



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:07 PM BST

PDB ID : 3JAG
EMDB ID: : EMD-3038
Title : Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UAA stop codon
Authors : Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.
Deposited on : 2015-06-10
Resolution : 3.65 Å(reported)
Based on PDB ID : 1DT9, 4V51, 3J7P, 3J92, 3BK7

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

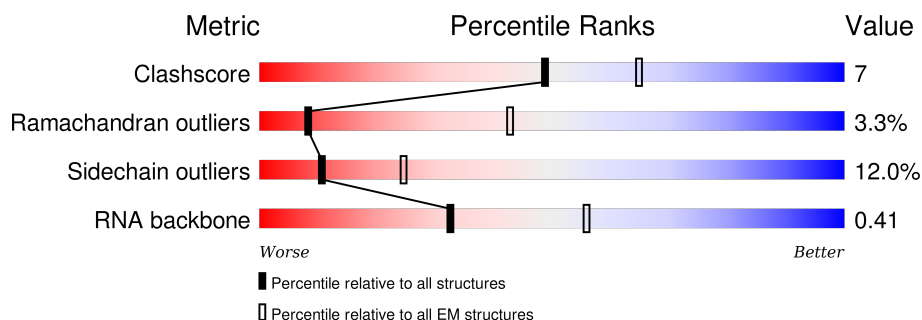
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	A	244	80% 16% .
2	B	394	81% 17% .
3	C	362	73% 24% .
4	D	292	83% 16% .
5	E	248	67% 24% . 5%
6	F	225	80% 17% .
7	G	241	78% 21% .
8	H	190	82% 16% .












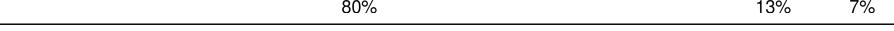

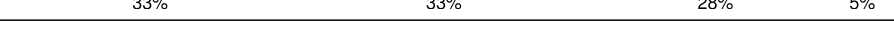





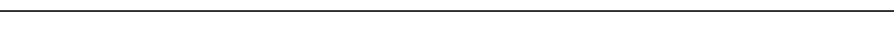

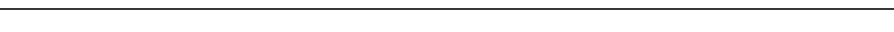
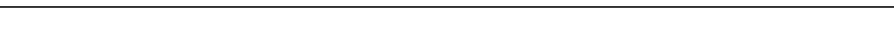


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Mol	Chain	Length	Quality of chain
9	I	213	 70%20%5% .
10	J	169	 81%18% .
11	L	210	 74%23% .
12	M	138	 73%25% .
13	N	203	 80%19% .
14	O	199	 79%17% .
15	P	153	 87%12% .
16	Q	187	 82%17% .
17	R	180	 76%21% .
18	S	175	 75%22% . .
19	T	159	 79%20% .
20	U	99	 83%15% .
21	V	131	 82%17% .
22	W	63	 89%10% .
23	X	119	 85%14% .
24	Y	134	 81%16% . .
25	Z	135	 78%21% .
26	a	147	 88%12% .
27	b	75	 92%8%
28	c	94	 88%12%
29	d	107	 83%15% .
30	e	128	 84%16%
31	f	109	 83%16% .
32	g	114	 88%12%
33	h	122	 88%11% .


























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Mol	Chain	Length	Quality of chain
34	i	102	 88% 9% ..
35	j	86	 88% 10% .
36	k	69	 88% 10% .
37	l	50	 80% 20%
38	m	52	 79% 19% .
39	n	23	 87% 13%
40	o	104	 86% 13% .
41	p	91	 93% 7%
42	r	125	 82% 17% .
43	s	198	 90% 9% .
44	t	163	 79% 20% .
45	1	15	 80% 13% 7%
46	2	76	 59% 32% 9%
47	3	75	 33% 33% 28% 5%
48	5	3662	 48% 38% 13% .
49	7	120	 65% 30% 5%
50	8	156	 45% 44% 11%
51	9	1719	 47% 41% 11% .
52	AA	208	 79% 17% .
53	BB	213	 77% 20% ..
54	CC	218	 75% 22% .
55	DD	227	 79% 19% .
56	EE	262	 75% 21% 5%
57	FF	191	 75% 21% .
58	GG	237	 75% 24% .





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Mol	Chain	Length	Quality of chain
59	HH	189	 78%18%.
60	II	206	 74%24%.
61	JJ	185	 78%17%..
62	KK	98	 68%30%.
63	LL	152	 80%17%..
64	MM	124	 77%22%.
65	NN	150	 79%19%.
66	OO	136	 67%24%7%.
67	PP	127	 77%20%.
68	QQ	141	 84%12%..
69	RR	129	 80%16%.
70	SS	137	 78%18%..
71	TT	141	 82%13%5%.
72	UU	104	 83%14%.
73	VV	83	 80%18%.
74	WW	129	 82%16%.
75	XX	141	 77%21%.
76	YY	126	 75%22%.
77	ZZ	75	 84%16%.
78	aa	98	 82%18%.
79	bb	83	 81%18%.
80	cc	61	 85%15%.
81	dd	53	 81%19%.
82	ee	57	 84%16%.
83	ff	69	 86%6%9%.

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Mol	Chain	Length	Quality of chain
84	gg	313	 90%10%
85	hh	12	 42%58%
86	ii	416	 91%9%
87	jj	594	 92%5% •

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 226469 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 protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

- Molecule 3 is a protein called uL4.

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	361	LYS	-	EXPRESSION TAG	UNP G1SVW5
C	362	SER	-	EXPRESSION TAG	UNP G1SVW5
C	363	ASP	-	EXPRESSION TAG	UNP G1SVW5

- Molecule 4 is a protein called uL18.

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

- Molecule 5 is a protein called eL6.

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

- Molecule 6 is a protein called uL30.

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

- Molecule 7 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called uL16.

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

- Molecule 10 is a protein called uL5.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	15	Total	C	N	O	S	0	0
			125	82	20	22	1		

- Molecule 46 is a RNA chain called tRNA(Val).

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 47 is a RNA chain called tRNA(Lys).

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3662	Total	C	N	O	P	0	0
			78486	34947	14363	25515	3661		

- Molecule 49 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 50 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	156	Total	C	N	O	P	0	0
			3314	1480	585	1094	155		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1719	Total	C	N	O	P	0	0
			36680	16371	6586	12005	1718		

- Molecule 52 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AA	208	Total	C	N	O	S	0	0
			1642	1045	289	300	8		

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	218	Total	C	N	O	S	0	0
			1694	1103	287	297	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	194	ARG	HIS	CONFLICT	UNP G1TUT9

- Molecule 55 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DD	227	Total	C	N	O	S	0	0
			1764	1124	317	315	8		

- Molecule 56 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	EE	262	Total	C	N	O	S	0	0
			2073	1323	384	357	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	25	GLY	SER	CONFLICT	UNP G1TK17

- Molecule 57 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	FF	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	HH	189	Total	C	N	O	S	0	0
			1521	969	280	271	1		

- Molecule 60 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	CONFLICT	UNP G1TJW1

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	KK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 63 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	LL	152	Total	C	N	O	S	0	0
			1238	788	232	212	6		

- Molecule 64 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	MM	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 65 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	NN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	PP	127	Total	C	N	O	S	0	0
			1060	673	201	179	7		

- Molecule 68 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	QQ	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 69 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	RR	129	Total	C	N	O	S	0	0
			1047	658	193	191	5		

- Molecule 70 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SS	137	Total	C	N	O	S	0	0
			1139	714	231	193	1		

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	TT	141	Total	C	N	O	S	0	0
			1102	692	212	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	CONFLICT	UNP G1TN62

- Molecule 72 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	UU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 73 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	VV	83	Total	C	N	O	S	0	0
			636	394	118	119	5		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
VV	3	ASN	SER	CONFLICT	UNP G1TM82
VV	4	ASP	ASN	CONFLICT	UNP G1TM82
VV	50	PHE	SER	CONFLICT	UNP G1TM82
VV	75	ALA	SER	CONFLICT	UNP G1TM82

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	YY	126	Total	C	N	O	S	0	0
			1023	646	200	172	5		

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	aa	98	Total	C	N	O	S	0	0
			781	486	161	129	5		

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	cc	61	Total	C	N	O	S	0	0
			475	290	92	91	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
cc	18	ILE	LEU	CONFLICT	UNP G1TIB4
cc	20	LYS	ARG	CONFLICT	UNP G1TIB4
cc	40	HIS	ARG	CONFLICT	UNP G1TIB4
cc	42	THR	ILE	CONFLICT	UNP G1TIB4

- Molecule 81 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	dd	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 82 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ee	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 83 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	ff	63	Total	C	N	O	S	0	0
			527	336	99	86	6		

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	12	Total	C	N	O	P	0	0
			256	115	46	83	12		

- Molecule 86 is a protein called eRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	416	Total	C	N	O	S	0	0
			3280	2087	559	623	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	183	ALA	GLY	ENGINEERED MUTATION	UNP P62495
ii	184	ALA	GLY	ENGINEERED MUTATION	UNP P62495

- Molecule 87 is a protein called ABCE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	577	Total	C	N	O	S	0	0
			4551	2910	780	830	31		

- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	P	1	Total	Mg	0
			1	1	
88	g	1	Total	Mg	0
			1	1	
88	Q	1	Total	Mg	0
			1	1	
88	I	1	Total	Mg	0
			1	1	
88	C	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	

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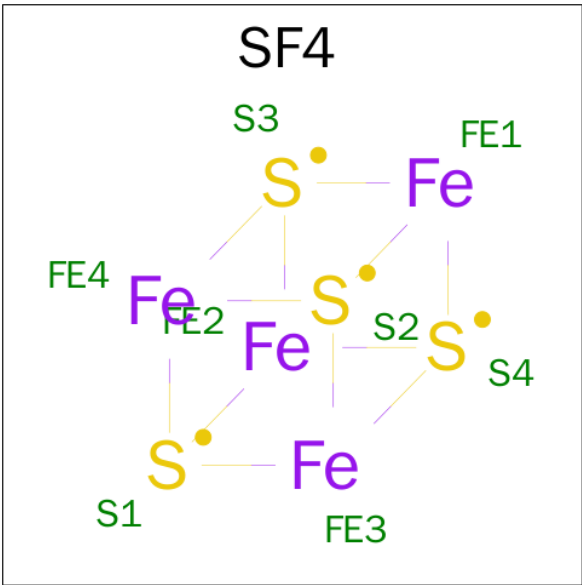
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Mol	Chain	Residues	Atoms		AltConf
88	7	5	Total 5	Mg 5	0
88	5	146	Total 146	Mg 146	0
88	8	2	Total 2	Mg 2	0
88	9	35	Total 35	Mg 35	0
88	hh	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

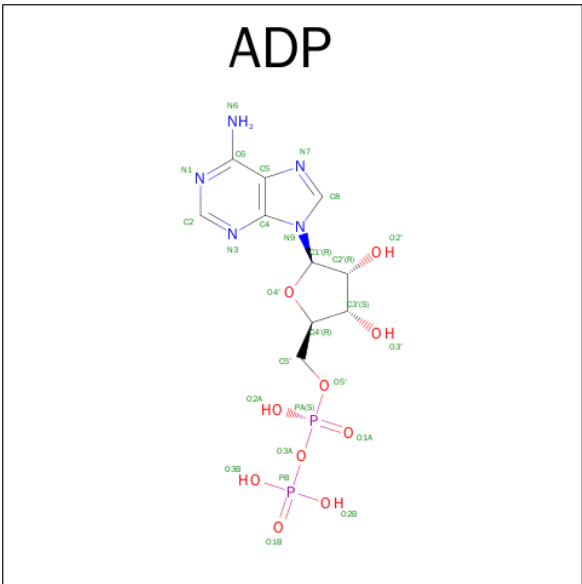
Mol	Chain	Residues	Atoms		AltConf
89	p	1	Total 1	Zn 1	0
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
90	jj	1	Total	Fe	S	0
			16	8	8	
90	jj	1	Total	Fe	S	0
			16	8	8	

- Molecule 91 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
91	jj	1	Total	C	N	O	P	0
			54	20	10	20	4	

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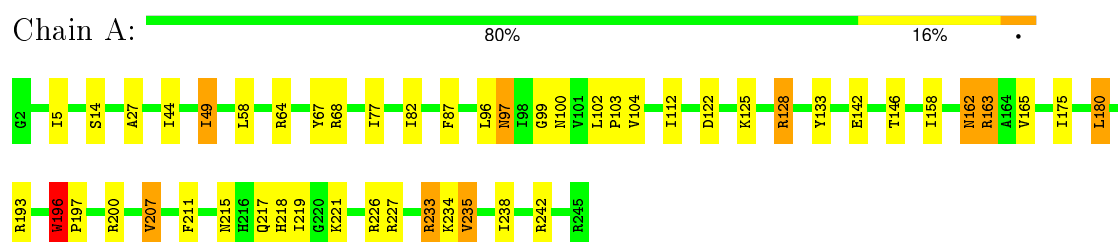
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
91	jj	1	54	20	10	20	4	0

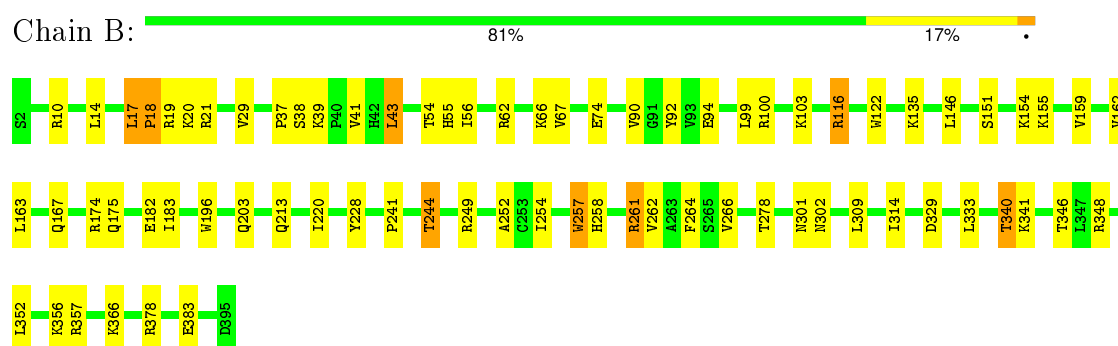
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

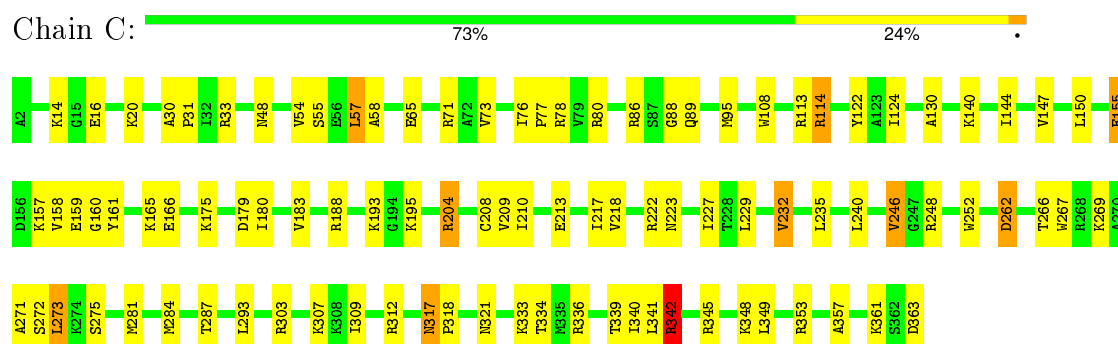
• Molecule 1: uL2



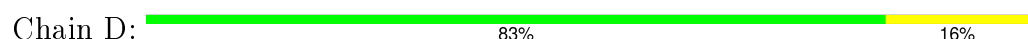
• Molecule 2: uL3

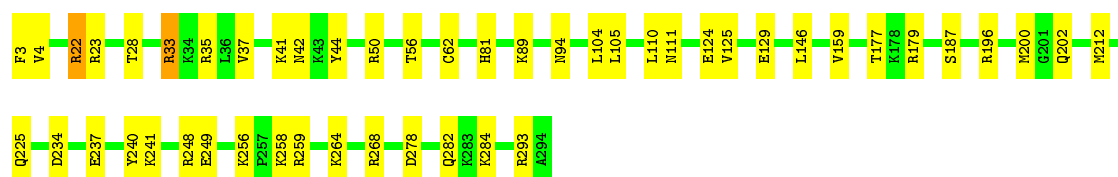


• Molecule 3: uL4

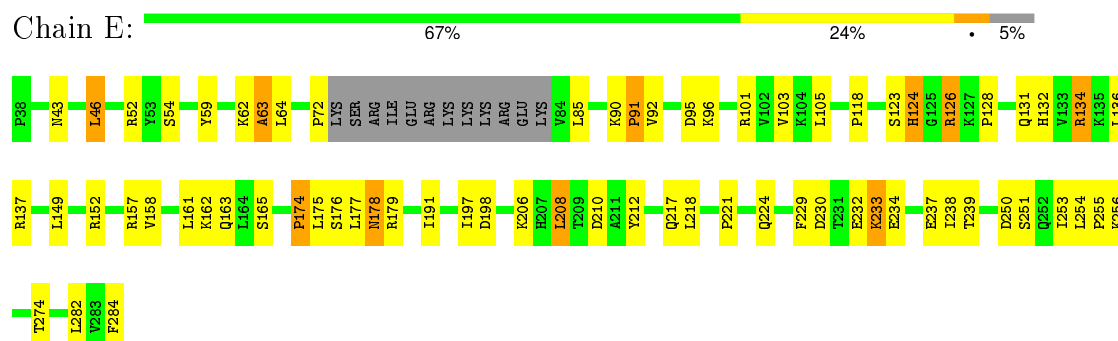


• Molecule 4: uL18

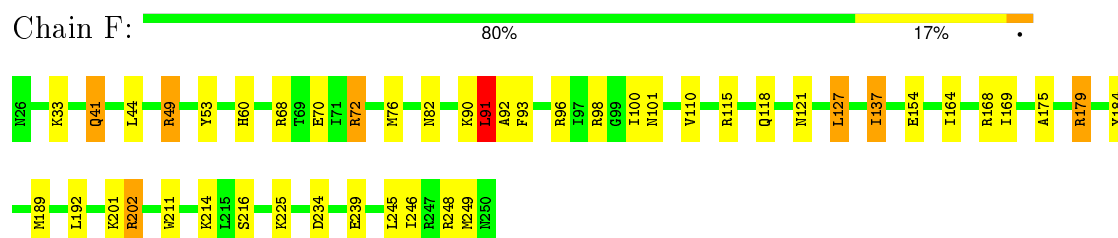




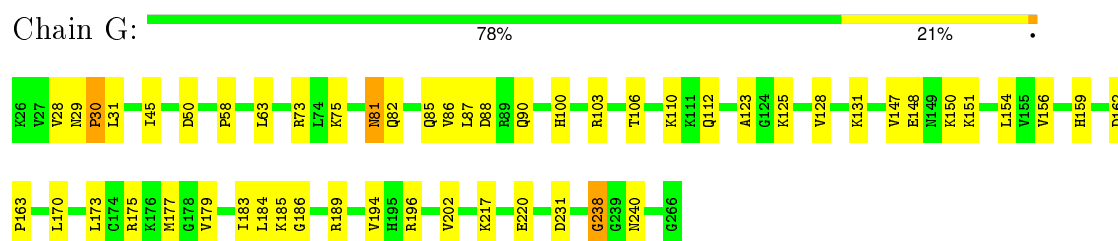
- Molecule 5: eL6



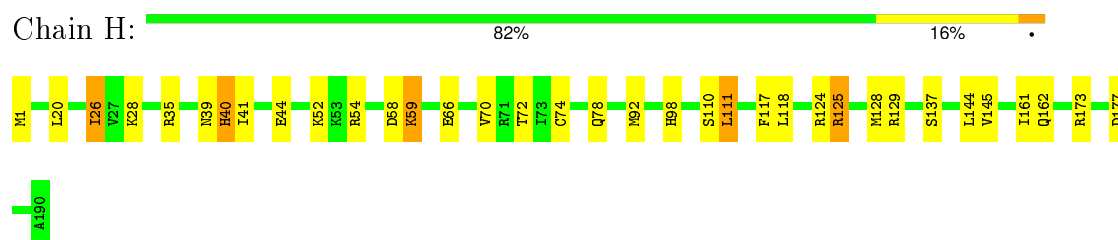
- Molecule 6: uL30



- Molecule 7: eL8

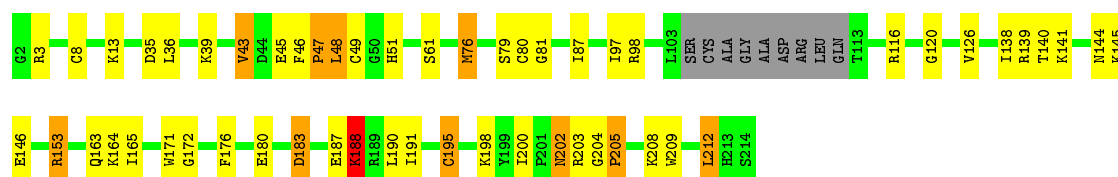


- Molecule 8: uL6



- Molecule 9: uL16





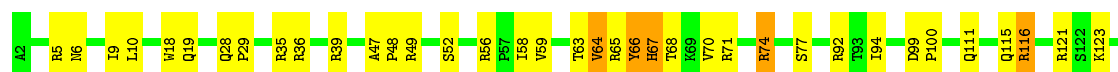
- Molecule 10: uL5

Chain J: 81% 18% .



- Molecule 11: eL13

Chain L: 74% 23% .



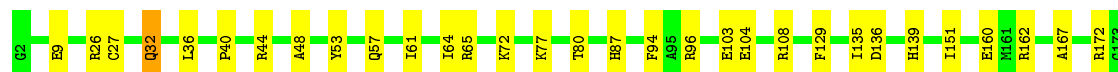
- Molecule 12: eL14

Chain M: 73% 25% .



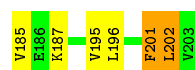
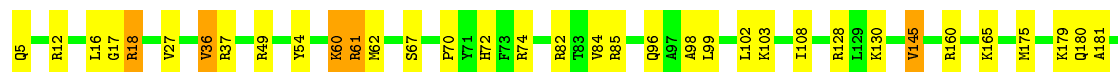
- Molecule 13: eL15

Chain N: 80% 19% .




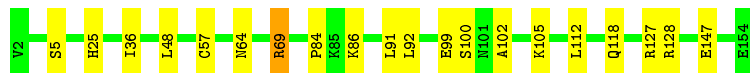
- Molecule 14: uL13

Chain O: 79% 17% .




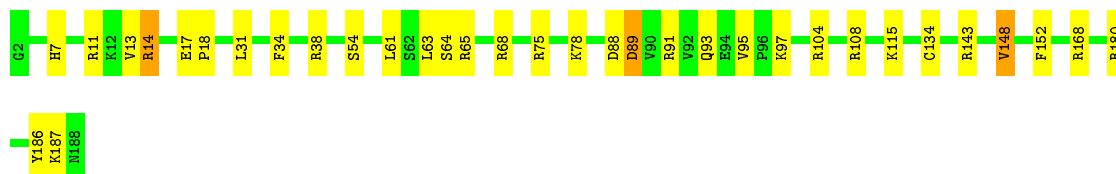
- Molecule 15: uL22

Chain P:  87% 12%



- Molecule 16: eL18

Chain Q:  82% 17%



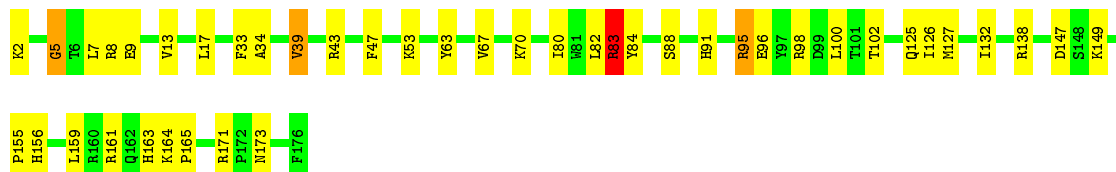
- Molecule 17: eL19

Chain R:  76% 21%




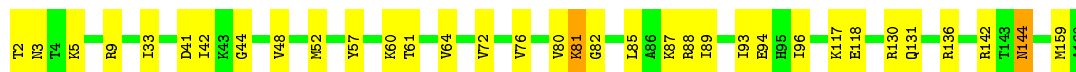
- Molecule 18: eL20

Chain S:  75% 22%




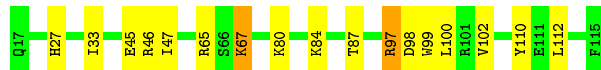
- Molecule 19: eL21

Chain T:  79% 20%

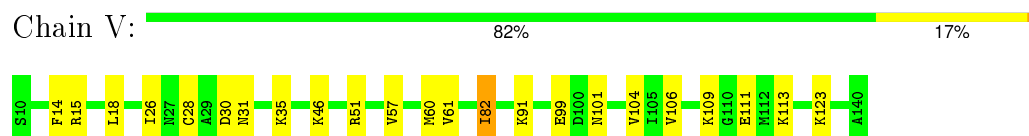


- Molecule 20: eL22

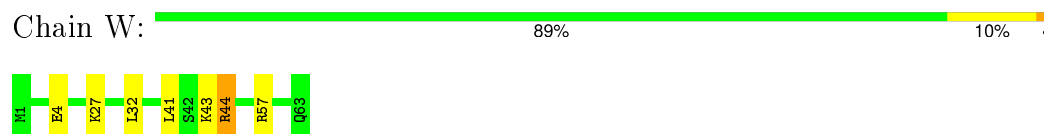
Chain U:  83% 15%



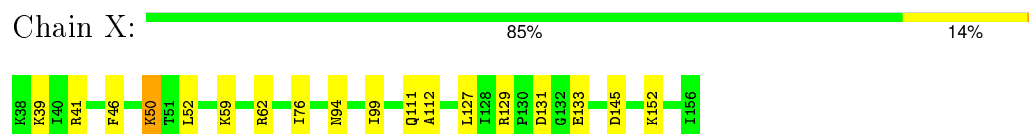
- Molecule 21: uL14



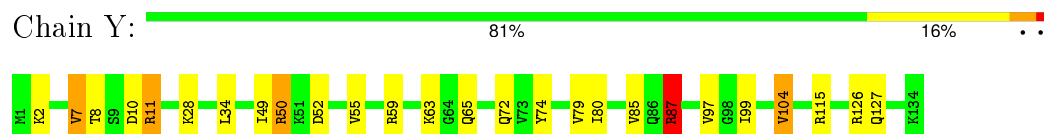
- Molecule 22: eL24



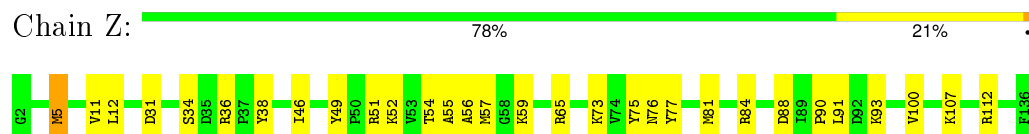
- Molecule 23: uL23



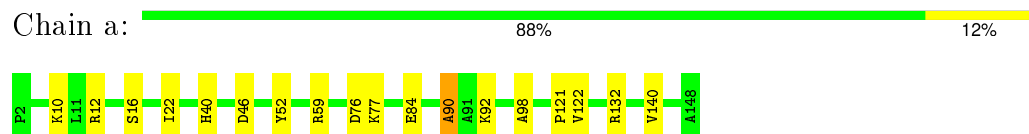
- Molecule 24: uL24



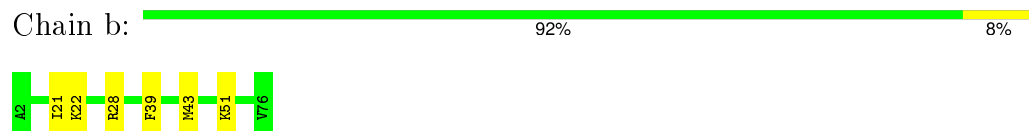
- Molecule 25: eL27



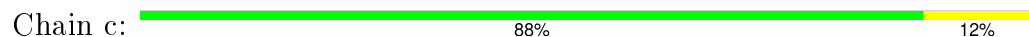
- Molecule 26: uL15



- Molecule 27: eL29



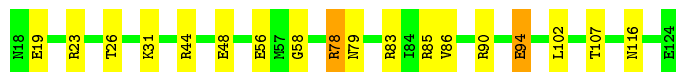
- Molecule 28: eL30





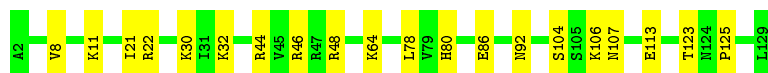
- Molecule 29: eL31

Chain d: 83% 15% .



- Molecule 30: eL32

Chain e: 84% 16%



- Molecule 31: eL33

Chain f: 83% 16% .



- Molecule 32: eL34

Chain g: 88% 12%



- Molecule 33: uL29

Chain h: 88% 11% .



- Molecule 34: eL36

Chain i: 88% 9% ..




- Molecule 35: eL37

Chain j: 88% 10% .




- Molecule 36: eL38

Chain k:  88% 10%




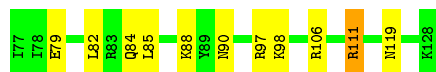
- Molecule 37: eL39

Chain l:  80% 20%




- Molecule 38: eL40

Chain m:  79% 19%




- Molecule 39: eL41

Chain n:  87% 13%



- Molecule 40: eL42

Chain o:  86% 13%




- Molecule 41: eL43

Chain p:  93% 7%



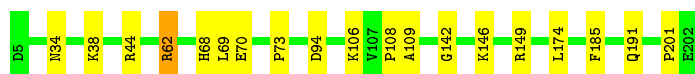
- Molecule 42: eL28

Chain r:  82% 17%

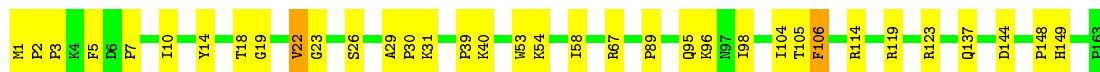
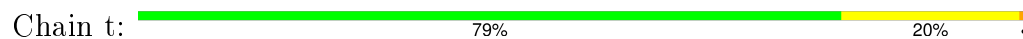


- Molecule 43: uL10

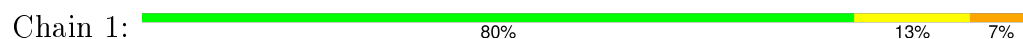
Chain s:  90% 9%



• Molecule 44: uL11



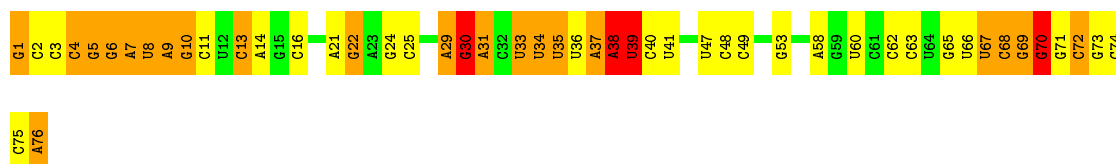
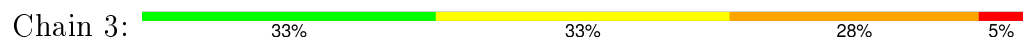
• Molecule 45: peptide



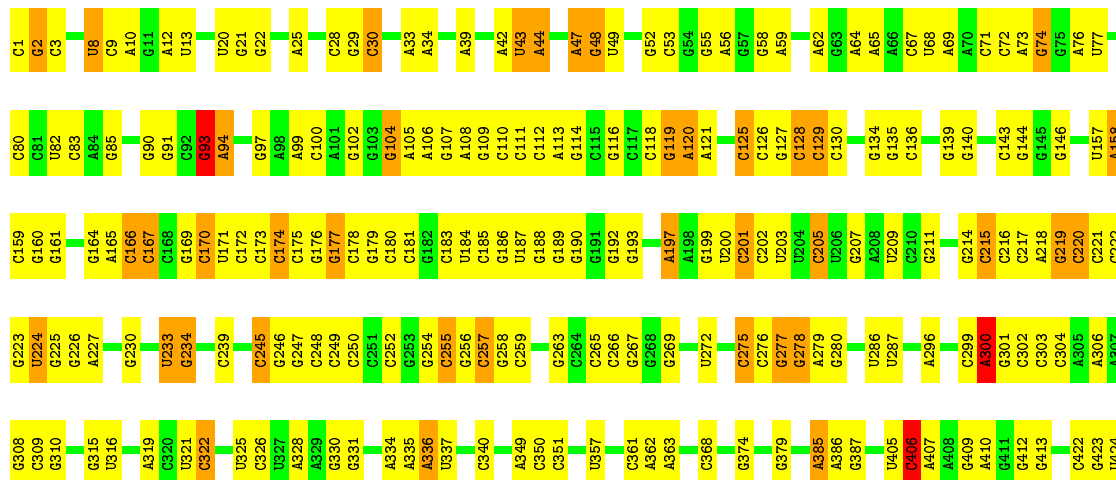
• Molecule 46: tRNA(Val)



• Molecule 47: tRNA(Lys)

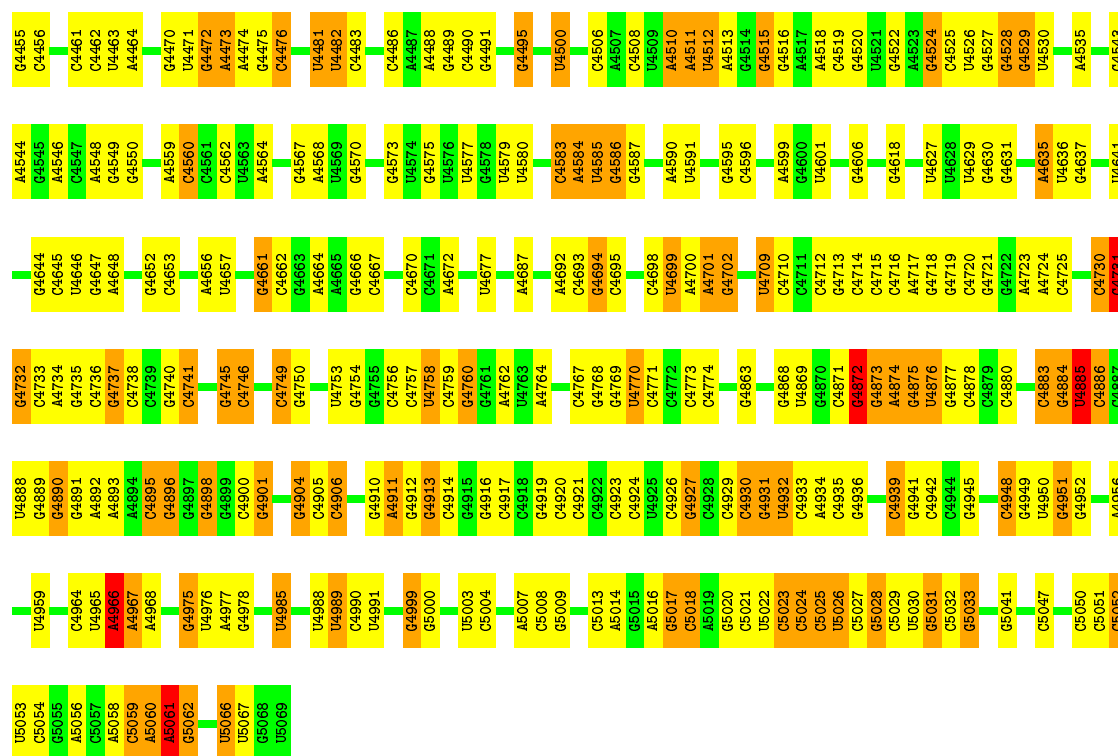


• Molecule 48: 28S ribosomal RNA



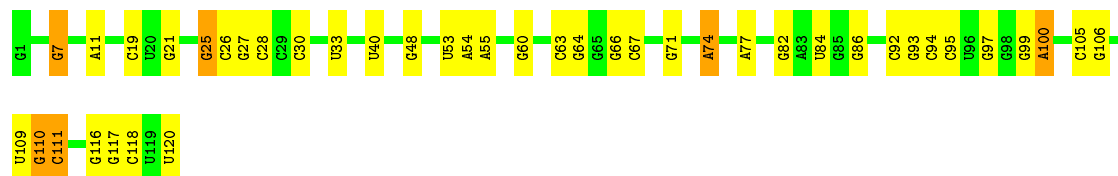
G2058	U1986	G1904	G1815	U1725	A1631	G1429	G1360	G1271	G1194	G994	G930	G703	U513	A429
C2059	C1987	A1907	G1818	U1726	A1632	C1430	G1361	C1272	G1195	C995	C931	C704	U514	A430
C2062	G1989	G1910	G1819	C1732	A1633	C1431	G1362	G1273	G1196	G1048	A932	C705	C515	G431
G2064	A1991	G1911	G1820	G1734	C1635	G1432	G1363	A1274	C1197	C1049	G933	C706	C516	U432
G2065	U1992	G1912	G1821	U1735	C1636	G1435	G1365	C1275	G1198	C1050	A935	C707	C517	A433
C2067	C1993	C1913	U1822	U1735	A1637	C1436	G1366	C1277	G1199	C1051	C936	A711	G518	A434
C2068	G1994	U1918	G1823	G1739	A1638	C1436	G1367	C1278	G1203	G1064	U937	C712	C519	C446
C2069	G1995	A1825	A1825	C1740	C1640	C1439	G1369	A1279	C1204	G1065	C938	G715	G642	C447
A2069	C1996	G1826	G1826	G1741	G1641	C1440	G1370	G1281	G1205	G1066	G939	C716	G643	G448
U2070	U1997	C1827	C1827	A1742	A1642	C1441	A1371	G1282	G1207	G1068	C941	U717	G645	C449
A2071	A1998	C1828	C1828	A1742	A1643	C1442	A1372	G1283	G1208	G1069	C942	C718	G646	C450
C2072	A1999	A1746	G1829	U1746	G1654	U1445	A1373	G1284	U1209	G1070	A943		G647	C451
C2073	G2000	U1747	G1830	U1747	C1655	C1446	G1374	U1285	G1210	C1071	A944	G721	A649	A452
G2076	G2001	U1748	G1831	U1748	C1655	C1446	G1375	C1286	G1211	C1072	U945	G722	A649	G453
C2077	A2002	A1749	C1832	U1750	U1656	C1447	C1376	G1287	G1212	C1073	C946	A723	U454	U454
G2078	G2003	G1750	G1833	G1750	C1661	G1448	C1377	G1288	G1213	G1074	C947	C724	G654	C455
G2079	U2004	A1751	U1834	A1751	C1661	C1449	C1378		G1214	G1075	C948	G725	G655	C456
G2080	G2005	G1752	G1835	G1752	C1662	C1450	C1379	G1291	G1215	C1076		G726	C656	C458
C2083	U2006	G1753	G1836	G1753	C1663		A1387	G1292			G951	G727	C657	C462
C2084	G2007	U1754	A1837	U1754	G1663	G1454	G1380	G1293	G1219	C1081	G952	U728	G663	C465
G2085	U2008	C1755	A1838	C1755	G1667	G1455	U1381	G1294	G1220	C1082	G953	G729	G664	A466
G2086	A2009	U1756	U1839	U1756	A1668	C1456	G1382	C1295	G1221	U1083	A956	G730	G665	U467
A2087	A2010	U1757	A1669	U1757	C1669	G1457	C1384	G1296	A1222	C1084	C957		G666	U468
A2088	C2011	G1758	G1670	G1758	G1670		A1387	U1297	G1232	C1085	G958	A733	G667	U469
G2089		G1759	U1671	G1759	U1671	C1464		C1301	G1233	C1086	G959		G668	U470
U2090	C2016	G1760	U1672	G1760	A1563	G1465	G1390	U1302	G1234	G1090	G960	G742	G670	A471
C2091	A2017	G1761	U1673	G1761	A1564	C1466	G1391	A1303	G1235	C1091	A961	G743	G671	C472
G2092	C2018	C1762	C1848	C1762	A1565	C1467	G1392	G1313	G1236	G1092	C962	G744	G672	C473
A2093	C2019	G1763	G1854	G1764	C1676	C1468	G1394		G1237	C1093	C963	G745	C673	C476
G2094	U2020	U1765	G1855	U1765	C1677		A1397	C1308	G1238	C1097	A964	G746	G674	G479
A2095	G2021	C1766	G1856	C1766	C1678	C1472	A1398	C1309	G1239	G1098	G965	A747	C675	C480
G2096	C2022	U1767	C1856	U1767	A1679	C1473	C1399	G1313	G1240	C1099	A966	G748	G676	G483
U2097	G2023	G1768	A1867	U1771	A1682	C1475	G1400		G1242	U1100	C967	G749	G677	C486
A2100	G2024	C1769	A1868	U1771	U1683	C1476	C1401	A1322	G1243	C1167	C968	U750	G678	G487
C2101	U2025	U1772	G1869	C1772	A1684	C1477			G1244		C969		C679	C488
G2107	A2026	A1776	G1885	A1776	G1685	C1478	G1404	A1326	G1245	G1170	G970	G751	G682	G489
C2109	U2027	C1777	C1885	C1777	C1686		C1405	C1327	G1246	G1171	U971	G752	G683	C493
G2110	C2028	A1874	A1873	U1777	U1687	C1481	G1406	G1328	U1247	C1172	G972		G684	C494
G2111	A2029	G1878	G1885	U1780	G1688	C1482	C1407	G1329	C1248	A1175	C974	G912	C685	C495
C2112	G2034	C1879	G1886	U1781	G1689	C1483	G1408	A1330	G1249	C1176	C975	U913	C686	C496
G2113	C2035	U1882	C1886	U1782	G1690	C1484	C1409	C1332		U1177	G976	U914	G688	C497
G2114	U2043	U1882	G1885	C1783	C1691	C1486	U1410	G1333	G1252		C977	A915	U688	C498
G2115	G2045	A1787	G1886	A1787	C1692		G1411		A1255	C1181	G978	C916	U689	C499
G2116	A2047	G1798	G1886	G1798	C1694	G1489	C1413	A1337	G1256	C1182	C979	G917	C690	C500
G2117	U2048	U1799	A1891	U1800	G1697	C1498	G1415	U1339	G1259	C1183	U982	C920	C693	C501
G2118	G2049	U1800	G1891	G1799	G1698	C1499	C1417	C1340	G1262	A1184	C983	C921	C694	C502
C2119	C2050	C1977	C1894	U1800	C1699	C1499	C1418	C1344	U1263	U1186	C984	C922	G695	C503
G2120	C2051	A1978	C1894	A1804	C1718	C1501	C1419	C1344	C1264	G1187	C985	C923	C696	C504
G2121	G2052	U1980	A1805	A1805	A1719	C1502	A1420	G1353	G1265	C1188	C986	C924	G697	C505
G2122	C2053	A1897	A1897	A1805	C1720	C1503	G1421	A1354	G1266	C1189	U989	C925	G698	C506
C2123	U2054	C1898	C1898	C1808	G1721	C1504	G1422	C1357	C1267	C1190	C990	G926	C699	C507
G2124	G2055	A1983	G1899	U1722	U1722	C1505	U1423	C1357	G1268	C1191	C991	G927	G700	A509
C2125	G2056	A1984	C1900	A1723	G1424	C1506	G1424	C1358	G1269	C1192	C992	C928	U702	C510
G2126	A2057	G1985		G1724	G1425	C1507	G1425	G1359	A1270	C1193	G993	A929		

U4372	G4276	C4171	G4106	A3905	U3814	A3719	A3624	G2847	G2756	G2673	C2583	C2505	G2483	G2314	C2127
A4376	A4280	G4182	G4107	A3906	G3815	G3722	G3625	G2855	A2757	A2676	G2586	G2506	G2424	G2315	G2128
A4377	A4281	G4183	G4108	G3907	A3816	A3723	G3626	G2856	G2758	A2677	G2587	A2507	U2425	G2322	G2129
A4378	A4282	G4184	C4110	U3912	U3818	A3724	G3628	A2858	G2759	G2681	G2588	A2511	A2428	G2323	G2130
A4379	A4283	G4185	C4111	G3913	G3819	A3725	G3629	G2859	G2761	G2682	C2589	A2512	A2429	C2324	C2131
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G4391	G4297	G4116	C4115	A3917	A3824	A3731	A3642	U2874	G2768	G2688	G2602	G2516	G2435	G2331	C2248
G4392	G4297	U4117	U4118	C3919	U3831	A3732	A3643	C2875	U2769	C2689	G2606	G2517	G2436	A2332	G2249
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A4398	G4305	U4210	C4123	G3933	U3838	A3743	A3648	G2896	G2775	A2696	G2611	U2526	C2445	C2337	G2254
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A4413	A4317	C4221	C4132	G3947	A3856	A3756	G3672	G2904	A2786	G2707	G2619	U2534	C2453	C2345	G2262
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U4432	C4332	A4238	C4147	A4085	A3877	G3777	G3688	G3595	G2811	G2722	U2638	U2549	C2468	C2360	G2277
U4433	C4333	G4239	C4148	G4086	A3878	G3778	G3689	G3596	G2812	G2723	U2639	U2550	C2469	C2361	G2278
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U4435	C4337	C4241	C4150	C4088	C3880	A3780	G3696	G3598	C2814	U2725	G2641	U2552	C2471	C2363	G2280
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U4441	C4350	U4255	C4156	G4094	G3886	A3786	G3707	C3604	U2827	G2731	U2647	U2558	C2477	C2369	G2286
U4442	C4351	G4256	C4157	G4095	C3887	U3787	G3708	C3605	U2828	G2732	C2654	U2559	C2478	C2370	G2287
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U4456	C4372	A4276	C4171	A4109	A3901	A3801	A3722	C3619	U2842	U2749	G2670	U2573	C2492	C2384	G2301
U4457	U4373	G4277	C4172	G4110	G3902	A3802	A3723	C3620	U2843	U2750	G2671	U2574	C2493	C2385	G2302
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U4468	C4384	G4287	C4183	G4119	G3913	A3813	A3734	C3631	U2854	U2761	G2682	U2585	C2504	C2396	G2313
U4469	U4385	U4288	C4184	G4120	G3914	A3814	A3735	C3632	U2855	U2762	G2683	U2586	C2505	C2397	G2314
U4470	A4386	A4289	C4185	G4121	G3915	A3815	A3736	C3633	U2856	U2763	G2684	U2587	C2506	C2398	G2315
U4471	C4387	G4290	C4186	G4122	G3916	A3816	A3737	C3634	U2857	U2764	G2685	U2588	C2507	C2399	G2316
U4472	U4388	U4291	C4187	G4123	G3917	A3817	A3738	C3635	U2858	U2765	G2686	U2589	C2508	C2400	G2317
U4473	A4389	A4292	C4188	G4124	G3918	A3818	A3739	C3636	U2859	U2766	G2687	U2590	C2509	C2401	G2318
U4474	C4390	G4293	C4189	G4125	G3919	A3819	A3740	C3637	U2860	U2767	G2688	U2591	C2510	C2402	G2319
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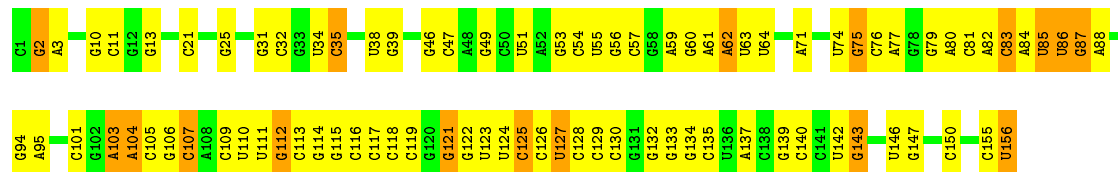
• Molecule 49: 5S ribosomal RNA

Chain 7: 65% 30% 5%



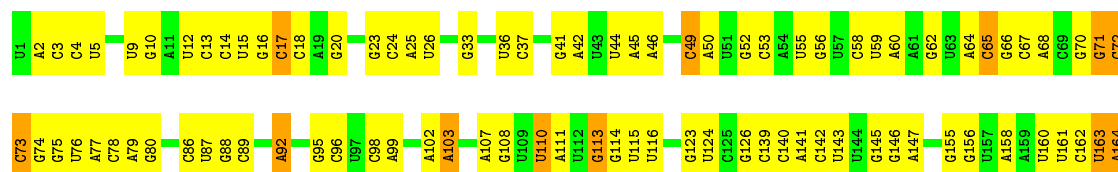
• Molecule 50: 5.8S ribosomal RNA

Chain 8: 45% 44% 11%



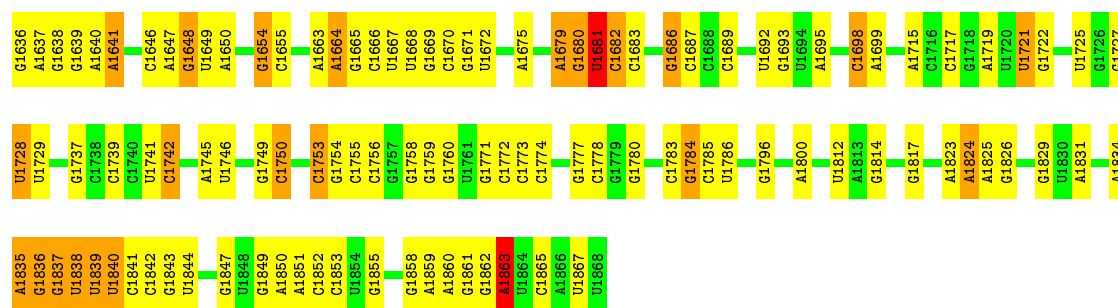
• Molecule 51: 18S ribosomal RNA

Chain 9: 47% 41% 11%

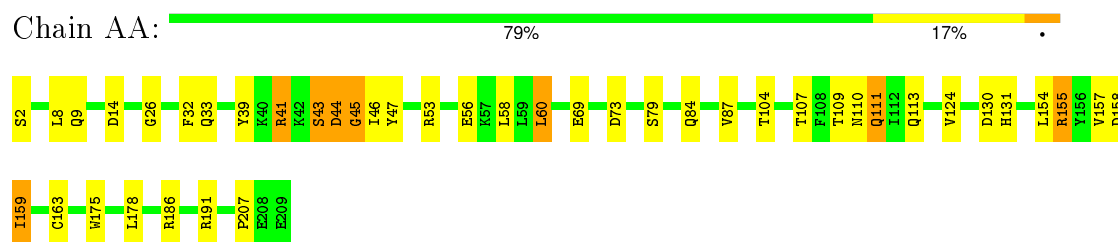



WORLDWIDE PDB
 PROTEIN DATA BANK

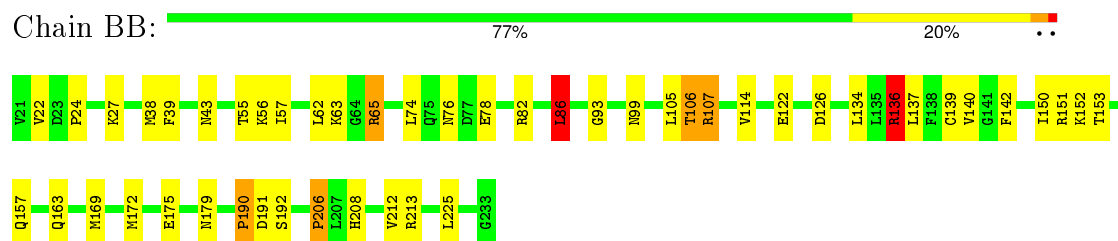
EMDataBank
 Unified Data Resource for 3DEM



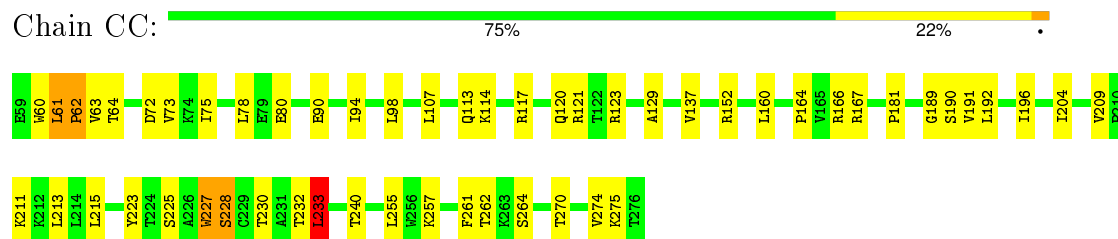
• Molecule 52: uS2



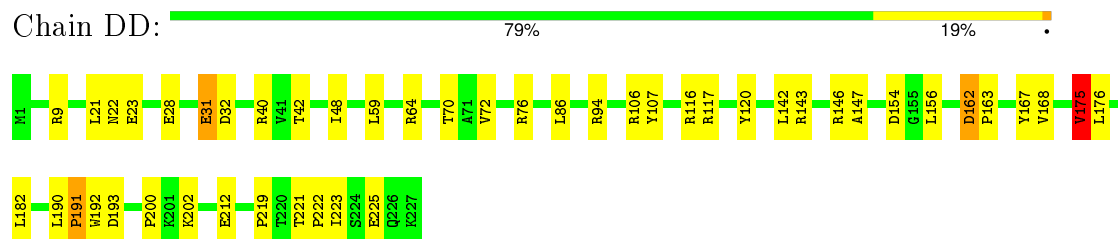
• Molecule 53: eS1




• Molecule 54: uS5

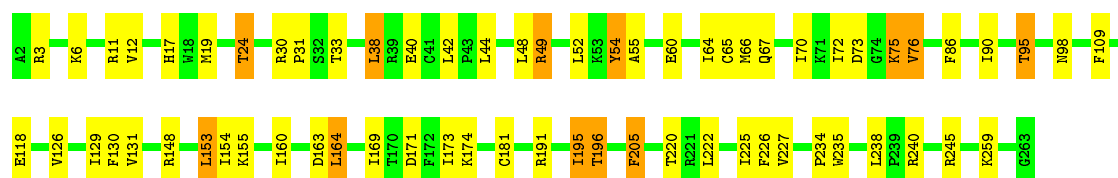


• Molecule 55: uS3




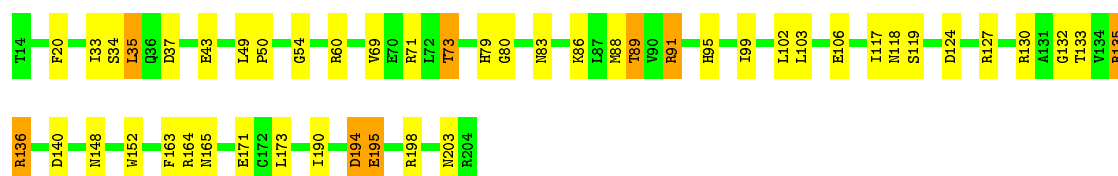
• Molecule 56: eS4

Chain EE: 




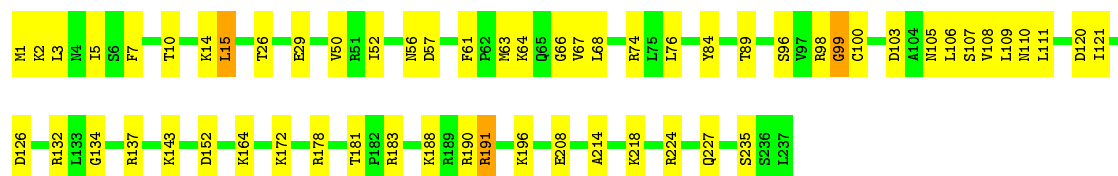
• Molecule 57: uS7

Chain FF: 




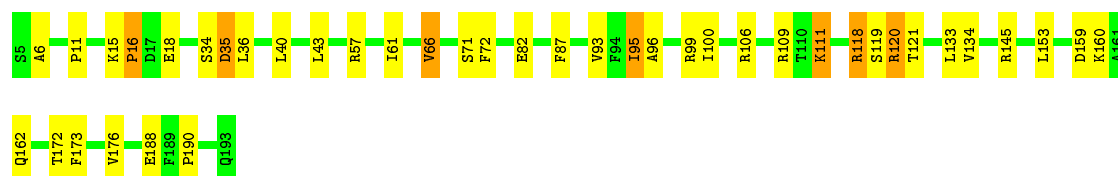
• Molecule 58: eS6

Chain GG: 



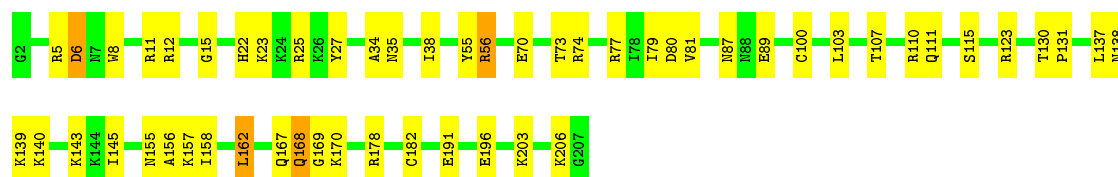
• Molecule 59: eS7

Chain HH: 




• Molecule 60: eS8

Chain II: 



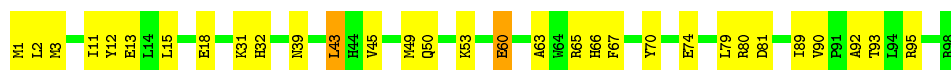
• Molecule 61: uS4

Chain JJ: 



- Molecule 62: eS10

Chain KK: 68% 30% .



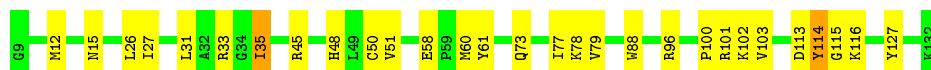
- Molecule 63: uS17

Chain LL: 80% 17% . .



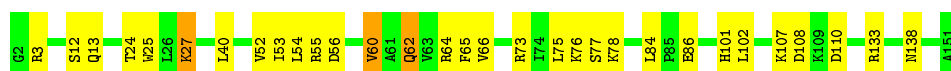
- Molecule 64: eS12

Chain MM: 77% 22% .



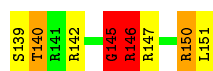
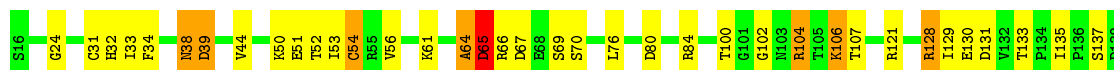
- Molecule 65: uS15

Chain NN: 79% 19% .



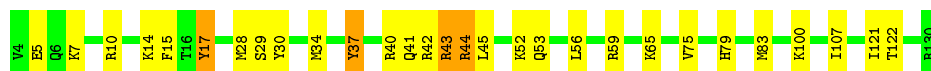
- Molecule 66: uS11

Chain OO: 67% 24% 7% .




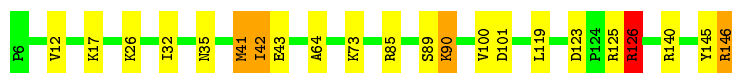
- Molecule 67: uS19

Chain PP: 77% 20% .




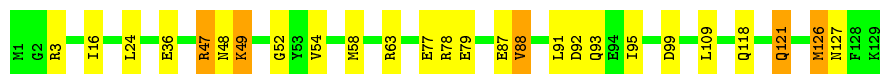
- Molecule 68: uS9

Chain QQ:  84% 12% ..




- Molecule 69: eS17

Chain RR:  80% 16% .




- Molecule 70: uS13

Chain SS:  78% 18% ..




- Molecule 71: eS19

Chain TT:  82% 13% 5%




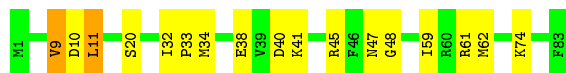
- Molecule 72: uS10

Chain UU:  83% 14% .




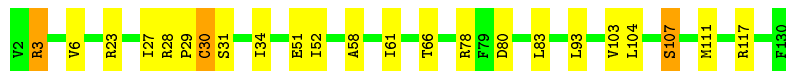
- Molecule 73: eS21

Chain VV:  80% 18% .




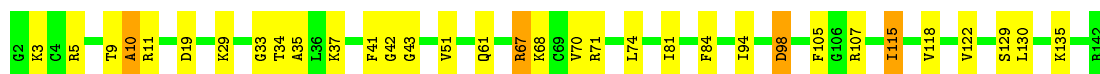
- Molecule 74: uS8

Chain WW:  82% 16% .



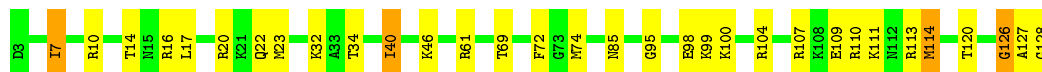
- Molecule 75: uS12

Chain XX:  77% 21% .



- Molecule 76: eS24

Chain YY: 75% 22%



- Molecule 77: eS25

Chain ZZ: 84% 16%



- Molecule 78: eS26

Chain aa: 82% 18%



- Molecule 79: eS27

Chain bb: 81% 18%



- Molecule 80: eS28

Chain cc: 85% 15%



- Molecule 81: uS14

Chain dd: 81% 19%




- Molecule 82: eS30

Chain ee: 84% 16%



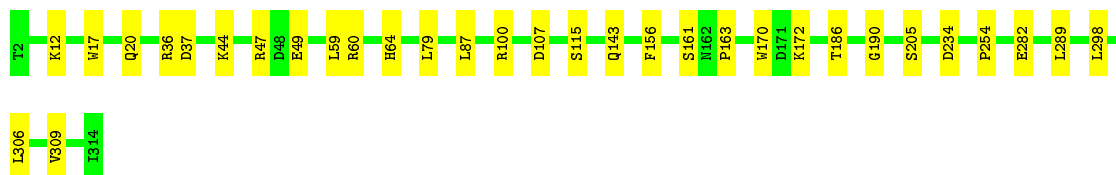
- Molecule 83: eS31

Chain ff:  86% 6% 9%



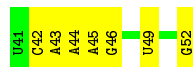
- Molecule 84: RACK1

Chain gg:  90% 10%



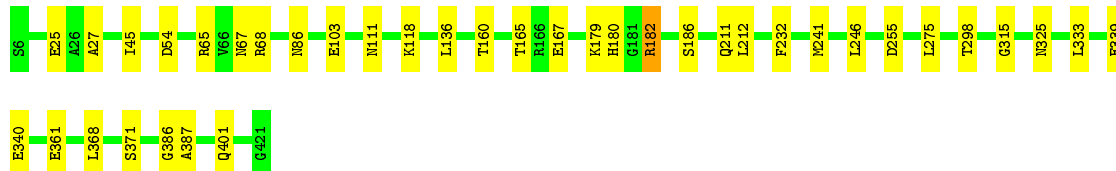
- Molecule 85: mRNA

Chain hh:  42% 58%



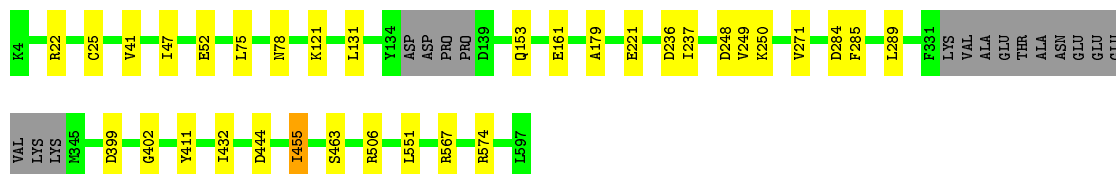
- Molecule 86: eRF1

Chain ii:  91% 9%



- Molecule 87: ABCE1

Chain jj:  92% 5% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	49979	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30, 30	Depositor
Minimum defocus (nm)	2000, 2000	Depositor
Maximum defocus (nm)	3600, 3600	Depositor
Magnification	59000, 59000	Depositor
Image detector	FEI FALCON II (4k 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, MG, SF4, ADP

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.47	0/1906	0.78	0/2556
10	J	0.43	0/1376	0.75	1/1841 (0.1%)
11	L	0.42	0/1734	0.80	0/2317
12	M	0.44	0/1158	0.74	0/1547
13	N	0.46	0/1746	0.79	0/2338
14	O	0.48	1/1671 (0.1%)	0.79	0/2234
15	P	0.49	0/1268	0.75	0/1700
16	Q	0.43	0/1530	0.81	0/2041
17	R	0.43	0/1524	0.80	3/2013 (0.1%)
18	S	0.48	0/1493	0.85	3/2002 (0.1%)
19	T	0.40	0/1326	0.70	0/1770
2	B	0.47	0/3216	0.77	2/4311 (0.0%)
20	U	0.40	0/822	0.64	0/1103
21	V	0.45	0/993	0.74	0/1332
22	W	0.47	0/541	0.81	1/720 (0.1%)
23	X	0.45	0/993	0.71	0/1334
24	Y	0.44	0/1132	0.79	1/1504 (0.1%)
25	Z	0.41	0/1130	0.71	0/1507
26	a	0.45	0/1191	0.77	0/1590
27	b	0.45	0/619	0.72	0/818
28	c	0.38	0/742	0.66	0/996
29	d	0.44	0/903	0.82	1/1216 (0.1%)
3	C	0.48	0/2937	0.81	6/3946 (0.2%)
30	e	0.52	0/1071	0.84	0/1429
31	f	0.48	0/895	0.87	0/1198
32	g	0.46	0/916	0.79	1/1220 (0.1%)
33	h	0.39	0/1021	0.75	1/1348 (0.1%)
34	i	0.53	1/841 (0.1%)	1.85	7/1112 (0.6%)
35	j	0.50	0/720	0.91	2/952 (0.2%)
36	k	0.39	0/575	0.68	0/761
37	l	0.49	0/454	0.83	0/599
38	m	0.41	0/435	0.79	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	n	0.46	0/223	0.89	0/284
4	D	0.40	0/2432	0.70	1/3257 (0.0%)
40	o	0.42	0/864	0.74	0/1140
41	p	0.46	0/718	0.72	0/953
42	r	0.49	0/1017	0.79	0/1364
43	s	0.38	0/1547	0.59	0/2088
44	t	0.41	0/1257	0.70	0/1697
45	1	0.48	0/129	0.61	0/173
46	2	0.26	0/1805	0.71	0/2809
47	3	0.39	1/1777 (0.1%)	0.97	8/2763 (0.3%)
48	5	0.39	2/87790 (0.0%)	0.78	87/136937 (0.1%)
49	7	0.32	0/2858	0.67	0/4455
5	E	0.46	0/1936	0.81	2/2600 (0.1%)
50	8	0.39	0/3701	0.73	0/5766
51	9	0.33	1/41013 (0.0%)	0.78	43/63919 (0.1%)
52	AA	0.41	0/1679	0.68	0/2283
53	BB	0.40	0/1756	0.76	4/2350 (0.2%)
54	CC	0.40	0/1732	0.75	2/2347 (0.1%)
55	DD	0.41	0/1792	0.72	0/2412
56	EE	0.38	0/2115	0.74	1/2843 (0.0%)
57	FF	0.42	1/1531 (0.1%)	0.74	2/2059 (0.1%)
58	GG	0.43	0/1946	0.75	0/2590
59	HH	0.40	0/1544	0.69	1/2068 (0.0%)
6	F	0.45	0/1905	0.75	1/2539 (0.0%)
60	II	0.44	0/1715	0.76	0/2287
61	JJ	0.44	0/1550	0.85	5/2069 (0.2%)
62	KK	0.41	0/851	0.72	0/1147
63	LL	0.44	0/1259	0.75	0/1684
64	MM	0.45	0/968	0.64	0/1296
65	NN	0.44	0/1232	0.75	0/1656
66	OO	0.41	0/1029	0.84	1/1380 (0.1%)
67	PP	0.43	0/1079	0.75	1/1437 (0.1%)
68	QQ	0.37	0/1142	0.73	1/1528 (0.1%)
69	RR	0.38	0/1060	0.70	0/1421
7	G	0.42	0/1967	0.75	2/2647 (0.1%)
70	SS	0.41	0/1157	0.83	2/1548 (0.1%)
71	TT	0.39	0/1120	0.77	2/1499 (0.1%)
72	UU	0.37	0/831	0.69	0/1115
73	VV	0.39	0/645	0.74	0/865
74	WW	0.44	0/1051	0.75	0/1406
75	XX	0.38	0/1116	0.74	0/1490
76	YY	0.40	0/1040	0.72	0/1382
77	ZZ	0.38	0/604	0.74	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	aa	0.39	0/794	0.76	0/1065
79	bb	0.39	0/665	0.64	0/891
8	H	0.40	0/1535	0.74	1/2063 (0.0%)
80	cc	0.36	0/478	0.76	0/640
81	dd	0.41	0/455	0.81	1/603 (0.2%)
82	ee	0.38	0/462	0.74	0/607
83	ff	0.41	0/538	0.61	0/713
84	gg	0.35	0/2493	0.63	0/3394
85	hh	0.32	0/286	0.74	0/443
86	ii	0.38	0/3333	0.62	1/4483 (0.0%)
87	jj	0.43	1/4633 (0.0%)	0.61	2/6249 (0.0%)
9	I	0.40	0/1693	0.68	1/2260 (0.0%)
All	All	0.40	8/242727 (0.0%)	0.77	201/355704 (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
1	A	0	1
11	L	0	1
17	R	0	1
18	S	0	3
2	B	0	2
24	Y	0	1
26	a	0	2
3	C	0	2
31	f	0	2
34	i	0	3
38	m	0	1
42	r	0	1
5	E	0	1
51	9	0	3
52	AA	0	2
56	EE	0	2
57	FF	0	1
59	HH	0	1
66	OO	0	1
68	QQ	0	1
70	SS	0	1
71	TT	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
72	UU	0	1
73	VV	0	1
74	WW	0	1
75	XX	0	1
86	ii	0	2
9	I	0	2
All	All	0	42

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
87	jj	121	LYS	CE-NZ	13.88	1.83	1.49
34	i	91	SER	C-N	-9.54	1.12	1.34
51	9	1306	U	O3'-P	-7.59	1.52	1.61
48	5	957	G	O3'-P	6.93	1.69	1.61
47	3	41	U	C3'-C2'	6.36	1.59	1.52
57	FF	195	GLU	CD-OE1	5.24	1.31	1.25
48	5	4390	A	O3'-P	-5.15	1.54	1.61
14	O	96	GLN	CD-OE1	5.14	1.35	1.24

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	92	SER	CA-C-N	-33.35	43.83	117.20
34	i	91	SER	O-C-N	-30.40	74.06	122.70
34	i	92	SER	C-N-CA	-30.10	46.45	121.70
47	3	70	G	N9-C1'-C2'	-11.69	98.81	114.00
48	5	3753	G	N9-C1'-C2'	-11.37	99.22	114.00
51	9	1305	C	N1-C1'-C2'	-11.22	99.41	114.00
51	9	909	G	N9-C1'-C2'	-10.94	99.78	114.00
51	9	1306	U	N1-C1'-C2'	-10.45	100.41	114.00
48	5	3718	A	N9-C1'-C2'	-10.34	100.56	114.00
51	9	321	C	N1-C1'-C2'	-10.32	100.59	114.00
51	9	1386	A	N9-C1'-C2'	-10.27	100.65	114.00
48	5	1357	C	C4'-C3'-O3'	10.12	133.25	113.00
48	5	1358	G	C4'-C3'-O3'	10.12	133.24	113.00
51	9	1235	G	N9-C1'-C2'	-10.00	101.00	112.00
24	Y	87	ARG	NE-CZ-NH2	9.95	125.27	120.30
51	9	1455	A	N9-C1'-C2'	-9.77	101.25	112.00
48	5	1964	A	N9-C1'-C2'	-9.53	101.52	112.00
51	9	1294	G	N9-C1'-C2'	-9.51	101.54	112.00
47	3	30	G	N9-C1'-C2'	-9.42	101.64	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	30	PRO	CA-N-CD	-8.98	98.92	111.50
35	j	63	ARG	NE-CZ-NH1	8.98	124.79	120.30
48	5	1965	G	N9-C1'-C2'	-8.94	102.17	112.00
51	9	1394	G	C2'-C3'-O3'	8.83	128.93	109.50
47	3	38	A	N9-C1'-C2'	-8.77	102.35	112.00
51	9	322	C	N1-C1'-C2'	-8.73	102.39	112.00
48	5	1969	G	N9-C1'-C2'	-8.73	102.39	112.00
87	jj	121	LYS	CD-CE-NZ	-8.64	91.82	111.70
18	S	83	ARG	NE-CZ-NH2	8.59	124.59	120.30
2	B	37	PRO	CA-N-CD	-8.58	99.48	111.50
22	W	44	ARG	NE-CZ-NH1	8.54	124.57	120.30
70	SS	113	ARG	NE-CZ-NH1	8.52	124.56	120.30
53	BB	136	ARG	NE-CZ-NH2	8.50	124.55	120.30
34	i	25	ARG	NE-CZ-NH1	8.48	124.54	120.30
51	9	908	A	N9-C1'-C2'	-8.44	102.72	112.00
51	9	1212	G	N9-C1'-C2'	-8.44	102.72	112.00
48	5	4975	G	C2'-C3'-O3'	8.41	127.99	109.50
48	5	1961	G	N9-C1'-C2'	-8.22	102.96	112.00
3	C	342	ARG	NE-CZ-NH1	8.17	124.39	120.30
48	5	2027	U	N1-C1'-C2'	-8.01	103.19	112.00
48	5	3888	G	C2'-C3'-O3'	8.01	127.13	109.50
48	5	125	C	C2'-C3'-O3'	8.01	127.11	109.50
51	9	1641	A	O5'-P-OP1	-7.73	98.74	105.70
51	9	1308	U	N1-C1'-C2'	-7.66	103.57	112.00
47	3	39	U	N1-C1'-C2'	-7.60	103.64	112.00
61	JJ	24	ARG	NE-CZ-NH1	7.58	124.09	120.30
48	5	1292	C	C2'-C3'-O3'	7.57	126.16	109.50
48	5	4528	G	C2'-C3'-O3'	7.57	126.15	109.50
48	5	1455	G	C2'-C3'-O3'	7.51	126.03	109.50
71	TT	56	ARG	NE-CZ-NH1	7.50	124.05	120.30
51	9	1305	C	C4'-C3'-O3'	7.49	127.98	113.00
48	5	3718	A	C4'-C3'-O3'	7.43	127.86	113.00
51	9	1234	C	N1-C1'-C2'	-7.43	103.83	112.00
34	i	91	SER	C-N-CA	7.41	140.23	121.70
51	9	1385	G	N9-C1'-C2'	-7.40	103.86	112.00
48	5	2046	G	C2'-C3'-O3'	7.38	125.73	109.50
61	JJ	127	ARG	NE-CZ-NH1	7.35	123.98	120.30
34	i	92	SER	O-C-N	-7.29	111.04	122.70
48	5	1211	G	C2'-C3'-O3'	7.28	125.51	109.50
48	5	1966	C	N1-C1'-C2'	-7.27	104.00	112.00
51	9	110	U	C2'-C3'-O3'	7.22	125.38	109.50
86	ii	182	ARG	NE-CZ-NH1	7.20	123.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	5061	A	C2'-C3'-O3'	7.17	125.27	109.50
48	5	5060	A	C2'-C3'-O3'	7.12	125.16	109.50
47	3	1	G	C5'-C4'-O4'	7.10	117.62	109.10
48	5	1500	A	C2'-C3'-O3'	7.09	125.10	109.50
48	5	1474	C	C2'-C3'-O3'	7.08	125.08	109.50
48	5	4872	G	C2'-C3'-O3'	7.05	125.02	109.50
48	5	2858	A	N9-C1'-C2'	-6.99	104.31	112.00
48	5	4975	G	C4'-C3'-O3'	-6.98	94.75	109.40
48	5	2695	A	C2'-C3'-O3'	6.93	124.80	113.70
29	d	78	ARG	NE-CZ-NH1	6.89	123.75	120.30
48	5	4885	U	C2'-C3'-O3'	6.88	124.71	113.70
48	5	4951	G	C2'-C3'-O3'	6.86	124.67	113.70
48	5	275	C	C2'-C3'-O3'	6.81	124.60	113.70
48	5	406	C	C2'-C3'-O3'	6.81	124.60	113.70
48	5	4948	C	C2'-C3'-O3'	6.76	124.52	113.70
48	5	215	C	C2'-C3'-O3'	6.73	124.47	113.70
48	5	1477	C	C2'-C3'-O3'	6.72	124.45	113.70
51	9	1235	G	C4'-C3'-O3'	6.72	126.43	113.00
48	5	1967	A	N9-C1'-C2'	-6.71	104.62	112.00
48	5	5059	C	C2'-C3'-O3'	6.68	124.38	113.70
68	QQ	126	ARG	NE-CZ-NH2	6.56	123.58	120.30
51	9	321	C	C4'-C3'-O3'	6.54	126.08	113.00
48	5	3697	U	C2'-C3'-O3'	6.52	124.14	113.70
51	9	1305	C	C1'-C2'-O2'	-6.52	91.05	110.60
48	5	1818	G	C2'-C3'-O3'	6.51	124.11	113.70
51	9	1308	U	C4'-C3'-O3'	6.48	125.96	113.00
48	5	2083	C	C4'-C3'-O3'	6.47	125.95	113.00
48	5	1958	A	N9-C1'-C2'	-6.44	104.92	112.00
48	5	1398	A	C2'-C3'-O3'	6.38	123.91	113.70
51	9	312	G	C2'-C3'-O3'	6.36	123.87	113.70
51	9	1681	U	N1-C1'-C2'	-6.31	105.06	112.00
48	5	1969	G	C4'-C3'-O3'	6.30	125.61	113.00
48	5	2028	C	N1-C1'-C2'	-6.28	105.10	112.00
48	5	1964	A	C4'-C3'-O3'	6.26	125.53	113.00
47	3	70	G	C4'-C3'-O3'	6.26	125.52	113.00
51	9	1419	C	C2'-C3'-O3'	6.24	123.69	113.70
48	5	2858	A	C4'-C3'-O3'	6.20	125.40	113.00
48	5	1279	A	C2'-C3'-O3'	6.17	123.57	113.70
61	JJ	131	ARG	NE-CZ-NH1	6.14	123.37	120.30
61	JJ	131	ARG	NE-CZ-NH2	-6.13	117.24	120.30
48	5	1696	C	C2'-C3'-O3'	6.12	123.49	113.70
51	9	1306	U	C5'-C4'-O4'	6.07	116.39	109.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	2123	C	C2'-C3'-O3'	6.05	123.37	113.70
6	F	91	LEU	CA-CB-CG	5.99	129.07	115.30
51	9	666	U	N1-C1'-C2'	5.93	121.71	114.00
34	i	85	ARG	NE-CZ-NH1	5.93	123.26	120.30
48	5	1072	C	N1-C1'-C2'	5.91	121.68	114.00
48	5	1961	G	C4'-C3'-O3'	5.87	124.74	113.00
48	5	2474	G	C2'-C3'-O3'	5.86	123.08	113.70
18	S	83	ARG	NE-CZ-NH1	-5.85	117.38	120.30
47	3	30	G	C4'-C3'-O3'	5.85	124.69	113.00
48	5	90	G	C2'-C3'-O3'	5.84	123.04	113.70
5	E	208	LEU	CA-CB-CG	5.81	128.65	115.30
48	5	957	G	P-O3'-C3'	5.77	126.63	119.70
81	dd	44	ARG	NE-CZ-NH1	5.76	123.18	120.30
54	CC	61	LEU	C-N-CD	5.76	140.49	128.40
5	E	72	PRO	N-CA-CB	5.74	110.19	103.30
48	5	300	A	N9-C1'-C2'	5.72	121.43	114.00
48	5	1236	C	C2'-C3'-O3'	5.69	122.81	113.70
48	5	47	A	C4'-C3'-O3'	5.68	124.35	113.00
51	9	1275	G	C2'-C3'-O3'	5.67	122.77	113.70
48	5	1672	U	N1-C1'-C2'	5.66	121.36	114.00
51	9	1386	A	C4'-C3'-O3'	5.65	124.30	113.00
51	9	1211	G	N9-C1'-C2'	-5.61	105.83	112.00
48	5	1962	A	N9-C1'-C2'	-5.58	105.87	112.00
51	9	1385	G	C4'-C3'-O3'	5.58	124.15	113.00
51	9	1824	A	C2'-C3'-O3'	5.57	122.62	113.70
51	9	1268	C	N1-C1'-C2'	-5.56	105.88	112.00
51	9	1447	G	N9-C1'-C2'	-5.54	105.90	112.00
48	5	2632	U	N1-C1'-C2'	5.53	121.18	114.00
48	5	4378	A	C2'-C3'-O3'	5.53	122.54	113.70
48	5	1848	C	C2'-C3'-O3'	5.52	122.53	113.70
57	FF	135	ARG	NE-CZ-NH2	-5.52	117.54	120.30
10	J	119	TYR	CA-CB-CG	5.51	123.87	113.40
35	j	63	ARG	NE-CZ-NH2	-5.51	117.55	120.30
48	5	1365	C	C4'-C3'-O3'	5.50	124.00	113.00
51	9	488	U	N1-C1'-C2'	5.49	121.14	114.00
53	BB	136	ARG	CG-CD-NE	5.46	123.26	111.80
87	jj	506	ARG	NE-CZ-NH2	-5.44	117.58	120.30
51	9	532	C	C2'-C3'-O3'	5.43	122.40	113.70
17	R	103	ARG	NE-CZ-NH1	5.43	123.02	120.30
48	5	2797	C	N1-C1'-C2'	-5.41	106.05	112.00
51	9	1535	U	N1-C1'-C2'	5.41	121.03	114.00
48	5	977	C	C2'-C3'-O3'	5.38	122.31	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4966	A	N9-C1'-C2'	5.38	121.00	114.00
3	C	232	VAL	CB-CA-C	-5.38	101.18	111.40
48	5	336	A	C1'-O4'-C4'	-5.38	105.60	109.90
17	R	103	ARG	NE-CZ-NH2	-5.34	117.63	120.30
48	5	1329	G	C2'-C3'-O3'	5.33	122.23	113.70
53	BB	136	ARG	NE-CZ-NH1	-5.30	117.65	120.30
48	5	385	A	C4'-C3'-O3'	5.27	123.54	113.00
48	5	3670	C	C4'-C3'-O3'	5.26	123.53	113.00
57	FF	91	ARG	NE-CZ-NH2	5.24	122.92	120.30
48	5	1847	C	C4'-C3'-O3'	-5.24	98.41	109.40
7	G	231	ASP	CB-CG-OD2	5.23	123.01	118.30
48	5	48	G	C2'-C3'-O3'	5.23	122.08	113.70
70	SS	113	ARG	NE-CZ-NH2	-5.23	117.68	120.30
51	9	844	U	O4'-C1'-N1	5.23	112.38	108.20
48	5	2068	C	C4'-C3'-O3'	5.22	123.44	113.00
48	5	4731	G	N9-C1'-C2'	5.22	120.79	114.00
66	OO	146	ARG	NE-CZ-NH2	-5.21	117.69	120.30
51	9	1477	U	C2'-C3'-O3'	5.21	122.04	113.70
48	5	486	C	C2'-C3'-O3'	5.21	122.04	113.70
48	5	2054	U	N1-C1'-C2'	5.20	120.76	114.00
48	5	2246	C	C2'-C3'-O3'	5.20	122.02	113.70
3	C	363	ASP	CB-CG-OD2	5.20	122.98	118.30
3	C	262	ASP	CB-CG-OD2	5.19	122.97	118.30
33	h	22	ASP	CB-CG-OD2	5.19	122.97	118.30
51	9	501	C	N1-C1'-C2'	5.18	120.73	114.00
9	I	183	ASP	CB-CG-OD2	5.17	122.96	118.30
17	R	108	ARG	NE-CZ-NH1	5.17	122.89	120.30
48	5	3715	U	N1-C1'-C2'	-5.15	106.33	112.00
61	JJ	38	ARG	NE-CZ-NH2	-5.15	117.72	120.30
32	g	24	ARG	NE-CZ-NH1	5.14	122.87	120.30
51	9	1863	A	N9-C1'-C2'	5.14	120.69	114.00
8	H	124	ARG	NE-CZ-NH1	5.14	122.87	120.30
48	5	1755	C	C2'-C3'-O3'	5.14	121.92	113.70
48	5	505	G	C2'-C3'-O3'	5.12	121.89	113.70
3	C	204	ARG	NE-CZ-NH2	5.12	122.86	120.30
67	PP	44	ARG	NE-CZ-NH1	5.12	122.86	120.30
54	CC	233	LEU	CA-CB-CG	5.12	127.06	115.30
51	9	1060	A	N9-C1'-C2'	5.11	120.64	114.00
2	B	258	HIS	N-CA-C	5.10	124.77	111.00
47	3	38	A	C4'-C3'-O3'	5.10	123.20	113.00
48	5	1563	A	N9-C1'-C2'	-5.09	106.40	112.00
53	BB	65	ARG	NE-CZ-NH1	5.09	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	S	83	ARG	CG-CD-NE	5.08	122.47	111.80
48	5	1266	G	C2'-C3'-O3'	5.07	121.81	113.70
4	D	22	ARG	NE-CZ-NH1	5.05	122.83	120.30
48	5	1279	A	N9-C1'-C2'	5.05	120.56	114.00
51	9	1234	C	C4'-C3'-O3'	5.04	123.08	113.00
56	EE	11	ARG	NE-CZ-NH2	5.04	122.82	120.30
71	TT	56	ARG	NE-CZ-NH2	-5.04	117.78	120.30
3	C	342	ARG	NE-CZ-NH2	-5.03	117.78	120.30
48	5	3753	G	C4'-C3'-O3'	5.02	123.04	113.00
59	HH	118	ARG	NE-CZ-NH1	5.01	122.80	120.30
48	5	1379	C	O4'-C1'-C2'	-5.01	100.79	105.80
48	5	93	G	C4'-C3'-O3'	5.00	123.01	113.00
48	5	979	C	C2'-C3'-O3'	5.00	121.70	113.70
48	5	3811	G	C2'-C3'-O3'	-5.00	98.50	109.50

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	9	1212	G	Sidechain
51	9	1308	U	Sidechain
51	9	909	G	Sidechain
1	A	196	TRP	Peptide
52	AA	163	CYS	Peptide
52	AA	73	ASP	Peptide
2	B	17	LEU	Peptide
2	B	257	TRP	Peptide
3	C	339	THR	Peptide
3	C	48	ASN	Peptide
5	E	123	SER	Peptide
56	EE	129	ILE	Peptide
56	EE	205	PHE	Peptide
57	FF	43	GLU	Peptide
59	HH	111	LYS	Peptide
9	I	188	LYS	Peptide
9	I	202	ASN	Peptide
11	L	66	TYR	Peptide
66	OO	145	GLY	Peptide
68	QQ	42	ILE	Peptide
17	R	19	LYS	Peptide
18	S	163	HIS	Peptide
18	S	164	LYS	Peptide

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Mol	Chain	Res	Type	Group
18	S	5	GLY	Peptide
70	SS	11	HIS	Peptide
71	TT	42	HIS	Peptide
72	UU	68	THR	Peptide
73	VV	32	ILE	Peptide
74	WW	27	ILE	Peptide
75	XX	98	ASP	Peptide
24	Y	7	VAL	Peptide
26	a	46	ASP	Peptide
26	a	90	ALA	Peptide
31	f	105	LEU	Peptide
31	f	106	TYR	Peptide
34	i	91	SER	Mainchain
34	i	92	SER	Mainchain,Peptide
86	ii	325	ASN	Peptide
86	ii	371	SER	Peptide
38	m	111	ARG	Peptide
42	r	70	GLN	Peptide

5.2 Too-close contacts ⓘ

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	A	1868	0	1959	19	0
2	B	3148	0	3267	30	0
3	C	2883	0	3053	41	0
4	D	2386	0	2419	23	0
5	E	1898	0	2035	34	0
6	F	1870	0	1994	18	0
7	G	1934	0	2087	36	0
8	H	1516	0	1597	10	0
9	I	1655	0	1704	36	0
10	J	1353	0	1386	16	0
11	L	1703	0	1820	22	0
12	M	1137	0	1211	23	0
13	N	1701	0	1749	16	0
14	O	1638	0	1777	23	0
15	P	1242	0	1274	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Q	1506	0	1623	10	0
17	R	1508	0	1664	34	0
18	S	1454	0	1496	11	0
19	T	1298	0	1366	11	0
20	U	808	0	831	3	0
21	V	979	0	1039	3	0
22	W	528	0	541	3	0
23	X	976	0	1053	6	0
24	Y	1115	0	1205	6	0
25	Z	1107	0	1182	11	0
26	a	1162	0	1209	0	0
27	b	609	0	650	0	0
28	c	732	0	769	0	0
29	d	888	0	930	0	0
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	1000	0	0
33	h	1013	0	1147	0	0
34	i	830	0	914	0	0
35	j	705	0	737	0	0
36	k	569	0	637	0	0
37	l	444	0	483	0	0
38	m	429	0	467	0	0
39	n	222	0	264	0	0
40	o	851	0	921	0	0
41	p	708	0	757	0	0
42	r	1001	0	1060	0	0
43	s	1523	0	1577	0	0
44	t	1238	0	1295	0	0
45	1	125	0	117	3	0
46	2	1616	0	824	15	0
47	3	1593	0	811	111	0
48	5	78486	0	39661	1252	0
49	7	2558	0	1296	26	0
50	8	3314	0	1683	48	0
51	9	36680	0	18530	603	0
52	AA	1642	0	1646	14	0
53	BB	1729	0	1803	9	0
54	CC	1694	0	1782	35	0
55	DD	1764	0	1863	8	0
56	EE	2073	0	2175	22	0
57	FF	1509	0	1563	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	GG	1923	0	2089	20	0
59	HH	1521	0	1616	14	0
60	II	1686	0	1772	30	0
61	JJ	1525	0	1640	18	0
62	KK	827	0	854	5	0
63	LL	1238	0	1315	11	0
64	MM	958	0	993	3	0
65	NN	1208	0	1294	6	0
66	OO	1016	0	1039	13	0
67	PP	1060	0	1120	12	0
68	QQ	1124	0	1193	6	0
69	RR	1047	0	1103	17	0
70	SS	1139	0	1191	11	0
71	TT	1102	0	1142	11	0
72	UU	821	0	883	1	0
73	VV	636	0	634	4	0
74	WW	1034	0	1080	5	0
75	XX	1098	0	1167	11	0
76	YY	1023	0	1090	7	0
77	ZZ	598	0	656	3	0
78	aa	781	0	828	0	0
79	bb	651	0	672	0	0
80	cc	475	0	497	0	0
81	dd	445	0	439	0	0
82	ee	457	0	502	0	0
83	ff	527	0	545	0	0
84	gg	2436	0	2393	0	0
85	hh	256	0	129	0	0
86	ii	3280	0	3326	0	0
87	jj	4551	0	4687	0	0
88	5	146	0	0	0	0
88	7	5	0	0	0	0
88	8	2	0	0	0	0
88	9	35	0	0	0	0
88	C	1	0	0	0	0
88	I	1	0	0	0	0
88	P	1	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
89	aa	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	dd	1	0	0	0	0
89	ff	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	16	0	0	0	0
91	jj	54	0	24	0	0
All	All	226469	0	169875	2584	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 7.

All (2584) 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)
61:JJ:121:LYS:NZ	61:JJ:121:LYS:CE	1.49	1.39
57:FF:194:ASP:O	57:FF:198:ARG:HG3	1.28	1.33
48:5:976:G:H2'	48:5:977:C:O4'	1.26	1.30
7:G:29:ASN:OD1	7:G:30:PRO:HD3	1.30	1.28
48:5:4213:A:N1	48:5:4218:U:O4	1.66	1.26
51:9:1454:A:OP1	69:RR:3:ARG:NE	1.71	1.22
48:5:2367:A:N1	48:5:2788:U:O4	1.72	1.21
9:I:191:ILE:CD1	9:I:200:ILE:HD12	1.71	1.21
48:5:2468:U:O4	48:5:2473:A:N1	1.72	1.20
48:5:1929:A:N1	48:5:2054:U:O4	1.73	1.20
54:CC:191:VAL:HA	54:CC:228:SER:OG	1.03	1.19
57:FF:194:ASP:OD1	57:FF:198:ARG:NE	1.77	1.18
48:5:1963:C:N3	48:5:4694:G:O6	1.74	1.17
9:I:191:ILE:HD12	9:I:200:ILE:CD1	1.78	1.14
57:FF:194:ASP:OD1	57:FF:198:ARG:CZ	1.95	1.14
5:E:59:TYR:CD2	5:E:64:LEU:HD12	1.84	1.12
56:EE:52:LEU:HD13	56:EE:54:TYR:CD2	1.85	1.11
7:G:30:PRO:HD2	7:G:31:LEU:H	1.13	1.08
54:CC:191:VAL:CA	54:CC:228:SER:OG	1.99	1.08
7:G:86:VAL:HG21	7:G:185:LYS:HE3	1.37	1.07
7:G:86:VAL:HG11	7:G:185:LYS:HG2	1.34	1.06
51:9:872:A:N1	51:9:914:U:O4	1.89	1.05
9:I:191:ILE:CD1	9:I:200:ILE:CD1	2.35	1.04
17:R:174:GLU:O	17:R:178:GLN:OE1	1.75	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:6:G:N2	47:3:67:U:O2	1.89	1.04
51:9:1454:A:P	69:RR:3:ARG:HE	1.80	1.03
48:5:1962:A:C2'	48:5:1963:C:H5'	1.88	1.02
48:5:2409:U:C4	48:5:2783:A:N1	2.28	1.02
48:5:1929:A:H61	48:5:2054:U:H3	1.04	1.02
51:9:1308:U:C4	51:9:1309:C:C6	2.49	1.01
17:R:178:GLN:OE1	17:R:178:GLN:N	1.94	1.01
48:5:1983:A:N1	48:5:2008:U:C4	2.30	1.00
9:I:191:ILE:HD11	9:I:200:ILE:HD12	1.38	1.00
48:5:1983:A:N1	48:5:2008:U:O4	1.95	0.99
51:9:830:A:N6	51:9:844:U:N3	2.08	0.99
7:G:156:VAL:HG11	7:G:184:LEU:HD12	1.40	0.99
54:CC:227:TRP:O	54:CC:228:SER:OG	1.80	0.99
48:5:4694:G:N2	48:5:4694:G:OP1	1.94	0.99
47:3:39:U:O4'	57:FF:135:ARG:NH2	1.97	0.98
47:3:5:G:H2'	47:3:6:G:C8	1.98	0.98
3:C:161:TYR:CD1	3:C:166:GLU:HB3	1.99	0.98
51:9:1448:A:O2'	51:9:1449:G:C5'	2.12	0.97
48:5:77:U:O4	48:5:335:A:N1	1.96	0.97
51:9:1144:A:H2'	51:9:1145:A:C8	1.99	0.97
10:J:80:GLU:OE2	10:J:170:TYR:OH	1.81	0.97
11:L:170:THR:HG22	11:L:173:GLU:HG3	1.46	0.97
47:3:35:U:C1'	51:9:1641:A:OP1	2.14	0.96
48:5:2409:U:O4	48:5:2783:A:N1	1.98	0.95
2:B:163:LEU:CD2	2:B:182:GLU:HG2	1.95	0.95
48:5:1563:A:N6	51:9:1028:A:N1	2.16	0.94
17:R:176:ARG:HB2	17:R:176:ARG:NH2	1.81	0.94
7:G:29:ASN:OD1	7:G:30:PRO:CD	2.16	0.94
51:9:872:A:N1	51:9:914:U:C4	2.36	0.93
54:CC:191:VAL:HA	54:CC:228:SER:CB	1.98	0.93
51:9:830:A:N1	51:9:844:U:O4	2.02	0.93
48:5:1278:C:H3'	48:5:1279:A:H4'	1.50	0.92
54:CC:60:TRP:O	54:CC:61:LEU:HD12	1.68	0.92
48:5:1968:G:H1	48:5:2018:C:H42	0.93	0.92
47:3:39:U:HO2'	47:3:40:C:H6	0.92	0.91
51:9:1681:U:O2'	51:9:1682:C:O4'	1.88	0.91
51:9:1407:U:H2'	51:9:1408:U:C5	2.05	0.91
48:5:976:G:C2'	48:5:977:C:O4'	2.18	0.91
47:3:6:G:H1	47:3:67:U:H3	1.18	0.91
56:EE:52:LEU:HD13	56:EE:54:TYR:HD2	1.28	0.91
47:3:68:C:O2'	47:3:69:G:O4'	1.88	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:5:G:N1	47:3:68:C:O2	2.05	0.90
51:9:1305:C:O2'	51:9:1306:U:H5'	1.72	0.90
48:5:1968:G:H1	48:5:2018:C:N4	1.69	0.90
51:9:1233:G:C2'	51:9:1234:C:H5'	2.02	0.90
9:I:191:ILE:HD12	9:I:200:ILE:HD11	1.55	0.89
57:FF:194:ASP:OD1	57:FF:198:ARG:NH1	2.05	0.89
54:CC:73:VAL:HG12	54:CC:73:VAL:O	1.71	0.88
11:L:164:GLU:N	11:L:164:GLU:OE2	2.06	0.88
4:D:33:ARG:NH2	49:7:7:G:O3'	2.06	0.88
48:5:2395:A:O2'	48:5:2806:A:H1'	1.72	0.88
48:5:2026:A:C2'	48:5:2027:U:H5'	2.04	0.88
47:3:66:U:C4	47:3:67:U:C5	2.61	0.88
47:3:5:G:C2	47:3:6:G:C5	2.61	0.87
51:9:1267:C:O2'	51:9:1268:C:H5'	1.72	0.87
2:B:163:LEU:HD23	2:B:182:GLU:HG2	1.57	0.87
48:5:957:G:H1'	48:5:958:G:OP2	1.75	0.87
47:3:67:U:O2'	47:3:68:C:H5'	1.74	0.87
7:G:30:PRO:HD2	7:G:31:LEU:N	1.90	0.86
51:9:1454:A:OP1	69:RR:3:ARG:CZ	2.23	0.86
5:E:238:ILE:O	5:E:239:THR:OG1	1.92	0.86
48:5:2027:U:O2'	48:5:2028:C:H5'	1.74	0.86
48:5:3753:G:OP2	48:5:3776:G:O2'	1.92	0.86
48:5:102:G:O2'	48:5:1381:U:O2'	1.93	0.86
48:5:1929:A:N6	48:5:2054:U:H3	1.72	0.86
48:5:2468:U:N3	48:5:2473:A:N6	2.24	0.85
51:9:1448:A:O2'	51:9:1449:G:H5''	1.76	0.85
51:9:1235:G:H2'	51:9:1236:G:H8	1.42	0.85
51:9:830:A:N6	51:9:844:U:H3	1.73	0.85
9:I:191:ILE:HD12	9:I:200:ILE:HD12	1.42	0.84
57:FF:194:ASP:O	57:FF:198:ARG:CG	2.20	0.84
51:9:1305:C:C2'	51:9:1306:U:H5'	2.06	0.84
48:5:1279:A:C3'	48:5:1280:C:H5''	2.08	0.83
17:R:172:ARG:CB	51:9:909:G:OP2	2.26	0.83
48:5:4694:G:H21	48:5:4694:G:P	2.00	0.83
48:5:1963:C:C4	48:5:4694:G:O6	2.31	0.83
51:9:1233:G:O2'	51:9:1234:C:H5'	1.79	0.82
48:5:5026:U:H5'	60:II:79:ILE:HD11	1.62	0.82
12:M:116:LYS:CG	14:O:196:LEU:HD21	2.10	0.82
48:5:3914:U:H3	48:5:4378:A:N6	1.76	0.81
61:JJ:121:LYS:NZ	61:JJ:121:LYS:CD	2.48	0.81
56:EE:52:LEU:HD13	56:EE:54:TYR:CE2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:723:A:H2	48:5:943:A:N1	1.79	0.81
48:5:4075:U:O2'	48:5:4076:G:H2'	1.80	0.81
7:G:156:VAL:HG11	7:G:184:LEU:CD1	2.10	0.81
48:5:3751:G:C2'	48:5:3752:C:H5'	2.11	0.81
17:R:176:ARG:HH21	17:R:176:ARG:HB2	1.46	0.81
48:5:1367:C:C2	48:5:1370:G:H2'	2.16	0.80
47:3:5:G:H2'	47:3:6:G:H8	1.41	0.80
2:B:163:LEU:HD21	2:B:182:GLU:HG2	1.63	0.80
51:9:321:C:O2'	51:9:322:C:H5'	1.82	0.80
47:3:38:A:C2	57:FF:135:ARG:NH1	2.50	0.79
47:3:4:C:C2	47:3:5:G:N7	2.50	0.79
47:3:6:G:O2'	47:3:7:A:O4'	1.99	0.79
7:G:156:VAL:CG1	7:G:184:LEU:HD12	2.13	0.79
59:HH:66:VAL:HG22	59:HH:96:ALA:HB1	1.64	0.79
51:9:1293:A:N6	51:9:1306:U:O2	2.16	0.79
51:9:1268:C:O2'	51:9:1269:G:O5'	2.00	0.79
51:9:1235:G:H2'	51:9:1236:G:C8	2.18	0.79
48:5:2026:A:O2'	48:5:2027:U:H5'	1.82	0.78
51:9:656:G:O2'	54:CC:227:TRP:NE1	2.15	0.78
48:5:723:A:C2	48:5:943:A:N1	2.51	0.78
48:5:504:G:N1	48:5:654:C:C2	2.52	0.78
48:5:919:C:N4	48:5:920:C:C4	2.52	0.78
51:9:1293:A:N6	51:9:1306:U:C2	2.52	0.78
51:9:1102:G:N2	51:9:1103:C:C2	2.50	0.78
48:5:1213:G:C6	48:5:1215:C:C2	2.71	0.78
9:I:48:LEU:HD21	9:I:145:LYS:HG2	1.63	0.78
48:5:1279:A:H3'	48:5:1280:C:H5"	1.64	0.78
17:R:176:ARG:NH1	51:9:909:G:OP1	2.17	0.77
48:5:1379:C:H4'	48:5:1380:G:O4'	1.84	0.77
51:9:1385:G:O2'	51:9:1386:A:H5'	1.85	0.77
48:5:1962:A:H2'	48:5:1963:C:H5'	1.66	0.77
7:G:86:VAL:HG21	7:G:185:LYS:CE	2.15	0.77
54:CC:211:LYS:O	54:CC:215:LEU:HG	1.84	0.77
48:5:4371:G:O2'	48:5:4372:U:OP2	2.03	0.77
12:M:116:LYS:HG3	14:O:196:LEU:HD21	1.67	0.77
17:R:174:GLU:O	17:R:178:GLN:CD	2.22	0.77
17:R:168:GLU:O	17:R:172:ARG:HG2	1.83	0.77
48:5:3914:U:H3	48:5:4378:A:H61	1.29	0.77
2:B:14:LEU:HD23	2:B:17:LEU:HD21	1.66	0.77
51:9:322:C:O2'	51:9:323:C:O5'	2.02	0.77
48:5:745:G:H2'	48:5:746:A:O4'	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:872:A:C6	51:9:914:U:O4	2.37	0.76
47:3:39:U:O2'	47:3:40:C:H6	1.67	0.76
47:3:35:U:O4'	51:9:1641:A:OP1	2.03	0.76
48:5:1563:A:C8	51:9:678:U:H4'	2.20	0.76
48:5:2468:U:C4	48:5:2473:A:N1	2.54	0.76
51:9:1420:G:HO2'	71:TT:4:VAL:N	1.84	0.76
51:9:643:A:OP2	61:JJ:38:ARG:NH2	2.18	0.76
5:E:217:GLN:NE2	5:E:233:LYS:HD2	2.01	0.76
70:SS:11:HIS:O	70:SS:12:ILE:HD12	1.85	0.76
7:G:86:VAL:HG12	7:G:87:LEU:N	2.00	0.76
51:9:913:A:OP1	59:HH:99:ARG:NH2	2.19	0.75
51:9:1293:A:C6	51:9:1306:U:C2	2.74	0.75
48:5:4723:A:H2'	48:5:4724:A:C8	2.21	0.75
48:5:166:C:O2	48:5:167:C:H5	1.69	0.75
48:5:3629:A:H4'	51:9:1721:U:O2	1.85	0.75
2:B:174:ARG:NH1	48:5:4985:U:O2	2.19	0.75
47:3:35:U:H1'	51:9:1641:A:OP1	1.84	0.75
48:5:504:G:C2	48:5:654:C:O2	2.39	0.75
54:CC:204:ILE:HD13	54:CC:215:LEU:CD2	2.16	0.75
48:5:2793:G:C6	48:5:2797:C:C4	2.75	0.75
7:G:30:PRO:CD	7:G:31:LEU:H	1.96	0.74
13:N:202:ARG:NH2	48:5:1372:A:OP1	2.21	0.74
51:9:872:A:C6	51:9:914:U:C4	2.76	0.74
51:9:1406:G:H3'	51:9:1407:U:H4'	1.69	0.74
51:9:1454:A:P	69:RR:3:ARG:NE	2.51	0.74
48:5:2769:U:C2	48:5:2770:C:C5	2.76	0.74
9:I:202:ASN:O	49:7:63:C:C5	2.40	0.74
9:I:49:CYS:SG	9:I:51:HIS:NE2	2.60	0.74
51:9:980:A:H2'	51:9:981:A:C8	2.23	0.74
47:3:33:U:P	57:FF:127:ARG:HH12	2.11	0.73
58:GG:3:LEU:HD13	58:GG:111:LEU:HD11	1.69	0.73
51:9:1211:G:C2'	51:9:1212:G:H5'	2.18	0.73
47:3:35:U:H1'	51:9:1641:A:P	2.28	0.73
54:CC:60:TRP:C	54:CC:61:LEU:HD12	2.08	0.73
4:D:200:MET:HE2	4:D:241:LYS:HG3	1.71	0.73
48:5:2367:A:N6	48:5:2798:A:O4'	2.21	0.73
51:9:1308:U:H3	51:9:1309:C:H1'	1.53	0.73
2:B:163:LEU:CD2	2:B:182:GLU:CG	2.65	0.73
48:5:3629:A:C4'	51:9:1721:U:O2	2.36	0.73
47:3:13:C:N3	47:3:22:G:O6	2.22	0.73
47:3:66:U:C5	47:3:67:U:C5	2.77	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:911:C:H2'	51:9:912:C:H5'	1.71	0.72
47:3:35:U:C1'	51:9:1641:A:P	2.77	0.72
51:9:309:G:N2	51:9:310:C:C2	2.58	0.72
4:D:200:MET:CE	4:D:241:LYS:HG3	2.19	0.72
48:5:166:C:O2	48:5:167:C:C5	2.42	0.72
51:9:1308:U:O2'	51:9:1309:C:O5'	2.08	0.72
11:L:170:THR:CG2	11:L:173:GLU:HG3	2.19	0.72
48:5:516:C:C2	48:5:646:G:N2	2.58	0.72
51:9:103:A:OP2	51:9:356:C:N4	2.22	0.71
51:9:1680:G:O2'	51:9:1681:U:H5'	1.89	0.71
51:9:1235:G:H5'	51:9:1247:C:H42	1.53	0.71
47:3:33:U:C5'	57:FF:127:ARG:HH12	2.02	0.71
59:HH:93:VAL:HG21	59:HH:133:LEU:HD23	1.72	0.71
47:3:35:U:O4'	51:9:1641:A:P	2.49	0.71
48:5:286:U:H2'	48:5:287:U:C6	2.26	0.71
3:C:161:TYR:CE1	3:C:166:GLU:HB3	2.25	0.71
51:9:751:G:C2	51:9:792:C:N3	2.58	0.71
48:5:4579:U:H2'	48:5:4580:U:C6	2.25	0.71
2:B:163:LEU:HD21	2:B:182:GLU:CG	2.20	0.71
51:9:911:C:C2'	51:9:912:C:H5'	2.20	0.71
51:9:1386:A:H2'	51:9:1387:G:C8	2.26	0.71
10:J:119:TYR:HB3	70:SS:12:ILE:HD13	1.72	0.71
48:5:1278:C:C3'	48:5:1279:A:H4'	2.19	0.71
48:5:1962:A:O2'	48:5:1963:C:H5'	1.89	0.71
48:5:4901:G:N2	48:5:4921:C:C2	2.59	0.71
48:5:973:G:N2	48:5:1282:G:O2'	2.23	0.71
47:3:76:A:N7	48:5:4371:G:C6	2.59	0.70
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.72	0.70
47:3:4:C:C2	47:3:5:G:C8	2.80	0.70
48:5:77:U:N3	48:5:335:A:N6	2.39	0.70
10:J:165:TRP:CH2	10:J:170:TYR:HE2	2.10	0.70
11:L:56:ARG:O	11:L:116:ARG:NH2	2.23	0.70
48:5:978:G:H2'	48:5:979:C:O4'	1.91	0.70
4:D:200:MET:HE1	4:D:241:LYS:N	2.06	0.70
48:5:22:G:N2	50:8:35:C:C2	2.59	0.70
48:5:3723:A:H2'	48:5:3724:A:C8	2.26	0.70
54:CC:204:ILE:HD13	54:CC:215:LEU:HD21	1.72	0.70
48:5:4213:A:N1	48:5:4218:U:C4	2.57	0.70
49:7:30:C:C2	49:7:48:G:N2	2.59	0.70
47:3:1:G:N2	47:3:2:C:C2	2.59	0.70
47:3:68:C:C2	47:3:69:G:C8	2.79	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:181:C:N3	48:5:256:G:C2	2.60	0.70
48:5:4453:C:C2	48:5:4529:G:C2	2.80	0.70
47:3:4:C:HO2'	47:3:5:G:H8	1.38	0.70
48:5:499:G:N2	48:5:656:C:C2	2.60	0.70
48:5:977:C:C2	48:5:978:G:C8	2.80	0.69
51:9:1386:A:O2'	51:9:1387:G:H5'	1.90	0.69
48:5:956:A:H4'	48:5:957:G:OP2	1.93	0.69
48:5:504:G:C6	48:5:654:C:N3	2.60	0.69
47:3:68:C:C2	47:3:69:G:N7	2.60	0.69
51:9:1102:G:N1	51:9:1103:C:C4	2.60	0.69
48:5:1958:A:C2	48:5:2026:A:C2	2.80	0.69
51:9:872:A:C2	51:9:914:U:O4	2.45	0.69
63:LL:131:CYS:SG	63:LL:132:ARG:N	2.64	0.69
48:5:1929:A:N1	48:5:2054:U:C4	2.59	0.69
3:C:161:TYR:CD1	3:C:166:GLU:CB	2.74	0.69
51:9:1407:U:H2'	51:9:1408:U:C6	2.28	0.69
47:3:76:A:C6	48:5:4371:G:C5	2.81	0.69
48:5:499:G:C2	48:5:656:C:C2	2.80	0.69
48:5:1964:A:C2'	48:5:1965:G:H5'	2.23	0.69
48:5:166:C:H2'	48:5:166:C:O2	1.92	0.69
48:5:3753:G:N2	48:5:3754:G:C4	2.61	0.69
48:5:1380:G:O2'	48:5:1381:U:O2	2.09	0.69
48:5:5024:C:H2'	60:II:168:GLN:HG3	1.75	0.69
5:E:251:SER:O	5:E:255:PRO:CD	2.41	0.68
48:5:497:G:N2	48:5:657:C:C2	2.61	0.68
9:I:203:ARG:NH2	49:7:105:C:OP2	2.25	0.68
48:5:2409:U:C4	48:5:2783:A:C2	2.80	0.68
7:G:87:LEU:HD23	7:G:184:LEU:CD2	2.23	0.68
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.26	0.68
48:5:2084:C:H3'	48:5:2085:G:H5'	1.76	0.68
48:5:642:G:N2	48:5:643:C:C2	2.61	0.68
47:3:5:G:N1	47:3:6:G:C6	2.61	0.68
48:5:3751:G:O2'	48:5:3752:C:H5'	1.92	0.68
48:5:2773:G:N2	48:5:2774:C:C2	2.62	0.68
48:5:1964:A:H2'	48:5:1965:G:H5'	1.75	0.68
17:R:176:ARG:NH1	51:9:909:G:H5'	2.09	0.67
4:D:200:MET:CE	4:D:237:GLU:O	2.43	0.67
48:5:1280:C:C4	48:5:1282:G:C6	2.82	0.67
10:J:83:LEU:HD12	10:J:170:TYR:OH	1.93	0.67
51:9:522:A:OP2	61:JJ:45:ARG:NH2	2.27	0.67
51:9:50:A:N1	51:9:488:U:O4	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:33:U:C5'	57:FF:127:ARG:NH1	2.57	0.67
48:5:2367:A:N1	48:5:2788:U:C4	2.61	0.67
51:9:1448:A:O2'	51:9:1449:G:O5'	2.12	0.67
48:5:1956:A:H2'	48:5:1957:U:C6	2.30	0.67
48:5:1264:C:H2'	48:5:1265:G:O4'	1.94	0.67
48:5:2632:U:H2'	48:5:2633:U:C6	2.29	0.67
48:5:1983:A:C2	48:5:2008:U:C4	2.82	0.67
47:3:34:U:O2	51:9:1641:A:H5'	1.94	0.67
51:9:1253:A:OP2	51:9:1526:G:N2	2.27	0.67
48:5:1968:G:O2'	48:5:1969:G:O5'	2.13	0.67
48:5:1635:C:C2'	48:5:1636:U:H5'	2.24	0.67
48:5:1358:G:C6	48:5:1379:C:N3	2.63	0.66
17:R:172:ARG:HB2	51:9:909:G:OP2	1.95	0.66
48:5:969:C:O2'	48:5:970:G:N3	2.28	0.66
48:5:1724:G:H4'	48:5:1725:U:OP2	1.95	0.66
47:3:13:C:O2	47:3:22:G:N1	2.27	0.66
74:WW:52:ILE:HG22	74:WW:61:ILE:HG12	1.76	0.66
48:5:2654:C:C2	48:5:2681:G:N2	2.64	0.66
51:9:1649:U:C4	51:9:1675:A:N1	2.63	0.66
56:EE:52:LEU:CD1	56:EE:54:TYR:HD2	2.04	0.66
47:3:66:U:C4	47:3:67:U:C4	2.83	0.66
48:5:1983:A:C6	48:5:2008:U:O4	2.49	0.66
12:M:116:LYS:HG2	14:O:196:LEU:HD21	1.76	0.66
9:I:187:GLU:O	9:I:188:LYS:HE3	1.95	0.66
51:9:1293:A:C6	51:9:1306:U:O2	2.48	0.66
48:5:2127:C:H2'	48:5:2128:G:C8	2.30	0.66
48:5:2367:A:N6	48:5:2788:U:N3	2.44	0.66
48:5:5026:U:OP2	60:II:79:ILE:HD13	1.94	0.66
12:M:126:GLU:HG3	14:O:181:ALA:CB	2.26	0.66
48:5:977:C:C2'	48:5:978:G:H5'	2.25	0.66
17:R:176:ARG:HH11	51:9:909:G:H4'	1.59	0.66
48:5:3712:A:C2	51:9:970:G:C6	2.84	0.66
48:5:986:C:C2	48:5:1068:G:N2	2.63	0.66
48:5:2288:G:N2	48:5:2290:C:C2	2.64	0.66
48:5:4481:U:H2'	48:5:4482:U:C6	2.30	0.66
48:5:1268:G:H4'	48:5:1269:G:OP1	1.96	0.66
7:G:87:LEU:HD23	7:G:184:LEU:HD21	1.77	0.66
51:9:913:A:H62	59:HH:120:ARG:HG3	1.61	0.66
47:3:37:A:C2'	47:3:38:A:H5'	2.25	0.65
2:B:261:ARG:HE	48:5:3870:C:H4'	1.61	0.65
48:5:1279:A:C2'	48:5:1280:C:H5''	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:83:LEU:HD12	10:J:170:TYR:CZ	2.30	0.65
16:Q:11:ARG:NH2	48:5:1690:C:OP2	2.29	0.65
45:1:57:ARG:NH2	48:5:3862:A:O2'	2.29	0.65
51:9:316:G:N2	51:9:317:C:C2	2.64	0.65
47:3:29:A:O2'	47:3:30:G:O5'	2.10	0.65
12:M:126:GLU:HG3	14:O:181:ALA:HB1	1.79	0.65
48:5:3668:C:C2	48:5:3675:G:C2	2.85	0.65
47:3:35:U:H1'	51:9:1640:A:O3'	1.97	0.65
51:9:1267:C:HO2'	51:9:1268:C:H5'	1.61	0.65
51:9:1444:U:H2'	51:9:1445:U:C6	2.31	0.65
51:9:1454:A:C2	51:9:1476:A:H4'	2.31	0.65
51:9:1454:A:O2'	51:9:1455:A:OP2	2.12	0.65
51:9:50:A:N1	51:9:488:U:C4	2.65	0.65
48:5:2367:A:N6	48:5:2788:U:H3	1.95	0.65
48:5:1958:A:N1	48:5:2026:A:N1	2.45	0.65
51:9:412:G:N2	51:9:429:C:C2	2.65	0.65
51:9:1109:C:O2	51:9:1109:C:H2'	1.94	0.65
47:3:66:U:H2'	47:3:67:U:O4'	1.97	0.65
4:D:200:MET:HE3	4:D:240:TYR:HB2	1.78	0.65
48:5:1359:G:H2'	48:5:1360:G:C8	2.32	0.65
48:5:2409:U:O4	48:5:2783:A:C6	2.50	0.64
48:5:1563:A:C8	48:5:1563:A:O5'	2.49	0.64
51:9:913:A:N6	59:HH:120:ARG:HG3	2.12	0.64
5:E:126:ARG:NH2	48:5:712:C:O2'	2.31	0.64
48:5:2258:C:O2	48:5:2258:C:H2'	1.96	0.64
51:9:200:G:N2	51:9:201:C:C2	2.65	0.64
48:5:1550:G:C2	48:5:1579:C:C2	2.85	0.64
48:5:482:G:H2'	48:5:483:G:C8	2.33	0.64
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.78	0.64
51:9:1406:G:C3'	51:9:1407:U:H4'	2.27	0.64
51:9:751:G:N2	51:9:792:C:C2	2.66	0.64
48:5:3662:A:H61	48:5:3680:U:H3	1.44	0.64
5:E:254:LEU:HD23	5:E:254:LEU:O	1.96	0.64
48:5:22:G:C2	50:8:35:C:N3	2.66	0.64
48:5:976:G:OP1	48:5:976:G:H4'	1.96	0.64
48:5:504:G:C6	48:5:654:C:C2	2.85	0.64
71:TT:33:TRP:O	71:TT:35:ASP:N	2.30	0.64
48:5:1962:A:C3'	48:5:1963:C:H5'	2.27	0.64
51:9:872:A:N6	51:9:914:U:C5	2.66	0.64
48:5:1358:G:H8	48:5:1358:G:H3'	1.61	0.64
47:3:76:A:N6	48:5:4371:G:N7	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2090:U:P	48:5:2090:U:O4'	2.56	0.64
47:3:38:A:C2	57:FF:135:ARG:CZ	2.81	0.63
51:9:1144:A:C2	51:9:1145:A:C2	2.85	0.63
3:C:114:ARG:HB2	3:C:114:ARG:CZ	2.28	0.63
48:5:1404:G:C2	48:5:1414:C:C2	2.85	0.63
48:5:111:C:C2	48:5:331:G:C2	2.86	0.63
48:5:1358:G:H2'	48:5:1359:G:O4'	1.97	0.63
48:5:1213:G:N1	48:5:1215:C:C2	2.67	0.63
48:5:1268:G:C2	48:5:1270:A:C8	2.86	0.63
48:5:5066:U:H2'	48:5:5067:U:C6	2.33	0.63
7:G:30:PRO:CD	7:G:31:LEU:N	2.59	0.63
48:5:1378:C:H3'	48:5:1379:C:C5'	2.29	0.63
51:9:200:G:N1	51:9:201:C:C4	2.66	0.63
48:5:3610:A:O2'	60:II:89:GLU:OE1	2.04	0.63
76:YY:110:ARG:O	76:YY:113:ARG:O	2.16	0.63
48:5:1279:A:H3'	48:5:1280:C:C5'	2.29	0.63
7:G:87:LEU:CD2	7:G:184:LEU:HD21	2.29	0.63
7:G:86:VAL:CG1	7:G:87:LEU:N	2.61	0.63
47:3:68:C:N3	47:3:69:G:N7	2.47	0.63
51:9:1453:C:H2'	51:9:1454:A:H4'	1.81	0.63
9:I:191:ILE:HD11	9:I:200:ILE:CD1	2.18	0.63
54:CC:73:VAL:CG1	54:CC:73:VAL:O	2.45	0.63
11:L:116:ARG:NH1	11:L:155:MET:O	2.29	0.63
48:5:1635:C:H2'	48:5:1636:U:H5'	1.79	0.63
48:5:2108:G:C6	48:5:2125:C:N4	2.66	0.63
48:5:1957:U:O2'	48:5:1958:A:H8	1.82	0.63
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.81	0.63
9:I:80:CYS:SG	9:I:81:GLY:N	2.71	0.63
47:3:67:U:C2'	47:3:68:C:H5'	2.29	0.62
49:7:30:C:N3	49:7:48:G:C2	2.67	0.62
10:J:83:LEU:CD1	10:J:170:TYR:CZ	2.82	0.62
7:G:86:VAL:HG12	7:G:87:LEU:H	1.65	0.62
12:M:126:GLU:CG	14:O:181:ALA:HB1	2.29	0.62
48:5:933:G:C2	48:5:940:C:C6	2.88	0.62
3:C:271:ALA:O	3:C:272:SER:OG	2.12	0.62
14:O:72:HIS:N	48:5:4586:G:OP1	2.30	0.62
48:5:1241:C:N4	48:5:1270:A:O2'	2.33	0.62
48:5:5000:G:C2	48:5:5051:C:C2	2.87	0.62
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.82	0.62
51:9:474:G:N2	51:9:475:C:C2	2.67	0.62
51:9:1842:C:C2	51:9:1858:G:C2	2.88	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4461:C:O2	48:5:4516:G:C2	2.53	0.62
51:9:1771:G:N2	51:9:1772:C:C2	2.67	0.62
51:9:1537:A:H2'	51:9:1538:C:O4'	2.00	0.62
51:9:1727:G:H2'	51:9:1728:U:O4'	1.99	0.62
51:9:1466:G:N2	51:9:1467:C:C2	2.68	0.62
48:5:106:A:H1'	48:5:336:A:C8	2.34	0.62
48:5:1358:G:O2'	48:5:1359:G:O4'	2.16	0.62
48:5:1367:C:N3	48:5:1369:C:OP2	2.32	0.62
48:5:1957:U:O2'	48:5:1958:A:OP2	2.18	0.62
48:5:2547:G:N2	48:5:2548:C:C2	2.68	0.62
48:5:1964:A:O2'	48:5:1965:G:H5'	1.99	0.61
7:G:156:VAL:CG1	7:G:184:LEU:CD1	2.75	0.61
51:9:1386:A:H2'	51:9:1387:G:H8	1.62	0.61
48:5:1358:G:H3'	48:5:1358:G:C8	2.35	0.61
48:5:1378:C:H3'	48:5:1379:C:H5'	1.81	0.61
48:5:222:C:H2'	48:5:223:G:O4'	2.00	0.61
7:G:86:VAL:CG1	7:G:87:LEU:H	2.13	0.61
47:3:4:C:O2'	47:3:5:G:H8	1.83	0.61
48:5:2468:U:H3	48:5:2473:A:N6	1.97	0.61
51:9:309:G:N1	51:9:310:C:C4	2.68	0.61
48:5:2905:C:C2	48:5:3590:G:N2	2.69	0.61
48:5:1213:G:C2	48:5:1215:C:O2	2.53	0.61
48:5:4901:G:C2	48:5:4921:C:N3	2.69	0.61
48:5:181:C:C2	48:5:256:G:N2	2.69	0.61
25:Z:5:MET:HG2	25:Z:77:TYR:CE1	2.36	0.61
1:A:27:ALA:O	1:A:128:ARG:NH2	2.34	0.61
51:9:1453:C:C2'	51:9:1454:A:H4'	2.30	0.61
48:5:3751:G:H2'	48:5:3752:C:H5'	1.83	0.61
48:5:167:C:C2	48:5:269:G:N2	2.69	0.61
48:5:3723:A:C2	48:5:3724:A:C6	2.89	0.61
45:1:68:VAL:C	46:2:76:A:O3'	2.39	0.61
18:S:80:ILE:HD11	18:S:126:ILE:HD12	1.83	0.61
51:9:1130:G:C2	51:9:1131:G:C8	2.89	0.61
48:5:199:G:C6	48:5:201:C:N4	2.68	0.61
48:5:1854:G:N2	48:5:4394:A:O4'	2.33	0.61
51:9:1454:A:C2	51:9:1476:A:C4'	2.84	0.60
48:5:1081:C:C2	48:5:1220:G:C2	2.88	0.60
48:5:1186:U:H2'	48:5:1187:G:O4'	2.01	0.60
55:DD:31:GLU:OE1	55:DD:106:ARG:NH2	2.34	0.60
48:5:4213:A:C2	48:5:4218:U:O4	2.50	0.60
5:E:126:ARG:HH12	48:5:1285:U:P	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1454:A:C2	51:9:1476:A:H5''	2.37	0.60
48:5:1964:A:C5	48:5:1965:G:C8	2.90	0.60
51:9:1129:G:H3'	51:9:1130:G:H8	1.66	0.60
48:5:1987:C:H2'	48:5:1987:C:O2	2.00	0.60
47:3:10:G:N2	47:3:11:C:C2	2.69	0.60
48:5:515:C:C2	48:5:647:G:C2	2.90	0.60
48:5:22:G:C2	50:8:35:C:C2	2.89	0.60
63:LL:66:VAL:HG23	63:LL:131:CYS:SG	2.41	0.60
48:5:3612:C:H1'	48:5:5016:A:C8	2.36	0.60
48:5:2616:C:C2	48:5:2722:G:C2	2.89	0.60
48:5:5061:A:O2'	48:5:5062:G:OP2	2.10	0.60
51:9:1454:A:OP1	69:RR:49:LYS:HD2	2.01	0.60
48:5:77:U:H3	48:5:335:A:N6	2.00	0.60
4:D:200:MET:CE	4:D:240:TYR:HB2	2.31	0.60
54:CC:227:TRP:O	54:CC:228:SER:CB	2.50	0.60
47:3:37:A:H2'	47:3:38:A:H5'	1.83	0.60
47:3:39:U:O4'	57:FF:135:ARG:CZ	2.49	0.60
48:5:1957:U:O2'	48:5:1958:A:H5'	2.01	0.60
49:7:30:C:C2	49:7:48:G:C2	2.90	0.60
48:5:2758:G:O2'	48:5:2764:A:N3	2.27	0.60
51:9:1416:C:H2'	51:9:1417:C:C2	2.37	0.60
48:5:1963:C:O2'	48:5:1964:A:OP1	2.20	0.59
48:5:1296:G:H1'	48:5:1297:U:P	2.42	0.59
48:5:4441:A:H8	48:5:4441:A:H5''	1.67	0.59
51:9:945:U:H2'	51:9:946:U:C6	2.38	0.59
51:9:1401:A:C2	51:9:1402:A:C6	2.89	0.59
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.84	0.59
48:5:1991:A:N6	48:5:2003:G:OP1	2.35	0.59
48:5:2446:C:C2	48:5:2515:G:C2	2.90	0.59
48:5:917:A:C2	48:5:919:C:C5	2.89	0.59
48:5:2084:C:H3'	48:5:2085:G:C5'	2.32	0.59
56:EE:163:ASP:O	56:EE:164:LEU:HB2	2.02	0.59
46:2:53:G:C2	46:2:62:C:C2	2.91	0.59
9:I:49:CYS:HB2	9:I:172:GLY:O	2.03	0.59
8:H:111:LEU:HD11	8:H:125:ARG:HB2	1.84	0.59
48:5:3594:C:H2'	48:5:3594:C:O2	2.02	0.59
47:3:76:A:N7	48:5:4371:G:N1	2.51	0.59
51:9:1212:G:O2'	51:9:1213:C:O5'	2.20	0.59
48:5:4411:G:C2	48:5:4432:C:C2	2.90	0.59
47:3:53:G:C2	47:3:62:C:C2	2.91	0.59
48:5:3712:A:C6	51:9:970:G:C2	2.91	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1074:G:C2	48:5:1238:A:C2	2.90	0.59
48:5:300:A:C2	48:5:301:G:C5	2.91	0.59
11:L:165:LYS:HB2	11:L:165:LYS:NZ	2.17	0.59
51:9:195:C:C2	51:9:205:G:N2	2.71	0.59
3:C:157:LYS:O	3:C:160:GLY:N	2.35	0.59
48:5:1278:C:C6	48:5:1279:A:H1'	2.38	0.59
48:5:919:C:C4	48:5:920:C:C5	2.91	0.59
48:5:1266:G:H5''	48:5:2112:G:C2	2.38	0.59
48:5:4213:A:N6	48:5:4218:U:H3	2.01	0.59
51:9:1405:A:H2'	51:9:1406:G:O4'	2.03	0.59
48:5:4182:G:H5''	48:5:4183:G:OP2	2.03	0.59
48:5:1279:A:C2	48:5:1280:C:C2	2.90	0.59
48:5:1965:G:O2'	48:5:1966:C:O5'	2.21	0.59
51:9:1308:U:N3	51:9:1309:C:C1'	2.66	0.59
9:I:183:ASP:O	9:I:187:GLU:HG3	2.03	0.59
48:5:1823:G:O3'	48:5:1825:A:P	2.60	0.59
48:5:665:C:O2	48:5:665:C:H2'	2.02	0.59
51:9:1144:A:C2'	51:9:1145:A:C8	2.83	0.58
51:9:322:C:O2'	51:9:323:C:P	2.61	0.58
48:5:642:G:N1	48:5:643:C:C4	2.71	0.58
51:9:164:A:O2'	51:9:165:G:O4'	2.21	0.58
48:5:2827:G:H2'	48:5:2827:G:N3	2.18	0.58
51:9:65:C:N4	58:GG:134:GLY:O	2.35	0.58
51:9:1408:U:O4	51:9:1409:A:N6	2.35	0.58
48:5:5024:C:O3'	60:II:170:LYS:HE2	2.02	0.58
48:5:1213:G:O6	48:5:1215:C:C4	2.56	0.58
48:5:2256:C:H2'	48:5:2256:C:O2	2.03	0.58
48:5:1268:G:C4	48:5:2111:G:C2	2.91	0.58
51:9:312:G:O2'	51:9:313:A:OP1	2.14	0.58
48:5:245:C:O2	48:5:245:C:O4'	2.21	0.58
51:9:1305:C:C2'	51:9:1306:U:C5'	2.80	0.58
51:9:321:C:HO2'	51:9:322:C:H5'	1.68	0.58
48:5:4723:A:C2	48:5:4724:A:C6	2.91	0.58
48:5:1074:G:N2	48:5:1075:G:C2	2.72	0.58
48:5:2026:A:H2'	48:5:2027:U:H5'	1.85	0.58
48:5:5026:U:C6	60:II:79:ILE:HG13	2.39	0.58
48:5:166:C:C2'	48:5:166:C:O2	2.51	0.58
51:9:960:U:O2'	51:9:962:A:N7	2.29	0.58
51:9:1531:A:H2'	51:9:1532:C:C6	2.38	0.58
5:E:198:ASP:O	5:E:256:LYS:HD3	2.02	0.58
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1358:G:C2'	48:5:1359:G:O4'	2.52	0.58
48:5:5026:U:C5	60:II:79:ILE:HG13	2.39	0.58
48:5:5026:U:OP2	60:II:79:ILE:CD1	2.52	0.58
9:I:202:ASN:O	49:7:63:C:C4	2.57	0.58
48:5:1840:G:H3'	48:5:1842:G:P	2.44	0.58
48:5:4892:A:N1	48:5:4927:G:O6	2.37	0.58
48:5:685:C:O2	48:5:685:C:H2'	2.04	0.58
51:9:750:C:H2'	51:9:750:C:O2	2.04	0.58
54:CC:64:THR:OG1	54:CC:90:GLU:HG3	2.04	0.58
51:9:1374:C:H2'	51:9:1375:G:O4'	2.03	0.58
48:5:1430:C:C2	48:5:1455:G:C2	2.91	0.58
53:BB:107:ARG:NH2	66:OO:133:THR:O	2.35	0.58
51:9:1102:G:N2	51:9:1130:G:N2	2.51	0.58
51:9:1859:A:C2	51:9:1860:A:C6	2.92	0.58
54:CC:75:ILE:HG23	54:CC:80:GLU:OE1	2.04	0.58
48:5:973:G:N2	48:5:1282:G:HO2'	2.00	0.58
48:5:4207:C:C2	48:5:4226:G:C2	2.92	0.58
51:9:1447:G:C6	51:9:1448:A:N6	2.71	0.58
51:9:1233:G:H2'	51:9:1234:C:H5'	1.82	0.58
48:5:2654:C:C2	48:5:2681:G:C2	2.92	0.58
51:9:1444:U:O2'	51:9:1580:A:N1	2.37	0.58
51:9:358:C:C2	51:9:405:G:C2	2.91	0.58
48:5:516:C:N3	48:5:646:G:C2	2.72	0.57
51:9:316:G:N1	51:9:317:C:C4	2.72	0.57
48:5:3593:C:H4'	48:5:3594:C:OP2	2.03	0.57
48:5:4757:C:O4'	48:5:4757:C:O2	2.22	0.57
51:9:841:G:N2	51:9:842:C:C2	2.72	0.57
51:9:1211:G:O2'	51:9:1212:G:H5'	2.03	0.57
76:YY:113:ARG:O	76:YY:114:MET:HB2	2.04	0.57
48:5:2623:A:C2	48:5:2624:G:C5	2.92	0.57
9:I:187:GLU:O	9:I:188:LYS:HB2	2.04	0.57
12:M:130:LEU:HD21	14:O:180:GLN:OE1	2.04	0.57
51:9:623:G:N2	51:9:624:C:C2	2.72	0.57
48:5:1541:C:C2	48:5:1619:G:C2	2.91	0.57
5:E:128:PRO:HD2	5:E:131:GLN:OE1	2.03	0.57
48:5:685:C:O2	48:5:685:C:C2'	2.52	0.57
48:5:1682:A:C2	48:5:1683:U:C2	2.92	0.57
48:5:2554:U:H4'	48:5:2555:G:OP1	2.03	0.57
12:M:126:GLU:CD	12:M:130:LEU:HD13	2.25	0.57
51:9:1760:G:C2	51:9:1773:C:C2	2.92	0.57
51:9:1613:G:C2	51:9:1627:C:C2	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1137:U:N3	51:9:1148:A:N6	2.51	0.57
7:G:87:LEU:CD2	7:G:184:LEU:CD2	2.83	0.57
47:3:5:G:N2	47:3:6:G:C4	2.72	0.57
48:5:1269:G:C6	48:5:2111:G:N2	2.72	0.57
48:5:4213:A:H61	48:5:4218:U:H3	1.50	0.57
17:R:172:ARG:HG3	51:9:909:G:OP2	2.05	0.57
48:5:1280:C:C2	48:5:1282:G:C5	2.93	0.57
51:9:1308:U:H3	51:9:1309:C:C1'	2.18	0.57
3:C:158:VAL:HA	3:C:161:TYR:CD2	2.40	0.57
51:9:1102:G:C2	51:9:1103:C:C4	2.92	0.57
48:5:127:G:N2	48:5:128:C:C2	2.73	0.57
48:5:1639:U:H3	48:5:1643:A:HO2'	1.51	0.57
48:5:1365:C:H4'	48:5:1366:G:OP1	2.05	0.57
51:9:1488:C:O2'	51:9:1490:G:OP2	2.20	0.57
48:5:1279:A:H2'	48:5:1280:C:H5''	1.86	0.57
51:9:1454:A:N1	51:9:1476:A:C5'	2.68	0.57
10:J:119:TYR:CB	70:SS:12:ILE:HD13	2.35	0.57
12:M:69:ARG:O	12:M:71:LYS:N	2.38	0.57
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.87	0.57
50:8:83:C:H4'	50:8:85:U:O2	2.03	0.57
47:3:68:C:HO2'	47:3:69:G:C1'	2.13	0.56
51:9:1526:G:N2	51:9:1527:C:C2	2.73	0.56
48:5:2089:G:N3	48:5:2089:G:H2'	2.20	0.56
48:5:1999:A:H1'	48:5:2017:A:N1	2.20	0.56
48:5:2301:G:N2	48:5:2302:C:C2	2.72	0.56
48:5:1279:A:C3'	48:5:1280:C:C5'	2.80	0.56
48:5:1279:A:O2'	48:5:1280:C:OP1	2.23	0.56
5:E:59:TYR:CE2	5:E:64:LEU:HD12	2.38	0.56
51:9:752:G:C6	51:9:790:C:N4	2.73	0.56
48:5:1757:U:H2'	48:5:1758:G:O4'	2.04	0.56
48:5:4769:G:H2'	48:5:4770:U:O4'	2.04	0.56
48:5:2297:G:N2	48:5:2338:C:C2	2.73	0.56
48:5:2256:C:O2	48:5:2256:C:C2'	2.53	0.56
3:C:183:VAL:HG22	3:C:204:ARG:HB2	1.88	0.56
48:5:3900:G:H5''	48:5:3901:A:H4'	1.87	0.56
48:5:677:G:N2	48:5:678:C:C2	2.74	0.56
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.39	0.56
48:5:4101:C:C2	48:5:4109:G:C2	2.94	0.56
48:5:2258:C:O2	48:5:2258:C:C2'	2.54	0.56
5:E:62:LYS:O	5:E:63:ALA:HB3	2.06	0.56
3:C:336:ARG:O	3:C:340:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:976:G:C2	48:5:977:C:C2	2.94	0.56
51:9:1455:A:O2'	51:9:1456:G:O5'	2.21	0.56
48:5:1358:G:C3'	48:5:1358:G:C8	2.87	0.56
48:5:2288:G:N1	48:5:2290:C:C4	2.73	0.56
48:5:199:G:C2	48:5:220:C:O2	2.58	0.56
51:9:434:G:H2'	51:9:435:A:C8	2.40	0.56
14:O:160:ARG:NH2	48:5:4759:C:OP1	2.38	0.56
48:5:2481:G:C2	48:5:2498:C:C2	2.94	0.56
17:R:173:ARG:O	17:R:176:ARG:HB3	2.05	0.56
51:9:217:A:C2	51:9:309:G:N1	2.74	0.56
48:5:2773:G:N1	48:5:2774:C:C4	2.73	0.56
48:5:1404:G:N2	48:5:1414:C:C2	2.74	0.56
51:9:407:G:H2'	51:9:407:G:N3	2.21	0.56
48:5:4583:C:C4	48:5:4718:G:C6	2.93	0.56
52:AA:104:THR:O	52:AA:107:THR:HG23	2.06	0.56
51:9:913:A:N3	59:HH:66:VAL:HG11	2.21	0.56
48:5:2028:C:O2'	48:5:2029:A:C5'	2.53	0.56
48:5:1360:G:C6	48:5:1361:G:C5	2.94	0.56
51:9:1760:G:N2	51:9:1773:C:C2	2.74	0.56
50:8:155:C:H2'	50:8:156:U:O4'	2.05	0.56
51:9:1117:C:O2	51:9:1117:C:O4'	2.24	0.56
48:5:1249:C:C2	48:5:1262:G:C2	2.94	0.56
48:5:746:A:O2'	48:5:747:A:O5'	2.20	0.56
48:5:4092:G:N2	48:5:4158:C:C2	2.74	0.56
48:5:976:G:C6	48:5:977:C:C4	2.93	0.56
51:9:1308:U:C5	51:9:1309:C:C6	2.94	0.56
56:EE:31:PRO:CD	56:EE:38:LEU:HD13	2.36	0.56
48:5:1067:G:H2'	48:5:1068:G:O4'	2.05	0.56
48:5:2089:G:O2'	48:5:2090:U:OP2	2.24	0.56
51:9:834:C:H3'	51:9:835:C:C4'	2.36	0.56
51:9:598:G:N2	51:9:639:C:C2	2.74	0.56
48:5:1672:U:H2'	48:5:1673:U:C6	2.41	0.56
4:D:129:GLU:HG3	4:D:177:THR:HG21	1.86	0.56
17:R:172:ARG:CG	51:9:909:G:OP2	2.54	0.56
54:CC:204:ILE:CD1	54:CC:215:LEU:HD23	2.36	0.56
48:5:4723:A:C2	48:5:4724:A:C5	2.94	0.56
48:5:516:C:C2	48:5:646:G:C2	2.94	0.56
51:9:1403:C:C2'	51:9:1403:C:O2	2.53	0.56
48:5:977:C:C4	48:5:978:G:N7	2.74	0.55
48:5:497:G:C2	48:5:657:C:C2	2.94	0.55
48:5:1468:C:C2	48:5:1498:G:C2	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:39:U:O2'	47:3:40:C:O5'	2.23	0.55
48:5:4583:C:N4	48:5:4718:G:C6	2.75	0.55
48:5:2688:G:N2	48:5:2689:C:C2	2.74	0.55
48:5:4730:C:O5'	48:5:4731:G:N2	2.39	0.55
5:E:208:LEU:O	5:E:208:LEU:HD12	2.06	0.55
48:5:2524:U:H5''	48:5:2711:G:C2	2.42	0.55
47:3:39:U:O2'	47:3:40:C:C6	2.49	0.55
47:3:34:U:O2	51:9:1641:A:OP1	2.24	0.55
51:9:322:C:HO2'	51:9:323:C:P	2.30	0.55
48:5:1205:G:N2	48:5:1206:C:C2	2.75	0.55
3:C:334:THR:HG21	6:F:53:TYR:OH	2.06	0.55
48:5:466:A:C2	48:5:467:U:C4	2.95	0.55
56:EE:55:ALA:HB1	56:EE:60:GLU:HB2	1.89	0.55
47:3:76:A:N6	48:5:4371:G:C5	2.75	0.55
48:5:2793:G:C5	48:5:2797:C:N4	2.74	0.55
48:5:5028:G:C6	48:5:5029:C:N4	2.75	0.55
48:5:1483:C:O4'	48:5:1483:C:O2	2.22	0.55
51:9:167:G:C6	51:9:168:C:C5	2.94	0.55
51:9:1351:G:O2'	51:9:1378:A:N1	2.35	0.55
51:9:350:C:O2'	51:9:383:G:N1	2.39	0.55
58:GG:188:LYS:HA	58:GG:191:ARG:HD3	1.87	0.55
75:XX:41:PHE:O	75:XX:43:GLY:N	2.39	0.55
17:R:176:ARG:CZ	17:R:176:ARG:HB2	2.37	0.55
48:5:4281:A:C2	48:5:4283:G:C5	2.95	0.55
48:5:3718:A:H2'	48:5:3719:A:C8	2.42	0.55
48:5:1771:U:H2'	48:5:1772:C:O4'	2.06	0.55
48:5:4416:G:N2	48:5:4417:C:C2	2.75	0.55
56:EE:234:PRO:HG3	56:EE:238:LEU:HD11	1.88	0.55
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.39	0.55
18:S:53:LYS:NZ	49:7:74:A:O2'	2.40	0.55
48:5:1983:A:C2	48:5:2008:U:O4	2.58	0.55
48:5:1956:A:O2'	48:5:1957:U:H5'	2.07	0.55
51:9:853:C:O2	51:9:853:C:O4'	2.25	0.55
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.54	0.55
51:9:1454:A:OP1	69:RR:3:ARG:NH1	2.38	0.55
51:9:1406:G:H2'	51:9:1407:U:O3'	2.07	0.55
10:J:119:TYR:CD1	70:SS:12:ILE:HG12	2.41	0.55
48:5:1266:G:H5''	48:5:2112:G:N3	2.22	0.55
51:9:1784:G:N2	51:9:1785:C:C2	2.75	0.55
48:5:1975:G:O4'	48:5:1984:A:H1'	2.06	0.55
48:5:181:C:N4	48:5:256:G:C6	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2905:C:C2	48:5:3590:G:C2	2.95	0.55
51:9:598:G:C2	51:9:639:C:C2	2.94	0.55
2:B:18:PRO:O	2:B:20:LYS:N	2.40	0.55
59:HH:43:LEU:HD22	59:HH:72:PHE:CD2	2.42	0.55
51:9:953:C:H2'	51:9:954:U:O4'	2.07	0.55
48:5:1929:A:C2	48:5:2054:U:O4	2.57	0.55
54:CC:204:ILE:CD1	54:CC:215:LEU:CD2	2.84	0.55
47:3:76:A:C5	48:5:4371:G:C5	2.95	0.55
17:R:59:SER:N	48:5:4646:U:OP1	2.39	0.55
15:P:118:GLN:NE2	48:5:423:G:N3	2.55	0.55
57:FF:35:LEU:HD13	57:FF:117:ILE:HG12	1.89	0.55
9:I:204:GLY:O	9:I:205:PRO:C	2.46	0.54
48:5:2027:U:C2'	48:5:2028:C:H5'	2.38	0.54
61:JJ:35:TYR:O	61:JJ:37:LEU:N	2.41	0.54
48:5:5000:G:N2	48:5:5051:C:C2	2.75	0.54
51:9:834:C:N3	51:9:841:G:C2	2.75	0.54
48:5:4281:A:C2	48:5:4283:G:C6	2.94	0.54
51:9:698:G:N1	51:9:733:C:C2	2.76	0.54
48:5:1268:G:C2	48:5:2111:G:N2	2.76	0.54
48:5:1297:U:O4'	48:5:1297:U:OP2	2.26	0.54
48:5:3617:G:O2'	48:5:3620:G:N7	2.36	0.54
51:9:216:C:O4'	51:9:216:C:O2	2.24	0.54
51:9:291:G:H21	51:9:292:A:HO2'	1.54	0.54
48:5:975:C:C3'	48:5:976:G:O4'	2.55	0.54
48:5:93:G:O2'	48:5:94:A:O4'	2.24	0.54
51:9:1447:G:N1	51:9:1448:A:C6	2.75	0.54
48:5:1265:G:C2'	48:5:1266:G:H5'	2.37	0.54
48:5:2547:G:N1	48:5:2548:C:C4	2.76	0.54
4:D:258:LYS:O	4:D:259:ARG:HG3	2.07	0.54
25:Z:52:LYS:O	25:Z:65:ARG:NH2	2.40	0.54
48:5:5023:C:O4'	48:5:5023:C:O2	2.23	0.54
6:F:93:PHE:CD2	6:F:246:ILE:HD11	2.42	0.54
48:5:3753:G:OP1	48:5:3777:G:H8	1.91	0.54
48:5:5025:C:OP2	60:II:170:LYS:HG3	2.06	0.54
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.41	0.54
3:C:357:ALA:O	3:C:361:LYS:HG3	2.08	0.54
51:9:1139:C:O2	51:9:1139:C:O4'	2.26	0.54
60:II:38:ILE:HD11	60:II:81:VAL:HG23	1.90	0.54
51:9:887:U:O2	51:9:887:U:O4'	2.26	0.54
5:E:174:PRO:O	5:E:176:SER:N	2.40	0.54
9:I:98:ARG:HB3	9:I:120:GLY:HA3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:VAL:HG13	7:G:183:ILE:O	2.07	0.54
48:5:2409:U:C5	48:5:2783:A:C2	2.95	0.54
51:9:830:A:N6	51:9:844:U:C2	2.74	0.54
51:9:643:A:OP1	51:9:643:A:H4'	2.08	0.54
48:5:986:C:C2	48:5:1068:G:C2	2.96	0.54
48:5:4913:G:O2'	48:5:4914:C:O4'	2.24	0.54
47:3:16:C:O2	47:3:16:C:O4'	2.26	0.54
47:3:66:U:C2	47:3:67:U:C6	2.96	0.54
51:9:751:G:O2'	51:9:752:G:O4'	2.25	0.54
48:5:2108:G:C2	48:5:2125:C:N3	2.76	0.54
51:9:1137:U:H3	51:9:1148:A:N6	2.06	0.54
48:5:4730:C:O4'	48:5:4730:C:O2	2.25	0.54
51:9:172:U:O2	51:9:172:U:C2'	2.56	0.54
51:9:1408:U:H2'	51:9:1409:A:C8	2.43	0.54
48:5:1381:U:O2	48:5:1381:U:O4'	2.26	0.54
51:9:1649:U:O4	51:9:1675:A:C2	2.60	0.54
48:5:2108:G:N1	48:5:2125:C:C4	2.76	0.54
48:5:112:C:C2	48:5:330:G:C2	2.96	0.54
47:3:38:A:O2'	47:3:39:U:H5'	2.08	0.54
47:3:39:U:O2'	47:3:40:C:C5'	2.56	0.54
17:R:172:ARG:HB3	51:9:909:G:OP2	2.08	0.54
47:3:76:A:C6	48:5:4371:G:N7	2.76	0.54
48:5:4885:U:H2'	48:5:4886:C:O4'	2.07	0.54
48:5:422:C:C2	50:8:13:G:C2	2.96	0.53
48:5:976:G:H2'	48:5:977:C:C1'	2.34	0.53
48:5:52:G:N2	48:5:53:C:C2	2.76	0.53
51:9:1654:G:N2	51:9:1655:C:C2	2.77	0.53
51:9:1126:G:N2	51:9:1127:C:C2	2.76	0.53
51:9:1454:A:C2	51:9:1476:A:C5'	2.91	0.53
48:5:5026:U:O4	60:II:103:LEU:HD13	2.08	0.53
51:9:1303:C:O2	51:9:1303:C:O4'	2.25	0.53
14:O:84:VAL:HG11	14:O:102:LEU:HD22	1.91	0.53
48:5:3641:U:H5	48:5:3646:A:N7	2.06	0.53
48:5:4138:C:C2	48:5:4147:G:C2	2.95	0.53
48:5:3782:C:N3	48:5:3811:G:C2	2.76	0.53
48:5:4543:G:H2'	48:5:4544:A:C8	2.43	0.53
51:9:1537:A:N1	51:9:1596:U:O4	2.41	0.53
48:5:4283:G:N2	48:5:4284:C:C2	2.77	0.53
49:7:66:G:C2	49:7:67:C:C2	2.96	0.53
48:5:1965:G:C2	48:5:1966:C:C2	2.96	0.53
47:3:33:U:P	57:FF:127:ARG:NH1	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:HH:95:ILE:HD11	59:HH:133:LEU:HG	1.91	0.53
48:5:181:C:C2	48:5:256:G:C2	2.97	0.53
51:9:944:A:C5	51:9:945:U:C5	2.96	0.53
48:5:2301:G:N1	48:5:2302:C:C4	2.77	0.53
48:5:4305:G:N3	48:5:4305:G:C2'	2.71	0.53
48:5:1811:G:N2	48:5:1812:C:C2	2.77	0.53
48:5:4093:G:C3'	48:5:4094:G:H5'	2.39	0.53
48:5:2045:G:O6	48:5:3870:C:O2'	2.25	0.53
48:5:3870:C:C2	48:5:3886:G:C2	2.95	0.53
12:M:133:ALA:O	12:M:136:LEU:HB3	2.07	0.53
51:9:384:U:O4	60:II:5:ARG:NH2	2.42	0.53
48:5:4213:A:N6	48:5:4218:U:N3	2.53	0.53
48:5:1983:A:C2	48:5:2010:A:H5''	2.44	0.53
48:5:3753:G:O2'	48:5:3754:G:C5'	2.56	0.53
48:5:3751:G:O2'	48:5:3775:A:N6	2.41	0.53
48:5:4579:U:H2'	48:5:4580:U:O4'	2.08	0.53
9:I:204:GLY:O	9:I:205:PRO:O	2.26	0.53
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.90	0.53
51:9:163:U:OP1	58:GG:84:TYR:HA	2.08	0.53
1:A:207:VAL:HG11	48:5:1633:G:C6	2.44	0.53
12:M:122:ILE:HG22	14:O:185:VAL:HG11	1.91	0.53
48:5:1213:G:C6	48:5:1215:C:N3	2.76	0.53
48:5:3662:A:N6	48:5:3680:U:H3	2.07	0.53
48:5:707:C:C2	48:5:1291:G:C2	2.97	0.53
51:9:1454:A:H5'	69:RR:49:LYS:NZ	2.23	0.53
51:9:1308:U:C4	51:9:1309:C:N1	2.75	0.53
51:9:1401:A:H2'	51:9:1402:A:C8	2.44	0.53
21:V:28:CYS:SG	21:V:30:ASP:OD1	2.67	0.53
48:5:2268:A:H4'	48:5:2269:C:H5'	1.90	0.53
48:5:2557:G:C2	48:5:2571:C:C2	2.96	0.53
51:9:1835:A:C4	51:9:1863:A:N7	2.77	0.53
48:5:1968:G:HO2'	48:5:1969:G:P	2.31	0.53
51:9:1102:G:C2	51:9:1130:G:N2	2.77	0.53
58:GG:5:ILE:HG12	58:GG:111:LEU:HD12	1.91	0.53
5:E:251:SER:O	5:E:255:PRO:HD2	2.08	0.53
51:9:522:A:O2'	61:JJ:131:ARG:NH2	2.41	0.53
48:5:2297:G:C2	48:5:2338:C:N3	2.77	0.53
47:3:31:A:H2'	57:FF:136:ARG:HH22	1.74	0.53
48:5:119:G:C8	48:5:119:G:H5''	2.44	0.53
51:9:55:U:O2	51:9:55:U:C2'	2.56	0.53
48:5:2110:C:OP1	48:5:2110:C:C6	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4260:U:H2'	48:5:4261:C:C6	2.44	0.53
2:B:163:LEU:HD23	2:B:182:GLU:CG	2.32	0.52
51:9:1839:U:H2'	51:9:1840:U:C6	2.43	0.52
48:5:3900:G:N2	48:5:4562:C:C2	2.77	0.52
51:9:1599:U:O2	51:9:1599:U:O4'	2.27	0.52
48:5:1485:C:O4'	48:5:1485:C:O2	2.26	0.52
51:9:1528:G:N2	51:9:1529:C:C2	2.78	0.52
48:5:1879:C:O2'	48:5:1891:A:N3	2.39	0.52
51:9:635:G:C6	51:9:636:C:C4	2.97	0.52
69:RR:126:MET:O	69:RR:127:ASN:ND2	2.43	0.52
51:9:1408:U:C4	51:9:1409:A:N6	2.77	0.52
48:5:2638:G:C2	48:5:2639:U:C4	2.98	0.52
48:5:1269:G:C5	48:5:2111:G:C2	2.98	0.52
55:DD:21:LEU:HD22	55:DD:48:ILE:HD11	1.90	0.52
51:9:1401:A:C2	51:9:1402:A:N1	2.77	0.52
48:5:3811:G:O2'	48:5:3814:U:OP2	2.28	0.52
48:5:2726:G:C6	48:5:2727:C:N4	2.77	0.52
48:5:4508:C:N3	48:5:4512:U:H5	2.07	0.52
48:5:4895:C:H1'	48:5:4896:G:C8	2.45	0.52
24:Y:49:ILE:HD13	24:Y:80:ILE:HD13	1.92	0.52
5:E:59:TYR:CZ	5:E:64:LEU:HB2	2.44	0.52
48:5:1958:A:C2	48:5:2026:A:N1	2.78	0.52
48:5:919:C:N4	48:5:920:C:C5	2.77	0.52
48:5:4371:G:C5	48:5:4372:U:C4	2.98	0.52
47:3:1:G:N1	47:3:2:C:C4	2.78	0.52
51:9:832:G:C2	51:9:843:C:C2	2.97	0.52
51:9:427:U:O2	51:9:427:U:O4'	2.28	0.52
5:E:157:ARG:O	5:E:178:ASN:OD1	2.28	0.52
48:5:85:G:O2'	48:5:97:G:O6	2.27	0.52
1:A:196:TRP:O	1:A:197:PRO:C	2.47	0.52
51:9:1448:A:O2'	51:9:1449:G:P	2.67	0.52
47:3:33:U:H5'	57:FF:127:ARG:NH1	2.24	0.52
19:T:2:THR:N	48:5:4220:A:OP2	2.43	0.52
48:5:1964:A:H2'	48:5:1965:G:C5'	2.40	0.52
51:9:1409:A:C6	51:9:1410:C:C5	2.98	0.52
48:5:4378:A:O2'	48:5:4379:A:H2'	2.09	0.52
47:3:76:A:C5	48:5:4371:G:C6	2.98	0.52
10:J:119:TYR:HE2	10:J:125:ILE:HD11	1.74	0.52
58:GG:214:ALA:O	58:GG:218:LYS:N	2.39	0.52
51:9:1859:A:H2'	51:9:1860:A:C8	2.44	0.52
48:5:256:G:N2	48:5:257:C:C2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3782:C:C2	48:5:3811:G:N2	2.77	0.52
51:9:1500:G:C6	51:9:1501:C:C4	2.97	0.52
18:S:95:ARG:NH2	48:5:1951:G:O2'	2.42	0.52
2:B:21:ARG:NH2	48:5:4568:A:O3'	2.43	0.52
48:5:1277:G:N2	48:5:1278:C:C2	2.78	0.52
51:9:1236:G:C6	51:9:1237:C:C4	2.97	0.52
48:5:5025:C:OP1	60:II:169:GLY:HA3	2.10	0.52
51:9:1384:C:C2'	51:9:1385:G:H5'	2.40	0.52
48:5:2627:C:O2	48:5:2627:C:O4'	2.27	0.52
51:9:73:C:O4'	51:9:73:C:O2	2.27	0.52
51:9:1149:A:N3	51:9:1149:A:H2'	2.23	0.52
6:F:49:ARG:NH1	48:5:974:C:O3'	2.43	0.52
51:9:1294:G:O2'	51:9:1295:A:O5'	2.22	0.52
48:5:3594:C:C2'	48:5:3594:C:O2	2.57	0.52
48:5:4735:G:C2	48:5:4736:C:C2	2.98	0.52
48:5:4939:C:O3'	48:5:4941:G:P	2.68	0.52
50:8:106:G:N2	50:8:107:C:C2	2.78	0.52
48:5:470:A:C5	48:5:471:A:C8	2.98	0.52
48:5:166:C:C2	48:5:167:C:H5	2.28	0.52
48:5:301:G:C6	48:5:302:C:C4	2.97	0.52
51:9:195:C:C2	51:9:205:G:C2	2.98	0.52
48:5:707:C:O2	48:5:1291:G:C2	2.63	0.52
51:9:1520:G:H2'	51:9:1520:G:N3	2.25	0.52
51:9:1553:C:O4'	51:9:1553:C:O2	2.25	0.52
58:GG:74:ARG:HA	58:GG:96:SER:HA	1.92	0.52
10:J:53:ALA:HB2	10:J:68:ILE:HD12	1.92	0.52
2:B:29:VAL:HG13	2:B:348:ARG:HD3	1.92	0.52
7:G:86:VAL:CG1	7:G:185:LYS:HG2	2.24	0.52
51:9:1385:G:HO2'	51:9:1386:A:H5'	1.74	0.52
48:5:44:A:N3	48:5:94:A:H2	2.08	0.52
48:5:2693:G:C6	48:5:2694:G:N1	2.78	0.52
51:9:1118:C:O4'	51:9:1118:C:O2	2.25	0.52
16:Q:186:TYR:CD2	48:5:4307:A:H4'	2.45	0.52
51:9:380:G:O6	60:II:178:ARG:NH2	2.43	0.52
50:8:55:U:O4	50:8:62:A:N1	2.43	0.52
51:9:1597:C:H4'	51:9:1603:G:C6	2.45	0.52
51:9:872:A:N6	51:9:914:U:C4	2.79	0.51
47:3:3:C:C2'	47:3:4:C:H5'	2.40	0.51
51:9:751:G:C6	51:9:792:C:N4	2.78	0.51
51:9:488:U:H2'	51:9:488:U:O2	2.08	0.51
48:5:4094:G:H2'	48:5:4095:G:O4'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:OO:106:LYS:HE3	66:OO:135:ILE:HG12	1.91	0.51
51:9:1398:G:N2	51:9:1399:C:C2	2.78	0.51
48:5:4906:C:C2	48:5:4916:G:C2	2.98	0.51
48:5:106:A:H2'	48:5:107:G:O4'	2.10	0.51
54:CC:61:LEU:N	54:CC:61:LEU:CD1	2.73	0.51
51:9:474:G:N1	51:9:475:C:C4	2.79	0.51
48:5:2826:U:H4'	48:5:2827:G:H5'	1.90	0.51
51:9:1617:G:N7	67:PP:43:ARG:NH1	2.58	0.51
55:DD:191:PRO:O	55:DD:193:ASP:N	2.44	0.51
67:PP:34:MET:HA	67:PP:34:MET:HE2	1.91	0.51
51:9:1448:A:C2'	51:9:1449:G:H5''	2.40	0.51
11:L:165:LYS:CB	11:L:165:LYS:NZ	2.73	0.51
46:2:16:C:O2	46:2:16:C:O4'	2.25	0.51
51:9:1698:C:O4'	51:9:1698:C:O2	2.24	0.51
51:9:501:C:C2'	51:9:501:C:O2	2.58	0.51
18:S:9:GLU:HG2	18:S:33:PHE:CE2	2.45	0.51
48:5:1171:G:C2	48:5:1191:C:C2	2.98	0.51
48:5:726:G:C6	48:5:727:C:N4	2.79	0.51
51:9:211:G:N2	51:9:212:C:C2	2.78	0.51
51:9:1130:G:N2	51:9:1131:G:C8	2.79	0.51
51:9:501:C:H2'	51:9:501:C:O2	2.11	0.51
57:FF:73:THR:HG22	57:FF:89:THR:HG23	1.93	0.51
48:5:1726:U:H3	48:5:1836:G:H1	1.59	0.51
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	1.92	0.51
25:Z:54:THR:O	25:Z:56:ALA:N	2.43	0.51
48:5:1398:A:H1'	48:5:1399:G:C8	2.45	0.51
48:5:2275:G:H5''	48:5:2275:G:H8	1.75	0.51
48:5:2505:C:O4'	48:5:2505:C:O2	2.28	0.51
48:5:962:C:OP2	48:5:2264:C:N3	2.43	0.51
48:5:4754:G:C2	48:5:4880:C:C2	2.99	0.51
51:9:71:G:H3'	51:9:72:C:H5''	1.92	0.51
47:3:35:U:O2'	47:3:36:U:H5'	2.11	0.51
47:3:10:G:N1	47:3:11:C:C4	2.78	0.51
51:9:1616:U:OP2	67:PP:43:ARG:NH2	2.42	0.51
48:5:1400:G:C6	48:5:1401:C:C4	2.99	0.51
13:N:65:ARG:HG3	13:N:129:PHE:CE2	2.46	0.51
48:5:2733:C:H2'	48:5:2734:U:O4'	2.11	0.51
48:5:4714:C:C5	48:5:4715:C:C5	2.99	0.51
3:C:108:TRP:HZ2	11:L:19:GLN:HE21	1.57	0.51
5:E:124:HIS:O	48:5:1282:G:O6	2.29	0.51
51:9:1448:A:O2'	51:9:1449:G:C4'	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:322:C:H6	51:9:322:C:OP2	1.94	0.51
48:5:986:C:N3	48:5:1068:G:C2	2.79	0.51
51:9:623:G:N1	51:9:624:C:C4	2.79	0.51
51:9:823:U:O2	51:9:823:U:O4'	2.28	0.51
6:F:92:ALA:CB	6:F:127:LEU:HD21	2.40	0.51
48:5:1072:C:C2'	48:5:1072:C:O2	2.59	0.51
51:9:1454:A:N1	51:9:1476:A:H5''	2.26	0.51
48:5:5026:U:C4	60:II:170:LYS:HE3	2.45	0.51
4:D:200:MET:HE1	4:D:241:LYS:HG3	1.93	0.51
48:5:1245:C:C4	48:5:1269:G:O6	2.64	0.51
48:5:1872:G:O2'	48:5:4219:A:N3	2.38	0.51
51:9:1500:G:C2	51:9:1501:C:C2	2.98	0.51
48:5:1398:A:O2'	48:5:1399:G:OP2	2.24	0.51
48:5:1086:C:C2	48:5:1212:G:C2	2.99	0.51
63:LL:37:TYR:CE1	63:LL:51:ILE:HG23	2.46	0.51
61:JJ:94:LEU:HD12	61:JJ:97:ILE:HD12	1.91	0.51
9:I:46:PHE:CD1	9:I:140:THR:HA	2.45	0.51
48:5:1378:C:OP1	48:5:1379:C:H3'	2.11	0.51
48:5:1269:G:C8	48:5:2111:G:C6	2.98	0.51
48:5:2108:G:N2	48:5:2125:C:C2	2.79	0.51
48:5:2043:A:O2'	48:5:4461:C:O2	2.27	0.51
51:9:833:C:H4'	51:9:834:C:OP1	2.10	0.51
48:5:4219:A:H2'	48:5:4220:A:C8	2.46	0.51
48:5:4749:C:O2	48:5:4749:C:O4'	2.27	0.51
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.38	0.51
48:5:671:G:C6	48:5:672:C:C4	2.98	0.51
51:9:830:A:N1	51:9:844:U:C4	2.78	0.51
51:9:1650:A:C4	51:9:1675:A:C6	2.99	0.51
21:V:82:ILE:HD12	21:V:104:VAL:HG22	1.93	0.51
51:9:1282:A:H3'	51:9:1283:C:C5'	2.40	0.51
48:5:1170:G:C2	48:5:1192:C:C2	2.98	0.51
48:5:77:U:C4	48:5:335:A:N1	2.75	0.51
48:5:3753:G:C2	48:5:3754:G:C8	2.99	0.51
9:I:49:CYS:SG	9:I:51:HIS:CE1	3.04	0.51
47:3:9:A:O2'	47:3:10:G:N7	2.44	0.51
71:TT:62:ARG:HD2	71:TT:62:ARG:C	2.31	0.51
3:C:342:ARG:HH11	3:C:342:ARG:HG3	1.76	0.51
6:F:245:LEU:HD23	6:F:249:MET:HG3	1.92	0.51
47:3:5:G:N3	47:3:6:G:C8	2.79	0.50
47:3:38:A:N1	57:FF:135:ARG:NH1	2.58	0.50
48:5:5026:U:C6	60:II:80:ASP:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2555:G:O6	48:5:2572:C:N4	2.42	0.50
48:5:3729:U:H2'	48:5:3730:U:C6	2.46	0.50
48:5:4692:A:C2	48:5:4693:C:N4	2.79	0.50
51:9:193:C:C2	51:9:207:G:C2	2.99	0.50
48:5:990:C:C4	48:5:1064:G:C2	2.99	0.50
48:5:1447:C:H2'	48:5:1448:G:O4'	2.10	0.50
9:I:191:ILE:CD1	9:I:200:ILE:HD11	2.21	0.50
51:9:1679:A:O2'	51:9:1680:G:OP2	2.19	0.50
51:9:981:A:H2'	51:9:982:G:C8	2.46	0.50
48:5:3724:A:N6	48:5:3725:G:C6	2.79	0.50
5:E:251:SER:O	5:E:255:PRO:HD3	2.10	0.50
51:9:62:G:O4'	51:9:172:U:N3	2.44	0.50
69:RR:126:MET:SD	69:RR:126:MET:N	2.85	0.50
51:9:1615:U:O4	67:PP:40:ARG:NH1	2.44	0.50
14:O:27:VAL:HG13	14:O:98:ALA:HB1	1.93	0.50
3:C:213:GLU:OE1	3:C:213:GLU:N	2.45	0.50
67:PP:17:TYR:OH	67:PP:37:TYR:HB3	2.11	0.50
48:5:1167:C:C2	48:5:1195:G:C2	2.99	0.50
48:5:3698:G:N2	48:5:3699:C:C2	2.79	0.50
11:L:65:ARG:HG2	11:L:66:TYR:CE2	2.47	0.50
48:5:2654:C:N3	48:5:2681:G:C2	2.79	0.50
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.92	0.50
48:5:484:U:C4	48:5:486:C:C5	3.00	0.50
48:5:2311:C:C2	48:5:2328:G:C2	2.99	0.50
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	1.92	0.50
48:5:960:A:N6	48:5:1283:G:O6	2.45	0.50
14:O:54:TYR:CE1	14:O:145:VAL:HG11	2.47	0.50
50:8:119:C:C2	50:8:132:G:C2	2.99	0.50
48:5:2494:U:H2'	48:5:2495:U:O4'	2.11	0.50
47:3:38:A:N3	57:FF:135:ARG:NH2	2.59	0.50
48:5:2557:G:C6	48:5:2558:C:C4	3.00	0.50
9:I:47:PRO:HB3	9:I:171:TRP:CE2	2.46	0.50
51:9:1364:U:O4'	51:9:1364:U:O2	2.28	0.50
20:U:100:LEU:HD22	20:U:112:LEU:HB3	1.92	0.50
5:E:59:TYR:CD2	5:E:64:LEU:CD1	2.76	0.50
17:R:176:ARG:HH11	51:9:909:G:C4'	2.24	0.50
54:CC:60:TRP:C	54:CC:61:LEU:CD1	2.77	0.50
48:5:4338:G:C4	48:5:4372:U:C5	3.00	0.50
48:5:1263:A:C6	48:5:1264:C:C4	3.00	0.50
51:9:1109:C:O2	51:9:1109:C:C2'	2.59	0.50
48:5:2712:G:N2	48:5:2713:C:C2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:43:U:H2'	48:5:44:A:O5'	2.11	0.50
51:9:1616:U:O4	67:PP:40:ARG:NH1	2.44	0.50
51:9:409:C:C2	51:9:432:G:N2	2.80	0.50
48:5:1910:G:N2	48:5:1911:C:C2	2.80	0.50
48:5:5026:U:OP2	60:II:77:ARG:NH2	2.45	0.50
51:9:113:G:N2	51:9:293:C:C2	2.80	0.50
48:5:1354:A:C5	48:5:1503:A:C2	3.00	0.50
48:5:4966:A:H2'	48:5:4967:A:C8	2.47	0.50
48:5:1886:G:N2	48:5:1894:C:C2	2.80	0.50
55:DD:175:VAL:HG13	55:DD:182:LEU:HB2	1.92	0.50
3:C:114:ARG:CZ	48:5:1358:G:H5''	2.41	0.50
47:3:33:U:OP1	57:FF:127:ARG:NH1	2.45	0.50
48:5:4758:U:H2'	48:5:4759:C:O4'	2.12	0.50
11:L:74:ARG:NH2	48:5:76:A:N7	2.59	0.50
3:C:266:THR:HG22	3:C:269:LYS:HB3	1.94	0.50
48:5:2065:G:H2'	48:5:2066:C:O4'	2.12	0.50
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.94	0.50
48:5:1412:G:N2	48:5:1413:C:C2	2.78	0.50
48:5:4462:C:C2	48:5:4515:G:C2	2.99	0.50
48:5:1400:G:C2	48:5:1401:C:C2	2.99	0.50
48:5:1886:G:C2	48:5:1894:C:C2	3.00	0.50
51:9:1116:C:O4'	51:9:1116:C:O2	2.29	0.50
48:5:3860:A:H61	48:5:4560:C:H5	1.60	0.50
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.47	0.50
48:5:1252:C:C2	48:5:1259:G:C2	3.00	0.50
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.46	0.50
48:5:28:C:C2	48:5:55:G:C2	3.00	0.50
52:AA:159:ILE:O	52:AA:159:ILE:HG23	2.12	0.50
48:5:1912:G:N2	48:5:1913:C:C2	2.80	0.50
48:5:977:C:N3	48:5:978:G:N7	2.59	0.50
48:5:2368:A:N6	48:5:2788:U:O2	2.45	0.50
47:3:4:C:C2'	47:3:5:G:H8	2.25	0.50
48:5:2586:G:C8	48:5:2770:C:H1'	2.46	0.50
48:5:2257:C:O2'	48:5:2258:C:O5'	2.25	0.50
51:9:1842:C:C2	51:9:1858:G:N2	2.79	0.50
48:5:1072:C:H1'	48:5:1073:G:C8	2.46	0.50
5:E:161:LEU:HD21	5:E:253:ILE:HD11	1.93	0.50
48:5:2046:G:C2	48:5:2047:A:C2	3.00	0.50
48:5:4699:U:C4	48:5:4702:G:C6	3.00	0.50
48:5:4510:A:O2'	48:5:4511:A:O4'	2.30	0.50
1:A:215:ASN:ND2	48:5:4546:A:N7	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3717:A:O2'	48:5:3718:A:O5'	2.30	0.49
48:5:4699:U:C4	48:5:4701:A:N6	2.80	0.49
65:NN:55:ARG:NH1	65:NN:56:ASP:OD1	2.45	0.49
51:9:1321:G:H2'	51:9:1322:G:O4'	2.12	0.49
48:5:1301:C:O2	48:5:1301:C:O4'	2.30	0.49
48:5:224:U:O4'	48:5:224:U:O2	2.26	0.49
23:X:127:LEU:HD12	23:X:127:LEU:C	2.32	0.49
68:QQ:41:MET:SD	68:QQ:41:MET:N	2.85	0.49
51:9:411:G:N2	51:9:430:C:C2	2.80	0.49
47:3:24:G:C6	47:3:25:C:C4	3.00	0.49
49:7:82:G:C2	49:7:95:C:C2	3.00	0.49
48:5:4709:U:C4	48:5:4710:C:C4	3.00	0.49
61:JJ:24:ARG:HH11	61:JJ:24:ARG:HG2	1.77	0.49
46:2:39:G:N2	46:2:40:C:C2	2.80	0.49
48:5:4583:C:C4	48:5:4718:G:N1	2.79	0.49
5:E:174:PRO:O	5:E:177:LEU:N	2.43	0.49
64:MM:113:ASP:O	64:MM:115:GLY:N	2.45	0.49
6:F:164:ILE:HB	6:F:169:ILE:HD12	1.94	0.49
48:5:2367:A:C2	48:5:2788:U:O4	2.60	0.49
56:EE:31:PRO:HD2	56:EE:38:LEU:HD13	1.93	0.49
48:5:93:G:O2'	48:5:94:A:O5'	2.31	0.49
51:9:635:G:C2	51:9:636:C:C2	3.00	0.49
48:5:965:G:H2'	48:5:965:G:N3	2.27	0.49
48:5:1776:A:C6	48:5:1777:C:C4	3.00	0.49
54:CC:204:ILE:HD13	54:CC:215:LEU:HD23	1.92	0.49
51:9:217:A:C2	51:9:218:U:C6	3.00	0.49
51:9:412:G:C2	51:9:429:C:C2	3.00	0.49
48:5:2557:G:C2	48:5:2558:C:C2	3.00	0.49
11:L:66:TYR:O	11:L:68:THR:N	2.44	0.49
3:C:341:LEU:HD21	5:E:46:LEU:HD21	1.94	0.49
64:MM:50:CYS:SG	64:MM:51:VAL:N	2.86	0.49
63:LL:82:MET:HB3	63:LL:85:THR:HG23	1.94	0.49
50:8:125:C:O4'	50:8:125:C:O2	2.30	0.49
58:GG:1:MET:HE3	58:GG:106:LEU:HB2	1.95	0.49
51:9:1551:U:O2	51:9:1551:U:O4'	2.29	0.49
47:3:69:G:C2	47:3:70:G:C5	3.00	0.49
47:3:5:G:C2	47:3:6:G:N7	2.81	0.49
48:5:4441:A:C8	48:5:4441:A:H5''	2.48	0.49
5:E:152:ARG:NH1	48:5:4939:C:OP1	2.46	0.49
48:5:2065:G:C6	48:5:2066:C:C4	3.01	0.49
48:5:937:U:H2'	48:5:937:U:O2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:698:G:N2	48:5:699:C:C2	2.81	0.49
17:R:35:ALA:O	17:R:37:SER:N	2.45	0.49
18:S:173:ASN:HA	48:5:4762:A:H2	1.78	0.49
48:5:984:C:C2	48:5:1070:G:C2	3.00	0.49
50:8:127:U:C4	50:8:128:C:C5	3.00	0.49
48:5:2586:G:N7	48:5:2587:A:C6	2.80	0.49
48:5:4583:C:N3	48:5:4718:G:C2	2.81	0.49
50:8:56:G:C4	50:8:62:A:C2	3.01	0.49
51:9:1315:U:O2	51:9:1315:U:O4'	2.29	0.49
13:N:135:ILE:HD12	13:N:151:ILE:HD13	1.95	0.49
49:7:93:G:C6	49:7:94:C:C4	3.00	0.49
48:5:202:C:C2	48:5:214:G:C2	3.00	0.49
51:9:1108:G:C2	51:9:1125:C:C2	3.00	0.49
51:9:1455:A:H5''	69:RR:52:GLY:HA2	1.95	0.49
48:5:1214:C:H1'	48:5:1215:C:OP2	2.12	0.49
48:5:497:G:C2	48:5:657:C:N3	2.81	0.49
51:9:1231:C:O2'	51:9:1253:A:N6	2.45	0.49
48:5:300:A:C2	48:5:301:G:C6	3.01	0.49
48:5:1984:A:N6	48:5:2011:C:O2'	2.46	0.49
7:G:81:ASN:OD1	7:G:238:GLY:N	2.46	0.49
51:9:191:A:H3'	51:9:192:C:H5''	1.94	0.49
48:5:4099:G:C6	48:5:4100:C:C4	3.00	0.49
7:G:156:VAL:HG13	7:G:184:LEU:HG	1.95	0.49
51:9:1145:A:C5	51:9:1146:C:H1'	2.48	0.49
51:9:1212:G:O2'	51:9:1213:C:O4'	2.30	0.49
48:5:3717:A:N1	48:5:3933:G:H1'	2.28	0.49
18:S:47:PHE:HE1	18:S:125:GLN:HG2	1.76	0.49
48:5:2020:U:H2'	48:5:2020:U:O2	2.12	0.49
48:5:209:U:C4	48:5:233:U:O4	2.66	0.49
51:9:1308:U:C4	51:9:1309:C:C5	2.99	0.49
47:3:35:U:C1'	51:9:1640:A:O3'	2.60	0.49
17:R:172:ARG:O	17:R:176:ARG:NH2	2.45	0.49
48:5:919:C:N4	48:5:920:C:N4	2.60	0.49
58:GG:52:ILE:O	58:GG:52:ILE:HG23	2.13	0.49
51:9:309:G:C2	51:9:310:C:C4	3.01	0.49
48:5:4735:G:C6	48:5:4736:C:C4	3.01	0.49
48:5:4559:A:O3'	48:5:4560:C:O2	2.31	0.49
48:5:742:G:N2	48:5:923:C:C2	2.81	0.49
51:9:14:C:O2	51:9:1198:G:C2	2.66	0.49
48:5:2517:A:N3	48:5:2539:C:O2'	2.46	0.49
48:5:4872:G:O2'	48:5:4873:G:OP1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1995:G:C6	48:5:1996:C:C4	3.01	0.49
2:B:252:ALA:HB1	48:5:4524:G:N3	2.28	0.49
51:9:1305:C:H2'	51:9:1306:U:C5'	2.43	0.49
48:5:2090:U:OP2	48:5:2090:U:O4'	2.31	0.49
6:F:168:ARG:HD2	6:F:211:TRP:CD1	2.48	0.49
48:5:2909:C:C2	48:5:3586:G:C2	3.00	0.49
47:3:5:G:N3	47:3:6:G:N7	2.61	0.48
48:5:3753:G:OP1	48:5:3777:G:C8	2.66	0.48
48:5:4586:G:H5''	48:5:4586:G:H8	1.77	0.48
51:9:1771:G:N1	51:9:1772:C:C4	2.82	0.48
6:F:92:ALA:HB3	6:F:127:LEU:HD21	1.94	0.48
51:9:88:G:C6	51:9:89:C:C4	3.01	0.48
48:5:2336:G:C6	48:5:2337:C:C4	3.01	0.48
1:A:44:ILE:HG22	1:A:87:PHE:CD1	2.47	0.48
48:5:4136:G:C6	48:5:4137:C:C4	3.00	0.48
5:E:149:LEU:HD11	5:E:191:ILE:HG13	1.94	0.48
48:5:2609:G:C2	48:5:2731:C:O2	2.66	0.48
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.95	0.48
51:9:1344:A:N6	51:9:1386:A:H5''	2.28	0.48
10:J:119:TYR:CB	70:SS:12:ILE:HG21	2.43	0.48
51:9:1466:G:N1	51:9:1467:C:C4	2.81	0.48
51:9:1489:A:H4'	51:9:1490:G:OP2	2.12	0.48
48:5:2297:G:C2	48:5:2338:C:C2	3.02	0.48
49:7:66:G:C6	49:7:67:C:C4	3.00	0.48
48:5:3715:U:H2'	48:5:3716:C:C6	2.48	0.48
16:Q:65:ARG:NH1	48:5:1502:G:OP1	2.46	0.48
48:5:505:G:C2	48:5:506:C:C2	3.01	0.48
48:5:1549:G:C2	48:5:1580:C:C2	3.01	0.48
70:SS:30:ILE:HD11	70:SS:45:LEU:HD21	1.95	0.48
51:9:1447:G:H2'	51:9:1448:A:C8	2.47	0.48
10:J:82:ILE:HG22	10:J:130:PHE:HE2	1.79	0.48
18:S:34:ALA:HB1	18:S:39:VAL:CG2	2.43	0.48
51:9:384:U:O2'	63:LL:135:SER:C	2.52	0.48
66:OO:102:GLY:O	66:OO:106:LYS:NZ	2.45	0.48
48:5:1072:C:O2	48:5:1072:C:H2'	2.13	0.48
48:5:1995:G:C2	48:5:1996:C:C2	3.01	0.48
51:9:963:A:H2'	51:9:964:A:O4'	2.14	0.48
2:B:378:ARG:HE	22:W:32:LEU:HD21	1.78	0.48
9:I:87:ILE:HG12	9:I:138:ILE:HG12	1.95	0.48
23:X:50:LYS:HG3	48:5:2475:G:C6	2.48	0.48
50:8:139:G:C6	50:8:140:C:C4	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:978:G:C6	48:5:979:C:C4	3.02	0.48
48:5:504:G:C2	48:5:654:C:C2	3.00	0.48
4:D:200:MET:HE3	4:D:237:GLU:O	2.13	0.48
48:5:1541:C:C2	48:5:1619:G:N2	2.81	0.48
48:5:3586:G:C6	48:5:3587:C:C4	3.02	0.48
48:5:505:G:C6	48:5:506:C:C4	3.01	0.48
51:9:185:G:N2	51:9:186:C:C2	2.82	0.48
47:3:39:U:H4'	66:OO:66:ARG:HH22	1.78	0.48
51:9:1236:G:C2	51:9:1237:C:C2	3.01	0.48
48:5:4183:G:N3	48:5:4183:G:H2'	2.28	0.48
48:5:1839:U:H2'	48:5:1840:G:O4'	2.14	0.48
15:P:69:ARG:NH2	48:5:4568:A:N3	2.62	0.48
48:5:4635:A:C2	48:5:4664:A:C5	3.02	0.48
47:3:24:G:H2'	47:3:25:C:O4'	2.13	0.48
51:9:88:G:C2	51:9:89:C:C2	3.01	0.48
48:5:1754:U:O4'	48:5:1754:U:O2	2.30	0.48
48:5:4767:C:C2	48:5:4868:G:C2	3.01	0.48
51:9:1190:A:H2'	51:9:1191:C:O4'	2.13	0.48
47:3:6:G:O2'	47:3:7:A:H5'	2.14	0.48
48:5:2028:C:O2'	48:5:2029:A:O4'	2.32	0.48
48:5:1270:A:H2'	48:5:1271:G:O5'	2.14	0.48
48:5:4276:G:N2	48:5:4333:C:C2	2.81	0.48
7:G:30:PRO:HD2	7:G:31:LEU:HD22	1.96	0.48
3:C:183:VAL:HG22	3:C:204:ARG:CB	2.44	0.48
48:5:4093:G:H3'	48:5:4094:G:H5'	1.94	0.48
53:BB:139:CYS:HB2	53:BB:172:MET:HE3	1.96	0.48
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.95	0.48
51:9:1717:C:C2	51:9:1817:G:C2	3.00	0.48
48:5:4079:C:C2	48:5:4168:G:C2	3.02	0.48
66:OO:145:GLY:O	66:OO:147:ARG:N	2.46	0.48
51:9:305:U:O2'	51:9:309:G:O4'	2.29	0.48
48:5:2128:G:C6	48:5:2129:C:C4	3.02	0.48
48:5:1075:G:C2	48:5:1076:C:C2	3.02	0.48
46:2:53:G:N2	46:2:62:C:C2	2.81	0.48
57:FF:35:LEU:HD13	57:FF:117:ILE:HG23	1.95	0.48
48:5:1448:G:N2	48:5:1449:C:C2	2.81	0.48
53:BB:62:LEU:HA	53:BB:65:ARG:HE	1.77	0.48
48:5:4989:U:O2	48:5:4989:U:O4'	2.30	0.48
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.44	0.48
50:8:103:A:C8	50:8:104:A:C8	3.02	0.48
56:EE:173:ILE:HD11	56:EE:235:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4152:G:N2	48:5:4153:C:C2	2.81	0.48
6:F:110:VAL:HG21	6:F:137:ILE:HD12	1.96	0.48
48:5:77:U:H3	48:5:336:A:N6	2.12	0.48
47:3:34:U:O2'	47:3:35:U:O4'	2.32	0.48
51:9:1406:G:C5	51:9:1407:U:H1'	2.48	0.48
51:9:1235:G:H5'	51:9:1247:C:N4	2.23	0.48
48:5:3629:A:C1'	51:9:1721:U:O2	2.61	0.48
48:5:499:G:H2'	48:5:499:G:N3	2.28	0.48
51:9:433:A:H2'	51:9:434:G:C8	2.49	0.48
67:PP:34:MET:CE	67:PP:42:ARG:HA	2.43	0.48
48:5:671:G:C2	48:5:672:C:C2	3.02	0.48
48:5:2315:G:C2	48:5:2325:C:C2	3.01	0.48
75:XX:67:ARG:HG2	75:XX:115:ILE:HD12	1.96	0.48
52:AA:157:VAL:HG23	52:AA:157:VAL:O	2.14	0.48
48:5:1751:A:C2	48:5:1780:A:C2	3.02	0.48
50:8:46:G:N2	50:8:47:C:C2	2.82	0.48
48:5:230:G:C2	48:5:239:C:C2	3.02	0.48
48:5:1964:A:C2'	48:5:1965:G:C5'	2.91	0.48
48:5:199:G:C6	48:5:220:C:N3	2.81	0.48
65:NN:60:VAL:HG23	65:NN:66:VAL:HG21	1.96	0.48
48:5:1400:G:H2'	48:5:1401:C:O4'	2.14	0.48
48:5:5020:G:C2	48:5:5021:C:C2	3.02	0.48
51:9:1046:U:H2'	51:9:1047:C:O4'	2.14	0.48
48:5:1822:U:O4'	48:5:1822:U:O2	2.29	0.48
51:9:15:U:H2'	51:9:16:G:O4'	2.14	0.48
60:II:11:ARG:NH1	60:II:15:GLY:O	2.41	0.48
48:5:4883:C:O2'	48:5:4884:G:P	2.72	0.48
51:9:1481:G:C6	51:9:1482:C:N3	2.82	0.48
66:OO:54:CYS:SG	66:OO:84:ARG:HG3	2.54	0.48
48:5:1198:G:H2'	48:5:1199:G:C8	2.48	0.48
6:F:118:GLN:HB2	6:F:121:ASN:HD21	1.78	0.48
51:9:1308:U:O4	51:9:1309:C:C6	2.65	0.47
46:2:40:C:H4'	47:3:36:U:H1'	1.96	0.47
48:5:3717:A:O2'	48:5:3718:A:O4'	2.32	0.47
51:9:71:G:O2'	51:9:72:C:OP1	2.24	0.47
51:9:1265:A:H2'	51:9:1265:A:N3	2.28	0.47
48:5:967:C:N3	48:5:2254:G:C6	2.81	0.47
48:5:4666:G:C6	48:5:4667:C:C4	3.01	0.47
48:5:2496:G:C2	48:5:2497:C:C2	3.02	0.47
47:3:5:G:C4	47:3:6:G:N7	2.81	0.47
51:9:1408:U:C4	51:9:1409:A:C6	3.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:499:G:C2	48:5:500:G:C8	3.02	0.47
51:9:1537:A:C2	51:9:1596:U:N3	2.82	0.47
48:5:1987:C:C2'	48:5:1987:C:O2	2.61	0.47
48:5:4305:G:N3	48:5:4305:G:H2'	2.29	0.47
48:5:3918:G:C6	48:5:3919:C:C4	3.02	0.47
48:5:4099:G:C2	48:5:4100:C:C2	3.02	0.47
48:5:1655:C:H2'	48:5:1656:U:H5''	1.96	0.47
75:XX:9:THR:O	75:XX:10:ALA:C	2.52	0.47
48:5:929:A:H3'	48:5:930:G:C5'	2.43	0.47
48:5:1221:G:O2'	48:5:1222:A:O5'	2.21	0.47
48:5:1904:G:C2	48:5:2073:C:C2	3.02	0.47
7:G:162:ASP:HB3	7:G:163:PRO:HD3	1.96	0.47
48:5:1189:G:C6	48:5:1190:C:C4	3.02	0.47
48:5:1240:G:C2	48:5:1241:C:C2	3.02	0.47
48:5:199:G:N1	48:5:220:C:C2	2.82	0.47
48:5:2097:U:O4'	48:5:2097:U:O2	2.32	0.47
48:5:2539:C:H2'	48:5:2540:C:C6	2.49	0.47
48:5:4119:C:O4'	48:5:4119:C:O2	2.30	0.47
46:2:30:G:C6	46:2:31:C:C4	3.02	0.47
60:II:162:LEU:HD11	60:II:191:GLU:HG2	1.97	0.47
48:5:1246:G:H2'	48:5:1247:U:O4'	2.14	0.47
51:9:1299:A:OP2	67:PP:59:ARG:NH2	2.47	0.47
51:9:666:U:H2'	51:9:667:U:C6	2.50	0.47
51:9:1308:U:N3	51:9:1309:C:H1'	2.23	0.47
48:5:1358:G:O6	48:5:1379:C:N3	2.47	0.47
48:5:4919:G:C2	48:5:4920:C:C2	3.02	0.47
49:7:71:G:C2	49:7:105:C:C2	3.03	0.47
48:5:1238:A:H2'	48:5:1239:C:C6	2.49	0.47
48:5:300:A:H2'	48:5:301:G:C8	2.50	0.47
48:5:2336:G:C2	48:5:2337:C:C2	3.03	0.47
48:5:100:C:O2	48:5:100:C:O4'	2.30	0.47
48:5:2267:U:O4'	48:5:2267:U:O2	2.33	0.47
3:C:303:ARG:O	16:Q:38:ARG:NH1	2.46	0.47
3:C:209:VAL:HB	3:C:229:LEU:HD13	1.97	0.47
14:O:17:GLY:HA3	48:5:2052:G:O3'	2.14	0.47
48:5:705:G:N2	48:5:706:C:C2	2.82	0.47
51:9:1847:G:N2	51:9:1853:C:C2	2.83	0.47
56:EE:54:TYR:CD1	76:YY:17:LEU:HD11	2.49	0.47
47:3:5:G:C2	47:3:6:G:C4	3.03	0.47
48:5:499:G:C2	48:5:656:C:N3	2.82	0.47
51:9:1650:A:C5	51:9:1675:A:N1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1240:G:C6	48:5:1241:C:C4	3.03	0.47
48:5:2089:G:C6	48:5:2262:G:H2'	2.49	0.47
51:9:832:G:N2	51:9:843:C:C2	2.82	0.47
48:5:4759:C:H2'	48:5:4760:G:O4'	2.14	0.47
48:5:2496:G:C6	48:5:2497:C:C4	3.03	0.47
48:5:1723:A:N1	48:5:1838:A:C2	2.83	0.47
51:9:1535:U:O2	51:9:1535:U:H2'	2.15	0.47
48:5:1584:G:C6	48:5:1585:C:C4	3.01	0.47
51:9:1344:A:N6	51:9:1386:A:C5'	2.77	0.47
51:9:1211:G:C3'	51:9:1212:G:H5'	2.43	0.47
57:FF:73:THR:HG22	57:FF:89:THR:CG2	2.45	0.47
48:5:1189:G:C2	48:5:1190:C:C2	3.03	0.47
69:RR:24:LEU:HD22	69:RR:54:VAL:HG11	1.95	0.47
51:9:92:A:C6	51:9:446:G:C6	3.03	0.47
19:T:57:TYR:CD1	19:T:76:VAL:HG21	2.49	0.47
1:A:162:ASN:C	1:A:162:ASN:HD22	2.18	0.47
48:5:978:G:C2	48:5:979:C:C2	3.02	0.47
51:9:1308:U:O4	51:9:1309:C:C4	2.67	0.47
3:C:86:ARG:HA	3:C:89:GLN:HG3	1.95	0.47
47:3:34:U:O2	51:9:1641:A:C5'	2.60	0.47
48:5:1367:C:H2'	48:5:1367:C:O2	2.14	0.47
2:B:220:ILE:HB	2:B:346:THR:HB	1.97	0.47
50:8:56:G:C2	50:8:57:C:C2	3.03	0.47
48:5:2065:G:C2	48:5:2066:C:C2	3.03	0.47
48:5:742:G:C2	48:5:923:C:C2	3.03	0.47
51:9:86:C:C4	51:9:87:U:C5	3.03	0.47
48:5:2542:G:C2	48:5:2775:C:C2	3.03	0.47
51:9:1115:U:O4'	51:9:1115:U:O2	2.32	0.47
51:9:1260:A:C4	51:9:1620:A:N7	2.82	0.47
51:9:1648:G:C8	68:QQ:125:ARG:HB3	2.50	0.47
48:5:2612:G:C6	48:5:2613:C:C4	3.02	0.47
4:D:35:ARG:HB2	48:5:4325:A:C2	2.49	0.47
48:5:1099:C:H2'	48:5:1100:U:O4'	2.15	0.47
48:5:4740:G:C2	48:5:4741:C:C2	3.03	0.47
48:5:4773:C:C2	48:5:4863:G:C2	3.03	0.47
52:AA:2:SER:OG	52:AA:56:GLU:O	2.29	0.47
48:5:2477:A:H2'	48:5:2478:C:C6	2.50	0.47
51:9:1754:G:C6	51:9:1755:C:C4	3.03	0.47
51:9:1666:C:H2'	51:9:1667:U:O4'	2.15	0.47
47:3:69:G:N1	47:3:70:G:C6	2.83	0.47
48:5:2128:G:C2	48:5:2129:C:C2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:126:GLU:OE2	12:M:130:LEU:HD13	2.14	0.47
48:5:4916:G:C2	48:5:4917:C:C2	3.02	0.47
51:9:1551:U:H2'	51:9:1552:G:C8	2.50	0.47
49:7:93:G:C2	49:7:94:C:C2	3.03	0.47
48:5:751:G:C2	48:5:752:G:N7	2.82	0.47
48:5:2698:G:C6	48:5:2699:C:C4	3.03	0.47
48:5:3709:U:O2'	48:5:3710:G:O4'	2.32	0.47
48:5:3896:C:O2	48:5:4564:A:N1	2.48	0.47
48:5:4472:G:C6	48:5:4473:A:N7	2.83	0.47
48:5:3628:G:C2	48:5:3834:C:C2	3.03	0.47
50:8:75:G:N2	50:8:76:C:C2	2.83	0.47
70:SS:82:TRP:O	70:SS:84:LEU:N	2.48	0.47
51:9:1454:A:HO2'	51:9:1455:A:P	2.37	0.47
58:GG:3:LEU:HD22	58:GG:109:LEU:HB2	1.96	0.47
59:HH:133:LEU:HD21	59:HH:176:VAL:HG11	1.97	0.47
48:5:1550:G:N1	48:5:1551:C:C2	2.83	0.47
48:5:2088:A:HO2'	48:5:2089:G:P	2.38	0.47
48:5:299:C:C4	48:5:300:A:N7	2.83	0.47
48:5:3717:A:OP2	48:5:3735:G:N2	2.48	0.47
48:5:2245:G:C2	48:5:2246:C:C2	3.03	0.47
51:9:12:U:H2'	51:9:13:C:C6	2.50	0.47
48:5:2907:G:H2'	48:5:2908:U:O4'	2.15	0.47
48:5:4102:C:C2	48:5:4108:G:C2	3.03	0.47
48:5:3597:G:C2	48:5:3598:C:C2	3.03	0.47
48:5:3629:A:O4'	51:9:1721:U:O2	2.33	0.47
5:E:126:ARG:HH21	48:5:712:C:C2'	2.28	0.47
48:5:4758:U:O4'	48:5:4758:U:O2	2.31	0.47
48:5:1995:G:C5	48:5:1996:C:C4	3.02	0.47
48:5:479:G:N2	48:5:480:C:C2	2.83	0.47
48:5:3626:G:C6	48:5:3836:A:C2	3.03	0.47
13:N:94:PHE:CE2	13:N:96:ARG:HB2	2.50	0.47
48:5:1613:A:H3'	48:5:1614:C:C5'	2.45	0.47
48:5:177:G:C2	48:5:178:C:C2	3.02	0.47
48:5:1557:C:C2	48:5:1571:G:C2	3.03	0.47
48:5:2028:C:O2'	48:5:2029:A:O5'	2.33	0.46
76:YY:113:ARG:O	76:YY:114:MET:CB	2.62	0.46
48:5:4411:G:C2	48:5:4432:C:O2	2.68	0.46
48:5:4092:G:C2	48:5:4158:C:C2	3.03	0.46
51:9:639:C:H2'	51:9:640:A:C8	2.50	0.46
48:5:1171:G:C6	48:5:1172:C:C4	3.03	0.46
68:QQ:42:ILE:HD12	68:QQ:42:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:105:LEU:HD12	17:R:138:LEU:HD13	1.97	0.46
48:5:2844:A:O2'	48:5:4631:G:H4'	2.14	0.46
48:5:105:A:C2	48:5:336:A:C8	3.04	0.46
48:5:497:G:H3'	48:5:498:C:H5''	1.97	0.46
48:5:1468:C:C2	48:5:1498:G:N2	2.83	0.46
51:9:1265:A:N3	51:9:1265:A:C2'	2.77	0.46
48:5:99:A:H2'	48:5:100:C:O2	2.14	0.46
48:5:177:G:C6	48:5:178:C:C4	3.02	0.46
48:5:3627:G:N2	48:5:3835:C:C2	2.83	0.46
50:8:53:G:C6	50:8:54:C:C4	3.03	0.46
48:5:4904:G:N2	48:5:4905:C:C2	2.84	0.46
48:5:1357:C:H5''	48:5:1358:G:OP1	2.16	0.46
48:5:181:C:C4	48:5:256:G:N1	2.84	0.46
11:L:165:LYS:HB2	11:L:165:LYS:HZ1	1.80	0.46
51:9:834:C:H3'	51:9:835:C:H4'	1.96	0.46
51:9:697:G:C2	51:9:734:C:C2	3.03	0.46
51:9:1141:G:N2	51:9:1147:C:C2	2.84	0.46
48:5:4652:G:N2	48:5:4653:C:C2	2.84	0.46
65:NN:40:LEU:HD21	65:NN:53:ILE:HG21	1.97	0.46
12:M:125:ASN:O	12:M:129:LYS:HG3	2.15	0.46
51:9:194:C:C2	51:9:206:G:C2	3.04	0.46
48:5:4489:G:C6	48:5:4490:C:C4	3.03	0.46
17:R:71:ARG:NH1	48:5:3605:C:OP2	2.38	0.46
61:JJ:118:GLY:O	61:JJ:120:ALA:N	2.48	0.46
47:3:37:A:N1	57:FF:133:THR:HG23	2.30	0.46
51:9:50:A:C2	51:9:488:U:O4	2.68	0.46
51:9:962:A:N1	51:9:1055:A:O2'	2.48	0.46
48:5:1661:C:C2	48:5:2345:G:N1	2.84	0.46
48:5:1448:G:C6	48:5:1449:C:N4	2.83	0.46
51:9:14:C:C2	51:9:1198:G:C2	3.04	0.46
48:5:488:G:N2	48:5:489:C:C2	2.84	0.46
51:9:1534:C:H1'	51:9:1536:G:C4	2.51	0.46
51:9:1459:G:C6	51:9:1460:C:C4	3.04	0.46
51:9:187:G:C6	51:9:188:C:C4	3.04	0.46
54:CC:94:ILE:HD11	54:CC:98:LEU:HD12	1.97	0.46
48:5:994:G:C2	48:5:1050:C:C2	3.03	0.46
51:9:987:A:C2	53:BB:114:VAL:HG21	2.51	0.46
48:5:977:C:O2'	48:5:978:G:H5'	2.16	0.46
51:9:1308:U:O4	51:9:1309:C:C2	2.68	0.46
17:R:176:ARG:HH12	51:9:909:G:H5'	1.81	0.46
48:5:4919:G:C6	48:5:4920:C:C4	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2088:A:O2'	48:5:2089:G:P	2.74	0.46
51:9:834:C:C2	51:9:841:G:N2	2.84	0.46
48:5:1998:A:O2'	48:5:1999:A:O4'	2.33	0.46
47:3:24:G:C2	47:3:25:C:C2	3.02	0.46
48:5:984:C:C2	48:5:1070:G:N2	2.83	0.46
48:5:209:U:N3	48:5:233:U:C4	2.83	0.46
13:N:172:ARG:NH1	48:5:62:A:OP1	2.49	0.46
51:9:1524:G:N2	51:9:1525:C:C2	2.83	0.46
48:5:1235:G:H2'	48:5:1236:C:H5'	1.96	0.46
51:9:123:G:C2	51:9:342:C:C2	3.03	0.46
48:5:2468:U:N3	48:5:2473:A:C6	2.83	0.46
5:E:59:TYR:CE1	5:E:64:LEU:HB2	2.50	0.46
48:5:504:G:O6	48:5:654:C:C4	2.69	0.46
51:9:1129:G:H3'	51:9:1130:G:C8	2.48	0.46
51:9:980:A:C2	51:9:981:A:C6	3.03	0.46
48:5:4916:G:C6	48:5:4917:C:C4	3.04	0.46
12:M:24:LEU:HB2	12:M:43:THR:HG21	1.98	0.46
48:5:3586:G:C2	48:5:3587:C:C2	3.03	0.46
48:5:4136:G:C2	48:5:4137:C:C2	3.04	0.46
48:5:2771:G:C6	48:5:2772:C:C4	3.04	0.46
51:9:1624:U:O2	51:9:1624:U:O4'	2.34	0.46
13:N:57:GLN:HB3	13:N:139:HIS:CE1	2.50	0.46
51:9:182:C:H2'	51:9:184:G:H1'	1.96	0.46
9:I:61:SER:HA	9:I:126:VAL:HG23	1.97	0.46
3:C:130:ALA:HB3	3:C:246:VAL:HG13	1.97	0.46
61:JJ:121:LYS:NZ	61:JJ:121:LYS:HG2	4.27	0.46
48:5:977:C:H2'	48:5:978:G:O4'	2.15	0.46
51:9:873:G:N1	51:9:914:U:C5	2.84	0.46
10:J:165:TRP:CH2	10:J:170:TYR:CE2	2.99	0.46
51:9:1537:A:C2	51:9:1538:C:C2	3.03	0.46
47:3:31:A:H2'	57:FF:136:ARG:NH2	2.31	0.46
48:5:1878:G:N2	48:5:1879:C:C2	2.83	0.46
19:T:130:ARG:NH2	48:5:1836:G:OP1	2.48	0.46
7:G:100:HIS:HA	7:G:103:ARG:HD2	1.98	0.46
66:OO:65:ASP:N	66:OO:65:ASP:OD1	2.48	0.46
48:5:721:G:C2	48:5:948:C:C2	3.03	0.46
48:5:4454:G:HO2'	48:5:4500:U:HO2'	1.59	0.46
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.98	0.46
56:EE:195:ILE:O	56:EE:196:THR:CB	2.64	0.46
51:9:321:C:H2'	51:9:322:C:C6	2.51	0.46
5:E:217:GLN:HE22	5:E:233:LYS:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:254:LEU:N	5:E:255:PRO:HD2	2.30	0.46
51:9:1231:C:H2'	51:9:1232:U:O4'	2.16	0.46
48:5:1241:C:C2'	48:5:1242:G:OP1	2.64	0.46
4:D:44:TYR:CD1	48:5:1823:G:H4'	2.51	0.46
48:5:4473:A:C2	48:5:4474:A:C5	3.03	0.46
48:5:4737:G:C2	48:5:4738:C:C2	3.03	0.46
3:C:218:VAL:HG12	3:C:218:VAL:O	2.14	0.46
53:BB:86:LEU:HA	53:BB:99:ASN:O	2.15	0.46
7:G:58:PRO:CD	23:X:46:PHE:HD2	2.28	0.46
48:5:1899:G:N2	48:5:1900:C:C2	2.83	0.46
48:5:1818:G:O2'	48:5:1819:G:OP1	2.23	0.46
48:5:1362:G:N2	48:5:1363:C:C2	2.83	0.46
51:9:1476:A:H3'	51:9:1477:U:C5'	2.46	0.46
48:5:1270:A:H2'	48:5:1271:G:O4'	2.16	0.46
51:9:1109:C:O2'	51:9:1110:G:O5'	2.16	0.46
48:5:4109:G:C6	48:5:4110:C:C4	3.04	0.46
48:5:4731:G:H4'	48:5:4732:G:H5'	1.98	0.46
6:F:91:LEU:HD22	6:F:92:ALA:N	2.31	0.46
48:5:1910:G:C6	48:5:1911:C:N4	2.84	0.46
70:SS:113:ARG:HG2	70:SS:113:ARG:HH11	1.80	0.46
51:9:437:G:C2	51:9:457:C:C2	3.03	0.46
51:9:1759:G:C2	51:9:1774:C:C2	3.04	0.46
48:5:1279:A:C4	48:5:1280:C:C4	3.04	0.46
48:5:1958:A:O2'	48:5:1959:U:H5''	2.15	0.46
48:5:4913:G:HO2'	48:5:4914:C:C1'	2.28	0.46
51:9:409:C:C2	51:9:432:G:C2	3.03	0.46
48:5:1995:G:C6	48:5:1996:C:N3	2.84	0.46
48:5:4524:G:N2	48:5:4525:C:C2	2.84	0.46
51:9:156:G:H4'	58:GG:108:VAL:HG23	1.97	0.46
14:O:18:ARG:NH1	48:5:2053:C:O3'	2.47	0.46
48:5:1098:G:C2	48:5:1099:C:C2	3.04	0.46
48:5:2898:G:C6	48:5:2899:C:C4	3.04	0.46
51:9:1347:U:H2'	51:9:1348:G:C8	2.50	0.46
48:5:1539:G:C6	48:5:1540:C:C4	3.03	0.46
48:5:2752:G:H2'	48:5:2753:G:O4'	2.16	0.46
61:JJ:120:ALA:O	61:JJ:121:LYS:CB	2.64	0.45
51:9:642:U:H4'	51:9:643:A:OP1	2.16	0.45
48:5:1399:G:H2'	48:5:1400:G:O4'	2.16	0.45
48:5:2729:C:H2'	48:5:2730:U:O4'	2.15	0.45
48:5:2:G:C2	48:5:3:C:C2	3.04	0.45
49:7:27:G:C2	49:7:28:C:C2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:GG:66:GLY:N	58:GG:100:CYS:SG	2.89	0.45
48:5:971:U:H2'	48:5:972:C:H5'	1.98	0.45
46:2:7:G:C6	46:2:49:C:N4	2.84	0.45
51:9:1275:G:O2'	51:9:1276:A:OP2	2.28	0.45
49:7:117:G:C2	49:7:118:C:C2	3.04	0.45
50:8:115:G:N2	50:8:116:C:C2	2.84	0.45
48:5:715:G:H1	48:5:953:C:H42	1.63	0.45
51:9:830:A:H2'	51:9:831:G:O4'	2.17	0.45
4:D:41:LYS:CG	19:T:93:ILE:HD11	2.46	0.45
48:5:747:A:C2	48:5:749:G:H1'	2.50	0.45
48:5:302:C:N4	48:5:303:C:N4	2.64	0.45
51:9:1835:A:N9	51:9:1863:A:N7	2.63	0.45
48:5:1613:A:H3'	48:5:1614:C:H5'	1.98	0.45
48:5:4303:C:O2	48:5:4303:C:O4'	2.34	0.45
46:2:34:A:O2'	46:2:35:A:O4'	2.31	0.45
51:9:52:G:C6	51:9:53:C:C4	3.05	0.45
48:5:2567:G:C2	48:5:2568:C:C2	3.04	0.45
48:5:4080:C:C2	48:5:4167:G:C2	3.04	0.45
60:II:34:ALA:HB2	60:II:56:ARG:HG3	1.98	0.45
48:5:3600:G:C2	48:5:3601:C:C2	3.05	0.45
48:5:744:G:C2	48:5:921:C:C2	3.04	0.45
48:5:918:G:H2'	48:5:918:G:N3	2.32	0.45
47:3:76:A:C8	48:5:4341:C:N4	2.82	0.45
48:5:1270:A:C5	48:5:1271:G:H1'	2.52	0.45
48:5:4583:C:C2	48:5:4718:G:N2	2.84	0.45
48:5:2640:G:N7	48:5:2694:G:O6	2.49	0.45
48:5:5020:G:C6	48:5:5021:C:C4	3.04	0.45
51:9:1229:G:C2	51:9:1230:C:C2	3.04	0.45
48:5:3705:G:C6	48:5:3706:C:C4	3.05	0.45
62:KK:12:TYR:CD2	62:KK:79:LEU:HD22	2.52	0.45
57:FF:20:PHE:CZ	57:FF:69:VAL:HG11	2.52	0.45
48:5:2768:C:O2	48:5:2768:C:O4'	2.31	0.45
48:5:4587:G:C2	48:5:4716:C:C2	3.05	0.45
24:Y:10:ASP:O	24:Y:11:ARG:C	2.54	0.45
48:5:2270:G:C6	48:5:2271:C:C4	3.05	0.45
48:5:2465:C:H2'	48:5:2466:G:O4'	2.16	0.45
48:5:179:G:C2	48:5:180:C:C2	3.05	0.45
51:9:1669:G:C6	51:9:1670:C:C4	3.04	0.45
48:5:278:G:H4'	48:5:279:A:OP2	2.16	0.45
66:OO:139:SER:OG	66:OO:140:THR:N	2.49	0.45
25:Z:46:ILE:HD11	25:Z:49:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1874:A:H5'	48:5:4218:U:O2	2.17	0.45
47:3:66:U:O4	47:3:67:U:C4	2.70	0.45
17:R:176:ARG:NH1	51:9:909:G:C5'	2.77	0.45
75:XX:94:ILE:HD11	75:XX:122:VAL:HG11	1.97	0.45
48:5:1823:G:C3'	48:5:1825:A:P	3.04	0.45
48:5:5020:G:H2'	48:5:5021:C:O4'	2.16	0.45
48:5:1584:G:C2	48:5:1585:C:C2	3.05	0.45
48:5:4740:G:C6	48:5:4741:C:C4	3.04	0.45
48:5:2245:G:C6	48:5:2246:C:C4	3.04	0.45
9:I:97:ILE:HD13	9:I:126:VAL:HG11	1.97	0.45
57:FF:49:LEU:HD13	57:FF:50:PRO:HD2	1.99	0.45
53:BB:212:VAL:HG23	53:BB:212:VAL:O	2.15	0.45
4:D:42:ASN:N	4:D:42:ASN:OD1	2.48	0.45
51:9:592:C:O4'	51:9:592:C:O2	2.33	0.45
51:9:916:A:C5	65:NN:73:ARG:HD3	2.52	0.45
48:5:325:U:H2'	48:5:326:C:C6	2.51	0.45
51:9:1038:U:O2'	51:9:1180:C:N3	2.49	0.45
58:GG:67:VAL:HG23	58:GG:99:GLY:HA2	1.98	0.45
59:HH:15:LYS:N	59:HH:16:PRO:HD2	2.32	0.45
47:3:3:C:H2'	47:3:4:C:H5'	1.99	0.45
51:9:1131:G:N1	51:9:1132:C:C4	2.84	0.45
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	1.98	0.45
74:WW:6:VAL:HG13	74:WW:29:PRO:HG2	1.97	0.45
48:5:3782:C:C2	48:5:3811:G:C2	3.05	0.45
48:5:469:C:C2	48:5:470:A:C8	3.05	0.45
50:8:56:G:C6	50:8:57:C:C4	3.05	0.45
48:5:4489:G:C2	48:5:4490:C:C2	3.04	0.45
48:5:3600:G:C6	48:5:3601:C:C4	3.05	0.45
51:9:1229:G:C6	51:9:1230:C:C4	3.05	0.45
2:B:100:ARG:NH1	48:5:4911:A:OP2	2.50	0.45
48:5:476:G:N2	48:5:679:C:C2	2.85	0.45
25:Z:100:VAL:HG13	25:Z:107:LYS:HA	1.97	0.45
63:LL:96:ILE:HD12	63:LL:96:ILE:N	2.32	0.45
1:A:97:ASN:N	1:A:97:ASN:OD1	2.49	0.45
3:C:78:ARG:HB3	3:C:88:GLY:HA2	1.98	0.45
51:9:443:U:O2'	58:GG:89:THR:HG22	2.17	0.45
50:8:118:C:C2	50:8:133:G:C2	3.04	0.45
51:9:1386:A:OP1	51:9:1483:A:N3	2.50	0.45
48:5:1297:U:O4'	48:5:1297:U:P	2.75	0.45
48:5:994:G:C2	48:5:995:C:C2	3.05	0.45
56:EE:86:PHE:HE2	56:EE:226:PHE:CD2	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:963:G:H2'	48:5:963:G:N3	2.32	0.45
51:9:1057:C:O2	51:9:1057:C:O4'	2.35	0.45
48:5:1855:G:C6	48:5:1856:C:C4	3.05	0.45
48:5:1732:C:C2	48:5:1798:G:C2	3.04	0.45
51:9:673:G:C2	51:9:674:C:C2	3.05	0.45
48:5:190:G:C2	48:5:252:C:C2	3.05	0.45
48:5:4482:U:N3	48:5:4483:C:C5	2.84	0.45
9:I:3:ARG:NH2	48:5:4431:U:OP2	2.50	0.45
51:9:841:G:N1	51:9:842:C:C4	2.85	0.45
58:GG:61:PHE:CE2	58:GG:96:SER:HB3	2.52	0.45
48:5:2909:C:O2	48:5:3586:G:C2	2.70	0.45
48:5:994:G:C6	48:5:995:C:C4	3.04	0.45
48:5:5031:G:N2	48:5:5032:C:C2	2.85	0.45
48:5:2618:G:C2	48:5:2720:C:C2	3.04	0.45
66:OO:31:CYS:HA	66:OO:44:VAL:HA	1.99	0.45
51:9:301:A:N3	60:II:73:THR:HG21	2.31	0.45
61:JJ:121:LYS:NZ	61:JJ:121:LYS:CG	3.85	0.45
48:5:1965:G:O2'	48:5:1966:C:P	2.74	0.45
51:9:1407:U:C2'	51:9:1408:U:C6	2.97	0.45
48:5:1213:G:C4	48:5:1215:C:H1'	2.52	0.45
3:C:262:ASP:O	3:C:271:ALA:O	2.34	0.45
48:5:1365:C:O2	48:5:1366:G:C8	2.70	0.45
48:5:4109:G:C2	48:5:4110:C:C2	3.05	0.45
50:8:53:G:C2	50:8:54:C:C2	3.05	0.45
48:5:2898:G:C2	48:5:2899:C:C2	3.05	0.45
7:G:63:LEU:HD12	13:N:32:GLN:HB3	1.99	0.45
51:9:1058:A:H2'	51:9:1059:G:C8	2.52	0.45
48:5:1416:G:N2	48:5:1417:C:C2	2.85	0.45
48:5:2559:G:C6	48:5:2560:C:C4	3.04	0.45
9:I:139:ARG:NH1	9:I:195:CYS:SG	2.90	0.45
63:LL:59:LYS:O	63:LL:141:ASN:ND2	2.46	0.45
48:5:3648:A:H1'	48:5:3785:A:N6	2.31	0.45
48:5:1196:G:C6	48:5:1197:C:C4	3.05	0.45
56:EE:55:ALA:HB2	56:EE:64:ILE:HD12	1.99	0.45
47:3:5:G:C6	47:3:6:G:O6	2.70	0.45
48:5:2408:U:C1'	48:5:2409:U:C5	3.00	0.45
51:9:1516:G:O3'	67:PP:122:THR:HG21	2.16	0.45
51:9:1386:A:O2'	51:9:1387:G:C5'	2.63	0.45
48:5:3662:A:N6	48:5:3680:U:N3	2.60	0.45
48:5:1404:G:C6	48:5:1405:C:C4	3.04	0.45
51:9:433:A:H5''	60:II:22:HIS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1448:G:C2	48:5:1449:C:C2	3.05	0.45
51:9:52:G:C2	51:9:53:C:C2	3.04	0.45
51:9:1228:A:H2'	51:9:1229:G:C8	2.51	0.45
3:C:76:ILE:HG22	3:C:77:PRO:HD2	1.98	0.45
48:5:1196:G:C2	48:5:1197:C:C2	3.04	0.45
48:5:4476:C:O2	48:5:4476:C:O4'	2.35	0.45
48:5:2715:G:C2	48:5:2716:C:C2	3.05	0.45
51:9:696:G:C2	51:9:735:C:C2	3.05	0.45
48:5:4142:C:C4	48:5:4143:G:N1	2.85	0.45
13:N:180:PHE:O	13:N:182:HIS:N	2.50	0.45
48:5:1963:C:HO2'	48:5:1964:A:P	2.40	0.45
48:5:917:A:C6	48:5:919:C:N4	2.85	0.45
51:9:832:G:C6	51:9:833:C:C4	3.05	0.45
51:9:1139:C:H2'	51:9:1140:G:O4'	2.17	0.45
51:9:1398:G:C6	51:9:1399:C:C4	3.05	0.45
51:9:1298:G:O2'	51:9:1299:A:O5'	2.35	0.45
49:7:117:G:C6	49:7:118:C:C4	3.05	0.45
56:EE:160:ILE:HG21	56:EE:169:ILE:HG22	1.99	0.45
1:A:211:PHE:CD1	1:A:219:ILE:HG23	2.53	0.45
48:5:5017:G:C2	48:5:5018:C:C2	3.05	0.45
47:3:5:G:O2'	47:3:6:G:H5'	2.17	0.44
51:9:1268:C:O2'	51:9:1269:G:P	2.75	0.44
51:9:322:C:C6	51:9:322:C:OP2	2.70	0.44
51:9:1131:G:N2	51:9:1132:C:C2	2.85	0.44
48:5:4461:C:N3	48:5:4516:G:C6	2.86	0.44
48:5:2730:U:H2'	48:5:2731:C:C6	2.52	0.44
50:8:75:G:C6	50:8:76:C:N4	2.85	0.44
11:L:18:TRP:CE3	13:N:198:LEU:HD12	2.53	0.44
14:O:61:ARG:HA	14:O:70:PRO:HD2	1.99	0.44
48:5:2858:A:O2'	48:5:2859:G:O4'	2.34	0.44
48:5:1280:C:N3	48:5:1282:G:C6	2.84	0.44
54:CC:191:VAL:CA	54:CC:228:SER:CB	2.81	0.44
51:9:1145:A:C6	51:9:1146:C:H1'	2.52	0.44
48:5:4075:U:H4'	48:5:4076:G:OP1	2.17	0.44
48:5:1245:C:C5	48:5:1269:G:C6	3.06	0.44
48:5:2089:G:HO2'	48:5:2090:U:P	2.39	0.44
48:5:4147:G:C6	48:5:4148:C:C4	3.05	0.44
48:5:1171:G:C2	48:5:1172:C:C2	3.05	0.44
51:9:1717:C:C2	51:9:1817:G:N2	2.86	0.44
51:9:1045:U:H2'	51:9:1046:U:O4'	2.17	0.44
8:H:137:SER:HB3	8:H:145:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:210:ILE:HD12	3:C:210:ILE:N	2.33	0.44
48:5:4495:G:C2	48:5:4506:C:C2	3.06	0.44
48:5:158:A:C4	48:5:277:G:C6	3.05	0.44
13:N:178:HIS:HA	13:N:181:HIS:CE1	2.53	0.44
23:X:76:ILE:HG21	23:X:112:ALA:HB2	1.99	0.44
3:C:158:VAL:HG12	3:C:217:ILE:HD12	1.98	0.44
48:5:654:C:H2'	48:5:654:C:O2	2.17	0.44
48:5:3723:A:C2	48:5:3724:A:C5	3.05	0.44
51:9:1526:G:N1	51:9:1527:C:C4	2.85	0.44
51:9:167:G:N1	51:9:168:C:C4	2.86	0.44
48:5:2315:G:C2	48:5:2325:C:O2	2.71	0.44
51:9:673:G:C6	51:9:674:C:C4	3.04	0.44
12:M:132:ARG:O	12:M:135:LEU:HB3	2.17	0.44
48:5:4584:A:H2'	48:5:4585:U:O4'	2.18	0.44
51:9:1739:C:C2	51:9:1796:G:C2	3.05	0.44
48:5:3941:G:H2'	48:5:3942:A:O4'	2.16	0.44
51:9:1749:G:C2	51:9:1750:C:C2	3.05	0.44
46:2:65:G:N2	46:2:66:C:C2	2.86	0.44
48:5:1466:G:N2	48:5:1467:C:C2	2.85	0.44
48:5:4212:A:C2	48:5:4218:U:C5	3.06	0.44
47:3:69:G:C2	47:3:70:G:C6	3.05	0.44
51:9:1267:C:C2	51:9:1516:G:N2	2.86	0.44
51:9:1649:U:C4	51:9:1675:A:C2	3.06	0.44
48:5:1268:G:O4'	48:5:2111:G:C5	2.71	0.44
51:9:1416:C:O3'	51:9:1417:C:O4'	2.36	0.44
48:5:1835:G:H4'	48:5:1836:G:O5'	2.18	0.44
61:JJ:144:ILE:HA	61:JJ:145:PRO:HD3	1.89	0.44
51:9:123:G:N2	51:9:342:C:C2	2.86	0.44
48:5:4303:C:O5'	48:5:4303:C:O2	2.34	0.44
48:5:1383:G:C6	48:5:1384:C:C4	3.05	0.44
8:H:39:ASN:O	8:H:40:HIS:HB3	2.17	0.44
51:9:797:C:O2	51:9:798:G:O2'	2.34	0.44
48:5:211:G:H4'	48:5:234:G:C8	2.52	0.44
11:L:58:ILE:HG23	11:L:70:VAL:CG1	2.47	0.44
63:LL:55:TYR:CE2	63:LL:115:PRO:HG2	2.52	0.44
48:5:2664:G:N2	48:5:2671:C:C2	2.86	0.44
51:9:303:C:H2'	51:9:304:C:O4'	2.17	0.44
48:5:2468:U:C4	48:5:2473:A:N6	2.80	0.44
51:9:1447:G:O6	51:9:1448:A:N6	2.51	0.44
48:5:744:G:H2'	48:5:745:G:C8	2.52	0.44
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1268:G:C4	48:5:2111:G:N2	2.86	0.44
48:5:939:G:N3	48:5:939:G:H2'	2.33	0.44
45:1:68:VAL:C	46:2:76:A:O2'	2.56	0.44
48:5:4583:C:C2	48:5:4718:G:C2	3.04	0.44
48:5:4717:A:H2'	48:5:4718:G:O4'	2.17	0.44
11:L:9:ILE:O	11:L:9:ILE:HG23	2.18	0.44
48:5:4966:A:H2'	48:5:4967:A:O4'	2.17	0.44
48:5:2612:G:C2	48:5:2613:C:C2	3.05	0.44
48:5:1308:C:H2'	48:5:1309:C:C6	2.53	0.44
17:R:99:MET:CE	17:R:128:LYS:HA	2.47	0.44
48:5:4876:U:O2	48:5:4876:U:O4'	2.35	0.44
48:5:2889:G:C6	48:5:2890:C:C4	3.05	0.44
48:5:2889:G:C2	48:5:2890:C:C2	3.05	0.44
51:9:1083:A:N7	51:9:1841:C:O2'	2.45	0.44
11:L:29:PRO:CB	48:5:1371:A:H2'	2.47	0.44
48:5:2457:G:C2	48:5:2458:C:C2	3.06	0.44
48:5:2779:C:O2'	50:8:112:G:OP1	2.25	0.44
7:G:147:VAL:HG13	7:G:179:VAL:HG21	2.00	0.44
48:5:2294:G:N2	48:5:2295:C:C2	2.85	0.44
51:9:1476:A:H3'	51:9:1477:U:H5''	2.00	0.44
7:G:86:VAL:CG2	7:G:185:LYS:HE3	2.26	0.44
3:C:161:TYR:HD1	3:C:166:GLU:CB	2.29	0.44
61:JJ:35:TYR:CD1	61:JJ:106:LEU:HD23	2.53	0.44
48:5:3724:A:C6	48:5:3725:G:C5	3.06	0.44
48:5:3680:U:O2	48:5:3680:U:H2'	2.17	0.44
51:9:1466:G:C6	51:9:1467:C:N4	2.86	0.44
48:5:2481:G:C6	48:5:2482:C:C4	3.05	0.44
48:5:4416:G:N1	48:5:4417:C:C4	2.86	0.44
55:DD:175:VAL:HG13	55:DD:182:LEU:CB	2.47	0.44
48:5:4462:C:C2	48:5:4515:G:N2	2.86	0.44
51:9:1229:G:H2'	51:9:1230:C:O4'	2.17	0.44
48:5:1855:G:C2	48:5:1856:C:C2	3.05	0.44
63:LL:55:TYR:CD2	63:LL:115:PRO:HG2	2.52	0.44
17:R:92:LYS:NZ	48:5:2606:G:O3'	2.50	0.44
48:5:4232:U:H1'	48:5:4233:A:OP2	2.18	0.44
48:5:4240:G:C6	48:5:4241:C:C4	3.05	0.44
48:5:4890:G:C2	48:5:4930:C:C2	3.05	0.44
48:5:1721:G:C6	48:5:1722:C:C4	3.06	0.44
50:8:134:G:C6	50:8:135:C:C4	3.06	0.44
48:5:2021:G:C6	48:5:2022:C:C4	3.06	0.44
57:FF:194:ASP:CG	57:FF:198:ARG:NH1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1679:A:H3'	57:FF:60:ARG:HD2	2.00	0.44
51:9:1267:C:C2	51:9:1516:G:C2	3.05	0.44
48:5:1358:G:H2'	48:5:1359:G:C8	2.53	0.44
48:5:642:G:C2	48:5:643:C:C4	3.05	0.44
48:5:1404:G:C2	48:5:1405:C:C2	3.06	0.44
48:5:223:G:H4'	48:5:225:G:C8	2.52	0.44
51:9:841:G:C2	51:9:842:C:C2	3.05	0.44
52:AA:155:ARG:NE	73:VV:61:ARG:O	2.48	0.44
51:9:1655:C:OP1	71:TT:92:PHE:N	2.46	0.44
50:8:139:G:C2	50:8:140:C:C2	3.05	0.44
52:AA:87:VAL:HG12	52:AA:175:TRP:CZ2	2.52	0.44
48:5:1236:C:O2'	48:5:1237:C:O5'	2.24	0.44
48:5:2594:C:O2	48:5:2752:G:C2	2.71	0.44
51:9:1749:G:C6	51:9:1750:C:C4	3.06	0.44
48:5:2021:G:C2	48:5:2022:C:C2	3.06	0.44
9:I:176:PHE:CE2	9:I:190:LEU:HD21	2.53	0.44
62:KK:15:LEU:O	62:KK:18:GLU:O	2.36	0.44
48:5:4898:G:N2	48:5:4923:C:C2	2.86	0.44
48:5:1667:G:H5'	48:5:1688:G:OP1	2.18	0.44
18:S:83:ARG:HH21	18:S:83:ARG:CG	2.30	0.44
51:9:190:G:O2'	51:9:209:A:N6	2.50	0.44
48:5:1431:C:C2	48:5:1454:G:C2	3.05	0.44
48:5:254:G:C2	48:5:255:C:C2	3.06	0.44
51:9:1563:G:C2	51:9:1564:C:C2	3.06	0.44
48:5:4433:G:N2	48:5:4434:C:C2	2.86	0.44
48:5:4250:G:C2	48:5:4259:C:C2	3.05	0.44
48:5:1826:G:C6	48:5:1827:C:C4	3.05	0.44
24:Y:99:ILE:HG21	24:Y:104:VAL:HG23	1.99	0.44
51:9:1777:G:C6	51:9:1778:C:C4	3.05	0.44
17:R:176:ARG:HH21	17:R:176:ARG:CB	2.23	0.44
51:9:1102:G:C2	51:9:1103:C:C5	3.06	0.44
51:9:752:G:N1	51:9:790:C:C4	2.85	0.44
48:5:1270:A:C2'	48:5:1271:G:O5'	2.66	0.44
51:9:200:G:C2	51:9:201:C:C4	3.06	0.44
12:M:62:LEU:HD23	12:M:82:ILE:HG13	1.99	0.44
48:5:688:U:H2'	48:5:689:U:C6	2.53	0.44
48:5:4666:G:C2	48:5:4667:C:C2	3.05	0.44
48:5:2542:G:N2	48:5:2775:C:C2	2.86	0.44
51:9:1754:G:C2	51:9:1755:C:C2	3.05	0.44
48:5:751:G:N2	48:5:912:G:C4	2.85	0.44
48:5:3597:G:C6	48:5:3598:C:C4	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:58:PRO:HD3	23:X:46:PHE:HD2	1.83	0.44
48:5:2567:G:C6	48:5:2568:C:C4	3.06	0.44
51:9:1669:G:C2	51:9:1670:C:C2	3.05	0.44
48:5:80:C:C2	48:5:104:G:C2	3.05	0.44
6:F:225:LYS:HE3	48:5:1907:A:H4'	2.00	0.44
50:8:10:G:C2	50:8:11:C:C2	3.06	0.44
48:5:1691:G:C6	48:5:1692:C:C4	3.06	0.44
57:FF:99:ILE:HG23	77:ZZ:67:LEU:HD21	2.00	0.44
51:9:1541:G:C6	51:9:1542:C:C4	3.06	0.44
51:9:1741:U:H2'	51:9:1742:C:O4'	2.17	0.44
48:5:4661:G:C6	48:5:4662:C:C4	3.04	0.44
48:5:174:C:C2	48:5:263:G:C2	3.05	0.44
4:D:282:GLN:OE1	48:5:1185:G:N2	2.51	0.44
47:3:4:C:O2'	47:3:5:G:O4'	2.35	0.44
48:5:956:A:H3'	48:5:957:G:C8	2.52	0.44
48:5:3752:C:H2'	48:5:3777:G:C8	2.53	0.44
51:9:323:C:H3'	51:9:324:C:C5'	2.48	0.44
48:5:1213:G:C6	48:5:1215:C:C4	3.06	0.44
48:5:4094:G:H2'	48:5:4095:G:C1'	2.48	0.44
51:9:636:C:C4	51:9:637:U:C4	3.06	0.44
51:9:1616:U:H2'	51:9:1617:G:O4'	2.18	0.44
51:9:187:G:C2	51:9:188:C:C2	3.05	0.44
48:5:205:C:C4	48:5:211:G:C6	3.06	0.44
48:5:2122:G:O2'	48:5:2123:C:P	2.76	0.44
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.99	0.44
48:5:1947:U:O2	48:5:1947:U:H2'	2.18	0.44
48:5:1048:G:C6	48:5:1049:C:C4	3.06	0.44
48:5:4139:G:C6	48:5:4140:C:C4	3.06	0.44
51:9:561:A:O2'	61:JJ:134:HIS:NE2	2.48	0.44
5:E:132:HIS:CE1	48:5:711:A:H1'	2.52	0.44
51:9:1121:G:C6	51:9:1122:A:C5	3.05	0.44
11:L:71:ARG:NH2	48:5:74:G:O3'	2.51	0.44
5:E:134:ARG:NH1	5:E:165:SER:O	2.51	0.44
51:9:1476:A:C8	69:RR:3:ARG:HB2	2.53	0.43
48:5:4919:G:N2	48:5:4920:C:C2	2.86	0.43
12:M:126:GLU:CG	14:O:181:ALA:CB	2.92	0.43
5:E:126:ARG:NH1	48:5:1285:U:P	2.89	0.43
48:5:933:G:C2	48:5:939:G:C2	3.06	0.43
48:5:1205:G:C2	48:5:1206:C:C2	3.06	0.43
48:5:1064:G:C2	48:5:1065:G:C4	3.06	0.43
48:5:4966:A:C2	48:5:4967:A:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2270:G:C2	48:5:2271:C:C2	3.06	0.43
48:5:4495:G:N2	48:5:4506:C:C2	2.86	0.43
51:9:1777:G:C2	51:9:1778:C:C2	3.05	0.43
48:5:1048:G:C2	48:5:1049:C:C2	3.05	0.43
71:TT:56:ARG:HH11	71:TT:56:ARG:HG2	1.83	0.43
51:9:145:G:N1	51:9:146:G:C6	2.86	0.43
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.81	0.43
48:5:2439:G:N3	48:5:2439:G:H2'	2.32	0.43
51:9:1258:A:C2	51:9:1664:A:C8	3.06	0.43
3:C:57:LEU:O	3:C:58:ALA:C	2.56	0.43
48:5:113:A:H2'	48:5:114:G:O4'	2.18	0.43
48:5:1424:G:H2'	48:5:1425:G:O4'	2.18	0.43
52:AA:43:SER:O	52:AA:45:GLY:N	2.51	0.43
53:BB:190:PRO:O	53:BB:192:SER:N	2.50	0.43
9:I:200:ILE:HD13	9:I:212:LEU:HD21	2.00	0.43
3:C:158:VAL:HA	3:C:161:TYR:HD2	1.82	0.43
48:5:1957:U:H3'	48:5:1957:U:OP2	2.18	0.43
48:5:2026:A:HO2'	48:5:2027:U:H5'	1.80	0.43
51:9:1675:A:N3	51:9:1675:A:O4'	2.51	0.43
12:M:126:GLU:CD	12:M:130:LEU:CD1	2.86	0.43
48:5:5029:C:H2'	48:5:5030:U:O4'	2.18	0.43
48:5:2614:C:O2	48:5:2726:G:C2	2.71	0.43
52:AA:60:LEU:HD13	52:AA:159:ILE:HD11	2.00	0.43
48:5:1721:G:C2	48:5:1722:C:C2	3.06	0.43
8:H:44:GLU:HB3	8:H:58:ASP:HB2	2.00	0.43
48:5:4423:U:O2	48:5:4423:U:O4'	2.37	0.43
51:9:996:A:H2'	51:9:997:A:C8	2.53	0.43
6:F:72:ARG:NH1	48:5:1209:U:O2'	2.51	0.43
57:FF:71:ARG:NH1	57:FF:148:ASN:OD1	2.50	0.43
48:5:2847:G:N2	48:5:3842:C:C2	2.87	0.43
25:Z:36:ARG:HG2	25:Z:38:TYR:CE1	2.53	0.43
48:5:915:A:HO2'	48:5:916:C:H6	1.63	0.43
56:EE:48:LEU:HD21	56:EE:70:ILE:HD11	2.00	0.43
48:5:1277:G:N1	48:5:1278:C:C4	2.86	0.43
48:5:1279:A:H3'	48:5:1280:C:C6	2.54	0.43
48:5:1280:C:C2	48:5:1282:G:C4	3.07	0.43
51:9:1454:A:OP1	69:RR:49:LYS:CD	2.65	0.43
48:5:1963:C:N3	48:5:4694:G:C6	2.74	0.43
48:5:917:A:C2	48:5:918:G:N2	2.86	0.43
51:9:1537:A:N1	51:9:1596:U:C4	2.86	0.43
48:5:665:C:O2	48:5:665:C:C2'	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1449:C:H2'	48:5:1450:C:O4'	2.18	0.43
48:5:2609:G:N1	48:5:2731:C:C2	2.87	0.43
48:5:1237:C:O2	48:5:1237:C:O4'	2.34	0.43
48:5:2862:G:N3	48:5:3624:A:H2'	2.33	0.43
16:Q:148:VAL:HG13	16:Q:152:PHE:CZ	2.53	0.43
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.54	0.43
48:5:82:U:H2'	48:5:83:C:O4'	2.18	0.43
51:9:922:A:OP1	74:WW:28:ARG:NH2	2.52	0.43
51:9:496:C:OP2	56:EE:49:ARG:NH1	2.52	0.43
54:CC:64:THR:OG1	54:CC:90:GLU:CG	2.66	0.43
48:5:2481:G:C2	48:5:2482:C:C2	3.07	0.43
48:5:5032:C:N4	48:5:5033:G:C6	2.87	0.43
48:5:2559:G:C2	48:5:2560:C:C2	3.06	0.43
48:5:4644:G:C6	48:5:4645:C:C4	3.07	0.43
67:PP:53:GLN:HE22	67:PP:83:MET:HG3	1.84	0.43
48:5:1755:C:C3'	48:5:1756:U:H5''	2.49	0.43
10:J:141:ILE:HD11	49:7:55:A:C2	2.53	0.43
48:5:4320:G:H2'	48:5:4321:U:O4'	2.18	0.43
48:5:4326:G:C6	48:5:4327:C:C4	3.06	0.43
48:5:258:G:C2	48:5:259:C:C2	3.06	0.43
52:AA:69:GLU:HB3	54:CC:270:THR:HG21	2.00	0.43
48:5:5003:U:H2'	48:5:5004:C:O4'	2.17	0.43
48:5:3905:A:C2	48:5:4449:A:C6	3.06	0.43
51:9:1333:U:H4'	55:DD:147:ALA:HB2	1.99	0.43
48:5:1563:A:N7	51:9:678:U:C4'	2.81	0.43
48:5:1563:A:N7	51:9:678:U:O4'	2.51	0.43
67:PP:34:MET:HA	67:PP:34:MET:CE	2.49	0.43
3:C:108:TRP:HB2	13:N:200:LEU:HD13	2.00	0.43
9:I:45:GLU:O	9:I:46:PHE:CG	2.72	0.43
50:8:86:U:O2'	50:8:87:G:H2'	2.18	0.43
48:5:2698:G:C2	48:5:2699:C:C2	3.07	0.43
48:5:1557:C:C2	48:5:1571:G:N2	2.86	0.43
50:8:115:G:C2	50:8:116:C:C2	3.07	0.43
48:5:1383:G:C2	48:5:1384:C:C2	3.07	0.43
48:5:2458:C:H2'	48:5:2459:G:O4'	2.19	0.43
4:D:3:PHE:HB2	48:5:1755:C:C6	2.53	0.43
51:9:1612:G:C2	51:9:1628:C:C2	3.07	0.43
54:CC:129:ALA:HB2	54:CC:213:LEU:HD11	2.00	0.43
48:5:322:C:O2	48:5:4356:G:C2	2.71	0.43
48:5:1422:G:C2	48:5:1464:C:C2	3.07	0.43
51:9:1035:A:H2'	51:9:1036:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1874:A:C5'	48:5:4218:U:O2	2.66	0.43
51:9:908:A:C2'	51:9:909:G:O5'	2.67	0.43
48:5:1265:G:OP1	48:5:2115:G:N1	2.52	0.43
48:5:1271:G:H3'	48:5:1272:C:H5'	2.00	0.43
48:5:1757:U:C2	48:5:1758:G:C8	3.06	0.43
48:5:423:G:H2'	48:5:424:U:O4'	2.18	0.43
48:5:4525:C:H2'	48:5:4526:U:O4'	2.19	0.43
51:9:194:C:C2	51:9:206:G:N2	2.87	0.43
48:5:2715:G:C6	48:5:2716:C:C4	3.07	0.43
48:5:2457:G:C6	48:5:2458:C:C4	3.07	0.43
48:5:3670:C:O2'	48:5:3671:G:O4'	2.36	0.43
48:5:1431:C:C2	48:5:1454:G:N2	2.86	0.43
58:GG:57:ASP:HB2	58:GG:98:ARG:HD2	2.01	0.43
48:5:4216:G:C2'	48:5:4217:G:H5'	2.48	0.43
51:9:5:U:C2	51:9:20:G:N2	2.86	0.43
15:P:102:ALA:CB	15:P:112:LEU:HD11	2.49	0.43
51:9:378:U:H2'	51:9:379:C:O4'	2.19	0.43
48:5:192:G:C2	48:5:250:C:C2	3.07	0.43
48:5:975:C:H2'	48:5:976:G:C1'	2.49	0.43
51:9:1308:U:N3	51:9:1309:C:N1	2.67	0.43
51:9:909:G:H2'	51:9:910:G:C8	2.54	0.43
51:9:1233:G:C6	51:9:1234:C:C4	3.06	0.43
48:5:1379:C:O2	48:5:1379:C:O4'	2.37	0.43
48:5:3870:C:C2	48:5:3886:G:N2	2.87	0.43
24:Y:50:ARG:NH2	50:8:83:C:O2	2.51	0.43
51:9:113:G:C2	51:9:293:C:C2	3.06	0.43
51:9:62:G:H1'	51:9:172:U:O2	2.18	0.43
48:5:1549:G:N2	48:5:1580:C:C2	2.87	0.43
25:Z:73:LYS:HG2	25:Z:75:TYR:CZ	2.53	0.43
48:5:2690:C:H2'	48:5:2691:U:O4'	2.19	0.43
57:FF:102:LEU:HD11	77:ZZ:100:VAL:HG21	2.00	0.43
50:8:2:G:N3	50:8:2:G:H2'	2.33	0.43
47:3:72:C:H5''	47:3:72:C:C6	2.54	0.43
48:5:674:G:C6	48:5:675:C:C4	3.07	0.43
51:9:1834:A:C2	51:9:1836:G:C4	3.06	0.43
48:5:4470:G:N2	48:5:4486:C:C2	2.87	0.43
58:GG:7:PHE:CD2	58:GG:10:THR:HG23	2.53	0.43
48:5:1075:G:C6	48:5:1076:C:C4	3.07	0.43
48:5:52:G:N1	48:5:53:C:C4	2.87	0.43
48:5:698:G:N1	48:5:699:C:C4	2.87	0.43
48:5:1723:A:N1	48:5:1838:A:N1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:5017:G:C6	48:5:5018:C:C4	3.06	0.43
48:5:2606:G:C6	48:5:2607:C:C4	3.07	0.43
51:9:1134:G:N2	51:9:1135:C:C2	2.87	0.43
51:9:1056:U:O2	51:9:1063:C:N4	2.52	0.43
74:WW:30:CYS:SG	74:WW:31:SER:N	2.91	0.43
51:9:1241:A:C2	51:9:1517:G:O4'	2.72	0.43
48:5:1436:C:O5'	48:5:2119:C:N4	2.52	0.43
47:3:8:U:H5	47:3:14:A:N7	2.16	0.43
7:G:194:VAL:HG21	7:G:196:ARG:NH1	2.33	0.43
14:O:12:ARG:O	18:S:171:ARG:NH2	2.52	0.43
51:9:910:G:C6	51:9:911:C:C4	3.07	0.43
10:J:119:TYR:HB3	70:SS:12:ILE:HG21	2.01	0.43
48:5:4901:G:N1	48:5:4921:C:C4	2.87	0.43
51:9:1650:A:C6	51:9:1675:A:C2	3.07	0.43
48:5:1239:C:O2'	48:5:1240:G:P	2.76	0.43
51:9:1843:G:H2'	51:9:1844:U:O4'	2.19	0.43
25:Z:51:ARG:HB2	25:Z:65:ARG:HD2	2.01	0.43
46:2:7:G:C2	46:2:49:C:C2	3.07	0.43
2:B:43:LEU:HG	2:B:183:ILE:HG21	2.01	0.43
8:H:59:LYS:HB2	8:H:70:VAL:HG22	2.01	0.43
51:9:1105:G:C2	51:9:1128:C:C2	3.07	0.43
51:9:1753:C:C2	51:9:1780:G:C2	3.07	0.43
48:5:4629:U:H2'	48:5:4630:G:O4'	2.18	0.43
50:8:142:U:H2'	50:8:143:G:O4'	2.19	0.43
48:5:1278:C:C2	48:5:1279:A:O2'	2.61	0.43
5:E:59:TYR:CE2	5:E:64:LEU:CD1	3.01	0.43
47:3:4:C:N3	47:3:5:G:N7	2.67	0.43
66:OO:64:ALA:O	66:OO:66:ARG:N	2.52	0.43
48:5:920:C:H2'	48:5:921:C:O4'	2.19	0.43
48:5:1085:C:C2	48:5:1213:G:N1	2.86	0.43
51:9:1771:G:C6	51:9:1772:C:N4	2.87	0.43
48:5:3590:G:C6	48:5:3591:C:C4	3.07	0.43
51:9:1784:G:N1	51:9:1785:C:C4	2.87	0.43
51:9:1315:U:C4	51:9:1316:C:C4	3.07	0.43
51:9:1481:G:C2	51:9:1482:C:C2	3.07	0.43
48:5:967:C:OP1	48:5:2254:G:N1	2.52	0.43
48:5:4904:G:C2	48:5:4905:C:C2	3.06	0.43
48:5:674:G:C2	48:5:675:C:C2	3.07	0.43
48:5:1739:G:C6	48:5:1740:C:N4	2.87	0.43
51:9:452:G:N2	51:9:453:C:C2	2.87	0.43
2:B:241:PRO:O	2:B:244:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:17:GLU:HB2	16:Q:18:PRO:HD2	2.00	0.43
48:5:1322:A:N6	48:5:4446:U:OP1	2.52	0.43
48:5:3938:G:O6	48:5:4172:A:N1	2.52	0.43
48:5:1277:G:C2	48:5:1278:C:C2	3.07	0.42
47:3:4:C:O2	47:3:5:G:C8	2.70	0.42
48:5:1968:G:N1	48:5:2018:C:N4	2.50	0.42
48:5:1358:G:H2'	48:5:1359:G:H8	1.83	0.42
48:5:1379:C:H4'	48:5:1380:G:C8	2.53	0.42
14:O:196:LEU:HB3	14:O:202:LEU:HD22	2.01	0.42
57:FF:127:ARG:HG3	57:FF:127:ARG:HH11	1.84	0.42
51:9:1771:G:C2	51:9:1772:C:C4	3.08	0.42
51:9:1466:G:C2	51:9:1467:C:C4	3.07	0.42
51:9:292:A:HO2'	51:9:293:C:P	2.39	0.42
48:5:4147:G:C2	48:5:4148:C:C2	3.07	0.42
11:L:65:ARG:HG2	11:L:66:TYR:CD2	2.54	0.42
75:XX:67:ARG:CG	75:XX:115:ILE:HD12	2.49	0.42
48:5:4737:G:C6	48:5:4738:C:C4	3.06	0.42
48:5:1466:G:C6	48:5:1467:C:C4	3.07	0.42
71:TT:56:ARG:HD2	71:TT:79:TYR:CE2	2.54	0.42
48:5:914:U:H2'	48:5:915:A:O4'	2.19	0.42
48:5:2034:G:C6	48:5:2035:C:C4	3.07	0.42
48:5:1846:G:C2	48:5:1847:C:C2	3.07	0.42
8:H:117:PHE:CZ	8:H:118:LEU:HD23	2.53	0.42
70:SS:81:ASP:N	70:SS:81:ASP:OD1	2.52	0.42
75:XX:84:PHE:HB2	75:XX:118:VAL:HG11	2.01	0.42
18:S:96:GLU:OE2	18:S:138:ARG:N	2.50	0.42
48:5:2703:G:C2	48:5:2704:C:C2	3.07	0.42
51:9:1335:G:C6	51:9:1336:C:C4	3.06	0.42
51:9:1568:C:H2'	51:9:1569:A:C8	2.54	0.42
9:I:153:ARG:HA	9:I:165:ILE:HD11	2.00	0.42
48:5:2468:U:O4	48:5:2473:A:C2	2.59	0.42
75:XX:70:VAL:HG21	75:XX:94:ILE:HG21	2.01	0.42
51:9:358:C:C2	51:9:405:G:N2	2.87	0.42
51:9:1500:G:H2'	51:9:1501:C:O4'	2.19	0.42
48:5:1070:G:C6	48:5:1071:C:N4	2.87	0.42
51:9:1459:G:C2	51:9:1460:C:C2	3.06	0.42
48:5:1808:C:C2	48:5:1831:G:C2	3.07	0.42
48:5:3670:C:O2'	48:5:3671:G:O5'	2.37	0.42
48:5:1826:G:C2	48:5:1827:C:C2	3.07	0.42
50:8:10:G:C6	50:8:11:C:C4	3.07	0.42
49:7:25:G:C6	49:7:26:C:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BB:136:ARG:HH21	53:BB:136:ARG:HG3	1.84	0.42
51:9:398:A:H5'	51:9:398:A:C8	2.54	0.42
49:7:110:G:C2	49:7:111:C:C2	3.07	0.42
48:5:4932:U:H2'	48:5:4933:C:O4'	2.18	0.42
66:OO:67:ASP:HB2	66:OO:70:SER:HB3	2.01	0.42
48:5:2569:G:H2'	48:5:2570:U:O4'	2.18	0.42
48:5:2473:A:C6	48:5:2506:G:N7	2.87	0.42
47:3:67:U:H2'	47:3:68:C:C6	2.54	0.42
48:5:3753:G:O2'	48:5:3754:G:H5'	2.19	0.42
48:5:3590:G:N1	48:5:3591:C:C2	2.87	0.42
51:9:164:A:H2'	51:9:165:G:C2	2.54	0.42
48:5:119:G:H3'	48:5:120:A:H5'	2.01	0.42
51:9:1298:G:O2'	51:9:1299:A:O4'	2.37	0.42
51:9:1134:G:C2	51:9:1135:C:C2	3.07	0.42
51:9:1452:A:C5'	69:RR:48:ASN:HD21	2.32	0.42
48:5:4291:G:H5''	48:5:4291:G:N3	2.34	0.42
51:9:448:A:H5''	60:II:25:ARG:HA	2.00	0.42
71:TT:28:LEU:O	71:TT:29:LYS:HB2	2.20	0.42
51:9:1571:G:C2	51:9:1572:C:C2	3.07	0.42
48:5:1275:G:N2	48:5:1276:C:C2	2.88	0.42
48:5:2793:G:C6	48:5:2797:C:N4	2.88	0.42
48:5:4461:C:C2	48:5:4516:G:C2	3.07	0.42
51:9:1530:U:H2'	51:9:1531:A:O4'	2.19	0.42
51:9:1126:G:C2	51:9:1127:C:C2	3.07	0.42
51:9:666:U:C5	51:9:1150:A:C5	3.08	0.42
48:5:179:G:C6	48:5:180:C:C4	3.06	0.42
48:5:2606:G:C2	48:5:2607:C:C2	3.07	0.42
48:5:1925:G:C6	48:5:1926:C:C4	3.08	0.42
71:TT:104:LEU:HD22	71:TT:121:ARG:HG2	2.00	0.42
75:XX:74:LEU:HD21	75:XX:81:ILE:HD12	2.00	0.42
51:9:999:G:C6	51:9:1000:C:C4	3.07	0.42
50:8:31:G:C6	50:8:32:C:C4	3.08	0.42
51:9:614:C:C2	51:9:626:G:C2	3.07	0.42
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.54	0.42
48:5:1332:C:C2	48:5:2355:G:N2	2.87	0.42
48:5:2086:G:C6	48:5:2087:C:C4	3.08	0.42
8:H:92:MET:SD	8:H:161:ILE:HD11	2.59	0.42
6:F:175:ALA:O	6:F:179:ARG:HB2	2.19	0.42
48:5:517:C:C2	48:5:645:G:N2	2.87	0.42
51:9:827:A:C5	51:9:828:G:C8	3.08	0.42
51:9:668:A:N1	51:9:1143:A:C5	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:CC:60:TRP:CE2	54:CC:62:PRO:HB3	2.54	0.42
51:9:1233:G:C2	51:9:1234:C:C2	3.08	0.42
48:5:165:A:H3'	48:5:166:C:H6	1.83	0.42
48:5:2256:C:H1'	48:5:2257:C:OP2	2.20	0.42
48:5:93:G:H2'	48:5:94:A:C8	2.55	0.42
48:5:469:C:H2'	48:5:470:A:O4'	2.20	0.42
51:9:211:G:C2	51:9:212:C:C2	3.08	0.42
48:5:28:C:C2	48:5:55:G:N2	2.88	0.42
48:5:3942:A:H2'	48:5:3943:A:O4'	2.19	0.42
48:5:1466:G:C2	48:5:1467:C:C2	3.08	0.42
51:9:1541:G:C2	51:9:1542:C:C2	3.07	0.42
25:Z:38:TYR:CE1	25:Z:76:ASN:OD1	2.73	0.42
48:5:4326:G:C2	48:5:4327:C:C2	3.08	0.42
58:GG:63:MET:HG3	58:GG:98:ARG:HD3	2.02	0.42
50:8:31:G:C2	50:8:32:C:C2	3.08	0.42
61:JJ:14:VAL:HG23	61:JJ:48:PHE:CD1	2.54	0.42
48:5:2424:G:O5'	48:5:2424:G:H8	2.02	0.42
51:9:839:C:C2'	51:9:839:C:O2	2.66	0.42
51:9:17:C:O2'	51:9:1194:A:N1	2.33	0.42
65:NN:62:GLN:HB2	65:NN:65:PHE:CD2	2.55	0.42
48:5:1748:U:C2	48:5:1783:C:C2	3.08	0.42
48:5:1787:A:N3	48:5:4210:U:O2'	2.52	0.42
73:VV:20:SER:HB3	73:VV:59:ILE:HD11	2.01	0.42
48:5:247:G:C2	48:5:248:C:C2	3.07	0.42
75:XX:33:GLY:O	75:XX:35:ALA:N	2.52	0.42
48:5:2391:G:N2	48:5:2392:C:C2	2.87	0.42
6:F:184:TYR:HB3	6:F:202:ARG:HG2	2.01	0.42
48:5:973:G:C6	48:5:974:C:C4	3.08	0.42
48:5:2793:G:H5''	48:5:2794:C:H5''	2.00	0.42
51:9:1137:U:HO2'	52:AA:155:ARG:HH22	1.66	0.42
48:5:2712:G:N1	48:5:2713:C:C4	2.87	0.42
51:9:1398:G:C2	51:9:1399:C:C2	3.08	0.42
75:XX:9:THR:O	75:XX:11:ARG:N	2.52	0.42
48:5:1904:G:N2	48:5:2073:C:C2	2.88	0.42
17:R:97:ARG:NH2	48:5:2725:A:OP1	2.53	0.42
56:EE:126:VAL:CG1	56:EE:160:ILE:HD11	2.49	0.42
13:N:48:ALA:HB1	13:N:53:TYR:HB3	2.01	0.42
48:5:4891:G:C2	48:5:4929:C:C2	3.08	0.42
17:R:11:ALA:HB1	17:R:50:ILE:HD13	2.02	0.42
48:5:1506:G:C2	48:5:1507:C:C2	3.08	0.42
48:5:4131:G:C2	48:5:4132:C:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2645:G:C6	48:5:2646:C:C4	3.07	0.42
49:7:86:G:C2	49:7:92:C:C2	3.08	0.42
51:9:1447:G:C6	51:9:1448:A:C6	3.07	0.42
48:5:5026:U:O4	60:II:103:LEU:CD1	2.68	0.42
48:5:4920:C:H2'	48:5:4921:C:C6	2.55	0.42
48:5:22:G:N1	50:8:35:C:C4	2.88	0.42
52:AA:111:GLN:O	54:CC:63:VAL:HG11	2.20	0.42
48:5:2712:G:C2	48:5:2713:C:C2	3.08	0.42
48:5:2322:G:C6	48:5:2323:C:C4	3.08	0.42
48:5:4433:G:C2	48:5:4434:C:C2	3.07	0.42
71:TT:56:ARG:HD2	71:TT:79:TYR:CD2	2.54	0.42
48:5:1755:C:H3'	48:5:1756:U:H5''	2.02	0.42
48:5:258:G:C6	48:5:259:C:C4	3.07	0.42
51:9:1834:A:C2'	51:9:1834:A:N3	2.82	0.42
51:9:1134:G:C6	51:9:1135:C:C4	3.06	0.42
52:AA:124:VAL:HG13	52:AA:130:ASP:HB2	2.01	0.42
51:9:1692:U:H2'	51:9:1693:G:C8	2.54	0.42
51:9:95:G:C6	51:9:96:C:C4	3.08	0.42
60:II:6:ASP:OD1	60:II:6:ASP:N	2.53	0.42
48:5:2396:A:N6	48:5:2814:C:O2	2.53	0.42
20:U:84:LYS:HB2	20:U:110:TYR:CE2	2.54	0.42
51:9:1207:G:C6	51:9:1837:G:C6	3.08	0.42
3:C:235:LEU:HD22	3:C:240:LEU:HD11	2.02	0.42
2:B:340:THR:OG1	2:B:341:LYS:N	2.52	0.42
51:9:1486:A:H2'	51:9:1487:A:O4'	2.19	0.42
51:9:947:G:C2	51:9:948:C:C2	3.08	0.42
48:5:973:G:N2	48:5:974:C:C2	2.88	0.42
51:9:912:C:H3'	51:9:913:A:H5''	2.01	0.42
51:9:751:G:N1	51:9:792:C:C4	2.88	0.42
48:5:4901:G:C2	48:5:4921:C:C2	3.07	0.42
48:5:4207:C:C2	48:5:4226:G:N2	2.88	0.42
48:5:1205:G:N1	48:5:1206:C:C4	2.88	0.42
51:9:211:G:C6	51:9:212:C:N4	2.88	0.42
51:9:666:U:C2	51:9:667:U:C5	3.07	0.42
68:QQ:125:ARG:O	68:QQ:126:ARG:NH2	2.53	0.42
47:3:72:C:H5''	47:3:72:C:H6	1.84	0.42
48:5:2339:G:C6	48:5:2340:C:C4	3.08	0.42
48:5:1662:C:H2'	48:5:1663:C:C6	2.55	0.42
51:9:993:G:C2	51:9:994:C:C2	3.08	0.42
48:5:3642:A:OP1	48:5:3644:U:OP1	2.38	0.42
58:GG:2:LYS:HB3	58:GG:15:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ARG:HD2	2:B:122:TRP:CD2	2.55	0.42
51:9:23:G:C2	51:9:24:C:C2	3.08	0.42
48:5:518:G:C6	48:5:519:C:C4	3.08	0.42
48:5:193:G:C2	48:5:249:C:C2	3.07	0.42
48:5:3765:G:O2'	48:5:3766:A:C8	2.63	0.42
50:8:60:G:N2	50:8:64:U:C2	2.87	0.42
10:J:33:LEU:CD2	10:J:70:VAL:HB	2.50	0.42
14:O:85:ARG:HG3	14:O:99:LEU:HD11	2.02	0.42
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	2.02	0.42
53:BB:39:PHE:CE2	53:BB:74:LEU:HD23	2.55	0.42
48:5:2576:G:C6	48:5:2577:C:C4	3.07	0.42
48:5:4455:G:C6	48:5:4456:C:C4	3.08	0.42
51:9:1309:C:O2'	51:9:1310:U:C5'	2.68	0.42
11:L:170:THR:HG23	11:L:173:GLU:H	1.85	0.42
48:5:3752:C:O2'	48:5:3753:G:P	2.78	0.42
48:5:744:G:H2'	48:5:745:G:H8	1.85	0.42
2:B:14:LEU:HD22	2:B:264:PHE:CE2	2.54	0.42
48:5:4724:A:C6	48:5:4725:C:C4	3.08	0.42
48:5:301:G:C2	48:5:302:C:C2	3.08	0.42
48:5:303:C:H2'	48:5:304:C:O4'	2.20	0.42
51:9:1481:G:C6	51:9:1482:C:C4	3.07	0.42
48:5:751:G:N2	48:5:752:G:C5	2.88	0.42
50:8:76:C:H2'	50:8:77:A:O4'	2.20	0.42
48:5:479:G:C2	48:5:480:C:C2	3.08	0.42
48:5:1539:G:C2	48:5:1540:C:C2	3.08	0.42
48:5:2:G:C6	48:5:3:C:C4	3.07	0.42
50:8:115:G:C6	50:8:116:C:C4	3.08	0.42
51:9:1563:G:C6	51:9:1564:C:C4	3.07	0.42
48:5:674:G:N2	48:5:675:C:C2	2.88	0.42
48:5:1275:G:C2	48:5:1276:C:C2	3.07	0.42
48:5:2645:G:C2	48:5:2646:C:C2	3.08	0.42
2:B:41:VAL:HG21	2:B:196:TRP:CG	2.55	0.42
13:N:103:GLU:OE1	13:N:167:ALA:HB3	2.19	0.42
51:9:1153:C:O4'	51:9:1153:C:O2	2.37	0.42
13:N:160:GLU:OE1	13:N:160:GLU:N	2.50	0.42
51:9:591:U:O4'	51:9:591:U:O2	2.36	0.42
54:CC:274:VAL:O	54:CC:274:VAL:HG13	2.20	0.42
51:9:1719:A:N6	51:9:1814:G:O2'	2.51	0.42
52:AA:41:ARG:HD3	52:AA:47:TYR:CZ	2.55	0.42
48:5:3816:A:O2'	48:5:3819:G:N3	2.42	0.42
8:H:26:ILE:HB	8:H:35:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2468:U:C2	48:5:2469:C:C5	3.08	0.42
14:O:201:PHE:HB2	14:O:202:LEU:HD13	2.02	0.42
48:5:199:G:C2	48:5:201:C:N3	2.88	0.42
48:5:127:G:C2	48:5:128:C:C2	3.08	0.42
48:5:3918:G:C2	48:5:3919:C:C2	3.08	0.42
48:5:2268:A:C4'	48:5:2269:C:H5'	2.50	0.42
19:T:80:VAL:O	19:T:82:GLY:N	2.53	0.42
48:5:2052:G:C6	48:5:2053:C:C4	3.08	0.42
48:5:2771:G:C2	48:5:2772:C:C2	3.08	0.42
48:5:1416:G:C2	48:5:1417:C:C2	3.07	0.42
60:II:156:ALA:O	60:II:158:ILE:N	2.53	0.42
50:8:134:G:C2	50:8:135:C:C2	3.08	0.42
13:N:48:ALA:HB1	13:N:53:TYR:CB	2.50	0.42
51:9:1838:U:O2	66:OO:150:ARG:HD2	2.20	0.42
51:9:339:A:C6	51:9:340:C:C4	3.08	0.42
48:5:207:G:O4'	48:5:406:C:H5'	2.19	0.42
48:5:717:U:H3	48:5:951:G:H1	1.68	0.42
48:5:351:C:C2	50:8:25:G:N2	2.88	0.42
48:5:5008:C:H2'	48:5:5009:G:O4'	2.20	0.42
3:C:195:LYS:NZ	50:8:21:C:OP1	2.52	0.42
61:JJ:114:VAL:HG12	61:JJ:120:ALA:HB2	2.00	0.41
48:5:1983:A:N1	48:5:2010:A:OP2	2.53	0.41
48:5:1359:G:C5	48:5:1360:G:C5	3.07	0.41
48:5:1213:G:C5	48:5:1215:C:N1	2.88	0.41
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	2.02	0.41
48:5:4453:C:C2	48:5:4529:G:N2	2.88	0.41
5:E:126:ARG:NH1	48:5:1285:U:OP2	2.53	0.41
48:5:1811:G:C2	48:5:1812:C:C2	3.08	0.41
67:PP:34:MET:HE3	67:PP:45:LEU:HD12	2.02	0.41
48:5:4713:G:C6	48:5:4714:C:C4	3.08	0.41
48:5:2066:C:O2'	48:5:2067:C:H5'	2.19	0.41
48:5:1412:G:C6	48:5:1413:C:C4	3.08	0.41
48:5:1098:G:C6	48:5:1099:C:C4	3.07	0.41
48:5:2618:G:N2	48:5:2720:C:C2	2.88	0.41
46:2:65:G:C2	46:2:66:C:C2	3.08	0.41
48:5:1612:G:H2'	48:5:1612:G:N3	2.35	0.41
48:5:1484:G:C2'	48:5:1484:G:N3	2.82	0.41
51:9:531:A:H3'	51:9:532:C:H5''	2.02	0.41
48:5:1970:A:C2	48:5:2016:C:C5	3.08	0.41
2:B:151:SER:O	2:B:155:LYS:HG3	2.20	0.41
51:9:936:G:C6	51:9:937:C:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:169:G:C2	48:5:170:C:C2	3.08	0.41
48:5:4269:G:C6	48:5:4270:C:C4	3.08	0.41
6:F:60:HIS:HA	48:5:944:A:N7	2.35	0.41
51:9:752:G:C2	51:9:790:C:N3	2.87	0.41
49:7:30:C:C4	49:7:48:G:N1	2.88	0.41
48:5:5028:G:C2	48:5:5029:C:C2	3.08	0.41
48:5:1448:G:C6	48:5:1449:C:C4	3.09	0.41
9:I:76:MET:HG3	9:I:87:ILE:HD11	2.02	0.41
48:5:4152:G:C2	48:5:4153:C:C2	3.09	0.41
48:5:4473:A:C2	48:5:4474:A:C4	3.08	0.41
48:5:1416:G:C6	48:5:1417:C:C4	3.08	0.41
62:KK:15:LEU:HD22	62:KK:49:MET:CE	2.50	0.41
48:5:254:G:C6	48:5:255:C:C4	3.08	0.41
48:5:4139:G:C2	48:5:4140:C:C2	3.07	0.41
51:9:999:G:C2	51:9:1000:C:C2	3.08	0.41
48:5:4131:G:C6	48:5:4132:C:C4	3.09	0.41
48:5:219:G:OP1	48:5:219:G:H4'	2.19	0.41
48:5:1090:G:C2	48:5:1091:C:C2	3.08	0.41
51:9:617:G:N2	51:9:618:C:C2	2.89	0.41
48:5:2076:G:C2	48:5:2077:C:C2	3.09	0.41
48:5:695:G:H3'	48:5:696:C:H5'	2.01	0.41
48:5:1203:G:C2	48:5:1204:C:C2	3.08	0.41
6:F:41:GLN:HG3	48:5:2095:A:N1	2.34	0.41
48:5:2468:U:C4	48:5:2473:A:C6	3.07	0.41
48:5:1957:U:O2'	48:5:1958:A:P	2.78	0.41
51:9:1613:G:N2	51:9:1627:C:C2	2.89	0.41
17:R:99:MET:HE3	17:R:127:VAL:HG12	2.01	0.41
51:9:839:C:O2	51:9:839:C:H2'	2.19	0.41
51:9:993:G:C6	51:9:994:C:C4	3.08	0.41
48:5:351:C:C2	50:8:25:G:C2	3.07	0.41
48:5:2076:G:C6	48:5:2077:C:C4	3.08	0.41
6:F:41:GLN:CG	48:5:2095:A:N1	2.83	0.41
13:N:40:PRO:HG3	48:5:8:U:H5''	2.02	0.41
48:5:2874:U:H4'	48:5:2875:C:OP2	2.20	0.41
51:9:630:U:C2'	51:9:630:U:O2	2.69	0.41
12:M:56:GLN:HE21	12:M:56:GLN:HB3	1.71	0.41
7:G:50:ASP:OD1	7:G:50:ASP:C	2.58	0.41
48:5:130:C:C2	48:5:139:G:N2	2.88	0.41
12:M:127:VAL:HG12	12:M:131:GLN:HE21	1.84	0.41
72:UU:46:LYS:HD3	72:UU:97:ILE:HG23	2.03	0.41
51:9:107:A:H2'	51:9:108:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:8:71:A:C2	50:8:88:A:H1'	2.56	0.41
51:9:1217:A:H2'	51:9:1218:C:C6	2.55	0.41
47:3:67:U:H2'	47:3:68:C:H6	1.86	0.41
3:C:114:ARG:NE	48:5:1358:G:O3'	2.50	0.41
48:5:199:G:C2	48:5:201:C:C4	3.08	0.41
48:5:2711:G:H3'	48:5:2712:G:H5''	2.03	0.41
57:FF:86:LYS:O	57:FF:89:THR:N	2.53	0.41
48:5:4967:A:C2	48:5:4968:A:C4	3.08	0.41
48:5:689:U:N3	48:5:690:C:C5	2.89	0.41
51:9:14:C:OP2	54:CC:232:THR:HG21	2.20	0.41
50:8:46:G:O2'	50:8:61:A:N1	2.48	0.41
48:5:479:G:C6	48:5:480:C:C4	3.08	0.41
48:5:3627:G:C2	48:5:3835:C:C2	3.09	0.41
48:5:2771:G:H2'	48:5:2772:C:O4'	2.21	0.41
3:C:30:ALA:HB1	3:C:31:PRO:HD2	2.03	0.41
71:TT:65:TYR:HA	71:TT:123:LEU:HD22	2.01	0.41
24:Y:87:ARG:HG3	24:Y:87:ARG:HH21	1.85	0.41
51:9:1518:C:O5'	51:9:1518:C:O2	2.38	0.41
48:5:4874:A:H3'	48:5:4875:G:C5'	2.50	0.41
48:5:1339:U:H2'	48:5:1340:C:C6	2.55	0.41
48:5:1981:G:O2'	48:5:1982:G:C8	2.73	0.41
52:AA:33:GLN:HB3	52:AA:154:LEU:HD12	2.02	0.41
48:5:1280:C:C2'	48:5:1282:G:C8	3.04	0.41
51:9:1308:U:C2'	51:9:1309:C:O5'	2.69	0.41
47:3:39:U:C2	47:3:40:C:C5	3.07	0.41
48:5:1358:G:N3	48:5:1359:G:N7	2.68	0.41
48:5:4579:U:O2	48:5:4580:U:C2	2.74	0.41
48:5:3712:A:N6	51:9:970:G:C2	2.88	0.41
48:5:1075:G:N2	48:5:1076:C:C2	2.89	0.41
48:5:3591:C:C4	48:5:3592:G:C8	3.08	0.41
51:9:832:G:C2	51:9:833:C:C2	3.08	0.41
2:B:29:VAL:HG23	2:B:346:THR:HG21	2.01	0.41
51:9:1260:A:C6	51:9:1619:A:C6	3.09	0.41
48:5:4587:G:N2	48:5:4716:C:C2	2.88	0.41
48:5:190:G:C2	48:5:252:C:O2	2.74	0.41
3:C:210:ILE:HG21	3:C:252:TRP:CZ3	2.56	0.41
51:9:17:C:H2'	51:9:18:C:C6	2.55	0.41
51:9:23:G:C6	51:9:24:C:C4	3.08	0.41
51:9:936:G:C2	51:9:937:C:C2	3.08	0.41
4:D:146:LEU:HD11	4:D:159:VAL:CG1	2.50	0.41
54:CC:164:PRO:HB2	73:VV:11:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:RR:36:GLU:HG2	69:RR:47:ARG:HD2	2.03	0.41
4:D:284:LYS:HD2	9:I:209:TRP:CZ2	2.55	0.41
48:5:4408:G:C6	48:5:4409:C:C4	3.08	0.41
25:Z:12:LEU:HB2	25:Z:81:MET:HB3	2.03	0.41
69:RR:91:LEU:HD12	69:RR:92:ASP:N	2.35	0.41
48:5:450:G:O2'	48:5:452:A:H4'	2.21	0.41
54:CC:190:SER:OG	54:CC:191:VAL:N	2.53	0.41
48:5:1360:G:H2'	48:5:1361:G:O4'	2.21	0.41
48:5:1264:C:C4	48:5:1265:G:N7	2.89	0.41
48:5:1075:G:H2'	48:5:1076:C:C6	2.55	0.41
48:5:1245:C:O2	48:5:2111:G:O2'	2.33	0.41
48:5:1550:G:C2	48:5:1579:C:O2	2.73	0.41
59:HH:43:LEU:HD21	59:HH:71:SER:HB3	2.01	0.41
48:5:1633:G:H5'	48:5:1634:A:OP1	2.20	0.41
51:9:1108:G:N2	51:9:1125:C:C2	2.88	0.41
48:5:2052:G:C2	48:5:2053:C:C2	3.09	0.41
48:5:4904:G:C6	48:5:4905:C:C4	3.08	0.41
48:5:4652:G:C2	48:5:4653:C:C2	3.08	0.41
48:5:1819:G:H5''	48:5:1819:G:C8	2.56	0.41
49:7:27:G:C6	49:7:28:C:C4	3.09	0.41
23:X:99:ILE:HG23	23:X:133:GLU:HB3	2.03	0.41
48:5:4413:C:O2	48:5:4413:C:O4'	2.39	0.41
48:5:129:C:C2	48:5:140:G:N2	2.89	0.41
48:5:1685:G:C6	48:5:1686:C:C4	3.09	0.41
19:T:64:VAL:HG13	19:T:72:VAL:HG13	2.03	0.41
24:Y:85:VAL:HG12	24:Y:97:VAL:HB	2.03	0.41
48:5:2050:G:C2	48:5:2051:C:C2	3.08	0.41
51:9:1473:G:N2	51:9:1475:G:OP2	2.51	0.41
48:5:3684:G:C6	48:5:3685:C:N4	2.89	0.41
17:R:4:LEU:HD11	17:R:29:THR:HG23	2.01	0.41
7:G:159:HIS:CE1	7:G:185:LYS:HE2	2.56	0.41
51:9:1448:A:HO2'	51:9:1449:G:C4'	2.33	0.41
48:5:1245:C:C5	48:5:1269:G:O6	2.72	0.41
48:5:730:G:N2	48:5:939:G:N2	2.68	0.41
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.56	0.41
48:5:93:G:O2'	48:5:94:A:C5'	2.69	0.41
51:9:172:U:O2	51:9:172:U:O2'	2.30	0.41
51:9:1654:G:C6	51:9:1655:C:C4	3.09	0.41
48:5:4093:G:C6	48:5:4094:G:N7	2.89	0.41
11:L:74:ARG:NH2	48:5:76:A:C8	2.89	0.41
48:5:1412:G:C2	48:5:1413:C:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:5031:G:C6	48:5:5032:C:C4	3.09	0.41
48:5:2703:G:C6	48:5:2704:C:C4	3.08	0.41
51:9:1518:C:O4'	51:9:1518:C:O2	2.37	0.41
64:MM:35:ILE:HD13	64:MM:61:TYR:CE1	2.56	0.41
48:5:1668:A:C4	48:5:2282:A:C2	3.09	0.41
2:B:54:THR:OG1	2:B:55:HIS:N	2.54	0.41
48:5:4931:G:H2'	48:5:4931:G:N3	2.36	0.41
19:T:41:ASP:HA	19:T:61:THR:HA	2.03	0.41
48:5:2058:G:C6	48:5:2059:C:C4	3.09	0.41
51:9:1089:G:C6	51:9:1090:C:C4	3.09	0.41
51:9:1097:G:C6	51:9:1098:C:C4	3.09	0.41
62:KK:53:LYS:HD3	62:KK:60:GLU:HG3	2.03	0.41
18:S:13:VAL:HG22	18:S:63:TYR:HB3	2.03	0.41
48:5:2006:U:H2'	48:5:2007:G:O4'	2.21	0.41
51:9:949:G:C2	51:9:950:C:C2	3.08	0.41
48:5:1374:G:C2	48:5:1375:C:C2	3.09	0.41
51:9:1308:U:O2'	51:9:1309:C:P	2.79	0.41
56:EE:64:ILE:HG23	76:YY:17:LEU:HD13	2.03	0.41
48:5:1075:G:C6	48:5:1076:C:N4	2.89	0.41
48:5:3612:C:H1'	48:5:5016:A:H8	1.85	0.41
51:9:1331:C:OP2	51:9:1490:G:OP1	2.38	0.41
48:5:2688:G:N1	48:5:2689:C:C4	2.88	0.41
48:5:990:C:C4	48:5:991:C:C5	3.09	0.41
46:2:30:G:C2	46:2:31:C:C2	3.08	0.41
48:5:2478:C:N4	48:5:2479:G:O6	2.54	0.41
51:9:1227:G:C2	51:9:1228:A:C8	3.09	0.41
48:5:1383:G:C5	48:5:1384:C:C4	3.09	0.41
63:LL:35:ARG:NH2	63:LL:55:TYR:O	2.50	0.41
57:FF:103:LEU:HD22	77:ZZ:67:LEU:HD22	2.02	0.41
48:5:1925:G:C2	48:5:1926:C:C2	3.08	0.41
8:H:144:LEU:HD22	8:H:161:ILE:CD1	2.51	0.41
49:7:19:C:C2	49:7:60:G:C2	3.09	0.41
76:YY:7:ILE:HD11	76:YY:40:ILE:CD1	2.50	0.41
48:5:4745:G:N2	48:5:4746:C:N4	2.69	0.41
51:9:385:G:H2'	51:9:385:G:N3	2.36	0.41
46:2:33:U:C5	68:QQ:146:ARG:NH1	2.88	0.41
1:A:233:ARG:O	1:A:235:VAL:N	2.53	0.41
2:B:92:TYR:HB2	2:B:159:VAL:HB	2.03	0.41
51:9:1573:G:C2	51:9:1574:C:C2	3.08	0.41
51:9:1455:A:H3'	51:9:1455:A:OP2	2.21	0.41
48:5:1957:U:O2'	48:5:1958:A:C8	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:5026:U:H3'	60:II:79:ILE:CD1	2.50	0.41
60:II:79:ILE:HG23	60:II:103:LEU:HB2	2.01	0.41
48:5:2767:U:C4	48:5:2769:U:O4	2.74	0.41
48:5:1550:G:C2	48:5:1551:C:C2	3.08	0.41
48:5:1550:G:C6	48:5:1551:C:C4	3.08	0.41
48:5:127:G:C6	48:5:128:C:C4	3.09	0.41
48:5:2481:G:N2	48:5:2498:C:C2	2.89	0.41
48:5:467:U:C4	48:5:468:U:C5	3.09	0.41
51:9:1654:G:C2	51:9:1655:C:C2	3.08	0.41
51:9:1654:G:N1	51:9:1655:C:C4	2.89	0.41
1:A:207:VAL:HG12	48:5:3919:C:H4'	2.02	0.41
2:B:220:ILE:HG12	2:B:278:THR:HG23	2.02	0.41
9:I:140:THR:OG1	9:I:141:LYS:N	2.51	0.41
14:O:60:LYS:HG2	48:5:2046:G:C5	2.56	0.41
50:8:128:C:C5	50:8:129:C:C5	3.09	0.41
48:5:4473:A:H2'	48:5:4474:A:C8	2.56	0.41
60:II:55:TYR:HB2	60:II:182:CYS:O	2.21	0.41
48:5:2465:C:H1'	48:5:3672:G:N2	2.36	0.41
48:5:476:G:C2	48:5:679:C:C2	3.09	0.41
48:5:258:G:N2	48:5:259:C:C2	2.89	0.41
51:9:1571:G:C6	51:9:1572:C:C4	3.09	0.41
48:5:517:C:C2	48:5:645:G:C2	3.09	0.41
48:5:2811:G:N1	48:5:2814:C:OP2	2.46	0.41
48:5:3685:C:H2'	48:5:3686:G:O4'	2.20	0.41
51:9:1097:G:C2	51:9:1098:C:C2	3.09	0.41
3:C:349:LEU:O	3:C:353:ARG:HG3	2.21	0.41
51:9:1411:G:H3'	51:9:1412:C:H4'	2.03	0.41
48:5:4595:G:C6	48:5:4596:C:C4	3.09	0.41
51:9:463:C:H2'	51:9:465:A:C8	2.56	0.41
51:9:1199:A:H2'	51:9:1200:A:C8	2.56	0.41
2:B:257:TRP:CE2	48:5:4518:A:N7	2.88	0.41
51:9:389:A:C6	51:9:390:C:C4	3.09	0.41
48:5:2743:A:H2'	48:5:2744:A:C8	2.56	0.41
50:8:121:G:C2	50:8:130:C:C2	3.09	0.41
59:HH:118:ARG:O	59:HH:121:THR:HG22	2.20	0.41
48:5:1092:G:C6	48:5:1093:C:C4	3.09	0.41
16:Q:64:SER:OG	16:Q:89:ASP:OD2	2.38	0.41
51:9:1686:G:C2	51:9:1687:C:C2	3.08	0.41
51:9:1686:G:N2	51:9:1687:C:C2	2.89	0.41
1:A:49:ILE:HG22	1:A:58:LEU:HB2	2.02	0.41
51:9:36:U:C2	51:9:520:A:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4999:G:C2	48:5:5052:C:C2	3.09	0.41
48:5:1328:G:O2'	48:5:2349:A:OP1	2.36	0.41
51:9:114:G:O6	51:9:351:G:H1'	2.21	0.41
48:5:4129:G:C6	48:5:4130:C:C4	3.08	0.41
48:5:4129:G:C2	48:5:4130:C:C2	3.08	0.41
15:P:64:ASN:HD21	48:5:3892:U:H4'	1.86	0.41
48:5:1699:A:N6	48:5:2094:G:O2'	2.54	0.41
48:5:4977:A:H2'	48:5:4978:G:O4'	2.20	0.41
51:9:929:G:C6	51:9:930:C:C4	3.08	0.41
51:9:1393:G:C6	51:9:1394:G:C6	3.09	0.41
48:5:975:C:N4	48:5:1279:A:C2	2.89	0.41
48:5:4371:G:C8	48:5:4372:U:C5	3.09	0.41
48:5:167:C:C2	48:5:269:G:C2	3.09	0.41
48:5:197:A:N1	48:5:225:G:O2'	2.43	0.41
51:9:841:G:C6	51:9:842:C:C4	3.09	0.41
51:9:832:G:C2	51:9:843:C:N3	2.89	0.41
51:9:1528:G:N1	51:9:1529:C:C4	2.89	0.41
48:5:176:G:H2'	48:5:177:G:O4'	2.20	0.41
48:5:3705:G:C2	48:5:3706:C:C2	3.09	0.41
19:T:48:VAL:HG21	19:T:94:GLU:HG2	2.02	0.41
48:5:80:C:C2	48:5:104:G:N2	2.89	0.41
48:5:1691:G:C2	48:5:1692:C:C2	3.08	0.41
8:H:117:PHE:CE1	8:H:118:LEU:HD23	2.56	0.41
48:5:4455:G:C2	48:5:4456:C:C2	3.09	0.41
48:5:1484:G:N3	48:5:1484:G:H2'	2.36	0.41
51:9:936:G:C2	51:9:1007:C:C2	3.09	0.41
48:5:2682:G:C2	48:5:2683:C:C2	3.09	0.41
51:9:223:C:C2	51:9:299:A:C2	3.09	0.41
48:5:961:G:C2'	48:5:961:G:N3	2.84	0.41
51:9:1040:G:H5''	51:9:1040:G:H8	1.85	0.41
48:5:3857:G:C6	48:5:3858:C:C4	3.08	0.41
51:9:49:C:O2	51:9:478:G:C2	2.73	0.41
51:9:480:G:C2	51:9:481:C:C2	3.09	0.41
48:5:33:A:C6	48:5:34:A:C6	3.09	0.41
48:5:1963:C:O2'	48:5:1964:A:P	2.79	0.40
56:EE:49:ARG:HB3	56:EE:55:ALA:HB3	2.03	0.40
51:9:1143:A:H2'	51:9:1144:A:C8	2.56	0.40
48:5:1563:A:N7	51:9:678:U:H4'	2.35	0.40
54:CC:233:LEU:C	54:CC:233:LEU:HD12	2.42	0.40
48:5:2322:G:C2	48:5:2323:C:C2	3.09	0.40
48:5:4462:C:N3	48:5:4515:G:C2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2363:A:C2	48:5:3860:A:C4	3.09	0.40
48:5:2581:A:H2'	48:5:2582:A:C8	2.55	0.40
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	2.03	0.40
48:5:952:G:C2	48:5:953:C:C2	3.09	0.40
60:II:139:LYS:HD2	60:II:145:ILE:HD12	2.02	0.40
48:5:2050:G:C6	48:5:2051:C:C4	3.09	0.40
51:9:1220:A:N6	51:9:1221:G:C6	2.89	0.40
73:VV:9:VAL:HG13	73:VV:10:ASP:N	2.36	0.40
48:5:701:G:H2'	48:5:701:G:N3	2.37	0.40
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.56	0.40
2:B:249:ARG:NH2	48:5:3845:A:OP2	2.54	0.40
48:5:4091:G:N2	48:5:4159:C:C2	2.89	0.40
68:QQ:12:VAL:HG11	68:QQ:90:LYS:HB3	2.02	0.40
16:Q:14:ARG:NH2	48:5:2083:C:OP2	2.54	0.40
48:5:368:C:C2	48:5:374:G:C2	3.09	0.40
48:5:2519:U:C2	48:5:2520:C:C5	3.09	0.40
48:5:977:C:H2'	48:5:978:G:H5'	2.02	0.40
17:R:177:LEU:HB2	17:R:178:GLN:OE1	2.21	0.40
47:3:4:C:O2'	47:3:5:G:P	2.79	0.40
48:5:1358:G:N1	48:5:1379:C:O2	2.54	0.40
54:CC:204:ILE:HD11	54:CC:215:LEU:HD23	2.03	0.40
51:9:310:C:H2'	51:9:311:C:C6	2.56	0.40
4:D:258:LYS:O	4:D:259:ARG:CG	2.70	0.40
51:9:1126:G:C6	51:9:1127:C:C4	3.09	0.40
48:5:1448:G:C2	48:5:2097:U:C4	3.09	0.40
48:5:1070:G:C2	48:5:1071:C:C2	3.09	0.40
48:5:4644:G:C2	48:5:4645:C:C2	3.09	0.40
51:9:452:G:C2	51:9:453:C:C2	3.10	0.40
48:5:1275:G:C6	48:5:1276:C:C4	3.09	0.40
48:5:2576:G:C2	48:5:2577:C:C2	3.09	0.40
48:5:1092:G:C2	48:5:1093:C:C2	3.09	0.40
51:9:1686:G:C6	51:9:1687:C:C4	3.08	0.40
48:5:2410:C:C2	48:5:2435:G:N2	2.89	0.40
1:A:67:TYR:HB3	48:5:4086:G:C6	2.57	0.40
51:9:878:G:C6	51:9:909:G:C6	3.09	0.40
51:9:1293:A:C2'	51:9:1294:G:O5'	2.70	0.40
48:5:1213:G:C2	48:5:1215:C:C2	3.10	0.40
48:5:199:G:C2	48:5:201:C:C2	3.09	0.40
48:5:5028:G:C2	48:5:5029:C:N3	2.89	0.40
25:Z:51:ARG:NH1	48:5:2755:A:OP2	2.54	0.40
51:9:1126:G:N1	51:9:1127:C:C4	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4713:G:C2	48:5:4714:C:C2	3.09	0.40
48:5:4699:U:O4	48:5:4702:G:C6	2.75	0.40
48:5:4709:U:C4	48:5:4710:C:N4	2.89	0.40
51:9:1855:G:OP2	66:OO:147:ARG:NH1	2.49	0.40
48:5:2123:C:O2'	48:5:2124:G:OP2	2.19	0.40
1:A:122:ASP:C	1:A:122:ASP:OD1	2.59	0.40
51:9:452:G:C6	51:9:453:C:C4	3.10	0.40
19:T:42:ILE:HD13	19:T:89:ILE:HD11	2.03	0.40
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.44	0.40
22:W:44:ARG:HH11	22:W:44:ARG:CG	2.33	0.40
22:W:44:ARG:HH11	22:W:44:ARG:HG2	1.87	0.40
48:5:1761:G:C2	48:5:1762:C:C2	3.09	0.40
49:7:77:A:C2	49:7:100:A:C4	3.09	0.40
3:C:180:ILE:HD11	3:C:227:ILE:HD11	2.03	0.40
48:5:4154:G:C2	48:5:4155:C:C2	3.09	0.40
48:5:29:G:C6	48:5:30:C:C4	3.09	0.40
48:5:462:G:C2	48:5:694:C:C2	3.10	0.40
48:5:4187:G:H2'	48:5:4188:U:O4'	2.21	0.40
48:5:975:C:H3'	48:5:976:G:O4'	2.21	0.40
48:5:2468:U:O2	48:5:2469:C:C5	2.75	0.40
48:5:4075:U:HO2'	48:5:4076:G:P	2.45	0.40
5:E:90:LYS:N	5:E:91:PRO:HD3	2.36	0.40
48:5:2622:G:C6	48:5:2623:A:N7	2.89	0.40
48:5:4276:G:C2	48:5:4333:C:C2	3.09	0.40
48:5:702:U:H2'	48:5:703:G:H4'	2.03	0.40
48:5:488:G:C6	48:5:489:C:C4	3.09	0.40
11:L:39:ARG:NH2	48:5:1362:G:OP1	2.55	0.40
48:5:158:A:C5	48:5:277:G:C6	3.09	0.40
48:5:4240:G:C2	48:5:4241:C:C2	3.09	0.40
48:5:1739:G:C2	48:5:1740:C:N3	2.90	0.40
48:5:2086:G:C2	48:5:2087:C:C2	3.09	0.40
48:5:247:G:C6	48:5:248:C:C4	3.09	0.40
48:5:1506:G:C6	48:5:1507:C:C4	3.10	0.40
48:5:1090:G:C2	48:5:1207:C:C2	3.10	0.40
48:5:1203:G:C6	48:5:1204:C:C4	3.09	0.40
48:5:1936:C:C5	49:7:84:U:C4	3.10	0.40
76:YY:126:GLY:O	76:YY:128:GLY:N	2.55	0.40
51:9:374:G:C2	51:9:391:C:C2	3.10	0.40
1:A:103:PRO:HA	1:A:163:ARG:HA	2.03	0.40
48:5:2831:G:C2	48:5:3855:C:C2	3.09	0.40
51:9:1559:C:C2	51:9:1577:G:C2	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4349:C:H3'	48:5:4350:C:C5'	2.50	0.40
15:P:36:ILE:HD12	15:P:48:LEU:HD11	2.04	0.40
47:3:5:G:N1	47:3:6:G:C5	2.83	0.40
51:9:830:A:C6	51:9:844:U:N3	2.82	0.40
17:R:176:ARG:HH11	51:9:909:G:C5'	2.35	0.40
48:5:102:G:C2'	48:5:1381:U:O2'	2.68	0.40
48:5:747:A:C2	48:5:918:G:N1	2.89	0.40
51:9:1403:C:H2'	51:9:1403:C:O2	2.22	0.40
48:5:4714:C:C6	48:5:4715:C:C5	3.10	0.40
51:9:1667:U:H2'	51:9:1668:U:C6	2.56	0.40
48:5:963:G:C2'	48:5:963:G:N3	2.84	0.40
51:9:1257:G:H4'	51:9:1258:A:C5'	2.52	0.40
56:EE:75:LYS:O	56:EE:76:VAL:HB	2.22	0.40
14:O:36:VAL:HG11	14:O:108:ILE:HD12	2.02	0.40
48:5:1693:U:H2'	48:5:1694:C:O4'	2.21	0.40
20:U:87:THR:HG23	20:U:102:VAL:HG21	2.02	0.40
3:C:317:ASN:HA	3:C:318:PRO:HD3	1.96	0.40
50:8:146:U:H2'	50:8:147:G:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/244 (99%)	215 (89%)	23 (10%)	4 (2%)	11	57
2	B	392/394 (100%)	354 (90%)	33 (8%)	5 (1%)	15	61
3	C	360/362 (99%)	322 (89%)	30 (8%)	8 (2%)	8	52
4	D	290/292 (99%)	263 (91%)	25 (9%)	2 (1%)	26	72
5	E	232/248 (94%)	179 (77%)	34 (15%)	19 (8%)	1	17
6	F	223/225 (99%)	206 (92%)	16 (7%)	1 (0%)	39	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	239/241 (99%)	206 (86%)	25 (10%)	8 (3%)	5	44
8	H	188/190 (99%)	170 (90%)	16 (8%)	2 (1%)	17	65
9	I	200/213 (94%)	181 (90%)	14 (7%)	5 (2%)	7	49
10	J	167/169 (99%)	144 (86%)	15 (9%)	8 (5%)	3	32
11	L	208/210 (99%)	182 (88%)	15 (7%)	11 (5%)	2	29
12	M	136/138 (99%)	124 (91%)	12 (9%)	0	100	100
13	N	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
14	O	197/199 (99%)	190 (96%)	7 (4%)	0	100	100
15	P	151/153 (99%)	141 (93%)	9 (6%)	1 (1%)	26	72
16	Q	185/187 (99%)	172 (93%)	11 (6%)	2 (1%)	17	65
17	R	178/180 (99%)	166 (93%)	10 (6%)	2 (1%)	17	65
18	S	173/175 (99%)	158 (91%)	11 (6%)	4 (2%)	8	52
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	10	55
20	U	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	2	30
21	V	129/131 (98%)	116 (90%)	12 (9%)	1 (1%)	24	70
22	W	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
23	X	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	21	68
24	Y	132/134 (98%)	115 (87%)	15 (11%)	2 (2%)	13	59
25	Z	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	3	34
26	a	145/147 (99%)	124 (86%)	16 (11%)	5 (3%)	5	44
27	b	73/75 (97%)	66 (90%)	6 (8%)	1 (1%)	14	60
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	d	105/107 (98%)	90 (86%)	13 (12%)	2 (2%)	10	55
30	e	126/128 (98%)	117 (93%)	6 (5%)	3 (2%)	7	51
31	f	107/109 (98%)	93 (87%)	9 (8%)	5 (5%)	3	33
32	g	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
33	h	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	5	44
34	i	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	4	38
35	j	84/86 (98%)	73 (87%)	10 (12%)	1 (1%)	16	63
36	k	67/69 (97%)	57 (85%)	7 (10%)	3 (4%)	3	34
37	l	48/50 (96%)	40 (83%)	4 (8%)	4 (8%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	m	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
39	n	21/23 (91%)	21 (100%)	0	0	100	100
40	o	102/104 (98%)	89 (87%)	10 (10%)	3 (3%)	6	47
41	p	89/91 (98%)	79 (89%)	10 (11%)	0	100	100
42	r	123/125 (98%)	100 (81%)	18 (15%)	5 (4%)	3	37
43	s	196/198 (99%)	162 (83%)	24 (12%)	10 (5%)	2	30
44	t	161/163 (99%)	100 (62%)	34 (21%)	27 (17%)	0	4
45	l	13/15 (87%)	10 (77%)	1 (8%)	2 (15%)	0	5
52	AA	206/208 (99%)	174 (84%)	23 (11%)	9 (4%)	3	34
53	BB	211/213 (99%)	172 (82%)	25 (12%)	14 (7%)	1	24
54	CC	216/218 (99%)	187 (87%)	22 (10%)	7 (3%)	5	45
55	DD	225/227 (99%)	187 (83%)	29 (13%)	9 (4%)	4	38
56	EE	260/262 (99%)	215 (83%)	29 (11%)	16 (6%)	2	26
57	FF	189/191 (99%)	163 (86%)	18 (10%)	8 (4%)	3	36
58	GG	235/237 (99%)	205 (87%)	27 (12%)	3 (1%)	15	61
59	HH	187/189 (99%)	153 (82%)	22 (12%)	12 (6%)	2	25
60	II	204/206 (99%)	171 (84%)	26 (13%)	7 (3%)	5	44
61	JJ	183/185 (99%)	156 (85%)	20 (11%)	7 (4%)	4	39
62	KK	96/98 (98%)	64 (67%)	21 (22%)	11 (12%)	0	9
63	LL	150/152 (99%)	131 (87%)	14 (9%)	5 (3%)	5	44
64	MM	122/124 (98%)	85 (70%)	29 (24%)	8 (7%)	1	24
65	NN	148/150 (99%)	126 (85%)	16 (11%)	6 (4%)	3	37
66	OO	134/136 (98%)	104 (78%)	15 (11%)	15 (11%)	0	9
67	PP	125/127 (98%)	111 (89%)	11 (9%)	3 (2%)	7	51
68	QQ	139/141 (99%)	116 (84%)	17 (12%)	6 (4%)	3	35
69	RR	127/129 (98%)	108 (85%)	14 (11%)	5 (4%)	4	38
70	SS	135/137 (98%)	116 (86%)	11 (8%)	8 (6%)	2	27
71	TT	139/141 (99%)	128 (92%)	8 (6%)	3 (2%)	8	52
72	UU	102/104 (98%)	88 (86%)	8 (8%)	6 (6%)	2	27
73	VV	81/83 (98%)	70 (86%)	7 (9%)	4 (5%)	3	32
74	WW	127/129 (98%)	110 (87%)	10 (8%)	7 (6%)	2	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	XX	139/141 (99%)	125 (90%)	10 (7%)	4 (3%)	6	47
76	YY	124/126 (98%)	102 (82%)	15 (12%)	7 (6%)	2	28
77	ZZ	73/75 (97%)	59 (81%)	12 (16%)	2 (3%)	6	48
78	aa	96/98 (98%)	78 (81%)	9 (9%)	9 (9%)	1	14
79	bb	81/83 (98%)	66 (82%)	9 (11%)	6 (7%)	1	20
80	cc	59/61 (97%)	48 (81%)	10 (17%)	1 (2%)	11	57
81	dd	51/53 (96%)	44 (86%)	6 (12%)	1 (2%)	9	54
82	ee	55/57 (96%)	40 (73%)	13 (24%)	2 (4%)	4	41
83	ff	59/69 (86%)	51 (86%)	6 (10%)	2 (3%)	5	44
84	gg	311/313 (99%)	269 (86%)	33 (11%)	9 (3%)	6	47
86	ii	414/416 (100%)	383 (92%)	25 (6%)	6 (1%)	14	60
87	jj	569/594 (96%)	518 (91%)	40 (7%)	11 (2%)	10	55
All	All	12494/12710 (98%)	10874 (87%)	1202 (10%)	418 (3%)	8	44

All (418) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	TRP
5	E	91	PRO
5	E	95	ASP
5	E	118	PRO
5	E	175	LEU
5	E	221	PRO
7	G	45	ILE
7	G	128	VAL
8	H	40	HIS
8	H	110	SER
9	I	188	LYS
11	L	64	VAL
11	L	67	HIS
16	Q	148	VAL
17	R	36	ASN
18	S	165	PRO
25	Z	84	ARG
26	a	90	ALA
29	d	94	GLU
30	e	92	ASN
31	f	80	ASN

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Mol	Chain	Res	Type
34	i	91	SER
34	i	92	SER
35	j	36	LYS
36	k	61	PRO
40	o	32	SER
42	r	86	ALA
43	s	201	PRO
44	t	29	ALA
44	t	30	PRO
44	t	31	LYS
44	t	53	TRP
44	t	89	PRO
44	t	144	ASP
44	t	148	PRO
44	t	149	HIS
52	AA	44	ASP
52	AA	186	ARG
53	BB	57	ILE
55	DD	192	TRP
55	DD	202	LYS
55	DD	223	ILE
56	EE	118	GLU
56	EE	164	LEU
57	FF	80	GLY
59	HH	18	GLU
59	HH	66	VAL
59	HH	159	ASP
59	HH	190	PRO
60	II	157	LYS
61	JJ	4	ALA
61	JJ	36	GLY
61	JJ	121	LYS
62	KK	95	ARG
64	MM	79	VAL
64	MM	102	LYS
64	MM	114	TYR
65	NN	24	THR
66	OO	56	VAL
66	OO	65	ASP
66	OO	140	THR
68	QQ	43	GLU
68	QQ	64	ALA

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Mol	Chain	Res	Type
69	RR	88	VAL
69	RR	93	GLN
71	TT	29	LYS
71	TT	34	VAL
72	UU	107	GLU
73	VV	33	PRO
75	XX	34	THR
76	YY	104	ARG
77	ZZ	113	THR
82	ee	9	VAL
84	gg	161	SER
84	gg	282	GLU
86	ii	298	THR
86	ii	386	GLY
86	ii	387	ALA
87	jj	455	ILE
1	A	217	GLN
2	B	18	PRO
2	B	302	ASN
3	C	16	GLU
3	C	73	VAL
3	C	273	LEU
3	C	275	SER
4	D	187	SER
5	E	85	LEU
5	E	92	VAL
5	E	96	LYS
5	E	210	ASP
5	E	234	GLU
9	I	47	PRO
10	J	116	GLY
10	J	155	HIS
11	L	143	GLU
16	Q	14	ARG
17	R	19	LYS
18	S	88	SER
18	S	155	PRO
19	T	44	GLY
19	T	81	LYS
20	U	98	ASP
23	X	131	ASP
25	Z	34	SER

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Mol	Chain	Res	Type
25	Z	55	ALA
30	e	44	ARG
31	f	79	GLY
31	f	107	PRO
33	h	7	ARG
33	h	74	LYS
37	l	49	LEU
42	r	67	ARG
42	r	71	ARG
42	r	107	ARG
43	s	62	ARG
43	s	69	LEU
43	s	70	GLU
43	s	106	LYS
43	s	109	ALA
44	t	5	PHE
44	t	22	VAL
44	t	26	SER
44	t	39	PRO
44	t	54	LYS
44	t	58	ILE
44	t	106	PHE
52	AA	45	GLY
52	AA	191	ARG
53	BB	86	LEU
53	BB	140	VAL
53	BB	152	LYS
53	BB	153	THR
53	BB	179	ASN
53	BB	191	ASP
54	CC	228	SER
55	DD	175	VAL
55	DD	219	PRO
56	EE	95	THR
56	EE	171	ASP
56	EE	196	THR
57	FF	34	SER
57	FF	54	GLY
58	GG	105	ASN
58	GG	152	ASP
59	HH	160	LYS
60	II	155	ASN

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Mol	Chain	Res	Type
62	KK	3	MET
62	KK	39	ASN
62	KK	63	ALA
62	KK	67	PHE
63	LL	66	VAL
64	MM	15	ASN
65	NN	138	ASN
66	OO	24	GLY
66	OO	104	ARG
66	OO	129	ILE
66	OO	146	ARG
67	PP	14	LYS
67	PP	75	VAL
68	QQ	35	ASN
68	QQ	100	VAL
70	SS	12	ILE
70	SS	133	GLY
71	TT	39	LEU
72	UU	50	VAL
72	UU	52	GLY
73	VV	41	LYS
74	WW	107	SER
75	XX	42	GLY
76	YY	34	THR
76	YY	95	GLY
76	YY	114	MET
76	YY	120	THR
76	YY	127	ALA
78	aa	9	GLY
78	aa	10	ARG
78	aa	25	ASN
78	aa	62	TYR
79	bb	4	ALA
79	bb	6	ASP
79	bb	82	LYS
84	gg	254	PRO
86	ii	315	GLY
87	jj	25	CYS
87	jj	47	ILE
1	A	14	SER
1	A	180	LEU
5	E	174	PRO

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Mol	Chain	Res	Type
5	E	232	GLU
7	G	85	GLN
10	J	11	PRO
11	L	63	THR
20	U	47	ILE
21	V	14	PHE
26	a	76	ASP
30	e	125	PRO
31	f	37	ASP
33	h	89	ARG
34	i	3	LEU
34	i	11	LEU
36	k	32	VAL
40	o	33	LEU
40	o	77	CYS
43	s	108	PRO
43	s	142	GLY
44	t	67	ARG
44	t	105	THR
44	t	137	GLN
53	BB	106	THR
53	BB	206	PRO
55	DD	200	PRO
56	EE	24	THR
56	EE	76	VAL
56	EE	98	ASN
56	EE	109	PHE
56	EE	153	LEU
56	EE	154	ILE
57	FF	37	ASP
57	FF	119	SER
57	FF	163	PHE
59	HH	16	PRO
59	HH	111	LYS
60	II	27	TYR
60	II	137	LEU
60	II	138	ASN
61	JJ	120	ALA
61	JJ	138	ARG
62	KK	31	LYS
62	KK	92	ALA
63	LL	28	THR

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Mol	Chain	Res	Type
63	LL	147	LYS
64	MM	100	PRO
65	NN	3	ARG
65	NN	108	ASP
66	OO	32	HIS
68	QQ	17	LYS
69	RR	63	ARG
70	SS	11	HIS
70	SS	83	PHE
73	VV	45	ARG
73	VV	48	GLY
74	WW	3	ARG
74	WW	30	CYS
74	WW	58	ALA
74	WW	78	ARG
75	XX	10	ALA
77	ZZ	112	ASN
78	aa	8	ASN
78	aa	15	ARG
78	aa	61	ALA
79	bb	75	GLU
80	cc	26	GLN
84	gg	12	LYS
84	gg	60	ARG
86	ii	27	ALA
87	jj	22	ARG
87	jj	179	ALA
3	C	155	GLU
3	C	222	ARG
3	C	248	ARG
5	E	224	GLN
9	I	79	SER
9	I	205	PRO
10	J	153	ALA
11	L	100	PRO
19	T	144	ASN
20	U	27	HIS
20	U	97	ARG
25	Z	31	ASP
25	Z	91	LEU
26	a	92	LYS
26	a	98	ALA

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Mol	Chain	Res	Type
29	d	58	GLY
37	l	39	SER
37	l	47	THR
42	r	33	LYS
44	t	2	PRO
44	t	18	THR
44	t	119	ARG
52	AA	207	PRO
54	CC	264	SER
55	DD	143	ARG
56	EE	30	ARG
60	II	143	LYS
61	JJ	5	ARG
61	JJ	147	PHE
62	KK	93	THR
66	OO	39	ASP
66	OO	64	ALA
66	OO	128	ARG
69	RR	121	GLN
70	SS	7	GLU
72	UU	48	LEU
72	UU	118	ASP
74	WW	66	THR
75	XX	129	SER
83	ff	85	LYS
87	jj	285	PHE
2	B	19	ARG
2	B	38	SER
2	B	301	ASN
3	C	309	ILE
5	E	54	SER
5	E	63	ALA
5	E	179	ARG
5	E	218	LEU
7	G	123	ALA
7	G	125	LYS
10	J	124	GLY
11	L	6	ASN
11	L	52	SER
11	L	134	PRO
20	U	67	LYS
24	Y	11	ARG

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Mol	Chain	Res	Type
24	Y	63	LYS
31	f	106	TYR
33	h	97	LYS
36	k	29	LYS
37	l	44	TRP
43	s	34	ASN
44	t	7	PRO
44	t	19	GLY
45	1	57	ARG
52	AA	43	SER
52	AA	110	ASN
53	BB	22	VAL
53	BB	76	ASN
54	CC	62	PRO
54	CC	255	LEU
54	CC	261	PHE
56	EE	40	GLU
56	EE	131	VAL
57	FF	132	GLY
58	GG	99	GLY
59	HH	6	ALA
59	HH	57	ARG
59	HH	100	ILE
60	II	131	PRO
62	KK	32	HIS
62	KK	43	LEU
63	LL	19	ASN
63	LL	32	LYS
64	MM	116	LYS
65	NN	27	LYS
66	OO	38	ASN
66	OO	54	CYS
67	PP	15	PHE
69	RR	95	ILE
70	SS	59	LEU
70	SS	92	ASP
72	UU	105	SER
74	WW	93	LEU
78	aa	65	PRO
79	bb	51	GLN
81	dd	11	PRO
82	ee	22	GLN

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Mol	Chain	Res	Type
84	gg	37	ASP
84	gg	205	SER
5	E	103	VAL
5	E	229	PHE
6	F	239	GLU
7	G	82	GLN
10	J	146	ARG
11	L	5	ARG
11	L	167	ARG
11	L	169	ILE
44	t	10	ILE
55	DD	191	PRO
59	HH	35	ASP
62	KK	90	VAL
64	MM	103	VAL
65	NN	60	VAL
68	QQ	32	ILE
70	SS	10	GLN
83	ff	117	PRO
87	jj	402	GLY
7	G	238	GLY
10	J	152	GLY
26	a	22	ILE
27	b	21	ILE
56	EE	90	ILE
57	FF	33	ILE
66	OO	33	ILE
66	OO	145	GLY
76	YY	126	GLY
79	bb	38	PRO
84	gg	163	PRO
84	gg	190	GLY
87	jj	237	ILE
7	G	186	GLY
25	Z	90	PRO
44	t	23	GLY
53	BB	24	PRO
64	MM	58	GLU
87	jj	41	VAL
87	jj	432	ILE
4	D	125	VAL
9	I	43	VAL

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Mol	Chain	Res	Type
18	S	5	GLY
43	s	73	PRO
44	t	3	PRO
45	1	64	PRO
53	BB	93	GLY
53	BB	190	PRO
86	ii	118	LYS
10	J	174	ILE
44	t	98	ILE
52	AA	159	ILE
54	CC	181	PRO
54	CC	189	GLY
55	DD	222	PRO
59	HH	11	PRO
78	aa	64	LEU
15	P	84	PRO
52	AA	26	GLY
56	EE	195	ILE
87	jj	249	VAL

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	
1	A	187/187 (100%)	160 (86%)	27 (14%)	4	27
2	B	336/342 (98%)	301 (90%)	35 (10%)	9	43
3	C	302/302 (100%)	260 (86%)	42 (14%)	4	29
4	D	247/247 (100%)	222 (90%)	25 (10%)	9	44
5	E	208/221 (94%)	184 (88%)	24 (12%)	7	37
6	F	194/195 (100%)	166 (86%)	28 (14%)	4	27
7	G	206/206 (100%)	183 (89%)	23 (11%)	7	39
8	H	169/169 (100%)	149 (88%)	20 (12%)	6	36
9	I	174/180 (97%)	155 (89%)	19 (11%)	8	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	142/142 (100%)	130 (92%)	12 (8%)	13	53
11	L	176/176 (100%)	147 (84%)	29 (16%)	3	20
12	M	117/117 (100%)	100 (86%)	17 (14%)	4	27
13	N	171/171 (100%)	151 (88%)	20 (12%)	7	36
14	O	171/171 (100%)	148 (86%)	23 (14%)	5	30
15	P	134/134 (100%)	121 (90%)	13 (10%)	10	46
16	Q	163/163 (100%)	141 (86%)	22 (14%)	5	30
17	R	159/159 (100%)	139 (87%)	20 (13%)	5	32
18	S	156/156 (100%)	133 (85%)	23 (15%)	4	26
19	T	139/139 (100%)	123 (88%)	16 (12%)	7	37
20	U	89/89 (100%)	81 (91%)	8 (9%)	12	50
21	V	101/101 (100%)	84 (83%)	17 (17%)	2	19
22	W	55/55 (100%)	50 (91%)	5 (9%)	12	50
23	X	107/107 (100%)	96 (90%)	11 (10%)	9	43
24	Y	124/124 (100%)	106 (86%)	18 (14%)	4	27
25	Z	117/117 (100%)	110 (94%)	7 (6%)	24	66
26	a	119/119 (100%)	107 (90%)	12 (10%)	9	44
27	b	62/62 (100%)	57 (92%)	5 (8%)	15	54
28	c	79/79 (100%)	68 (86%)	11 (14%)	4	29
29	d	98/98 (100%)	81 (83%)	17 (17%)	2	17
30	e	114/114 (100%)	97 (85%)	17 (15%)	4	26
31	f	88/88 (100%)	76 (86%)	12 (14%)	5	30
32	g	98/98 (100%)	85 (87%)	13 (13%)	5	31
33	h	109/109 (100%)	97 (89%)	12 (11%)	8	40
34	i	86/86 (100%)	79 (92%)	7 (8%)	15	54
35	j	73/73 (100%)	64 (88%)	9 (12%)	6	34
36	k	64/64 (100%)	58 (91%)	6 (9%)	11	48
37	l	47/47 (100%)	41 (87%)	6 (13%)	5	32
38	m	48/48 (100%)	37 (77%)	11 (23%)	1	8
39	n	22/22 (100%)	19 (86%)	3 (14%)	5	30
40	o	92/92 (100%)	79 (86%)	13 (14%)	4	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	p	74/74 (100%)	68 (92%)	6 (8%)	15	54
42	r	109/109 (100%)	90 (83%)	19 (17%)	2	17
43	s	166/166 (100%)	156 (94%)	10 (6%)	24	66
44	t	136/136 (100%)	126 (93%)	10 (7%)	17	58
45	1	13/13 (100%)	13 (100%)	0	100	100
52	AA	174/174 (100%)	154 (88%)	20 (12%)	7	37
53	BB	194/194 (100%)	166 (86%)	28 (14%)	4	27
54	CC	184/184 (100%)	161 (88%)	23 (12%)	6	33
55	DD	190/190 (100%)	160 (84%)	30 (16%)	3	23
56	EE	223/223 (100%)	191 (86%)	32 (14%)	4	28
57	FF	161/161 (100%)	138 (86%)	23 (14%)	4	28
58	GG	207/207 (100%)	177 (86%)	30 (14%)	4	27
59	HH	169/169 (100%)	153 (90%)	16 (10%)	11	47
60	II	178/178 (100%)	155 (87%)	23 (13%)	5	32
61	JJ	161/161 (100%)	140 (87%)	21 (13%)	5	32
62	KK	89/89 (100%)	76 (85%)	13 (15%)	4	27
63	LL	136/136 (100%)	119 (88%)	17 (12%)	6	33
64	MM	104/104 (100%)	87 (84%)	17 (16%)	3	20
65	NN	130/130 (100%)	112 (86%)	18 (14%)	4	29
66	OO	106/106 (100%)	81 (76%)	25 (24%)	1	7
67	PP	116/116 (100%)	98 (84%)	18 (16%)	3	24
68	QQ	117/117 (100%)	104 (89%)	13 (11%)	8	40
69	RR	117/117 (100%)	104 (89%)	13 (11%)	8	40
70	SS	119/119 (100%)	100 (84%)	19 (16%)	3	22
71	TT	112/112 (100%)	98 (88%)	14 (12%)	6	33
72	UU	94/94 (100%)	82 (87%)	12 (13%)	5	32
73	VV	67/67 (100%)	59 (88%)	8 (12%)	6	35
74	WW	112/112 (100%)	102 (91%)	10 (9%)	12	51
75	XX	113/113 (100%)	98 (87%)	15 (13%)	5	31
76	YY	108/108 (100%)	87 (81%)	21 (19%)	2	12
77	ZZ	66/66 (100%)	58 (88%)	8 (12%)	6	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	aa	85/85 (100%)	76 (89%)	9 (11%)	8	42
79	bb	75/75 (100%)	64 (85%)	11 (15%)	4	26
80	cc	54/54 (100%)	46 (85%)	8 (15%)	4	26
81	dd	47/47 (100%)	39 (83%)	8 (17%)	2	18
82	ee	47/47 (100%)	40 (85%)	7 (15%)	4	26
83	ff	59/62 (95%)	57 (97%)	2 (3%)	44	79
84	gg	272/272 (100%)	249 (92%)	23 (8%)	13	53
86	ii	358/358 (100%)	328 (92%)	30 (8%)	14	53
87	jj	507/522 (97%)	486 (96%)	21 (4%)	37	76
All	All	10892/10936 (100%)	9583 (88%)	1309 (12%)	11	35

All (1309) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	49	ILE
1	A	64	ARG
1	A	68	ARG
1	A	96	LEU
1	A	97	ASN
1	A	100	ASN
1	A	102	LEU
1	A	125	LYS
1	A	128	ARG
1	A	142	GLU
1	A	158	ILE
1	A	162	ASN
1	A	163	ARG
1	A	165	VAL
1	A	175	ILE
1	A	180	LEU
1	A	193	ARG
1	A	200	ARG
1	A	207	VAL
1	A	218	HIS
1	A	221	LYS
1	A	226	ARG
1	A	227	ARG
1	A	233	ARG

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Mol	Chain	Res	Type
1	A	235	VAL
1	A	242	ARG
2	B	10	ARG
2	B	39	LYS
2	B	43	LEU
2	B	56	ILE
2	B	62	ARG
2	B	66	LYS
2	B	67	VAL
2	B	74	GLU
2	B	90	VAL
2	B	94	GLU
2	B	99	LEU
2	B	103	LYS
2	B	116	ARG
2	B	135	LYS
2	B	146	LEU
2	B	154	LYS
2	B	162	VAL
2	B	167	GLN
2	B	175	GLN
2	B	203	GLN
2	B	213	GLN
2	B	228	TYR
2	B	244	THR
2	B	261	ARG
2	B	262	VAL
2	B	309	LEU
2	B	314	ILE
2	B	329	ASP
2	B	333	LEU
2	B	340	THR
2	B	352	LEU
2	B	356	LYS
2	B	357	ARG
2	B	366	LYS
2	B	383	GLU
3	C	14	LYS
3	C	20	LYS
3	C	33	ARG
3	C	54	VAL
3	C	55	SER

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Mol	Chain	Res	Type
3	C	57	LEU
3	C	65	GLU
3	C	71	ARG
3	C	80	ARG
3	C	95	MET
3	C	113	ARG
3	C	114	ARG
3	C	122	TYR
3	C	124	ILE
3	C	140	LYS
3	C	144	ILE
3	C	147	VAL
3	C	150	LEU
3	C	155	GLU
3	C	159	GLU
3	C	165	LYS
3	C	175	LYS
3	C	179	ASP
3	C	188	ARG
3	C	193	LYS
3	C	208	CYS
3	C	223	ASN
3	C	232	VAL
3	C	246	VAL
3	C	267	TRP
3	C	273	LEU
3	C	281	MET
3	C	284	MET
3	C	287	THR
3	C	307	LYS
3	C	312	ARG
3	C	317	ASN
3	C	321	ASN
3	C	333	LYS
3	C	342	ARG
3	C	345	ARG
3	C	348	LYS
4	D	4	VAL
4	D	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	56	THR

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Mol	Chain	Res	Type
4	D	81	HIS
4	D	89	LYS
4	D	94	ASN
4	D	104	LEU
4	D	110	LEU
4	D	111	ASN
4	D	124	GLU
4	D	179	ARG
4	D	196	ARG
4	D	202	GLN
4	D	212	MET
4	D	225	GLN
4	D	234	ASP
4	D	248	ARG
4	D	249	GLU
4	D	256	LYS
4	D	264	LYS
4	D	268	ARG
4	D	278	ASP
4	D	293	ARG
5	E	43	ASN
5	E	46	LEU
5	E	52	ARG
5	E	101	ARG
5	E	105	LEU
5	E	124	HIS
5	E	126	ARG
5	E	134	ARG
5	E	136	LEU
5	E	137	ARG
5	E	158	VAL
5	E	162	LYS
5	E	163	GLN
5	E	178	ASN
5	E	197	ILE
5	E	206	LYS
5	E	212	TYR
5	E	230	ASP
5	E	233	LYS
5	E	237	GLU
5	E	250	ASP
5	E	274	THR

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Mol	Chain	Res	Type
5	E	282	LEU
5	E	284	PHE
6	F	33	LYS
6	F	41	GLN
6	F	44	LEU
6	F	49	ARG
6	F	68	ARG
6	F	70	GLU
6	F	72	ARG
6	F	76	MET
6	F	82	ASN
6	F	90	LYS
6	F	91	LEU
6	F	96	ARG
6	F	98	ARG
6	F	100	ILE
6	F	101	ASN
6	F	115	ARG
6	F	127	LEU
6	F	137	ILE
6	F	154	GLU
6	F	179	ARG
6	F	189	MET
6	F	192	LEU
6	F	201	LYS
6	F	202	ARG
6	F	214	LYS
6	F	216	SER
6	F	234	ASP
6	F	248	ARG
7	G	28	VAL
7	G	73	ARG
7	G	75	LYS
7	G	81	ASN
7	G	88	ASP
7	G	90	GLN
7	G	106	THR
7	G	110	LYS
7	G	112	GLN
7	G	131	LYS
7	G	148	GLU
7	G	150	LYS

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Mol	Chain	Res	Type
7	G	151	LYS
7	G	154	LEU
7	G	170	LEU
7	G	173	LEU
7	G	175	ARG
7	G	177	MET
7	G	189	ARG
7	G	202	VAL
7	G	217	LYS
7	G	220	GLU
7	G	240	ASN
8	H	1	MET
8	H	20	LEU
8	H	26	ILE
8	H	28	LYS
8	H	41	ILE
8	H	52	LYS
8	H	54	ARG
8	H	59	LYS
8	H	66	GLU
8	H	72	THR
8	H	74	CYS
8	H	78	GLN
8	H	98	HIS
8	H	111	LEU
8	H	125	ARG
8	H	128	MET
8	H	129	ARG
8	H	162	GLN
8	H	173	ARG
8	H	177	ASP
9	I	8	CYS
9	I	13	LYS
9	I	35	ASP
9	I	36	LEU
9	I	39	LYS
9	I	43	VAL
9	I	48	LEU
9	I	76	MET
9	I	116	ARG
9	I	144	ASN
9	I	146	GLU

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Mol	Chain	Res	Type
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	180	GLU
9	I	195	CYS
9	I	198	LYS
9	I	208	LYS
9	I	212	LEU
10	J	15	LEU
10	J	16	ARG
10	J	18	ARG
10	J	33	LEU
10	J	34	THR
10	J	49	VAL
10	J	55	TYR
10	J	81	GLU
10	J	90	ARG
10	J	113	ILE
10	J	151	ILE
10	J	168	GLN
11	L	10	LEU
11	L	28	GLN
11	L	35	ARG
11	L	36	ARG
11	L	49	ARG
11	L	59	VAL
11	L	64	VAL
11	L	67	HIS
11	L	74	ARG
11	L	77	SER
11	L	92	ARG
11	L	94	ILE
11	L	99	ASP
11	L	111	GLN
11	L	115	GLN
11	L	116	ARG
11	L	121	ARG
11	L	123	LYS
11	L	130	LYS
11	L	143	GLU
11	L	158	ARG
11	L	162	LYS

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Mol	Chain	Res	Type
11	L	165	LYS
11	L	174	LYS
11	L	186	ARG
11	L	190	ARG
11	L	195	ARG
11	L	198	ARG
11	L	201	GLU
12	M	4	ARG
12	M	5	ARG
12	M	8	GLU
12	M	25	VAL
12	M	29	ASP
12	M	32	ASP
12	M	33	GLN
12	M	38	VAL
12	M	43	THR
12	M	48	GLN
12	M	56	GLN
12	M	57	LEU
12	M	61	ILE
12	M	96	GLU
12	M	105	THR
12	M	118	MET
12	M	119	ARG
13	N	9	GLU
13	N	26	ARG
13	N	27	CYS
13	N	32	GLN
13	N	36	LEU
13	N	44	ARG
13	N	61	ILE
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	80	THR
13	N	87	HIS
13	N	104	GLU
13	N	108	ARG
13	N	136	ASP
13	N	162	ARG
13	N	174	LEU
13	N	189	ARG

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Mol	Chain	Res	Type
13	N	199	GLN
13	N	202	ARG
14	O	5	GLN
14	O	16	LEU
14	O	18	ARG
14	O	36	VAL
14	O	37	ARG
14	O	49	ARG
14	O	60	LYS
14	O	61	ARG
14	O	62	MET
14	O	67	SER
14	O	74	ARG
14	O	82	ARG
14	O	103	LYS
14	O	128	ARG
14	O	130	LYS
14	O	145	VAL
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	187	LYS
14	O	195	VAL
14	O	201	PHE
14	O	202	LEU
15	P	5	SER
15	P	25	HIS
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	92	LEU
15	P	99	GLU
15	P	100	SER
15	P	105	LYS
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	7	HIS
16	Q	13	VAL
16	Q	31	LEU
16	Q	54	SER

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Mol	Chain	Res	Type
16	Q	61	LEU
16	Q	63	LEU
16	Q	68	ARG
16	Q	75	ARG
16	Q	78	LYS
16	Q	88	ASP
16	Q	89	ASP
16	Q	91	ARG
16	Q	93	GLN
16	Q	95	VAL
16	Q	97	LYS
16	Q	108	ARG
16	Q	115	LYS
16	Q	134	CYS
16	Q	143	ARG
16	Q	168	ARG
16	Q	180	ARG
16	Q	187	LYS
17	R	10	LEU
17	R	15	LEU
17	R	34	ASN
17	R	39	GLN
17	R	40	GLN
17	R	43	LYS
17	R	50	ILE
17	R	52	ARG
17	R	75	HIS
17	R	89	MET
17	R	98	ARG
17	R	99	MET
17	R	106	LEU
17	R	107	ARG
17	R	113	LYS
17	R	123	LEU
17	R	133	LYS
17	R	138	LEU
17	R	176	ARG
17	R	180	LYS
18	S	2	LYS
18	S	7	LEU
18	S	8	ARG
18	S	17	LEU

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Mol	Chain	Res	Type
18	S	39	VAL
18	S	43	ARG
18	S	67	VAL
18	S	70	LYS
18	S	82	LEU
18	S	83	ARG
18	S	84	TYR
18	S	91	HIS
18	S	95	ARG
18	S	98	ARG
18	S	100	LEU
18	S	102	THR
18	S	127	MET
18	S	132	ILE
18	S	147	ASP
18	S	149	LYS
18	S	156	HIS
18	S	159	LEU
18	S	161	ARG
19	T	3	ASN
19	T	5	LYS
19	T	9	ARG
19	T	33	ILE
19	T	52	MET
19	T	60	LYS
19	T	81	LYS
19	T	88	ARG
19	T	96	ILE
19	T	117	LYS
19	T	118	GLU
19	T	131	GLN
19	T	136	ARG
19	T	142	ARG
19	T	144	ASN
19	T	159	MET
20	U	33	ILE
20	U	45	GLU
20	U	46	ARG
20	U	65	ARG
20	U	67	LYS
20	U	80	LYS
20	U	97	ARG

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Mol	Chain	Res	Type
20	U	99	TRP
21	V	15	ARG
21	V	18	LEU
21	V	31	ASN
21	V	35	LYS
21	V	46	LYS
21	V	51	ARG
21	V	57	VAL
21	V	60	MET
21	V	61	VAL
21	V	82	ILE
21	V	91	LYS
21	V	99	GLU
21	V	106	VAL
21	V	109	LYS
21	V	111	GLU
21	V	113	LYS
21	V	123	LYS
22	W	4	GLU
22	W	27	LYS
22	W	41	LEU
22	W	43	LYS
22	W	57	ARG
23	X	39	LYS
23	X	41	ARG
23	X	50	LYS
23	X	52	LEU
23	X	59	LYS
23	X	62	ARG
23	X	94	ASN
23	X	111	GLN
23	X	129	ARG
23	X	145	ASP
23	X	152	LYS
24	Y	2	LYS
24	Y	7	VAL
24	Y	8	THR
24	Y	28	LYS
24	Y	34	LEU
24	Y	50	ARG
24	Y	52	ASP
24	Y	55	VAL

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Mol	Chain	Res	Type
24	Y	59	ARG
24	Y	65	GLN
24	Y	72	GLN
24	Y	74	TYR
24	Y	79	VAL
24	Y	87	ARG
24	Y	104	VAL
24	Y	115	ARG
24	Y	126	ARG
24	Y	127	GLN
25	Z	5	MET
25	Z	11	VAL
25	Z	57	MET
25	Z	59	LYS
25	Z	88	ASP
25	Z	93	LYS
25	Z	112	ARG
26	a	10	LYS
26	a	12	ARG
26	a	16	SER
26	a	40	HIS
26	a	52	TYR
26	a	59	ARG
26	a	77	LYS
26	a	84	GLU
26	a	121	PRO
26	a	122	VAL
26	a	132	ARG
26	a	140	VAL
27	b	22	LYS
27	b	28	ARG
27	b	39	PHE
27	b	43	MET
27	b	51	LYS
28	c	28	VAL
28	c	37	MET
28	c	40	GLN
28	c	50	ASN
28	c	61	GLU
28	c	77	ASN
28	c	78	ASN
28	c	81	LEU

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Mol	Chain	Res	Type
28	c	90	ARG
28	c	91	VAL
28	c	94	LEU
29	d	19	GLU
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	44	ARG
29	d	48	GLU
29	d	56	GLU
29	d	78	ARG
29	d	79	ASN
29	d	83	ARG
29	d	85	ARG
29	d	86	VAL
29	d	90	ARG
29	d	94	GLU
29	d	102	LEU
29	d	107	THR
29	d	116	ASN
30	e	8	VAL
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	30	LYS
30	e	32	LYS
30	e	46	ARG
30	e	48	ARG
30	e	64	LYS
30	e	78	LEU
30	e	80	HIS
30	e	86	GLU
30	e	104	SER
30	e	106	LYS
30	e	107	ASN
30	e	113	GLU
30	e	123	THR
31	f	16	ARG
31	f	21	GLN
31	f	33	VAL
31	f	36	ARG
31	f	46	ARG

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Mol	Chain	Res	Type
31	f	52	LYS
31	f	56	ASN
31	f	64	PRO
31	f	69	VAL
31	f	84	VAL
31	f	100	ARG
31	f	101	ILE
32	g	5	LEU
32	g	11	LEU
32	g	14	ASN
32	g	15	THR
32	g	54	ARG
32	g	60	ARG
32	g	64	LEU
32	g	66	ARG
32	g	71	LYS
32	g	73	HIS
32	g	90	ARG
32	g	100	GLN
32	g	115	LYS
33	h	10	ARG
33	h	28	LEU
33	h	48	ARG
33	h	65	GLN
33	h	67	GLU
33	h	69	LEU
33	h	88	THR
33	h	89	ARG
33	h	97	LYS
33	h	98	HIS
33	h	104	THR
33	h	122	LYS
34	i	18	THR
34	i	25	ARG
34	i	33	LEU
34	i	86	LYS
34	i	87	ARG
34	i	89	GLU
34	i	103	LYS
35	j	2	THR
35	j	3	LYS
35	j	15	THR

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Mol	Chain	Res	Type
35	j	20	ARG
35	j	25	LYS
35	j	29	LEU
35	j	63	ARG
35	j	68	LYS
35	j	79	ARG
36	k	18	LYS
36	k	29	LYS
36	k	31	ASN
36	k	57	LYS
36	k	69	LEU
36	k	70	LYS
37	l	3	SER
37	l	8	ARG
37	l	16	LYS
37	l	17	GLN
37	l	36	ARG
37	l	46	ARG
38	m	79	GLU
38	m	82	LEU
38	m	84	GLN
38	m	85	LEU
38	m	88	LYS
38	m	90	ASN
38	m	97	ARG
38	m	98	LYS
38	m	106	ARG
38	m	111	ARG
38	m	119	ASN
39	n	2	ARG
39	n	9	ARG
39	n	21	ARG
40	o	17	LYS
40	o	24	THR
40	o	26	TYR
40	o	33	LEU
40	o	36	GLN
40	o	43	ARG
40	o	55	ILE
40	o	61	LYS
40	o	69	ARG
40	o	82	MET

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Mol	Chain	Res	Type
40	o	89	LYS
40	o	99	ARG
40	o	102	GLN
41	p	16	THR
41	p	24	LYS
41	p	49	ARG
41	p	54	ILE
41	p	60	CYS
41	p	84	ARG
42	r	10	VAL
42	r	17	LEU
42	r	18	ILE
42	r	20	ARG
42	r	21	ASN
42	r	26	SER
42	r	28	GLU
42	r	31	ASN
42	r	32	LEU
42	r	37	SER
42	r	39	ARG
42	r	67	ARG
42	r	80	THR
42	r	83	ASN
42	r	103	HIS
42	r	105	ASP
42	r	107	ARG
42	r	108	MET
42	r	118	LEU
43	s	38	LYS
43	s	44	ARG
43	s	62	ARG
43	s	68	HIS
43	s	94	ASP
43	s	146	LYS
43	s	149	ARG
43	s	174	LEU
43	s	185	PHE
43	s	191	GLN
44	t	1	MET
44	t	14	TYR
44	t	22	VAL
44	t	40	LYS

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Mol	Chain	Res	Type
44	t	95	GLN
44	t	96	LYS
44	t	104	ILE
44	t	106	PHE
44	t	114	ARG
44	t	123	ARG
52	AA	8	LEU
52	AA	9	GLN
52	AA	14	ASP
52	AA	32	PHE
52	AA	39	TYR
52	AA	41	ARG
52	AA	44	ASP
52	AA	46	ILE
52	AA	53	ARG
52	AA	58	LEU
52	AA	60	LEU
52	AA	79	SER
52	AA	84	GLN
52	AA	109	THR
52	AA	111	GLN
52	AA	113	GLN
52	AA	131	HIS
52	AA	155	ARG
52	AA	158	ASP
52	AA	178	LEU
53	BB	27	LYS
53	BB	38	MET
53	BB	43	ASN
53	BB	55	THR
53	BB	56	LYS
53	BB	63	LYS
53	BB	78	GLU
53	BB	82	ARG
53	BB	86	LEU
53	BB	105	LEU
53	BB	106	THR
53	BB	107	ARG
53	BB	122	GLU
53	BB	126	ASP
53	BB	134	LEU
53	BB	136	ARG

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Mol	Chain	Res	Type
53	BB	137	LEU
53	BB	142	PHE
53	BB	150	ILE
53	BB	151	ARG
53	BB	157	GLN
53	BB	163	GLN
53	BB	169	MET
53	BB	175	GLU
53	BB	206	PRO
53	BB	208	HIS
53	BB	213	ARG
53	BB	225	LEU
54	CC	72	ASP
54	CC	78	LEU
54	CC	107	LEU
54	CC	113	GLN
54	CC	114	LYS
54	CC	117	ARG
54	CC	120	GLN
54	CC	121	ARG
54	CC	123	ARG
54	CC	137	VAL
54	CC	152	ARG
54	CC	160	LEU
54	CC	166	ARG
54	CC	167	ARG
54	CC	192	LEU
54	CC	225	SER
54	CC	227	TRP
54	CC	230	THR
54	CC	233	LEU
54	CC	240	THR
54	CC	257	LYS
54	CC	262	THR
54	CC	275	LYS
55	DD	9	ARG
55	DD	22	ASN
55	DD	23	GLU
55	DD	28	GLU
55	DD	31	GLU
55	DD	32	ASP
55	DD	40	ARG

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Mol	Chain	Res	Type
55	DD	42	THR
55	DD	59	LEU
55	DD	64	ARG
55	DD	72	VAL
55	DD	76	ARG
55	DD	94	ARG
55	DD	107	TYR
55	DD	116	ARG
55	DD	117	ARG
55	DD	120	TYR
55	DD	142	LEU
55	DD	146	ARG
55	DD	154	ASP
55	DD	156	LEU
55	DD	162	ASP
55	DD	167	TYR
55	DD	168	VAL
55	DD	175	VAL
55	DD	176	LEU
55	DD	190	LEU
55	DD	212	GLU
55	DD	221	THR
55	DD	225	GLU
56	EE	3	ARG
56	EE	6	LYS
56	EE	12	VAL
56	EE	17	HIS
56	EE	19	MET
56	EE	24	THR
56	EE	33	THR
56	EE	38	LEU
56	EE	42	LEU
56	EE	49	ARG
56	EE	54	TYR
56	EE	65	CYS
56	EE	66	MET
56	EE	67	GLN
56	EE	73	ASP
56	EE	75	LYS
56	EE	95	THR
56	EE	130	PHE
56	EE	148	ARG

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Mol	Chain	Res	Type
56	EE	153	LEU
56	EE	155	LYS
56	EE	174	LYS
56	EE	181	CYS
56	EE	191	ARG
56	EE	205	PHE
56	EE	220	THR
56	EE	222	LEU
56	EE	225	ILE
56	EE	227	VAL
56	EE	240	ARG
56	EE	245	ARG
56	EE	259	LYS
57	FF	35	LEU
57	FF	73	THR
57	FF	79	HIS
57	FF	83	ASN
57	FF	88	MET
57	FF	89	THR
57	FF	91	ARG
57	FF	95	HIS
57	FF	106	GLU
57	FF	118	ASN
57	FF	124	ASP
57	FF	130	ARG
57	FF	136	ARG
57	FF	140	ASP
57	FF	152	TRP
57	FF	164	ARG
57	FF	165	ASN
57	FF	171	GLU
57	FF	173	LEU
57	FF	190	ILE
57	FF	194	ASP
57	FF	195	GLU
57	FF	203	ASN
58	GG	14	LYS
58	GG	15	LEU
58	GG	26	THR
58	GG	29	GLU
58	GG	50	VAL
58	GG	56	ASN

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Mol	Chain	Res	Type
58	GG	64	LYS
58	GG	68	LEU
58	GG	76	LEU
58	GG	103	ASP
58	GG	107	SER
58	GG	110	ASN
58	GG	120	ASP
58	GG	121	ILE
58	GG	126	ASP
58	GG	132	ARG
58	GG	137	ARG
58	GG	143	LYS
58	GG	164	LYS
58	GG	172	LYS
58	GG	178	ARG
58	GG	181	THR
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	196	LYS
58	GG	208	GLU
58	GG	224	ARG
58	GG	227	GLN
58	GG	235	SER
59	HH	34	SER
59	HH	35	ASP
59	HH	36	LEU
59	HH	40	LEU
59	HH	82	GLU
59	HH	87	PHE
59	HH	95	ILE
59	HH	106	ARG
59	HH	109	ARG
59	HH	119	SER
59	HH	120	ARG
59	HH	145	ARG
59	HH	153	LEU
59	HH	162	GLN
59	HH	172	THR
59	HH	188	GLU
60	II	6	ASP
60	II	8	TRP

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Mol	Chain	Res	Type
60	II	12	ARG
60	II	23	LYS
60	II	35	ASN
60	II	56	ARG
60	II	70	GLU
60	II	74	ARG
60	II	87	ASN
60	II	100	CYS
60	II	107	THR
60	II	110	ARG
60	II	111	GLN
60	II	115	SER
60	II	123	ARG
60	II	130	THR
60	II	140	LYS
60	II	162	LEU
60	II	167	GLN
60	II	168	GLN
60	II	196	GLU
60	II	203	LYS
60	II	206	LYS
61	JJ	15	THR
61	JJ	24	ARG
61	JJ	29	LEU
61	JJ	39	ASN
61	JJ	42	GLU
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	65	GLU
61	JJ	67	ASP
61	JJ	69	ARG
61	JJ	101	LYS
61	JJ	109	ARG
61	JJ	110	LEU
61	JJ	116	LYS
61	JJ	127	ARG
61	JJ	131	ARG
61	JJ	135	ILE
61	JJ	136	ARG
61	JJ	138	ARG
61	JJ	162	ARG
61	JJ	172	ARG

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Mol	Chain	Res	Type
62	KK	1	MET
62	KK	2	LEU
62	KK	13	GLU
62	KK	43	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	65	ARG
62	KK	66	HIS
62	KK	70	TYR
62	KK	74	GLU
62	KK	80	ARG
62	KK	81	ASP
62	KK	89	ILE
63	LL	8	ARG
63	LL	16	ILE
63	LL	22	ARG
63	LL	31	GLU
63	LL	40	ILE
63	LL	66	VAL
63	LL	67	SER
63	LL	69	ARG
63	LL	85	THR
63	LL	90	ARG
63	LL	91	ASP
63	LL	97	ARG
63	LL	121	GLN
63	LL	131	CYS
63	LL	134	LEU
63	LL	135	SER
63	LL	147	LYS
64	MM	12	MET
64	MM	26	LEU
64	MM	27	ILE
64	MM	31	LEU
64	MM	33	ARG
64	MM	35	ILE
64	MM	45	ARG
64	MM	48	HIS
64	MM	60	MET
64	MM	73	GLN
64	MM	77	ILE
64	MM	78	LYS

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Mol	Chain	Res	Type
64	MM	88	TRP
64	MM	96	ARG
64	MM	101	ARG
64	MM	114	TYR
64	MM	127	TYR
65	NN	12	SER
65	NN	13	GLN
65	NN	25	TRP
65	NN	27	LYS
65	NN	52	VAL
65	NN	62	GLN
65	NN	64	ARG
65	NN	75	LEU
65	NN	76	LYS
65	NN	77	SER
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	101	HIS
65	NN	102	LEU
65	NN	107	LYS
65	NN	110	ASP
65	NN	133	ARG
66	OO	34	PHE
66	OO	38	ASN
66	OO	39	ASP
66	OO	50	LYS
66	OO	51	GLU
66	OO	52	THR
66	OO	53	ILE
66	OO	61	LYS
66	OO	65	ASP
66	OO	69	SER
66	OO	76	LEU
66	OO	80	ASP
66	OO	100	THR
66	OO	104	ARG
66	OO	106	LYS
66	OO	107	THR
66	OO	121	ARG
66	OO	128	ARG
66	OO	130	GLU

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Mol	Chain	Res	Type
66	OO	131	ASP
66	OO	137	SER
66	OO	142	ARG
66	OO	146	ARG
66	OO	150	ARG
66	OO	151	LEU
67	PP	5	GLU
67	PP	7	LYS
67	PP	10	ARG
67	PP	17	TYR
67	PP	28	MET
67	PP	29	SER
67	PP	30	TYR
67	PP	37	TYR
67	PP	41	GLN
67	PP	43	ARG
67	PP	44	ARG
67	PP	52	LYS
67	PP	56	LEU
67	PP	65	LYS
67	PP	79	HIS
67	PP	100	LYS
67	PP	107	ILE
67	PP	121	ILE
68	QQ	26	LYS
68	QQ	41	MET
68	QQ	73	LYS
68	QQ	85	ARG
68	QQ	89	SER
68	QQ	90	LYS
68	QQ	101	ASP
68	QQ	119	LEU
68	QQ	123	ASP
68	QQ	126	ARG
68	QQ	140	ARG
68	QQ	145	TYR
68	QQ	146	ARG
69	RR	47	ARG
69	RR	49	LYS
69	RR	58	MET
69	RR	77	GLU
69	RR	78	ARG

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Mol	Chain	Res	Type
69	RR	79	GLU
69	RR	87	GLU
69	RR	88	VAL
69	RR	99	ASP
69	RR	109	LEU
69	RR	118	GLN
69	RR	121	GLN
69	RR	126	MET
70	SS	8	LYS
70	SS	13	LEU
70	SS	14	ARG
70	SS	34	LYS
70	SS	52	LEU
70	SS	63	GLU
70	SS	78	LYS
70	SS	81	ASP
70	SS	82	TRP
70	SS	86	ARG
70	SS	92	ASP
70	SS	95	TYR
70	SS	113	ARG
70	SS	115	LYS
70	SS	118	ARG
70	SS	125	HIS
70	SS	131	VAL
70	SS	134	GLN
70	SS	136	THR
71	TT	16	ARG
71	TT	28	LEU
71	TT	39	LEU
71	TT	62	ARG
71	TT	67	ARG
71	TT	74	SER
71	TT	82	ARG
71	TT	84	ARG
71	TT	93	SER
71	TT	102	ARG
71	TT	121	ARG
71	TT	123	LEU
71	TT	124	THR
71	TT	128	GLN
72	UU	33	GLU

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Mol	Chain	Res	Type
72	UU	36	CYS
72	UU	44	LYS
72	UU	48	LEU
72	UU	49	LYS
72	UU	51	LYS
72	UU	56	MET
72	UU	68	THR
72	UU	84	ILE
72	UU	93	SER
72	UU	111	GLU
72	UU	118	ASP
73	VV	9	VAL
73	VV	11	LEU
73	VV	34	MET
73	VV	38	GLU
73	VV	40	ASP
73	VV	47	ASN
73	VV	62	MET
73	VV	74	LYS
74	WW	3	ARG
74	WW	23	ARG
74	WW	51	GLU
74	WW	80	ASP
74	WW	83	LEU
74	WW	103	VAL
74	WW	104	LEU
74	WW	107	SER
74	WW	111	MET
74	WW	117	ARG
75	XX	3	LYS
75	XX	5	ARG
75	XX	19	ASP
75	XX	29	LYS
75	XX	37	LYS
75	XX	61	GLN
75	XX	67	ARG
75	XX	68	LYS
75	XX	71	ARG
75	XX	98	ASP
75	XX	105	PHE
75	XX	107	ARG
75	XX	115	ILE

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Mol	Chain	Res	Type
75	XX	130	LEU
75	XX	135	LYS
76	YY	7	ILE
76	YY	10	ARG
76	YY	14	THR
76	YY	16	ARG
76	YY	20	ARG
76	YY	22	GLN
76	YY	23	MET
76	YY	32	LYS
76	YY	40	ILE
76	YY	46	LYS
76	YY	61	ARG
76	YY	69	THR
76	YY	72	PHE
76	YY	74	MET
76	YY	85	ASN
76	YY	98	GLU
76	YY	99	LYS
76	YY	100	LYS
76	YY	107	ARG
76	YY	109	GLU
76	YY	111	LYS
77	ZZ	44	LEU
77	ZZ	74	SER
77	ZZ	83	LEU
77	ZZ	89	GLN
77	ZZ	93	SER
77	ZZ	99	LEU
77	ZZ	110	THR
77	ZZ	114	LYS
78	aa	18	VAL
78	aa	19	GLN
78	aa	23	CYS
78	aa	26	CYS
78	aa	41	ILE
78	aa	51	ARG
78	aa	52	ASP
78	aa	74	CYS
78	aa	95	ARG
79	bb	3	LEU
79	bb	17	ARG

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Mol	Chain	Res	Type
79	bb	27	SER
79	bb	36	LYS
79	bb	37	CYS
79	bb	40	CYS
79	bb	51	GLN
79	bb	60	SER
79	bb	63	LEU
79	bb	72	ARG
79	bb	84	HIS
80	cc	31	ARG
80	cc	34	PHE
80	cc	44	ARG
80	cc	60	GLU
80	cc	61	SER
80	cc	62	GLU
80	cc	63	ARG
80	cc	67	ARG
81	dd	5	GLN
81	dd	6	LEU
81	dd	21	CYS
81	dd	26	ASN
81	dd	27	ARG
81	dd	32	ARG
81	dd	39	CYS
81	dd	56	ASP
82	ee	15	GLN
82	ee	16	THR
82	ee	18	LYS
82	ee	24	LYS
82	ee	26	LYS
82	ee	37	GLN
82	ee	52	LYS
83	ff	81	THR
83	ff	130	HIS
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	44	LYS
84	gg	47	ARG
84	gg	49	GLU
84	gg	59	LEU
84	gg	64	HIS

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Mol	Chain	Res	Type
84	gg	79	LEU
84	gg	87	LEU
84	gg	100	ARG
84	gg	107	ASP
84	gg	115	SER
84	gg	143	GLN
84	gg	156	PHE
84	gg	170	TRP
84	gg	172	LYS
84	gg	186	THR
84	gg	234	ASP
84	gg	289	LEU
84	gg	298	LEU
84	gg	306	LEU
84	gg	309	VAL
86	ii	25	GLU
86	ii	45	ILE
86	ii	54	ASP
86	ii	65	ARG
86	ii	67	ASN
86	ii	68	ARG
86	ii	86	ASN
86	ii	103	GLU
86	ii	111	ASN
86	ii	136	LEU
86	ii	160	THR
86	ii	165	THR
86	ii	167	GLU
86	ii	179	LYS
86	ii	180	HIS
86	ii	182	ARG
86	ii	186	SER
86	ii	211	GLN
86	ii	212	LEU
86	ii	232	PHE
86	ii	241	MET
86	ii	246	LEU
86	ii	255	ASP
86	ii	275	LEU
86	ii	333	LEU
86	ii	339	GLU
86	ii	340	GLU

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Mol	Chain	Res	Type
86	ii	361	GLU
86	ii	368	LEU
86	ii	401	GLN
87	jj	52	GLU
87	jj	75	LEU
87	jj	78	ASN
87	jj	131	LEU
87	jj	153	GLN
87	jj	161	GLU
87	jj	221	GLU
87	jj	236	ASP
87	jj	248	ASP
87	jj	250	LYS
87	jj	271	VAL
87	jj	284	ASP
87	jj	289	LEU
87	jj	399	ASP
87	jj	411	TYR
87	jj	444	ASP
87	jj	455	ILE
87	jj	463	SER
87	jj	551	LEU
87	jj	567	ARG
87	jj	574	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	217	GLN
12	M	131	GLN
80	cc	40	HIS
86	ii	325	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	22 (29%)	1 (1%)
47	3	72/75 (96%)	36 (50%)	13 (18%)
48	5	3645/3662 (99%)	1161 (31%)	270 (7%)
49	7	119/120 (99%)	19 (15%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	8	155/156 (99%)	47 (30%)	6 (3%)
51	9	1710/1719 (99%)	559 (32%)	113 (6%)
85	hh	11/12 (91%)	7 (63%)	0
All	All	5786/5820 (99%)	1851 (31%)	404 (6%)

All (1851) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	5	C
46	2	7	G
46	2	8	U
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G
46	2	20	U
46	2	20(A)	U
46	2	21	A
46	2	31	C
46	2	35	A
46	2	42	A
46	2	47	U
46	2	49	C
46	2	58	A
46	2	60	A
46	2	61	C
46	2	67	G
46	2	72	C
46	2	75	C
46	2	76	A
47	3	4	C
47	3	5	G
47	3	6	G
47	3	7	A
47	3	8	U
47	3	9	A
47	3	10	G
47	3	13	C
47	3	21	A
47	3	22	G
47	3	29	A
47	3	30	G

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Mol	Chain	Res	Type
47	3	31	A
47	3	33	U
47	3	34	U
47	3	35	U
47	3	37	A
47	3	38	A
47	3	39	U
47	3	47	U
47	3	48	C
47	3	49	C
47	3	58	A
47	3	60	U
47	3	63	C
47	3	65	G
47	3	67	U
47	3	68	C
47	3	69	G
47	3	70	G
47	3	71	G
47	3	72	C
47	3	73	G
47	3	74	C
47	3	75	C
47	3	76	A
48	5	2	G
48	5	8	U
48	5	9	C
48	5	10	A
48	5	12	A
48	5	13	U
48	5	20	U
48	5	21	G
48	5	25	A
48	5	30	C
48	5	39	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A

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Mol	Chain	Res	Type
48	5	64	A
48	5	65	A
48	5	67	C
48	5	68	U
48	5	69	A
48	5	71	C
48	5	72	C
48	5	73	A
48	5	74	G
48	5	91	G
48	5	93	G
48	5	94	A
48	5	104	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	116	G
48	5	118	C
48	5	119	G
48	5	120	A
48	5	121	A
48	5	126	C
48	5	128	C
48	5	129	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	146	G
48	5	157	U
48	5	158	A
48	5	159	C
48	5	160	G
48	5	161	G
48	5	164	G
48	5	166	C
48	5	167	C
48	5	170	C
48	5	171	U
48	5	172	C
48	5	173	C

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Mol	Chain	Res	Type
48	5	174	C
48	5	175	C
48	5	177	G
48	5	183	C
48	5	184	U
48	5	185	C
48	5	186	G
48	5	187	U
48	5	188	G
48	5	189	G
48	5	197	A
48	5	200	U
48	5	201	C
48	5	203	U
48	5	205	C
48	5	216	C
48	5	217	C
48	5	218	A
48	5	219	G
48	5	220	C
48	5	221	C
48	5	224	U
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	246	G
48	5	255	C
48	5	257	C
48	5	265	C
48	5	266	C
48	5	267	G
48	5	272	U
48	5	276	C
48	5	277	G
48	5	278	G
48	5	280	G
48	5	296	A
48	5	300	A
48	5	306	A
48	5	309	C
48	5	310	G

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Mol	Chain	Res	Type
48	5	315	G
48	5	316	U
48	5	319	A
48	5	321	U
48	5	322	C
48	5	328	A
48	5	334	A
48	5	337	U
48	5	340	C
48	5	349	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	362	A
48	5	363	A
48	5	379	G
48	5	385	A
48	5	386	A
48	5	387	G
48	5	405	U
48	5	406	C
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	429	A
48	5	431	G
48	5	432	U
48	5	433	A
48	5	434	A
48	5	446	C
48	5	448	G
48	5	449	C
48	5	451	C
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	458	C
48	5	465	G
48	5	467	U

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Mol	Chain	Res	Type
48	5	468	U
48	5	469	C
48	5	470	A
48	5	473	C
48	5	485	C
48	5	486	C
48	5	487	G
48	5	498	C
48	5	499	G
48	5	500	G
48	5	502	C
48	5	503	C
48	5	504	G
48	5	506	C
48	5	509	A
48	5	510	U
48	5	513	U
48	5	514	U
48	5	515	C
48	5	519	C
48	5	649	A
48	5	654	C
48	5	655	C
48	5	663	G
48	5	664	G
48	5	665	C
48	5	666	G
48	5	667	A
48	5	668	C
48	5	669	C
48	5	682	G
48	5	684	G
48	5	685	C
48	5	686	A
48	5	689	U
48	5	690	C
48	5	694	C
48	5	695	G
48	5	696	C
48	5	697	G
48	5	701	G
48	5	703	G

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Mol	Chain	Res	Type
48	5	707	C
48	5	718	C
48	5	721	G
48	5	722	G
48	5	723	A
48	5	724	C
48	5	728	U
48	5	729	G
48	5	730	G
48	5	737	C
48	5	742	G
48	5	745	G
48	5	746	A
48	5	747	A
48	5	748	G
48	5	749	G
48	5	911	U
48	5	914	U
48	5	915	A
48	5	918	G
48	5	919	C
48	5	920	C
48	5	925	C
48	5	927	G
48	5	928	C
48	5	929	A
48	5	930	G
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	935	A
48	5	936	C
48	5	937	U
48	5	938	C
48	5	939	G
48	5	940	C
48	5	942	G
48	5	944	A
48	5	945	U
48	5	946	C
48	5	957	G

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Mol	Chain	Res	Type
48	5	958	G
48	5	960	A
48	5	961	G
48	5	962	C
48	5	963	G
48	5	964	A
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C
48	5	969	C
48	5	970	G
48	5	971	U
48	5	972	C
48	5	973	G
48	5	975	C
48	5	976	G
48	5	977	C
48	5	978	G
48	5	979	C
48	5	982	U
48	5	983	C
48	5	984	C
48	5	989	U
48	5	990	C
48	5	992	C
48	5	1051	G
48	5	1070	G
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1083	U
48	5	1097	C
48	5	1175	A
48	5	1176	C
48	5	1177	U
48	5	1181	C
48	5	1182	C
48	5	1183	C
48	5	1193	C
48	5	1195	G

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Mol	Chain	Res	Type
48	5	1204	C
48	5	1209	U
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1219	G
48	5	1221	G
48	5	1222	A
48	5	1233	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1240	G
48	5	1241	C
48	5	1242	G
48	5	1243	C
48	5	1244	G
48	5	1245	C
48	5	1255	A
48	5	1256	G
48	5	1259	G
48	5	1266	G
48	5	1267	C
48	5	1268	G
48	5	1269	G
48	5	1270	A
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1279	A
48	5	1280	C
48	5	1281	G
48	5	1285	U
48	5	1287	G
48	5	1288	G
48	5	1293	G
48	5	1294	A

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Mol	Chain	Res	Type
48	5	1295	C
48	5	1296	G
48	5	1297	U
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1330	A
48	5	1337	A
48	5	1344	C
48	5	1354	A
48	5	1358	G
48	5	1364	U
48	5	1365	C
48	5	1366	G
48	5	1367	C
48	5	1368	A
48	5	1369	C
48	5	1370	G
48	5	1371	A
48	5	1372	A
48	5	1376	C
48	5	1377	G
48	5	1378	C
48	5	1379	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1390	G
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1399	G
48	5	1407	C
48	5	1408	G
48	5	1409	C
48	5	1410	U
48	5	1411	C
48	5	1413	C
48	5	1414	C
48	5	1416	G

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Mol	Chain	Res	Type
48	5	1418	C
48	5	1420	A
48	5	1429	C
48	5	1432	G
48	5	1435	G
48	5	1436	C
48	5	1439	C
48	5	1440	U
48	5	1441	C
48	5	1442	C
48	5	1445	U
48	5	1446	C
48	5	1448	G
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1472	C
48	5	1475	G
48	5	1477	C
48	5	1478	C
48	5	1481	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1501	C
48	5	1502	G
48	5	1503	A
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1524	A
48	5	1525	A
48	5	1534	A
48	5	1535	C
48	5	1547	A

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Mol	Chain	Res	Type
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1578	U
48	5	1582	U
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1636	U
48	5	1638	A
48	5	1641	G
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1670	G
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1691	G
48	5	1692	C
48	5	1696	C
48	5	1697	G
48	5	1698	C
48	5	1699	A
48	5	1719	A
48	5	1720	C
48	5	1721	G
48	5	1722	C
48	5	1724	G
48	5	1725	U
48	5	1733	G
48	5	1734	G
48	5	1735	U
48	5	1741	G

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Mol	Chain	Res	Type
48	5	1742	A
48	5	1746	A
48	5	1750	G
48	5	1753	G
48	5	1754	U
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1758	G
48	5	1760	G
48	5	1761	G
48	5	1764	G
48	5	1767	A
48	5	1768	C
48	5	1772	C
48	5	1776	A
48	5	1777	C
48	5	1781	U
48	5	1787	A
48	5	1799	G
48	5	1800	U
48	5	1804	A
48	5	1805	A
48	5	1812	C
48	5	1815	G
48	5	1818	G
48	5	1819	G
48	5	1820	C
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1830	G
48	5	1832	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1840	G
48	5	1847	C
48	5	1848	C
48	5	1855	G
48	5	1867	A

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Mol	Chain	Res	Type
48	5	1869	G
48	5	1882	U
48	5	1885	G
48	5	1897	A
48	5	1898	C
48	5	1899	G
48	5	1900	C
48	5	1910	G
48	5	1918	U
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1932	A
48	5	1947	U
48	5	1952	G
48	5	1955	G
48	5	1956	A
48	5	1957	U
48	5	1958	A
48	5	1959	U
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1964	A
48	5	1965	G
48	5	1966	C
48	5	1967	A
48	5	1968	G
48	5	1969	G
48	5	1975	G
48	5	1976	G
48	5	1977	C
48	5	1979	A
48	5	1980	U
48	5	1981	G
48	5	1983	A
48	5	1984	A
48	5	1985	G
48	5	1986	U
48	5	1987	C

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Mol	Chain	Res	Type
48	5	1988	G
48	5	1990	A
48	5	1991	A
48	5	1992	U
48	5	1993	C
48	5	1997	U
48	5	1998	A
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2010	A
48	5	2011	C
48	5	2019	C
48	5	2020	U
48	5	2021	G
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2027	U
48	5	2028	C
48	5	2044	U
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2068	C
48	5	2069	A
48	5	2070	U
48	5	2071	A
48	5	2079	G
48	5	2084	C
48	5	2085	G
48	5	2089	G
48	5	2090	U
48	5	2091	C
48	5	2092	G

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Mol	Chain	Res	Type
48	5	2093	A
48	5	2094	G
48	5	2095	A
48	5	2097	U
48	5	2100	A
48	5	2101	C
48	5	2107	C
48	5	2108	G
48	5	2109	G
48	5	2110	C
48	5	2111	G
48	5	2112	G
48	5	2113	G
48	5	2114	G
48	5	2115	G
48	5	2116	C
48	5	2117	G
48	5	2118	G
48	5	2119	C
48	5	2120	G
48	5	2121	C
48	5	2122	G
48	5	2123	C
48	5	2124	G
48	5	2125	C
48	5	2126	G
48	5	2127	C
48	5	2129	C
48	5	2130	G
48	5	2131	C
48	5	2247	C
48	5	2248	C
48	5	2250	C
48	5	2251	G
48	5	2252	G
48	5	2253	A
48	5	2254	G
48	5	2255	C
48	5	2256	C
48	5	2257	C
48	5	2258	C
48	5	2259	G

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Mol	Chain	Res	Type
48	5	2260	C
48	5	2261	G
48	5	2262	G
48	5	2263	A
48	5	2264	C
48	5	2265	G
48	5	2266	C
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2274	C
48	5	2275	G
48	5	2277	C
48	5	2279	A
48	5	2288	G
48	5	2289	C
48	5	2299	G
48	5	2300	A
48	5	2301	G
48	5	2312	U
48	5	2313	A
48	5	2314	G
48	5	2331	G
48	5	2332	A
48	5	2333	G
48	5	2335	C
48	5	2337	C
48	5	2348	G
48	5	2351	C
48	5	2360	A
48	5	2364	G
48	5	2370	A
48	5	2374	A
48	5	2382	A
48	5	2395	A
48	5	2396	A
48	5	2399	G
48	5	2417	A
48	5	2422	C
48	5	2424	G
48	5	2425	U

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Mol	Chain	Res	Type
48	5	2428	A
48	5	2429	A
48	5	2433	G
48	5	2434	G
48	5	2440	U
48	5	2441	C
48	5	2450	G
48	5	2458	C
48	5	2469	C
48	5	2471	G
48	5	2474	G
48	5	2475	G
48	5	2485	U
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2499	C
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2507	A
48	5	2511	A
48	5	2512	A
48	5	2513	A
48	5	2514	G
48	5	2521	G
48	5	2527	A
48	5	2530	U
48	5	2537	A
48	5	2544	G
48	5	2546	G
48	5	2547	G
48	5	2553	A
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2568	C

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Mol	Chain	Res	Type
48	5	2571	C
48	5	2575	U
48	5	2577	C
48	5	2583	C
48	5	2586	G
48	5	2587	A
48	5	2588	C
48	5	2589	C
48	5	2601	A
48	5	2602	G
48	5	2611	A
48	5	2620	G
48	5	2623	A
48	5	2627	C
48	5	2638	G
48	5	2640	G
48	5	2643	G
48	5	2647	A
48	5	2658	G
48	5	2661	U
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2673	G
48	5	2676	A
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2694	G
48	5	2695	A
48	5	2696	A
48	5	2704	C
48	5	2708	U
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2733	C

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Mol	Chain	Res	Type
48	5	2740	U
48	5	2743	A
48	5	2752	G
48	5	2754	G
48	5	2755	A
48	5	2756	G
48	5	2760	G
48	5	2761	U
48	5	2762	G
48	5	2767	U
48	5	2768	C
48	5	2769	U
48	5	2770	C
48	5	2772	C
48	5	2787	A
48	5	2788	U
48	5	2789	A
48	5	2790	U
48	5	2795	A
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2824	C
48	5	2825	A
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2838	G
48	5	2839	U
48	5	2842	G
48	5	2855	G
48	5	2859	G
48	5	2862	G
48	5	2869	U
48	5	2896	G
48	5	2897	G
48	5	2898	G
48	5	2904	U
48	5	2905	C

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Mol	Chain	Res	Type
48	5	2910	G
48	5	3594	C
48	5	3596	A
48	5	3597	G
48	5	3598	C
48	5	3605	C
48	5	3606	U
48	5	3615	G
48	5	3617	G
48	5	3625	G
48	5	3626	G
48	5	3627	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3659	G
48	5	3662	A
48	5	3668	C
48	5	3671	G
48	5	3673	C
48	5	3674	G
48	5	3680	U
48	5	3681	G
48	5	3682	A
48	5	3692	A
48	5	3696	C
48	5	3698	G
48	5	3710	G
48	5	3711	A
48	5	3712	A
48	5	3715	U
48	5	3716	C
48	5	3717	A
48	5	3718	A
48	5	3722	G
48	5	3728	A
48	5	3729	U
48	5	3732	A
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3752	C

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Mol	Chain	Res	Type
48	5	3753	G
48	5	3756	A
48	5	3759	A
48	5	3760	A
48	5	3764	U
48	5	3769	C
48	5	3773	U
48	5	3774	A
48	5	3775	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3784	A
48	5	3786	U
48	5	3787	G
48	5	3798	U
48	5	3799	A
48	5	3809	G
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3824	A
48	5	3831	U
48	5	3836	A
48	5	3838	U
48	5	3840	U
48	5	3859	G
48	5	3867	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3882	C
48	5	3889	G
48	5	3897	G
48	5	3898	G
48	5	3900	G
48	5	3901	A

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Mol	Chain	Res	Type
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3912	U
48	5	3915	U
48	5	3916	G
48	5	3917	A
48	5	3918	G
48	5	3925	U
48	5	3926	C
48	5	3927	U
48	5	3938	G
48	5	3939	G
48	5	3943	A
48	5	3946	G
48	5	4069	U
48	5	4070	U
48	5	4073	A
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4091	G
48	5	4092	G
48	5	4093	G
48	5	4094	G
48	5	4097	G
48	5	4104	G
48	5	4105	A
48	5	4107	G
48	5	4112	C
48	5	4114	C
48	5	4115	G
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C

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Mol	Chain	Res	Type
48	5	4127	A
48	5	4143	G
48	5	4144	C
48	5	4145	C
48	5	4161	G
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4165	C
48	5	4166	G
48	5	4168	G
48	5	4170	A
48	5	4171	C
48	5	4182	G
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4203	A
48	5	4208	U
48	5	4212	A
48	5	4213	A
48	5	4216	G
48	5	4217	G
48	5	4218	U
48	5	4225	G
48	5	4226	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4235	G
48	5	4238	G
48	5	4239	A
48	5	4241	C
48	5	4251	A
48	5	4254	G
48	5	4267	G
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4276	G
48	5	4291	G
48	5	4297	G

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Mol	Chain	Res	Type
48	5	4302	U
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4311	A
48	5	4313	A
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4329	G
48	5	4330	G
48	5	4331	G
48	5	4332	C
48	5	4336	A
48	5	4337	C
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4360	U
48	5	4367	G
48	5	4372	U
48	5	4376	A
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4394	A
48	5	4395	U
48	5	4398	C
48	5	4405	G
48	5	4419	U
48	5	4420	U
48	5	4421	C
48	5	4422	A
48	5	4424	A
48	5	4426	C
48	5	4433	G
48	5	4438	U
48	5	4439	U

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Mol	Chain	Res	Type
48	5	4441	A
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4464	A
48	5	4471	U
48	5	4472	G
48	5	4473	A
48	5	4475	G
48	5	4476	C
48	5	4481	U
48	5	4482	U
48	5	4488	A
48	5	4491	G
48	5	4495	G
48	5	4500	U
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4522	G
48	5	4524	G
48	5	4527	G
48	5	4528	G
48	5	4529	G
48	5	4530	U
48	5	4535	A
48	5	4548	A
48	5	4549	G
48	5	4550	G
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4577	U
48	5	4583	C
48	5	4584	A

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Mol	Chain	Res	Type
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4591	U
48	5	4599	A
48	5	4601	U
48	5	4606	G
48	5	4618	G
48	5	4627	U
48	5	4635	A
48	5	4636	U
48	5	4637	G
48	5	4641	U
48	5	4647	G
48	5	4648	A
48	5	4656	A
48	5	4657	U
48	5	4661	G
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4687	A
48	5	4694	G
48	5	4695	C
48	5	4698	C
48	5	4700	A
48	5	4701	A
48	5	4702	G
48	5	4709	U
48	5	4712	C
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4730	C
48	5	4731	G
48	5	4732	G
48	5	4733	C
48	5	4734	A
48	5	4737	G
48	5	4741	C
48	5	4745	G
48	5	4746	C

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Mol	Chain	Res	Type
48	5	4749	C
48	5	4750	G
48	5	4753	U
48	5	4756	C
48	5	4758	U
48	5	4760	G
48	5	4764	A
48	5	4768	G
48	5	4770	U
48	5	4771	C
48	5	4774	C
48	5	4869	U
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	U
48	5	4877	G
48	5	4878	C
48	5	4883	C
48	5	4884	G
48	5	4885	U
48	5	4886	C
48	5	4889	G
48	5	4890	G
48	5	4893	A
48	5	4895	C
48	5	4896	G
48	5	4898	G
48	5	4900	C
48	5	4901	G
48	5	4904	G
48	5	4906	C
48	5	4910	G
48	5	4911	A
48	5	4912	G
48	5	4913	G
48	5	4924	C
48	5	4926	C
48	5	4927	G
48	5	4930	C

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Mol	Chain	Res	Type
48	5	4931	G
48	5	4932	U
48	5	4934	A
48	5	4936	G
48	5	4939	C
48	5	4942	C
48	5	4945	G
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4952	G
48	5	4956	A
48	5	4959	U
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4976	U
48	5	4985	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4991	U
48	5	4999	G
48	5	5007	A
48	5	5013	C
48	5	5014	A
48	5	5017	G
48	5	5018	C
48	5	5022	U
48	5	5023	C
48	5	5024	C
48	5	5025	C
48	5	5026	U
48	5	5027	C
48	5	5028	G
48	5	5031	G
48	5	5033	G
48	5	5041	G
48	5	5047	C
48	5	5050	C

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Mol	Chain	Res	Type
48	5	5052	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5058	A
48	5	5060	A
48	5	5061	A
48	5	5062	G
48	5	5066	U
49	7	7	G
49	7	11	A
49	7	21	G
49	7	25	G
49	7	33	U
49	7	40	U
49	7	53	U
49	7	54	A
49	7	64	G
49	7	74	A
49	7	97	G
49	7	99	G
49	7	100	A
49	7	106	G
49	7	109	U
49	7	110	G
49	7	111	C
49	7	116	G
49	7	120	U
50	8	2	G
50	8	3	A
50	8	34	U
50	8	35	C
50	8	38	U
50	8	39	G
50	8	49	G
50	8	51	U
50	8	59	A
50	8	62	A
50	8	63	U
50	8	74	U
50	8	75	G
50	8	79	G

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Mol	Chain	Res	Type
50	8	80	A
50	8	81	C
50	8	82	A
50	8	83	C
50	8	84	A
50	8	85	U
50	8	86	U
50	8	87	G
50	8	94	G
50	8	95	A
50	8	101	C
50	8	103	A
50	8	104	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	113	C
50	8	114	G
50	8	117	C
50	8	121	G
50	8	122	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	150	C
50	8	156	U
51	9	3	C
51	9	4	C
51	9	9	U
51	9	10	G
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C

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Mol	Chain	Res	Type
51	9	41	G
51	9	42	A
51	9	44	U
51	9	45	A
51	9	46	A
51	9	49	C
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	64	A
51	9	65	C
51	9	66	G
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	72	C
51	9	73	C
51	9	74	G
51	9	75	G
51	9	76	U
51	9	77	A
51	9	78	C
51	9	79	A
51	9	80	G
51	9	99	A
51	9	103	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	140	C
51	9	141	A
51	9	142	C
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A

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Mol	Chain	Res	Type
51	9	161	U
51	9	162	C
51	9	163	U
51	9	164	A
51	9	165	G
51	9	167	G
51	9	168	C
51	9	172	U
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	190	G
51	9	191	A
51	9	192	C
51	9	202	G
51	9	206	G
51	9	213	G
51	9	214	U
51	9	216	C
51	9	217	A
51	9	225	G
51	9	289	G
51	9	291	G
51	9	292	A
51	9	293	C
51	9	302	A
51	9	304	C
51	9	305	U
51	9	306	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	310	C
51	9	312	G
51	9	313	A
51	9	314	U
51	9	316	G
51	9	320	G
51	9	322	C
51	9	324	C
51	9	326	C

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Mol	Chain	Res	Type
51	9	327	G
51	9	328	U
51	9	338	G
51	9	339	A
51	9	347	G
51	9	350	C
51	9	351	G
51	9	355	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	369	C
51	9	370	G
51	9	371	A
51	9	377	G
51	9	379	C
51	9	384	U
51	9	385	G
51	9	386	C
51	9	398	A
51	9	400	C
51	9	407	G
51	9	408	A
51	9	409	C
51	9	416	U
51	9	417	C
51	9	418	A
51	9	435	A
51	9	438	G
51	9	441	C
51	9	448	A
51	9	449	A
51	9	450	C
51	9	453	C
51	9	459	C
51	9	460	A
51	9	464	A
51	9	465	A
51	9	466	G
51	9	469	A
51	9	472	C

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Mol	Chain	Res	Type
51	9	473	A
51	9	474	G
51	9	482	G
51	9	487	U
51	9	488	U
51	9	489	A
51	9	492	C
51	9	500	A
51	9	501	C
51	9	503	C
51	9	508	A
51	9	511	U
51	9	512	A
51	9	517	C
51	9	523	A
51	9	525	A
51	9	530	U
51	9	532	C
51	9	533	A
51	9	535	G
51	9	539	C
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	552	G
51	9	554	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	563	G
51	9	568	C
51	9	576	A
51	9	583	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U

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Mol	Chain	Res	Type
51	9	592	C
51	9	593	C
51	9	594	A
51	9	595	U
51	9	603	C
51	9	605	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	614	C
51	9	617	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	631	U
51	9	632	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	654	A
51	9	655	A
51	9	659	G
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	683	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	698	G
51	9	731	G
51	9	735	C
51	9	737	G
51	9	738	C
51	9	747	U
51	9	748	C

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Mol	Chain	Res	Type
51	9	749	U
51	9	752	G
51	9	753	C
51	9	788	G
51	9	789	G
51	9	791	C
51	9	794	A
51	9	796	G
51	9	797	C
51	9	798	G
51	9	799	U
51	9	800	U
51	9	810	A
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	833	C
51	9	834	C
51	9	835	C
51	9	836	G
51	9	837	A
51	9	838	G
51	9	839	C
51	9	840	C
51	9	844	U
51	9	845	G
51	9	847	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	873	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	879	C
51	9	880	G
51	9	887	U
51	9	888	U
51	9	890	U

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Mol	Chain	Res	Type
51	9	892	U
51	9	893	U
51	9	901	G
51	9	902	G
51	9	903	A
51	9	908	A
51	9	910	G
51	9	912	C
51	9	913	A
51	9	914	U
51	9	917	U
51	9	920	A
51	9	921	G
51	9	930	C
51	9	933	G
51	9	934	G
51	9	938	A
51	9	943	U
51	9	944	A
51	9	955	A
51	9	956	G
51	9	971	G
51	9	985	G
51	9	990	A
51	9	992	A
51	9	996	A
51	9	999	G
51	9	1008	A
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1033	G
51	9	1040	G
51	9	1041	G
51	9	1044	G
51	9	1049	A
51	9	1060	A
51	9	1067	C
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1096	G

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Mol	Chain	Res	Type
51	9	1100	A
51	9	1109	C
51	9	1110	G
51	9	1111	U
51	9	1113	A
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1118	C
51	9	1120	U
51	9	1121	G
51	9	1131	G
51	9	1133	A
51	9	1138	C
51	9	1139	C
51	9	1144	A
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1157	G
51	9	1158	G
51	9	1166	G
51	9	1168	G
51	9	1170	A
51	9	1175	G
51	9	1181	A
51	9	1195	A
51	9	1196	A
51	9	1207	G
51	9	1208	A
51	9	1210	G
51	9	1211	G
51	9	1212	G
51	9	1213	C
51	9	1215	C
51	9	1216	C
51	9	1224	G
51	9	1234	C
51	9	1235	G
51	9	1240	A
51	9	1242	U

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Mol	Chain	Res	Type
51	9	1243	U
51	9	1250	A
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1258	A
51	9	1259	A
51	9	1260	A
51	9	1265	A
51	9	1266	C
51	9	1267	C
51	9	1268	C
51	9	1270	G
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1276	A
51	9	1280	G
51	9	1282	A
51	9	1283	C
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1288	U
51	9	1289	U
51	9	1290	G
51	9	1291	A
51	9	1292	C
51	9	1293	A
51	9	1294	G
51	9	1295	A
51	9	1299	A
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1304	U
51	9	1305	C
51	9	1308	U
51	9	1309	C
51	9	1310	U

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Mol	Chain	Res	Type
51	9	1312	G
51	9	1314	U
51	9	1315	U
51	9	1316	C
51	9	1318	G
51	9	1322	G
51	9	1330	G
51	9	1331	C
51	9	1342	U
51	9	1348	G
51	9	1364	U
51	9	1371	U
51	9	1372	U
51	9	1378	A
51	9	1385	G
51	9	1386	A
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1398	G
51	9	1402	A
51	9	1403	C
51	9	1404	U
51	9	1405	A
51	9	1407	U
51	9	1408	U
51	9	1410	C
51	9	1412	C
51	9	1413	G
51	9	1414	A
51	9	1417	C
51	9	1418	C
51	9	1419	C
51	9	1420	G
51	9	1422	G
51	9	1424	G
51	9	1426	U
51	9	1427	C
51	9	1432	U
51	9	1433	C
51	9	1434	C

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Mol	Chain	Res	Type
51	9	1437	C
51	9	1438	A
51	9	1439	A
51	9	1440	C
51	9	1442	U
51	9	1447	G
51	9	1448	A
51	9	1449	G
51	9	1452	A
51	9	1454	A
51	9	1455	A
51	9	1456	G
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1464	C
51	9	1466	G
51	9	1473	G
51	9	1474	A
51	9	1475	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1490	G
51	9	1494	U
51	9	1495	G
51	9	1498	A
51	9	1507	G
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1523	C
51	9	1531	A
51	9	1533	A
51	9	1535	U
51	9	1536	G
51	9	1544	C
51	9	1545	A
51	9	1546	G
51	9	1548	G
51	9	1552	G
51	9	1553	C

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Mol	Chain	Res	Type
51	9	1554	C
51	9	1555	U
51	9	1556	A
51	9	1558	C
51	9	1560	U
51	9	1564	C
51	9	1567	G
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1582	C
51	9	1585	U
51	9	1586	U
51	9	1587	G
51	9	1588	A
51	9	1589	A
51	9	1595	U
51	9	1596	U
51	9	1599	U
51	9	1601	A
51	9	1603	G
51	9	1604	G
51	9	1606	G
51	9	1612	G
51	9	1618	C
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1639	G
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1672	U
51	9	1680	G

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Mol	Chain	Res	Type
51	9	1681	U
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1725	U
51	9	1728	U
51	9	1729	U
51	9	1737	G
51	9	1742	C
51	9	1745	A
51	9	1746	U
51	9	1750	C
51	9	1753	C
51	9	1756	C
51	9	1758	G
51	9	1783	C
51	9	1784	G
51	9	1786	U
51	9	1800	A
51	9	1812	U
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1839	U
51	9	1840	U
51	9	1849	G
51	9	1850	A
51	9	1851	A
51	9	1852	C

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Mol	Chain	Res	Type
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
85	hh	42	C
85	hh	43	A
85	hh	44	A
85	hh	45	A
85	hh	46	G
85	hh	49	U
85	hh	52	G

All (404) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	2	34	A
47	3	4	C
47	3	5	G
47	3	6	G
47	3	7	A
47	3	9	A
47	3	29	A
47	3	30	G
47	3	38	A
47	3	60	U
47	3	67	U
47	3	68	C
47	3	69	G
47	3	74	C
48	5	1	C
48	5	12	A
48	5	20	U
48	5	42	A
48	5	47	A
48	5	48	G
48	5	58	G
48	5	64	A
48	5	72	C
48	5	93	G
48	5	119	G
48	5	120	A
48	5	125	C

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Mol	Chain	Res	Type
48	5	126	C
48	5	134	G
48	5	143	C
48	5	157	U
48	5	159	C
48	5	170	C
48	5	187	U
48	5	200	U
48	5	215	C
48	5	216	C
48	5	218	A
48	5	219	G
48	5	224	U
48	5	226	G
48	5	245	C
48	5	265	C
48	5	266	C
48	5	275	C
48	5	296	A
48	5	308	G
48	5	315	G
48	5	361	C
48	5	385	A
48	5	387	G
48	5	406	C
48	5	409	G
48	5	451	C
48	5	454	U
48	5	486	C
48	5	497	G
48	5	502	C
48	5	505	G
48	5	664	G
48	5	684	G
48	5	693	C
48	5	728	U
48	5	733	A
48	5	746	A
48	5	747	A
48	5	917	A
48	5	930	G
48	5	931	C

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Mol	Chain	Res	Type
48	5	932	A
48	5	935	A
48	5	943	A
48	5	956	A
48	5	957	G
48	5	965	G
48	5	977	C
48	5	978	G
48	5	989	U
48	5	1071	C
48	5	1211	G
48	5	1214	C
48	5	1232	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1241	C
48	5	1266	G
48	5	1268	G
48	5	1272	C
48	5	1279	A
48	5	1280	C
48	5	1292	C
48	5	1296	G
48	5	1329	G
48	5	1357	C
48	5	1365	C
48	5	1368	A
48	5	1370	G
48	5	1371	A
48	5	1376	C
48	5	1379	C
48	5	1380	G
48	5	1390	G
48	5	1398	A
48	5	1407	C
48	5	1410	U
48	5	1419	G
48	5	1420	A
48	5	1435	G
48	5	1440	U

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Mol	Chain	Res	Type
48	5	1445	U
48	5	1455	G
48	5	1474	C
48	5	1477	C
48	5	1481	C
48	5	1485	C
48	5	1502	G
48	5	1523	A
48	5	1533	A
48	5	1563	A
48	5	1601	A
48	5	1625	G
48	5	1633	G
48	5	1654	G
48	5	1678	C
48	5	1696	C
48	5	1697	G
48	5	1724	G
48	5	1733	G
48	5	1746	A
48	5	1755	C
48	5	1756	U
48	5	1804	A
48	5	1818	G
48	5	1819	G
48	5	1835	G
48	5	1891	A
48	5	1921	C
48	5	1956	A
48	5	1957	U
48	5	1958	A
48	5	1961	G
48	5	1964	A
48	5	1965	G
48	5	1966	C
48	5	1967	A
48	5	1968	G
48	5	1974	U
48	5	1975	G
48	5	1986	U
48	5	2009	A
48	5	2019	C

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Mol	Chain	Res	Type
48	5	2028	C
48	5	2046	G
48	5	2068	C
48	5	2083	C
48	5	2084	C
48	5	2088	A
48	5	2089	G
48	5	2093	A
48	5	2107	C
48	5	2110	C
48	5	2116	C
48	5	2119	C
48	5	2123	C
48	5	2125	C
48	5	2246	C
48	5	2251	G
48	5	2253	A
48	5	2256	C
48	5	2257	C
48	5	2260	C
48	5	2262	G
48	5	2263	A
48	5	2265	G
48	5	2266	C
48	5	2269	C
48	5	2278	G
48	5	2313	A
48	5	2370	A
48	5	2396	A
48	5	2398	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2473	A
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	G
48	5	2505	C
48	5	2506	G
48	5	2513	A
48	5	2530	U

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Mol	Chain	Res	Type
48	5	2546	G
48	5	2553	A
48	5	2554	U
48	5	2586	G
48	5	2588	C
48	5	2661	U
48	5	2687	U
48	5	2695	A
48	5	2696	A
48	5	2754	G
48	5	2760	G
48	5	2769	U
48	5	2782	U
48	5	2794	C
48	5	2806	A
48	5	2827	G
48	5	2858	A
48	5	3593	C
48	5	3625	G
48	5	3648	A
48	5	3670	C
48	5	3673	C
48	5	3697	U
48	5	3709	U
48	5	3710	G
48	5	3713	U
48	5	3715	U
48	5	3717	A
48	5	3752	C
48	5	3753	G
48	5	3809	G
48	5	3810	C
48	5	3811	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	4069	U
48	5	4075	U
48	5	4084	G
48	5	4086	G
48	5	4115	G
48	5	4119	C

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Mol	Chain	Res	Type
48	5	4120	U
48	5	4121	G
48	5	4124	G
48	5	4144	C
48	5	4170	A
48	5	4221	C
48	5	4232	U
48	5	4254	G
48	5	4272	G
48	5	4331	G
48	5	4378	A
48	5	4395	U
48	5	4404	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4475	G
48	5	4510	A
48	5	4527	G
48	5	4528	G
48	5	4548	A
48	5	4560	C
48	5	4583	C
48	5	4656	A
48	5	4694	G
48	5	4699	U
48	5	4719	G
48	5	4730	C
48	5	4872	G
48	5	4885	U
48	5	4888	U
48	5	4889	G
48	5	4895	C
48	5	4900	C
48	5	4926	C
48	5	4935	C
48	5	4948	C
48	5	4951	G
48	5	4965	U
48	5	4975	G
48	5	4990	C
48	5	5022	U

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Mol	Chain	Res	Type
48	5	5026	U
48	5	5027	C
48	5	5059	C
48	5	5060	A
48	5	5061	A
49	7	109	U
50	8	2	G
50	8	51	U
50	8	94	G
50	8	110	U
50	8	111	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	72	C
51	9	92	A
51	9	98	C
51	9	102	A
51	9	110	U
51	9	113	G
51	9	139	C
51	9	140	C
51	9	160	U
51	9	164	A
51	9	181	A
51	9	183	G
51	9	215	G
51	9	291	G
51	9	292	A
51	9	304	C
51	9	305	U
51	9	311	C
51	9	312	G
51	9	322	C
51	9	327	G
51	9	369	C
51	9	385	G
51	9	400	C
51	9	407	G
51	9	434	G
51	9	448	A
51	9	464	A

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Mol	Chain	Res	Type
51	9	465	A
51	9	473	A
51	9	488	U
51	9	500	A
51	9	532	C
51	9	550	C
51	9	559	G
51	9	589	G
51	9	594	A
51	9	620	G
51	9	627	U
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U
51	9	746	C
51	9	747	U
51	9	752	G
51	9	797	C
51	9	798	G
51	9	810	A
51	9	833	C
51	9	867	G
51	9	868	G
51	9	869	A
51	9	870	A
51	9	887	U
51	9	912	C
51	9	913	A
51	9	1016	U
51	9	1087	A
51	9	1109	C
51	9	1113	A
51	9	1115	U
51	9	1137	U
51	9	1165	G
51	9	1212	G
51	9	1253	A
51	9	1265	A
51	9	1275	G
51	9	1283	C
51	9	1294	G

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Mol	Chain	Res	Type
51	9	1298	G
51	9	1302	G
51	9	1308	U
51	9	1309	C
51	9	1312	G
51	9	1313	A
51	9	1330	G
51	9	1342	U
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1407	U
51	9	1418	C
51	9	1419	C
51	9	1432	U
51	9	1448	A
51	9	1454	A
51	9	1455	A
51	9	1475	G
51	9	1477	U
51	9	1489	A
51	9	1508	A
51	9	1534	C
51	9	1555	U
51	9	1580	A
51	9	1622	U
51	9	1623	A
51	9	1632	G
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1647	A
51	9	1663	A
51	9	1664	A
51	9	1679	A
51	9	1680	G
51	9	1721	U
51	9	1824	A
51	9	1835	A
51	9	1837	G
51	9	1867	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 207 ligands modelled in this entry, 203 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
90	SF4	jj	600	87	0,12,12	0.00	-	0,24,24	0.00	-
90	SF4	jj	601	87	0,12,12	0.00	-	0,24,24	0.00	-
91	ADP	jj	602	-	24,29,29	1.07	1 (4%)	23,45,45	1.93	1 (4%)
91	ADP	jj	603	-	24,29,29	1.08	2 (8%)	23,45,45	1.90	1 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	SF4	jj	600	87	-	0/0/48/48	0/6/5/5
90	SF4	jj	601	87	-	0/0/48/48	0/6/5/5
91	ADP	jj	602	-	-	0/12/32/32	0/3/3/3
91	ADP	jj	603	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	603	ADP	C2-N3	2.02	1.35	1.32
91	jj	603	ADP	C5-C4	3.28	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	602	ADP	C5-C4	3.31	1.48	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	jj	602	ADP	N3-C2-N1	-7.77	122.77	128.87
91	jj	603	ADP	N3-C2-N1	-7.64	122.87	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.