60:916:G:H8     | 1.80                     | 0.47              |
| 55:RG0:144:LYS:HD2 | 55:RG0:144:LYS:N    | 2.30                     | 0.47              |
| 42:S60:1110:C:H5'  | 68:ST0:54:THR:HG22  | 1.97                     | 0.47              |
| 50:SDD:8:TYR:CE2   | 75:SP0:72:ARG:NE    | 2.82                     | 0.47              |
| 63:SN0:128:TYR:HE1 | 63:SN0:132:LYS:HZ2  | 1.61                     | 0.47              |
| 42:R60:995:A:C8    | 42:R60:996:G:C8     | 3.03                     | 0.47              |
| 43:RA0:10:ASP:CB   | 66:RR0:112:ASN:HD21 | 2.28                     | 0.47              |
| 43:RA0:52:LYS:HB2  | 66:RR0:109:TYR:CE2  | 2.49                     | 0.47              |
| 46:RBB:24:PHE:CZ   | 71:RW0:51:ILE:HG23  | 2.49                     | 0.47              |
| 4:LAA:127:GLN:HE22 | 19:LII:7:ASN:H      | 1.63                     | 0.46              |
| 42:S60:384:A:C2    | 59:SJ0:169:ARG:HB2  | 2.50                     | 0.46              |
| 42:S60:1068:U:H5'  | 49:SD0:207:ILE:HD11 | 1.96                     | 0.46              |
| 43:SA0:50:ASP:CG   | 66:SR0:109:TYR:HH   | 2.22                     | 0.46              |
| 43:SA0:197:ARG:HD3 | 66:SR0:91:LEU:CB    | 2.46                     | 0.46              |
| 63:SN0:66:VAL:HG23 | 63:SN0:67:THR:HG23  | 1.97                     | 0.46              |
| 42:R60:517:U:H5'   | 51:RE0:219:SER:O    | 2.15                     | 0.46              |
| 42:R60:932:A:C6    | 42:R60:933:G:C6     | 3.03                     | 0.46              |
| 42:R60:958:A:OP1   | 47:RC0:111:ARG:CZ   | 2.63                     | 0.46              |
| 42:R60:1018:U:H4'  | 42:R60:1019:C:OP2   | 2.15                     | 0.46              |
| 44:SAA:51:ASP:OD2  | 48:SCC:57:GLU:C     | 2.57                     | 0.46              |
| 46:SBB:24:PHE:CZ   | 71:SW0:51:ILE:HG23  | 2.49                     | 0.46              |
| 49:SD0:36:ARG:NH1  | 69:SU0:112:GLU:OE1  | 2.48                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 55:SG0:144:LYS:N    | 55:SG0:144:LYS:HD2  | 2.30                     | 0.46              |
| 67:SS0:20:MET:CE    | 67:SS0:29:ASP:OD1   | 2.63                     | 0.46              |
| 42:R60:909:G:O6     | 62:RM0:37:ARG:HB3   | 2.15                     | 0.46              |
| 42:R60:997:A:C2     | 42:R60:998:U:H1'    | 2.50                     | 0.46              |
| 49:RD0:36:ARG:NH1   | 69:RU0:112:GLU:OE1  | 2.48                     | 0.46              |
| 54:RFF:128:VAL:HG21 | 54:RFF:141:ARG:HE   | 1.80                     | 0.46              |
| 1:L50:1878:G:H2'    | 1:L50:1879:A:C8     | 2.50                     | 0.46              |
| 3:LA0:238:LYS:HZ3   | 42:S60:714:U:P      | 2.38                     | 0.46              |
| 10:LE0:39:ILE:HG22  | 13:LFF:107:ASN:ND2  | 2.30                     | 0.46              |
| 47:SC0:216:PHE:HZ   | 71:SW0:128:TYR:CD1  | 2.33                     | 0.46              |
| 1:K50:2060:A:H2'    | 1:K50:2060:A:N3     | 2.29                     | 0.46              |
| 42:R60:1126:A:H8    | 42:R60:1164:G:H21   | 1.61                     | 0.46              |
| 1:L50:2140:A:O2'    | 1:L50:2141:U:H2'    | 2.15                     | 0.46              |
| 42:S60:63:G:H2'     | 42:S60:76:A:C2      | 2.50                     | 0.46              |
| 42:S60:86:A:H1'     | 51:SE0:7:LYS:HD2    | 1.97                     | 0.46              |
| 42:S60:517:U:H5'    | 51:SE0:219:SER:O    | 2.15                     | 0.46              |
| 67:SS0:55:ARG:HH22  | 68:ST0:32:ASN:ND2   | 2.13                     | 0.46              |
| 1:K50:2140:A:O2'    | 1:K50:2141:U:H2'    | 2.15                     | 0.46              |
| 42:R60:705:A:C2     | 42:R60:706:G:N1     | 2.83                     | 0.46              |
| 2:L70:1:A:H61       | 2:L70:118:U:H3      | 1.63                     | 0.46              |
| 42:S60:662:U:H1'    | 63:SN0:52:ASN:ND2   | 2.29                     | 0.46              |
| 42:R60:396:A:H2'    | 42:R60:397:A:C8     | 2.51                     | 0.46              |
| 42:S60:396:A:H2'    | 42:S60:397:A:C8     | 2.51                     | 0.46              |
| 42:S60:1018:U:H4'   | 42:S60:1019:C:OP2   | 2.15                     | 0.46              |
| 43:SA0:52:LYS:HB2   | 66:SR0:109:TYR:CE2  | 2.50                     | 0.46              |
| 42:R60:964:G:N2     | 42:R60:966:G:H3'    | 2.31                     | 0.46              |
| 62:RM0:15:LEU:C     | 62:RM0:15:LEU:HD12  | 2.41                     | 0.46              |
| 42:S60:997:A:C2     | 42:S60:998:U:H1'    | 2.50                     | 0.46              |
| 54:SFF:99:LYS:HB3   | 54:RFF:104:THR:HG21 | 1.98                     | 0.46              |
| 67:SS0:10:PHE:CD1   | 74:SZ0:81:PHE:CD2   | 3.03                     | 0.46              |
| 1:K50:1308:A:H61    | 1:K50:2434:A:H2     | 1.63                     | 0.46              |
| 42:R60:86:A:H1'     | 51:RE0:7:LYS:HD2    | 1.97                     | 0.46              |
| 42:R60:864:A:N1     | 75:RP0:118:ARG:HB2  | 2.31                     | 0.46              |
| 63:RN0:66:VAL:HG23  | 63:RN0:67:THR:HG23  | 1.97                     | 0.46              |
| 1:L50:303:C:H2'     | 1:L50:304:U:C6      | 2.51                     | 0.46              |
| 43:SA0:10:ASP:CB    | 66:SR0:112:ASN:HD21 | 2.28                     | 0.46              |
| 47:SC0:50:HIS:HA    | 70:SV0:6:ARG:HD2    | 1.98                     | 0.46              |
| 53:SF0:40:LEU:HD23  | 65:SQ0:43:PHE:HE1   | 1.73                     | 0.46              |
| 1:K50:202:G:O2'     | 17:KHH:105:THR:HG22 | 2.16                     | 0.46              |
| 2:K70:1:A:H61       | 2:K70:118:U:H3      | 1.63                     | 0.46              |
| 42:R60:349:A:OP1    | 51:RE0:57:ASN:ND2   | 2.48                     | 0.46              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 47:RC0:148:VAL:HG21 | 71:RW0:97:PHE:CE1   | 2.51                     | 0.46              |
| 1:L50:202:G:O2'     | 17:LHH:105:THR:HG22 | 2.16                     | 0.46              |
| 42:S60:970:U:H6     | 42:S60:970:U:H5''   | 1.80                     | 0.46              |
| 1:K50:303:C:H2'     | 1:K50:304:U:C6      | 2.51                     | 0.46              |
| 10:KE0:39:ILE:HG22  | 13:KFF:107:ASN:ND2  | 2.30                     | 0.46              |
| 42:R60:910:A:H62    | 42:R60:922:G:N2     | 2.11                     | 0.46              |
| 42:R60:1110:C:H5'   | 68:RT0:54:THR:HG22  | 1.97                     | 0.46              |
| 42:S60:989:G:H5'    | 43:SA0:104:ILE:HG23 | 1.98                     | 0.46              |
| 47:SC0:130:PRO:CB   | 70:SV0:4:PHE:CE1    | 2.98                     | 0.46              |
| 49:SD0:34:LYS:HD3   | 69:SU0:62:CYS:HB3   | 1.98                     | 0.46              |
| 22:KL0:25:GLN:HB3   | 22:KL0:26:PRO:HD3   | 1.97                     | 0.46              |
| 29:KP0:70:THR:HG22  | 29:KP0:72:GLN:H     | 1.81                     | 0.46              |
| 42:R60:131:U:H2'    | 42:R60:132:C:C6     | 2.51                     | 0.46              |
| 42:R60:384:A:C2     | 59:RJ0:169:ARG:HB2  | 2.51                     | 0.46              |
| 42:S60:466:C:H4'    | 72:SX0:100:GLU:HG2  | 1.97                     | 0.45              |
| 42:R60:864:A:C2     | 75:RP0:118:ARG:HB2  | 2.51                     | 0.45              |
| 43:RA0:197:ARG:HD3  | 66:RR0:91:LEU:CB    | 2.45                     | 0.45              |
| 22:LL0:25:GLN:HB3   | 22:LL0:26:PRO:HD3   | 1.97                     | 0.45              |
| 42:S60:244:U:H2'    | 42:S60:245:A:H8     | 1.81                     | 0.45              |
| 42:S60:1085:G:H4'   | 75:SP0:140:THR:CG2  | 2.47                     | 0.45              |
| 42:S60:1109:A:H2'   | 42:S60:1110:C:C6    | 2.52                     | 0.45              |
| 47:SC0:148:VAL:HG21 | 71:SW0:97:PHE:CE1   | 2.51                     | 0.45              |
| 42:R60:662:U:H1'    | 63:RN0:52:ASN:ND2   | 2.29                     | 0.45              |
| 42:S60:131:U:H2'    | 42:S60:132:C:C6     | 2.51                     | 0.45              |
| 42:S60:864:A:N1     | 75:SP0:118:ARG:HB2  | 2.31                     | 0.45              |
| 54:SFF:128:VAL:HG21 | 54:SFF:141:ARG:HE   | 1.80                     | 0.45              |
| 4:KAA:127:GLN:HE22  | 19:KII:7:ASN:H      | 1.63                     | 0.45              |
| 42:R60:474:A:O2'    | 47:RC0:193:LYS:NZ   | 2.49                     | 0.45              |
| 49:RD0:239:ILE:CA   | 66:RR0:19:ARG:NH1   | 2.77                     | 0.45              |
| 73:RY0:116:ARG:NH1  | 73:RY0:120:LYS:HZ2  | 2.15                     | 0.45              |
| 3:LA0:238:LYS:HZ2   | 42:S60:714:U:H5''   | 1.81                     | 0.45              |
| 37:LW0:98:ASN:HD22  | 55:SG0:147:PHE:N    | 2.10                     | 0.45              |
| 42:S60:864:A:C4     | 75:SP0:118:ARG:HD3  | 2.51                     | 0.45              |
| 42:S60:909:G:O6     | 62:SM0:37:ARG:HB3   | 2.15                     | 0.45              |
| 42:R60:1085:G:OP1   | 75:RP0:99:ARG:NE    | 2.46                     | 0.45              |
| 49:RD0:34:LYS:HD3   | 69:RU0:62:CYS:HB3   | 1.98                     | 0.45              |
| 54:RFF:96:GLN:OE1   | 54:RFF:96:GLN:N     | 2.50                     | 0.45              |
| 1:L50:1308:A:H61    | 1:L50:2434:A:H2     | 1.63                     | 0.45              |
| 1:L50:2416:G:H5''   | 1:L50:2416:G:H8     | 1.82                     | 0.45              |
| 6:LC0:322:VAL:O     | 12:LF0:140:ARG:NH2  | 2.49                     | 0.45              |
| 29:LP0:70:THR:HG22  | 29:LP0:72:GLN:H     | 1.81                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 31:LQ0:21:ARG:HB3   | 31:LQ0:57:THR:HG21  | 1.98                     | 0.45              |
| 62:SM0:15:LEU:C     | 62:SM0:15:LEU:HD12  | 2.41                     | 0.45              |
| 1:K50:158:A:N6      | 1:K50:168:G:H1'     | 2.32                     | 0.45              |
| 1:K50:2267:C:O2     | 1:K50:2267:C:O4'    | 2.33                     | 0.45              |
| 3:KA0:238:LYS:HZ3   | 42:R60:714:U:P      | 2.39                     | 0.45              |
| 42:R60:1194:U:H2'   | 42:R60:1196:U:C5    | 2.51                     | 0.45              |
| 43:RA0:10:ASP:HB3   | 66:RR0:112:ASN:OD1  | 2.16                     | 0.45              |
| 47:RC0:50:HIS:HA    | 70:RV0:6:ARG:HD2    | 1.98                     | 0.45              |
| 47:RC0:130:PRO:CB   | 70:RV0:4:PHE:CE1    | 2.98                     | 0.45              |
| 54:RFF:93:LYS:HB3   | 54:RFF:94:PRO:CD    | 2.42                     | 0.45              |
| 1:L50:1032:A:H8     | 1:L50:1032:A:H5''   | 1.82                     | 0.45              |
| 1:L50:1691:A:H62    | 42:S60:1248:G:H4'   | 1.71                     | 0.45              |
| 42:S60:661:A:H5'    | 63:SN0:15:VAL:O     | 2.17                     | 0.45              |
| 42:S60:864:A:C2     | 75:SP0:118:ARG:HB2  | 2.52                     | 0.45              |
| 12:KF0:69:LYS:HG3   | 34:KT0:142:MET:O    | 2.17                     | 0.45              |
| 42:R60:1085:G:H4'   | 75:RP0:140:THR:CG2  | 2.47                     | 0.45              |
| 43:RA0:218:GLN:HB3  | 66:RR0:84:PHE:CE2   | 2.51                     | 0.45              |
| 67:RS0:24:PHE:CE2   | 67:RS0:107:ILE:HG12 | 2.52                     | 0.45              |
| 1:L50:158:A:N6      | 1:L50:168:G:H1'     | 2.32                     | 0.45              |
| 42:S60:55:G:H5'     | 73:SY0:123:ARG:NH1  | 2.32                     | 0.45              |
| 42:S60:1194:U:H2'   | 42:S60:1196:U:C5    | 2.51                     | 0.45              |
| 67:SS0:24:PHE:CE2   | 67:SS0:107:ILE:HG12 | 2.52                     | 0.45              |
| 6:KC0:322:VAL:O     | 12:KF0:140:ARG:NH2  | 2.49                     | 0.45              |
| 51:RE0:183:LEU:HD22 | 51:RE0:191:CYS:HB2  | 1.98                     | 0.45              |
| 73:RY0:116:ARG:CZ   | 73:RY0:120:LYS:HZ2  | 2.30                     | 0.45              |
| 42:S60:478:C:O2     | 61:SL0:93:LYS:HE2   | 2.17                     | 0.45              |
| 42:S60:964:G:N2     | 42:S60:966:G:H3'    | 2.31                     | 0.45              |
| 1:K50:1032:A:H5''   | 1:K50:1032:A:H8     | 1.82                     | 0.45              |
| 42:S60:899:A:O2'    | 60:SK0:50:SER:OG    | 2.18                     | 0.45              |
| 42:S60:1082:A:H2'   | 42:S60:1083:U:C6    | 2.52                     | 0.45              |
| 59:SJ0:84:MET:HE2   | 59:SJ0:84:MET:HA    | 1.99                     | 0.45              |
| 67:SS0:127:LEU:HD22 | 75:SP0:132:ARG:NH2  | 2.32                     | 0.45              |
| 6:KC0:103:VAL:HG13  | 22:KL0:23:PHE:CZ    | 2.52                     | 0.45              |
| 37:KW0:99:LYS:O     | 37:KW0:102:LYS:CG   | 2.64                     | 0.45              |
| 43:RA0:50:ASP:OD1   | 66:RR0:109:TYR:OH   | 2.33                     | 0.45              |
| 43:RA0:50:ASP:CG    | 66:RR0:109:TYR:HH   | 2.23                     | 0.45              |
| 47:RC0:167:GLY:HA3  | 59:RJ0:103:LEU:O    | 2.17                     | 0.45              |
| 67:RS0:127:LEU:HD22 | 75:RP0:132:ARG:NH2  | 2.32                     | 0.45              |
| 1:L50:316:A:OP1     | 26:LN0:50:MET:HE1   | 2.17                     | 0.45              |
| 6:LC0:103:VAL:HG13  | 22:LL0:23:PHE:CZ    | 2.52                     | 0.45              |
| 43:SA0:85:LYS:NZ    | 66:SR0:82:GLU:OE2   | 2.48                     | 0.45              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 48:SCC:45:ILE:HG12  | 53:SF0:133:SER:HB3  | 1.99                     | 0.45              |
| 51:SE0:183:LEU:HD22 | 51:SE0:191:CYS:HB2  | 1.98                     | 0.45              |
| 54:SFF:93:LYS:HB3   | 54:SFF:94:PRO:CD    | 2.42                     | 0.45              |
| 73:SY0:22:GLU:C     | 73:SY0:23:LEU:HG    | 2.33                     | 0.45              |
| 1:K50:316:A:OP1     | 26:KN0:50:MET:HE1   | 2.17                     | 0.45              |
| 1:K50:2416:G:H8     | 1:K50:2416:G:H5''   | 1.82                     | 0.45              |
| 42:R60:864:A:C4     | 75:RP0:118:ARG:HD3  | 2.52                     | 0.45              |
| 42:R60:989:G:H5'    | 43:RA0:104:ILE:HG23 | 1.98                     | 0.45              |
| 1:L50:1885:G:H1     | 1:L50:1933:C:H42    | 1.66                     | 0.44              |
| 6:LC0:328:ILE:HG13  | 12:LF0:53:ILE:HG22  | 1.99                     | 0.44              |
| 42:S60:94:U:H3'     | 42:S60:263:A:H61    | 1.83                     | 0.44              |
| 58:SI0:69:THR:HG21  | 61:SL0:22:TYR:CE2   | 2.52                     | 0.44              |
| 71:RW0:26:ARG:O     | 71:RW0:26:ARG:HG2   | 2.18                     | 0.44              |
| 1:L50:2267:C:O2     | 1:L50:2267:C:O4'    | 2.33                     | 0.44              |
| 42:S60:431:G:H2'    | 42:S60:445:U:N3     | 2.32                     | 0.44              |
| 43:SA0:10:ASP:HB3   | 66:SR0:112:ASN:OD1  | 2.16                     | 0.44              |
| 43:SA0:51:ILE:CD1   | 66:SR0:105:MET:CE   | 2.89                     | 0.44              |
| 47:SC0:148:VAL:HG21 | 71:SW0:97:PHE:CZ    | 2.53                     | 0.44              |
| 51:SE0:175:LEU:HD22 | 51:SE0:222:PHE:CD1  | 2.52                     | 0.44              |
| 35:KU0:39:ILE:HG23  | 35:KU0:48:LEU:HD21  | 2.00                     | 0.44              |
| 42:R60:1109:A:H2'   | 42:R60:1110:C:C6    | 2.51                     | 0.44              |
| 43:RA0:52:LYS:HB2   | 66:RR0:109:TYR:CD1  | 2.51                     | 0.44              |
| 64:RO0:27:HIS:HE1   | 64:RO0:36:THR:HG23  | 1.82                     | 0.44              |
| 42:S60:1107:U:H2'   | 42:S60:1108:C:C6    | 2.53                     | 0.44              |
| 43:SA0:218:GLN:HB3  | 66:SR0:84:PHE:CE2   | 2.51                     | 0.44              |
| 73:SY0:116:ARG:CZ   | 73:SY0:120:LYS:NZ   | 2.80                     | 0.44              |
| 2:K70:70:U:H3       | 2:K70:105:G:H1      | 1.65                     | 0.44              |
| 31:KQ0:21:ARG:HB3   | 31:KQ0:57:THR:HG21  | 1.98                     | 0.44              |
| 42:R60:478:C:O2     | 61:RL0:93:LYS:HE2   | 2.17                     | 0.44              |
| 42:R60:661:A:H5'    | 63:RN0:15:VAL:O     | 2.17                     | 0.44              |
| 42:R60:1144:G:O2'   | 42:R60:1145:G:H5'   | 2.17                     | 0.44              |
| 51:RE0:175:LEU:HD22 | 51:RE0:222:PHE:CD1  | 2.52                     | 0.44              |
| 42:S60:662:U:H1'    | 63:SN0:52:ASN:HD21  | 1.83                     | 0.44              |
| 42:S60:995:A:C3'    | 42:S60:996:G:H8     | 2.23                     | 0.44              |
| 42:S60:1010:G:OP1   | 69:SU0:52:LYS:CE    | 2.65                     | 0.44              |
| 3:KA0:238:LYS:NZ    | 42:R60:714:U:H5''   | 2.32                     | 0.44              |
| 42:R60:171:U:H5'    | 42:R60:172:U:H6     | 1.82                     | 0.44              |
| 42:R60:1010:G:OP1   | 69:RU0:52:LYS:CE    | 2.65                     | 0.44              |
| 58:RI0:69:THR:HG21  | 61:RL0:22:TYR:CE2   | 2.52                     | 0.44              |
| 1:L50:188:G:OP2     | 4:LAA:34:LYS:HG2    | 2.17                     | 0.44              |
| 12:LF0:69:LYS:HG3   | 34:LT0:142:MET:O    | 2.17                     | 0.44              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 42:S60:997:A:H3'    | 42:S60:998:U:C6    | 2.53                     | 0.44              |
| 67:SS0:24:PHE:CE2   | 67:SS0:79:ILE:HG21 | 2.53                     | 0.44              |
| 42:R60:55:G:H5'     | 73:RY0:123:ARG:NH1 | 2.32                     | 0.44              |
| 42:R60:244:U:H2'    | 42:R60:245:A:H8    | 1.81                     | 0.44              |
| 47:RC0:148:VAL:HG21 | 71:RW0:97:PHE:CZ   | 2.53                     | 0.44              |
| 35:LU0:39:ILE:HG23  | 35:LU0:48:LEU:HD21 | 1.99                     | 0.44              |
| 43:SA0:63:ARG:CD    | 70:SV0:30:LEU:CG   | 2.95                     | 0.44              |
| 42:R60:1082:A:H2'   | 42:R60:1083:U:C6   | 2.52                     | 0.44              |
| 42:R60:1121:A:H3'   | 42:R60:1122:A:H8   | 1.82                     | 0.44              |
| 10:LE0:11:ILE:HD12  | 11:LEE:91:ALA:HB1  | 1.98                     | 0.44              |
| 37:LW0:69:GLU:O     | 37:LW0:70:LYS:C    | 2.61                     | 0.44              |
| 44:SAA:47:ALA:HB2   | 48:SCC:61:ARG:HE   | 1.71                     | 0.44              |
| 54:SFF:132:ARG:C    | 42:R60:918:A:H4'   | 2.41                     | 0.44              |
| 34:KT0:126:PRO:HB2  | 34:KT0:128:LEU:CD2 | 2.47                     | 0.44              |
| 73:RY0:116:ARG:CZ   | 73:RY0:120:LYS:NZ  | 2.80                     | 0.44              |
| 1:L50:2551:C:H2'    | 1:L50:2552:G:O4'   | 2.18                     | 0.44              |
| 2:L70:70:U:H3       | 2:L70:105:G:H1     | 1.65                     | 0.44              |
| 42:S60:171:U:H5'    | 42:S60:172:U:H6    | 1.82                     | 0.44              |
| 42:S60:1149:U:C5    | 67:SS0:140:ARG:CZ  | 3.00                     | 0.44              |
| 51:SE0:54:VAL:CG2   | 73:SY0:23:LEU:HD11 | 2.47                     | 0.44              |
| 10:KE0:11:ILE:HD12  | 11:KEE:91:ALA:HB1  | 1.99                     | 0.44              |
| 42:R60:914:U:C5     | 42:R60:916:G:C5    | 3.06                     | 0.44              |
| 43:RA0:33:LEU:HD13  | 43:RA0:150:THR:HA  | 2.00                     | 0.44              |
| 43:RA0:117:ARG:CZ   | 47:RC0:243:GLU:OE2 | 2.65                     | 0.44              |
| 47:RC0:166:LYS:O    | 59:RJ0:103:LEU:HB3 | 2.18                     | 0.44              |
| 56:RGG:228:LYS:HZ3  | 66:RR0:25:THR:CG2  | 2.29                     | 0.44              |
| 41:MD1:106:TYR:HE2  | 41:MD1:108:GLU:HA  | 1.83                     | 0.44              |
| 42:S60:517:U:C5'    | 51:SE0:219:SER:O   | 2.66                     | 0.44              |
| 64:SO0:27:HIS:HE1   | 64:SO0:36:THR:HG23 | 1.82                     | 0.44              |
| 1:K50:188:G:OP2     | 4:KAA:34:LYS:HG2   | 2.17                     | 0.44              |
| 1:K50:2551:C:H2'    | 1:K50:2552:G:O4'   | 2.18                     | 0.44              |
| 41:MD2:106:TYR:HE2  | 41:MD2:108:GLU:HA  | 1.83                     | 0.44              |
| 42:S60:1160:A:P     | 75:SP0:62:SER:HG   | 2.40                     | 0.43              |
| 47:SC0:148:VAL:HG22 | 71:SW0:94:SER:HB2  | 2.00                     | 0.43              |
| 17:KHH:113:LYS:HE2  | 22:KL0:46:ASN:HD22 | 1.83                     | 0.43              |
| 37:KW0:69:GLU:O     | 37:KW0:70:LYS:C    | 2.60                     | 0.43              |
| 41:MD2:17:ILE:HD12  | 41:MD2:95:TYR:CD2  | 2.53                     | 0.43              |
| 3:LA0:238:LYS:NZ    | 42:S60:714:U:H5''  | 2.32                     | 0.43              |
| 42:S60:218:A:H4'    | 42:S60:219:U:H5''  | 2.00                     | 0.43              |
| 42:S60:1144:G:O2'   | 42:S60:1145:G:H5'  | 2.17                     | 0.43              |
| 69:SU0:116:THR:O    | 69:SU0:117:LEU:HG  | 2.18                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:R60:94:U:H3'     | 42:R60:263:A:H61    | 1.83                     | 0.43              |
| 42:R60:1149:U:C5    | 67:RS0:140:ARG:CZ   | 3.00                     | 0.43              |
| 43:RA0:63:ARG:CD    | 70:RV0:30:LEU:CG    | 2.95                     | 0.43              |
| 49:RD0:30:ALA:HB2   | 69:RU0:60:PHE:CE2   | 2.53                     | 0.43              |
| 42:S60:132:C:H3'    | 42:S60:133:A:C8     | 2.53                     | 0.43              |
| 42:S60:1121:A:H3'   | 42:S60:1122:A:H8    | 1.82                     | 0.43              |
| 42:S60:1160:A:OP1   | 75:SP0:62:SER:OG    | 2.22                     | 0.43              |
| 43:SA0:33:LEU:HD13  | 43:SA0:150:THR:HA   | 2.00                     | 0.43              |
| 47:SC0:167:GLY:HA3  | 59:SJ0:103:LEU:O    | 2.17                     | 0.43              |
| 54:SFF:96:GLN:OE1   | 54:SFF:96:GLN:N     | 2.50                     | 0.43              |
| 71:SW0:26:ARG:HG2   | 71:SW0:26:ARG:O     | 2.18                     | 0.43              |
| 1:K50:1875:G:H2'    | 1:K50:1876:A:C8     | 2.53                     | 0.43              |
| 42:R60:995:A:C3'    | 42:R60:996:G:H8     | 2.23                     | 0.43              |
| 51:RE0:54:VAL:CG2   | 73:RY0:23:LEU:HD11  | 2.47                     | 0.43              |
| 69:RU0:116:THR:O    | 69:RU0:117:LEU:HG   | 2.18                     | 0.43              |
| 14:LG0:119:ASP:CG   | 14:LG0:145:THR:HA   | 2.44                     | 0.43              |
| 41:MD1:52:LYS:CG    | 42:S60:606:G:N2     | 2.74                     | 0.43              |
| 43:SA0:214:LEU:HD13 | 66:SR0:86:PRO:HG3   | 2.00                     | 0.43              |
| 58:SI0:123:ASP:HB2  | 61:SL0:22:TYR:HE1   | 1.84                     | 0.43              |
| 1:K50:32:G:H21      | 1:K50:377:A:H62     | 1.66                     | 0.43              |
| 1:K50:1089:U:H2'    | 1:K50:1090:A:H8     | 1.84                     | 0.43              |
| 27:KO0:84:LYS:HE2   | 27:KO0:89:HIS:CD2   | 2.54                     | 0.43              |
| 42:R60:1107:U:H2'   | 42:R60:1108:C:C6    | 2.53                     | 0.43              |
| 1:L50:32:G:H21      | 1:L50:377:A:H62     | 1.66                     | 0.43              |
| 1:L50:2525:G:H5'    | 29:LP0:71:PRO:HD3   | 2.00                     | 0.43              |
| 5:LB0:133:LEU:H     | 5:LB0:133:LEU:HG    | 1.69                     | 0.43              |
| 11:LEE:133:LEU:O    | 11:LEE:133:LEU:HG   | 2.19                     | 0.43              |
| 42:S60:50:U:H2'     | 42:S60:51:G:C8      | 2.54                     | 0.43              |
| 42:S60:705:A:H2'    | 42:S60:707:A:N7     | 2.34                     | 0.43              |
| 42:S60:1230:U:O3'   | 44:SAA:88:SER:HA    | 2.18                     | 0.43              |
| 43:SA0:52:LYS:HB2   | 66:SR0:109:TYR:CD1  | 2.52                     | 0.43              |
| 4:KAA:144:VAL:HG21  | 22:KL0:163:TYR:O    | 2.19                     | 0.43              |
| 41:MD2:52:LYS:CG    | 42:R60:606:G:N2     | 2.74                     | 0.43              |
| 42:R60:218:A:H4'    | 42:R60:219:U:H5''   | 2.00                     | 0.43              |
| 42:R60:517:U:C5'    | 51:RE0:219:SER:O    | 2.66                     | 0.43              |
| 42:R60:1230:U:O3'   | 44:RAA:88:SER:HA    | 2.18                     | 0.43              |
| 63:RN0:122:LEU:C    | 63:RN0:122:LEU:HD23 | 2.44                     | 0.43              |
| 1:L50:597:A:H4'     | 63:SN0:123:TYR:CD1  | 2.53                     | 0.43              |
| 14:LG0:174:PHE:CE2  | 14:LG0:178:ILE:HD11 | 2.53                     | 0.43              |
| 34:LT0:126:PRO:HB2  | 34:LT0:128:LEU:CD2  | 2.47                     | 0.43              |
| 42:S60:189:A:H2'    | 42:S60:190:A:H4'    | 2.01                     | 0.43              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 63:SN0:122:LEU:HD23 | 63:SN0:122:LEU:C    | 2.44                     | 0.43              |
| 1:K50:1885:G:H1     | 1:K50:1933:C:H42    | 1.66                     | 0.43              |
| 42:R60:916:G:O3'    | 42:R60:917:U:O2     | 2.37                     | 0.43              |
| 43:RA0:50:ASP:OD1   | 66:RR0:109:TYR:CE2  | 2.72                     | 0.43              |
| 48:RCC:45:ILE:HG12  | 53:RF0:133:SER:HB3  | 1.99                     | 0.43              |
| 59:RJ0:84:MET:HE2   | 59:RJ0:84:MET:HA    | 1.99                     | 0.43              |
| 62:RM0:15:LEU:HB3   | 62:RM0:122:PHE:CE2  | 2.52                     | 0.43              |
| 12:LF0:69:LYS:HD3   | 34:LT0:141:GLU:CG   | 2.49                     | 0.43              |
| 42:S60:914:U:C5     | 42:S60:916:G:C5     | 3.06                     | 0.43              |
| 10:KE0:100:ILE:CD1  | 24:KM0:102:PHE:HB2  | 2.36                     | 0.43              |
| 14:KG0:119:ASP:CG   | 14:KG0:145:THR:HA   | 2.43                     | 0.43              |
| 14:KG0:174:PHE:CE2  | 14:KG0:178:ILE:HD11 | 2.53                     | 0.43              |
| 42:R60:431:G:H2'    | 42:R60:445:U:N3     | 2.32                     | 0.43              |
| 42:R60:997:A:H3'    | 42:R60:998:U:C6     | 2.53                     | 0.43              |
| 43:RA0:85:LYS:NZ    | 66:RR0:82:GLU:OE2   | 2.48                     | 0.43              |
| 1:L50:21:U:H5'      | 1:L50:1087:G:OP1    | 2.19                     | 0.43              |
| 26:LN0:14:LYS:HE2   | 26:LN0:120:TRP:CZ3  | 2.53                     | 0.43              |
| 42:S60:502:A:O3'    | 71:SW0:4:LYS:NZ     | 2.52                     | 0.43              |
| 42:S60:933:G:H8     | 42:S60:933:G:O5'    | 2.02                     | 0.43              |
| 50:SDD:16:PHE:HE1   | 75:SP0:66:GLY:HA3   | 1.82                     | 0.43              |
| 58:SI0:69:THR:HG22  | 61:SL0:20:ASN:OD1   | 2.18                     | 0.43              |
| 1:K50:2462:A:H2'    | 1:K50:2463:A:C8     | 2.54                     | 0.43              |
| 12:KF0:69:LYS:HD3   | 34:KT0:141:GLU:CG   | 2.49                     | 0.43              |
| 37:KW0:80:VAL:O     | 37:KW0:81:ARG:C     | 2.62                     | 0.43              |
| 42:R60:790:G:H5''   | 42:R60:790:G:H8     | 1.84                     | 0.43              |
| 42:R60:1107:U:H2'   | 42:R60:1108:C:H6    | 1.84                     | 0.43              |
| 1:L50:1698:A:H1'    | 42:S60:1247:C:H1'   | 2.01                     | 0.43              |
| 43:SA0:43:GLU:HG2   | 66:SR0:120:LYS:HE2  | 2.01                     | 0.43              |
| 47:SC0:149:LYS:HB3  | 71:SW0:93:PRO:HA    | 2.01                     | 0.43              |
| 49:SD0:30:ALA:HB2   | 69:SU0:60:PHE:CE2   | 2.53                     | 0.43              |
| 6:KC0:2:SER:O       | 6:KC0:3:ARG:HG2     | 2.19                     | 0.43              |
| 42:R60:830:G:O3'    | 42:R60:831:G:H8     | 2.02                     | 0.43              |
| 50:RDD:16:PHE:HE1   | 75:RP0:66:GLY:HA3   | 1.82                     | 0.43              |
| 55:RG0:144:LYS:C    | 55:RG0:146:GLY:H    | 2.27                     | 0.43              |
| 1:L50:88:A:H5'      | 21:LJJ:75:ALA:HB2   | 2.01                     | 0.43              |
| 1:L50:1441:U:H4'    | 38:LX0:64:ILE:CD1   | 2.49                     | 0.43              |
| 1:L50:1875:G:H2'    | 1:L50:1876:A:C8     | 2.53                     | 0.43              |
| 17:LHH:113:LYS:HE2  | 22:LL0:46:ASN:HD22  | 1.83                     | 0.43              |
| 42:S60:790:G:H5''   | 42:S60:790:G:H8     | 1.84                     | 0.43              |
| 42:S60:1262:A:C8    | 42:S60:1262:A:H5''  | 2.54                     | 0.43              |
| 53:SF0:42:HIS:ND1   | 65:SQ0:79:TYR:OH    | 2.36                     | 0.43              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:K50:597:A:H4'     | 63:RN0:123:TYR:CD1 | 2.53                     | 0.43              |
| 42:R60:1208:G:H2'   | 42:R60:1209:C:H5'  | 2.01                     | 0.43              |
| 58:RI0:123:ASP:HB2  | 61:RL0:22:TYR:HE1  | 1.84                     | 0.43              |
| 1:L50:1691:A:C2     | 42:S60:1248:G:H1'  | 2.55                     | 0.42              |
| 24:LM0:71:ILE:O     | 24:LM0:71:ILE:HG13 | 2.18                     | 0.42              |
| 27:LO0:84:LYS:HE2   | 27:LO0:89:HIS:CD2  | 2.54                     | 0.42              |
| 37:LW0:67:HIS:HB2   | 42:S60:1282:A:N3   | 2.34                     | 0.42              |
| 41:MD1:17:ILE:HD12  | 41:MD1:95:TYR:CD2  | 2.53                     | 0.42              |
| 58:SI0:8:ARG:HH11   | 58:SI0:8:ARG:HD3   | 1.72                     | 0.42              |
| 1:K50:21:U:H5'      | 1:K50:1087:G:OP1   | 2.19                     | 0.42              |
| 1:K50:1441:U:H4'    | 38:KX0:64:ILE:CD1  | 2.49                     | 0.42              |
| 43:RA0:10:ASP:CB    | 66:RR0:112:ASN:OD1 | 2.67                     | 0.42              |
| 47:RC0:148:VAL:HG22 | 71:RW0:94:SER:HB2  | 2.00                     | 0.42              |
| 42:S60:999:C:O2'    | 42:S60:1000:C:H5'  | 2.20                     | 0.42              |
| 43:SA0:10:ASP:CB    | 66:SR0:112:ASN:OD1 | 2.67                     | 0.42              |
| 49:SD0:34:LYS:CE    | 69:SU0:60:PHE:HB3  | 2.49                     | 0.42              |
| 1:K50:145:A:H5''    | 21:KJJ:46:LYS:HD2  | 2.01                     | 0.42              |
| 6:KC0:328:ILE:HG13  | 12:KF0:53:ILE:HG22 | 1.99                     | 0.42              |
| 37:KW0:67:HIS:HB2   | 42:R60:1282:A:N3   | 2.34                     | 0.42              |
| 42:R60:502:A:O3'    | 71:RW0:4:LYS:NZ    | 2.52                     | 0.42              |
| 43:RA0:118:GLU:OE2  | 47:RC0:31:THR:CA   | 2.61                     | 0.42              |
| 58:RI0:68:LYS:HE2   | 58:RI0:152:TYR:CD2 | 2.54                     | 0.42              |
| 67:RS0:24:PHE:CE2   | 67:RS0:79:ILE:HG21 | 2.53                     | 0.42              |
| 1:L50:145:A:H5''    | 21:LJJ:46:LYS:HD2  | 2.01                     | 0.42              |
| 1:L50:1933:C:H2'    | 1:L50:1934:C:C6    | 2.55                     | 0.42              |
| 1:L50:2170:A:C8     | 28:LOO:54:PRO:HB3  | 2.55                     | 0.42              |
| 4:LAA:144:VAL:HG21  | 22:LL0:163:TYR:O   | 2.19                     | 0.42              |
| 37:LW0:99:LYS:O     | 37:LW0:102:LYS:CG  | 2.64                     | 0.42              |
| 54:SFF:93:LYS:CB    | 54:SFF:94:PRO:HD2  | 2.43                     | 0.42              |
| 42:R60:50:U:H2'     | 42:R60:51:G:C8     | 2.54                     | 0.42              |
| 42:R60:662:U:H1'    | 63:RN0:52:ASN:HD21 | 1.83                     | 0.42              |
| 42:R60:1230:U:O3'   | 44:RAA:88:SER:CB   | 2.67                     | 0.42              |
| 42:R60:1231:U:H4'   | 44:RAA:86:VAL:CG1  | 2.50                     | 0.42              |
| 49:RD0:34:LYS:CE    | 69:RU0:60:PHE:HB3  | 2.49                     | 0.42              |
| 58:RI0:69:THR:HG22  | 61:RL0:20:ASN:OD1  | 2.18                     | 0.42              |
| 1:L50:555:G:H1'     | 6:LC0:71:ARG:NH1   | 2.34                     | 0.42              |
| 1:L50:2160:G:H5''   | 28:LOO:65:LYS:HD2  | 2.02                     | 0.42              |
| 43:SA0:50:ASP:OD1   | 66:SR0:109:TYR:CE2 | 2.72                     | 0.42              |
| 47:SC0:166:LYS:O    | 59:SJ0:103:LEU:HB3 | 2.18                     | 0.42              |
| 1:K50:2525:G:H5'    | 29:KP0:71:PRO:HD3  | 2.00                     | 0.42              |
| 26:KN0:14:LYS:HE2   | 26:KN0:120:TRP:CZ3 | 2.53                     | 0.42              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:R60:996:G:H2'    | 42:R60:997:A:O4'    | 2.20                     | 0.42              |
| 42:R60:1023:A:P     | 66:RR0:3:GLN:OE1    | 2.78                     | 0.42              |
| 42:R60:1262:A:C8    | 42:R60:1262:A:H5''  | 2.54                     | 0.42              |
| 43:RA0:70:ASN:N     | 47:RC0:240:ILE:CD1  | 2.78                     | 0.42              |
| 43:RA0:184:TYR:CD2  | 70:RV0:35:ARG:HD3   | 2.54                     | 0.42              |
| 43:RA0:214:LEU:HD13 | 66:RR0:86:PRO:HG3   | 2.00                     | 0.42              |
| 56:RGG:147:ASN:HD22 | 56:RGG:147:ASN:N    | 2.17                     | 0.42              |
| 1:L50:2462:A:H2'    | 1:L50:2463:A:C8     | 2.54                     | 0.42              |
| 17:LHH:6:LYS:HG3    | 17:LHH:7:ASP:OD1    | 2.19                     | 0.42              |
| 42:S60:916:G:O3'    | 42:S60:917:U:O2     | 2.37                     | 0.42              |
| 42:S60:1033:A:H2'   | 42:S60:1034:A:H5'   | 2.00                     | 0.42              |
| 42:S60:1208:G:H2'   | 42:S60:1209:C:H5'   | 2.01                     | 0.42              |
| 42:S60:1231:U:H4'   | 44:SAA:86:VAL:CG1   | 2.50                     | 0.42              |
| 43:SA0:70:ASN:N     | 47:SC0:240:ILE:CD1  | 2.78                     | 0.42              |
| 43:SA0:184:TYR:CD2  | 70:SV0:35:ARG:HD3   | 2.54                     | 0.42              |
| 66:SR0:103:MET:SD   | 66:SR0:117:LEU:HG   | 2.60                     | 0.42              |
| 5:KB0:265:ARG:NH1   | 27:KOO:62:SER:OG    | 2.53                     | 0.42              |
| 11:KEE:133:LEU:HG   | 11:KEE:133:LEU:O    | 2.19                     | 0.42              |
| 17:KHH:66:LEU:HD12  | 38:KX0:22:ILE:HD11  | 2.01                     | 0.42              |
| 42:R60:189:A:H2'    | 42:R60:190:A:H4'    | 2.01                     | 0.42              |
| 42:R60:705:A:H2'    | 42:R60:707:A:N7     | 2.34                     | 0.42              |
| 43:RA0:215:TYR:CE1  | 66:RR0:84:PHE:CZ    | 3.08                     | 0.42              |
| 66:RR0:103:MET:SD   | 66:RR0:117:LEU:HG   | 2.60                     | 0.42              |
| 37:LW0:80:VAL:O     | 37:LW0:81:ARG:C     | 2.62                     | 0.42              |
| 42:S60:926:G:H2'    | 42:S60:927:G:C8     | 2.54                     | 0.42              |
| 43:SA0:118:GLU:OE2  | 47:SC0:31:THR:CA    | 2.61                     | 0.42              |
| 43:SA0:120:ARG:HE   | 47:SC0:232:ILE:HG22 | 1.75                     | 0.42              |
| 49:SD0:184:ILE:HD12 | 49:SD0:215:MET:CE   | 2.50                     | 0.42              |
| 1:K50:1933:C:H2'    | 1:K50:1934:C:C6     | 2.55                     | 0.42              |
| 1:K50:2160:G:H5''   | 28:KOO:65:LYS:HD2   | 2.02                     | 0.42              |
| 31:KQ0:164:TYR:CE2  | 31:KQ0:177:ARG:HD2  | 2.55                     | 0.42              |
| 42:R60:696:G:H1     | 42:R60:712:A:H2     | 1.68                     | 0.42              |
| 42:R60:1199:C:OP2   | 50:RDD:41:ARG:NH2   | 2.47                     | 0.42              |
| 46:RBB:69:LYS:HB2   | 46:RBB:69:LYS:HE3   | 1.85                     | 0.42              |
| 6:LC0:2:SER:O       | 6:LC0:3:ARG:HG2     | 2.19                     | 0.42              |
| 42:S60:830:G:O3'    | 42:S60:831:G:H8     | 2.02                     | 0.42              |
| 42:S60:967:A:H5''   | 42:S60:968:C:C6     | 2.55                     | 0.42              |
| 43:SA0:50:ASP:OD1   | 66:SR0:109:TYR:OH   | 2.33                     | 0.42              |
| 43:SA0:215:TYR:CG   | 66:SR0:84:PHE:CE2   | 3.05                     | 0.42              |
| 56:SGG:147:ASN:HD22 | 56:SGG:147:ASN:N    | 2.17                     | 0.42              |
| 34:LT0:112:ASN:C    | 34:LT0:112:ASN:ND2  | 2.76                     | 0.42              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 42:S60:552:G:O2'    | 71:SW0:105:SER:HB3 | 2.20                     | 0.42              |
| 42:S60:1023:A:P     | 66:SR0:3:GLN:OE1   | 2.78                     | 0.42              |
| 42:S60:1230:U:O3'   | 44:SAA:88:SER:CB   | 2.68                     | 0.42              |
| 43:SA0:64:MET:HB3   | 70:SV0:27:MET:CG   | 2.28                     | 0.42              |
| 43:SA0:215:TYR:CE1  | 66:SR0:84:PHE:CZ   | 3.08                     | 0.42              |
| 67:SS0:127:LEU:HD22 | 75:SP0:132:ARG:CZ  | 2.50                     | 0.42              |
| 1:K50:88:A:H5'      | 21:KJJ:75:ALA:HB2  | 2.01                     | 0.42              |
| 1:K50:2211:A:H5''   | 1:K50:2212:G:N2    | 2.35                     | 0.42              |
| 42:R60:1024:G:C2    | 42:R60:1025:G:C8   | 3.08                     | 0.42              |
| 47:RC0:149:LYS:HB3  | 71:RW0:93:PRO:HA   | 2.01                     | 0.42              |
| 1:L50:222:A:H2'     | 1:L50:223:A:C8     | 2.55                     | 0.42              |
| 1:L50:2026:G:C2     | 28:LOO:5:PRO:HG2   | 2.55                     | 0.42              |
| 42:S60:173:A:N7     | 51:SE0:131:VAL:CG1 | 2.82                     | 0.42              |
| 42:S60:915:A:N3     | 54:RFF:150:LYS:CD  | 2.83                     | 0.42              |
| 42:S60:1168:A:H3'   | 42:S60:1169:G:C8   | 2.55                     | 0.42              |
| 1:K50:2026:G:C2     | 28:KOO:5:PRO:HG2   | 2.55                     | 0.42              |
| 42:R60:1033:A:H2'   | 42:R60:1034:A:H5'  | 2.00                     | 0.42              |
| 42:R60:1108:C:H5'   | 68:RT0:44:THR:OG1  | 2.20                     | 0.42              |
| 47:RC0:230:ASN:N    | 70:RV0:24:GLN:NE2  | 2.45                     | 0.42              |
| 31:LQ0:164:TYR:CE2  | 31:LQ0:177:ARG:HD2 | 2.55                     | 0.42              |
| 42:S60:1024:G:C2    | 42:S60:1025:G:C8   | 3.08                     | 0.42              |
| 43:SA0:57:LYS:NZ    | 70:SV0:60:TYR:CD1  | 2.84                     | 0.42              |
| 47:SC0:228:GLU:O    | 70:SV0:42:ILE:HG21 | 2.20                     | 0.42              |
| 49:SD0:94:GLN:NE2   | 60:SK0:19:SER:CB   | 2.81                     | 0.42              |
| 54:SFF:99:LYS:HE2   | 54:SFF:102:ILE:CG1 | 2.40                     | 0.42              |
| 1:K50:1325:G:H1     | 1:K50:1370:U:H3    | 1.67                     | 0.42              |
| 1:K50:1691:A:C2     | 42:R60:1248:G:H1'  | 2.55                     | 0.42              |
| 1:K50:1698:A:H1'    | 42:R60:1247:C:H1'  | 2.01                     | 0.42              |
| 1:K50:2170:A:C8     | 28:KOO:54:PRO:HB3  | 2.55                     | 0.42              |
| 1:K50:2573:U:H2'    | 1:K50:2574:A:C8    | 2.55                     | 0.42              |
| 42:R60:156:U:H2'    | 42:R60:157:A:C8    | 2.55                     | 0.42              |
| 42:R60:933:G:H8     | 42:R60:933:G:O5'   | 2.02                     | 0.42              |
| 42:R60:954:G:H5'    | 42:R60:980:G:OP1   | 2.20                     | 0.42              |
| 42:S60:924:U:H1'    | 42:S60:925:A:C8    | 2.55                     | 0.41              |
| 1:K50:1298:A:H5'    | 1:K50:1299:A:OP2   | 2.20                     | 0.41              |
| 1:K50:2610:U:H2'    | 1:K50:2611:C:C6    | 2.55                     | 0.41              |
| 42:R60:375:G:H5''   | 42:R60:375:G:H8    | 1.85                     | 0.41              |
| 42:R60:899:A:O2'    | 60:RK0:50:SER:OG   | 2.18                     | 0.41              |
| 42:R60:967:A:H5''   | 42:R60:968:C:C6    | 2.55                     | 0.41              |
| 43:RA0:81:ASP:C     | 43:RA0:83:GLY:H    | 2.28                     | 0.41              |
| 57:RH0:53:LEU:HB3   | 57:RH0:54:PRO:HD3  | 2.02                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:L50:1325:G:H1     | 1:L50:1370:U:H3    | 1.67                     | 0.41              |
| 1:L50:2211:A:H5''   | 1:L50:2212:G:N2    | 2.35                     | 0.41              |
| 5:LB0:265:ARG:NH1   | 27:LO0:62:SER:OG   | 2.53                     | 0.41              |
| 8:LD0:214:LEU:HD23  | 8:LD0:214:LEU:HA   | 1.94                     | 0.41              |
| 42:S60:954:G:H5'    | 42:S60:980:G:OP1   | 2.20                     | 0.41              |
| 42:S60:1107:U:H2'   | 42:S60:1108:C:H6   | 1.84                     | 0.41              |
| 1:K50:506:G:H2'     | 1:K50:508:A:N7     | 2.36                     | 0.41              |
| 17:KHH:6:LYS:HG3    | 17:KHH:7:ASP:OD1   | 2.19                     | 0.41              |
| 42:R60:924:U:H1'    | 42:R60:925:A:C8    | 2.55                     | 0.41              |
| 42:R60:926:G:H2'    | 42:R60:927:G:C8    | 2.54                     | 0.41              |
| 42:R60:995:A:H2'    | 42:R60:996:G:H5'   | 2.02                     | 0.41              |
| 42:R60:999:C:O2'    | 42:R60:1000:C:H5'  | 2.20                     | 0.41              |
| 55:RG0:156:GLU:O    | 55:RG0:160:LYS:HG3 | 2.20                     | 0.41              |
| 1:L50:1298:A:H5'    | 1:L50:1299:A:OP2   | 2.20                     | 0.41              |
| 42:S60:864:A:C6     | 75:SP0:118:ARG:HB2 | 2.55                     | 0.41              |
| 42:S60:996:G:H2'    | 42:S60:997:A:O4'   | 2.20                     | 0.41              |
| 47:SC0:229:LEU:CD1  | 70:SV0:42:ILE:HG12 | 2.50                     | 0.41              |
| 55:SG0:144:LYS:C    | 55:SG0:146:GLY:H   | 2.27                     | 0.41              |
| 58:SI0:68:LYS:HE2   | 58:SI0:152:TYR:CD2 | 2.54                     | 0.41              |
| 43:RA0:43:GLU:HG2   | 66:RR0:120:LYS:HE2 | 2.01                     | 0.41              |
| 47:RC0:228:GLU:O    | 70:RV0:42:ILE:HG21 | 2.20                     | 0.41              |
| 49:RD0:184:ILE:HD12 | 49:RD0:215:MET:HE3 | 2.03                     | 0.41              |
| 51:RE0:35:PRO:HD2   | 51:RE0:83:PRO:HG2  | 2.03                     | 0.41              |
| 62:RM0:15:LEU:CB    | 62:RM0:122:PHE:HE2 | 2.31                     | 0.41              |
| 1:L50:885:G:C8      | 1:L50:885:G:H5''   | 2.56                     | 0.41              |
| 1:L50:1089:U:H2'    | 1:L50:1090:A:H8    | 1.84                     | 0.41              |
| 8:LD0:262:ASP:C     | 8:LD0:264:SER:H    | 2.29                     | 0.41              |
| 37:LW0:102:LYS:HB3  | 55:SG0:150:ASP:HB3 | 2.03                     | 0.41              |
| 42:S60:1090:C:O2    | 75:SP0:146:HIS:HE1 | 2.02                     | 0.41              |
| 42:S60:1262:A:H61   | 42:S60:1301:U:H3   | 1.68                     | 0.41              |
| 61:SL0:144:ILE:HD13 | 61:SL0:147:LYS:HE2 | 2.03                     | 0.41              |
| 1:K50:1424:A:H4'    | 15:KGG:77:GLY:H    | 1.85                     | 0.41              |
| 1:K50:2492:U:H2'    | 1:K50:2493:G:C8    | 2.55                     | 0.41              |
| 42:R60:552:G:O2'    | 71:RW0:105:SER:HB3 | 2.20                     | 0.41              |
| 47:RC0:130:PRO:CG   | 70:RV0:4:PHE:CE1   | 3.03                     | 0.41              |
| 1:L50:1488:U:H6     | 1:L50:1488:U:H2'   | 1.65                     | 0.41              |
| 1:L50:1940:C:H2'    | 1:L50:1941:A:H8    | 1.86                     | 0.41              |
| 42:S60:1085:G:OP1   | 75:SP0:99:ARG:NE   | 2.46                     | 0.41              |
| 49:SD0:184:ILE:HD12 | 49:SD0:215:MET:HE3 | 2.03                     | 0.41              |
| 8:KD0:47:GLN:HB2    | 34:KT0:68:ASN:O    | 2.21                     | 0.41              |
| 14:KG0:16:PRO:HG2   | 26:KN0:32:GLN:HE21 | 1.86                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 47:RC0:149:LYS:HB2  | 71:RW0:93:PRO:O    | 2.21                     | 0.41              |
| 47:RC0:229:LEU:CD1  | 70:RV0:42:ILE:HG12 | 2.50                     | 0.41              |
| 28:LOO:64:LYS:HE2   | 28:LOO:64:LYS:HB3  | 1.92                     | 0.41              |
| 42:S60:474:A:O2'    | 47:SC0:193:LYS:NZ  | 2.48                     | 0.41              |
| 42:S60:696:G:H1     | 42:S60:712:A:H2    | 1.68                     | 0.41              |
| 42:S60:1054:G:H2'   | 42:S60:1055:A:O4'  | 2.21                     | 0.41              |
| 42:S60:1199:C:OP2   | 50:SDD:41:ARG:NH2  | 2.47                     | 0.41              |
| 50:SDD:13:GLU:OE2   | 75:SP0:76:LYS:NZ   | 2.37                     | 0.41              |
| 1:K50:1642:G:H2'    | 1:K50:1643:G:C8    | 2.56                     | 0.41              |
| 34:KT0:112:ASN:C    | 34:KT0:112:ASN:ND2 | 2.76                     | 0.41              |
| 43:RA0:64:MET:HB3   | 70:RV0:27:MET:CG   | 2.29                     | 0.41              |
| 1:L50:2610:U:H2'    | 1:L50:2611:C:C6    | 2.55                     | 0.41              |
| 14:LG0:16:PRO:HG2   | 26:LN0:32:GLN:HE21 | 1.86                     | 0.41              |
| 50:SDD:7:LYS:CA     | 75:SP0:67:PHE:O    | 2.68                     | 0.41              |
| 53:SF0:49:THR:O     | 53:SF0:49:THR:HG22 | 2.20                     | 0.41              |
| 1:K50:222:A:H2'     | 1:K50:223:A:C8     | 2.55                     | 0.41              |
| 1:K50:1078:G:O2'    | 11:KEE:80:LYS:NZ   | 2.54                     | 0.41              |
| 4:KAA:70:THR:OG1    | 19:KII:5:LYS:HB2   | 2.21                     | 0.41              |
| 18:KI0:30:LYS:HE2   | 18:KI0:66:GLU:HG2  | 2.02                     | 0.41              |
| 42:R60:918:A:C5     | 42:R60:919:C:C4    | 3.09                     | 0.41              |
| 42:R60:1090:C:O2    | 75:RP0:146:HIS:HE1 | 2.02                     | 0.41              |
| 67:RS0:127:LEU:HD22 | 75:RP0:132:ARG:CZ  | 2.50                     | 0.41              |
| 1:L50:506:G:H2'     | 1:L50:508:A:N7     | 2.36                     | 0.41              |
| 1:L50:1296:C:H6     | 1:L50:1296:C:H5''  | 1.85                     | 0.41              |
| 10:LE0:59:ALA:O     | 10:LE0:60:SER:HB2  | 2.21                     | 0.41              |
| 42:S60:999:C:C4     | 42:S60:1000:C:C4   | 3.09                     | 0.41              |
| 42:S60:1108:C:H5'   | 68:ST0:44:THR:OG1  | 2.20                     | 0.41              |
| 47:SC0:230:ASN:CB   | 70:SV0:24:GLN:NE2  | 2.84                     | 0.41              |
| 57:SH0:53:LEU:HB3   | 57:SH0:54:PRO:HD3  | 2.02                     | 0.41              |
| 1:K50:186:G:H2'     | 1:K50:187:A:C8     | 2.56                     | 0.41              |
| 1:K50:555:G:H1'     | 6:KC0:71:ARG:NH1   | 2.34                     | 0.41              |
| 2:K70:34:C:O2'      | 8:KD0:206:GLU:OE1  | 2.27                     | 0.41              |
| 17:KHH:66:LEU:CD1   | 38:KX0:22:ILE:HD11 | 2.51                     | 0.41              |
| 42:R60:173:A:N7     | 51:RE0:131:VAL:CG1 | 2.82                     | 0.41              |
| 42:R60:864:A:C6     | 75:RP0:118:ARG:HB2 | 2.55                     | 0.41              |
| 42:R60:1054:G:H2'   | 42:R60:1055:A:O4'  | 2.21                     | 0.41              |
| 47:RC0:219:PRO:CB   | 71:RW0:66:ARG:HH21 | 2.31                     | 0.41              |
| 1:L50:885:G:H5''    | 1:L50:885:G:H8     | 1.86                     | 0.41              |
| 1:L50:1642:G:H2'    | 1:L50:1643:G:C8    | 2.56                     | 0.41              |
| 1:L50:2492:U:H2'    | 1:L50:2493:G:C8    | 2.55                     | 0.41              |
| 1:L50:2573:U:H2'    | 1:L50:2574:A:C8    | 2.55                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 42:S60:375:G:H8     | 42:S60:375:G:H5''   | 1.85                     | 0.41              |
| 47:SC0:149:LYS:HB2  | 71:SW0:93:PRO:O     | 2.21                     | 0.41              |
| 51:SE0:35:PRO:HD2   | 51:SE0:83:PRO:HG2   | 2.03                     | 0.41              |
| 1:K50:885:G:H8      | 1:K50:885:G:H5''    | 1.85                     | 0.41              |
| 1:K50:1133:C:H4'    | 1:K50:1134:A:H5'    | 2.02                     | 0.41              |
| 10:KE0:59:ALA:O     | 10:KE0:60:SER:HB2   | 2.21                     | 0.41              |
| 42:R60:132:C:H3'    | 42:R60:133:A:C8     | 2.53                     | 0.41              |
| 42:R60:999:C:C4     | 42:R60:1000:C:C4    | 3.09                     | 0.41              |
| 42:R60:1024:G:O2'   | 42:R60:1025:G:H5'   | 2.21                     | 0.41              |
| 43:RA0:120:ARG:HH11 | 47:RC0:232:ILE:HD13 | 1.84                     | 0.41              |
| 49:RD0:184:ILE:HD12 | 49:RD0:215:MET:CE   | 2.50                     | 0.41              |
| 53:RF0:49:THR:O     | 53:RF0:49:THR:HG22  | 2.20                     | 0.41              |
| 61:RL0:144:ILE:HD13 | 61:RL0:147:LYS:HE2  | 2.03                     | 0.41              |
| 74:RZ0:58:ILE:O     | 74:RZ0:58:ILE:HG13  | 2.21                     | 0.41              |
| 1:L50:1078:G:O2'    | 11:LEE:80:LYS:NZ    | 2.54                     | 0.41              |
| 27:LO0:80:MET:C     | 27:LO0:80:MET:SD    | 3.04                     | 0.41              |
| 42:S60:156:U:H2'    | 42:S60:157:A:C8     | 2.55                     | 0.41              |
| 42:S60:574:A:H1'    | 46:SBB:67:GLY:CA    | 2.51                     | 0.41              |
| 42:S60:910:A:N6     | 42:S60:922:G:H21    | 2.15                     | 0.41              |
| 42:S60:1143:A:C5    | 67:SS0:36:LYS:HB2   | 2.56                     | 0.41              |
| 46:SBB:81:ILE:CD1   | 63:SN0:25:TYR:HB2   | 2.51                     | 0.41              |
| 42:R60:1262:A:H61   | 42:R60:1301:U:H3    | 1.69                     | 0.41              |
| 46:RBB:81:ILE:CD1   | 63:RN0:25:TYR:HB2   | 2.51                     | 0.41              |
| 1:L50:186:G:H2'     | 1:L50:187:A:C8      | 2.56                     | 0.40              |
| 1:L50:401:A:N1      | 6:LC0:80:THR:CG2    | 2.84                     | 0.40              |
| 1:L50:763:U:H2'     | 1:L50:764:U:O4'     | 2.22                     | 0.40              |
| 18:LI0:30:LYS:HE2   | 18:LI0:66:GLU:HG2   | 2.02                     | 0.40              |
| 42:S60:405:A:H2'    | 42:S60:406:U:H6     | 1.84                     | 0.40              |
| 42:S60:995:A:H2'    | 42:S60:996:G:H5'    | 2.02                     | 0.40              |
| 43:SA0:117:ARG:CZ   | 47:SC0:243:GLU:OE2  | 2.65                     | 0.40              |
| 47:SC0:130:PRO:CG   | 70:SV0:4:PHE:CE1    | 3.03                     | 0.40              |
| 1:K50:1296:C:H5''   | 1:K50:1296:C:H6     | 1.85                     | 0.40              |
| 1:K50:1738:G:N3     | 42:R60:1306:A:C2    | 2.89                     | 0.40              |
| 6:KC0:323:GLU:HG2   | 6:KC0:324:ILE:N     | 2.36                     | 0.40              |
| 21:KJJ:40:PRO:O     | 38:KX0:3:LYS:HE3    | 2.21                     | 0.40              |
| 42:R60:910:A:N6     | 42:R60:922:G:H21    | 2.15                     | 0.40              |
| 43:RA0:51:ILE:CG1   | 66:RR0:105:MET:CE   | 2.99                     | 0.40              |
| 55:RG0:176:LYS:CD   | 55:RG0:176:LYS:N    | 2.84                     | 0.40              |
| 73:RY0:116:ARG:NH2  | 73:RY0:120:LYS:NZ   | 2.69                     | 0.40              |
| 1:L50:1133:C:H4'    | 1:L50:1134:A:H5'    | 2.02                     | 0.40              |
| 1:L50:1424:A:H4'    | 15:LGG:77:GLY:H     | 1.85                     | 0.40              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 10:LE0:17:TYR:CE1   | 11:LEE:79:ARG:HD3   | 2.56                     | 0.40              |
| 17:LHH:66:LEU:HD12  | 38:LX0:22:ILE:HD11  | 2.01                     | 0.40              |
| 21:LJJ:40:PRO:O     | 38:LX0:3:LYS:HE3    | 2.21                     | 0.40              |
| 42:S60:918:A:C5     | 42:S60:919:C:C4     | 3.09                     | 0.40              |
| 55:SG0:156:GLU:O    | 55:SG0:160:LYS:HG3  | 2.20                     | 0.40              |
| 56:SGG:65:PHE:CZ    | 66:SR0:29:TYR:OH    | 2.62                     | 0.40              |
| 62:SM0:60:ARG:NH1   | 54:RFF:100:GLN:HE22 | 2.19                     | 0.40              |
| 1:K50:1142:A:H4'    | 9:KDD:58:LYS:HE3    | 2.03                     | 0.40              |
| 1:K50:1344:G:H4'    | 32:KR0:116:LYS:HD2  | 2.04                     | 0.40              |
| 10:KE0:17:TYR:CE1   | 11:KEE:79:ARG:HD3   | 2.56                     | 0.40              |
| 27:K00:80:MET:C     | 27:K00:80:MET:SD    | 3.04                     | 0.40              |
| 37:KW0:102:LYS:HB3  | 55:RG0:150:ASP:HB3  | 2.03                     | 0.40              |
| 43:RA0:6:VAL:HA     | 43:RA0:7:PRO:HD3    | 1.97                     | 0.40              |
| 43:RA0:140:VAL:O    | 43:RA0:141:ASN:CG   | 2.65                     | 0.40              |
| 49:RD0:94:GLN:NE2   | 60:RK0:19:SER:CB    | 2.81                     | 0.40              |
| 17:LHH:66:LEU:CD1   | 38:LX0:22:ILE:HD11  | 2.51                     | 0.40              |
| 18:LI0:41:ALA:HA    | 18:LI0:42:PRO:HD3   | 2.00                     | 0.40              |
| 42:S60:899:A:C6     | 42:S60:932:A:H1'    | 2.57                     | 0.40              |
| 47:SC0:166:LYS:CB   | 59:SJ0:100:GLU:OE2  | 2.69                     | 0.40              |
| 1:K50:101:C:H2'     | 1:K50:102:A:C8      | 2.56                     | 0.40              |
| 1:K50:885:G:H5''    | 1:K50:885:G:C8      | 2.56                     | 0.40              |
| 1:K50:1874:U:H3     | 1:K50:1944:A:H61    | 1.69                     | 0.40              |
| 14:KG0:131:THR:O    | 14:KG0:135:LYS:HG2  | 2.21                     | 0.40              |
| 42:R60:1146:G:H5'   | 68:RT0:90:GLY:HA3   | 2.03                     | 0.40              |
| 47:RC0:166:LYS:CB   | 59:RJ0:100:GLU:OE2  | 2.69                     | 0.40              |
| 55:RG0:169:VAL:HG11 | 55:RG0:176:LYS:HG2  | 2.04                     | 0.40              |
| 59:RJ0:55:LYS:O     | 59:RJ0:59:ILE:HG12  | 2.21                     | 0.40              |
| 1:L50:158:A:H61     | 1:L50:168:G:H1'     | 1.86                     | 0.40              |
| 1:L50:2473:G:H2'    | 1:L50:2474:A:O4'    | 2.21                     | 0.40              |
| 8:LD0:47:GLN:HB2    | 34:LT0:68:ASN:O     | 2.21                     | 0.40              |
| 22:LL0:7:LEU:HA     | 22:LL0:8:PRO:HD3    | 1.90                     | 0.40              |
| 31:LQ0:57:THR:O     | 31:LQ0:57:THR:HG22  | 2.22                     | 0.40              |
| 53:SF0:95:THR:CG2   | 53:SF0:169:ILE:HG12 | 2.52                     | 0.40              |
| 1:K50:158:A:H61     | 1:K50:168:G:H1'     | 1.87                     | 0.40              |
| 4:KAA:68:ASP:OD2    | 19:KII:3:ILE:HG23   | 2.22                     | 0.40              |
| 29:KP0:61:PHE:CE1   | 29:KP0:78:THR:HG21  | 2.57                     | 0.40              |
| 47:RC0:230:ASN:CB   | 70:RV0:24:GLN:NE2   | 2.84                     | 0.40              |
| 1:L50:101:C:H2'     | 1:L50:102:A:C8      | 2.56                     | 0.40              |
| 1:L50:1322:A:H5'    | 15:LGG:33:GLN:NE2   | 2.37                     | 0.40              |
| 4:LAA:70:THR:OG1    | 19:LII:5:LYS:HB2    | 2.21                     | 0.40              |
| 42:S60:960:U:C4     | 42:S60:961:G:N7     | 2.89                     | 0.40              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 42:S60:1146:G:H5'   | 68:ST0:90:GLY:HA3 | 2.03                     | 0.40              |
| 55:SG0:176:LYS:CD   | 55:SG0:176:LYS:N  | 2.84                     | 0.40              |
| 1:K50:401:A:N1      | 6:KC0:80:THR:CG2  | 2.84                     | 0.40              |
| 1:K50:2492:U:H2'    | 1:K50:2493:G:H8   | 1.87                     | 0.40              |
| 42:R60:132:C:O2     | 42:R60:132:C:H2'  | 2.21                     | 0.40              |
| 42:R60:574:A:H1'    | 46:RBB:67:GLY:CA  | 2.51                     | 0.40              |
| 42:R60:933:G:C8     | 42:R60:933:G:O5'  | 2.74                     | 0.40              |
| 42:R60:1023:A:H5''  | 66:RR0:3:GLN:CG   | 2.52                     | 0.40              |
| 43:RA0:184:TYR:O    | 70:RV0:35:ARG:CZ  | 2.69                     | 0.40              |
| 56:RGG:105:ARG:HH22 | 66:RR0:37:ASP:N   | 2.20                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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 |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 3   | KA0   | 243/246 (99%) | 236 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 3   | LA0   | 243/246 (99%) | 236 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 4   | KAA   | 145/147 (99%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 4   | LAA   | 145/147 (99%) | 142 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 5   | KB0   | 381/392 (97%) | 372 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 5   | LB0   | 381/392 (97%) | 372 (98%) | 9 (2%)  | 0        | 100         | 100 |
| 6   | KC0   | 325/328 (99%) | 313 (96%) | 11 (3%) | 1 (0%)   | 36          | 72  |
| 6   | LC0   | 325/328 (99%) | 313 (96%) | 11 (3%) | 1 (0%)   | 36          | 72  |
| 7   | KCC   | 97/110 (88%)  | 94 (97%)  | 2 (2%)  | 1 (1%)   | 12          | 49  |
| 7   | LCC   | 97/110 (88%)  | 94 (97%)  | 2 (2%)  | 1 (1%)   | 12          | 49  |
| 8   | KD0   | 279/291 (96%) | 274 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 8   | LD0   | 279/291 (96%) | 274 (98%) | 5 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 9   | KDD   | 107/110 (97%) | 104 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 9   | LDD   | 107/110 (97%) | 104 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 10  | KE0   | 163/171 (95%) | 154 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 10  | LE0   | 163/171 (95%) | 154 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 11  | KEE   | 133/139 (96%) | 127 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 11  | LEE   | 133/139 (96%) | 127 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 12  | KF0   | 229/235 (97%) | 224 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 12  | LF0   | 229/235 (97%) | 224 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 13  | KFF   | 109/111 (98%) | 106 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 13  | LFF   | 109/111 (98%) | 106 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 14  | KG0   | 197/206 (96%) | 194 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 14  | LG0   | 197/206 (96%) | 194 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 15  | KGG   | 102/106 (96%) | 96 (94%)   | 5 (5%)  | 1 (1%)   | 12          | 49  |
| 15  | LGG   | 102/106 (96%) | 96 (94%)   | 5 (5%)  | 1 (1%)   | 12          | 49  |
| 16  | KH0   | 181/187 (97%) | 177 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 16  | LH0   | 181/187 (97%) | 177 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 17  | KHH   | 117/119 (98%) | 109 (93%)  | 8 (7%)  | 0        | 100         | 100 |
| 17  | LHH   | 117/119 (98%) | 109 (93%)  | 8 (7%)  | 0        | 100         | 100 |
| 18  | KI0   | 215/218 (99%) | 213 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 18  | LI0   | 215/218 (99%) | 214 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 19  | KII   | 95/98 (97%)   | 91 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 19  | LII   | 95/98 (97%)   | 91 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 20  | KJ0   | 165/171 (96%) | 156 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 20  | LJ0   | 165/171 (96%) | 156 (94%)  | 9 (6%)  | 0        | 100         | 100 |
| 21  | KJJ   | 87/92 (95%)   | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 21  | LJJ   | 87/92 (95%)   | 86 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 22  | KL0   | 162/165 (98%) | 155 (96%)  | 6 (4%)  | 1 (1%)   | 21          | 59  |
| 22  | LL0   | 162/165 (98%) | 155 (96%)  | 6 (4%)  | 1 (1%)   | 21          | 59  |
| 23  | KLL   | 49/52 (94%)   | 48 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 23  | LLL   | 49/52 (94%)   | 48 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 24  | KM0   | 113/115 (98%) | 106 (94%)  | 6 (5%)  | 1 (1%)   | 14          | 51  |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 24  | LM0   | 113/115 (98%) | 106 (94%) | 6 (5%)  | 1 (1%)   | 14          | 51  |
| 25  | KMM   | 50/127 (39%)  | 50 (100%) | 0       | 0        | 100         | 100 |
| 25  | LMM   | 50/127 (39%)  | 50 (100%) | 0       | 0        | 100         | 100 |
| 26  | KN0   | 201/204 (98%) | 195 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 26  | LN0   | 201/204 (98%) | 195 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 27  | KO0   | 196/198 (99%) | 193 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 27  | LO0   | 196/198 (99%) | 193 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 28  | KOO   | 98/104 (94%)  | 96 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 28  | LOO   | 98/104 (94%)  | 96 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 29  | KP0   | 152/167 (91%) | 145 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 29  | LP0   | 152/167 (91%) | 145 (95%) | 7 (5%)  | 0        | 100         | 100 |
| 30  | KPP   | 85/89 (96%)   | 80 (94%)  | 4 (5%)  | 1 (1%)   | 10          | 44  |
| 30  | LPP   | 85/89 (96%)   | 80 (94%)  | 4 (5%)  | 1 (1%)   | 10          | 44  |
| 31  | KQ0   | 180/183 (98%) | 175 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 31  | LQ0   | 180/183 (98%) | 175 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 32  | KR0   | 162/168 (96%) | 160 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 32  | LR0   | 162/168 (96%) | 160 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 33  | KS0   | 168/171 (98%) | 159 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 33  | LS0   | 168/171 (98%) | 159 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 34  | KT0   | 154/158 (98%) | 145 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 34  | LT0   | 154/158 (98%) | 145 (94%) | 9 (6%)  | 0        | 100         | 100 |
| 35  | KU0   | 98/113 (87%)  | 93 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 35  | LU0   | 98/113 (87%)  | 93 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 36  | KV0   | 139/142 (98%) | 137 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 36  | LV0   | 139/142 (98%) | 137 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 37  | KW0   | 100/131 (76%) | 93 (93%)  | 6 (6%)  | 1 (1%)   | 12          | 49  |
| 37  | LW0   | 100/131 (76%) | 93 (93%)  | 6 (6%)  | 1 (1%)   | 12          | 49  |
| 38  | KX0   | 110/113 (97%) | 106 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 38  | LX0   | 110/113 (97%) | 106 (96%) | 4 (4%)  | 0        | 100         | 100 |
| 39  | KY0   | 129/131 (98%) | 123 (95%) | 6 (5%)  | 0        | 100         | 100 |
| 39  | LY0   | 129/131 (98%) | 123 (95%) | 6 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 40  | KZ0   | 116/153 (76%) | 116 (100%) | 0       | 0        | 100         | 100 |
| 40  | LZ0   | 116/153 (76%) | 116 (100%) | 0       | 0        | 100         | 100 |
| 41  | MD1   | 149/151 (99%) | 144 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 41  | MD2   | 149/151 (99%) | 144 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 43  | RA0   | 218/233 (94%) | 206 (94%)  | 12 (6%) | 0        | 100         | 100 |
| 43  | SA0   | 218/233 (94%) | 206 (94%)  | 12 (6%) | 0        | 100         | 100 |
| 44  | RAA   | 99/102 (97%)  | 98 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 44  | SAA   | 99/102 (97%)  | 98 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 45  | RB0   | 202/230 (88%) | 197 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 45  | SB0   | 202/230 (88%) | 197 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 46  | RBB   | 79/82 (96%)   | 77 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 46  | SBB   | 79/82 (96%)   | 77 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 47  | RC0   | 224/248 (90%) | 220 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 47  | SC0   | 224/248 (90%) | 220 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 48  | RCC   | 60/65 (92%)   | 57 (95%)   | 3 (5%)  | 0        | 100         | 100 |
| 48  | SCC   | 60/65 (92%)   | 57 (95%)   | 3 (5%)  | 0        | 100         | 100 |
| 49  | RD0   | 214/242 (88%) | 212 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 49  | SD0   | 214/242 (88%) | 212 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 50  | RDD   | 63/65 (97%)   | 58 (92%)   | 5 (8%)  | 0        | 100         | 100 |
| 50  | SDD   | 63/65 (97%)   | 58 (92%)   | 5 (8%)  | 0        | 100         | 100 |
| 51  | RE0   | 258/280 (92%) | 247 (96%)  | 11 (4%) | 0        | 100         | 100 |
| 51  | SE0   | 258/280 (92%) | 247 (96%)  | 11 (4%) | 0        | 100         | 100 |
| 52  | REE   | 54/60 (90%)   | 53 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 52  | SEE   | 54/60 (90%)   | 53 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 53  | RF0   | 190/195 (97%) | 181 (95%)  | 9 (5%)  | 0        | 100         | 100 |
| 53  | SF0   | 190/195 (97%) | 180 (95%)  | 10 (5%) | 0        | 100         | 100 |
| 54  | RFF   | 56/150 (37%)  | 52 (93%)   | 4 (7%)  | 0        | 100         | 100 |
| 54  | SFF   | 56/150 (37%)  | 52 (93%)   | 4 (7%)  | 0        | 100         | 100 |
| 55  | RG0   | 227/230 (99%) | 214 (94%)  | 13 (6%) | 0        | 100         | 100 |
| 55  | SG0   | 227/230 (99%) | 214 (94%)  | 13 (6%) | 0        | 100         | 100 |
| 56  | RGG   | 315/326 (97%) | 295 (94%)  | 19 (6%) | 1 (0%)   | 36          | 72  |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 56  | SGG   | 315/326 (97%) | 295 (94%)  | 19 (6%) | 1 (0%)   | 36          | 72  |
| 57  | RH0   | 161/164 (98%) | 156 (97%)  | 4 (2%)  | 1 (1%)   | 21          | 59  |
| 57  | SH0   | 161/164 (98%) | 156 (97%)  | 4 (2%)  | 1 (1%)   | 21          | 59  |
| 58  | RI0   | 165/173 (95%) | 161 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 58  | SI0   | 165/173 (95%) | 161 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 59  | RJ0   | 166/184 (90%) | 165 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 59  | SJ0   | 166/184 (90%) | 165 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 60  | RK0   | 86/107 (80%)  | 81 (94%)   | 4 (5%)  | 1 (1%)   | 10          | 44  |
| 60  | SK0   | 86/107 (80%)  | 81 (94%)   | 4 (5%)  | 1 (1%)   | 10          | 44  |
| 61  | RL0   | 148/155 (96%) | 141 (95%)  | 7 (5%)  | 0        | 100         | 100 |
| 61  | SL0   | 148/155 (96%) | 141 (95%)  | 7 (5%)  | 0        | 100         | 100 |
| 62  | RM0   | 109/130 (84%) | 106 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 62  | SM0   | 109/130 (84%) | 106 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 63  | RN0   | 140/143 (98%) | 134 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 63  | SN0   | 140/143 (98%) | 134 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 64  | RO0   | 127/135 (94%) | 120 (94%)  | 7 (6%)  | 0        | 100         | 100 |
| 64  | SO0   | 127/135 (94%) | 120 (94%)  | 7 (6%)  | 0        | 100         | 100 |
| 65  | RQ0   | 140/143 (98%) | 134 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 65  | SQ0   | 140/143 (98%) | 134 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 66  | RR0   | 117/120 (98%) | 113 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 66  | SR0   | 117/120 (98%) | 113 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 67  | RS0   | 142/160 (89%) | 137 (96%)  | 4 (3%)  | 1 (1%)   | 18          | 56  |
| 67  | SS0   | 142/160 (89%) | 137 (96%)  | 4 (3%)  | 1 (1%)   | 18          | 56  |
| 68  | RT0   | 140/143 (98%) | 140 (100%) | 0       | 0        | 100         | 100 |
| 68  | ST0   | 140/143 (98%) | 140 (100%) | 0       | 0        | 100         | 100 |
| 69  | RU0   | 98/119 (82%)  | 94 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 69  | SU0   | 98/119 (82%)  | 94 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 70  | RV0   | 63/67 (94%)   | 62 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 70  | SV0   | 63/67 (94%)   | 62 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 71  | RW0   | 126/128 (98%) | 124 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 71  | SW0   | 126/128 (98%) | 124 (98%)  | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 72  | RX0   | 138/141 (98%)     | 136 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 72  | SX0   | 138/141 (98%)     | 136 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 73  | RY0   | 134/146 (92%)     | 121 (90%)   | 11 (8%)  | 2 (2%)   | 8           | 40  |
| 73  | SY0   | 134/146 (92%)     | 122 (91%)   | 10 (8%)  | 2 (2%)   | 8           | 40  |
| 74  | RZ0   | 74/128 (58%)      | 69 (93%)    | 5 (7%)   | 0        | 100         | 100 |
| 74  | SZ0   | 74/128 (58%)      | 69 (93%)    | 5 (7%)   | 0        | 100         | 100 |
| 75  | RP0   | 115/163 (71%)     | 113 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 75  | SP0   | 115/163 (71%)     | 113 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| All | All   | 21258/22938 (93%) | 20523 (96%) | 709 (3%) | 26 (0%)  | 49          | 83  |

All (26) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | LGG   | 78  | GLY  |
| 73  | SY0   | 134 | LYS  |
| 15  | KGG   | 78  | GLY  |
| 73  | RY0   | 134 | LYS  |
| 30  | LPP   | 18  | TYR  |
| 37  | LW0   | 81  | ARG  |
| 67  | SS0   | 24  | PHE  |
| 73  | SY0   | 37  | ASN  |
| 30  | KPP   | 18  | TYR  |
| 37  | KW0   | 81  | ARG  |
| 67  | RS0   | 24  | PHE  |
| 73  | RY0   | 37  | ASN  |
| 56  | SGG   | 61  | GLY  |
| 56  | RGG   | 61  | GLY  |
| 24  | LM0   | 48  | GLY  |
| 57  | SH0   | 107 | PHE  |
| 24  | KM0   | 48  | GLY  |
| 57  | RH0   | 107 | PHE  |
| 60  | SK0   | 71  | GLY  |
| 60  | RK0   | 71  | GLY  |
| 7   | LCC   | 64  | ILE  |
| 22  | LL0   | 8   | PRO  |
| 7   | KCC   | 64  | ILE  |
| 22  | KL0   | 8   | PRO  |
| 6   | LC0   | 297 | ILE  |
| 6   | KC0   | 297 | ILE  |



### 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 |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | KA0   | 202/203 (100%) | 199 (98%)  | 3 (2%)   | 57          | 72  |
| 3   | LA0   | 202/203 (100%) | 199 (98%)  | 3 (2%)   | 57          | 72  |
| 4   | KAA   | 123/123 (100%) | 119 (97%)  | 4 (3%)   | 33          | 55  |
| 4   | LAA   | 123/123 (100%) | 119 (97%)  | 4 (3%)   | 33          | 55  |
| 5   | KB0   | 328/336 (98%)  | 319 (97%)  | 9 (3%)   | 39          | 61  |
| 5   | LB0   | 328/336 (98%)  | 319 (97%)  | 9 (3%)   | 39          | 61  |
| 6   | KC0   | 277/278 (100%) | 274 (99%)  | 3 (1%)   | 65          | 76  |
| 6   | LC0   | 277/278 (100%) | 274 (99%)  | 3 (1%)   | 65          | 76  |
| 7   | KCC   | 87/97 (90%)    | 85 (98%)   | 2 (2%)   | 44          | 64  |
| 7   | LCC   | 87/97 (90%)    | 85 (98%)   | 2 (2%)   | 44          | 64  |
| 8   | KD0   | 251/261 (96%)  | 249 (99%)  | 2 (1%)   | 73          | 80  |
| 8   | LD0   | 251/261 (96%)  | 249 (99%)  | 2 (1%)   | 73          | 80  |
| 9   | KDD   | 99/100 (99%)   | 99 (100%)  | 0        | 100         | 100 |
| 9   | LDD   | 99/100 (99%)   | 99 (100%)  | 0        | 100         | 100 |
| 10  | KE0   | 153/159 (96%)  | 150 (98%)  | 3 (2%)   | 48          | 66  |
| 10  | LE0   | 153/159 (96%)  | 150 (98%)  | 3 (2%)   | 48          | 66  |
| 11  | KEE   | 118/122 (97%)  | 118 (100%) | 0        | 100         | 100 |
| 11  | LEE   | 118/122 (97%)  | 118 (100%) | 0        | 100         | 100 |
| 12  | KF0   | 212/216 (98%)  | 211 (100%) | 1 (0%)   | 81          | 83  |
| 12  | LF0   | 212/216 (98%)  | 211 (100%) | 1 (0%)   | 81          | 83  |
| 13  | KFF   | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 13  | LFF   | 98/98 (100%)   | 98 (100%)  | 0        | 100         | 100 |
| 14  | KG0   | 183/190 (96%)  | 183 (100%) | 0        | 100         | 100 |
| 14  | LG0   | 183/190 (96%)  | 183 (100%) | 0        | 100         | 100 |
| 15  | KGG   | 88/90 (98%)    | 86 (98%)   | 2 (2%)   | 44          | 64  |
| 15  | LGG   | 88/90 (98%)    | 86 (98%)   | 2 (2%)   | 44          | 64  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 16  | KH0   | 165/169 (98%)  | 161 (98%)  | 4 (2%)   | 43          | 64  |
| 16  | LH0   | 165/169 (98%)  | 161 (98%)  | 4 (2%)   | 43          | 64  |
| 17  | KHH   | 110/110 (100%) | 109 (99%)  | 1 (1%)   | 70          | 79  |
| 17  | LHH   | 110/110 (100%) | 109 (99%)  | 1 (1%)   | 70          | 79  |
| 18  | KI0   | 188/189 (100%) | 188 (100%) | 0        | 100         | 100 |
| 18  | LI0   | 188/189 (100%) | 188 (100%) | 0        | 100         | 100 |
| 19  | KII   | 84/84 (100%)   | 82 (98%)   | 2 (2%)   | 43          | 64  |
| 19  | LII   | 84/84 (100%)   | 82 (98%)   | 2 (2%)   | 43          | 64  |
| 20  | KJ0   | 146/149 (98%)  | 144 (99%)  | 2 (1%)   | 59          | 72  |
| 20  | LJ0   | 146/149 (98%)  | 144 (99%)  | 2 (1%)   | 59          | 72  |
| 21  | KJJ   | 78/81 (96%)    | 77 (99%)   | 1 (1%)   | 61          | 74  |
| 21  | LJJ   | 78/81 (96%)    | 77 (99%)   | 1 (1%)   | 61          | 74  |
| 22  | KL0   | 148/149 (99%)  | 142 (96%)  | 6 (4%)   | 27          | 49  |
| 22  | LL0   | 148/149 (99%)  | 142 (96%)  | 6 (4%)   | 27          | 49  |
| 23  | KLL   | 46/47 (98%)    | 46 (100%)  | 0        | 100         | 100 |
| 23  | LLL   | 46/47 (98%)    | 46 (100%)  | 0        | 100         | 100 |
| 24  | KM0   | 110/110 (100%) | 110 (100%) | 0        | 100         | 100 |
| 24  | LM0   | 110/110 (100%) | 110 (100%) | 0        | 100         | 100 |
| 25  | KMM   | 46/112 (41%)   | 46 (100%)  | 0        | 100         | 100 |
| 25  | LMM   | 46/112 (41%)   | 46 (100%)  | 0        | 100         | 100 |
| 26  | KN0   | 175/176 (99%)  | 171 (98%)  | 4 (2%)   | 44          | 64  |
| 26  | LN0   | 175/176 (99%)  | 171 (98%)  | 4 (2%)   | 44          | 64  |
| 27  | KO0   | 178/178 (100%) | 177 (99%)  | 1 (1%)   | 78          | 83  |
| 27  | LO0   | 178/178 (100%) | 177 (99%)  | 1 (1%)   | 78          | 83  |
| 28  | KOO   | 85/89 (96%)    | 85 (100%)  | 0        | 100         | 100 |
| 28  | LOO   | 85/89 (96%)    | 85 (100%)  | 0        | 100         | 100 |
| 29  | KP0   | 135/147 (92%)  | 132 (98%)  | 3 (2%)   | 45          | 64  |
| 29  | LP0   | 135/147 (92%)  | 132 (98%)  | 3 (2%)   | 45          | 64  |
| 30  | KPP   | 75/77 (97%)    | 73 (97%)   | 2 (3%)   | 39          | 61  |
| 30  | LPP   | 75/77 (97%)    | 73 (97%)   | 2 (3%)   | 39          | 61  |
| 31  | KQ0   | 165/166 (99%)  | 165 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 31  | LQ0   | 165/166 (99%)  | 165 (100%) | 0        | 100         | 100 |
| 32  | KR0   | 142/145 (98%)  | 141 (99%)  | 1 (1%)   | 76          | 81  |
| 32  | LR0   | 142/145 (98%)  | 141 (99%)  | 1 (1%)   | 76          | 81  |
| 33  | KS0   | 155/156 (99%)  | 152 (98%)  | 3 (2%)   | 50          | 67  |
| 33  | LS0   | 155/156 (99%)  | 152 (98%)  | 3 (2%)   | 50          | 67  |
| 34  | KT0   | 140/142 (99%)  | 138 (99%)  | 2 (1%)   | 59          | 72  |
| 34  | LT0   | 140/142 (99%)  | 138 (99%)  | 2 (1%)   | 59          | 72  |
| 35  | KU0   | 89/98 (91%)    | 88 (99%)   | 1 (1%)   | 65          | 76  |
| 35  | LU0   | 89/98 (91%)    | 88 (99%)   | 1 (1%)   | 65          | 76  |
| 36  | KV0   | 113/114 (99%)  | 112 (99%)  | 1 (1%)   | 70          | 79  |
| 36  | LV0   | 113/114 (99%)  | 112 (99%)  | 1 (1%)   | 70          | 79  |
| 37  | KW0   | 93/120 (78%)   | 89 (96%)   | 4 (4%)   | 26          | 47  |
| 37  | LW0   | 93/120 (78%)   | 89 (96%)   | 4 (4%)   | 26          | 47  |
| 38  | KX0   | 92/93 (99%)    | 91 (99%)   | 1 (1%)   | 65          | 76  |
| 38  | LX0   | 92/93 (99%)    | 91 (99%)   | 1 (1%)   | 65          | 76  |
| 39  | KY0   | 116/116 (100%) | 114 (98%)  | 2 (2%)   | 53          | 69  |
| 39  | LY0   | 116/116 (100%) | 114 (98%)  | 2 (2%)   | 53          | 69  |
| 40  | KZ0   | 106/141 (75%)  | 106 (100%) | 0        | 100         | 100 |
| 40  | LZ0   | 106/141 (75%)  | 106 (100%) | 0        | 100         | 100 |
| 41  | MD1   | 139/139 (100%) | 139 (100%) | 0        | 100         | 100 |
| 41  | MD2   | 139/139 (100%) | 139 (100%) | 0        | 100         | 100 |
| 43  | RA0   | 194/206 (94%)  | 191 (98%)  | 3 (2%)   | 57          | 72  |
| 43  | SA0   | 194/206 (94%)  | 191 (98%)  | 3 (2%)   | 57          | 72  |
| 44  | RAA   | 92/93 (99%)    | 92 (100%)  | 0        | 100         | 100 |
| 44  | SAA   | 92/93 (99%)    | 92 (100%)  | 0        | 100         | 100 |
| 45  | RB0   | 182/203 (90%)  | 182 (100%) | 0        | 100         | 100 |
| 45  | SB0   | 182/203 (90%)  | 182 (100%) | 0        | 100         | 100 |
| 46  | RBB   | 72/73 (99%)    | 71 (99%)   | 1 (1%)   | 59          | 72  |
| 46  | SBB   | 72/73 (99%)    | 71 (99%)   | 1 (1%)   | 59          | 72  |
| 47  | RC0   | 187/209 (90%)  | 185 (99%)  | 2 (1%)   | 65          | 76  |
| 47  | SC0   | 187/209 (90%)  | 185 (99%)  | 2 (1%)   | 65          | 76  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 48  | RCC   | 51/54 (94%)    | 51 (100%)  | 0        | 100         | 100 |
| 48  | SCC   | 51/54 (94%)    | 51 (100%)  | 0        | 100         | 100 |
| 49  | RD0   | 189/215 (88%)  | 189 (100%) | 0        | 100         | 100 |
| 49  | SD0   | 189/215 (88%)  | 189 (100%) | 0        | 100         | 100 |
| 50  | RDD   | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 50  | SDD   | 57/57 (100%)   | 57 (100%)  | 0        | 100         | 100 |
| 51  | RE0   | 231/251 (92%)  | 229 (99%)  | 2 (1%)   | 70          | 79  |
| 51  | SE0   | 231/251 (92%)  | 229 (99%)  | 2 (1%)   | 70          | 79  |
| 52  | REE   | 44/47 (94%)    | 44 (100%)  | 0        | 100         | 100 |
| 52  | SEE   | 44/47 (94%)    | 44 (100%)  | 0        | 100         | 100 |
| 53  | RF0   | 167/170 (98%)  | 163 (98%)  | 4 (2%)   | 43          | 64  |
| 53  | SF0   | 167/170 (98%)  | 163 (98%)  | 4 (2%)   | 43          | 64  |
| 54  | RFF   | 45/136 (33%)   | 44 (98%)   | 1 (2%)   | 45          | 64  |
| 54  | SFF   | 46/136 (34%)   | 45 (98%)   | 1 (2%)   | 45          | 64  |
| 55  | RG0   | 199/199 (100%) | 195 (98%)  | 4 (2%)   | 48          | 66  |
| 55  | SG0   | 199/199 (100%) | 195 (98%)  | 4 (2%)   | 48          | 66  |
| 56  | RGG   | 282/288 (98%)  | 278 (99%)  | 4 (1%)   | 59          | 72  |
| 56  | SGG   | 282/288 (98%)  | 278 (99%)  | 4 (1%)   | 59          | 72  |
| 57  | RH0   | 153/154 (99%)  | 153 (100%) | 0        | 100         | 100 |
| 57  | SH0   | 153/154 (99%)  | 153 (100%) | 0        | 100         | 100 |
| 58  | RI0   | 147/153 (96%)  | 147 (100%) | 0        | 100         | 100 |
| 58  | SI0   | 147/153 (96%)  | 147 (100%) | 0        | 100         | 100 |
| 59  | RJ0   | 152/165 (92%)  | 150 (99%)  | 2 (1%)   | 61          | 74  |
| 59  | SJ0   | 152/165 (92%)  | 150 (99%)  | 2 (1%)   | 61          | 74  |
| 60  | RK0   | 83/99 (84%)    | 82 (99%)   | 1 (1%)   | 63          | 75  |
| 60  | SK0   | 83/99 (84%)    | 82 (99%)   | 1 (1%)   | 63          | 75  |
| 61  | RL0   | 140/145 (97%)  | 139 (99%)  | 1 (1%)   | 76          | 81  |
| 61  | SL0   | 140/145 (97%)  | 139 (99%)  | 1 (1%)   | 76          | 81  |
| 62  | RM0   | 99/114 (87%)   | 99 (100%)  | 0        | 100         | 100 |
| 62  | SM0   | 99/114 (87%)   | 99 (100%)  | 0        | 100         | 100 |
| 63  | RN0   | 126/127 (99%)  | 126 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 63  | SN0   | 126/127 (99%)     | 126 (100%)  | 0        | 100         | 100 |
| 64  | RO0   | 102/108 (94%)     | 101 (99%)   | 1 (1%)   | 68          | 78  |
| 64  | SO0   | 102/108 (94%)     | 101 (99%)   | 1 (1%)   | 68          | 78  |
| 65  | RQ0   | 120/121 (99%)     | 119 (99%)   | 1 (1%)   | 73          | 80  |
| 65  | SQ0   | 120/121 (99%)     | 119 (99%)   | 1 (1%)   | 73          | 80  |
| 66  | RR0   | 109/111 (98%)     | 108 (99%)   | 1 (1%)   | 70          | 79  |
| 66  | SR0   | 109/111 (98%)     | 108 (99%)   | 1 (1%)   | 70          | 79  |
| 67  | RS0   | 125/138 (91%)     | 124 (99%)   | 1 (1%)   | 73          | 80  |
| 67  | SS0   | 125/138 (91%)     | 124 (99%)   | 1 (1%)   | 73          | 80  |
| 68  | RT0   | 129/130 (99%)     | 127 (98%)   | 2 (2%)   | 55          | 70  |
| 68  | ST0   | 129/130 (99%)     | 127 (98%)   | 2 (2%)   | 55          | 70  |
| 69  | RU0   | 92/110 (84%)      | 92 (100%)   | 0        | 100         | 100 |
| 69  | SU0   | 92/110 (84%)      | 92 (100%)   | 0        | 100         | 100 |
| 70  | RV0   | 61/63 (97%)       | 61 (100%)   | 0        | 100         | 100 |
| 70  | SV0   | 61/63 (97%)       | 61 (100%)   | 0        | 100         | 100 |
| 71  | RW0   | 111/111 (100%)    | 110 (99%)   | 1 (1%)   | 70          | 79  |
| 71  | SW0   | 111/111 (100%)    | 110 (99%)   | 1 (1%)   | 70          | 79  |
| 72  | RX0   | 115/116 (99%)     | 115 (100%)  | 0        | 100         | 100 |
| 72  | SX0   | 115/116 (99%)     | 115 (100%)  | 0        | 100         | 100 |
| 73  | RY0   | 126/136 (93%)     | 121 (96%)   | 5 (4%)   | 28          | 49  |
| 73  | SY0   | 126/136 (93%)     | 121 (96%)   | 5 (4%)   | 28          | 49  |
| 74  | RZ0   | 73/118 (62%)      | 73 (100%)   | 0        | 100         | 100 |
| 74  | SZ0   | 73/118 (62%)      | 73 (100%)   | 0        | 100         | 100 |
| 75  | RP0   | 107/144 (74%)     | 106 (99%)   | 1 (1%)   | 70          | 79  |
| 75  | SP0   | 107/144 (74%)     | 106 (99%)   | 1 (1%)   | 70          | 79  |
| All | All   | 19001/20268 (94%) | 18785 (99%) | 216 (1%) | 63          | 76  |

All (216) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | LA0   | 44  | GLU  |
| 3   | LA0   | 189 | ARG  |
| 3   | LA0   | 222 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | LAA   | 22  | VAL  |
| 4   | LAA   | 26  | ARG  |
| 4   | LAA   | 39  | LYS  |
| 4   | LAA   | 54  | ARG  |
| 5   | LB0   | 10  | ARG  |
| 5   | LB0   | 23  | LYS  |
| 5   | LB0   | 86  | VAL  |
| 5   | LB0   | 122 | ARG  |
| 5   | LB0   | 132 | LYS  |
| 5   | LB0   | 133 | LEU  |
| 5   | LB0   | 134 | MET  |
| 5   | LB0   | 135 | PHE  |
| 5   | LB0   | 336 | ARG  |
| 6   | LC0   | 103 | VAL  |
| 6   | LC0   | 207 | THR  |
| 6   | LC0   | 328 | ILE  |
| 7   | LCC   | 64  | ILE  |
| 7   | LCC   | 76  | SER  |
| 8   | LD0   | 85  | THR  |
| 8   | LD0   | 285 | GLN  |
| 10  | LE0   | 15  | LYS  |
| 10  | LE0   | 17  | TYR  |
| 10  | LE0   | 30  | LEU  |
| 12  | LF0   | 42  | ARG  |
| 15  | LGG   | 32  | PHE  |
| 15  | LGG   | 101 | MET  |
| 16  | LH0   | 34  | VAL  |
| 16  | LH0   | 62  | GLN  |
| 16  | LH0   | 64  | ARG  |
| 16  | LH0   | 149 | ASP  |
| 17  | LHH   | 107 | LEU  |
| 19  | LII   | 47  | ARG  |
| 19  | LII   | 90  | GLU  |
| 20  | LJ0   | 106 | HIS  |
| 20  | LJ0   | 144 | ARG  |
| 21  | LJJ   | 2   | SER  |
| 22  | LL0   | 5   | GLN  |
| 22  | LL0   | 30  | LEU  |
| 22  | LL0   | 44  | TYR  |
| 22  | LL0   | 90  | VAL  |
| 22  | LL0   | 97  | ARG  |
| 22  | LL0   | 98  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | LN0   | 65  | ARG  |
| 26  | LN0   | 112 | ASN  |
| 26  | LN0   | 135 | VAL  |
| 26  | LN0   | 155 | VAL  |
| 27  | LO0   | 105 | ASP  |
| 29  | LP0   | 30  | ARG  |
| 29  | LP0   | 60  | VAL  |
| 29  | LP0   | 120 | ASN  |
| 30  | LPP   | 8   | VAL  |
| 30  | LPP   | 18  | TYR  |
| 32  | LR0   | 19  | ARG  |
| 33  | LS0   | 52  | PRO  |
| 33  | LS0   | 157 | ARG  |
| 33  | LS0   | 171 | ASN  |
| 34  | LT0   | 55  | LYS  |
| 34  | LT0   | 112 | ASN  |
| 35  | LU0   | 92  | ARG  |
| 36  | LV0   | 28  | LEU  |
| 37  | LW0   | 80  | VAL  |
| 37  | LW0   | 81  | ARG  |
| 37  | LW0   | 91  | VAL  |
| 37  | LW0   | 92  | GLU  |
| 38  | LX0   | 40  | HIS  |
| 39  | LY0   | 1   | MET  |
| 39  | LY0   | 114 | ARG  |
| 43  | SA0   | 8   | LEU  |
| 43  | SA0   | 102 | ARG  |
| 43  | SA0   | 154 | ILE  |
| 46  | SBB   | 58  | CYS  |
| 47  | SC0   | 156 | SER  |
| 47  | SC0   | 221 | VAL  |
| 51  | SE0   | 211 | VAL  |
| 51  | SE0   | 213 | LYS  |
| 53  | SF0   | 18  | TYR  |
| 53  | SF0   | 61  | GLU  |
| 53  | SF0   | 92  | GLU  |
| 53  | SF0   | 97  | GLN  |
| 54  | SFF   | 93  | LYS  |
| 55  | SG0   | 92  | ARG  |
| 55  | SG0   | 100 | SER  |
| 55  | SG0   | 129 | VAL  |
| 55  | SG0   | 222 | TRP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | SGG   | 76  | ASP  |
| 56  | SGG   | 106 | ASP  |
| 56  | SGG   | 150 | THR  |
| 56  | SGG   | 305 | ASP  |
| 59  | SJ0   | 62  | ASP  |
| 59  | SJ0   | 130 | GLN  |
| 60  | SK0   | 80  | TYR  |
| 61  | SL0   | 148 | LYS  |
| 64  | SO0   | 122 | ASP  |
| 65  | SQ0   | 99  | GLU  |
| 66  | SR0   | 84  | PHE  |
| 67  | SS0   | 24  | PHE  |
| 68  | ST0   | 17  | LEU  |
| 68  | ST0   | 28  | VAL  |
| 71  | SW0   | 110 | ASP  |
| 73  | SY0   | 11  | PHE  |
| 73  | SY0   | 37  | ASN  |
| 73  | SY0   | 39  | MET  |
| 73  | SY0   | 135 | ARG  |
| 73  | SY0   | 143 | LYS  |
| 3   | KA0   | 44  | GLU  |
| 3   | KA0   | 189 | ARG  |
| 3   | KA0   | 222 | VAL  |
| 4   | KAA   | 22  | VAL  |
| 4   | KAA   | 26  | ARG  |
| 4   | KAA   | 39  | LYS  |
| 4   | KAA   | 54  | ARG  |
| 5   | KB0   | 10  | ARG  |
| 5   | KB0   | 23  | LYS  |
| 5   | KB0   | 86  | VAL  |
| 5   | KB0   | 122 | ARG  |
| 5   | KB0   | 132 | LYS  |
| 5   | KB0   | 133 | LEU  |
| 5   | KB0   | 134 | MET  |
| 5   | KB0   | 135 | PHE  |
| 5   | KB0   | 336 | ARG  |
| 6   | KC0   | 103 | VAL  |
| 6   | KC0   | 207 | THR  |
| 6   | KC0   | 328 | ILE  |
| 7   | KCC   | 64  | ILE  |
| 7   | KCC   | 76  | SER  |
| 8   | KD0   | 85  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | KD0   | 285 | GLN  |
| 10  | KE0   | 15  | LYS  |
| 10  | KE0   | 17  | TYR  |
| 10  | KE0   | 30  | LEU  |
| 12  | KF0   | 42  | ARG  |
| 15  | KGG   | 32  | PHE  |
| 15  | KGG   | 101 | MET  |
| 16  | KH0   | 34  | VAL  |
| 16  | KH0   | 62  | GLN  |
| 16  | KH0   | 64  | ARG  |
| 16  | KH0   | 149 | ASP  |
| 17  | KHH   | 107 | LEU  |
| 19  | KII   | 47  | ARG  |
| 19  | KII   | 90  | GLU  |
| 20  | KJ0   | 106 | HIS  |
| 20  | KJ0   | 144 | ARG  |
| 21  | KJJ   | 2   | SER  |
| 22  | KL0   | 5   | GLN  |
| 22  | KL0   | 30  | LEU  |
| 22  | KL0   | 44  | TYR  |
| 22  | KL0   | 90  | VAL  |
| 22  | KL0   | 97  | ARG  |
| 22  | KL0   | 98  | ARG  |
| 26  | KN0   | 65  | ARG  |
| 26  | KN0   | 112 | ASN  |
| 26  | KN0   | 135 | VAL  |
| 26  | KN0   | 155 | VAL  |
| 27  | KO0   | 105 | ASP  |
| 29  | KP0   | 30  | ARG  |
| 29  | KP0   | 60  | VAL  |
| 29  | KP0   | 120 | ASN  |
| 30  | KPP   | 8   | VAL  |
| 30  | KPP   | 18  | TYR  |
| 32  | KR0   | 19  | ARG  |
| 33  | KS0   | 52  | PRO  |
| 33  | KS0   | 157 | ARG  |
| 33  | KS0   | 171 | ASN  |
| 34  | KT0   | 55  | LYS  |
| 34  | KT0   | 112 | ASN  |
| 35  | KU0   | 92  | ARG  |
| 36  | KV0   | 28  | LEU  |
| 37  | KW0   | 80  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 37  | KW0   | 81  | ARG  |
| 37  | KW0   | 91  | VAL  |
| 37  | KW0   | 92  | GLU  |
| 38  | KX0   | 40  | HIS  |
| 39  | KY0   | 1   | MET  |
| 39  | KY0   | 114 | ARG  |
| 43  | RA0   | 8   | LEU  |
| 43  | RA0   | 102 | ARG  |
| 43  | RA0   | 154 | ILE  |
| 46  | RBB   | 58  | CYS  |
| 47  | RC0   | 156 | SER  |
| 47  | RC0   | 221 | VAL  |
| 51  | RE0   | 211 | VAL  |
| 51  | RE0   | 213 | LYS  |
| 53  | RF0   | 18  | TYR  |
| 53  | RF0   | 61  | GLU  |
| 53  | RF0   | 92  | GLU  |
| 53  | RF0   | 97  | GLN  |
| 54  | RFF   | 93  | LYS  |
| 55  | RG0   | 92  | ARG  |
| 55  | RG0   | 100 | SER  |
| 55  | RG0   | 129 | VAL  |
| 55  | RG0   | 222 | TRP  |
| 56  | RGG   | 76  | ASP  |
| 56  | RGG   | 106 | ASP  |
| 56  | RGG   | 150 | THR  |
| 56  | RGG   | 305 | ASP  |
| 59  | RJ0   | 62  | ASP  |
| 59  | RJ0   | 130 | GLN  |
| 60  | RK0   | 80  | TYR  |
| 61  | RL0   | 148 | LYS  |
| 64  | RO0   | 122 | ASP  |
| 65  | RQ0   | 99  | GLU  |
| 66  | RR0   | 84  | PHE  |
| 67  | RS0   | 24  | PHE  |
| 68  | RT0   | 17  | LEU  |
| 68  | RT0   | 28  | VAL  |
| 71  | RW0   | 110 | ASP  |
| 73  | RY0   | 11  | PHE  |
| 73  | RY0   | 37  | ASN  |
| 73  | RY0   | 39  | MET  |
| 73  | RY0   | 135 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 73  | RY0   | 143 | LYS  |
| 75  | SP0   | 135 | ARG  |
| 75  | RP0   | 135 | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | K50   | 2494/2618 (95%) | 748 (29%)         | 103 (4%)        |
| 1   | L50   | 2494/2618 (95%) | 748 (29%)         | 102 (4%)        |
| 2   | K70   | 118/119 (99%)   | 36 (30%)          | 4 (3%)          |
| 2   | L70   | 118/119 (99%)   | 36 (30%)          | 4 (3%)          |
| 42  | R60   | 1352/1368 (98%) | 525 (38%)         | 70 (5%)         |
| 42  | S60   | 1352/1368 (98%) | 524 (38%)         | 70 (5%)         |
| All | All   | 7928/8210 (96%) | 2617 (33%)        | 353 (4%)        |

All (2617) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 2   | U    |
| 1   | L50   | 3   | A    |
| 1   | L50   | 13  | A    |
| 1   | L50   | 15  | G    |
| 1   | L50   | 21  | U    |
| 1   | L50   | 22  | U    |
| 1   | L50   | 23  | U    |
| 1   | L50   | 24  | G    |
| 1   | L50   | 25  | G    |
| 1   | L50   | 31  | G    |
| 1   | L50   | 39  | G    |
| 1   | L50   | 43  | G    |
| 1   | L50   | 48  | A    |
| 1   | L50   | 51  | A    |
| 1   | L50   | 52  | G    |
| 1   | L50   | 59  | A    |
| 1   | L50   | 62  | U    |
| 1   | L50   | 63  | G    |
| 1   | L50   | 68  | G    |
| 1   | L50   | 70  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 71  | G    |
| 1   | L50   | 73  | A    |
| 1   | L50   | 74  | G    |
| 1   | L50   | 75  | C    |
| 1   | L50   | 76  | A    |
| 1   | L50   | 77  | G    |
| 1   | L50   | 82  | G    |
| 1   | L50   | 87  | C    |
| 1   | L50   | 88  | A    |
| 1   | L50   | 98  | A    |
| 1   | L50   | 99  | U    |
| 1   | L50   | 100 | A    |
| 1   | L50   | 101 | C    |
| 1   | L50   | 108 | G    |
| 1   | L50   | 113 | G    |
| 1   | L50   | 114 | G    |
| 1   | L50   | 118 | A    |
| 1   | L50   | 123 | U    |
| 1   | L50   | 132 | A    |
| 1   | L50   | 135 | A    |
| 1   | L50   | 136 | U    |
| 1   | L50   | 137 | A    |
| 1   | L50   | 151 | G    |
| 1   | L50   | 152 | A    |
| 1   | L50   | 157 | A    |
| 1   | L50   | 158 | A    |
| 1   | L50   | 159 | A    |
| 1   | L50   | 160 | C    |
| 1   | L50   | 165 | G    |
| 1   | L50   | 167 | G    |
| 1   | L50   | 169 | A    |
| 1   | L50   | 178 | G    |
| 1   | L50   | 181 | G    |
| 1   | L50   | 184 | G    |
| 1   | L50   | 186 | G    |
| 1   | L50   | 188 | G    |
| 1   | L50   | 191 | A    |
| 1   | L50   | 194 | A    |
| 1   | L50   | 201 | A    |
| 1   | L50   | 202 | G    |
| 1   | L50   | 204 | C    |
| 1   | L50   | 209 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 210 | G    |
| 1   | L50   | 211 | U    |
| 1   | L50   | 212 | G    |
| 1   | L50   | 213 | U    |
| 1   | L50   | 214 | A    |
| 1   | L50   | 215 | A    |
| 1   | L50   | 216 | U    |
| 1   | L50   | 221 | A    |
| 1   | L50   | 224 | U    |
| 1   | L50   | 225 | G    |
| 1   | L50   | 226 | A    |
| 1   | L50   | 233 | G    |
| 1   | L50   | 234 | U    |
| 1   | L50   | 237 | A    |
| 1   | L50   | 238 | A    |
| 1   | L50   | 239 | A    |
| 1   | L50   | 240 | G    |
| 1   | L50   | 241 | G    |
| 1   | L50   | 242 | A    |
| 1   | L50   | 246 | A    |
| 1   | L50   | 247 | G    |
| 1   | L50   | 255 | U    |
| 1   | L50   | 258 | G    |
| 1   | L50   | 265 | A    |
| 1   | L50   | 266 | A    |
| 1   | L50   | 267 | G    |
| 1   | L50   | 268 | C    |
| 1   | L50   | 273 | C    |
| 1   | L50   | 276 | U    |
| 1   | L50   | 277 | A    |
| 1   | L50   | 284 | G    |
| 1   | L50   | 285 | A    |
| 1   | L50   | 286 | U    |
| 1   | L50   | 287 | A    |
| 1   | L50   | 289 | U    |
| 1   | L50   | 298 | G    |
| 1   | L50   | 309 | U    |
| 1   | L50   | 311 | C    |
| 1   | L50   | 312 | G    |
| 1   | L50   | 314 | U    |
| 1   | L50   | 315 | G    |
| 1   | L50   | 316 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 317 | G    |
| 1   | L50   | 330 | G    |
| 1   | L50   | 331 | U    |
| 1   | L50   | 332 | A    |
| 1   | L50   | 333 | A    |
| 1   | L50   | 340 | G    |
| 1   | L50   | 343 | A    |
| 1   | L50   | 345 | G    |
| 1   | L50   | 346 | A    |
| 1   | L50   | 347 | G    |
| 1   | L50   | 352 | C    |
| 1   | L50   | 353 | A    |
| 1   | L50   | 358 | G    |
| 1   | L50   | 366 | G    |
| 1   | L50   | 373 | U    |
| 1   | L50   | 382 | A    |
| 1   | L50   | 384 | A    |
| 1   | L50   | 385 | C    |
| 1   | L50   | 392 | C    |
| 1   | L50   | 396 | G    |
| 1   | L50   | 397 | A    |
| 1   | L50   | 400 | U    |
| 1   | L50   | 416 | A    |
| 1   | L50   | 434 | G    |
| 1   | L50   | 438 | A    |
| 1   | L50   | 449 | U    |
| 1   | L50   | 450 | C    |
| 1   | L50   | 453 | G    |
| 1   | L50   | 454 | C    |
| 1   | L50   | 467 | A    |
| 1   | L50   | 478 | A    |
| 1   | L50   | 488 | C    |
| 1   | L50   | 495 | A    |
| 1   | L50   | 499 | G    |
| 1   | L50   | 503 | A    |
| 1   | L50   | 504 | G    |
| 1   | L50   | 507 | G    |
| 1   | L50   | 508 | A    |
| 1   | L50   | 509 | A    |
| 1   | L50   | 510 | G    |
| 1   | L50   | 517 | A    |
| 1   | L50   | 523 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 524 | G    |
| 1   | L50   | 527 | A    |
| 1   | L50   | 530 | A    |
| 1   | L50   | 533 | G    |
| 1   | L50   | 534 | A    |
| 1   | L50   | 535 | A    |
| 1   | L50   | 536 | A    |
| 1   | L50   | 542 | G    |
| 1   | L50   | 553 | C    |
| 1   | L50   | 556 | A    |
| 1   | L50   | 562 | U    |
| 1   | L50   | 563 | U    |
| 1   | L50   | 564 | G    |
| 1   | L50   | 567 | A    |
| 1   | L50   | 568 | A    |
| 1   | L50   | 569 | C    |
| 1   | L50   | 570 | U    |
| 1   | L50   | 580 | U    |
| 1   | L50   | 581 | G    |
| 1   | L50   | 587 | A    |
| 1   | L50   | 601 | C    |
| 1   | L50   | 612 | C    |
| 1   | L50   | 618 | G    |
| 1   | L50   | 620 | C    |
| 1   | L50   | 625 | U    |
| 1   | L50   | 630 | U    |
| 1   | L50   | 631 | G    |
| 1   | L50   | 642 | G    |
| 1   | L50   | 643 | C    |
| 1   | L50   | 646 | A    |
| 1   | L50   | 647 | A    |
| 1   | L50   | 658 | G    |
| 1   | L50   | 659 | G    |
| 1   | L50   | 660 | G    |
| 1   | L50   | 661 | G    |
| 1   | L50   | 665 | A    |
| 1   | L50   | 667 | G    |
| 1   | L50   | 668 | A    |
| 1   | L50   | 675 | G    |
| 1   | L50   | 676 | A    |
| 1   | L50   | 684 | A    |
| 1   | L50   | 685 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 688 | G    |
| 1   | L50   | 689 | C    |
| 1   | L50   | 695 | C    |
| 1   | L50   | 710 | A    |
| 1   | L50   | 711 | U    |
| 1   | L50   | 714 | G    |
| 1   | L50   | 715 | G    |
| 1   | L50   | 720 | C    |
| 1   | L50   | 726 | C    |
| 1   | L50   | 729 | A    |
| 1   | L50   | 732 | G    |
| 1   | L50   | 736 | A    |
| 1   | L50   | 739 | A    |
| 1   | L50   | 741 | G    |
| 1   | L50   | 742 | G    |
| 1   | L50   | 749 | A    |
| 1   | L50   | 750 | U    |
| 1   | L50   | 763 | U    |
| 1   | L50   | 764 | U    |
| 1   | L50   | 765 | A    |
| 1   | L50   | 766 | A    |
| 1   | L50   | 767 | G    |
| 1   | L50   | 768 | G    |
| 1   | L50   | 772 | C    |
| 1   | L50   | 776 | C    |
| 1   | L50   | 778 | A    |
| 1   | L50   | 779 | A    |
| 1   | L50   | 781 | U    |
| 1   | L50   | 782 | G    |
| 1   | L50   | 784 | G    |
| 1   | L50   | 795 | U    |
| 1   | L50   | 796 | C    |
| 1   | L50   | 801 | A    |
| 1   | L50   | 802 | U    |
| 1   | L50   | 803 | G    |
| 1   | L50   | 806 | A    |
| 1   | L50   | 816 | G    |
| 1   | L50   | 822 | U    |
| 1   | L50   | 828 | A    |
| 1   | L50   | 830 | G    |
| 1   | L50   | 834 | G    |
| 1   | L50   | 838 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 840  | C    |
| 1   | L50   | 843  | A    |
| 1   | L50   | 848  | A    |
| 1   | L50   | 849  | A    |
| 1   | L50   | 852  | A    |
| 1   | L50   | 853  | A    |
| 1   | L50   | 854  | C    |
| 1   | L50   | 858  | G    |
| 1   | L50   | 859  | C    |
| 1   | L50   | 865  | G    |
| 1   | L50   | 866  | C    |
| 1   | L50   | 867  | U    |
| 1   | L50   | 871  | G    |
| 1   | L50   | 877  | A    |
| 1   | L50   | 878  | A    |
| 1   | L50   | 879  | U    |
| 1   | L50   | 885  | G    |
| 1   | L50   | 889  | G    |
| 1   | L50   | 893  | C    |
| 1   | L50   | 900  | A    |
| 1   | L50   | 905  | G    |
| 1   | L50   | 910  | A    |
| 1   | L50   | 980  | A    |
| 1   | L50   | 990  | U    |
| 1   | L50   | 998  | U    |
| 1   | L50   | 1001 | A    |
| 1   | L50   | 1002 | U    |
| 1   | L50   | 1010 | A    |
| 1   | L50   | 1017 | A    |
| 1   | L50   | 1018 | U    |
| 1   | L50   | 1021 | G    |
| 1   | L50   | 1022 | A    |
| 1   | L50   | 1023 | U    |
| 1   | L50   | 1024 | G    |
| 1   | L50   | 1030 | U    |
| 1   | L50   | 1032 | A    |
| 1   | L50   | 1033 | G    |
| 1   | L50   | 1034 | C    |
| 1   | L50   | 1037 | G    |
| 1   | L50   | 1050 | U    |
| 1   | L50   | 1053 | C    |
| 1   | L50   | 1055 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1056 | C    |
| 1   | L50   | 1061 | G    |
| 1   | L50   | 1062 | A    |
| 1   | L50   | 1070 | G    |
| 1   | L50   | 1075 | A    |
| 1   | L50   | 1082 | G    |
| 1   | L50   | 1085 | G    |
| 1   | L50   | 1087 | G    |
| 1   | L50   | 1089 | U    |
| 1   | L50   | 1090 | A    |
| 1   | L50   | 1096 | A    |
| 1   | L50   | 1099 | G    |
| 1   | L50   | 1100 | C    |
| 1   | L50   | 1102 | G    |
| 1   | L50   | 1105 | C    |
| 1   | L50   | 1111 | G    |
| 1   | L50   | 1117 | A    |
| 1   | L50   | 1118 | G    |
| 1   | L50   | 1120 | G    |
| 1   | L50   | 1121 | A    |
| 1   | L50   | 1123 | A    |
| 1   | L50   | 1124 | A    |
| 1   | L50   | 1130 | C    |
| 1   | L50   | 1131 | U    |
| 1   | L50   | 1133 | C    |
| 1   | L50   | 1134 | A    |
| 1   | L50   | 1135 | G    |
| 1   | L50   | 1136 | C    |
| 1   | L50   | 1142 | A    |
| 1   | L50   | 1144 | A    |
| 1   | L50   | 1148 | A    |
| 1   | L50   | 1149 | G    |
| 1   | L50   | 1150 | G    |
| 1   | L50   | 1151 | A    |
| 1   | L50   | 1155 | G    |
| 1   | L50   | 1163 | U    |
| 1   | L50   | 1169 | C    |
| 1   | L50   | 1170 | A    |
| 1   | L50   | 1171 | U    |
| 1   | L50   | 1172 | A    |
| 1   | L50   | 1173 | A    |
| 1   | L50   | 1175 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1177 | G    |
| 1   | L50   | 1181 | G    |
| 1   | L50   | 1182 | A    |
| 1   | L50   | 1183 | G    |
| 1   | L50   | 1189 | U    |
| 1   | L50   | 1191 | U    |
| 1   | L50   | 1192 | A    |
| 1   | L50   | 1193 | A    |
| 1   | L50   | 1194 | G    |
| 1   | L50   | 1196 | G    |
| 1   | L50   | 1213 | A    |
| 1   | L50   | 1217 | A    |
| 1   | L50   | 1218 | A    |
| 1   | L50   | 1221 | A    |
| 1   | L50   | 1224 | A    |
| 1   | L50   | 1231 | U    |
| 1   | L50   | 1232 | G    |
| 1   | L50   | 1233 | A    |
| 1   | L50   | 1235 | A    |
| 1   | L50   | 1236 | U    |
| 1   | L50   | 1237 | U    |
| 1   | L50   | 1243 | G    |
| 1   | L50   | 1247 | G    |
| 1   | L50   | 1250 | C    |
| 1   | L50   | 1252 | G    |
| 1   | L50   | 1254 | C    |
| 1   | L50   | 1256 | U    |
| 1   | L50   | 1257 | A    |
| 1   | L50   | 1264 | C    |
| 1   | L50   | 1267 | G    |
| 1   | L50   | 1268 | U    |
| 1   | L50   | 1269 | A    |
| 1   | L50   | 1270 | U    |
| 1   | L50   | 1274 | C    |
| 1   | L50   | 1277 | G    |
| 1   | L50   | 1278 | U    |
| 1   | L50   | 1282 | C    |
| 1   | L50   | 1283 | A    |
| 1   | L50   | 1284 | C    |
| 1   | L50   | 1296 | C    |
| 1   | L50   | 1299 | A    |
| 1   | L50   | 1304 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1305 | A    |
| 1   | L50   | 1308 | A    |
| 1   | L50   | 1309 | C    |
| 1   | L50   | 1317 | G    |
| 1   | L50   | 1318 | U    |
| 1   | L50   | 1327 | A    |
| 1   | L50   | 1332 | G    |
| 1   | L50   | 1333 | A    |
| 1   | L50   | 1340 | A    |
| 1   | L50   | 1341 | G    |
| 1   | L50   | 1342 | A    |
| 1   | L50   | 1346 | A    |
| 1   | L50   | 1350 | U    |
| 1   | L50   | 1355 | C    |
| 1   | L50   | 1356 | G    |
| 1   | L50   | 1359 | G    |
| 1   | L50   | 1361 | G    |
| 1   | L50   | 1362 | G    |
| 1   | L50   | 1374 | U    |
| 1   | L50   | 1375 | G    |
| 1   | L50   | 1384 | U    |
| 1   | L50   | 1385 | G    |
| 1   | L50   | 1386 | A    |
| 1   | L50   | 1387 | G    |
| 1   | L50   | 1395 | U    |
| 1   | L50   | 1396 | G    |
| 1   | L50   | 1402 | G    |
| 1   | L50   | 1411 | C    |
| 1   | L50   | 1412 | C    |
| 1   | L50   | 1414 | U    |
| 1   | L50   | 1416 | A    |
| 1   | L50   | 1427 | A    |
| 1   | L50   | 1429 | A    |
| 1   | L50   | 1430 | U    |
| 1   | L50   | 1431 | G    |
| 1   | L50   | 1432 | G    |
| 1   | L50   | 1440 | G    |
| 1   | L50   | 1447 | C    |
| 1   | L50   | 1449 | A    |
| 1   | L50   | 1450 | A    |
| 1   | L50   | 1453 | G    |
| 1   | L50   | 1454 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1455 | A    |
| 1   | L50   | 1457 | C    |
| 1   | L50   | 1458 | A    |
| 1   | L50   | 1466 | A    |
| 1   | L50   | 1467 | A    |
| 1   | L50   | 1468 | G    |
| 1   | L50   | 1474 | G    |
| 1   | L50   | 1475 | A    |
| 1   | L50   | 1479 | U    |
| 1   | L50   | 1485 | G    |
| 1   | L50   | 1486 | G    |
| 1   | L50   | 1488 | U    |
| 1   | L50   | 1489 | G    |
| 1   | L50   | 1490 | U    |
| 1   | L50   | 1491 | U    |
| 1   | L50   | 1492 | U    |
| 1   | L50   | 1499 | U    |
| 1   | L50   | 1513 | G    |
| 1   | L50   | 1524 | G    |
| 1   | L50   | 1527 | U    |
| 1   | L50   | 1533 | C    |
| 1   | L50   | 1534 | G    |
| 1   | L50   | 1535 | G    |
| 1   | L50   | 1536 | G    |
| 1   | L50   | 1538 | G    |
| 1   | L50   | 1547 | G    |
| 1   | L50   | 1554 | U    |
| 1   | L50   | 1555 | G    |
| 1   | L50   | 1556 | U    |
| 1   | L50   | 1557 | G    |
| 1   | L50   | 1563 | A    |
| 1   | L50   | 1564 | U    |
| 1   | L50   | 1565 | U    |
| 1   | L50   | 1566 | G    |
| 1   | L50   | 1568 | G    |
| 1   | L50   | 1569 | A    |
| 1   | L50   | 1571 | A    |
| 1   | L50   | 1573 | G    |
| 1   | L50   | 1574 | G    |
| 1   | L50   | 1575 | G    |
| 1   | L50   | 1583 | A    |
| 1   | L50   | 1591 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1592 | U    |
| 1   | L50   | 1602 | G    |
| 1   | L50   | 1610 | A    |
| 1   | L50   | 1611 | A    |
| 1   | L50   | 1612 | G    |
| 1   | L50   | 1613 | A    |
| 1   | L50   | 1614 | G    |
| 1   | L50   | 1617 | A    |
| 1   | L50   | 1619 | G    |
| 1   | L50   | 1624 | G    |
| 1   | L50   | 1626 | G    |
| 1   | L50   | 1638 | G    |
| 1   | L50   | 1643 | G    |
| 1   | L50   | 1644 | U    |
| 1   | L50   | 1645 | C    |
| 1   | L50   | 1646 | G    |
| 1   | L50   | 1649 | A    |
| 1   | L50   | 1651 | A    |
| 1   | L50   | 1653 | G    |
| 1   | L50   | 1665 | A    |
| 1   | L50   | 1668 | A    |
| 1   | L50   | 1674 | G    |
| 1   | L50   | 1675 | G    |
| 1   | L50   | 1680 | A    |
| 1   | L50   | 1682 | G    |
| 1   | L50   | 1685 | G    |
| 1   | L50   | 1686 | G    |
| 1   | L50   | 1689 | G    |
| 1   | L50   | 1692 | A    |
| 1   | L50   | 1693 | C    |
| 1   | L50   | 1697 | G    |
| 1   | L50   | 1698 | A    |
| 1   | L50   | 1699 | C    |
| 1   | L50   | 1705 | U    |
| 1   | L50   | 1708 | G    |
| 1   | L50   | 1709 | G    |
| 1   | L50   | 1710 | U    |
| 1   | L50   | 1711 | A    |
| 1   | L50   | 1717 | A    |
| 1   | L50   | 1718 | C    |
| 1   | L50   | 1720 | C    |
| 1   | L50   | 1724 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1733 | A    |
| 1   | L50   | 1735 | G    |
| 1   | L50   | 1739 | A    |
| 1   | L50   | 1742 | C    |
| 1   | L50   | 1743 | G    |
| 1   | L50   | 1746 | U    |
| 1   | L50   | 1749 | A    |
| 1   | L50   | 1751 | G    |
| 1   | L50   | 1755 | U    |
| 1   | L50   | 1760 | A    |
| 1   | L50   | 1770 | U    |
| 1   | L50   | 1772 | U    |
| 1   | L50   | 1797 | A    |
| 1   | L50   | 1799 | U    |
| 1   | L50   | 1800 | U    |
| 1   | L50   | 1801 | C    |
| 1   | L50   | 1808 | A    |
| 1   | L50   | 1809 | A    |
| 1   | L50   | 1810 | C    |
| 1   | L50   | 1811 | G    |
| 1   | L50   | 1820 | C    |
| 1   | L50   | 1821 | G    |
| 1   | L50   | 1822 | G    |
| 1   | L50   | 1828 | G    |
| 1   | L50   | 1832 | A    |
| 1   | L50   | 1833 | A    |
| 1   | L50   | 1835 | G    |
| 1   | L50   | 1836 | A    |
| 1   | L50   | 1837 | A    |
| 1   | L50   | 1838 | G    |
| 1   | L50   | 1839 | A    |
| 1   | L50   | 1846 | U    |
| 1   | L50   | 1854 | A    |
| 1   | L50   | 1858 | U    |
| 1   | L50   | 1860 | G    |
| 1   | L50   | 1868 | A    |
| 1   | L50   | 1869 | A    |
| 1   | L50   | 1870 | G    |
| 1   | L50   | 1872 | U    |
| 1   | L50   | 1873 | G    |
| 1   | L50   | 1874 | U    |
| 1   | L50   | 1881 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1883 | A    |
| 1   | L50   | 1885 | G    |
| 1   | L50   | 1887 | G    |
| 1   | L50   | 1888 | A    |
| 1   | L50   | 1931 | C    |
| 1   | L50   | 1934 | C    |
| 1   | L50   | 1935 | A    |
| 1   | L50   | 1937 | G    |
| 1   | L50   | 1938 | A    |
| 1   | L50   | 1939 | U    |
| 1   | L50   | 1940 | C    |
| 1   | L50   | 1941 | A    |
| 1   | L50   | 1942 | U    |
| 1   | L50   | 1943 | C    |
| 1   | L50   | 1946 | G    |
| 1   | L50   | 1949 | A    |
| 1   | L50   | 1950 | C    |
| 1   | L50   | 1955 | G    |
| 1   | L50   | 1956 | U    |
| 1   | L50   | 1957 | U    |
| 1   | L50   | 1958 | U    |
| 1   | L50   | 1959 | A    |
| 1   | L50   | 1960 | A    |
| 1   | L50   | 1961 | G    |
| 1   | L50   | 1963 | A    |
| 1   | L50   | 1966 | A    |
| 1   | L50   | 1967 | A    |
| 1   | L50   | 1968 | G    |
| 1   | L50   | 1973 | G    |
| 1   | L50   | 1977 | G    |
| 1   | L50   | 1978 | G    |
| 1   | L50   | 1985 | G    |
| 1   | L50   | 1991 | G    |
| 1   | L50   | 1995 | G    |
| 1   | L50   | 1997 | A    |
| 1   | L50   | 2007 | A    |
| 1   | L50   | 2008 | A    |
| 1   | L50   | 2011 | A    |
| 1   | L50   | 2013 | A    |
| 1   | L50   | 2015 | C    |
| 1   | L50   | 2016 | G    |
| 1   | L50   | 2019 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2020 | U    |
| 1   | L50   | 2022 | G    |
| 1   | L50   | 2023 | A    |
| 1   | L50   | 2027 | A    |
| 1   | L50   | 2030 | G    |
| 1   | L50   | 2031 | U    |
| 1   | L50   | 2032 | A    |
| 1   | L50   | 2036 | A    |
| 1   | L50   | 2037 | C    |
| 1   | L50   | 2039 | G    |
| 1   | L50   | 2042 | A    |
| 1   | L50   | 2043 | G    |
| 1   | L50   | 2045 | C    |
| 1   | L50   | 2046 | G    |
| 1   | L50   | 2047 | A    |
| 1   | L50   | 2048 | G    |
| 1   | L50   | 2049 | A    |
| 1   | L50   | 2052 | A    |
| 1   | L50   | 2057 | U    |
| 1   | L50   | 2059 | U    |
| 1   | L50   | 2060 | A    |
| 1   | L50   | 2061 | G    |
| 1   | L50   | 2062 | A    |
| 1   | L50   | 2063 | G    |
| 1   | L50   | 2065 | A    |
| 1   | L50   | 2067 | A    |
| 1   | L50   | 2073 | U    |
| 1   | L50   | 2075 | A    |
| 1   | L50   | 2076 | A    |
| 1   | L50   | 2077 | G    |
| 1   | L50   | 2078 | A    |
| 1   | L50   | 2085 | G    |
| 1   | L50   | 2087 | G    |
| 1   | L50   | 2093 | G    |
| 1   | L50   | 2096 | C    |
| 1   | L50   | 2097 | U    |
| 1   | L50   | 2098 | A    |
| 1   | L50   | 2099 | C    |
| 1   | L50   | 2108 | U    |
| 1   | L50   | 2109 | G    |
| 1   | L50   | 2110 | A    |
| 1   | L50   | 2111 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2114 | G    |
| 1   | L50   | 2122 | G    |
| 1   | L50   | 2124 | C    |
| 1   | L50   | 2130 | G    |
| 1   | L50   | 2131 | A    |
| 1   | L50   | 2136 | A    |
| 1   | L50   | 2140 | A    |
| 1   | L50   | 2141 | U    |
| 1   | L50   | 2142 | A    |
| 1   | L50   | 2145 | A    |
| 1   | L50   | 2146 | G    |
| 1   | L50   | 2149 | A    |
| 1   | L50   | 2150 | C    |
| 1   | L50   | 2152 | U    |
| 1   | L50   | 2160 | G    |
| 1   | L50   | 2162 | G    |
| 1   | L50   | 2164 | G    |
| 1   | L50   | 2167 | A    |
| 1   | L50   | 2168 | G    |
| 1   | L50   | 2169 | A    |
| 1   | L50   | 2170 | A    |
| 1   | L50   | 2171 | A    |
| 1   | L50   | 2177 | C    |
| 1   | L50   | 2178 | C    |
| 1   | L50   | 2185 | A    |
| 1   | L50   | 2189 | C    |
| 1   | L50   | 2211 | A    |
| 1   | L50   | 2212 | G    |
| 1   | L50   | 2213 | A    |
| 1   | L50   | 2217 | C    |
| 1   | L50   | 2221 | G    |
| 1   | L50   | 2224 | G    |
| 1   | L50   | 2228 | U    |
| 1   | L50   | 2229 | U    |
| 1   | L50   | 2234 | U    |
| 1   | L50   | 2235 | C    |
| 1   | L50   | 2239 | G    |
| 1   | L50   | 2240 | A    |
| 1   | L50   | 2241 | U    |
| 1   | L50   | 2243 | U    |
| 1   | L50   | 2253 | C    |
| 1   | L50   | 2254 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2255 | A    |
| 1   | L50   | 2256 | G    |
| 1   | L50   | 2257 | C    |
| 1   | L50   | 2260 | G    |
| 1   | L50   | 2262 | C    |
| 1   | L50   | 2266 | G    |
| 1   | L50   | 2272 | G    |
| 1   | L50   | 2275 | G    |
| 1   | L50   | 2279 | A    |
| 1   | L50   | 2286 | G    |
| 1   | L50   | 2291 | U    |
| 1   | L50   | 2293 | C    |
| 1   | L50   | 2296 | C    |
| 1   | L50   | 2303 | C    |
| 1   | L50   | 2304 | A    |
| 1   | L50   | 2306 | G    |
| 1   | L50   | 2309 | A    |
| 1   | L50   | 2310 | C    |
| 1   | L50   | 2313 | G    |
| 1   | L50   | 2319 | G    |
| 1   | L50   | 2322 | U    |
| 1   | L50   | 2323 | U    |
| 1   | L50   | 2325 | G    |
| 1   | L50   | 2337 | A    |
| 1   | L50   | 2339 | A    |
| 1   | L50   | 2340 | G    |
| 1   | L50   | 2345 | G    |
| 1   | L50   | 2347 | U    |
| 1   | L50   | 2351 | U    |
| 1   | L50   | 2355 | A    |
| 1   | L50   | 2358 | G    |
| 1   | L50   | 2364 | A    |
| 1   | L50   | 2376 | A    |
| 1   | L50   | 2377 | G    |
| 1   | L50   | 2379 | G    |
| 1   | L50   | 2394 | A    |
| 1   | L50   | 2399 | A    |
| 1   | L50   | 2401 | C    |
| 1   | L50   | 2410 | A    |
| 1   | L50   | 2412 | C    |
| 1   | L50   | 2413 | U    |
| 1   | L50   | 2416 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2419 | G    |
| 1   | L50   | 2420 | C    |
| 1   | L50   | 2423 | C    |
| 1   | L50   | 2424 | G    |
| 1   | L50   | 2432 | G    |
| 1   | L50   | 2434 | A    |
| 1   | L50   | 2436 | G    |
| 1   | L50   | 2437 | U    |
| 1   | L50   | 2441 | A    |
| 1   | L50   | 2447 | A    |
| 1   | L50   | 2451 | U    |
| 1   | L50   | 2452 | A    |
| 1   | L50   | 2453 | C    |
| 1   | L50   | 2459 | C    |
| 1   | L50   | 2460 | U    |
| 1   | L50   | 2473 | G    |
| 1   | L50   | 2475 | A    |
| 1   | L50   | 2476 | G    |
| 1   | L50   | 2477 | C    |
| 1   | L50   | 2482 | A    |
| 1   | L50   | 2487 | A    |
| 1   | L50   | 2490 | A    |
| 1   | L50   | 2491 | A    |
| 1   | L50   | 2501 | A    |
| 1   | L50   | 2503 | U    |
| 1   | L50   | 2508 | A    |
| 1   | L50   | 2509 | A    |
| 1   | L50   | 2518 | G    |
| 1   | L50   | 2519 | G    |
| 1   | L50   | 2520 | A    |
| 1   | L50   | 2529 | C    |
| 1   | L50   | 2532 | A    |
| 1   | L50   | 2533 | G    |
| 1   | L50   | 2534 | U    |
| 1   | L50   | 2535 | U    |
| 1   | L50   | 2538 | C    |
| 1   | L50   | 2539 | A    |
| 1   | L50   | 2548 | G    |
| 1   | L50   | 2555 | A    |
| 1   | L50   | 2558 | A    |
| 1   | L50   | 2559 | G    |
| 1   | L50   | 2562 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2563 | U    |
| 1   | L50   | 2565 | U    |
| 1   | L50   | 2568 | U    |
| 1   | L50   | 2578 | G    |
| 1   | L50   | 2588 | G    |
| 1   | L50   | 2593 | A    |
| 1   | L50   | 2595 | U    |
| 1   | L50   | 2596 | G    |
| 1   | L50   | 2597 | G    |
| 1   | L50   | 2598 | U    |
| 1   | L50   | 2600 | G    |
| 1   | L50   | 2605 | C    |
| 1   | L50   | 2606 | A    |
| 1   | L50   | 2612 | G    |
| 2   | L70   | 2    | G    |
| 2   | L70   | 10   | C    |
| 2   | L70   | 14   | U    |
| 2   | L70   | 15   | C    |
| 2   | L70   | 18   | C    |
| 2   | L70   | 22   | A    |
| 2   | L70   | 25   | A    |
| 2   | L70   | 27   | A    |
| 2   | L70   | 32   | A    |
| 2   | L70   | 33   | U    |
| 2   | L70   | 35   | C    |
| 2   | L70   | 41   | G    |
| 2   | L70   | 42   | A    |
| 2   | L70   | 49   | A    |
| 2   | L70   | 50   | A    |
| 2   | L70   | 51   | G    |
| 2   | L70   | 53   | U    |
| 2   | L70   | 63   | A    |
| 2   | L70   | 64   | G    |
| 2   | L70   | 65   | A    |
| 2   | L70   | 67   | C    |
| 2   | L70   | 69   | A    |
| 2   | L70   | 88   | C    |
| 2   | L70   | 89   | G    |
| 2   | L70   | 91   | C    |
| 2   | L70   | 93   | A    |
| 2   | L70   | 100  | A    |
| 2   | L70   | 101  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L70   | 104 | C    |
| 2   | L70   | 105 | G    |
| 2   | L70   | 107 | G    |
| 2   | L70   | 108 | G    |
| 2   | L70   | 109 | U    |
| 2   | L70   | 110 | G    |
| 2   | L70   | 115 | A    |
| 2   | L70   | 119 | U    |
| 42  | S60   | 7   | U    |
| 42  | S60   | 8   | U    |
| 42  | S60   | 14  | U    |
| 42  | S60   | 17  | C    |
| 42  | S60   | 26  | A    |
| 42  | S60   | 32  | G    |
| 42  | S60   | 37  | A    |
| 42  | S60   | 39  | A    |
| 42  | S60   | 40  | G    |
| 42  | S60   | 41  | A    |
| 42  | S60   | 43  | U    |
| 42  | S60   | 44  | U    |
| 42  | S60   | 45  | A    |
| 42  | S60   | 48  | C    |
| 42  | S60   | 52  | C    |
| 42  | S60   | 54  | U    |
| 42  | S60   | 55  | G    |
| 42  | S60   | 56  | U    |
| 42  | S60   | 66  | G    |
| 42  | S60   | 70  | U    |
| 42  | S60   | 71  | U    |
| 42  | S60   | 72  | A    |
| 42  | S60   | 73  | G    |
| 42  | S60   | 75  | G    |
| 42  | S60   | 76  | A    |
| 42  | S60   | 77  | A    |
| 42  | S60   | 83  | G    |
| 42  | S60   | 86  | A    |
| 42  | S60   | 88  | G    |
| 42  | S60   | 92  | A    |
| 42  | S60   | 94  | U    |
| 42  | S60   | 97  | C    |
| 42  | S60   | 98  | G    |
| 42  | S60   | 99  | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | S60   | 102 | G    |
| 42  | S60   | 104 | G    |
| 42  | S60   | 106 | A    |
| 42  | S60   | 107 | U    |
| 42  | S60   | 110 | A    |
| 42  | S60   | 112 | U    |
| 42  | S60   | 116 | U    |
| 42  | S60   | 118 | G    |
| 42  | S60   | 119 | A    |
| 42  | S60   | 120 | A    |
| 42  | S60   | 121 | C    |
| 42  | S60   | 124 | G    |
| 42  | S60   | 127 | A    |
| 42  | S60   | 128 | A    |
| 42  | S60   | 132 | C    |
| 42  | S60   | 133 | A    |
| 42  | S60   | 134 | G    |
| 42  | S60   | 138 | A    |
| 42  | S60   | 140 | A    |
| 42  | S60   | 141 | G    |
| 42  | S60   | 142 | A    |
| 42  | S60   | 147 | A    |
| 42  | S60   | 148 | A    |
| 42  | S60   | 150 | A    |
| 42  | S60   | 153 | G    |
| 42  | S60   | 155 | G    |
| 42  | S60   | 157 | A    |
| 42  | S60   | 161 | G    |
| 42  | S60   | 167 | G    |
| 42  | S60   | 172 | U    |
| 42  | S60   | 173 | A    |
| 42  | S60   | 174 | G    |
| 42  | S60   | 180 | G    |
| 42  | S60   | 181 | A    |
| 42  | S60   | 184 | A    |
| 42  | S60   | 186 | A    |
| 42  | S60   | 187 | A    |
| 42  | S60   | 189 | A    |
| 42  | S60   | 190 | A    |
| 42  | S60   | 191 | C    |
| 42  | S60   | 192 | A    |
| 42  | S60   | 193 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | S60   | 197 | A    |
| 42  | S60   | 198 | G    |
| 42  | S60   | 199 | G    |
| 42  | S60   | 204 | U    |
| 42  | S60   | 206 | A    |
| 42  | S60   | 219 | U    |
| 42  | S60   | 220 | C    |
| 42  | S60   | 222 | G    |
| 42  | S60   | 226 | G    |
| 42  | S60   | 227 | U    |
| 42  | S60   | 228 | A    |
| 42  | S60   | 238 | A    |
| 42  | S60   | 241 | G    |
| 42  | S60   | 242 | C    |
| 42  | S60   | 247 | U    |
| 42  | S60   | 254 | U    |
| 42  | S60   | 255 | A    |
| 42  | S60   | 256 | G    |
| 42  | S60   | 259 | G    |
| 42  | S60   | 262 | U    |
| 42  | S60   | 263 | A    |
| 42  | S60   | 264 | C    |
| 42  | S60   | 268 | G    |
| 42  | S60   | 271 | U    |
| 42  | S60   | 283 | U    |
| 42  | S60   | 284 | C    |
| 42  | S60   | 290 | A    |
| 42  | S60   | 292 | G    |
| 42  | S60   | 299 | G    |
| 42  | S60   | 300 | A    |
| 42  | S60   | 303 | G    |
| 42  | S60   | 304 | A    |
| 42  | S60   | 305 | C    |
| 42  | S60   | 307 | G    |
| 42  | S60   | 311 | C    |
| 42  | S60   | 314 | G    |
| 42  | S60   | 315 | G    |
| 42  | S60   | 318 | C    |
| 42  | S60   | 319 | A    |
| 42  | S60   | 320 | A    |
| 42  | S60   | 326 | G    |
| 42  | S60   | 327 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | S60   | 328 | A    |
| 42  | S60   | 329 | G    |
| 42  | S60   | 335 | G    |
| 42  | S60   | 338 | A    |
| 42  | S60   | 339 | A    |
| 42  | S60   | 340 | A    |
| 42  | S60   | 341 | A    |
| 42  | S60   | 342 | U    |
| 42  | S60   | 344 | A    |
| 42  | S60   | 345 | C    |
| 42  | S60   | 347 | G    |
| 42  | S60   | 348 | A    |
| 42  | S60   | 355 | C    |
| 42  | S60   | 356 | A    |
| 42  | S60   | 357 | A    |
| 42  | S60   | 358 | G    |
| 42  | S60   | 362 | G    |
| 42  | S60   | 363 | C    |
| 42  | S60   | 364 | G    |
| 42  | S60   | 367 | A    |
| 42  | S60   | 368 | G    |
| 42  | S60   | 371 | A    |
| 42  | S60   | 372 | A    |
| 42  | S60   | 373 | G    |
| 42  | S60   | 374 | A    |
| 42  | S60   | 375 | G    |
| 42  | S60   | 377 | C    |
| 42  | S60   | 378 | G    |
| 42  | S60   | 380 | G    |
| 42  | S60   | 382 | A    |
| 42  | S60   | 383 | A    |
| 42  | S60   | 384 | A    |
| 42  | S60   | 385 | C    |
| 42  | S60   | 388 | G    |
| 42  | S60   | 395 | U    |
| 42  | S60   | 396 | A    |
| 42  | S60   | 398 | A    |
| 42  | S60   | 399 | A    |
| 42  | S60   | 402 | C    |
| 42  | S60   | 407 | G    |
| 42  | S60   | 408 | A    |
| 42  | S60   | 409 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | S60   | 412 | A    |
| 42  | S60   | 414 | U    |
| 42  | S60   | 416 | G    |
| 42  | S60   | 422 | A    |
| 42  | S60   | 424 | G    |
| 42  | S60   | 425 | G    |
| 42  | S60   | 426 | C    |
| 42  | S60   | 431 | G    |
| 42  | S60   | 432 | C    |
| 42  | S60   | 437 | A    |
| 42  | S60   | 441 | G    |
| 42  | S60   | 444 | G    |
| 42  | S60   | 445 | U    |
| 42  | S60   | 446 | A    |
| 42  | S60   | 449 | A    |
| 42  | S60   | 450 | C    |
| 42  | S60   | 452 | A    |
| 42  | S60   | 453 | G    |
| 42  | S60   | 454 | C    |
| 42  | S60   | 461 | A    |
| 42  | S60   | 471 | A    |
| 42  | S60   | 473 | G    |
| 42  | S60   | 474 | A    |
| 42  | S60   | 476 | U    |
| 42  | S60   | 477 | G    |
| 42  | S60   | 478 | C    |
| 42  | S60   | 481 | C    |
| 42  | S60   | 482 | G    |
| 42  | S60   | 486 | A    |
| 42  | S60   | 487 | A    |
| 42  | S60   | 490 | G    |
| 42  | S60   | 491 | G    |
| 42  | S60   | 501 | G    |
| 42  | S60   | 506 | A    |
| 42  | S60   | 509 | G    |
| 42  | S60   | 510 | U    |
| 42  | S60   | 511 | A    |
| 42  | S60   | 512 | C    |
| 42  | S60   | 521 | A    |
| 42  | S60   | 527 | G    |
| 42  | S60   | 530 | U    |
| 42  | S60   | 535 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | S60   | 536 | G    |
| 42  | S60   | 540 | C    |
| 42  | S60   | 541 | G    |
| 42  | S60   | 543 | A    |
| 42  | S60   | 544 | U    |
| 42  | S60   | 547 | A    |
| 42  | S60   | 550 | G    |
| 42  | S60   | 553 | A    |
| 42  | S60   | 554 | A    |
| 42  | S60   | 565 | U    |
| 42  | S60   | 566 | A    |
| 42  | S60   | 567 | A    |
| 42  | S60   | 568 | G    |
| 42  | S60   | 575 | A    |
| 42  | S60   | 578 | A    |
| 42  | S60   | 579 | G    |
| 42  | S60   | 590 | U    |
| 42  | S60   | 593 | A    |
| 42  | S60   | 598 | C    |
| 42  | S60   | 599 | G    |
| 42  | S60   | 600 | A    |
| 42  | S60   | 601 | G    |
| 42  | S60   | 602 | A    |
| 42  | S60   | 608 | A    |
| 42  | S60   | 609 | A    |
| 42  | S60   | 610 | U    |
| 42  | S60   | 616 | G    |
| 42  | S60   | 621 | G    |
| 42  | S60   | 622 | C    |
| 42  | S60   | 623 | U    |
| 42  | S60   | 624 | U    |
| 42  | S60   | 625 | A    |
| 42  | S60   | 630 | U    |
| 42  | S60   | 633 | C    |
| 42  | S60   | 635 | G    |
| 42  | S60   | 637 | G    |
| 42  | S60   | 644 | G    |
| 42  | S60   | 647 | C    |
| 42  | S60   | 661 | A    |
| 42  | S60   | 662 | U    |
| 42  | S60   | 665 | G    |
| 42  | S60   | 668 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | S60   | 671 | C    |
| 42  | S60   | 673 | A    |
| 42  | S60   | 686 | G    |
| 42  | S60   | 687 | A    |
| 42  | S60   | 688 | G    |
| 42  | S60   | 690 | A    |
| 42  | S60   | 694 | A    |
| 42  | S60   | 700 | A    |
| 42  | S60   | 702 | U    |
| 42  | S60   | 705 | A    |
| 42  | S60   | 706 | G    |
| 42  | S60   | 707 | A    |
| 42  | S60   | 722 | G    |
| 42  | S60   | 724 | A    |
| 42  | S60   | 725 | G    |
| 42  | S60   | 727 | A    |
| 42  | S60   | 728 | A    |
| 42  | S60   | 730 | C    |
| 42  | S60   | 731 | G    |
| 42  | S60   | 733 | U    |
| 42  | S60   | 734 | G    |
| 42  | S60   | 738 | A    |
| 42  | S60   | 740 | G    |
| 42  | S60   | 749 | G    |
| 42  | S60   | 752 | A    |
| 42  | S60   | 753 | U    |
| 42  | S60   | 754 | G    |
| 42  | S60   | 755 | A    |
| 42  | S60   | 757 | C    |
| 42  | S60   | 771 | A    |
| 42  | S60   | 775 | U    |
| 42  | S60   | 776 | A    |
| 42  | S60   | 777 | G    |
| 42  | S60   | 780 | G    |
| 42  | S60   | 788 | G    |
| 42  | S60   | 789 | G    |
| 42  | S60   | 790 | G    |
| 42  | S60   | 791 | A    |
| 42  | S60   | 795 | U    |
| 42  | S60   | 806 | G    |
| 42  | S60   | 810 | U    |
| 42  | S60   | 817 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | S60   | 818 | A    |
| 42  | S60   | 820 | G    |
| 42  | S60   | 821 | G    |
| 42  | S60   | 823 | A    |
| 42  | S60   | 825 | U    |
| 42  | S60   | 831 | G    |
| 42  | S60   | 836 | A    |
| 42  | S60   | 839 | C    |
| 42  | S60   | 840 | C    |
| 42  | S60   | 841 | A    |
| 42  | S60   | 846 | G    |
| 42  | S60   | 848 | G    |
| 42  | S60   | 866 | U    |
| 42  | S60   | 868 | U    |
| 42  | S60   | 871 | C    |
| 42  | S60   | 872 | U    |
| 42  | S60   | 874 | A    |
| 42  | S60   | 875 | A    |
| 42  | S60   | 877 | G    |
| 42  | S60   | 878 | C    |
| 42  | S60   | 880 | G    |
| 42  | S60   | 881 | G    |
| 42  | S60   | 883 | C    |
| 42  | S60   | 884 | A    |
| 42  | S60   | 890 | C    |
| 42  | S60   | 898 | G    |
| 42  | S60   | 899 | A    |
| 42  | S60   | 905 | G    |
| 42  | S60   | 908 | U    |
| 42  | S60   | 909 | G    |
| 42  | S60   | 911 | G    |
| 42  | S60   | 915 | A    |
| 42  | S60   | 916 | G    |
| 42  | S60   | 917 | U    |
| 42  | S60   | 918 | A    |
| 42  | S60   | 919 | C    |
| 42  | S60   | 924 | U    |
| 42  | S60   | 925 | A    |
| 42  | S60   | 926 | G    |
| 42  | S60   | 927 | G    |
| 42  | S60   | 928 | U    |
| 42  | S60   | 929 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | S60   | 930  | A    |
| 42  | S60   | 932  | A    |
| 42  | S60   | 933  | G    |
| 42  | S60   | 934  | A    |
| 42  | S60   | 935  | G    |
| 42  | S60   | 936  | U    |
| 42  | S60   | 940  | G    |
| 42  | S60   | 941  | C    |
| 42  | S60   | 942  | A    |
| 42  | S60   | 952  | A    |
| 42  | S60   | 953  | C    |
| 42  | S60   | 955  | A    |
| 42  | S60   | 957  | G    |
| 42  | S60   | 958  | A    |
| 42  | S60   | 959  | G    |
| 42  | S60   | 962  | G    |
| 42  | S60   | 966  | G    |
| 42  | S60   | 967  | A    |
| 42  | S60   | 968  | C    |
| 42  | S60   | 970  | U    |
| 42  | S60   | 971  | U    |
| 42  | S60   | 972  | U    |
| 42  | S60   | 974  | G    |
| 42  | S60   | 976  | U    |
| 42  | S60   | 978  | A    |
| 42  | S60   | 980  | G    |
| 42  | S60   | 981  | U    |
| 42  | S60   | 987  | A    |
| 42  | S60   | 991  | A    |
| 42  | S60   | 995  | A    |
| 42  | S60   | 998  | U    |
| 42  | S60   | 999  | C    |
| 42  | S60   | 1003 | A    |
| 42  | S60   | 1006 | A    |
| 42  | S60   | 1007 | U    |
| 42  | S60   | 1008 | A    |
| 42  | S60   | 1011 | A    |
| 42  | S60   | 1012 | A    |
| 42  | S60   | 1013 | A    |
| 42  | S60   | 1014 | G    |
| 42  | S60   | 1017 | A    |
| 42  | S60   | 1018 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | S60   | 1019 | C    |
| 42  | S60   | 1021 | A    |
| 42  | S60   | 1023 | A    |
| 42  | S60   | 1024 | G    |
| 42  | S60   | 1028 | U    |
| 42  | S60   | 1029 | U    |
| 42  | S60   | 1033 | A    |
| 42  | S60   | 1039 | G    |
| 42  | S60   | 1041 | A    |
| 42  | S60   | 1042 | A    |
| 42  | S60   | 1045 | A    |
| 42  | S60   | 1046 | A    |
| 42  | S60   | 1047 | G    |
| 42  | S60   | 1052 | A    |
| 42  | S60   | 1053 | A    |
| 42  | S60   | 1054 | G    |
| 42  | S60   | 1056 | A    |
| 42  | S60   | 1057 | C    |
| 42  | S60   | 1058 | A    |
| 42  | S60   | 1059 | G    |
| 42  | S60   | 1060 | G    |
| 42  | S60   | 1062 | C    |
| 42  | S60   | 1063 | A    |
| 42  | S60   | 1064 | G    |
| 42  | S60   | 1066 | G    |
| 42  | S60   | 1075 | A    |
| 42  | S60   | 1076 | G    |
| 42  | S60   | 1077 | A    |
| 42  | S60   | 1078 | U    |
| 42  | S60   | 1088 | U    |
| 42  | S60   | 1089 | G    |
| 42  | S60   | 1090 | C    |
| 42  | S60   | 1092 | C    |
| 42  | S60   | 1094 | C    |
| 42  | S60   | 1099 | U    |
| 42  | S60   | 1100 | A    |
| 42  | S60   | 1102 | A    |
| 42  | S60   | 1103 | G    |
| 42  | S60   | 1104 | U    |
| 42  | S60   | 1105 | G    |
| 42  | S60   | 1106 | G    |
| 42  | S60   | 1111 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | S60   | 1112 | G    |
| 42  | S60   | 1116 | A    |
| 42  | S60   | 1117 | A    |
| 42  | S60   | 1118 | A    |
| 42  | S60   | 1119 | C    |
| 42  | S60   | 1120 | A    |
| 42  | S60   | 1121 | A    |
| 42  | S60   | 1122 | A    |
| 42  | S60   | 1123 | U    |
| 42  | S60   | 1124 | A    |
| 42  | S60   | 1125 | G    |
| 42  | S60   | 1126 | A    |
| 42  | S60   | 1127 | A    |
| 42  | S60   | 1128 | G    |
| 42  | S60   | 1129 | U    |
| 42  | S60   | 1130 | A    |
| 42  | S60   | 1135 | U    |
| 42  | S60   | 1136 | G    |
| 42  | S60   | 1137 | A    |
| 42  | S60   | 1139 | C    |
| 42  | S60   | 1141 | A    |
| 42  | S60   | 1142 | G    |
| 42  | S60   | 1146 | G    |
| 42  | S60   | 1152 | G    |
| 42  | S60   | 1154 | A    |
| 42  | S60   | 1158 | U    |
| 42  | S60   | 1159 | A    |
| 42  | S60   | 1160 | A    |
| 42  | S60   | 1161 | U    |
| 42  | S60   | 1162 | G    |
| 42  | S60   | 1170 | G    |
| 42  | S60   | 1171 | A    |
| 42  | S60   | 1175 | A    |
| 42  | S60   | 1176 | G    |
| 42  | S60   | 1177 | G    |
| 42  | S60   | 1179 | A    |
| 42  | S60   | 1182 | G    |
| 42  | S60   | 1185 | A    |
| 42  | S60   | 1191 | C    |
| 42  | S60   | 1192 | G    |
| 42  | S60   | 1194 | U    |
| 42  | S60   | 1195 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | S60   | 1196 | U    |
| 42  | S60   | 1202 | U    |
| 42  | S60   | 1203 | A    |
| 42  | S60   | 1204 | A    |
| 42  | S60   | 1205 | G    |
| 42  | S60   | 1210 | G    |
| 42  | S60   | 1211 | A    |
| 42  | S60   | 1214 | A    |
| 42  | S60   | 1216 | U    |
| 42  | S60   | 1217 | G    |
| 42  | S60   | 1219 | G    |
| 42  | S60   | 1223 | C    |
| 42  | S60   | 1225 | G    |
| 42  | S60   | 1227 | U    |
| 42  | S60   | 1230 | U    |
| 42  | S60   | 1237 | C    |
| 42  | S60   | 1238 | A    |
| 42  | S60   | 1239 | C    |
| 42  | S60   | 1240 | C    |
| 42  | S60   | 1241 | G    |
| 42  | S60   | 1243 | C    |
| 42  | S60   | 1246 | U    |
| 42  | S60   | 1249 | U    |
| 42  | S60   | 1250 | U    |
| 42  | S60   | 1251 | A    |
| 42  | S60   | 1260 | G    |
| 42  | S60   | 1262 | A    |
| 42  | S60   | 1263 | A    |
| 42  | S60   | 1264 | C    |
| 42  | S60   | 1266 | A    |
| 42  | S60   | 1267 | G    |
| 42  | S60   | 1270 | G    |
| 42  | S60   | 1274 | A    |
| 42  | S60   | 1275 | C    |
| 42  | S60   | 1276 | A    |
| 42  | S60   | 1280 | G    |
| 42  | S60   | 1282 | A    |
| 42  | S60   | 1283 | A    |
| 42  | S60   | 1284 | G    |
| 42  | S60   | 1287 | A    |
| 42  | S60   | 1294 | G    |
| 42  | S60   | 1295 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | S60   | 1296 | A    |
| 42  | S60   | 1297 | G    |
| 42  | S60   | 1301 | U    |
| 42  | S60   | 1302 | C    |
| 42  | S60   | 1307 | U    |
| 42  | S60   | 1310 | G    |
| 42  | S60   | 1314 | C    |
| 42  | S60   | 1315 | A    |
| 42  | S60   | 1316 | A    |
| 42  | S60   | 1317 | G    |
| 42  | S60   | 1320 | G    |
| 42  | S60   | 1322 | A    |
| 42  | S60   | 1326 | A    |
| 42  | S60   | 1327 | G    |
| 42  | S60   | 1328 | G    |
| 42  | S60   | 1329 | C    |
| 42  | S60   | 1331 | G    |
| 42  | S60   | 1340 | G    |
| 42  | S60   | 1341 | A    |
| 42  | S60   | 1342 | A    |
| 42  | S60   | 1343 | C    |
| 42  | S60   | 1348 | A    |
| 42  | S60   | 1352 | G    |
| 42  | S60   | 1353 | G    |
| 42  | S60   | 1354 | A    |
| 42  | S60   | 1355 | U    |
| 42  | S60   | 1356 | C    |
| 42  | S60   | 1357 | A    |
| 1   | K50   | 2    | U    |
| 1   | K50   | 3    | A    |
| 1   | K50   | 13   | A    |
| 1   | K50   | 15   | G    |
| 1   | K50   | 21   | U    |
| 1   | K50   | 22   | U    |
| 1   | K50   | 23   | U    |
| 1   | K50   | 24   | G    |
| 1   | K50   | 25   | G    |
| 1   | K50   | 31   | G    |
| 1   | K50   | 39   | G    |
| 1   | K50   | 43   | G    |
| 1   | K50   | 48   | A    |
| 1   | K50   | 51   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 52  | G    |
| 1   | K50   | 59  | A    |
| 1   | K50   | 62  | U    |
| 1   | K50   | 63  | G    |
| 1   | K50   | 68  | G    |
| 1   | K50   | 70  | A    |
| 1   | K50   | 71  | G    |
| 1   | K50   | 73  | A    |
| 1   | K50   | 74  | G    |
| 1   | K50   | 75  | C    |
| 1   | K50   | 76  | A    |
| 1   | K50   | 77  | G    |
| 1   | K50   | 82  | G    |
| 1   | K50   | 87  | C    |
| 1   | K50   | 88  | A    |
| 1   | K50   | 98  | A    |
| 1   | K50   | 99  | U    |
| 1   | K50   | 100 | A    |
| 1   | K50   | 101 | C    |
| 1   | K50   | 108 | G    |
| 1   | K50   | 113 | G    |
| 1   | K50   | 114 | G    |
| 1   | K50   | 118 | A    |
| 1   | K50   | 123 | U    |
| 1   | K50   | 132 | A    |
| 1   | K50   | 135 | A    |
| 1   | K50   | 136 | U    |
| 1   | K50   | 137 | A    |
| 1   | K50   | 151 | G    |
| 1   | K50   | 152 | A    |
| 1   | K50   | 157 | A    |
| 1   | K50   | 158 | A    |
| 1   | K50   | 159 | A    |
| 1   | K50   | 160 | C    |
| 1   | K50   | 165 | G    |
| 1   | K50   | 167 | G    |
| 1   | K50   | 169 | A    |
| 1   | K50   | 178 | G    |
| 1   | K50   | 181 | G    |
| 1   | K50   | 184 | G    |
| 1   | K50   | 186 | G    |
| 1   | K50   | 188 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 191 | A    |
| 1   | K50   | 194 | A    |
| 1   | K50   | 201 | A    |
| 1   | K50   | 202 | G    |
| 1   | K50   | 204 | C    |
| 1   | K50   | 209 | A    |
| 1   | K50   | 210 | G    |
| 1   | K50   | 211 | U    |
| 1   | K50   | 212 | G    |
| 1   | K50   | 213 | U    |
| 1   | K50   | 214 | A    |
| 1   | K50   | 215 | A    |
| 1   | K50   | 216 | U    |
| 1   | K50   | 221 | A    |
| 1   | K50   | 224 | U    |
| 1   | K50   | 225 | G    |
| 1   | K50   | 226 | A    |
| 1   | K50   | 233 | G    |
| 1   | K50   | 234 | U    |
| 1   | K50   | 237 | A    |
| 1   | K50   | 238 | A    |
| 1   | K50   | 239 | A    |
| 1   | K50   | 240 | G    |
| 1   | K50   | 241 | G    |
| 1   | K50   | 242 | A    |
| 1   | K50   | 246 | A    |
| 1   | K50   | 247 | G    |
| 1   | K50   | 255 | U    |
| 1   | K50   | 258 | G    |
| 1   | K50   | 265 | A    |
| 1   | K50   | 266 | A    |
| 1   | K50   | 267 | G    |
| 1   | K50   | 268 | C    |
| 1   | K50   | 273 | C    |
| 1   | K50   | 276 | U    |
| 1   | K50   | 277 | A    |
| 1   | K50   | 284 | G    |
| 1   | K50   | 285 | A    |
| 1   | K50   | 286 | U    |
| 1   | K50   | 287 | A    |
| 1   | K50   | 289 | U    |
| 1   | K50   | 298 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 309 | U    |
| 1   | K50   | 311 | C    |
| 1   | K50   | 312 | G    |
| 1   | K50   | 314 | U    |
| 1   | K50   | 315 | G    |
| 1   | K50   | 316 | A    |
| 1   | K50   | 317 | G    |
| 1   | K50   | 330 | G    |
| 1   | K50   | 331 | U    |
| 1   | K50   | 332 | A    |
| 1   | K50   | 333 | A    |
| 1   | K50   | 340 | G    |
| 1   | K50   | 343 | A    |
| 1   | K50   | 345 | G    |
| 1   | K50   | 346 | A    |
| 1   | K50   | 347 | G    |
| 1   | K50   | 352 | C    |
| 1   | K50   | 353 | A    |
| 1   | K50   | 358 | G    |
| 1   | K50   | 366 | G    |
| 1   | K50   | 373 | U    |
| 1   | K50   | 382 | A    |
| 1   | K50   | 384 | A    |
| 1   | K50   | 385 | C    |
| 1   | K50   | 392 | C    |
| 1   | K50   | 396 | G    |
| 1   | K50   | 397 | A    |
| 1   | K50   | 400 | U    |
| 1   | K50   | 416 | A    |
| 1   | K50   | 434 | G    |
| 1   | K50   | 438 | A    |
| 1   | K50   | 449 | U    |
| 1   | K50   | 450 | C    |
| 1   | K50   | 453 | G    |
| 1   | K50   | 454 | C    |
| 1   | K50   | 467 | A    |
| 1   | K50   | 478 | A    |
| 1   | K50   | 488 | C    |
| 1   | K50   | 495 | A    |
| 1   | K50   | 499 | G    |
| 1   | K50   | 503 | A    |
| 1   | K50   | 504 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 507 | G    |
| 1   | K50   | 508 | A    |
| 1   | K50   | 509 | A    |
| 1   | K50   | 510 | G    |
| 1   | K50   | 517 | A    |
| 1   | K50   | 523 | A    |
| 1   | K50   | 524 | G    |
| 1   | K50   | 527 | A    |
| 1   | K50   | 530 | A    |
| 1   | K50   | 533 | G    |
| 1   | K50   | 534 | A    |
| 1   | K50   | 535 | A    |
| 1   | K50   | 536 | A    |
| 1   | K50   | 542 | G    |
| 1   | K50   | 553 | C    |
| 1   | K50   | 556 | A    |
| 1   | K50   | 562 | U    |
| 1   | K50   | 563 | U    |
| 1   | K50   | 564 | G    |
| 1   | K50   | 567 | A    |
| 1   | K50   | 568 | A    |
| 1   | K50   | 569 | C    |
| 1   | K50   | 570 | U    |
| 1   | K50   | 580 | U    |
| 1   | K50   | 581 | G    |
| 1   | K50   | 587 | A    |
| 1   | K50   | 601 | C    |
| 1   | K50   | 612 | C    |
| 1   | K50   | 618 | G    |
| 1   | K50   | 620 | C    |
| 1   | K50   | 625 | U    |
| 1   | K50   | 630 | U    |
| 1   | K50   | 631 | G    |
| 1   | K50   | 642 | G    |
| 1   | K50   | 643 | C    |
| 1   | K50   | 646 | A    |
| 1   | K50   | 647 | A    |
| 1   | K50   | 658 | G    |
| 1   | K50   | 659 | G    |
| 1   | K50   | 660 | G    |
| 1   | K50   | 661 | G    |
| 1   | K50   | 665 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K50   | 667 | G    |
| 1   | K50   | 668 | A    |
| 1   | K50   | 675 | G    |
| 1   | K50   | 676 | A    |
| 1   | K50   | 684 | A    |
| 1   | K50   | 685 | G    |
| 1   | K50   | 688 | G    |
| 1   | K50   | 689 | C    |
| 1   | K50   | 695 | C    |
| 1   | K50   | 710 | A    |
| 1   | K50   | 711 | U    |
| 1   | K50   | 714 | G    |
| 1   | K50   | 715 | G    |
| 1   | K50   | 720 | C    |
| 1   | K50   | 726 | C    |
| 1   | K50   | 729 | A    |
| 1   | K50   | 732 | G    |
| 1   | K50   | 736 | A    |
| 1   | K50   | 739 | A    |
| 1   | K50   | 741 | G    |
| 1   | K50   | 742 | G    |
| 1   | K50   | 749 | A    |
| 1   | K50   | 750 | U    |
| 1   | K50   | 763 | U    |
| 1   | K50   | 764 | U    |
| 1   | K50   | 765 | A    |
| 1   | K50   | 766 | A    |
| 1   | K50   | 767 | G    |
| 1   | K50   | 768 | G    |
| 1   | K50   | 772 | C    |
| 1   | K50   | 776 | C    |
| 1   | K50   | 778 | A    |
| 1   | K50   | 779 | A    |
| 1   | K50   | 781 | U    |
| 1   | K50   | 782 | G    |
| 1   | K50   | 784 | G    |
| 1   | K50   | 795 | U    |
| 1   | K50   | 796 | C    |
| 1   | K50   | 801 | A    |
| 1   | K50   | 802 | U    |
| 1   | K50   | 803 | G    |
| 1   | K50   | 806 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 816  | G    |
| 1   | K50   | 822  | U    |
| 1   | K50   | 828  | A    |
| 1   | K50   | 830  | G    |
| 1   | K50   | 834  | G    |
| 1   | K50   | 838  | G    |
| 1   | K50   | 840  | C    |
| 1   | K50   | 843  | A    |
| 1   | K50   | 848  | A    |
| 1   | K50   | 849  | A    |
| 1   | K50   | 852  | A    |
| 1   | K50   | 853  | A    |
| 1   | K50   | 854  | C    |
| 1   | K50   | 858  | G    |
| 1   | K50   | 859  | C    |
| 1   | K50   | 865  | G    |
| 1   | K50   | 866  | C    |
| 1   | K50   | 867  | U    |
| 1   | K50   | 871  | G    |
| 1   | K50   | 877  | A    |
| 1   | K50   | 878  | A    |
| 1   | K50   | 879  | U    |
| 1   | K50   | 885  | G    |
| 1   | K50   | 889  | G    |
| 1   | K50   | 893  | C    |
| 1   | K50   | 900  | A    |
| 1   | K50   | 905  | G    |
| 1   | K50   | 910  | A    |
| 1   | K50   | 980  | A    |
| 1   | K50   | 990  | U    |
| 1   | K50   | 998  | U    |
| 1   | K50   | 1001 | A    |
| 1   | K50   | 1002 | U    |
| 1   | K50   | 1010 | A    |
| 1   | K50   | 1017 | A    |
| 1   | K50   | 1018 | U    |
| 1   | K50   | 1021 | G    |
| 1   | K50   | 1022 | A    |
| 1   | K50   | 1023 | U    |
| 1   | K50   | 1024 | G    |
| 1   | K50   | 1030 | U    |
| 1   | K50   | 1032 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1033 | G    |
| 1   | K50   | 1034 | C    |
| 1   | K50   | 1037 | G    |
| 1   | K50   | 1050 | U    |
| 1   | K50   | 1053 | C    |
| 1   | K50   | 1055 | A    |
| 1   | K50   | 1056 | C    |
| 1   | K50   | 1061 | G    |
| 1   | K50   | 1062 | A    |
| 1   | K50   | 1070 | G    |
| 1   | K50   | 1075 | A    |
| 1   | K50   | 1082 | G    |
| 1   | K50   | 1085 | G    |
| 1   | K50   | 1087 | G    |
| 1   | K50   | 1089 | U    |
| 1   | K50   | 1090 | A    |
| 1   | K50   | 1096 | A    |
| 1   | K50   | 1099 | G    |
| 1   | K50   | 1100 | C    |
| 1   | K50   | 1102 | G    |
| 1   | K50   | 1105 | C    |
| 1   | K50   | 1111 | G    |
| 1   | K50   | 1117 | A    |
| 1   | K50   | 1118 | G    |
| 1   | K50   | 1120 | G    |
| 1   | K50   | 1121 | A    |
| 1   | K50   | 1123 | A    |
| 1   | K50   | 1124 | A    |
| 1   | K50   | 1130 | C    |
| 1   | K50   | 1131 | U    |
| 1   | K50   | 1133 | C    |
| 1   | K50   | 1134 | A    |
| 1   | K50   | 1135 | G    |
| 1   | K50   | 1136 | C    |
| 1   | K50   | 1142 | A    |
| 1   | K50   | 1144 | A    |
| 1   | K50   | 1148 | A    |
| 1   | K50   | 1149 | G    |
| 1   | K50   | 1150 | G    |
| 1   | K50   | 1151 | A    |
| 1   | K50   | 1155 | G    |
| 1   | K50   | 1163 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1169 | C    |
| 1   | K50   | 1170 | A    |
| 1   | K50   | 1171 | U    |
| 1   | K50   | 1172 | A    |
| 1   | K50   | 1173 | A    |
| 1   | K50   | 1175 | A    |
| 1   | K50   | 1177 | G    |
| 1   | K50   | 1181 | G    |
| 1   | K50   | 1182 | A    |
| 1   | K50   | 1183 | G    |
| 1   | K50   | 1189 | U    |
| 1   | K50   | 1191 | U    |
| 1   | K50   | 1192 | A    |
| 1   | K50   | 1193 | A    |
| 1   | K50   | 1194 | G    |
| 1   | K50   | 1196 | G    |
| 1   | K50   | 1213 | A    |
| 1   | K50   | 1217 | A    |
| 1   | K50   | 1218 | A    |
| 1   | K50   | 1221 | A    |
| 1   | K50   | 1224 | A    |
| 1   | K50   | 1231 | U    |
| 1   | K50   | 1232 | G    |
| 1   | K50   | 1233 | A    |
| 1   | K50   | 1235 | A    |
| 1   | K50   | 1236 | U    |
| 1   | K50   | 1237 | U    |
| 1   | K50   | 1243 | G    |
| 1   | K50   | 1247 | G    |
| 1   | K50   | 1250 | C    |
| 1   | K50   | 1252 | G    |
| 1   | K50   | 1254 | C    |
| 1   | K50   | 1256 | U    |
| 1   | K50   | 1257 | A    |
| 1   | K50   | 1264 | C    |
| 1   | K50   | 1267 | G    |
| 1   | K50   | 1268 | U    |
| 1   | K50   | 1269 | A    |
| 1   | K50   | 1270 | U    |
| 1   | K50   | 1274 | C    |
| 1   | K50   | 1277 | G    |
| 1   | K50   | 1278 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1282 | C    |
| 1   | K50   | 1283 | A    |
| 1   | K50   | 1284 | C    |
| 1   | K50   | 1296 | C    |
| 1   | K50   | 1299 | A    |
| 1   | K50   | 1304 | A    |
| 1   | K50   | 1305 | A    |
| 1   | K50   | 1308 | A    |
| 1   | K50   | 1309 | C    |
| 1   | K50   | 1317 | G    |
| 1   | K50   | 1318 | U    |
| 1   | K50   | 1327 | A    |
| 1   | K50   | 1332 | G    |
| 1   | K50   | 1333 | A    |
| 1   | K50   | 1340 | A    |
| 1   | K50   | 1341 | G    |
| 1   | K50   | 1342 | A    |
| 1   | K50   | 1346 | A    |
| 1   | K50   | 1350 | U    |
| 1   | K50   | 1355 | C    |
| 1   | K50   | 1356 | G    |
| 1   | K50   | 1359 | G    |
| 1   | K50   | 1361 | G    |
| 1   | K50   | 1362 | G    |
| 1   | K50   | 1374 | U    |
| 1   | K50   | 1375 | G    |
| 1   | K50   | 1384 | U    |
| 1   | K50   | 1385 | G    |
| 1   | K50   | 1386 | A    |
| 1   | K50   | 1387 | G    |
| 1   | K50   | 1395 | U    |
| 1   | K50   | 1396 | G    |
| 1   | K50   | 1402 | G    |
| 1   | K50   | 1411 | C    |
| 1   | K50   | 1412 | C    |
| 1   | K50   | 1414 | U    |
| 1   | K50   | 1416 | A    |
| 1   | K50   | 1427 | A    |
| 1   | K50   | 1429 | A    |
| 1   | K50   | 1430 | U    |
| 1   | K50   | 1431 | G    |
| 1   | K50   | 1432 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1440 | G    |
| 1   | K50   | 1447 | C    |
| 1   | K50   | 1449 | A    |
| 1   | K50   | 1450 | A    |
| 1   | K50   | 1453 | G    |
| 1   | K50   | 1454 | U    |
| 1   | K50   | 1455 | A    |
| 1   | K50   | 1457 | C    |
| 1   | K50   | 1458 | A    |
| 1   | K50   | 1466 | A    |
| 1   | K50   | 1467 | A    |
| 1   | K50   | 1468 | G    |
| 1   | K50   | 1474 | G    |
| 1   | K50   | 1475 | A    |
| 1   | K50   | 1479 | U    |
| 1   | K50   | 1485 | G    |
| 1   | K50   | 1486 | G    |
| 1   | K50   | 1488 | U    |
| 1   | K50   | 1489 | G    |
| 1   | K50   | 1490 | U    |
| 1   | K50   | 1491 | U    |
| 1   | K50   | 1492 | U    |
| 1   | K50   | 1499 | U    |
| 1   | K50   | 1513 | G    |
| 1   | K50   | 1524 | G    |
| 1   | K50   | 1527 | U    |
| 1   | K50   | 1533 | C    |
| 1   | K50   | 1534 | G    |
| 1   | K50   | 1535 | G    |
| 1   | K50   | 1536 | G    |
| 1   | K50   | 1538 | G    |
| 1   | K50   | 1547 | G    |
| 1   | K50   | 1554 | U    |
| 1   | K50   | 1555 | G    |
| 1   | K50   | 1556 | U    |
| 1   | K50   | 1557 | G    |
| 1   | K50   | 1563 | A    |
| 1   | K50   | 1564 | U    |
| 1   | K50   | 1565 | U    |
| 1   | K50   | 1566 | G    |
| 1   | K50   | 1568 | G    |
| 1   | K50   | 1569 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1571 | A    |
| 1   | K50   | 1573 | G    |
| 1   | K50   | 1574 | G    |
| 1   | K50   | 1575 | G    |
| 1   | K50   | 1583 | A    |
| 1   | K50   | 1591 | G    |
| 1   | K50   | 1592 | U    |
| 1   | K50   | 1602 | G    |
| 1   | K50   | 1610 | A    |
| 1   | K50   | 1611 | A    |
| 1   | K50   | 1612 | G    |
| 1   | K50   | 1613 | A    |
| 1   | K50   | 1614 | G    |
| 1   | K50   | 1617 | A    |
| 1   | K50   | 1619 | G    |
| 1   | K50   | 1624 | G    |
| 1   | K50   | 1626 | G    |
| 1   | K50   | 1638 | G    |
| 1   | K50   | 1643 | G    |
| 1   | K50   | 1644 | U    |
| 1   | K50   | 1645 | C    |
| 1   | K50   | 1646 | G    |
| 1   | K50   | 1649 | A    |
| 1   | K50   | 1651 | A    |
| 1   | K50   | 1653 | G    |
| 1   | K50   | 1665 | A    |
| 1   | K50   | 1668 | A    |
| 1   | K50   | 1674 | G    |
| 1   | K50   | 1675 | G    |
| 1   | K50   | 1680 | A    |
| 1   | K50   | 1682 | G    |
| 1   | K50   | 1685 | G    |
| 1   | K50   | 1686 | G    |
| 1   | K50   | 1689 | G    |
| 1   | K50   | 1692 | A    |
| 1   | K50   | 1693 | C    |
| 1   | K50   | 1697 | G    |
| 1   | K50   | 1698 | A    |
| 1   | K50   | 1699 | C    |
| 1   | K50   | 1705 | U    |
| 1   | K50   | 1708 | G    |
| 1   | K50   | 1709 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1710 | U    |
| 1   | K50   | 1711 | A    |
| 1   | K50   | 1717 | A    |
| 1   | K50   | 1718 | C    |
| 1   | K50   | 1720 | C    |
| 1   | K50   | 1724 | G    |
| 1   | K50   | 1733 | A    |
| 1   | K50   | 1735 | G    |
| 1   | K50   | 1739 | A    |
| 1   | K50   | 1742 | C    |
| 1   | K50   | 1743 | G    |
| 1   | K50   | 1746 | U    |
| 1   | K50   | 1749 | A    |
| 1   | K50   | 1751 | G    |
| 1   | K50   | 1755 | U    |
| 1   | K50   | 1760 | A    |
| 1   | K50   | 1770 | U    |
| 1   | K50   | 1772 | U    |
| 1   | K50   | 1797 | A    |
| 1   | K50   | 1799 | U    |
| 1   | K50   | 1800 | U    |
| 1   | K50   | 1801 | C    |
| 1   | K50   | 1808 | A    |
| 1   | K50   | 1809 | A    |
| 1   | K50   | 1810 | C    |
| 1   | K50   | 1811 | G    |
| 1   | K50   | 1820 | C    |
| 1   | K50   | 1821 | G    |
| 1   | K50   | 1822 | G    |
| 1   | K50   | 1828 | G    |
| 1   | K50   | 1832 | A    |
| 1   | K50   | 1833 | A    |
| 1   | K50   | 1835 | G    |
| 1   | K50   | 1836 | A    |
| 1   | K50   | 1837 | A    |
| 1   | K50   | 1838 | G    |
| 1   | K50   | 1839 | A    |
| 1   | K50   | 1846 | U    |
| 1   | K50   | 1854 | A    |
| 1   | K50   | 1858 | U    |
| 1   | K50   | 1860 | G    |
| 1   | K50   | 1868 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1869 | A    |
| 1   | K50   | 1870 | G    |
| 1   | K50   | 1872 | U    |
| 1   | K50   | 1873 | G    |
| 1   | K50   | 1874 | U    |
| 1   | K50   | 1881 | U    |
| 1   | K50   | 1883 | A    |
| 1   | K50   | 1885 | G    |
| 1   | K50   | 1887 | G    |
| 1   | K50   | 1888 | A    |
| 1   | K50   | 1931 | C    |
| 1   | K50   | 1934 | C    |
| 1   | K50   | 1935 | A    |
| 1   | K50   | 1937 | G    |
| 1   | K50   | 1938 | A    |
| 1   | K50   | 1939 | U    |
| 1   | K50   | 1940 | C    |
| 1   | K50   | 1941 | A    |
| 1   | K50   | 1942 | U    |
| 1   | K50   | 1943 | C    |
| 1   | K50   | 1946 | G    |
| 1   | K50   | 1949 | A    |
| 1   | K50   | 1950 | C    |
| 1   | K50   | 1955 | G    |
| 1   | K50   | 1956 | U    |
| 1   | K50   | 1957 | U    |
| 1   | K50   | 1958 | U    |
| 1   | K50   | 1959 | A    |
| 1   | K50   | 1960 | A    |
| 1   | K50   | 1961 | G    |
| 1   | K50   | 1963 | A    |
| 1   | K50   | 1966 | A    |
| 1   | K50   | 1967 | A    |
| 1   | K50   | 1968 | G    |
| 1   | K50   | 1973 | G    |
| 1   | K50   | 1977 | G    |
| 1   | K50   | 1978 | G    |
| 1   | K50   | 1985 | G    |
| 1   | K50   | 1991 | G    |
| 1   | K50   | 1995 | G    |
| 1   | K50   | 1997 | A    |
| 1   | K50   | 2007 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2008 | A    |
| 1   | K50   | 2011 | A    |
| 1   | K50   | 2013 | A    |
| 1   | K50   | 2015 | C    |
| 1   | K50   | 2016 | G    |
| 1   | K50   | 2019 | G    |
| 1   | K50   | 2020 | U    |
| 1   | K50   | 2022 | G    |
| 1   | K50   | 2023 | A    |
| 1   | K50   | 2027 | A    |
| 1   | K50   | 2030 | G    |
| 1   | K50   | 2031 | U    |
| 1   | K50   | 2032 | A    |
| 1   | K50   | 2036 | A    |
| 1   | K50   | 2037 | C    |
| 1   | K50   | 2039 | G    |
| 1   | K50   | 2042 | A    |
| 1   | K50   | 2043 | G    |
| 1   | K50   | 2045 | C    |
| 1   | K50   | 2046 | G    |
| 1   | K50   | 2047 | A    |
| 1   | K50   | 2048 | G    |
| 1   | K50   | 2049 | A    |
| 1   | K50   | 2052 | A    |
| 1   | K50   | 2057 | U    |
| 1   | K50   | 2059 | U    |
| 1   | K50   | 2060 | A    |
| 1   | K50   | 2061 | G    |
| 1   | K50   | 2062 | A    |
| 1   | K50   | 2063 | G    |
| 1   | K50   | 2065 | A    |
| 1   | K50   | 2067 | A    |
| 1   | K50   | 2073 | U    |
| 1   | K50   | 2075 | A    |
| 1   | K50   | 2076 | A    |
| 1   | K50   | 2077 | G    |
| 1   | K50   | 2078 | A    |
| 1   | K50   | 2085 | G    |
| 1   | K50   | 2087 | G    |
| 1   | K50   | 2093 | G    |
| 1   | K50   | 2096 | C    |
| 1   | K50   | 2097 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2098 | A    |
| 1   | K50   | 2099 | C    |
| 1   | K50   | 2108 | U    |
| 1   | K50   | 2109 | G    |
| 1   | K50   | 2110 | A    |
| 1   | K50   | 2111 | G    |
| 1   | K50   | 2114 | G    |
| 1   | K50   | 2122 | G    |
| 1   | K50   | 2124 | C    |
| 1   | K50   | 2130 | G    |
| 1   | K50   | 2131 | A    |
| 1   | K50   | 2136 | A    |
| 1   | K50   | 2140 | A    |
| 1   | K50   | 2141 | U    |
| 1   | K50   | 2142 | A    |
| 1   | K50   | 2145 | A    |
| 1   | K50   | 2146 | G    |
| 1   | K50   | 2149 | A    |
| 1   | K50   | 2150 | C    |
| 1   | K50   | 2152 | U    |
| 1   | K50   | 2160 | G    |
| 1   | K50   | 2162 | G    |
| 1   | K50   | 2164 | G    |
| 1   | K50   | 2167 | A    |
| 1   | K50   | 2168 | G    |
| 1   | K50   | 2169 | A    |
| 1   | K50   | 2170 | A    |
| 1   | K50   | 2171 | A    |
| 1   | K50   | 2177 | C    |
| 1   | K50   | 2178 | C    |
| 1   | K50   | 2185 | A    |
| 1   | K50   | 2189 | C    |
| 1   | K50   | 2211 | A    |
| 1   | K50   | 2212 | G    |
| 1   | K50   | 2213 | A    |
| 1   | K50   | 2217 | C    |
| 1   | K50   | 2221 | G    |
| 1   | K50   | 2224 | G    |
| 1   | K50   | 2228 | U    |
| 1   | K50   | 2229 | U    |
| 1   | K50   | 2234 | U    |
| 1   | K50   | 2235 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2239 | G    |
| 1   | K50   | 2240 | A    |
| 1   | K50   | 2241 | U    |
| 1   | K50   | 2243 | U    |
| 1   | K50   | 2253 | C    |
| 1   | K50   | 2254 | U    |
| 1   | K50   | 2255 | A    |
| 1   | K50   | 2256 | G    |
| 1   | K50   | 2257 | C    |
| 1   | K50   | 2260 | G    |
| 1   | K50   | 2262 | C    |
| 1   | K50   | 2266 | G    |
| 1   | K50   | 2272 | G    |
| 1   | K50   | 2275 | G    |
| 1   | K50   | 2279 | A    |
| 1   | K50   | 2286 | G    |
| 1   | K50   | 2291 | U    |
| 1   | K50   | 2293 | C    |
| 1   | K50   | 2296 | C    |
| 1   | K50   | 2303 | C    |
| 1   | K50   | 2304 | A    |
| 1   | K50   | 2306 | G    |
| 1   | K50   | 2309 | A    |
| 1   | K50   | 2310 | C    |
| 1   | K50   | 2313 | G    |
| 1   | K50   | 2319 | G    |
| 1   | K50   | 2322 | U    |
| 1   | K50   | 2323 | U    |
| 1   | K50   | 2325 | G    |
| 1   | K50   | 2337 | A    |
| 1   | K50   | 2339 | A    |
| 1   | K50   | 2340 | G    |
| 1   | K50   | 2345 | G    |
| 1   | K50   | 2347 | U    |
| 1   | K50   | 2351 | U    |
| 1   | K50   | 2355 | A    |
| 1   | K50   | 2358 | G    |
| 1   | K50   | 2364 | A    |
| 1   | K50   | 2376 | A    |
| 1   | K50   | 2377 | G    |
| 1   | K50   | 2379 | G    |
| 1   | K50   | 2394 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2399 | A    |
| 1   | K50   | 2401 | C    |
| 1   | K50   | 2410 | A    |
| 1   | K50   | 2412 | C    |
| 1   | K50   | 2413 | U    |
| 1   | K50   | 2416 | G    |
| 1   | K50   | 2419 | G    |
| 1   | K50   | 2420 | C    |
| 1   | K50   | 2423 | C    |
| 1   | K50   | 2424 | G    |
| 1   | K50   | 2432 | G    |
| 1   | K50   | 2434 | A    |
| 1   | K50   | 2436 | G    |
| 1   | K50   | 2437 | U    |
| 1   | K50   | 2441 | A    |
| 1   | K50   | 2447 | A    |
| 1   | K50   | 2451 | U    |
| 1   | K50   | 2452 | A    |
| 1   | K50   | 2453 | C    |
| 1   | K50   | 2459 | C    |
| 1   | K50   | 2460 | U    |
| 1   | K50   | 2473 | G    |
| 1   | K50   | 2475 | A    |
| 1   | K50   | 2476 | G    |
| 1   | K50   | 2477 | C    |
| 1   | K50   | 2482 | A    |
| 1   | K50   | 2487 | A    |
| 1   | K50   | 2490 | A    |
| 1   | K50   | 2491 | A    |
| 1   | K50   | 2501 | A    |
| 1   | K50   | 2503 | U    |
| 1   | K50   | 2508 | A    |
| 1   | K50   | 2509 | A    |
| 1   | K50   | 2518 | G    |
| 1   | K50   | 2519 | G    |
| 1   | K50   | 2520 | A    |
| 1   | K50   | 2529 | C    |
| 1   | K50   | 2532 | A    |
| 1   | K50   | 2533 | G    |
| 1   | K50   | 2534 | U    |
| 1   | K50   | 2535 | U    |
| 1   | K50   | 2538 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 2539 | A    |
| 1   | K50   | 2548 | G    |
| 1   | K50   | 2555 | A    |
| 1   | K50   | 2558 | A    |
| 1   | K50   | 2559 | G    |
| 1   | K50   | 2562 | U    |
| 1   | K50   | 2563 | U    |
| 1   | K50   | 2565 | U    |
| 1   | K50   | 2568 | U    |
| 1   | K50   | 2578 | G    |
| 1   | K50   | 2588 | G    |
| 1   | K50   | 2593 | A    |
| 1   | K50   | 2595 | U    |
| 1   | K50   | 2596 | G    |
| 1   | K50   | 2597 | G    |
| 1   | K50   | 2598 | U    |
| 1   | K50   | 2600 | G    |
| 1   | K50   | 2605 | C    |
| 1   | K50   | 2606 | A    |
| 1   | K50   | 2612 | G    |
| 2   | K70   | 2    | G    |
| 2   | K70   | 10   | C    |
| 2   | K70   | 14   | U    |
| 2   | K70   | 15   | C    |
| 2   | K70   | 18   | C    |
| 2   | K70   | 22   | A    |
| 2   | K70   | 25   | A    |
| 2   | K70   | 27   | A    |
| 2   | K70   | 32   | A    |
| 2   | K70   | 33   | U    |
| 2   | K70   | 35   | C    |
| 2   | K70   | 41   | G    |
| 2   | K70   | 42   | A    |
| 2   | K70   | 49   | A    |
| 2   | K70   | 50   | A    |
| 2   | K70   | 51   | G    |
| 2   | K70   | 53   | U    |
| 2   | K70   | 63   | A    |
| 2   | K70   | 64   | G    |
| 2   | K70   | 65   | A    |
| 2   | K70   | 67   | C    |
| 2   | K70   | 69   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | K70   | 88  | C    |
| 2   | K70   | 89  | G    |
| 2   | K70   | 91  | C    |
| 2   | K70   | 93  | A    |
| 2   | K70   | 100 | A    |
| 2   | K70   | 101 | A    |
| 2   | K70   | 104 | C    |
| 2   | K70   | 105 | G    |
| 2   | K70   | 107 | G    |
| 2   | K70   | 108 | G    |
| 2   | K70   | 109 | U    |
| 2   | K70   | 110 | G    |
| 2   | K70   | 115 | A    |
| 2   | K70   | 119 | U    |
| 42  | R60   | 7   | U    |
| 42  | R60   | 8   | U    |
| 42  | R60   | 14  | U    |
| 42  | R60   | 17  | C    |
| 42  | R60   | 26  | A    |
| 42  | R60   | 32  | G    |
| 42  | R60   | 37  | A    |
| 42  | R60   | 39  | A    |
| 42  | R60   | 40  | G    |
| 42  | R60   | 41  | A    |
| 42  | R60   | 43  | U    |
| 42  | R60   | 44  | U    |
| 42  | R60   | 45  | A    |
| 42  | R60   | 48  | C    |
| 42  | R60   | 52  | C    |
| 42  | R60   | 54  | U    |
| 42  | R60   | 55  | G    |
| 42  | R60   | 56  | U    |
| 42  | R60   | 66  | G    |
| 42  | R60   | 70  | U    |
| 42  | R60   | 71  | U    |
| 42  | R60   | 72  | A    |
| 42  | R60   | 73  | G    |
| 42  | R60   | 75  | G    |
| 42  | R60   | 76  | A    |
| 42  | R60   | 77  | A    |
| 42  | R60   | 83  | G    |
| 42  | R60   | 86  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | R60   | 88  | G    |
| 42  | R60   | 92  | A    |
| 42  | R60   | 94  | U    |
| 42  | R60   | 97  | C    |
| 42  | R60   | 98  | G    |
| 42  | R60   | 99  | G    |
| 42  | R60   | 102 | G    |
| 42  | R60   | 104 | G    |
| 42  | R60   | 106 | A    |
| 42  | R60   | 107 | U    |
| 42  | R60   | 110 | A    |
| 42  | R60   | 112 | U    |
| 42  | R60   | 116 | U    |
| 42  | R60   | 118 | G    |
| 42  | R60   | 119 | A    |
| 42  | R60   | 120 | A    |
| 42  | R60   | 121 | C    |
| 42  | R60   | 124 | G    |
| 42  | R60   | 127 | A    |
| 42  | R60   | 128 | A    |
| 42  | R60   | 132 | C    |
| 42  | R60   | 133 | A    |
| 42  | R60   | 134 | G    |
| 42  | R60   | 138 | A    |
| 42  | R60   | 140 | A    |
| 42  | R60   | 141 | G    |
| 42  | R60   | 142 | A    |
| 42  | R60   | 147 | A    |
| 42  | R60   | 148 | A    |
| 42  | R60   | 150 | A    |
| 42  | R60   | 153 | G    |
| 42  | R60   | 155 | G    |
| 42  | R60   | 157 | A    |
| 42  | R60   | 161 | G    |
| 42  | R60   | 167 | G    |
| 42  | R60   | 172 | U    |
| 42  | R60   | 173 | A    |
| 42  | R60   | 174 | G    |
| 42  | R60   | 180 | G    |
| 42  | R60   | 181 | A    |
| 42  | R60   | 184 | A    |
| 42  | R60   | 186 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | R60   | 187 | A    |
| 42  | R60   | 189 | A    |
| 42  | R60   | 190 | A    |
| 42  | R60   | 191 | C    |
| 42  | R60   | 192 | A    |
| 42  | R60   | 193 | G    |
| 42  | R60   | 197 | A    |
| 42  | R60   | 198 | G    |
| 42  | R60   | 199 | G    |
| 42  | R60   | 204 | U    |
| 42  | R60   | 206 | A    |
| 42  | R60   | 219 | U    |
| 42  | R60   | 220 | C    |
| 42  | R60   | 222 | G    |
| 42  | R60   | 226 | G    |
| 42  | R60   | 227 | U    |
| 42  | R60   | 228 | A    |
| 42  | R60   | 238 | A    |
| 42  | R60   | 241 | G    |
| 42  | R60   | 242 | C    |
| 42  | R60   | 247 | U    |
| 42  | R60   | 254 | U    |
| 42  | R60   | 255 | A    |
| 42  | R60   | 256 | G    |
| 42  | R60   | 259 | G    |
| 42  | R60   | 262 | U    |
| 42  | R60   | 263 | A    |
| 42  | R60   | 264 | C    |
| 42  | R60   | 268 | G    |
| 42  | R60   | 271 | U    |
| 42  | R60   | 273 | A    |
| 42  | R60   | 283 | U    |
| 42  | R60   | 284 | C    |
| 42  | R60   | 290 | A    |
| 42  | R60   | 292 | G    |
| 42  | R60   | 299 | G    |
| 42  | R60   | 300 | A    |
| 42  | R60   | 303 | G    |
| 42  | R60   | 304 | A    |
| 42  | R60   | 305 | C    |
| 42  | R60   | 307 | G    |
| 42  | R60   | 311 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | R60   | 314 | G    |
| 42  | R60   | 315 | G    |
| 42  | R60   | 318 | C    |
| 42  | R60   | 319 | A    |
| 42  | R60   | 320 | A    |
| 42  | R60   | 326 | G    |
| 42  | R60   | 327 | C    |
| 42  | R60   | 328 | A    |
| 42  | R60   | 329 | G    |
| 42  | R60   | 335 | G    |
| 42  | R60   | 338 | A    |
| 42  | R60   | 339 | A    |
| 42  | R60   | 340 | A    |
| 42  | R60   | 341 | A    |
| 42  | R60   | 342 | U    |
| 42  | R60   | 344 | A    |
| 42  | R60   | 345 | C    |
| 42  | R60   | 347 | G    |
| 42  | R60   | 348 | A    |
| 42  | R60   | 355 | C    |
| 42  | R60   | 356 | A    |
| 42  | R60   | 357 | A    |
| 42  | R60   | 358 | G    |
| 42  | R60   | 362 | G    |
| 42  | R60   | 363 | C    |
| 42  | R60   | 364 | G    |
| 42  | R60   | 367 | A    |
| 42  | R60   | 368 | G    |
| 42  | R60   | 371 | A    |
| 42  | R60   | 372 | A    |
| 42  | R60   | 373 | G    |
| 42  | R60   | 374 | A    |
| 42  | R60   | 375 | G    |
| 42  | R60   | 377 | C    |
| 42  | R60   | 378 | G    |
| 42  | R60   | 380 | G    |
| 42  | R60   | 382 | A    |
| 42  | R60   | 383 | A    |
| 42  | R60   | 384 | A    |
| 42  | R60   | 385 | C    |
| 42  | R60   | 388 | G    |
| 42  | R60   | 395 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | R60   | 396 | A    |
| 42  | R60   | 398 | A    |
| 42  | R60   | 399 | A    |
| 42  | R60   | 402 | C    |
| 42  | R60   | 407 | G    |
| 42  | R60   | 408 | A    |
| 42  | R60   | 409 | G    |
| 42  | R60   | 412 | A    |
| 42  | R60   | 414 | U    |
| 42  | R60   | 416 | G    |
| 42  | R60   | 422 | A    |
| 42  | R60   | 424 | G    |
| 42  | R60   | 425 | G    |
| 42  | R60   | 426 | C    |
| 42  | R60   | 431 | G    |
| 42  | R60   | 432 | C    |
| 42  | R60   | 437 | A    |
| 42  | R60   | 441 | G    |
| 42  | R60   | 444 | G    |
| 42  | R60   | 445 | U    |
| 42  | R60   | 446 | A    |
| 42  | R60   | 449 | A    |
| 42  | R60   | 450 | C    |
| 42  | R60   | 452 | A    |
| 42  | R60   | 453 | G    |
| 42  | R60   | 454 | C    |
| 42  | R60   | 461 | A    |
| 42  | R60   | 471 | A    |
| 42  | R60   | 473 | G    |
| 42  | R60   | 474 | A    |
| 42  | R60   | 476 | U    |
| 42  | R60   | 477 | G    |
| 42  | R60   | 478 | C    |
| 42  | R60   | 481 | C    |
| 42  | R60   | 482 | G    |
| 42  | R60   | 486 | A    |
| 42  | R60   | 487 | A    |
| 42  | R60   | 490 | G    |
| 42  | R60   | 491 | G    |
| 42  | R60   | 501 | G    |
| 42  | R60   | 506 | A    |
| 42  | R60   | 509 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | R60   | 510 | U    |
| 42  | R60   | 511 | A    |
| 42  | R60   | 512 | C    |
| 42  | R60   | 521 | A    |
| 42  | R60   | 527 | G    |
| 42  | R60   | 530 | U    |
| 42  | R60   | 535 | A    |
| 42  | R60   | 536 | G    |
| 42  | R60   | 540 | C    |
| 42  | R60   | 541 | G    |
| 42  | R60   | 543 | A    |
| 42  | R60   | 544 | U    |
| 42  | R60   | 547 | A    |
| 42  | R60   | 550 | G    |
| 42  | R60   | 553 | A    |
| 42  | R60   | 554 | A    |
| 42  | R60   | 565 | U    |
| 42  | R60   | 566 | A    |
| 42  | R60   | 567 | A    |
| 42  | R60   | 568 | G    |
| 42  | R60   | 575 | A    |
| 42  | R60   | 578 | A    |
| 42  | R60   | 579 | G    |
| 42  | R60   | 590 | U    |
| 42  | R60   | 593 | A    |
| 42  | R60   | 598 | C    |
| 42  | R60   | 599 | G    |
| 42  | R60   | 600 | A    |
| 42  | R60   | 601 | G    |
| 42  | R60   | 602 | A    |
| 42  | R60   | 608 | A    |
| 42  | R60   | 609 | A    |
| 42  | R60   | 610 | U    |
| 42  | R60   | 616 | G    |
| 42  | R60   | 621 | G    |
| 42  | R60   | 622 | C    |
| 42  | R60   | 623 | U    |
| 42  | R60   | 624 | U    |
| 42  | R60   | 625 | A    |
| 42  | R60   | 630 | U    |
| 42  | R60   | 633 | C    |
| 42  | R60   | 635 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | R60   | 637 | G    |
| 42  | R60   | 644 | G    |
| 42  | R60   | 647 | C    |
| 42  | R60   | 661 | A    |
| 42  | R60   | 662 | U    |
| 42  | R60   | 665 | G    |
| 42  | R60   | 668 | G    |
| 42  | R60   | 671 | C    |
| 42  | R60   | 673 | A    |
| 42  | R60   | 686 | G    |
| 42  | R60   | 687 | A    |
| 42  | R60   | 688 | G    |
| 42  | R60   | 690 | A    |
| 42  | R60   | 694 | A    |
| 42  | R60   | 700 | A    |
| 42  | R60   | 702 | U    |
| 42  | R60   | 705 | A    |
| 42  | R60   | 706 | G    |
| 42  | R60   | 707 | A    |
| 42  | R60   | 722 | G    |
| 42  | R60   | 724 | A    |
| 42  | R60   | 725 | G    |
| 42  | R60   | 727 | A    |
| 42  | R60   | 728 | A    |
| 42  | R60   | 730 | C    |
| 42  | R60   | 731 | G    |
| 42  | R60   | 733 | U    |
| 42  | R60   | 734 | G    |
| 42  | R60   | 738 | A    |
| 42  | R60   | 740 | G    |
| 42  | R60   | 749 | G    |
| 42  | R60   | 752 | A    |
| 42  | R60   | 753 | U    |
| 42  | R60   | 754 | G    |
| 42  | R60   | 755 | A    |
| 42  | R60   | 757 | C    |
| 42  | R60   | 771 | A    |
| 42  | R60   | 775 | U    |
| 42  | R60   | 776 | A    |
| 42  | R60   | 777 | G    |
| 42  | R60   | 780 | G    |
| 42  | R60   | 788 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | R60   | 789 | G    |
| 42  | R60   | 790 | G    |
| 42  | R60   | 791 | A    |
| 42  | R60   | 795 | U    |
| 42  | R60   | 806 | G    |
| 42  | R60   | 810 | U    |
| 42  | R60   | 817 | A    |
| 42  | R60   | 818 | A    |
| 42  | R60   | 820 | G    |
| 42  | R60   | 821 | G    |
| 42  | R60   | 823 | A    |
| 42  | R60   | 825 | U    |
| 42  | R60   | 831 | G    |
| 42  | R60   | 836 | A    |
| 42  | R60   | 839 | C    |
| 42  | R60   | 840 | C    |
| 42  | R60   | 841 | A    |
| 42  | R60   | 846 | G    |
| 42  | R60   | 848 | G    |
| 42  | R60   | 866 | U    |
| 42  | R60   | 868 | U    |
| 42  | R60   | 871 | C    |
| 42  | R60   | 872 | U    |
| 42  | R60   | 874 | A    |
| 42  | R60   | 875 | A    |
| 42  | R60   | 877 | G    |
| 42  | R60   | 878 | C    |
| 42  | R60   | 880 | G    |
| 42  | R60   | 881 | G    |
| 42  | R60   | 883 | C    |
| 42  | R60   | 884 | A    |
| 42  | R60   | 890 | C    |
| 42  | R60   | 898 | G    |
| 42  | R60   | 899 | A    |
| 42  | R60   | 905 | G    |
| 42  | R60   | 908 | U    |
| 42  | R60   | 909 | G    |
| 42  | R60   | 911 | G    |
| 42  | R60   | 915 | A    |
| 42  | R60   | 916 | G    |
| 42  | R60   | 917 | U    |
| 42  | R60   | 918 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | R60   | 919  | C    |
| 42  | R60   | 924  | U    |
| 42  | R60   | 925  | A    |
| 42  | R60   | 926  | G    |
| 42  | R60   | 927  | G    |
| 42  | R60   | 928  | U    |
| 42  | R60   | 929  | C    |
| 42  | R60   | 930  | A    |
| 42  | R60   | 932  | A    |
| 42  | R60   | 933  | G    |
| 42  | R60   | 934  | A    |
| 42  | R60   | 935  | G    |
| 42  | R60   | 936  | U    |
| 42  | R60   | 940  | G    |
| 42  | R60   | 941  | C    |
| 42  | R60   | 942  | A    |
| 42  | R60   | 952  | A    |
| 42  | R60   | 953  | C    |
| 42  | R60   | 955  | A    |
| 42  | R60   | 957  | G    |
| 42  | R60   | 958  | A    |
| 42  | R60   | 959  | G    |
| 42  | R60   | 962  | G    |
| 42  | R60   | 966  | G    |
| 42  | R60   | 967  | A    |
| 42  | R60   | 968  | C    |
| 42  | R60   | 970  | U    |
| 42  | R60   | 971  | U    |
| 42  | R60   | 972  | U    |
| 42  | R60   | 974  | G    |
| 42  | R60   | 976  | U    |
| 42  | R60   | 978  | A    |
| 42  | R60   | 980  | G    |
| 42  | R60   | 981  | U    |
| 42  | R60   | 987  | A    |
| 42  | R60   | 991  | A    |
| 42  | R60   | 995  | A    |
| 42  | R60   | 998  | U    |
| 42  | R60   | 999  | C    |
| 42  | R60   | 1003 | A    |
| 42  | R60   | 1006 | A    |
| 42  | R60   | 1007 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | R60   | 1008 | A    |
| 42  | R60   | 1011 | A    |
| 42  | R60   | 1012 | A    |
| 42  | R60   | 1013 | A    |
| 42  | R60   | 1014 | G    |
| 42  | R60   | 1017 | A    |
| 42  | R60   | 1018 | U    |
| 42  | R60   | 1019 | C    |
| 42  | R60   | 1021 | A    |
| 42  | R60   | 1023 | A    |
| 42  | R60   | 1024 | G    |
| 42  | R60   | 1028 | U    |
| 42  | R60   | 1029 | U    |
| 42  | R60   | 1033 | A    |
| 42  | R60   | 1039 | G    |
| 42  | R60   | 1041 | A    |
| 42  | R60   | 1042 | A    |
| 42  | R60   | 1045 | A    |
| 42  | R60   | 1046 | A    |
| 42  | R60   | 1047 | G    |
| 42  | R60   | 1052 | A    |
| 42  | R60   | 1053 | A    |
| 42  | R60   | 1054 | G    |
| 42  | R60   | 1056 | A    |
| 42  | R60   | 1057 | C    |
| 42  | R60   | 1058 | A    |
| 42  | R60   | 1059 | G    |
| 42  | R60   | 1060 | G    |
| 42  | R60   | 1062 | C    |
| 42  | R60   | 1063 | A    |
| 42  | R60   | 1064 | G    |
| 42  | R60   | 1066 | G    |
| 42  | R60   | 1075 | A    |
| 42  | R60   | 1076 | G    |
| 42  | R60   | 1077 | A    |
| 42  | R60   | 1078 | U    |
| 42  | R60   | 1088 | U    |
| 42  | R60   | 1089 | G    |
| 42  | R60   | 1090 | C    |
| 42  | R60   | 1092 | C    |
| 42  | R60   | 1094 | C    |
| 42  | R60   | 1099 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | R60   | 1100 | A    |
| 42  | R60   | 1102 | A    |
| 42  | R60   | 1103 | G    |
| 42  | R60   | 1104 | U    |
| 42  | R60   | 1105 | G    |
| 42  | R60   | 1106 | G    |
| 42  | R60   | 1111 | A    |
| 42  | R60   | 1112 | G    |
| 42  | R60   | 1116 | A    |
| 42  | R60   | 1117 | A    |
| 42  | R60   | 1118 | A    |
| 42  | R60   | 1119 | C    |
| 42  | R60   | 1120 | A    |
| 42  | R60   | 1121 | A    |
| 42  | R60   | 1122 | A    |
| 42  | R60   | 1123 | U    |
| 42  | R60   | 1124 | A    |
| 42  | R60   | 1125 | G    |
| 42  | R60   | 1126 | A    |
| 42  | R60   | 1127 | A    |
| 42  | R60   | 1128 | G    |
| 42  | R60   | 1129 | U    |
| 42  | R60   | 1130 | A    |
| 42  | R60   | 1135 | U    |
| 42  | R60   | 1136 | G    |
| 42  | R60   | 1137 | A    |
| 42  | R60   | 1139 | C    |
| 42  | R60   | 1141 | A    |
| 42  | R60   | 1142 | G    |
| 42  | R60   | 1146 | G    |
| 42  | R60   | 1152 | G    |
| 42  | R60   | 1154 | A    |
| 42  | R60   | 1158 | U    |
| 42  | R60   | 1159 | A    |
| 42  | R60   | 1160 | A    |
| 42  | R60   | 1161 | U    |
| 42  | R60   | 1162 | G    |
| 42  | R60   | 1170 | G    |
| 42  | R60   | 1171 | A    |
| 42  | R60   | 1175 | A    |
| 42  | R60   | 1176 | G    |
| 42  | R60   | 1177 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | R60   | 1179 | A    |
| 42  | R60   | 1182 | G    |
| 42  | R60   | 1185 | A    |
| 42  | R60   | 1191 | C    |
| 42  | R60   | 1192 | G    |
| 42  | R60   | 1194 | U    |
| 42  | R60   | 1195 | A    |
| 42  | R60   | 1196 | U    |
| 42  | R60   | 1202 | U    |
| 42  | R60   | 1203 | A    |
| 42  | R60   | 1204 | A    |
| 42  | R60   | 1205 | G    |
| 42  | R60   | 1210 | G    |
| 42  | R60   | 1211 | A    |
| 42  | R60   | 1214 | A    |
| 42  | R60   | 1216 | U    |
| 42  | R60   | 1217 | G    |
| 42  | R60   | 1219 | G    |
| 42  | R60   | 1223 | C    |
| 42  | R60   | 1225 | G    |
| 42  | R60   | 1227 | U    |
| 42  | R60   | 1230 | U    |
| 42  | R60   | 1237 | C    |
| 42  | R60   | 1238 | A    |
| 42  | R60   | 1239 | C    |
| 42  | R60   | 1240 | C    |
| 42  | R60   | 1241 | G    |
| 42  | R60   | 1243 | C    |
| 42  | R60   | 1246 | U    |
| 42  | R60   | 1249 | U    |
| 42  | R60   | 1250 | U    |
| 42  | R60   | 1251 | A    |
| 42  | R60   | 1260 | G    |
| 42  | R60   | 1262 | A    |
| 42  | R60   | 1263 | A    |
| 42  | R60   | 1264 | C    |
| 42  | R60   | 1266 | A    |
| 42  | R60   | 1267 | G    |
| 42  | R60   | 1270 | G    |
| 42  | R60   | 1274 | A    |
| 42  | R60   | 1275 | C    |
| 42  | R60   | 1276 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | R60   | 1280 | G    |
| 42  | R60   | 1282 | A    |
| 42  | R60   | 1283 | A    |
| 42  | R60   | 1284 | G    |
| 42  | R60   | 1287 | A    |
| 42  | R60   | 1294 | G    |
| 42  | R60   | 1295 | C    |
| 42  | R60   | 1296 | A    |
| 42  | R60   | 1297 | G    |
| 42  | R60   | 1301 | U    |
| 42  | R60   | 1302 | C    |
| 42  | R60   | 1307 | U    |
| 42  | R60   | 1310 | G    |
| 42  | R60   | 1314 | C    |
| 42  | R60   | 1315 | A    |
| 42  | R60   | 1316 | A    |
| 42  | R60   | 1317 | G    |
| 42  | R60   | 1320 | G    |
| 42  | R60   | 1322 | A    |
| 42  | R60   | 1326 | A    |
| 42  | R60   | 1327 | G    |
| 42  | R60   | 1328 | G    |
| 42  | R60   | 1329 | C    |
| 42  | R60   | 1331 | G    |
| 42  | R60   | 1340 | G    |
| 42  | R60   | 1341 | A    |
| 42  | R60   | 1342 | A    |
| 42  | R60   | 1343 | C    |
| 42  | R60   | 1348 | A    |
| 42  | R60   | 1352 | G    |
| 42  | R60   | 1353 | G    |
| 42  | R60   | 1354 | A    |
| 42  | R60   | 1355 | U    |
| 42  | R60   | 1356 | C    |
| 42  | R60   | 1357 | A    |

All (353) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | L50   | 2   | U    |
| 1   | L50   | 3   | A    |
| 1   | L50   | 21  | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 22   | U    |
| 1   | L50   | 73   | A    |
| 1   | L50   | 75   | C    |
| 1   | L50   | 135  | A    |
| 1   | L50   | 211  | U    |
| 1   | L50   | 214  | A    |
| 1   | L50   | 225  | G    |
| 1   | L50   | 236  | A    |
| 1   | L50   | 265  | A    |
| 1   | L50   | 276  | U    |
| 1   | L50   | 308  | A    |
| 1   | L50   | 330  | G    |
| 1   | L50   | 351  | G    |
| 1   | L50   | 363  | U    |
| 1   | L50   | 396  | G    |
| 1   | L50   | 424  | G    |
| 1   | L50   | 463  | A    |
| 1   | L50   | 466  | C    |
| 1   | L50   | 523  | A    |
| 1   | L50   | 535  | A    |
| 1   | L50   | 550  | G    |
| 1   | L50   | 563  | U    |
| 1   | L50   | 567  | A    |
| 1   | L50   | 600  | G    |
| 1   | L50   | 657  | A    |
| 1   | L50   | 659  | G    |
| 1   | L50   | 667  | G    |
| 1   | L50   | 710  | A    |
| 1   | L50   | 712  | C    |
| 1   | L50   | 732  | G    |
| 1   | L50   | 741  | G    |
| 1   | L50   | 778  | A    |
| 1   | L50   | 782  | G    |
| 1   | L50   | 853  | A    |
| 1   | L50   | 996  | A    |
| 1   | L50   | 1000 | G    |
| 1   | L50   | 1008 | U    |
| 1   | L50   | 1017 | A    |
| 1   | L50   | 1018 | U    |
| 1   | L50   | 1032 | A    |
| 1   | L50   | 1061 | G    |
| 1   | L50   | 1089 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 1134 | A    |
| 1   | L50   | 1148 | A    |
| 1   | L50   | 1172 | A    |
| 1   | L50   | 1182 | A    |
| 1   | L50   | 1256 | U    |
| 1   | L50   | 1277 | G    |
| 1   | L50   | 1384 | U    |
| 1   | L50   | 1394 | U    |
| 1   | L50   | 1395 | U    |
| 1   | L50   | 1449 | A    |
| 1   | L50   | 1454 | U    |
| 1   | L50   | 1474 | G    |
| 1   | L50   | 1485 | G    |
| 1   | L50   | 1491 | U    |
| 1   | L50   | 1564 | U    |
| 1   | L50   | 1596 | A    |
| 1   | L50   | 1611 | A    |
| 1   | L50   | 1644 | U    |
| 1   | L50   | 1697 | G    |
| 1   | L50   | 1709 | G    |
| 1   | L50   | 1717 | A    |
| 1   | L50   | 1743 | G    |
| 1   | L50   | 1749 | A    |
| 1   | L50   | 1798 | U    |
| 1   | L50   | 1800 | U    |
| 1   | L50   | 1808 | A    |
| 1   | L50   | 1809 | A    |
| 1   | L50   | 1835 | G    |
| 1   | L50   | 1838 | G    |
| 1   | L50   | 1931 | C    |
| 1   | L50   | 1942 | U    |
| 1   | L50   | 1945 | C    |
| 1   | L50   | 1959 | A    |
| 1   | L50   | 1966 | A    |
| 1   | L50   | 1967 | A    |
| 1   | L50   | 2015 | C    |
| 1   | L50   | 2036 | A    |
| 1   | L50   | 2051 | C    |
| 1   | L50   | 2060 | A    |
| 1   | L50   | 2075 | A    |
| 1   | L50   | 2212 | G    |
| 1   | L50   | 2240 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | L50   | 2254 | U    |
| 1   | L50   | 2255 | A    |
| 1   | L50   | 2347 | U    |
| 1   | L50   | 2351 | U    |
| 1   | L50   | 2363 | A    |
| 1   | L50   | 2419 | G    |
| 1   | L50   | 2420 | C    |
| 1   | L50   | 2447 | A    |
| 1   | L50   | 2452 | A    |
| 1   | L50   | 2476 | G    |
| 1   | L50   | 2481 | U    |
| 1   | L50   | 2519 | G    |
| 1   | L50   | 2532 | A    |
| 1   | L50   | 2596 | G    |
| 1   | L50   | 2597 | G    |
| 2   | L70   | 32   | A    |
| 2   | L70   | 41   | G    |
| 2   | L70   | 62   | A    |
| 2   | L70   | 109  | U    |
| 42  | S60   | 71   | U    |
| 42  | S60   | 76   | A    |
| 42  | S60   | 118  | G    |
| 42  | S60   | 127  | A    |
| 42  | S60   | 180  | G    |
| 42  | S60   | 186  | A    |
| 42  | S60   | 190  | A    |
| 42  | S60   | 191  | C    |
| 42  | S60   | 218  | A    |
| 42  | S60   | 225  | A    |
| 42  | S60   | 226  | G    |
| 42  | S60   | 256  | G    |
| 42  | S60   | 262  | U    |
| 42  | S60   | 283  | U    |
| 42  | S60   | 303  | G    |
| 42  | S60   | 328  | A    |
| 42  | S60   | 339  | A    |
| 42  | S60   | 355  | C    |
| 42  | S60   | 372  | A    |
| 42  | S60   | 383  | A    |
| 42  | S60   | 407  | G    |
| 42  | S60   | 408  | A    |
| 42  | S60   | 424  | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | S60   | 425  | G    |
| 42  | S60   | 445  | U    |
| 42  | S60   | 473  | G    |
| 42  | S60   | 509  | G    |
| 42  | S60   | 511  | A    |
| 42  | S60   | 553  | A    |
| 42  | S60   | 565  | U    |
| 42  | S60   | 598  | C    |
| 42  | S60   | 661  | A    |
| 42  | S60   | 724  | A    |
| 42  | S60   | 753  | U    |
| 42  | S60   | 776  | A    |
| 42  | S60   | 788  | G    |
| 42  | S60   | 819  | A    |
| 42  | S60   | 877  | G    |
| 42  | S60   | 914  | U    |
| 42  | S60   | 916  | G    |
| 42  | S60   | 917  | U    |
| 42  | S60   | 918  | A    |
| 42  | S60   | 923  | A    |
| 42  | S60   | 925  | A    |
| 42  | S60   | 927  | G    |
| 42  | S60   | 934  | A    |
| 42  | S60   | 954  | G    |
| 42  | S60   | 970  | U    |
| 42  | S60   | 980  | G    |
| 42  | S60   | 1007 | U    |
| 42  | S60   | 1018 | U    |
| 42  | S60   | 1021 | A    |
| 42  | S60   | 1023 | A    |
| 42  | S60   | 1045 | A    |
| 42  | S60   | 1057 | C    |
| 42  | S60   | 1077 | A    |
| 42  | S60   | 1088 | U    |
| 42  | S60   | 1089 | G    |
| 42  | S60   | 1103 | G    |
| 42  | S60   | 1105 | G    |
| 42  | S60   | 1125 | G    |
| 42  | S60   | 1135 | U    |
| 42  | S60   | 1141 | A    |
| 42  | S60   | 1175 | A    |
| 42  | S60   | 1176 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | S60   | 1262 | A    |
| 42  | S60   | 1314 | C    |
| 42  | S60   | 1321 | U    |
| 42  | S60   | 1328 | G    |
| 42  | S60   | 1356 | C    |
| 1   | K50   | 2    | U    |
| 1   | K50   | 3    | A    |
| 1   | K50   | 21   | U    |
| 1   | K50   | 22   | U    |
| 1   | K50   | 73   | A    |
| 1   | K50   | 75   | C    |
| 1   | K50   | 135  | A    |
| 1   | K50   | 211  | U    |
| 1   | K50   | 214  | A    |
| 1   | K50   | 225  | G    |
| 1   | K50   | 236  | A    |
| 1   | K50   | 265  | A    |
| 1   | K50   | 276  | U    |
| 1   | K50   | 308  | A    |
| 1   | K50   | 330  | G    |
| 1   | K50   | 351  | G    |
| 1   | K50   | 363  | U    |
| 1   | K50   | 396  | G    |
| 1   | K50   | 424  | G    |
| 1   | K50   | 463  | A    |
| 1   | K50   | 466  | C    |
| 1   | K50   | 523  | A    |
| 1   | K50   | 535  | A    |
| 1   | K50   | 550  | G    |
| 1   | K50   | 563  | U    |
| 1   | K50   | 567  | A    |
| 1   | K50   | 600  | G    |
| 1   | K50   | 657  | A    |
| 1   | K50   | 659  | G    |
| 1   | K50   | 667  | G    |
| 1   | K50   | 710  | A    |
| 1   | K50   | 712  | C    |
| 1   | K50   | 732  | G    |
| 1   | K50   | 741  | G    |
| 1   | K50   | 778  | A    |
| 1   | K50   | 782  | G    |
| 1   | K50   | 853  | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 996  | A    |
| 1   | K50   | 1000 | G    |
| 1   | K50   | 1008 | U    |
| 1   | K50   | 1017 | A    |
| 1   | K50   | 1018 | U    |
| 1   | K50   | 1032 | A    |
| 1   | K50   | 1061 | G    |
| 1   | K50   | 1089 | U    |
| 1   | K50   | 1134 | A    |
| 1   | K50   | 1148 | A    |
| 1   | K50   | 1172 | A    |
| 1   | K50   | 1182 | A    |
| 1   | K50   | 1256 | U    |
| 1   | K50   | 1277 | G    |
| 1   | K50   | 1384 | U    |
| 1   | K50   | 1394 | U    |
| 1   | K50   | 1395 | U    |
| 1   | K50   | 1449 | A    |
| 1   | K50   | 1454 | U    |
| 1   | K50   | 1474 | G    |
| 1   | K50   | 1485 | G    |
| 1   | K50   | 1491 | U    |
| 1   | K50   | 1564 | U    |
| 1   | K50   | 1596 | A    |
| 1   | K50   | 1611 | A    |
| 1   | K50   | 1614 | G    |
| 1   | K50   | 1644 | U    |
| 1   | K50   | 1697 | G    |
| 1   | K50   | 1709 | G    |
| 1   | K50   | 1717 | A    |
| 1   | K50   | 1743 | G    |
| 1   | K50   | 1749 | A    |
| 1   | K50   | 1798 | U    |
| 1   | K50   | 1800 | U    |
| 1   | K50   | 1808 | A    |
| 1   | K50   | 1809 | A    |
| 1   | K50   | 1835 | G    |
| 1   | K50   | 1838 | G    |
| 1   | K50   | 1931 | C    |
| 1   | K50   | 1942 | U    |
| 1   | K50   | 1945 | C    |
| 1   | K50   | 1959 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | K50   | 1966 | A    |
| 1   | K50   | 1967 | A    |
| 1   | K50   | 2015 | C    |
| 1   | K50   | 2036 | A    |
| 1   | K50   | 2051 | C    |
| 1   | K50   | 2060 | A    |
| 1   | K50   | 2075 | A    |
| 1   | K50   | 2212 | G    |
| 1   | K50   | 2240 | A    |
| 1   | K50   | 2254 | U    |
| 1   | K50   | 2255 | A    |
| 1   | K50   | 2347 | U    |
| 1   | K50   | 2351 | U    |
| 1   | K50   | 2363 | A    |
| 1   | K50   | 2419 | G    |
| 1   | K50   | 2420 | C    |
| 1   | K50   | 2447 | A    |
| 1   | K50   | 2452 | A    |
| 1   | K50   | 2476 | G    |
| 1   | K50   | 2481 | U    |
| 1   | K50   | 2519 | G    |
| 1   | K50   | 2532 | A    |
| 1   | K50   | 2596 | G    |
| 1   | K50   | 2597 | G    |
| 2   | K70   | 32   | A    |
| 2   | K70   | 41   | G    |
| 2   | K70   | 62   | A    |
| 2   | K70   | 109  | U    |
| 42  | R60   | 71   | U    |
| 42  | R60   | 76   | A    |
| 42  | R60   | 118  | G    |
| 42  | R60   | 127  | A    |
| 42  | R60   | 180  | G    |
| 42  | R60   | 186  | A    |
| 42  | R60   | 190  | A    |
| 42  | R60   | 191  | C    |
| 42  | R60   | 218  | A    |
| 42  | R60   | 225  | A    |
| 42  | R60   | 226  | G    |
| 42  | R60   | 256  | G    |
| 42  | R60   | 262  | U    |
| 42  | R60   | 283  | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | R60   | 303  | G    |
| 42  | R60   | 328  | A    |
| 42  | R60   | 339  | A    |
| 42  | R60   | 355  | C    |
| 42  | R60   | 372  | A    |
| 42  | R60   | 383  | A    |
| 42  | R60   | 407  | G    |
| 42  | R60   | 408  | A    |
| 42  | R60   | 424  | G    |
| 42  | R60   | 425  | G    |
| 42  | R60   | 445  | U    |
| 42  | R60   | 473  | G    |
| 42  | R60   | 509  | G    |
| 42  | R60   | 511  | A    |
| 42  | R60   | 553  | A    |
| 42  | R60   | 565  | U    |
| 42  | R60   | 598  | C    |
| 42  | R60   | 661  | A    |
| 42  | R60   | 724  | A    |
| 42  | R60   | 753  | U    |
| 42  | R60   | 776  | A    |
| 42  | R60   | 788  | G    |
| 42  | R60   | 819  | A    |
| 42  | R60   | 877  | G    |
| 42  | R60   | 914  | U    |
| 42  | R60   | 916  | G    |
| 42  | R60   | 917  | U    |
| 42  | R60   | 918  | A    |
| 42  | R60   | 923  | A    |
| 42  | R60   | 925  | A    |
| 42  | R60   | 927  | G    |
| 42  | R60   | 934  | A    |
| 42  | R60   | 954  | G    |
| 42  | R60   | 970  | U    |
| 42  | R60   | 980  | G    |
| 42  | R60   | 1007 | U    |
| 42  | R60   | 1018 | U    |
| 42  | R60   | 1021 | A    |
| 42  | R60   | 1023 | A    |
| 42  | R60   | 1045 | A    |
| 42  | R60   | 1057 | C    |
| 42  | R60   | 1077 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 42  | R60   | 1088 | U    |
| 42  | R60   | 1089 | G    |
| 42  | R60   | 1103 | G    |
| 42  | R60   | 1105 | G    |
| 42  | R60   | 1125 | G    |
| 42  | R60   | 1135 | U    |
| 42  | R60   | 1141 | A    |
| 42  | R60   | 1175 | A    |
| 42  | R60   | 1176 | G    |
| 42  | R60   | 1262 | A    |
| 42  | R60   | 1314 | C    |
| 42  | R60   | 1321 | U    |
| 42  | R60   | 1328 | G    |
| 42  | R60   | 1356 | 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 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17457. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

### 6.1 Orthogonal projections

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

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

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 Mask visualisation

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

## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

## 8 Fourier-Shell correlation

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

## 9 Map-model fit

This section was not generated.