



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 12:39 pm GMT

PDB ID : 3JAH
EMDB ID: : EMD-3039
Title : Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UAG stop codon
Authors : Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.
Deposited on : 2015-06-10
Resolution : 3.45 Å(reported)
Based on PDB ID : 1DT9, 4V51, 3J7P, 3J92, 3BK7

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

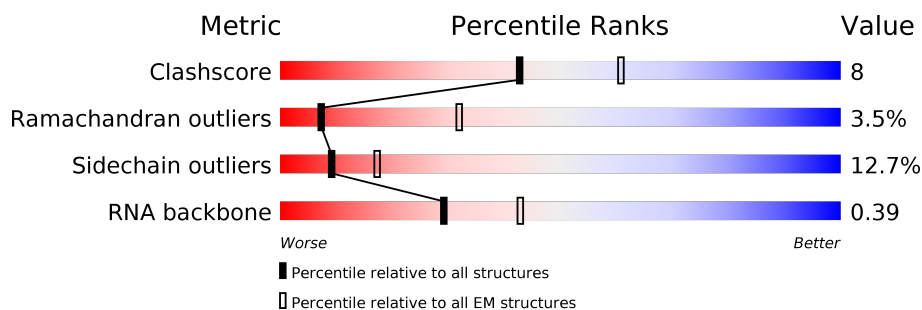
MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

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 3.45 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	76% 18% 5%
2	B	394	76% 21% .
3	C	362	71% 26% .
4	D	292	79% 18% .
5	E	248	65% 25% 5% 5%
6	F	225	76% 20% . .
7	G	241	78% 22% .
8	H	190	81% 17% .














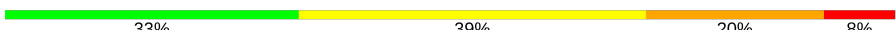











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Mol	Chain	Length	Quality of chain
9	I	213	
10	J	169	
11	L	210	
12	M	138	
13	N	203	
14	O	199	
15	P	153	
16	Q	187	
17	R	180	
18	S	175	
19	T	159	
20	U	99	
21	V	131	
22	W	63	
23	X	119	
24	Y	134	
25	Z	135	
26	a	147	
27	b	75	
28	c	94	
29	d	107	
30	e	128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


























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Mol	Chain	Length	Quality of chain
34	i	102	
35	j	86	
36	k	69	
37	l	50	
38	m	52	
39	n	23	
40	o	104	
41	p	91	
42	r	125	
43	s	198	
44	t	163	
45	1	15	
46	2	76	
47	3	75	
48	5	3662	
49	7	120	
50	8	156	
51	9	1719	
52	AA	208	
53	BB	213	
54	CC	218	
55	DD	227	
56	EE	262	
57	FF	191	
58	GG	237	





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Mol	Chain	Length	Quality of chain
59	HH	189	 71% 24% 5%
60	II	206	 69% 30% .
61	JJ	185	 75% 18% 6% .
62	KK	98	 71% 27% .
63	LL	152	 70% 24% . .
64	MM	124	 75% 24% .
65	NN	150	 76% 22% .
66	OO	136	 67% 23% 7% .
67	PP	127	 75% 21% .
68	QQ	141	 77% 20% .
69	RR	129	 78% 19% .
70	SS	137	 74% 20% . .
71	TT	141	 79% 16% 5% .
72	UU	104	 75% 22% . .
73	VV	83	 73% 24% .
74	WW	129	 65% 29% 5% .
75	XX	141	 72% 23% 5%
76	YY	126	 73% 22% 5%
77	ZZ	75	 77% 23%
78	aa	98	 81% 19%
79	bb	83	 80% 20%
80	cc	61	 80% 20%
81	dd	53	 81% 19%
82	ee	57	 82% 16% .
83	ff	68	 87% . 9%

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Mol	Chain	Length	Quality of chain
84	gg	313	 90% 9%
85	hh	12	 42% 58%
86	ii	416	 89% 10%
87	jj	594	 91% 5% •

2 Entry composition [i](#)

There are 91 unique types of molecules in this entry. The entry contains 226454 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
			2884	1814	578	478	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	LYS	-	EXPRESSION TAG	UNP G1SVW5
C	363	SER	-	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	776	241	216	9		

- Molecule 16 is a protein called uL14.

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
			1692	1102	287	296	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CC	194	ARG	HIS	CONFLICT	UNP G1TUT9
CC	228	GLY	SER	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	62	Total	C	N	O	S	0	0
			520	331	98	85	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ff	?	-	VAL	DELETION	UNP G1SK22

- 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
			257	115	46	84	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	576	Total	C	N	O	S	0	0
			4543	2904	779	829	31		

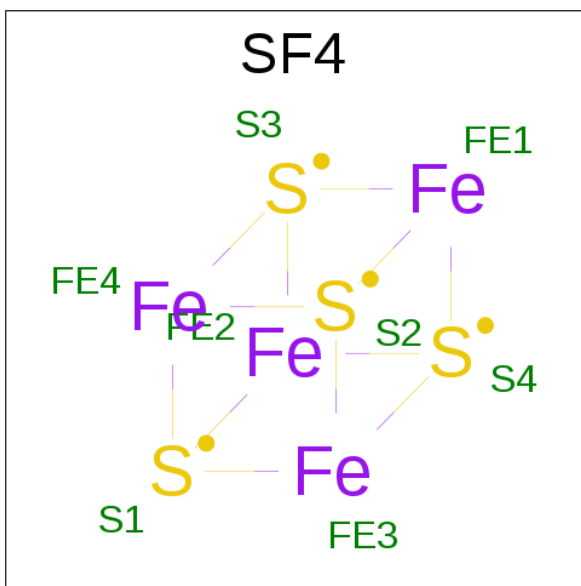
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	P	1	Total 1	Mg 1	0
88	g	1	Total 1	Mg 1	0
88	LL	1	Total 1	Mg 1	0
88	B	1	Total 1	Mg 1	0
88	I	1	Total 1	Mg 1	0
88	C	1	Total 1	Mg 1	0
88	V	1	Total 1	Mg 1	0
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	34	Total 34	Mg 34	0
88	hh	1	Total 1	Mg 1	0

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

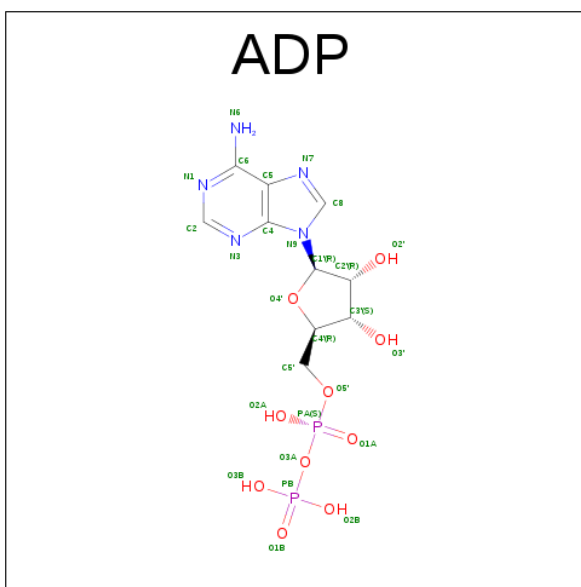
Mol	Chain	Residues	Atoms		AltConf
89	p	1	Total 1	Zn 1	0
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 91 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

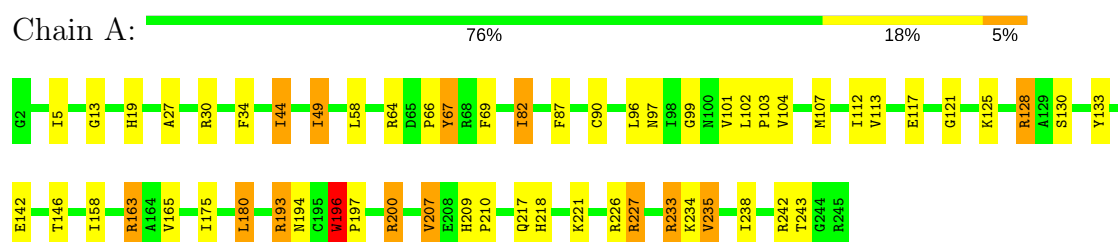


Mol	Chain	Residues	Atoms					AltConf
91	jj	1	Total	C	N	O	P	0
			54	20	10	20	4	
91	jj	1	Total	C	N	O	P	0
			54	20	10	20	4	

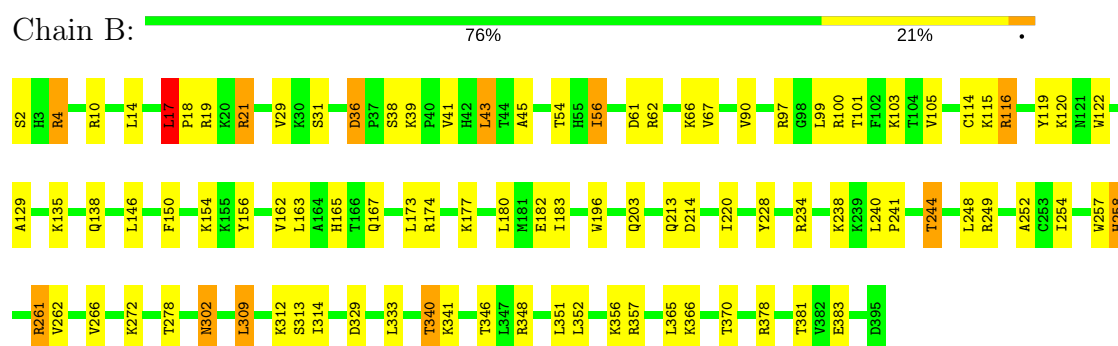
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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



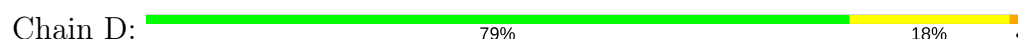
• Molecule 2: uL3

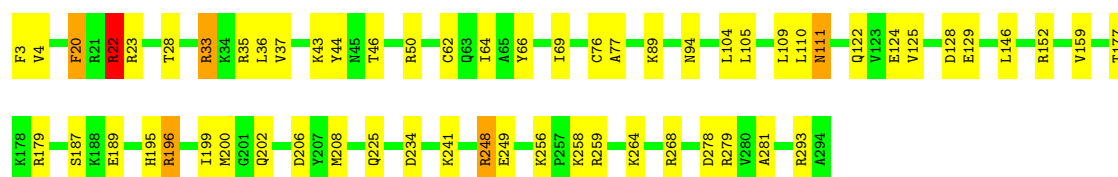


• Molecule 3: uL4

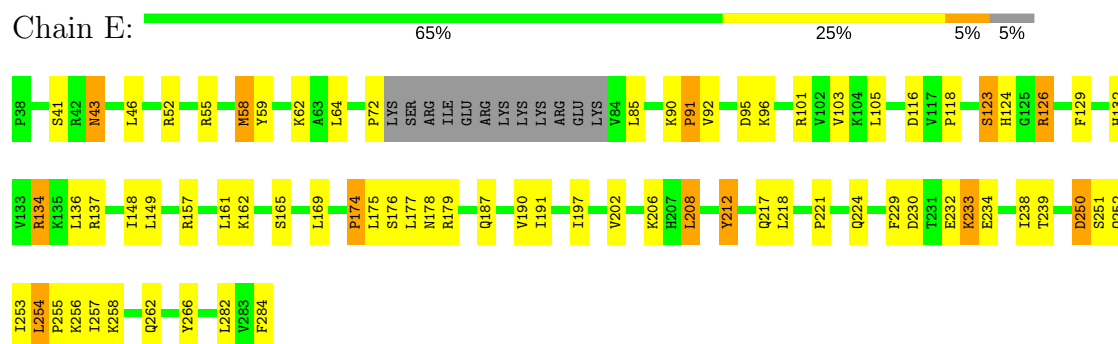


• Molecule 4: uL18

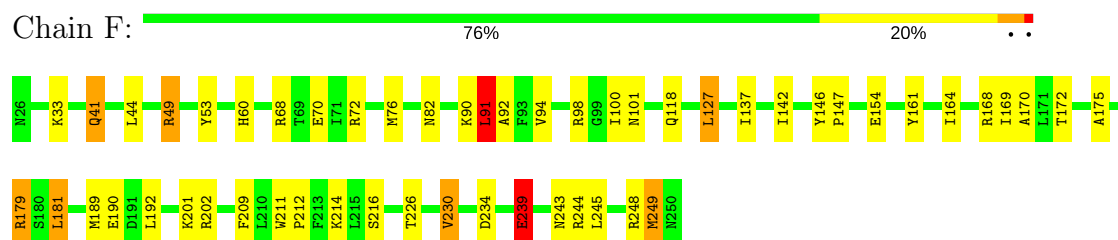




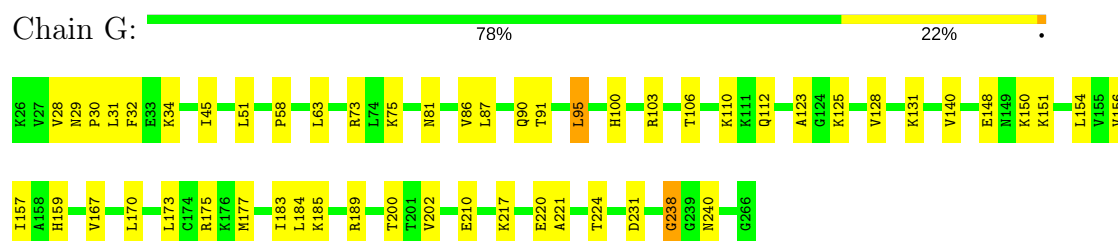
• Molecule 5: eL6



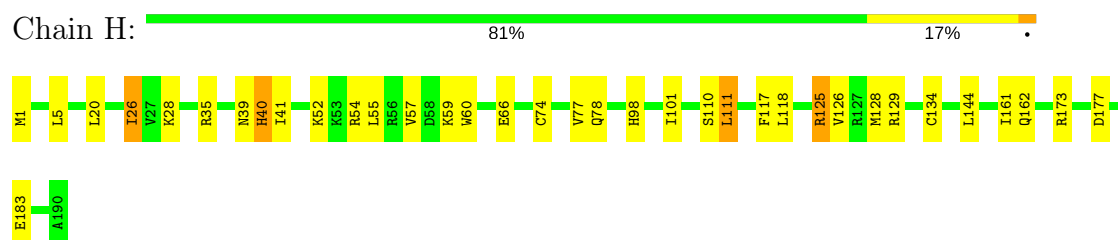
• Molecule 6: uL30



• Molecule 7: eL8

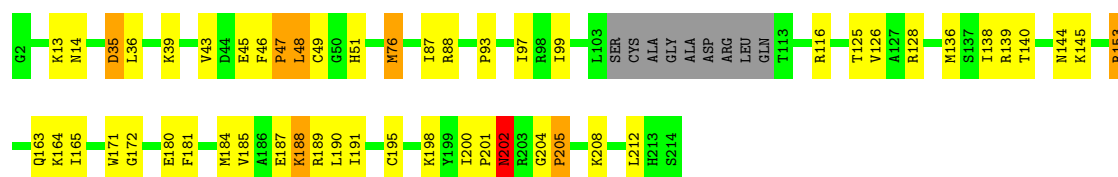


• Molecule 8: uL6



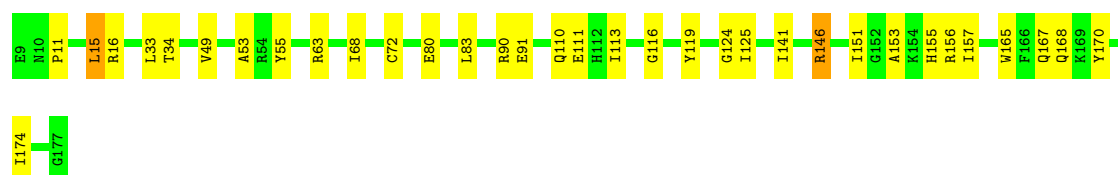
• Molecule 9: uL16





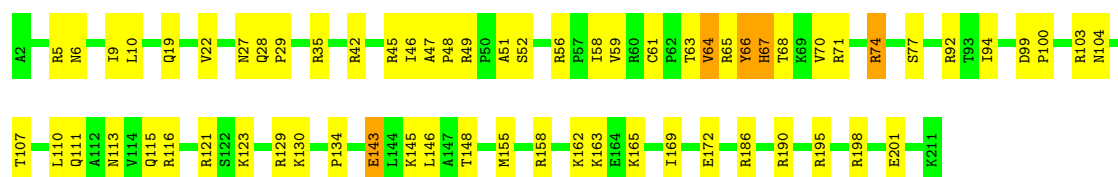
• Molecule 10: uL5

Chain J: 80% 19%



• Molecule 11: eL13

Chain L: 69% 29%



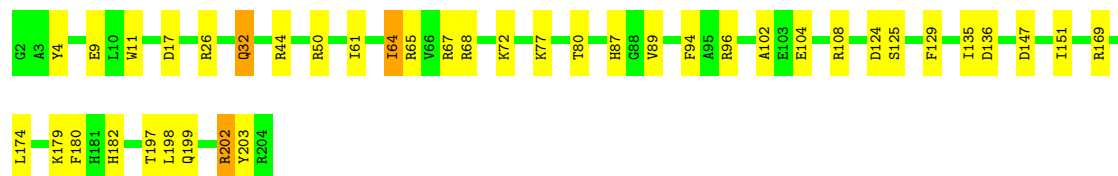
• Molecule 12: eL14

Chain M: 79% 20%



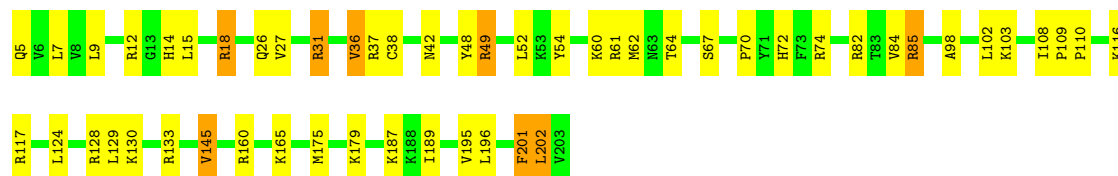
• Molecule 13: eL15

Chain N: 80% 18%




• Molecule 14: uL13

Chain O: 73% 23%




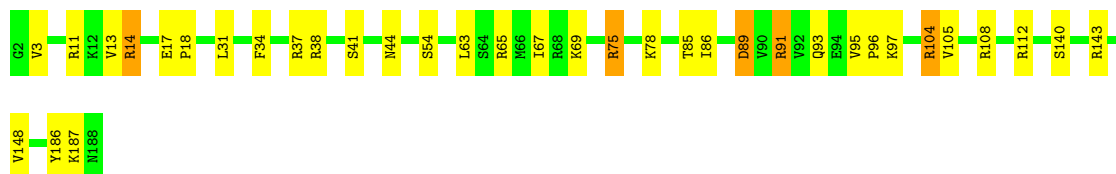
- Molecule 15: uL22

Chain P:  84% 14%



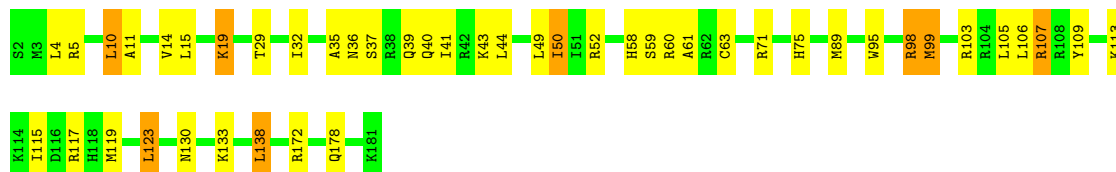
- Molecule 16: uL14

Chain Q:  81% 17%




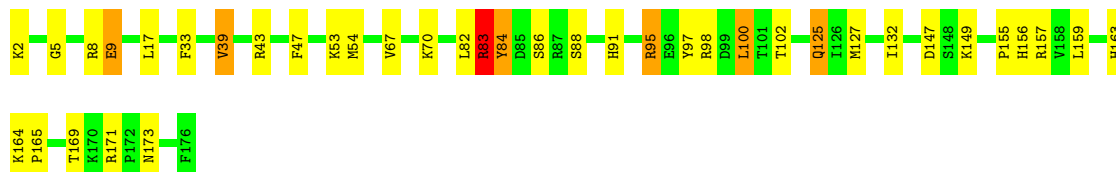
- Molecule 17: eL19

Chain R:  74% 21%




- Molecule 18: eL20

Chain S:  78% 18%




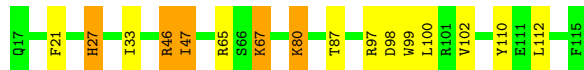
- Molecule 19: eL21

Chain T:  80% 19%




- Molecule 20: eL22

Chain U:  84% 11% 5%




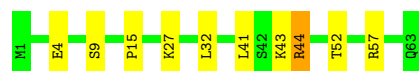
- Molecule 21: uL14

Chain V:  81% 18%




- Molecule 22: eL24

Chain W:  84% 14%




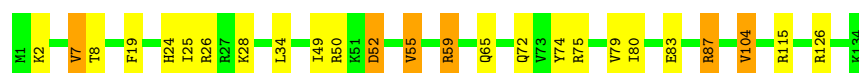
- Molecule 23: uL23

Chain X:  82% 16%



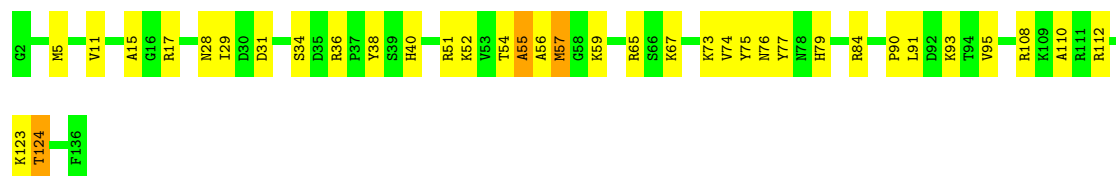
- Molecule 24: uL24

Chain Y:  81% 14%




- Molecule 25: eL27

Chain Z:  73% 24%



- Molecule 26: uL15

Chain a:  89% 11%




- Molecule 27: eL29

Chain b:  92% 8%




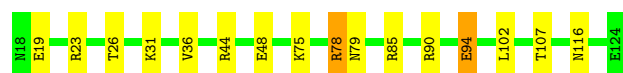
- Molecule 28: eL30

Chain c:  86% 14%




- Molecule 29: eL31

Chain d:  85% 13%




- Molecule 30: eL32

Chain e:  84% 16%




- Molecule 31: eL33

Chain f:  83% 17%




- Molecule 32: eL34

Chain g:  86% 13%



- Molecule 33: uL29

Chain h:  88% 11%




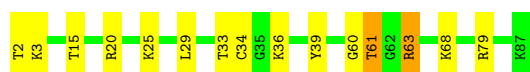
- Molecule 34: eL36

Chain i:  91% 9%

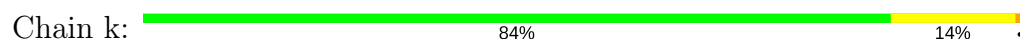


- Molecule 35: eL37

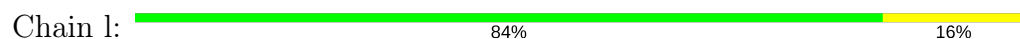
Chain j:  83% 15%



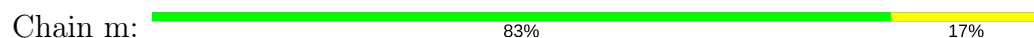
• Molecule 36: eL38



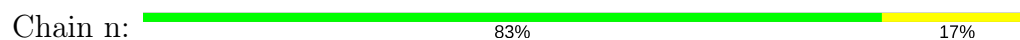
• Molecule 37: eL39



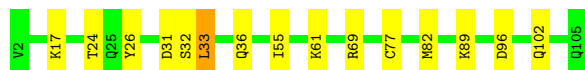
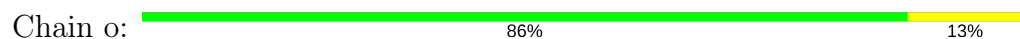
• Molecule 38: eL40



• Molecule 39: eL41



• Molecule 40: eL42



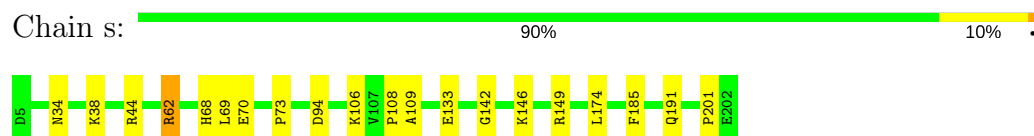
• Molecule 41: eL43



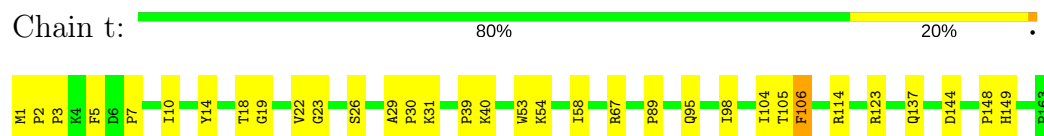
• Molecule 42: eL28



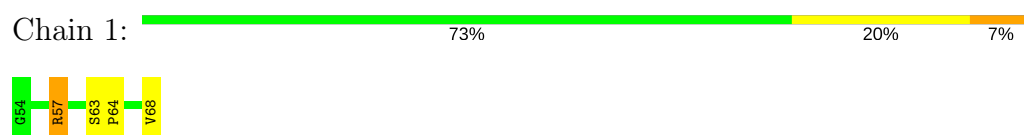
• Molecule 43: uL10



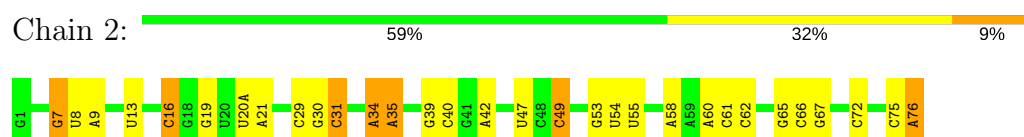
- Molecule 44: uL11



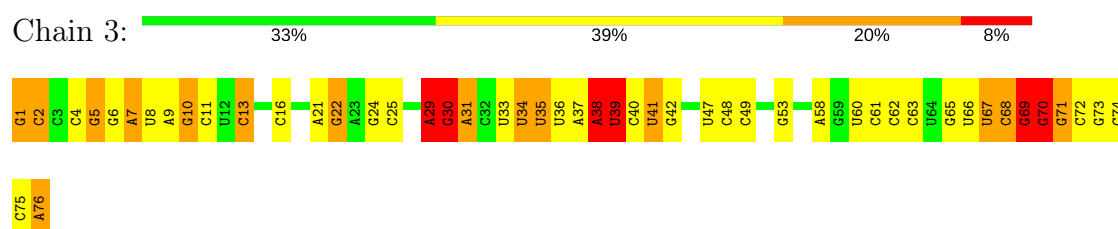
- Molecule 45: peptide



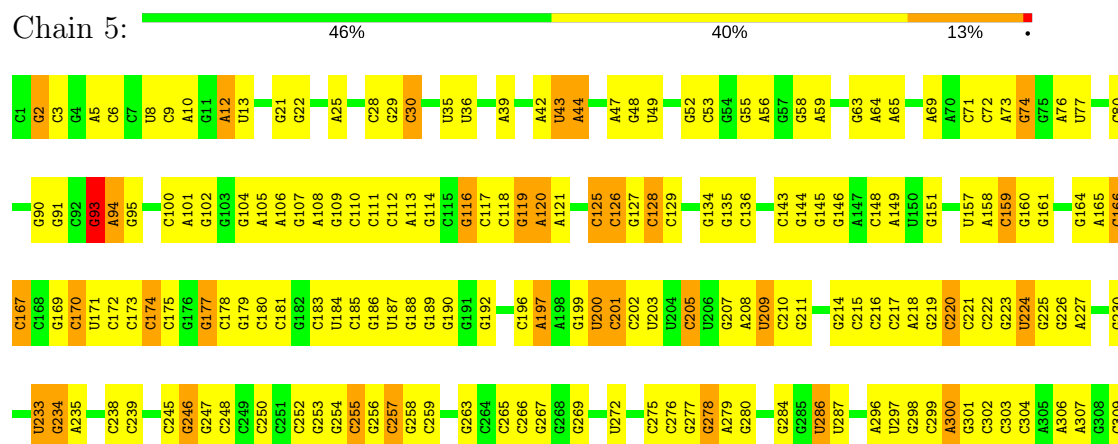
- Molecule 46: tRNA(Val)



- Molecule 47: tRNA(Lys)

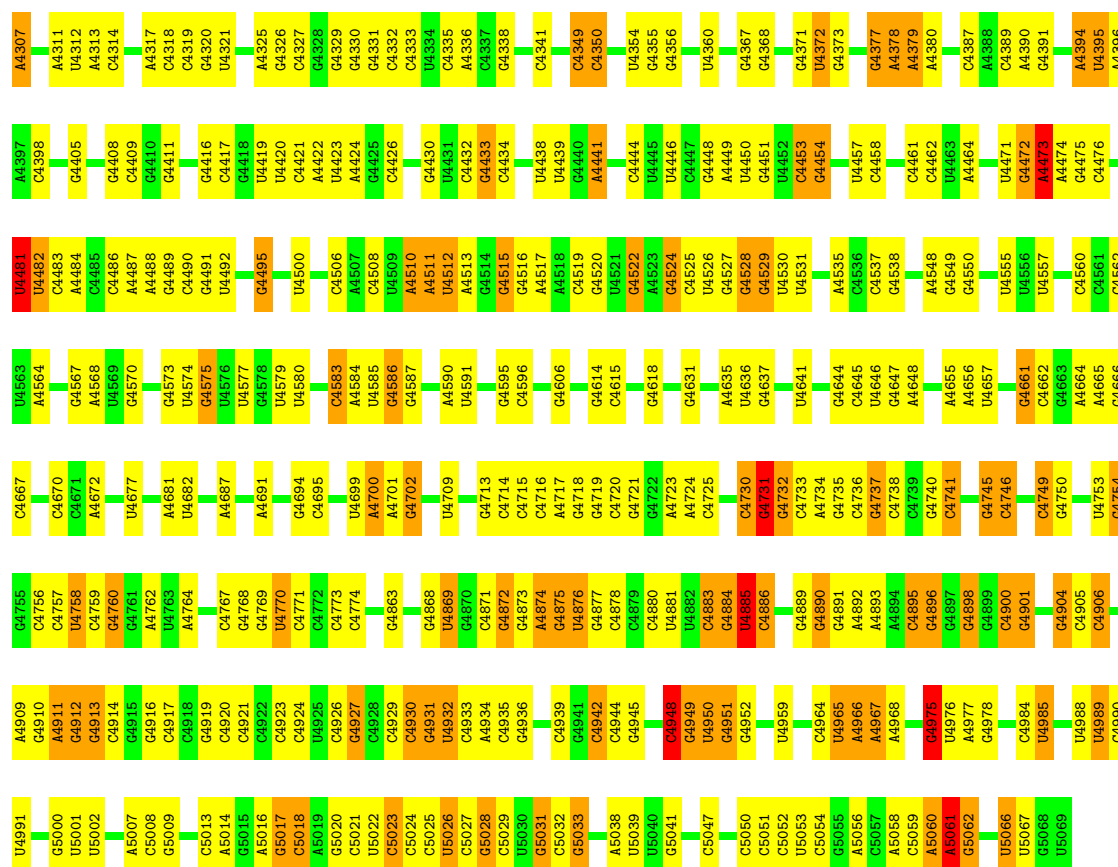


- Molecule 48: 28S ribosomal RNA

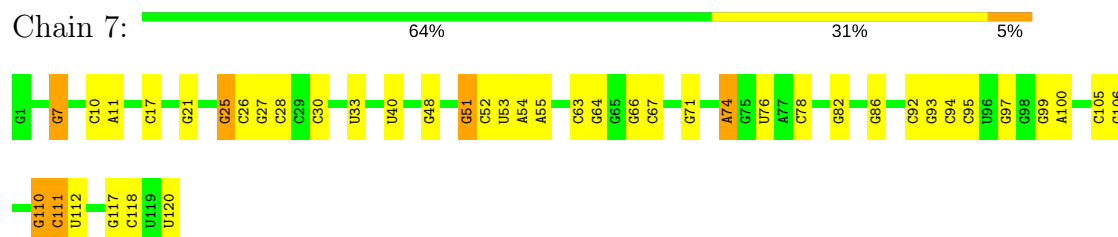




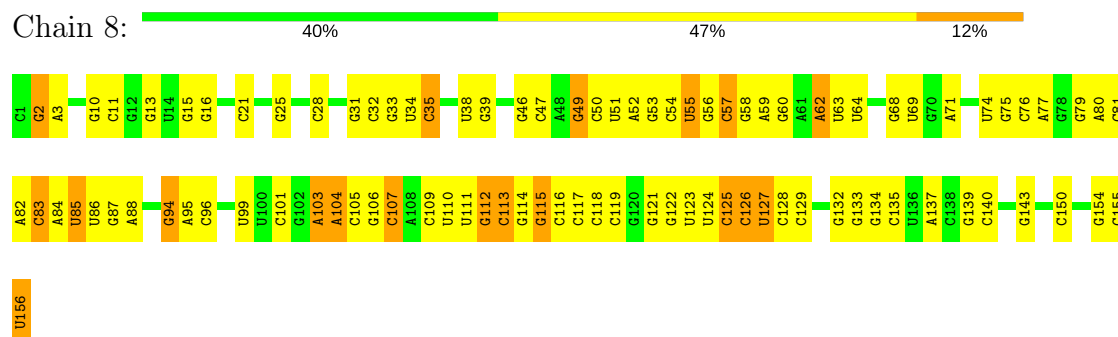

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G4226	G4143		G3777	U3697	C3605	U2827	C2733	C2654	G2568	G2495	U2408	G2297	G2116	U2048
U4229	G4144		G3778	G3698	U3606	U2828	U2734	U2661	G2569	G2496	U2409	G2298	G2117	G2049
U4232	G4145		A3779		G3606	G2830	U2740	U2662	G2571	C2498	A2417	A2300	G2118	G2050
A4233	G4146		G3780	A3702	A3610	G2831	U2740	G2663	C2572	C2499		G2301	G2119	C2051
	G4147		G3781		A3611		A2743	G2664	U2575	G2503	C2422	C2302	G2120	G2052
	C4148		C3782	G3705	C3612	A2835	A2744	C2669	G2576	C2504	G2423	C2311	G2121	G2053
G4238	G4152		A3783	G3706	G3615	G2838	G2752	C2670	G2577	C2505	G2424	G2312	G2122	U2054
A4239	G4153		A3784	U3707	G3616	U2839	G2753	G2671	C2578	G2506	G2425	G2313	G2123	G2055
G4240	G4154		U3786	G3708	G3617	G2842	G2754	G2672	G2589	G2507	U2426	G2314	G2124	G2056
C4241	C4155		G3787	G3710	C3618	G2843	G2755	G2673	C2583		A2428	G2315	G2125	A2057
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G4246	C4158		U3798	G3712	G3621	A2845	G2757	A2676	G2587	A2512		G2322	G2127	C2062
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C4258	C4165		A3724	G3725	U3641	U2869	G2769	G2689	G2606	U2525		G2331	G2249	A2070
C4259	G4166		G3726	G3727	A3642	A2870	G2770	G2690	G2607	G2526		G2332	G2250	A2071
U4260	G4167		A3727	A3728	U3644	G2871	G2771	G2691	G2608	A2527		G2333	G2251	G2072
C4261	G4168		G3728	A3729	U3645	G2872	G2772	G2692	G2609			G2334	G2252	G2073
C4262	G4169		U3729	G3730	A3646	G2873	G2773	G2693	G2610			G2335	G2253	G2074
C4263	A4170		U3730	A3731	A3653	G2874	G2774	G2694	G2611			G2336	G2254	G2075
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G4266	G4173		G3736	G3736	G3659	G2877	G2777	G2697	G2614			G2339	G2257	G2078
G4267	U4181		U3822	A3737	U3660	G2878	G2778	G2703	G2615			G2340	G2258	G2079
G4268	G4182		U3831	G3738	A3662	G2879	G2779	G2704	G2616			G2341	G2259	
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C4270	G4184		C3833	G3740	G3664	G2881	G2781	C2709	G2618			G2343	G2261	C2084
A4271	U4187		C3834	G3741	G3665	G2882	G2782	G2710	G2619			G2344	G2262	C2085
G4272	G4188		G3835	G3742	G3666	G2883	G2783	G2711	G2620			G2345	G2263	A2088
A4273			U3836	G3743	U3667	G2884	G2784	G2712	G2621			G2346	G2264	U2089
G4274	G4191		G3837	G3744	U3668	G2885	G2785	G2713	G2622			G2347	G2265	U2090
G4275			U3838	G3745	U3669	G2886	G2786	G2714	G2623			G2348	G2266	C2091
G4276	G4201		G3839	G3746	G3670	G2887	G2787	G2715	G2624			G2349	G2267	G2092
G4277	U4202		U3840	G3747	G3671	G2888	G2788	G2716	G2625			G2350	G2268	A2093
A4278	A4203		G3841	G3748	G3672	G2889	G2789	G2717	G2626			G2351	G2269	G2094
			C3842	G3749	G3673	G2890	G2790	G2718	G2627			G2352	G2270	A2095
A4280	C4207		A3843	G3750	G3674	G2891	G2791	G2719	G2628			G2353	G2271	G2096
A4281	U4208		G3844	G3751	G3675	G2892	G2792	G2720	G2629			G2354	G2272	U2097
A4282	G4209		U3845	G3752	G3676	G2893	G2793	G2721				G2355	G2273	A2100
G4283	U4210		A3846	G3753	G3677	G2894	G2794	G2722				G2356	G2274	G2101
C4284	C4211		C3847	G3754	G3678	G2895	G2795	G2723				G2357	G2275	G2102
	A4212		C3848	G3755	G3679	G2896	G2796	G2724				G2358	G2276	G2103
	G4213		C3849	G3756	G3680	G2897	G2797	G2725				G2359	G2277	
			C3850	G3757	U3681	G2898	G2798	G2726				G2360	G2278	C2107
G4291	G4216		C3851	G3758	U3682	G2899	G2799	G2727				G2361	G2279	C2108
	C4217		U3852	G3759	A3682	G2900	G2800	G2728				G2362	G2280	G2109
G4297	G4218		A3853	G3760	G3683	G2901	A2801	G2729				G2363	G2281	C2110
U4301	U4219		G3854	G3761	G3684	G2902	C2814	G2730				G2364	G2282	G2111
U4302	A4219		U4070	G3762	G3685	G2903	G2815	G2731				G2365	G2283	G2112
C4303	C4220		C4072	G3763	G3686	G2904	G2816	G2732				G2366	G2284	G2113
A4304	G4222		A4073	G3764	G3687	G2905	G2817	G2733				G2367	G2285	
			C3868	G3765	G3688	G2906	G2818	G2734				G2368	G2286	
U4306	C4223		C3870	G3766	G3689	G2907	C2819	G2735				G2369	G2287	
				G3767	G3690	G2908	G2820	G2736				G2370	G2288	
				G3768	G3691	G2909	A2821	G2737				G2371	G2289	
				G3769	G3692	G2910	G2822	G2738				G2372	G2290	
				G3770	G3693	G2911	G2823	G2739				G2373	G2291	
				G3771	G3694	G2912	G2824	G2740				G2374	G2292	
				G3772	G3695	G2913	G2825	G2741				G2375	G2293	
				G3773	G3696	G2914	G2826	G2742				G2376	G2294	
				G3774	G3697	G2915	G2827	G2743				G2377	G2295	
				G3775	G3698	G2916	G2828	G2744				G2378	G2296	
				G3776	G3699	G2917	G2829	G2745				G2379	G2297	
				G3777	G3700	G2918	G2830	G2746				G2380	G2298	
				G3778	G3701	G2919	G2831	G2747				G2381	G2299	
				G3779	G3702	G2920	G2832	G2748				G2382	G2300	
				G3780	G3703	G2921	G2833	G2749				G2383	G2301	
				G3781	G3704	G2922	G2834	G2750				G2384	G2302	
				G3782	G3705	G2923	G2835	G2751				G2385	G2303	
				G3783	G3706	G2924	G2836	G2752				G2386	G2304	
				G3784	G3707	G2925	G2837	G2753				G2387	G2305	
				G3785	G3708	G2926	G2838	G2754				G2388	G2306	
				G3786	G3709	G2927	G2839	G2755				G2389	G2307	
				G3787	G3710	G2928	G2840	G2756				G2390	G2308	
				G3788	G3711	G2929	G2841	G2757				G2391	G2309	
				G3789	G3712	G2930	G2842	G2758				G2392	G2310	
				G3790	G3713	G2931	G2843	G2759				G2393	G2311	
				G3791	G3714	G2932	G2844	G2760				G2394	G2312	
				G3792	G3715	G2933	G2845	G2761				G2395	G2313	
				G3793	G3716	G2934	G2846	G2762				G2396	G2314	
				G3794	G3717	G2935	G2847	G2763				G2397	G2315	
				G3795	G3718	G2936	G2848	G2764				G2398	G2316	
				G3796	G3719	G2937	G2849	G2765				G2399	G2317	
				G3797	G3720	G2938	G2850	G2766				G2400	G2318	
				G3798	G3721	G2939	G2851	G2767				G2401	G2319	
				G3799	G3722	G2940	G2852	G2768				G2402	G2320	
				G3800	G3723	G2941	G2853	G2769				G2403	G2321	
				G3801	G3724	G2942	G2854	G2770				G2404	G2322	
				G3802	G3725	G2943	G2855	G2771				G2405	G2323	
				G3803	G3726	G2944	G2856	G2772				G2406	G2324	
				G3804	G3727	G2945	G2857	G2773				G2407	G2325	
				G3805	G3728	G2946	G2858	G2774				G2408	G2326	
				G3806	G3729	G2947	G2859	G2775				G2409	G2327	
				G3807	G3730	G2948	G2860	G2776				G2410	G2328	
				G3808	G3731	G2949	G2861	G2777				G2411	G2329	
				G3809	G3732	G2950	G2862	G2778				G2412	G2330	
				G3810	G3733	G2951	G2863	G2779				G2413	G2331	
				G3811	G3734	G2952	G2864	G2780				G2414	G2332	
				G3812	G3735	G2953	G2865	G2781				G2415	G2333	
				G3813	G3736	G2954	G2866	G2782				G2416	G2334	
				G3814	G3737	G2955	G2867	G2783				G2417	G2335	
				G3815	G3738	G2956								



- Molecule 49: 5S ribosomal RNA



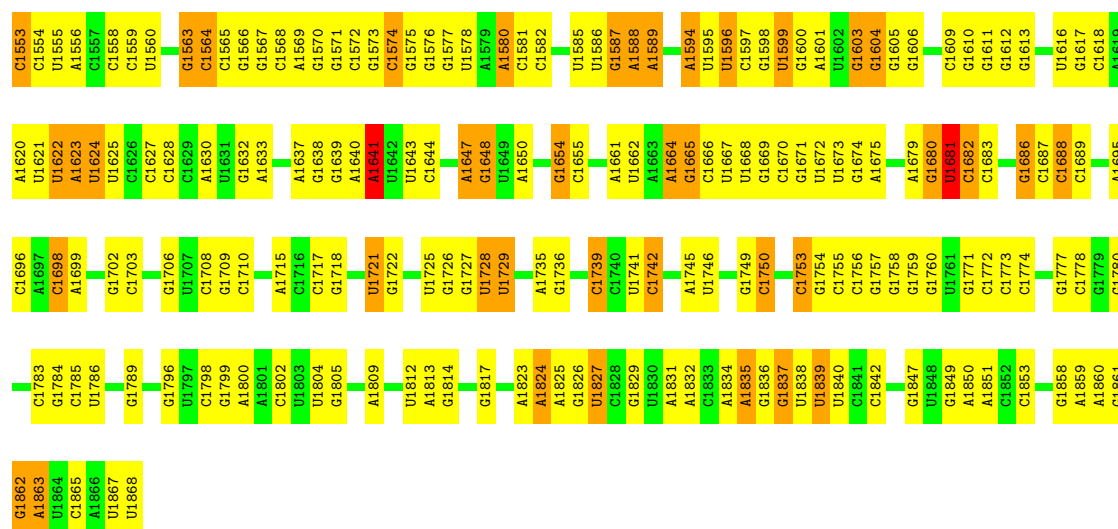
- Molecule 50: 5.8S ribosomal RNA



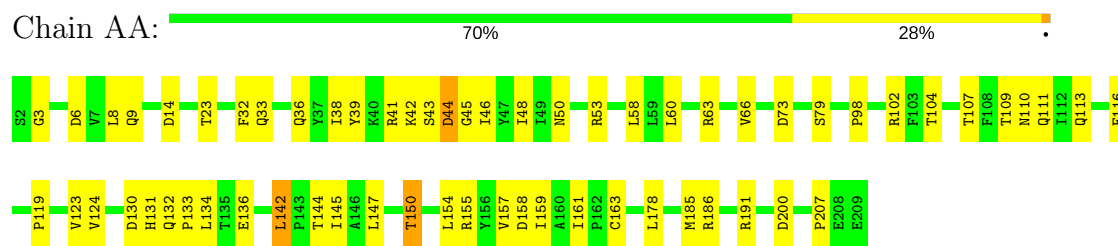
- Molecule 51: 18S ribosomal RNA



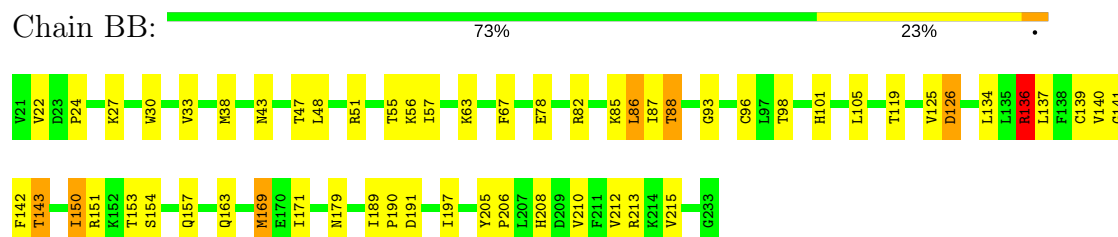
U1485	G1330	G1256	G1181	G1098	G971	G878	C790	U637	A555	G380	A301	U157	G70	U1
A1486	C1331	G1257	A1181	G1099	G978	C879	C791	G638	U556	G383	A302	A158	G71	A2
A1487	U1332	A1258	G1184	A1100	G980	G880	C792	C639	U557	U384	C303	A159	C72	C3
A1488	U1333	A1259	C1185	U1101	G979	G881	C793	A640	G558	G385	U305	U161	C73	C4
A1489	G1334	A1260	C1186	C1102	A980	U887	A794	A641	G559	C386	U306	U162	G74	U5
A1490	G1335	A1261	A1189	G1103	A981	U888	A795	A642	A560	C387	C307	U163	G75	G6
G1491	C1336	C1262	A1190	C1104	G982	U889	C796	A643	A561	C391	G308	U164	U76	U9
U1492	G1337	C1263	A1191	G1105	G983	U890	C797	G644	U562	C392	G309	U165	A77	G10
C1493	U1342	C1264	A1192	C1106	G984	U891	C798	A654	U563	A398	C310	A166	C78	A11
U1494	G1343	C1265	A1193	U1110	A990	U892	U799	U658	G564	C400	C311	C168	A79	A12
G1495	U1344	G1270	A1194	U1111	A991	U893	U800	C659	C568	U401	G312	U172	G80	G14
U1496	G1345	C1271	G1198	U1112	A992	G901	A810	C660	A576	G405	A313	A173	C86	U15
C1497	U1346	C1272	G1207	U1113	G993	G902	A811	C661	U577	U406	U314	C178	U87	G16
A1498	U1347	G1274	A1207	U1114	G994	A903	A812	C662	C578	U407	C315	G180	G88	C17
U1499	G1348	A1275	A1208	U1115	G995	G904	U821	C663	C579	U408	C316	A181	C89	C18
G1500	U1349	A1276	A1209	U1116	A996	U905	U822	C664	A583	C409	C317	U182	A92	A19
U1501	G1351	C1273	G1210	U1117	A997	G906	U823	U665	U584	G412	G320	G183	U93	G23
G1502	U1352	C1274	G1211	U1118	A998	G907	U824	U666	A585	U413	C321	G184	U94	G24
U1503	G1354	C1275	G1212	U1119	A999	G908	U825	U667	A586	U414	C322	G185	U95	A25
C1504	U1355	C1276	G1213	U1120	G1000	G909	U826	C668	U587	U415	C323	G186	U96	U26
U1505	G1356	C1277	C1214	U1121	U1002	U914	G828	C669	G589	U416	C324	G187	C96	
G1516	U1371	G1285	C1215	U1122	U1003	U915	G829	A671	U591	U417	C325	U188	A99	G29
U1517	U1372	G1286	C1216	U1123	G1007	A916	A830	A672	C592	U418	C326	U189	U100	C30
G1518	C1373	A1287	C1217	U1124	A1008	U917	C831	C673	C593	U419	C327	G190	U101	U31
U1519	U1374	U1288	C1218	U1125	A1009	U918	G832	C674	U594	U420	U328	A191	A102	U32
G1520	G1375	U1289	C1219	U1126	U1010	A919	C833	C675	U595	U421	U329	C192	A103	G33
C1521	U1376	U1290	C1220	U1127	U1011	U920	C834	U678	U596	U422	G338	C193	A104	U34
U1522	U1377	G1291	C1221	U1128	U1012	G921	C835	U679	U597	U423	A339	C194	U107	C37
G1523	G1378	A1292	C1222	U1129	U1013	A922	G836	G684	G598	U424	C340	C195	G108	
U1524	U1379	C1293	G1223	U1130	A1023	U923	A837	G685	U599	U425	C341	G200	U109	G41
C1525	G1380	C1294	G1224	U1131	G1033	C930	G838	U686	G600	U426	A343	C201	U110	A42
U1526	U1381	A1295	G1225	U1132	U1034	G933	C940	C687	C603	U427	G347	G202	A111	U43
G1527	G1382	C1296	C1226	U1133	G1035	U934	G941	U688	A604	U428	G348	U210	U112	U44
U1528	U1383	C1297	C1227	U1134	G1036	G935	C942	U689	A605	U429	U438	G211	G113	A45
C1529	G1384	C1298	C1228	U1135	G1037	U936	C943	U690	G606	U430	C441	G212	G114	A46
U1530	U1385	C1299	G1229	U1136	G1038	G937	C944	U691	U607	U431	C442	G213	G115	C47
A1531	G1386	C1300	C1230	U1137	G1039	U938	C945	U692	U608	U432	C350	G214	G116	C48
C1532	U1387	C1301	C1231	U1138	G1040	U939	C946	U693	C609	U433	C351	G215	U119	U51
U1533	G1388	C1302	C1232	U1139	G1041	G940	C947	U694	U609	U434	C352	G216	G123	G52
G1534	U1389	C1303	C1233	U1140	G1042	U941	C948	U695	G613	U435	C353	G217	U124	C53
U1535	C1390	C1304	C1234	U1141	G1043	U942	C949	U696	C614	U436	C354	G218	U125	A94
G1536	U1391	C1305	C1235	U1142	G1044	U943	C950	U697	G620	U437	C355	U219	G126	U55
C1537	U1392	C1306	C1236	U1143	G1045	U944	C951	U698	C621	U438	C356	G220	U127	G56
U1538	G1393	C1307	C1237	U1144	G1046	U945	C952	U699	G622	U439	C357	G221	G128	U57
G1539	U1394	C1308	C1238	U1145	G1047	U946	C953	U700	G623	U440	C358	G222	A141	C58
U1540	C1395	C1309	C1239	U1146	G1048	U947	C954	U701	G624	U441	C359	U218	G142	U59
C1541	U1396	C1310	C1240	U1147	G1049	U948	C955	U702	C625	U442	C360	G225	G145	A60
U1542	G1397	C1311	C1241	U1148	G1050	U949	C956	U703	C626	U443	C361	G226	G146	A61
G1543	U1398	C1312	C1242	U1149	G1051	U950	C957	U704	C627	U444	C362	G227	G147	G62
U1544	C1399	C1313	C1243	U1150	G1052	U951	C958	U705	C628	U445	C363	G228	A147	U63
A1545	U1400	C1314	C1244	U1151	G1053	U952	C959	U706	C629	U446	C364	G229	G148	A64
G1546	U1401	C1315	C1245	U1152	G1054	U953	C960	U707	C630	U447	C365	G230	A149	G65
U1547	C1402	C1316	C1246	U1153	G1055	U954	C961	U708	C631	U448	C366	G231	G150	C66
C1548	U1403	C1317	C1247	U1154	G1056	U955	C962	U709	C632	U449	C367	G232	C151	G67
U1549	U1404	C1318	C1248	U1155	G1057	U956	C963	U710	C633	U450	C368	G233	A152	C68
G1550	U1405	C1319	C1249	U1156	G1058	U957	C964	U711	C634	U451	C369	G234	G153	
U1551	C1406	C1320	C1250	U1157	G1059	U958	C965	U712	C635	U452	C370	G235	G154	A62
G1552	U1407	C1321	C1251	U1158	G1060	U959	C966	U713	C636	U453	C371	G236	A147	U63
C1553	U1408	C1322	C1252	U1159	G1061	U960	C967	U714	C637	U454	C372	G237	G155	A64
U1554	U1409	C1323	C1253	U1160	G1062	U961	C968	U715	C638	U455	C373	G238	A150	G65
G1555	C1410	C1324	C1254	U1161	G1063	U962	C969	U716	C639	U456	C374	G239	G156	C66
U1556	U1411	C1325	C1255	U1162	G1064	U963	C970	U717	C640	U457	C375	G240	G157	C67
G1557	C1412	C1326	C1256	U1163	G1065	U964	C971	U718	C641	U458	C376	G241	G158	A68
U1558	U1413	C1327	C1257	U1164	G1066	U965	C972	U719	C642	U459	C377	G242	G159	C69



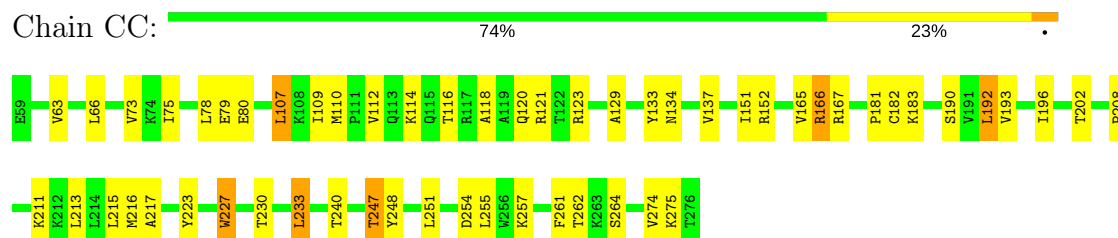
• Molecule 52: uS2



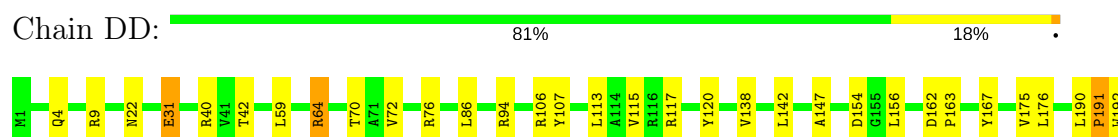
• Molecule 53: eS1



• Molecule 54: uS5

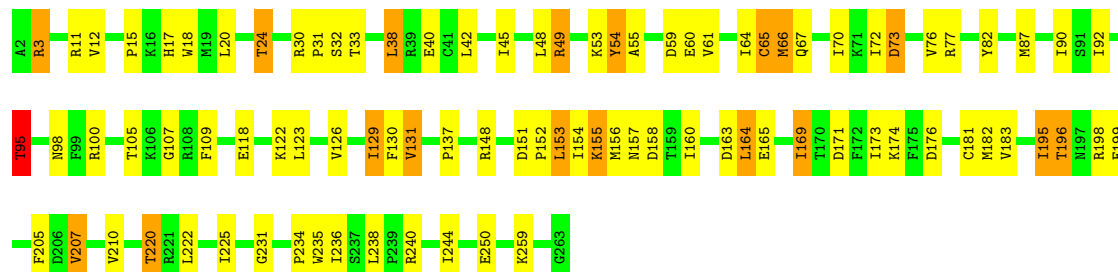


• Molecule 55: uS3

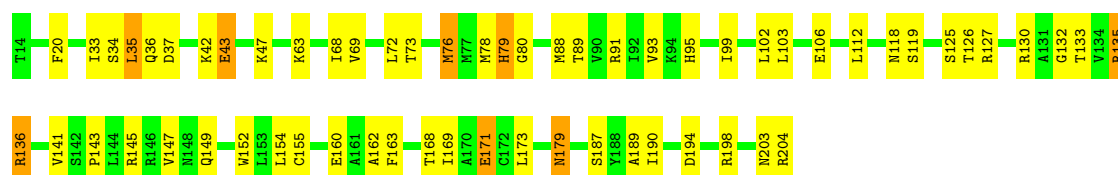




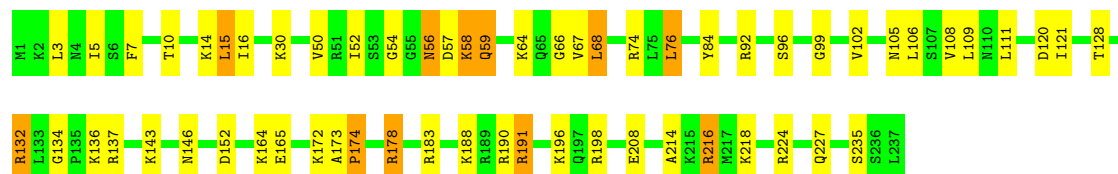
• Molecule 56: eS4



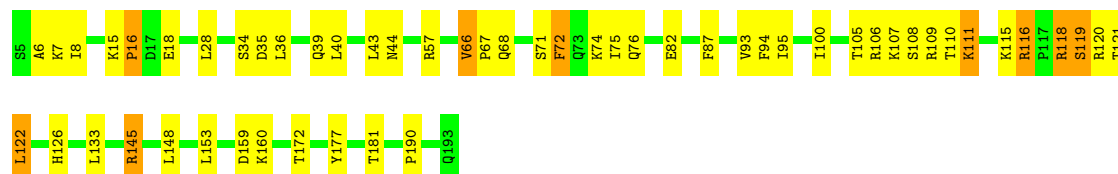
• Molecule 57: uS7



• Molecule 58: eS6

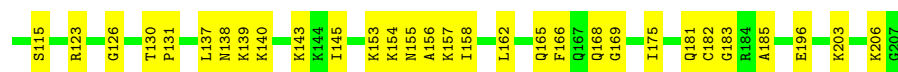


• Molecule 59: eS7

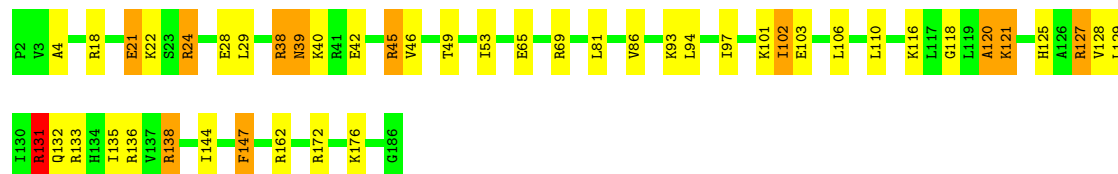


• Molecule 60: eS8





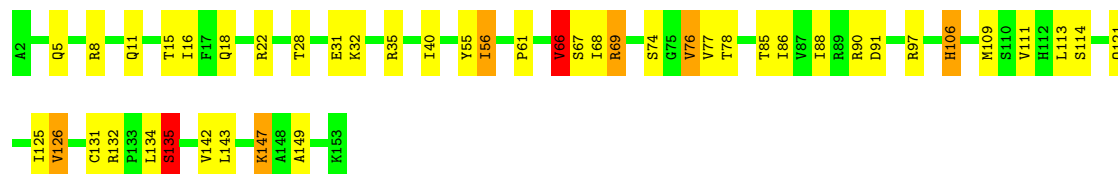
• Molecule 61: uS4



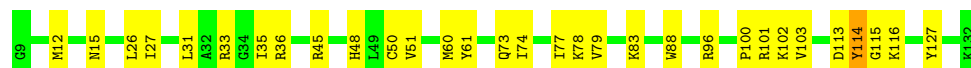
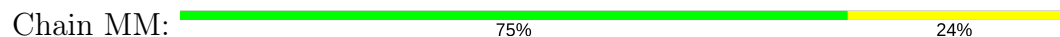
• Molecule 62: eS10



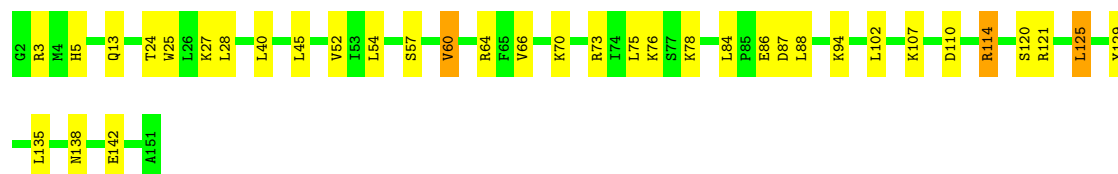
• Molecule 63: uS17



• Molecule 64: eS12

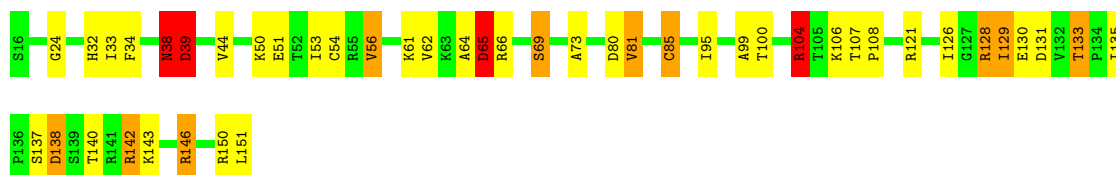


• Molecule 65: uS15



• Molecule 66: uS11





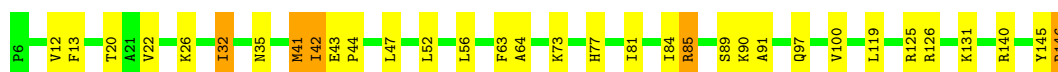
- Molecule 67: uS19

Chain PP: 75% 21% •



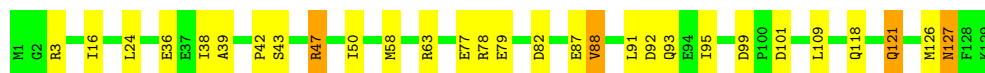
- Molecule 68: uS9

Chain QQ: 77% 20% •



- Molecule 69: eS17

Chain RR: 78% 19% •



- Molecule 70: uS13

Chain SS: 74% 20% • •



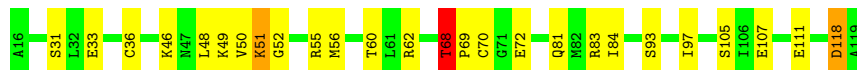
- Molecule 71: eS19

Chain TT: 79% 16% 5% •




- Molecule 72: uS10

Chain UU: 75% 22% • •



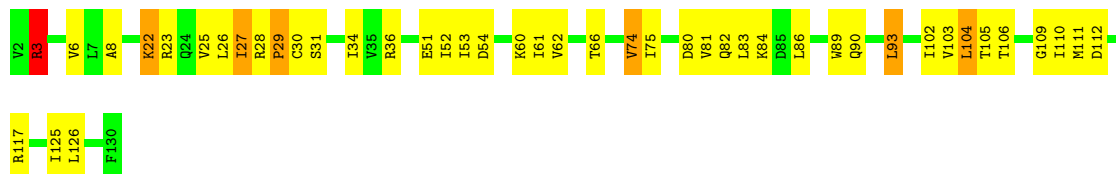
- Molecule 73: eS21

Chain VV:  73% 24% .



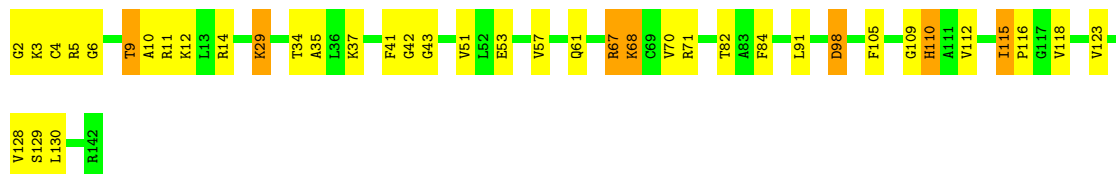
- Molecule 74: uS8

Chain WW:  65% 29% 5% .




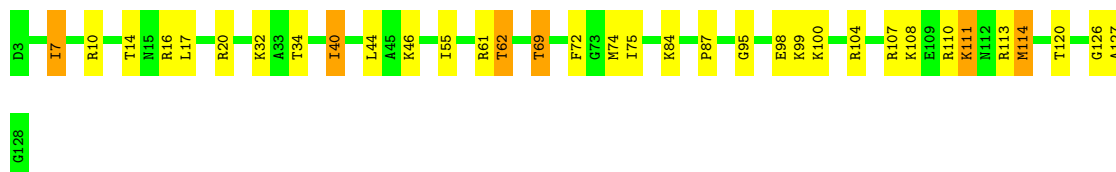
- Molecule 75: uS12

Chain XX:  72% 23% 5%




- Molecule 76: eS24

Chain YY:  73% 22% 5%




- Molecule 77: eS25

Chain ZZ:  77% 23%



- Molecule 78: eS26

Chain aa:  81% 19%



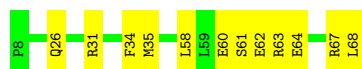
- Molecule 79: eS27

Chain bb:  80% 20%



• Molecule 80: eS28

Chain cc: 80% 20%



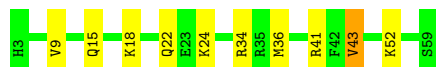
• Molecule 81: uS14

Chain dd: 81% 19%



• Molecule 82: eS30

Chain ee: 82% 16%



• Molecule 83: eS31

Chain ff: 87% 9%



• Molecule 84: RACK1

Chain gg: 90% 9%



• Molecule 85: mRNA

Chain hh: 42% 58%



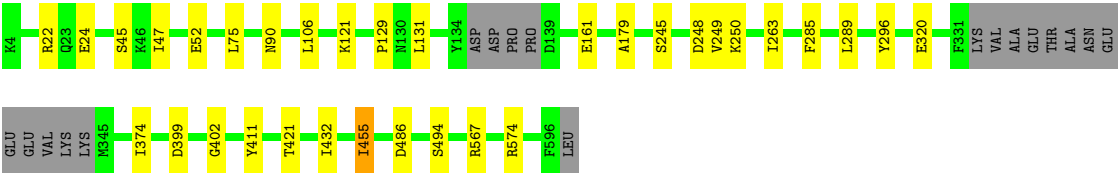
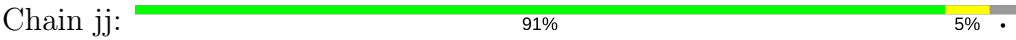
• Molecule 86: eRF1

Chain ii: 89% 10%





● Molecule 87: ABCE1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	20515	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	104478	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	0.46	0/1906	0.79	0/2556
10	J	0.38	0/1376	0.73	0/1841
11	L	0.41	0/1734	0.79	0/2317
12	M	0.37	0/1158	0.74	0/1547
13	N	0.43	0/1746	0.83	0/2338
14	O	0.40	0/1671	0.77	0/2234
15	P	0.42	0/1268	0.75	0/1701
16	Q	0.41	0/1530	0.81	1/2041 (0.0%)
17	R	0.41	0/1524	0.79	0/2013
18	S	0.40	0/1493	0.85	3/2002 (0.1%)
19	T	0.41	0/1326	0.72	0/1770
2	B	0.40	0/3216	0.78	1/4311 (0.0%)
20	U	0.41	0/822	0.68	0/1103
21	V	0.40	0/993	0.73	0/1332
22	W	0.48	0/541	0.83	1/720 (0.1%)
23	X	0.42	0/993	0.74	0/1334
24	Y	0.37	0/1132	0.80	2/1504 (0.1%)
25	Z	0.39	0/1130	0.72	0/1507
26	a	0.40	0/1191	0.79	0/1590
27	b	0.44	0/619	0.73	0/818
28	c	0.36	0/742	0.69	0/996
29	d	0.38	0/903	0.81	1/1216 (0.1%)
3	C	0.43	0/2938	0.80	5/3946 (0.1%)
30	e	0.47	0/1071	0.85	0/1429
31	f	0.52	0/895	0.87	0/1198
32	g	0.42	0/916	0.81	1/1220 (0.1%)
33	h	0.36	0/1021	0.77	1/1348 (0.1%)
34	i	0.40	0/841	0.82	2/1112 (0.2%)
35	j	0.45	0/720	0.93	1/952 (0.1%)
36	k	0.37	0/575	0.68	0/761
37	l	0.50	0/454	0.84	0/599
38	m	0.37	0/435	0.76	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	n	0.41	0/223	0.91	0/284
4	D	0.37	0/2432	0.70	2/3257 (0.1%)
40	o	0.39	0/864	0.75	0/1140
41	p	0.42	0/718	0.71	0/953
42	r	0.48	0/1017	0.80	1/1364 (0.1%)
43	s	0.38	0/1547	0.58	0/2088
44	t	0.41	0/1257	0.69	0/1697
45	1	0.45	0/129	0.72	0/173
46	2	0.26	0/1805	0.72	1/2809 (0.0%)
47	3	0.36	0/1777	0.97	10/2763 (0.4%)
48	5	0.37	4/87790 (0.0%)	0.79	75/136937 (0.1%)
49	7	0.30	0/2858	0.69	0/4455
5	E	0.46	0/1936	0.82	2/2600 (0.1%)
50	8	0.36	0/3701	0.74	0/5766
51	9	0.32	1/41013 (0.0%)	0.79	45/63919 (0.1%)
52	AA	0.36	0/1679	0.70	0/2283
53	BB	0.38	0/1756	0.77	4/2350 (0.2%)
54	CC	0.41	0/1730	0.76	1/2344 (0.0%)
55	DD	0.37	0/1792	0.72	0/2412
56	EE	0.39	0/2115	0.78	0/2843
57	FF	0.49	0/1531	0.78	1/2059 (0.0%)
58	GG	0.37	0/1946	0.78	0/2590
59	HH	0.44	0/1544	0.72	1/2068 (0.0%)
6	F	0.40	0/1905	0.75	1/2539 (0.0%)
60	II	0.41	0/1715	0.78	0/2287
61	JJ	0.41	0/1550	0.88	4/2069 (0.2%)
62	KK	0.47	0/851	0.73	0/1147
63	LL	0.40	0/1259	0.78	0/1684
64	MM	0.42	0/968	0.64	0/1296
65	NN	0.39	0/1232	0.77	0/1656
66	OO	0.42	0/1029	0.88	1/1380 (0.1%)
67	PP	0.39	0/1079	0.76	0/1437
68	QQ	0.37	0/1142	0.70	0/1528
69	RR	0.42	0/1060	0.71	0/1421
7	G	0.38	0/1967	0.73	1/2647 (0.0%)
70	SS	0.38	0/1157	0.84	1/1548 (0.1%)
71	TT	0.43	0/1120	0.78	2/1499 (0.1%)
72	UU	0.36	0/831	0.71	0/1115
73	VV	0.39	0/645	0.75	0/865
74	WW	0.38	0/1051	0.79	0/1406
75	XX	0.38	0/1116	0.80	0/1490
76	YY	0.39	0/1040	0.74	0/1382
77	ZZ	0.37	0/604	0.75	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	aa	0.39	0/794	0.83	0/1065
79	bb	0.37	0/665	0.67	0/891
8	H	0.37	0/1535	0.71	0/2063
80	cc	0.36	0/478	0.78	0/640
81	dd	0.40	0/455	0.80	0/603
82	ee	0.46	0/462	0.75	0/607
83	ff	0.39	0/531	0.62	0/703
84	gg	0.37	0/2493	0.65	0/3394
85	hh	0.29	0/287	0.76	0/445
86	ii	0.39	0/3333	0.63	2/4483 (0.0%)
87	jj	0.47	1/4625 (0.0%)	0.58	0/6238
9	I	0.41	0/1693	0.69	0/2260
All	All	0.38	6/242712 (0.0%)	0.78	174/355683 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
11	L	0	3
17	R	0	1
18	S	0	2
19	T	0	1
2	B	0	4
20	U	0	1
24	Y	0	1
3	C	0	2
31	f	0	1
4	D	0	1
42	r	0	2
48	5	0	1
5	E	0	1
51	9	0	1
52	AA	0	1
56	EE	0	2
57	FF	0	2
59	HH	0	1
60	II	0	1
61	JJ	0	2
66	OO	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
68	QQ	0	1
7	G	0	1
70	SS	0	1
71	TT	0	1
72	UU	0	2
73	VV	0	1
74	WW	0	2
75	XX	0	1
78	aa	0	1
86	ii	0	3
9	I	0	2
All	All	0	49

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	1965	G	O3'-P	-23.01	1.33	1.61
87	jj	121	LYS	CE-NZ	19.94	1.99	1.49
51	9	908	A	O3'-P	8.98	1.72	1.61
48	5	1847	C	O3'-P	-6.16	1.53	1.61
48	5	957	G	O3'-P	5.62	1.67	1.61
48	5	1358	G	O3'-P	5.10	1.67	1.61

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	909	G	O5'-P-OP2	-16.21	91.11	105.70
47	3	70	G	N9-C1'-C2'	-13.18	96.87	114.00
48	5	3753	G	N9-C1'-C2'	-11.91	98.52	114.00
51	9	1235	G	N9-C1'-C2'	-11.46	99.11	114.00
48	5	3718	A	N9-C1'-C2'	-10.30	100.61	114.00
48	5	1358	G	C4'-C3'-O3'	10.21	133.41	113.00
51	9	1386	A	N9-C1'-C2'	-10.19	100.76	114.00
51	9	1212	G	N9-C1'-C2'	-10.02	100.98	114.00
48	5	1357	C	C4'-C3'-O3'	9.68	132.37	113.00
24	Y	87	ARG	NE-CZ-NH2	9.17	124.89	120.30
48	5	4975	G	C2'-C3'-O3'	8.96	129.21	109.50
51	9	1294	G	N9-C1'-C2'	-8.95	102.15	112.00
47	3	38	A	N9-C1'-C2'	-8.89	102.22	112.00
47	3	30	G	N9-C1'-C2'	-8.83	102.28	112.00
53	BB	136	ARG	NE-CZ-NH2	8.82	124.71	120.30
22	W	44	ARG	NE-CZ-NH1	8.56	124.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	90	G	C2'-C3'-O3'	8.38	127.95	109.50
48	5	4528	G	C2'-C3'-O3'	8.37	127.90	109.50
48	5	3888	G	C2'-C3'-O3'	8.31	127.79	109.50
47	3	70	G	C4'-C3'-O3'	8.30	129.60	113.00
51	9	1394	G	C2'-C3'-O3'	8.28	127.71	109.50
48	5	1969	G	N9-C1'-C2'	-8.26	102.91	112.00
70	SS	113	ARG	NE-CZ-NH1	8.20	124.40	120.30
61	JJ	127	ARG	NE-CZ-NH1	8.12	124.36	120.30
48	5	4948	C	C2'-C3'-O3'	8.04	127.19	109.50
51	9	1385	G	N9-C1'-C2'	-8.01	103.19	112.00
18	S	83	ARG	NE-CZ-NH2	7.99	124.29	120.30
48	5	1211	G	C2'-C3'-O3'	7.95	126.98	109.50
48	5	3697	U	C2'-C3'-O3'	7.90	126.87	109.50
35	j	63	ARG	NE-CZ-NH1	7.84	124.22	120.30
48	5	1455	G	C2'-C3'-O3'	7.78	126.60	109.50
51	9	1235	G	C4'-C3'-O3'	7.73	128.47	113.00
61	JJ	131	ARG	NE-CZ-NH1	7.71	124.15	120.30
48	5	2858	A	N9-C1'-C2'	-7.65	103.59	112.00
48	5	2858	A	C4'-C3'-O3'	7.62	128.23	113.00
47	3	39	U	N1-C1'-C2'	-7.58	103.66	112.00
51	9	1681	U	N1-C1'-C2'	-7.56	103.68	112.00
48	5	1292	C	C2'-C3'-O3'	7.52	126.05	109.50
3	C	342	ARG	NE-CZ-NH1	7.51	124.05	120.30
48	5	3718	A	C4'-C3'-O3'	7.50	128.00	113.00
51	9	322	C	N1-C1'-C2'	-7.45	103.80	112.00
51	9	1448	A	N9-C1'-C2'	-7.42	103.84	112.00
51	9	1641	A	O5'-P-OP1	-7.38	99.06	105.70
48	5	275	C	C2'-C3'-O3'	7.36	125.68	109.50
48	5	5060	A	C2'-C3'-O3'	7.33	125.62	109.50
48	5	125	C	C2'-C3'-O3'	7.32	125.61	109.50
48	5	1477	C	C2'-C3'-O3'	7.27	125.50	109.50
48	5	2797	C	N1-C1'-C2'	-7.26	104.02	112.00
71	TT	56	ARG	NE-CZ-NH1	7.26	123.93	120.30
61	JJ	24	ARG	NE-CZ-NH1	7.24	123.92	120.30
48	5	5061	A	C2'-C3'-O3'	7.19	125.33	109.50
51	9	1144	A	N9-C1'-C2'	7.18	123.34	114.00
48	5	47	A	C4'-C3'-O3'	7.18	127.36	113.00
48	5	2695	A	C2'-C3'-O3'	7.14	125.21	109.50
51	9	1268	C	N1-C1'-C2'	-7.13	104.15	112.00
48	5	406	C	C2'-C3'-O3'	7.13	125.19	109.50
48	5	2027	U	N1-C1'-C2'	-7.13	104.16	112.00
48	5	5059	C	C2'-C3'-O3'	7.13	125.18	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	ii	182	ARG	NE-CZ-NH1	7.12	123.86	120.30
47	3	1	G	C5'-C4'-O4'	7.08	117.59	109.10
51	9	1455	A	N9-C1'-C2'	-7.07	104.22	112.00
51	9	102	A	C2'-C3'-O3'	7.04	124.99	109.50
48	5	1485	C	C2'-C3'-O3'	6.93	124.80	113.70
61	JJ	131	ARG	NE-CZ-NH2	-6.91	116.85	120.30
51	9	642	U	C4'-C3'-O3'	6.88	126.76	113.00
51	9	666	U	N1-C1'-C2'	6.84	122.89	114.00
48	5	1279	A	C2'-C3'-O3'	6.80	124.58	113.70
48	5	2046	G	C2'-C3'-O3'	6.76	124.52	113.70
48	5	1236	C	C2'-C3'-O3'	6.71	124.43	113.70
48	5	977	C	C2'-C3'-O3'	6.68	124.39	113.70
48	5	4885	U	C2'-C3'-O3'	6.66	124.35	113.70
48	5	93	G	C4'-C3'-O3'	6.64	126.29	113.00
34	i	25	ARG	NE-CZ-NH1	6.54	123.57	120.30
51	9	312	G	C2'-C3'-O3'	6.53	124.15	113.70
48	5	1818	G	C2'-C3'-O3'	6.51	124.12	113.70
51	9	1447	G	N9-C1'-C2'	-6.49	104.86	112.00
48	5	2083	C	C4'-C3'-O3'	6.44	125.87	113.00
51	9	1386	A	C4'-C3'-O3'	6.44	125.88	113.00
51	9	1060	A	N9-C1'-C2'	6.42	122.34	114.00
48	5	93	G	N9-C1'-C2'	-6.39	104.97	112.00
47	3	69	G	O4'-C1'-N9	6.39	113.31	108.20
48	5	3657	U	C2'-C3'-O3'	6.36	123.87	113.70
4	D	22	ARG	NE-CZ-NH1	6.34	123.47	120.30
48	5	1474	C	C2'-C3'-O3'	6.32	123.82	113.70
5	E	208	LEU	CA-CB-CG	6.32	129.84	115.30
48	5	1500	A	C2'-C3'-O3'	6.29	123.76	113.70
51	9	1	U	C5'-C4'-O4'	6.29	116.64	109.10
48	5	1398	A	C2'-C3'-O3'	6.28	123.74	113.70
51	9	110	U	C2'-C3'-O3'	6.28	123.74	113.70
48	5	2123	C	C2'-C3'-O3'	6.23	123.67	113.70
48	5	1380	G	N9-C1'-C2'	6.22	122.09	114.00
48	5	1969	G	C4'-C3'-O3'	6.22	125.45	113.00
48	5	1239	C	C2'-C3'-O3'	6.21	123.64	113.70
48	5	2632	U	N1-C1'-C2'	6.17	122.02	114.00
51	9	322	C	C2'-C3'-O3'	-6.15	95.97	109.50
51	9	1211	G	N9-C1'-C2'	-6.12	105.27	112.00
51	9	62	G	C2'-C3'-O3'	6.09	123.45	113.70
51	9	434	G	C2'-C3'-O3'	6.05	123.38	113.70
48	5	1072	C	N1-C1'-C2'	6.03	121.84	114.00
48	5	1672	U	N1-C1'-C2'	6.02	121.83	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1848	C	C2'-C3'-O3'	6.01	123.31	113.70
29	d	78	ARG	NE-CZ-NH1	5.98	123.29	120.30
48	5	1390	G	C2'-C3'-O3'	5.93	123.19	113.70
34	i	85	ARG	NE-CZ-NH1	5.93	123.26	120.30
48	5	1965	G	P-O3'-C3'	5.90	126.78	119.70
48	5	1696	C	C2'-C3'-O3'	5.90	123.13	113.70
51	9	1419	C	C2'-C3'-O3'	5.89	123.12	113.70
16	Q	104	ARG	NE-CZ-NH1	5.87	123.23	120.30
48	5	978	G	C2'-C3'-O3'	5.81	123.00	113.70
48	5	4872	G	C2'-C3'-O3'	5.78	122.95	113.70
5	E	72	PRO	N-CA-CB	5.78	110.24	103.30
48	5	4951	G	C2'-C3'-O3'	5.77	122.93	113.70
48	5	1329	G	C2'-C3'-O3'	5.76	122.91	113.70
48	5	4975	G	C4'-C3'-O3'	-5.72	97.39	109.40
48	5	215	C	C2'-C3'-O3'	5.69	122.80	113.70
51	9	1824	A	C2'-C3'-O3'	5.67	122.77	113.70
3	C	98	GLY	N-CA-C	-5.65	98.97	113.10
47	3	1	G	C5'-C4'-C3'	5.63	125.00	116.00
51	9	1	U	C5'-C4'-C3'	5.62	124.99	116.00
51	9	1234	C	N1-C1'-C2'	-5.60	105.83	112.00
6	F	91	LEU	CA-CB-CG	5.54	128.05	115.30
18	S	83	ARG	NE-CZ-NH1	-5.51	117.55	120.30
2	B	36	ASP	C-N-CD	5.50	139.96	128.40
51	9	1137	U	C2'-C3'-O3'	5.49	122.48	113.70
57	FF	135	ARG	NE-CZ-NH2	-5.48	117.56	120.30
47	3	29	A	N9-C1'-C2'	-5.46	105.99	112.00
48	5	979	C	C2'-C3'-O3'	5.46	122.44	113.70
48	5	4473	A	N9-C1'-C2'	5.46	121.09	114.00
48	5	2054	U	N1-C1'-C2'	5.45	121.08	114.00
53	BB	136	ARG	CG-CD-NE	5.45	123.23	111.80
71	TT	56	ARG	NE-CZ-NH2	-5.42	117.59	120.30
47	3	30	G	C4'-C3'-O3'	5.41	123.82	113.00
48	5	2028	C	N1-C1'-C2'	-5.41	106.05	112.00
48	5	957	G	P-O3'-C3'	5.40	126.19	119.70
51	9	1385	G	C4'-C3'-O3'	5.38	123.77	113.00
59	HH	118	ARG	NE-CZ-NH1	5.38	122.99	120.30
24	Y	75	ARG	NE-CZ-NH1	5.38	122.99	120.30
48	5	1365	C	C4'-C3'-O3'	5.37	123.75	113.00
51	9	1144	A	C8-N9-C1'	-5.35	118.07	127.70
51	9	844	U	C5'-C4'-O4'	5.34	115.51	109.10
86	ii	372	MET	C-N-CD	5.33	139.60	128.40
66	OO	146	ARG	NE-CZ-NH2	-5.31	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1212	G	C4'-C3'-O3'	5.29	123.59	113.00
53	BB	136	ARG	NE-CZ-NH1	-5.29	117.65	120.30
48	5	486	C	C2'-C3'-O3'	5.29	122.16	113.70
51	9	909	G	O5'-P-OP1	5.29	117.05	110.70
48	5	1266	G	C2'-C3'-O3'	5.28	122.15	113.70
48	5	3715	U	N1-C1'-C2'	-5.27	106.20	112.00
48	5	2586	G	N9-C1'-C2'	5.25	120.82	114.00
3	C	262	ASP	CB-CG-OD2	5.23	123.00	118.30
18	S	83	ARG	CG-CD-NE	5.22	122.76	111.80
33	h	22	ASP	CB-CG-OD2	5.21	122.98	118.30
51	9	1647	A	C2'-C3'-O3'	5.18	122.00	113.70
51	9	1144	A	C4-N9-C1'	5.16	135.58	126.30
7	G	231	ASP	CB-CG-OD2	5.15	122.94	118.30
51	9	1408	U	O5'-P-OP1	-5.13	101.09	105.70
48	5	4731	G	N9-C1'-C2'	5.11	120.65	114.00
42	r	17	LEU	CA-CB-CG	5.11	127.05	115.30
48	5	2661	U	C2'-C3'-O3'	5.11	121.88	113.70
53	BB	136	ARG	CD-NE-CZ	5.10	130.74	123.60
48	5	4481	U	C5'-C4'-O4'	5.09	115.21	109.10
48	5	4965	U	C2'-C3'-O3'	5.07	121.81	113.70
51	9	532	C	C2'-C3'-O3'	5.06	121.79	113.70
51	9	1109	C	N1-C1'-C2'	5.05	120.57	114.00
3	C	67	TRP	N-CA-C	-5.04	97.39	111.00
48	5	1755	C	C2'-C3'-O3'	5.04	121.77	113.70
51	9	488	U	N1-C1'-C2'	5.04	120.55	114.00
3	C	45	ARG	NE-CZ-NH1	5.04	122.82	120.30
32	g	66	ARG	NE-CZ-NH1	5.04	122.82	120.30
46	2	34	A	N9-C1'-C2'	-5.03	106.46	112.00
54	CC	233	LEU	CA-CB-CG	5.03	126.87	115.30
51	9	1354	G	C2'-C3'-O3'	5.03	121.75	113.70
4	D	22	ARG	CG-CD-NE	5.02	122.33	111.80
48	5	2246	C	C2'-C3'-O3'	5.01	121.72	113.70

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	2793	G	Sidechain
51	9	1448	A	Sidechain
1	A	196	TRP	Peptide
52	AA	73	ASP	Peptide
2	B	17	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	B	257	TRP	Peptide
2	B	258	HIS	Peptide
2	B	351	LEU	Peptide
3	C	245	HIS	Peptide
3	C	339	THR	Peptide
4	D	36	LEU	Peptide
5	E	123	SER	Peptide
56	EE	129	ILE	Peptide
56	EE	155	LYS	Peptide
57	FF	42	LYS	Peptide
57	FF	43	GLU	Peptide
7	G	238	GLY	Peptide
59	HH	111	LYS	Peptide
9	I	188	LYS	Peptide
9	I	202	ASN	Peptide
60	II	154	LYS	Peptide
61	JJ	38	ARG	Peptide
61	JJ	93	LYS	Peptide
11	L	27	ASN	Peptide
11	L	46	ILE	Peptide
11	L	66	TYR	Peptide
66	OO	104	ARG	Peptide
68	QQ	42	ILE	Peptide
17	R	19	LYS	Peptide
18	S	163	HIS	Peptide
18	S	164	LYS	Peptide
70	SS	11	HIS	Peptide
19	T	26	PRO	Peptide
71	TT	42	HIS	Peptide
20	U	27	HIS	Peptide
72	UU	68	THR	Peptide
72	UU	72	GLU	Peptide
73	VV	32	ILE	Peptide
74	WW	27	ILE	Peptide
74	WW	54	ASP	Peptide
75	XX	98	ASP	Peptide
24	Y	7	VAL	Peptide
78	aa	7	ASN	Peptide
31	f	105	LEU	Peptide
86	ii	325	ASN	Peptide
86	ii	371	SER	Peptide
86	ii	373	PRO	Peptide

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Mol	Chain	Res	Type	Group
42	r	106	LEU	Peptide
42	r	70	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1868	0	1959	31	0
2	B	3148	0	3267	55	0
3	C	2884	0	3062	45	0
4	D	2386	0	2419	31	0
5	E	1898	0	2035	66	0
6	F	1870	0	1994	27	0
7	G	1934	0	2087	32	0
8	H	1516	0	1597	10	0
9	I	1655	0	1704	45	0
10	J	1353	0	1386	16	0
11	L	1703	0	1820	22	0
12	M	1137	0	1211	16	0
13	N	1701	0	1749	18	0
14	O	1638	0	1777	31	0
15	P	1242	0	1269	12	0
16	Q	1506	0	1623	14	0
17	R	1508	0	1664	31	0
18	S	1454	0	1496	14	0
19	T	1298	0	1366	11	0
20	U	808	0	831	5	0
21	V	979	0	1039	5	0
22	W	528	0	541	5	0
23	X	976	0	1053	8	0
24	Y	1115	0	1205	6	0
25	Z	1107	0	1182	16	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	g	906	0	999	0	0
33	h	1013	0	1147	0	0
34	i	830	0	916	0	0
35	j	705	0	738	0	0
36	k	569	0	637	0	0
37	l	444	0	483	0	0
38	m	429	0	466	0	0
39	n	222	0	264	0	0
40	o	851	0	921	0	0
41	p	708	0	756	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	18	0
47	3	1593	0	811	79	0
48	5	78486	0	39663	1322	0
49	7	2558	0	1296	27	0
50	8	3314	0	1683	53	0
51	9	36680	0	18529	615	0
52	AA	1642	0	1646	22	0
53	BB	1729	0	1803	15	0
54	CC	1692	0	1780	22	0
55	DD	1764	0	1863	8	0
56	EE	2073	0	2175	45	0
57	FF	1509	0	1562	28	0
58	GG	1923	0	2089	29	0
59	HH	1521	0	1616	20	0
60	II	1686	0	1772	30	0
61	JJ	1525	0	1640	22	0
62	KK	827	0	854	7	0
63	LL	1238	0	1315	17	0
64	MM	958	0	993	3	0
65	NN	1208	0	1294	8	0
66	OO	1016	0	1039	14	0
67	PP	1060	0	1120	13	0
68	QQ	1124	0	1193	11	0
69	RR	1047	0	1103	9	0
70	SS	1139	0	1191	17	0
71	TT	1102	0	1142	11	0
72	UU	821	0	883	6	0
73	VV	636	0	634	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	WW	1034	0	1080	23	0
75	XX	1098	0	1167	11	0
76	YY	1023	0	1090	11	0
77	ZZ	598	0	656	6	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	520	0	536	0	0
84	gg	2436	0	2393	0	0
85	hh	257	0	129	0	0
86	ii	3280	0	3326	0	0
87	jj	4543	0	4674	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	34	0	0	0	0
88	B	1	0	0	0	0
88	C	1	0	0	0	0
88	I	1	0	0	0	0
88	LL	1	0	0	0	0
88	P	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
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	226454	0	169855	2802	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 8.

All (2802) 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)
51:9:1137:U:O4	51:9:1148:A:N1	1.61	1.34
48:5:976:G:H2'	48:5:977:C:O4'	1.26	1.32
17:R:172:ARG:NH1	51:9:908:A:H5''	1.47	1.29
48:5:2367:A:N1	48:5:2788:U:O4	1.66	1.29
5:E:126:ARG:NH1	48:5:712:C:H1'	1.49	1.27
61:JJ:121:LYS:CE	61:JJ:121:LYS:NZ	1.49	1.26
51:9:872:A:N1	51:9:914:U:O4	1.72	1.22
48:5:4213:A:N1	48:5:4218:U:O4	1.72	1.21
48:5:1958:A:H5''	48:5:1962:A:O2'	1.03	1.20
12:M:116:LYS:CG	14:O:196:LEU:HD21	1.72	1.20
17:R:172:ARG:NH1	51:9:908:A:C5'	2.03	1.20
48:5:1929:A:N1	48:5:2054:U:O4	1.75	1.19
48:5:2468:U:O4	48:5:2473:A:N1	1.73	1.19
5:E:202:VAL:HG13	5:E:256:LYS:NZ	1.55	1.18
51:9:322:C:O2'	51:9:323:C:P	2.01	1.17
9:I:191:ILE:CD1	9:I:200:ILE:HD12	1.74	1.16
7:G:156:VAL:HG11	7:G:184:LEU:HD12	1.28	1.14
5:E:59:TYR:CD2	5:E:64:LEU:HD12	1.83	1.13
5:E:254:LEU:HD23	5:E:257:ILE:HD11	1.24	1.13
17:R:172:ARG:HH11	51:9:908:A:H5''	0.98	1.13
51:9:1137:U:C4	51:9:1148:A:N1	2.18	1.12
9:I:191:ILE:HD11	9:I:200:ILE:HD12	1.29	1.12
48:5:1958:A:C5'	48:5:1962:A:O2'	1.95	1.11
11:L:163:LYS:HE2	48:5:509:A:H4'	1.16	1.11
12:M:116:LYS:HG3	14:O:196:LEU:HD21	1.33	1.09
5:E:126:ARG:HH11	48:5:712:C:C1'	1.65	1.09
5:E:126:ARG:NH1	48:5:712:C:C1'	2.14	1.08
9:I:191:ILE:HD12	9:I:200:ILE:CD1	1.84	1.07
5:E:202:VAL:CG1	5:E:256:LYS:NZ	2.17	1.07
9:I:191:ILE:CD1	9:I:200:ILE:CD1	2.33	1.07
11:L:42:ARG:NH1	11:L:51:ALA:O	1.88	1.06
5:E:62:LYS:NZ	48:5:978:G:OP2	1.88	1.06
5:E:202:VAL:CG1	5:E:256:LYS:HZ2	1.68	1.05
48:5:2409:U:C4	48:5:2783:A:N1	2.25	1.05
47:3:67:U:C2'	47:3:68:C:H5'	1.86	1.04
5:E:62:LYS:HE3	48:5:978:G:OP1	1.54	1.04
5:E:202:VAL:HG13	5:E:256:LYS:HZ2	1.05	1.04
47:3:41:U:O3'	57:FF:198:ARG:HD3	1.55	1.04
51:9:322:C:O2'	51:9:323:C:O5'	1.73	1.03
5:E:62:LYS:CE	48:5:978:G:P	2.46	1.03
51:9:1307:U:C2'	51:9:1308:U:H5''	1.87	1.03
51:9:872:A:N1	51:9:914:U:C4	2.27	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1307:U:H2'	51:9:1308:U:H5''	1.04	1.02
48:5:3751:G:C2'	48:5:3752:C:H5'	1.90	1.02
5:E:126:ARG:HH11	48:5:712:C:H1'	0.92	1.02
51:9:1137:U:O4	51:9:1148:A:C2	2.12	1.01
47:3:67:U:H2'	47:3:68:C:H5'	1.42	1.00
48:5:1929:A:H61	48:5:2054:U:H3	1.10	1.00
9:I:202:ASN:O	49:7:63:C:C5	2.15	0.99
5:E:126:ARG:NH1	48:5:712:C:C2'	2.26	0.99
5:E:62:LYS:CE	48:5:978:G:OP2	2.10	0.98
51:9:911:C:C2'	51:9:912:C:H5'	1.91	0.98
47:3:41:U:O2'	57:FF:198:ARG:NH2	1.94	0.98
10:J:80:GLU:OE2	10:J:170:TYR:OH	1.82	0.98
48:5:77:U:O4	48:5:335:A:N1	1.98	0.97
48:5:1968:G:H1	48:5:2018:C:H42	1.12	0.97
48:5:3751:G:O2'	48:5:3752:C:H5'	1.65	0.96
51:9:911:C:H2'	51:9:912:C:H5'	1.44	0.96
2:B:163:LEU:HD21	2:B:182:GLU:CG	1.95	0.96
48:5:1278:C:H3'	48:5:1279:A:H4'	1.48	0.95
48:5:1983:A:N1	48:5:2008:U:C4	2.35	0.95
48:5:4278:C:HO2'	48:5:4281:A:H8	1.06	0.95
48:5:1983:A:N1	48:5:2008:U:O4	2.00	0.95
48:5:957:G:H1'	48:5:958:G:OP2	1.67	0.94
2:B:163:LEU:CD2	2:B:182:GLU:HG2	1.96	0.94
5:E:126:ARG:HH12	48:5:712:C:C2'	1.81	0.94
51:9:830:A:N6	51:9:844:U:N3	2.16	0.94
51:9:830:A:N1	51:9:844:U:O4	2.01	0.94
17:R:172:ARG:HH12	51:9:908:A:H5'	1.29	0.94
17:R:98:ARG:NH2	17:R:107:ARG:HH12	15.83	0.94
48:5:2409:U:O4	48:5:2783:A:N1	1.99	0.93
51:9:1235:G:H5'	51:9:1247:C:H42	1.30	0.93
51:9:1407:U:H2'	51:9:1408:U:C5	2.04	0.92
9:I:48:LEU:HD21	9:I:145:LYS:HG2	1.49	0.92
17:R:98:ARG:HH22	17:R:107:ARG:HH12	16.44	0.92
5:E:126:ARG:NH1	48:5:712:C:O2'	2.03	0.92
54:CC:63:VAL:O	54:CC:63:VAL:HG12	1.67	0.92
48:5:976:G:C2'	48:5:977:C:O4'	2.17	0.92
17:R:98:ARG:NH2	17:R:107:ARG:NH1	16.17	0.92
2:B:163:LEU:CD2	2:B:182:GLU:CG	2.48	0.92
12:M:116:LYS:HG2	14:O:196:LEU:HD21	1.49	0.91
70:SS:11:HIS:O	70:SS:12:ILE:HD12	1.69	0.91
48:5:2468:U:N3	48:5:2473:A:N6	2.17	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:ARG:NH1	48:5:4985:U:O2	2.05	0.90
48:5:1958:A:O2'	48:5:1959:U:H5''	1.72	0.90
9:I:191:ILE:HD12	9:I:200:ILE:HD11	1.52	0.90
5:E:251:SER:O	5:E:255:PRO:CD	2.20	0.89
5:E:62:LYS:CE	48:5:978:G:OP1	2.20	0.88
48:5:102:G:O2'	48:5:1381:U:O2'	1.90	0.88
11:L:163:LYS:CE	48:5:509:A:H4'	2.04	0.88
54:CC:73:VAL:HG12	54:CC:73:VAL:O	1.73	0.87
48:5:1279:A:H3'	48:5:1280:C:H5''	1.57	0.87
51:9:1455:A:O2'	51:9:1456:G:O5'	1.91	0.87
2:B:156:TYR:CD1	48:5:4909:A:H2'	2.10	0.86
51:9:872:A:C2	51:9:914:U:O4	2.26	0.86
48:5:2027:U:O2'	48:5:2028:C:H5'	1.75	0.86
9:I:49:CYS:SG	9:I:51:HIS:NE2	2.48	0.86
5:E:238:ILE:O	5:E:239:THR:OG1	1.93	0.85
5:E:62:LYS:HE2	48:5:978:G:OP2	1.76	0.85
5:E:62:LYS:HE2	48:5:978:G:P	2.15	0.85
51:9:1267:C:O2'	51:9:1268:C:H5'	1.76	0.85
5:E:254:LEU:CD2	5:E:257:ILE:HD11	2.05	0.85
9:I:184:MET:HE2	9:I:190:LEU:HG	1.57	0.85
48:5:1279:A:C3'	48:5:1280:C:H5''	2.07	0.85
48:5:1956:A:O2'	48:5:1957:U:H5'	1.77	0.84
7:G:156:VAL:HG11	7:G:184:LEU:CD1	2.05	0.84
47:3:68:C:O2'	47:3:69:G:O4'	1.95	0.84
48:5:1957:U:O2'	48:5:1958:A:C8	2.29	0.84
17:R:172:ARG:NH1	51:9:908:A:H5'	1.89	0.84
54:CC:192:LEU:HD23	54:CC:227:TRP:NE1	1.93	0.83
51:9:1385:G:O2'	51:9:1386:A:H5'	1.79	0.83
47:3:29:A:O2'	47:3:30:G:O5'	1.97	0.83
51:9:872:A:C6	51:9:914:U:O4	2.30	0.83
4:D:33:ARG:NH2	49:7:7:G:O3'	2.10	0.82
48:5:3629:A:H4'	51:9:1721:U:O2	1.80	0.82
7:G:86:VAL:HG21	7:G:185:LYS:HE3	1.62	0.82
51:9:1406:G:H3'	51:9:1407:U:H4'	1.62	0.82
9:I:202:ASN:O	49:7:63:C:C4	2.32	0.81
5:E:157:ARG:O	5:E:178:ASN:ND2	2.13	0.81
7:G:87:LEU:HD23	7:G:184:LEU:CD2	2.10	0.81
54:CC:211:LYS:O	54:CC:215:LEU:HG	1.80	0.81
51:9:1681:U:O2'	51:9:1682:C:O4'	1.98	0.81
47:3:67:U:C3'	47:3:68:C:H5'	2.10	0.81
48:5:1367:C:C2	48:5:1370:G:H2'	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:81:ASP:OD1	12:M:84:THR:HG23	1.80	0.81
48:5:1379:C:H4'	48:5:1380:G:O4'	1.81	0.81
15:P:127:ARG:NH2	48:5:2422:C:OP1	2.14	0.81
51:9:1420:G:HO2'	71:TT:4:VAL:N	1.79	0.80
2:B:163:LEU:HD21	2:B:182:GLU:HG3	1.61	0.80
54:CC:192:LEU:HD23	54:CC:227:TRP:CD1	2.16	0.80
51:9:523:A:OP2	61:JJ:38:ARG:HD3	1.81	0.80
5:E:251:SER:O	5:E:255:PRO:HD2	1.81	0.80
2:B:156:TYR:CE1	48:5:4909:A:H2'	2.17	0.80
7:G:86:VAL:HG12	7:G:87:LEU:N	1.96	0.80
2:B:163:LEU:HD23	2:B:182:GLU:HG2	1.64	0.79
48:5:745:G:H2'	48:5:746:A:O4'	1.82	0.79
48:5:919:C:N4	48:5:920:C:C4	2.51	0.79
48:5:4723:A:H2'	48:5:4724:A:C8	2.17	0.79
48:5:957:G:N2	48:5:959:G:O6	2.15	0.79
51:9:292:A:O2'	51:9:293:C:OP2	2.01	0.79
48:5:2395:A:O2'	48:5:2806:A:H1'	1.82	0.79
48:5:3629:A:C4'	51:9:1721:U:O2	2.30	0.79
7:G:87:LEU:HD23	7:G:184:LEU:HD21	1.64	0.79
51:9:1144:A:H2'	51:9:1145:A:C8	2.17	0.79
48:5:1958:A:H5''	48:5:1962:A:HO2'	0.98	0.79
17:R:172:ARG:HH11	51:9:908:A:C5'	1.77	0.79
48:5:2026:A:C2'	48:5:2027:U:H5'	2.14	0.78
48:5:1929:A:N6	48:5:2054:U:H3	1.80	0.78
48:5:3751:G:H2'	48:5:3752:C:H5'	1.65	0.78
50:8:55:U:O4	50:8:62:A:N1	2.16	0.78
2:B:163:LEU:HD21	2:B:182:GLU:HG2	1.59	0.78
48:5:504:G:N1	48:5:654:C:C2	2.52	0.78
48:5:1213:G:C6	48:5:1215:C:C2	2.71	0.78
51:9:1454:A:OP1	69:RR:3:ARG:NE	2.16	0.77
48:5:77:U:N3	48:5:335:A:N6	2.32	0.77
48:5:1563:A:C8	51:9:678:U:H4'	2.19	0.77
48:5:2769:U:C2	48:5:2770:C:C5	2.72	0.77
48:5:3723:A:H2'	48:5:3724:A:C8	2.20	0.77
51:9:1137:U:O4	51:9:1148:A:C6	2.37	0.77
48:5:2793:G:C6	48:5:2797:C:C4	2.74	0.76
5:E:202:VAL:CG1	5:E:256:LYS:HZ1	1.97	0.76
51:9:1235:G:H5'	51:9:1247:C:N4	2.00	0.76
2:B:36:ASP:OD2	2:B:39:LYS:HE2	1.83	0.76
9:I:184:MET:HE1	9:I:190:LEU:HD11	1.67	0.76
48:5:2468:U:C4	48:5:2473:A:N1	2.54	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1268:C:O2'	51:9:1269:G:O5'	2.04	0.76
51:9:945:U:H2'	51:9:946:U:C6	2.21	0.75
47:3:35:U:C1'	51:9:1641:A:OP1	2.34	0.75
4:D:35:ARG:HB2	48:5:4325:A:C2	2.21	0.75
51:9:643:A:OP2	61:JJ:38:ARG:NH2	2.19	0.75
9:I:184:MET:CE	9:I:190:LEU:CD1	2.64	0.75
63:LL:131:CYS:SG	63:LL:132:ARG:N	2.60	0.75
48:5:2779:C:O2'	50:8:112:G:OP1	2.05	0.75
51:9:1102:G:N2	51:9:1103:C:C2	2.54	0.75
45:1:57:ARG:NH2	48:5:3862:A:O2'	2.20	0.74
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.69	0.74
51:9:1307:U:H2'	51:9:1308:U:C5'	2.01	0.74
51:9:1407:U:H2'	51:9:1408:U:C6	2.22	0.74
3:C:158:VAL:HA	3:C:161:TYR:CE2	2.22	0.74
3:C:159:GLU:OE1	3:C:159:GLU:N	2.20	0.74
9:I:184:MET:CE	9:I:190:LEU:HG	2.16	0.74
48:5:504:G:C2	48:5:654:C:O2	2.39	0.74
4:D:200:MET:HE1	4:D:241:LYS:CG	2.17	0.74
9:I:191:ILE:HD11	9:I:200:ILE:CD1	2.08	0.74
51:9:1405:A:H2'	51:9:1406:G:O4'	1.88	0.74
51:9:1680:G:O2'	51:9:1681:U:H5'	1.88	0.74
48:5:4371:G:O2'	48:5:4372:U:OP2	2.05	0.74
51:9:872:A:C6	51:9:914:U:C4	2.75	0.74
7:G:86:VAL:HG11	7:G:185:LYS:HG2	1.68	0.74
48:5:1279:A:H3'	48:5:1280:C:C5'	2.18	0.74
48:5:22:G:N2	50:8:35:C:C2	2.56	0.73
48:5:1278:C:C3'	48:5:1279:A:H4'	2.18	0.73
48:5:3914:U:H3	48:5:4378:A:N6	1.86	0.73
11:L:116:ARG:NH1	11:L:155:MET:O	2.21	0.73
48:5:956:A:H4'	48:5:957:G:OP2	1.89	0.73
51:9:1386:A:O2'	51:9:1387:G:H5'	1.89	0.72
47:3:76:A:N7	48:5:4371:G:C6	2.58	0.72
48:5:1280:C:C4	48:5:1282:G:C6	2.77	0.72
3:C:157:LYS:O	3:C:160:GLY:N	2.20	0.72
5:E:62:LYS:HE3	48:5:978:G:P	2.20	0.72
5:E:254:LEU:HD22	5:E:258:LYS:HE3	1.72	0.72
56:EE:154:ILE:O	56:EE:155:LYS:HG3	1.89	0.71
7:G:86:VAL:HG12	7:G:87:LEU:H	1.55	0.71
48:5:2367:A:N1	48:5:2788:U:C4	2.57	0.71
51:9:65:C:N4	58:GG:134:GLY:O	2.24	0.71
48:5:977:C:C2'	48:5:978:G:H5'	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2367:A:N6	48:5:2788:U:H3	1.88	0.71
48:5:1958:A:H4'	48:5:1962:A:H1'	1.72	0.71
48:5:2632:U:H2'	48:5:2633:U:C6	2.25	0.71
5:E:251:SER:O	5:E:255:PRO:HD3	1.91	0.71
48:5:2026:A:O2'	48:5:2027:U:H5'	1.90	0.71
48:5:3752:C:O2'	48:5:3753:G:OP2	2.09	0.71
48:5:516:C:C2	48:5:646:G:N2	2.59	0.71
51:9:1444:U:H2'	51:9:1445:U:C6	2.26	0.71
7:G:86:VAL:CG1	7:G:87:LEU:H	2.04	0.71
48:5:723:A:C2	48:5:943:A:N1	2.59	0.71
54:CC:192:LEU:HB3	54:CC:227:TRP:CD1	2.26	0.71
48:5:1724:G:H4'	48:5:1725:U:OP2	1.89	0.71
48:5:977:C:C2	48:5:978:G:C8	2.79	0.71
51:9:1235:G:H2'	51:9:1236:G:C8	2.26	0.71
5:E:217:GLN:NE2	5:E:233:LYS:HD2	2.05	0.71
48:5:181:C:N3	48:5:256:G:C2	2.59	0.70
47:3:39:U:O4'	57:FF:135:ARG:NH2	2.23	0.70
7:G:87:LEU:CD2	7:G:184:LEU:HD21	2.20	0.70
48:5:499:G:N2	48:5:656:C:C2	2.60	0.70
51:9:751:G:C2	51:9:792:C:N3	2.59	0.70
9:I:87:ILE:HG12	9:I:138:ILE:HG12	1.74	0.70
51:9:1455:A:HO2'	51:9:1456:G:P	2.15	0.70
48:5:1958:A:C5'	48:5:1962:A:HO2'	1.88	0.70
51:9:1212:G:O2'	51:9:1213:C:O5'	2.10	0.70
48:5:482:G:H2'	48:5:483:G:C8	2.27	0.69
48:5:4901:G:N2	48:5:4921:C:C2	2.60	0.69
57:FF:35:LEU:HD23	57:FF:147:VAL:HG22	1.73	0.69
48:5:2773:G:N2	48:5:2774:C:C2	2.61	0.69
48:5:4510:A:O2'	48:5:4511:A:O4'	2.11	0.69
54:CC:63:VAL:CG1	54:CC:63:VAL:O	2.41	0.69
48:5:1279:A:C2'	48:5:1280:C:H5''	2.21	0.69
48:5:1968:G:H1	48:5:2018:C:N4	1.89	0.69
9:I:187:GLU:OE1	9:I:189:ARG:NE	2.24	0.69
2:B:163:LEU:CD2	2:B:182:GLU:HG3	2.17	0.69
48:5:166:C:O2	48:5:166:C:H2'	1.90	0.69
48:5:4075:U:O2'	48:5:4076:G:H2'	1.91	0.69
48:5:2367:A:N6	48:5:2788:U:N3	2.40	0.69
48:5:4481:U:H2'	48:5:4482:U:C6	2.27	0.69
48:5:499:G:C2	48:5:656:C:C2	2.81	0.69
4:D:69:ILE:HD11	19:T:28:ALA:HB1	1.75	0.69
7:G:156:VAL:CG1	7:G:184:LEU:HD12	2.14	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1635:C:H2'	48:5:1636:U:H5'	1.75	0.69
51:9:309:G:N2	51:9:310:C:C2	2.61	0.69
48:5:1929:A:N1	48:5:2054:U:C4	2.59	0.68
2:B:261:ARG:HE	48:5:3870:C:H4'	1.57	0.68
48:5:1367:C:N3	48:5:1369:C:OP2	2.26	0.68
47:3:1:G:N2	47:3:2:C:C2	2.61	0.68
48:5:166:C:O2	48:5:167:C:H5	1.76	0.68
48:5:504:G:C6	48:5:654:C:N3	2.61	0.68
48:5:978:G:H2'	48:5:979:C:O4'	1.92	0.68
51:9:289:G:OP1	56:EE:155:LYS:HE3	1.94	0.68
47:3:13:C:N3	47:3:22:G:O6	2.26	0.68
48:5:1991:A:N6	48:5:2003:G:OP1	2.25	0.68
48:5:1380:G:O2'	48:5:1381:U:O2	2.10	0.68
48:5:1958:A:O2'	48:5:1959:U:C5'	2.41	0.68
47:3:39:U:O2'	47:3:40:C:H6	1.77	0.68
66:OO:95:ILE:HD11	66:OO:126:ILE:HD12	1.75	0.68
47:3:76:A:N6	48:5:4371:G:N7	2.41	0.68
47:3:76:A:C6	48:5:4371:G:C5	2.81	0.68
51:9:1235:G:H2'	51:9:1236:G:H8	1.59	0.68
51:9:1253:A:OP2	51:9:1526:G:N2	2.26	0.68
48:5:497:G:N2	48:5:657:C:C2	2.62	0.67
51:9:1406:G:C3'	51:9:1407:U:H4'	2.24	0.67
3:C:313:VAL:HG11	6:F:172:THR:HG21	1.76	0.67
48:5:2409:U:C4	48:5:2783:A:C2	2.82	0.67
48:5:2288:G:N2	48:5:2290:C:C2	2.63	0.67
48:5:4453:C:C2	48:5:4529:G:C2	2.82	0.67
48:5:642:G:N2	48:5:643:C:C2	2.62	0.67
51:9:1109:C:O2	51:9:1109:C:H2'	1.93	0.67
51:9:1137:U:N3	51:9:1148:A:N6	2.42	0.67
58:GG:67:VAL:HG23	58:GG:99:GLY:HA2	1.74	0.67
48:5:1358:G:H8	48:5:1358:G:H3'	1.58	0.67
48:5:166:C:O2	48:5:167:C:C5	2.48	0.67
48:5:3914:U:H3	48:5:4378:A:H61	1.37	0.67
51:9:1137:U:C4	51:9:1148:A:C6	2.82	0.67
6:F:245:LEU:HD23	6:F:249:MET:HG3	1.77	0.67
48:5:973:G:N2	48:5:1282:G:O2'	2.28	0.67
3:C:210:ILE:HG21	3:C:252:TRP:CZ3	2.30	0.67
48:5:5026:U:OP2	60:II:79:ILE:HD13	1.95	0.67
47:3:39:U:H4'	66:OO:66:ARG:HH22	1.60	0.67
48:5:1268:G:H4'	48:5:1269:G:OP1	1.95	0.67
51:9:1447:G:H2'	51:9:1448:A:C8	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1264:C:H2'	48:5:1265:G:O4'	1.95	0.67
51:9:446:G:OP2	60:II:47:ARG:NH1	2.27	0.67
11:L:56:ARG:O	11:L:116:ARG:NH2	2.28	0.66
5:E:161:LEU:HD21	5:E:253:ILE:HD11	1.76	0.66
48:5:1359:G:H2'	48:5:1360:G:C8	2.30	0.66
48:5:1957:U:O2'	48:5:1958:A:H8	1.78	0.66
48:5:22:G:C2	50:8:35:C:N3	2.64	0.66
51:9:1466:G:N2	51:9:1467:C:C2	2.63	0.66
10:J:83:LEU:HD12	10:J:170:TYR:OH	1.96	0.66
51:9:103:A:OP2	51:9:356:C:N4	2.29	0.66
47:3:33:U:P	57:FF:127:ARG:HH12	2.19	0.66
48:5:1957:U:C2'	48:5:1958:A:C8	2.79	0.66
25:Z:52:LYS:O	25:Z:65:ARG:NH2	2.29	0.66
48:5:2826:U:H4'	48:5:2827:G:H5'	1.77	0.66
51:9:1308:U:H2'	51:9:1309:C:O4'	1.96	0.66
10:J:83:LEU:HD12	10:J:170:TYR:CZ	2.31	0.66
48:5:1358:G:C6	48:5:1379:C:N3	2.64	0.66
48:5:199:G:C6	48:5:201:C:N4	2.64	0.66
51:9:316:G:N2	51:9:317:C:C2	2.64	0.66
5:E:202:VAL:HG13	5:E:256:LYS:HZ1	1.50	0.65
76:YY:110:ARG:O	76:YY:113:ARG:O	2.14	0.65
51:9:1526:G:N2	51:9:1527:C:C2	2.65	0.65
51:9:15:U:H2'	51:9:16:G:O4'	1.95	0.65
71:TT:38:LYS:O	71:TT:39:LEU:HB2	1.95	0.65
48:5:1958:A:H3'	48:5:1958:A:OP2	1.96	0.65
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.29	0.65
9:I:184:MET:HG2	9:I:189:ARG:HD2	1.79	0.65
48:5:723:A:H2	48:5:943:A:N1	1.93	0.65
51:9:1727:G:H2'	51:9:1728:U:O4'	1.97	0.65
48:5:1635:C:C2'	48:5:1636:U:H5'	2.27	0.65
51:9:1679:A:O2'	51:9:1680:G:OP2	2.09	0.65
3:C:271:ALA:O	3:C:272:SER:OG	2.11	0.65
47:3:39:U:O2'	47:3:40:C:O5'	2.14	0.65
2:B:14:LEU:HD23	2:B:17:LEU:HD21	1.77	0.65
48:5:1378:C:H3'	48:5:1379:C:C5'	2.26	0.65
2:B:45:ALA:HB3	2:B:183:ILE:HG23	1.79	0.65
4:D:200:MET:CE	4:D:241:LYS:HE3	2.26	0.65
48:5:1969:G:O2'	48:5:1970:A:H5'	1.97	0.65
51:9:164:A:O2'	51:9:165:G:O4'	2.15	0.65
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.78	0.65
51:9:1102:G:N1	51:9:1103:C:C4	2.65	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1681:U:O2'	51:9:1682:C:O5'	2.14	0.64
51:9:1416:C:H2'	51:9:1417:C:C2	2.33	0.64
51:9:200:G:N2	51:9:201:C:C2	2.65	0.64
51:9:980:A:H2'	51:9:981:A:C8	2.32	0.64
48:5:1358:G:C8	48:5:1358:G:H3'	2.32	0.64
48:5:2258:C:H2'	48:5:2258:C:O2	1.96	0.64
48:5:2468:U:H3	48:5:2473:A:N6	1.91	0.64
51:9:1401:A:C2	51:9:1402:A:C6	2.85	0.64
9:I:191:ILE:CD1	9:I:200:ILE:HD11	2.14	0.64
48:5:2090:U:P	48:5:2090:U:O4'	2.56	0.64
9:I:184:MET:CE	9:I:190:LEU:HD11	2.27	0.64
48:5:1404:G:C2	48:5:1414:C:C2	2.85	0.64
51:9:50:A:N1	51:9:488:U:O4	2.30	0.64
51:9:522:A:O3'	61:JJ:131:ARG:NH2	2.31	0.64
68:QQ:12:VAL:HG21	68:QQ:91:ALA:HA	1.80	0.64
48:5:986:C:C2	48:5:1068:G:N2	2.65	0.64
51:9:1617:G:N7	67:PP:43:ARG:NH1	2.46	0.64
14:O:201:PHE:HB2	14:O:202:LEU:HD13	1.80	0.64
48:5:2084:C:H3'	48:5:2085:G:C5'	2.27	0.64
48:5:5066:U:H2'	48:5:5067:U:C6	2.32	0.64
49:7:30:C:C2	49:7:48:G:N2	2.65	0.64
51:9:1835:A:C4	51:9:1863:A:N7	2.66	0.64
56:EE:31:PRO:CD	56:EE:38:LEU:HD13	2.28	0.64
48:5:1682:A:C2	48:5:1683:U:C2	2.85	0.64
48:5:2268:A:H4'	48:5:2269:C:H5'	1.80	0.64
51:9:1211:G:O2'	51:9:1212:G:H5'	1.97	0.64
51:9:1384:C:C2'	51:9:1385:G:H5'	2.28	0.64
56:EE:163:ASP:O	56:EE:164:LEU:HB2	1.97	0.64
9:I:184:MET:HE1	9:I:190:LEU:CD1	2.27	0.64
48:5:969:C:O2'	48:5:970:G:N3	2.31	0.63
7:G:86:VAL:HG13	7:G:183:ILE:O	1.98	0.63
51:9:1859:A:C2	51:9:1860:A:C6	2.85	0.63
51:9:200:G:N1	51:9:201:C:C4	2.66	0.63
71:TT:33:TRP:O	71:TT:35:ASP:N	2.31	0.63
48:5:1213:G:N1	48:5:1215:C:C2	2.67	0.63
48:5:4213:A:N1	48:5:4218:U:C4	2.61	0.63
48:5:4579:U:H2'	48:5:4580:U:C6	2.33	0.63
48:5:4723:A:C2	48:5:4724:A:C6	2.86	0.63
48:5:1378:C:H3'	48:5:1379:C:H5'	1.81	0.63
48:5:167:C:C2	48:5:269:G:N2	2.66	0.63
48:5:1823:G:O3'	48:5:1825:A:P	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:107:A:H2'	51:9:108:G:C8	2.33	0.63
4:D:200:MET:HE1	4:D:241:LYS:HG3	1.80	0.63
48:5:976:G:OP1	48:5:976:G:H4'	1.98	0.63
4:D:200:MET:HE2	4:D:241:LYS:HE3	1.80	0.63
47:3:37:A:C2'	47:3:38:A:H5'	2.28	0.63
47:3:41:U:O3'	57:FF:198:ARG:CD	2.40	0.63
54:CC:73:VAL:CG1	54:CC:73:VAL:O	2.47	0.63
48:5:1550:G:C2	48:5:1579:C:C2	2.86	0.63
5:E:254:LEU:HD23	5:E:257:ILE:CD1	2.14	0.63
17:R:107:ARG:C	17:R:107:ARG:HD2	3.55	0.63
48:5:504:G:C6	48:5:654:C:C2	2.87	0.63
51:9:830:A:N6	51:9:844:U:H3	1.97	0.63
6:F:161:TYR:CE2	6:F:170:ALA:HB2	2.34	0.63
9:I:184:MET:HE2	9:I:190:LEU:CG	2.27	0.63
48:5:22:G:C2	50:8:35:C:C2	2.87	0.62
11:L:65:ARG:HG2	11:L:66:TYR:CE2	2.34	0.62
48:5:1983:A:C6	48:5:2008:U:O4	2.52	0.62
48:5:2547:G:N2	48:5:2548:C:C2	2.68	0.62
47:3:35:U:H1'	51:9:1641:A:OP1	1.98	0.62
51:9:1842:C:C2	51:9:1858:G:C2	2.87	0.62
3:C:158:VAL:HA	3:C:161:TYR:CD2	2.33	0.62
9:I:204:GLY:O	9:I:205:PRO:O	2.16	0.62
48:5:1879:C:O2'	48:5:1891:A:N3	2.29	0.62
48:5:2108:G:C6	48:5:2125:C:N4	2.67	0.62
48:5:3668:C:C2	48:5:3675:G:C2	2.87	0.62
51:9:1211:G:C2'	51:9:1212:G:H5'	2.29	0.62
3:C:32:ILE:HD12	3:C:130:ALA:HB2	1.82	0.62
48:5:1339:U:H2'	48:5:1340:C:C6	2.34	0.62
48:5:3900:G:N2	48:5:4562:C:C2	2.67	0.62
7:G:87:LEU:CD2	7:G:184:LEU:CD2	2.77	0.62
51:9:448:A:H5''	60:II:25:ARG:HA	1.80	0.62
4:D:200:MET:CE	4:D:241:LYS:HG3	2.28	0.62
48:5:3783:A:H4'	48:5:3784:A:H5''	1.81	0.62
48:5:4769:G:H2'	48:5:4770:U:O4'	2.00	0.62
53:BB:30:TRP:CZ2	53:BB:48:LEU:HD23	2.35	0.62
7:G:86:VAL:CG1	7:G:87:LEU:N	2.57	0.62
12:M:81:ASP:OD1	12:M:84:THR:CG2	2.47	0.62
51:9:1408:U:O4	51:9:1409:A:N6	2.33	0.62
48:5:2409:U:O4	48:5:2783:A:C6	2.52	0.62
9:I:184:MET:CE	9:I:190:LEU:CG	2.78	0.62
48:5:3765:G:O2'	48:5:3766:A:C8	2.49	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:217:A:C2	51:9:309:G:N1	2.67	0.62
48:5:1081:C:C2	48:5:1220:G:C2	2.87	0.61
48:5:2905:C:C2	48:5:3590:G:N2	2.68	0.61
48:5:3723:A:C2	48:5:3724:A:C6	2.88	0.61
51:9:33:G:O6	51:9:522:A:H2	1.83	0.61
51:9:751:G:N2	51:9:792:C:C2	2.68	0.61
51:9:1771:G:N2	51:9:1772:C:C2	2.67	0.61
51:9:488:U:H2'	51:9:488:U:O2	2.00	0.61
24:Y:49:ILE:HD13	24:Y:80:ILE:HD13	1.82	0.61
48:5:1241:C:N4	48:5:1270:A:O2'	2.34	0.61
48:5:1296:G:H1'	48:5:1297:U:P	2.41	0.61
16:Q:65:ARG:NH1	48:5:1502:G:OP1	2.32	0.61
48:5:1723:A:N1	48:5:1838:A:C2	2.67	0.61
48:5:2045:G:O6	48:5:3870:C:O2'	2.17	0.61
48:5:77:U:H3	48:5:335:A:N6	1.97	0.61
48:5:1186:U:H2'	48:5:1187:G:O4'	2.00	0.61
48:5:1358:G:C8	48:5:1358:G:C3'	2.84	0.61
48:5:4885:U:H2'	48:5:4886:C:O4'	1.99	0.61
51:9:1233:G:O2'	51:9:1234:C:H5'	1.99	0.61
51:9:834:C:N3	51:9:841:G:C2	2.68	0.61
5:E:59:TYR:CD2	5:E:64:LEU:CD1	2.73	0.61
48:5:1983:A:C2	48:5:2008:U:C4	2.87	0.61
48:5:2127:C:H2'	48:5:2128:G:C8	2.36	0.61
51:9:1616:U:OP2	67:PP:43:ARG:NH2	2.33	0.61
74:WW:6:VAL:HG13	74:WW:29:PRO:HG2	1.83	0.61
47:3:38:A:O2'	47:3:39:U:H5'	2.00	0.61
48:5:1999:A:H1'	48:5:2017:A:N1	2.16	0.61
48:5:2758:G:O2'	48:5:2764:A:N3	2.26	0.61
48:5:977:C:C4	48:5:978:G:N7	2.69	0.61
58:GG:3:LEU:HD13	58:GG:111:LEU:HD11	1.82	0.61
18:S:9:GLU:HG2	18:S:33:PHE:CE2	2.36	0.61
48:5:1957:U:C2'	48:5:1958:A:H8	2.14	0.61
51:9:409:C:C2	51:9:432:G:N2	2.68	0.61
48:5:197:A:N1	48:5:225:G:O2'	2.25	0.61
48:5:1987:C:H2'	48:5:1987:C:O2	2.00	0.61
48:5:2554:U:H4'	48:5:2555:G:OP1	2.01	0.61
48:5:2623:A:C2	48:5:2624:G:C5	2.89	0.61
48:5:3594:C:H2'	48:5:3594:C:O2	2.01	0.61
48:5:4411:G:C2	48:5:4432:C:C2	2.89	0.61
51:9:1351:G:O2'	51:9:1378:A:N1	2.20	0.61
51:9:1531:A:H2'	51:9:1532:C:C6	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.83	0.60
2:B:163:LEU:HD23	2:B:182:GLU:CG	2.24	0.60
63:LL:77:VAL:HG22	63:LL:86:ILE:HD12	1.83	0.60
48:5:181:C:C2	48:5:256:G:N2	2.69	0.60
48:5:111:C:C2	48:5:331:G:C2	2.89	0.60
51:9:474:G:N2	51:9:475:C:C2	2.70	0.60
2:B:120:LYS:N	48:5:4968:A:OP1	2.33	0.60
51:9:301:A:N3	60:II:73:THR:HG21	2.15	0.60
48:5:3629:A:O4'	51:9:1721:U:O2	2.19	0.60
3:C:114:ARG:HB2	3:C:114:ARG:CZ	2.31	0.60
3:C:45:ARG:NH2	48:5:2295:C:O2'	2.34	0.60
48:5:515:C:C2	48:5:647:G:C2	2.90	0.60
3:C:76:ILE:HG22	3:C:77:PRO:HD2	1.84	0.60
65:NN:125:LEU:HD22	65:NN:129:TYR:CE2	2.36	0.60
48:5:1213:G:C2	48:5:1215:C:O2	2.54	0.60
48:5:286:U:H2'	48:5:287:U:C6	2.37	0.60
48:5:1268:G:C2	48:5:1270:A:C8	2.90	0.60
13:N:202:ARG:NH2	48:5:1372:A:OP1	2.34	0.60
48:5:1672:U:H2'	48:5:1673:U:C6	2.36	0.60
48:5:2288:G:N1	48:5:2290:C:C4	2.70	0.60
48:5:106:A:H1'	48:5:336:A:C8	2.36	0.60
48:5:4207:C:C2	48:5:4226:G:C2	2.90	0.60
56:EE:173:ILE:HD11	56:EE:235:TRP:CE3	2.36	0.60
48:5:2616:C:C2	48:5:2722:G:C2	2.89	0.60
51:9:1130:G:C2	51:9:1131:G:C8	2.89	0.60
75:XX:41:PHE:O	75:XX:43:GLY:N	2.34	0.60
48:5:1839:U:H2'	48:5:1840:G:O4'	2.00	0.60
48:5:2793:G:C5	48:5:2797:C:N4	2.69	0.60
48:5:4283:G:N2	48:5:4284:C:C2	2.70	0.60
63:LL:66:VAL:HG23	63:LL:131:CYS:SG	2.42	0.60
48:5:4901:G:C2	48:5:4921:C:N3	2.70	0.60
51:9:1551:U:H2'	51:9:1552:G:C8	2.37	0.60
51:9:293:C:O2	51:9:293:C:H2'	2.02	0.60
56:EE:183:VAL:HG11	56:EE:220:THR:HG21	1.82	0.60
56:EE:48:LEU:HD21	56:EE:70:ILE:HD11	1.84	0.60
48:5:4092:G:N2	48:5:4158:C:C2	2.70	0.59
48:5:4892:A:N1	48:5:4927:G:O6	2.35	0.59
48:5:5000:G:C2	48:5:5051:C:C2	2.89	0.59
51:9:598:G:C2	51:9:639:C:C2	2.90	0.59
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.36	0.59
46:2:53:G:C2	46:2:62:C:C2	2.90	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1074:G:N2	48:5:1075:G:C2	2.71	0.59
48:5:3617:G:O2'	48:5:3620:G:N7	2.35	0.59
51:9:1528:G:N2	51:9:1529:C:C2	2.70	0.59
62:KK:15:LEU:HD22	62:KK:49:MET:CE	2.32	0.59
62:KK:15:LEU:HD22	62:KK:49:MET:HE3	1.84	0.59
48:5:2827:G:H2'	48:5:2827:G:N3	2.18	0.59
55:DD:64:ARG:NH2	62:KK:73:ASN:OD1	2.35	0.59
73:VV:55:ILE:HD11	73:VV:69:ILE:HD11	1.83	0.59
48:5:166:C:O2	48:5:166:C:C2'	2.49	0.59
48:5:222:C:H2'	48:5:223:G:O4'	2.03	0.59
51:9:834:C:H3'	51:9:835:C:C4'	2.33	0.59
2:B:154:LYS:HB2	2:B:154:LYS:NZ	2.18	0.59
9:I:204:GLY:O	9:I:205:PRO:C	2.41	0.59
47:3:5:G:N2	47:3:6:G:C4	2.71	0.59
3:C:108:TRP:HZ2	11:L:19:GLN:HE21	1.51	0.59
12:M:116:LYS:HG3	14:O:196:LEU:CD2	2.20	0.59
18:S:53:LYS:NZ	49:7:74:A:O2'	2.35	0.59
48:5:1266:G:H5''	48:5:2112:G:C2	2.37	0.59
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.50	0.59
48:5:1541:C:C2	48:5:1619:G:C2	2.90	0.59
48:5:3662:A:H61	48:5:3680:U:H3	1.48	0.59
48:5:917:A:C2	48:5:919:C:C5	2.90	0.59
47:3:41:U:C3'	57:FF:198:ARG:HD3	2.32	0.59
49:7:30:C:N3	49:7:48:G:C2	2.71	0.59
58:GG:188:LYS:HA	58:GG:191:ARG:HD3	1.85	0.59
48:5:2446:C:C2	48:5:2515:G:C2	2.90	0.59
51:9:190:G:O2'	51:9:209:A:N6	2.36	0.59
48:5:113:A:H2'	48:5:114:G:O4'	2.03	0.59
48:5:1957:U:H2'	48:5:1958:A:C8	2.38	0.59
14:O:18:ARG:NH2	48:5:2057:A:OP1	2.36	0.59
51:9:50:A:N1	51:9:488:U:C4	2.71	0.59
3:C:357:ALA:O	3:C:361:LYS:HG3	2.03	0.59
48:5:2084:C:H3'	48:5:2085:G:H5'	1.84	0.58
48:5:2654:C:C2	48:5:2681:G:N2	2.71	0.58
61:JJ:53:ILE:HD13	61:JJ:81:LEU:HD21	1.85	0.58
51:9:1398:G:N2	51:9:1399:C:C2	2.71	0.58
74:WW:106:THR:HG1	74:WW:109:GLY:H	1.52	0.58
48:5:4219:A:H2'	48:5:4220:A:C8	2.37	0.58
51:9:217:A:C2	51:9:218:U:C6	2.90	0.58
47:3:10:G:N2	47:3:11:C:C2	2.71	0.58
48:5:4441:A:H8	48:5:4441:A:H5''	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:976:G:C2	48:5:977:C:C2	2.92	0.58
51:9:309:G:N1	51:9:310:C:C4	2.71	0.58
10:J:119:TYR:HE2	10:J:125:ILE:HD11	1.67	0.58
47:3:53:G:C2	47:3:62:C:C2	2.92	0.58
48:5:1074:G:C2	48:5:1238:A:C2	2.91	0.58
48:5:1957:U:H2'	48:5:1958:A:H8	1.67	0.58
48:5:919:C:C4	48:5:920:C:C5	2.92	0.58
51:9:1488:C:O2'	51:9:1490:G:OP2	2.22	0.58
51:9:752:G:C6	51:9:790:C:N4	2.71	0.58
51:9:872:A:N6	51:9:914:U:C5	2.72	0.58
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	1.86	0.58
48:5:1213:G:O6	48:5:1215:C:C4	2.57	0.58
48:5:642:G:N1	48:5:643:C:C4	2.71	0.58
20:U:87:THR:HG23	20:U:102:VAL:HG21	1.85	0.58
75:XX:67:ARG:HG2	75:XX:115:ILE:HD12	1.85	0.58
47:3:13:C:O2	47:3:22:G:N1	2.32	0.58
48:5:300:A:C2	48:5:301:G:C5	2.92	0.58
48:5:707:C:C2	48:5:1291:G:C2	2.92	0.58
51:9:412:G:N2	51:9:429:C:C2	2.72	0.58
57:FF:72:LEU:HD22	57:FF:112:LEU:HD11	1.86	0.58
48:5:4754:G:C2	48:5:4880:C:C2	2.92	0.58
48:5:685:C:H2'	48:5:685:C:O2	2.04	0.58
56:EE:55:ALA:HB2	56:EE:64:ILE:HD12	1.85	0.58
48:5:1279:A:C3'	48:5:1280:C:C5'	2.78	0.58
52:AA:38:ILE:HD11	52:AA:150:THR:HG22	1.86	0.58
56:EE:156:MET:O	56:EE:157:ASN:ND2	2.37	0.58
17:R:10:LEU:O	17:R:14:VAL:HG23	2.03	0.58
47:3:76:A:C6	48:5:4371:G:N7	2.72	0.58
48:5:4757:C:O4'	48:5:4757:C:O2	2.21	0.58
51:9:31:U:O2'	51:9:643:A:N1	2.33	0.58
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.34	0.58
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	1.86	0.58
48:5:1280:C:C2	48:5:1282:G:C5	2.93	0.57
48:5:1358:G:H2'	48:5:1359:G:O4'	2.04	0.57
48:5:245:C:O4'	48:5:245:C:O2	2.22	0.57
51:9:1543:U:HO2'	68:QQ:77:HIS:HE2	1.52	0.57
1:A:207:VAL:HG11	48:5:1633:G:C6	2.38	0.57
48:5:1757:U:H2'	48:5:1758:G:O4'	2.03	0.57
48:5:1840:G:H3'	48:5:1842:G:P	2.44	0.57
48:5:1959:U:H1'	48:5:1961:G:C1'	2.35	0.57
51:9:643:A:OP1	51:9:643:A:H4'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:202:VAL:HG12	5:E:256:LYS:NZ	2.17	0.57
59:HH:93:VAL:HG21	59:HH:133:LEU:HD23	1.84	0.57
48:5:5026:U:H3'	60:II:79:ILE:CD1	2.34	0.57
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.86	0.57
11:L:71:ARG:NH2	48:5:74:G:O3'	2.36	0.57
50:8:83:C:H4'	50:8:85:U:O2	2.03	0.57
51:9:1233:G:C2'	51:9:1234:C:H5'	2.34	0.57
11:L:42:ARG:HG3	11:L:45:ARG:HH12	1.69	0.57
74:WW:30:CYS:SG	74:WW:31:SER:N	2.77	0.57
48:5:3751:G:O2'	48:5:3775:A:N6	2.37	0.57
48:5:4461:C:O2	48:5:4516:G:C2	2.58	0.57
51:9:1406:G:H2'	51:9:1407:U:O3'	2.04	0.57
6:F:91:LEU:HD22	6:F:92:ALA:N	2.20	0.57
48:5:2256:C:H2'	48:5:2256:C:O2	2.04	0.57
48:5:4975:G:N2	48:5:4984:C:C2	2.72	0.57
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.86	0.57
48:5:2367:A:N6	48:5:2798:A:O4'	2.37	0.57
51:9:1212:G:O2'	51:9:1213:C:O4'	2.22	0.57
51:9:1233:G:C6	51:9:1234:C:C4	2.93	0.57
48:5:1639:U:N3	48:5:1643:A:O2'	2.37	0.57
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.87	0.57
14:O:7:LEU:HD22	14:O:9:LEU:HD21	1.86	0.57
51:9:316:G:N1	51:9:317:C:C4	2.72	0.57
48:5:1279:A:OP1	48:5:1279:A:O3'	2.22	0.57
48:5:3870:C:C2	48:5:3886:G:C2	2.92	0.57
51:9:1347:U:H2'	51:9:1348:G:C8	2.39	0.57
48:5:2408:U:C1'	48:5:2409:U:C5	2.88	0.57
50:8:55:U:C4	50:8:62:A:N1	2.72	0.57
51:9:195:C:C2	51:9:205:G:N2	2.73	0.57
51:9:322:C:O2'	51:9:323:C:OP2	2.21	0.57
3:C:313:VAL:CG1	6:F:172:THR:HG21	2.35	0.57
48:5:1365:C:H4'	48:5:1366:G:OP1	2.05	0.56
48:5:2773:G:N1	48:5:2774:C:C4	2.73	0.56
48:5:685:C:O2	48:5:685:C:C2'	2.53	0.56
47:3:35:U:O4'	51:9:1641:A:OP1	2.22	0.56
53:BB:141:GLY:HA2	53:BB:210:VAL:HG22	1.87	0.56
3:C:336:ARG:O	3:C:340:ILE:HG12	2.05	0.56
61:JJ:125:HIS:NE2	61:JJ:129:LEU:HD21	2.20	0.56
76:YY:113:ARG:O	76:YY:114:MET:HB2	2.05	0.56
48:5:2409:U:C5	48:5:2783:A:C2	2.93	0.56
51:9:1137:U:H3	51:9:1148:A:N6	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1760:G:C2	51:9:1773:C:C2	2.93	0.56
7:G:156:VAL:CG1	7:G:184:LEU:CD1	2.78	0.56
48:5:665:C:H2'	48:5:665:C:O2	2.05	0.56
49:7:66:G:C2	49:7:67:C:C2	2.93	0.56
7:G:86:VAL:HG22	7:G:183:ILE:HG22	1.87	0.56
10:J:83:LEU:CD1	10:J:170:TYR:CZ	2.87	0.56
23:X:139:ARG:NH2	48:5:2533:C:OP1	2.38	0.56
48:5:3709:U:O2'	48:5:3710:G:O4'	2.21	0.56
48:5:516:C:N3	48:5:646:G:C2	2.74	0.56
51:9:911:C:O2'	51:9:912:C:H5'	2.05	0.56
58:GG:214:ALA:O	58:GG:218:LYS:N	2.36	0.56
47:3:39:U:O2'	47:3:40:C:C6	2.57	0.56
48:5:1278:C:C6	48:5:1279:A:H1'	2.40	0.56
48:5:1398:A:O2'	48:5:1399:G:OP2	2.20	0.56
51:9:167:G:C6	51:9:168:C:C5	2.94	0.56
51:9:830:A:N1	51:9:844:U:C4	2.74	0.56
51:9:1009:A:O2'	65:NN:114:ARG:HG3	2.05	0.56
19:T:64:VAL:HG13	19:T:72:VAL:HG13	1.88	0.56
48:5:2258:C:C2'	48:5:2258:C:O2	2.54	0.56
48:5:2524:U:H5''	48:5:2711:G:C2	2.40	0.56
48:5:2640:G:N7	48:5:2694:G:O6	2.37	0.56
48:5:4101:C:C2	48:5:4109:G:C2	2.94	0.56
48:5:1666:C:O2'	48:5:1688:G:OP1	2.21	0.56
48:5:1268:G:C4	48:5:2111:G:C2	2.93	0.56
48:5:3759:A:N1	51:9:1708:C:O2'	2.30	0.56
48:5:4260:U:H2'	48:5:4261:C:C6	2.40	0.56
48:5:746:A:O2'	48:5:747:A:O5'	2.20	0.56
51:9:1545:A:H2'	51:9:1546:G:C8	2.41	0.56
17:R:60:ARG:NH1	17:R:63:CYS:SG	2.79	0.56
49:7:30:C:C2	49:7:48:G:C2	2.94	0.56
53:BB:85:LYS:HB3	53:BB:101:HIS:HB3	1.88	0.56
6:F:146:TYR:CE2	6:F:239:GLU:HB3	2.41	0.56
48:5:1279:A:H2'	48:5:1280:C:H5''	1.88	0.56
48:5:1360:G:C6	48:5:1361:G:C5	2.94	0.56
48:5:4416:G:N2	48:5:4417:C:C2	2.74	0.56
48:5:976:G:C6	48:5:977:C:C4	2.93	0.56
51:9:1231:C:H2'	51:9:1232:U:O4'	2.05	0.56
51:9:1643:U:H2'	51:9:1644:C:C6	2.40	0.56
51:9:434:G:H2'	51:9:435:A:C8	2.41	0.56
3:C:114:ARG:CZ	48:5:1358:G:H5''	2.36	0.56
48:5:1404:G:N2	48:5:1414:C:C2	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2555:G:O6	48:5:2572:C:N4	2.37	0.56
48:5:370:U:C6	48:5:1637:A:C2	2.93	0.56
49:7:82:G:C2	49:7:95:C:C2	2.94	0.56
50:8:155:C:H2'	50:8:156:U:O4'	2.05	0.56
51:9:1613:G:C2	51:9:1627:C:C2	2.93	0.56
59:HH:39:GLN:HG3	59:HH:75:ILE:HD12	1.87	0.56
48:5:1959:U:H1'	48:5:1961:G:N9	2.21	0.56
48:5:2028:C:O2'	48:5:2029:A:O5'	2.24	0.56
48:5:3593:C:H4'	48:5:3594:C:OP2	2.05	0.56
48:5:466:A:C2	48:5:467:U:C4	2.94	0.56
48:5:1269:G:C6	48:5:2111:G:N2	2.74	0.55
48:5:2481:G:C2	48:5:2498:C:C2	2.94	0.55
51:9:1117:C:O2	51:9:1117:C:O4'	2.25	0.55
51:9:1500:G:C6	51:9:1501:C:C4	2.94	0.55
51:9:1520:G:N3	51:9:1520:G:H2'	2.20	0.55
47:3:41:U:H4'	57:FF:198:ARG:HD3	1.88	0.55
15:P:36:ILE:HD12	15:P:48:LEU:HD11	1.88	0.55
48:5:2256:C:O2	48:5:2256:C:C2'	2.54	0.55
14:O:18:ARG:NH1	48:5:2053:C:O3'	2.38	0.55
17:R:10:LEU:HB3	17:R:41:ILE:HD13	1.88	0.55
47:3:39:U:O2'	47:3:40:C:C5'	2.54	0.55
48:5:1277:G:N2	48:5:1278:C:C2	2.75	0.55
48:5:2547:G:N1	48:5:2548:C:C4	2.75	0.55
48:5:4586:G:H5''	48:5:4586:G:H8	1.70	0.55
54:CC:75:ILE:HG23	54:CC:80:GLU:OE1	2.06	0.55
47:3:37:A:H2'	47:3:38:A:H5'	1.88	0.55
48:5:106:A:H2'	48:5:107:G:O4'	2.06	0.55
48:5:2557:G:C2	48:5:2571:C:C2	2.94	0.55
48:5:3612:C:H1'	48:5:5016:A:C8	2.41	0.55
48:5:181:C:N4	48:5:256:G:C6	2.74	0.55
15:P:69:ARG:NH2	48:5:4568:A:N3	2.55	0.55
48:5:497:G:C2	48:5:657:C:C2	2.94	0.55
51:9:642:U:H4'	51:9:643:A:OP1	2.05	0.55
15:P:48:LEU:HD12	15:P:92:LEU:HD13	1.87	0.55
48:5:2408:U:O4'	48:5:2409:U:C5	2.60	0.55
48:5:4524:G:N2	48:5:4525:C:C2	2.75	0.55
48:5:937:U:H2'	48:5:937:U:O2	2.07	0.55
51:9:1282:A:H3'	51:9:1283:C:C5'	2.36	0.55
51:9:145:G:N7	58:GG:178:ARG:NH1	2.54	0.55
3:C:158:VAL:HG22	3:C:161:TYR:HE2	1.71	0.55
45:1:68:VAL:C	46:2:76:A:O2'	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1279:A:C2	48:5:1280:C:C2	2.95	0.55
48:5:1371:A:N6	50:8:28:C:O2'	2.40	0.55
48:5:1743:A:C5	48:5:1744:U:C5	2.95	0.55
48:5:1751:A:C2	48:5:1780:A:C2	2.95	0.55
51:9:1741:U:H2'	51:9:1742:C:O4'	2.06	0.55
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	1.88	0.55
48:5:3641:U:H5	48:5:3646:A:N7	2.04	0.55
48:5:919:C:N4	48:5:920:C:C5	2.75	0.55
48:5:933:G:C2	48:5:940:C:C6	2.95	0.55
48:5:422:C:C2	50:8:13:G:C2	2.94	0.55
51:9:115:U:H2'	51:9:116:U:C6	2.41	0.55
51:9:1408:U:C4	51:9:1409:A:N6	2.74	0.55
51:9:1698:C:O2	51:9:1698:C:O4'	2.23	0.55
56:EE:55:ALA:HB1	56:EE:60:GLU:HB2	1.88	0.55
48:5:1975:G:O4'	48:5:1984:A:H1'	2.07	0.55
48:5:962:C:OP2	48:5:2264:C:N3	2.40	0.55
51:9:1102:G:N2	51:9:1130:G:N2	2.55	0.55
51:9:1616:U:O4	67:PP:40:ARG:NH1	2.40	0.55
51:9:1137:U:HO2'	52:AA:155:ARG:HH22	1.55	0.55
3:C:168:VAL:HG13	3:C:177:TRP:CZ3	2.41	0.55
5:E:238:ILE:C	5:E:239:THR:HG1	1.99	0.55
47:3:76:A:C5	48:5:4371:G:C5	2.94	0.55
48:5:1249:C:C2	48:5:1262:G:C2	2.95	0.55
48:5:127:G:N2	48:5:128:C:C2	2.75	0.55
48:5:1483:C:O4'	48:5:1483:C:O2	2.23	0.55
48:5:1485:C:O4'	48:5:1485:C:O2	2.23	0.55
48:5:2089:G:O2'	48:5:2090:U:OP2	2.25	0.55
17:R:71:ARG:NH1	48:5:3605:C:OP2	2.36	0.55
48:5:3816:A:O2'	48:5:3819:G:N3	2.39	0.55
51:9:1526:G:N1	51:9:1527:C:C4	2.75	0.55
51:9:698:G:N1	51:9:733:C:C2	2.75	0.55
56:EE:64:ILE:HG23	76:YY:17:LEU:HD13	1.89	0.55
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	1.89	0.55
48:5:2688:G:N2	48:5:2689:C:C2	2.75	0.54
51:9:1265:A:H2'	51:9:1265:A:N3	2.21	0.54
51:9:1760:G:N2	51:9:1773:C:C2	2.76	0.54
51:9:832:G:C2	51:9:843:C:C2	2.95	0.54
52:AA:42:LYS:CG	52:AA:48:ILE:HD11	2.36	0.54
48:5:1205:G:N2	48:5:1206:C:C2	2.76	0.54
51:9:1568:C:O2'	51:9:1569:A:O4'	2.24	0.54
51:9:164:A:C2	51:9:165:G:C8	2.95	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.89	0.54
46:2:34:A:O2'	46:2:35:A:O4'	2.25	0.54
48:5:4389:C:H2'	48:5:4390:A:C8	2.43	0.54
6:F:230:VAL:HA	18:S:39:VAL:HG12	1.89	0.54
72:UU:60:THR:HG22	72:UU:83:ARG:HG2	1.89	0.54
48:5:1968:G:O2'	48:5:1969:G:O5'	2.20	0.54
9:I:184:MET:HE2	9:I:190:LEU:CD1	2.36	0.54
14:O:36:VAL:HG11	14:O:108:ILE:HD12	1.89	0.54
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.39	0.54
48:5:1563:A:C8	48:5:1563:A:O5'	2.60	0.54
48:5:1664:U:H2'	48:5:1665:C:C6	2.42	0.54
48:5:2490:U:O2'	48:5:2491:C:O4'	2.23	0.54
48:5:2905:C:C2	48:5:3590:G:C2	2.96	0.54
48:5:3751:G:O2'	48:5:3752:C:C5'	2.47	0.54
51:9:1220:A:N6	51:9:1221:G:C6	2.75	0.54
51:9:1384:C:H2'	51:9:1385:G:H5'	1.89	0.54
51:9:1839:U:H2'	51:9:1840:U:O4'	2.08	0.54
47:3:16:C:O2	47:3:16:C:O4'	2.25	0.54
48:5:5023:C:O2	48:5:5023:C:O4'	2.23	0.54
2:B:163:LEU:HD23	2:B:182:GLU:HA	1.89	0.54
53:BB:88:THR:HG22	53:BB:96:CYS:HB3	1.88	0.54
56:EE:195:ILE:O	56:EE:196:THR:CB	2.55	0.54
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.87	0.54
75:XX:68:LYS:HB3	75:XX:91:LEU:HD22	1.88	0.54
51:9:1598:G:H3'	77:ZZ:80:ARG:HD2	1.89	0.54
47:3:38:A:C2	57:FF:135:ARG:NH1	2.75	0.54
48:5:2089:G:N3	48:5:2089:G:H2'	2.23	0.54
48:5:4213:A:H61	48:5:4218:U:H3	1.55	0.54
48:5:4730:C:O4'	48:5:4730:C:O2	2.24	0.54
48:5:516:C:C2	48:5:646:G:C2	2.95	0.54
51:9:1129:G:H3'	51:9:1130:G:H8	1.72	0.54
51:9:1144:A:C2	51:9:1145:A:C2	2.95	0.54
51:9:1403:C:O2	51:9:1403:C:C2'	2.54	0.54
65:NN:40:LEU:HD22	65:NN:45:LEU:HD12	1.90	0.54
48:5:1067:G:H2'	48:5:1068:G:O4'	2.07	0.54
3:C:114:ARG:NE	48:5:1358:G:O3'	2.37	0.54
48:5:3662:A:N6	48:5:3680:U:H3	2.06	0.54
51:9:1241:A:C2	51:9:1517:G:O4'	2.61	0.54
16:Q:69:LYS:O	16:Q:75:ARG:NH1	2.39	0.54
48:5:1380:G:H4'	48:5:1381:U:OP1	2.07	0.54
48:5:2367:A:C2	48:5:2788:U:O4	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:76:A:N7	48:5:4371:G:N1	2.56	0.54
48:5:4895:C:H1'	48:5:4896:G:C8	2.43	0.54
48:5:5061:A:O2'	48:5:5062:G:OP2	2.11	0.54
13:N:135:ILE:HD12	13:N:151:ILE:HD13	1.90	0.54
47:3:76:A:C8	48:5:4341:C:N4	2.74	0.54
48:5:1959:U:H4'	48:5:1961:G:C4'	2.37	0.54
49:7:66:G:C6	49:7:67:C:C4	2.95	0.54
51:9:1374:C:H2'	51:9:1375:G:O4'	2.08	0.54
51:9:669:A:N3	51:9:1164:G:O2'	2.38	0.54
1:A:196:TRP:O	1:A:197:PRO:C	2.46	0.54
2:B:116:ARG:HD2	2:B:122:TRP:CD2	2.43	0.54
67:PP:17:TYR:OH	67:PP:37:TYR:HB3	2.08	0.54
48:5:1468:C:C2	48:5:1498:G:C2	2.96	0.53
48:5:301:G:C6	48:5:302:C:C4	2.96	0.53
53:BB:119:THR:H	53:BB:143:THR:HG1	1.54	0.53
74:WW:52:ILE:HG22	74:WW:61:ILE:HG12	1.89	0.53
47:3:76:A:N6	48:5:4371:G:C5	2.77	0.53
48:5:1357:C:H5''	48:5:1358:G:OP1	2.08	0.53
48:5:3718:A:H2'	48:5:3719:A:C8	2.43	0.53
48:5:4717:A:H2'	48:5:4718:G:O4'	2.07	0.53
51:9:750:C:H2'	51:9:750:C:O2	2.08	0.53
51:9:522:A:O2'	61:JJ:131:ARG:NH2	2.42	0.53
51:9:522:A:OP2	61:JJ:45:ARG:NH2	2.42	0.53
19:T:48:VAL:HG21	19:T:94:GLU:HG2	1.90	0.53
48:5:1358:G:O2'	48:5:1359:G:O4'	2.20	0.53
48:5:1430:C:C2	48:5:1455:G:C2	2.96	0.53
48:5:1668:A:C4	48:5:2282:A:C2	2.96	0.53
48:5:2301:G:N2	48:5:2302:C:C2	2.76	0.53
51:9:71:G:O2'	51:9:72:C:OP1	2.20	0.53
56:EE:126:VAL:HG22	56:EE:158:ASP:O	2.08	0.53
47:3:34:U:O2	51:9:1641:A:OP1	2.26	0.53
48:5:3914:U:N3	48:5:4378:A:N6	2.48	0.53
48:5:4635:A:C2	48:5:4664:A:C5	2.96	0.53
51:9:1348:G:H1	51:9:1381:G:H22	1.57	0.53
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.41	0.53
51:9:216:C:O4'	51:9:216:C:O2	2.24	0.53
51:9:823:U:O4'	51:9:823:U:O2	2.25	0.53
48:5:1086:C:C2	48:5:1212:G:C2	2.97	0.53
48:5:4583:C:C4	48:5:4718:G:C6	2.96	0.53
48:5:4723:A:C2	48:5:4724:A:C5	2.97	0.53
51:9:501:C:H2'	51:9:501:C:O2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:686:U:O2	59:HH:118:ARG:NH2	2.32	0.53
10:J:119:TYR:HB3	70:SS:12:ILE:HD13	1.89	0.53
48:5:1297:U:O4'	48:5:1297:U:OP2	2.27	0.53
48:5:2108:G:N1	48:5:2125:C:C4	2.77	0.53
48:5:4977:A:H2'	48:5:4978:G:O4'	2.08	0.53
6:F:244:ARG:NH1	48:5:942:G:OP2	2.42	0.53
50:8:15:G:C6	50:8:16:G:N1	2.76	0.53
51:9:1386:A:H2'	51:9:1387:G:C8	2.43	0.53
53:BB:143:THR:HG22	53:BB:205:TYR:CD1	2.43	0.53
5:E:126:ARG:HH12	48:5:712:C:H2'	1.69	0.53
5:E:202:VAL:HB	5:E:252:GLN:OE1	2.09	0.53
48:5:1398:A:H1'	48:5:1399:G:C8	2.43	0.53
48:5:199:G:C2	48:5:220:C:O2	2.62	0.53
3:C:130:ALA:HB1	3:C:136:LEU:HD12	1.91	0.53
56:EE:31:PRO:HD3	56:EE:38:LEU:HD13	1.90	0.53
48:5:5026:U:H5'	60:II:79:ILE:HD11	1.90	0.53
48:5:2693:G:C6	48:5:2694:G:N1	2.77	0.53
51:9:167:G:N1	51:9:168:C:C4	2.77	0.53
51:9:71:G:H3'	51:9:72:C:H5''	1.91	0.53
7:G:156:VAL:HG13	7:G:184:LEU:HG	1.89	0.53
48:5:1213:G:C6	48:5:1215:C:N3	2.77	0.53
48:5:1447:C:H2'	48:5:1448:G:O4'	2.08	0.53
48:5:986:C:C2	48:5:1068:G:C2	2.97	0.53
51:9:1599:U:O2	51:9:1599:U:O4'	2.24	0.53
46:2:39:G:N2	46:2:40:C:C2	2.76	0.53
48:5:2654:C:C2	48:5:2681:G:C2	2.97	0.53
14:O:72:HIS:N	48:5:4586:G:OP1	2.39	0.53
48:5:5028:G:C6	48:5:5029:C:N4	2.77	0.53
48:5:677:G:N2	48:5:678:C:C2	2.77	0.53
51:9:55:U:C2'	51:9:55:U:O2	2.56	0.53
7:G:29:ASN:HB2	7:G:32:PHE:CE2	2.43	0.53
10:J:53:ALA:HB2	10:J:68:ILE:HD12	1.91	0.53
17:R:95:TRP:CH2	17:R:99:MET:HE2	2.44	0.53
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	1.91	0.53
48:5:1822:U:O2	48:5:1822:U:O4'	2.27	0.52
48:5:256:G:N2	48:5:257:C:C2	2.77	0.52
48:5:3594:C:O2	48:5:3594:C:C2'	2.56	0.52
51:9:944:A:C5	51:9:945:U:C5	2.97	0.52
8:H:26:ILE:HB	8:H:35:ARG:HG2	1.91	0.52
11:L:9:ILE:O	11:L:9:ILE:HG23	2.09	0.52
25:Z:29:ILE:HG21	25:Z:40:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:707:C:O2	48:5:1291:G:C2	2.63	0.52
48:5:2043:A:O2'	48:5:4461:C:O2	2.25	0.52
48:5:4579:U:H2'	48:5:4580:U:O4'	2.08	0.52
48:5:4759:C:H2'	48:5:4760:G:O4'	2.09	0.52
48:5:4883:C:HO2'	48:5:4884:G:P	2.32	0.52
48:5:977:C:N3	48:5:978:G:N7	2.57	0.52
51:9:834:C:C2	51:9:841:G:N2	2.78	0.52
66:OO:56:VAL:HG12	66:OO:81:VAL:HG23	1.92	0.52
17:R:35:ALA:O	17:R:37:SER:N	2.41	0.52
48:5:1899:G:N2	48:5:1900:C:C2	2.77	0.52
48:5:2110:C:C6	48:5:2110:C:OP1	2.62	0.52
48:5:2108:G:C2	48:5:2125:C:N3	2.77	0.52
48:5:4138:C:C2	48:5:4147:G:C2	2.96	0.52
48:5:4281:A:C2	48:5:4283:G:C5	2.98	0.52
51:9:1553:C:O2	51:9:1553:C:O4'	2.25	0.52
51:9:409:C:C2	51:9:432:G:C2	2.97	0.52
51:9:50:A:C2	51:9:488:U:O4	2.63	0.52
11:L:58:ILE:HG23	11:L:70:VAL:CG1	2.39	0.52
48:5:43:U:H2'	48:5:44:A:O5'	2.09	0.52
48:5:4441:A:C8	48:5:4441:A:H5''	2.44	0.52
51:9:873:G:N1	51:9:914:U:C5	2.77	0.52
63:LL:113:LEU:HD23	63:LL:142:VAL:HG21	1.90	0.52
48:5:112:C:C2	48:5:330:G:C2	2.97	0.52
17:R:59:SER:N	48:5:4646:U:OP1	2.42	0.52
47:3:6:G:N2	47:3:67:U:O2	2.42	0.52
48:5:12:A:H8	48:5:12:A:H5''	1.75	0.52
48:5:1378:C:OP1	48:5:1379:C:H3'	2.09	0.52
48:5:181:C:C2	48:5:256:G:C2	2.98	0.52
48:5:2733:C:H2'	48:5:2734:U:O4'	2.10	0.52
51:9:1265:A:C2'	51:9:1265:A:N3	2.73	0.52
51:9:853:C:O4'	51:9:853:C:O2	2.28	0.52
52:AA:123:VAL:HG13	52:AA:145:ILE:HB	1.92	0.52
54:CC:165:VAL:HG21	54:CC:217:ALA:HB1	1.91	0.52
70:SS:27:ALA:HB1	70:SS:42:HIS:CE1	2.43	0.52
48:5:2638:G:C2	48:5:2639:U:C4	2.98	0.52
48:5:300:A:H2'	48:5:301:G:C8	2.45	0.52
51:9:350:C:HO2'	51:9:383:G:N2	2.06	0.52
4:D:129:GLU:HG3	4:D:177:THR:HG21	1.90	0.52
56:EE:129:ILE:HD13	56:EE:155:LYS:HA	1.90	0.52
48:5:1874:A:H5'	48:5:4218:U:O2	2.10	0.52
48:5:1912:G:N2	48:5:1913:C:C2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4338:G:C4	48:5:4372:U:C5	2.98	0.52
48:5:1854:G:N2	48:5:4394:A:O4'	2.42	0.52
48:5:52:G:N2	48:5:53:C:C2	2.78	0.52
51:9:1696:C:HO2'	51:9:1702:G:HO2'	1.57	0.52
59:HH:43:LEU:HD21	59:HH:71:SER:HB3	1.92	0.52
48:5:1266:G:H5''	48:5:2112:G:N3	2.25	0.52
51:9:49:C:O2	51:9:478:G:C2	2.63	0.52
51:9:751:G:C6	51:9:792:C:N4	2.78	0.52
51:9:834:C:H3'	51:9:835:C:H4'	1.91	0.52
2:B:29:VAL:HG13	2:B:348:ARG:HD3	1.91	0.52
5:E:62:LYS:HE2	48:5:979:C:OP2	2.10	0.52
56:EE:49:ARG:HB3	56:EE:55:ALA:HB3	1.92	0.52
57:FF:102:LEU:HD11	77:ZZ:100:VAL:HG21	1.92	0.52
17:R:95:TRP:CZ2	17:R:99:MET:HE2	2.45	0.52
48:5:1549:G:C2	48:5:1580:C:C2	2.98	0.52
48:5:211:G:H4'	48:5:234:G:C8	2.45	0.52
48:5:4735:G:C2	48:5:4736:C:C2	2.98	0.52
51:9:1407:U:C2'	51:9:1408:U:C6	2.91	0.52
51:9:1386:A:OP1	51:9:1483:A:N3	2.43	0.52
51:9:312:G:O2'	51:9:313:A:OP1	2.19	0.52
51:9:437:G:C2	51:9:457:C:C2	2.98	0.52
51:9:507:G:OP1	76:YY:108:LYS:NZ	2.40	0.52
51:9:980:A:C2	51:9:981:A:C6	2.98	0.52
2:B:154:LYS:HB2	2:B:154:LYS:HZ2	1.75	0.52
56:EE:11:ARG:HD2	56:EE:20:LEU:HB3	1.90	0.52
48:5:2525:U:P	48:5:2711:G:H1	2.33	0.51
47:3:76:A:C5	48:5:4371:G:C6	2.98	0.51
48:5:915:A:HO2'	48:5:916:C:H6	1.58	0.51
51:9:1235:G:C5'	51:9:1247:C:H42	2.13	0.51
51:9:963:A:H2'	51:9:964:A:O4'	2.09	0.51
48:5:1771:U:H2'	48:5:1772:C:O4'	2.10	0.51
48:5:1904:G:C2	48:5:2073:C:C2	2.98	0.51
50:8:119:C:C2	50:8:132:G:C2	2.98	0.51
51:9:1118:C:O2	51:9:1118:C:O4'	2.25	0.51
51:9:398:A:H5'	51:9:398:A:C8	2.46	0.51
4:D:196:ARG:O	4:D:200:MET:HG2	2.10	0.51
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	1.92	0.51
48:5:1358:G:H2'	48:5:1359:G:H8	1.75	0.51
48:5:1736:A:N3	49:7:78:C:O2'	2.42	0.51
48:5:1268:G:C2	48:5:2111:G:N2	2.78	0.51
2:B:21:ARG:NH2	48:5:4568:A:O3'	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4966:A:H2'	48:5:4967:A:C8	2.45	0.51
48:5:5000:G:N2	48:5:5051:C:C2	2.78	0.51
5:E:250:ASP:O	5:E:254:LEU:HB2	2.10	0.51
25:Z:51:ARG:HB2	25:Z:65:ARG:HD2	1.92	0.51
46:2:16:C:O2	46:2:16:C:O4'	2.24	0.51
48:5:1723:A:N1	48:5:1838:A:N1	2.58	0.51
48:5:2297:G:N2	48:5:2338:C:C2	2.79	0.51
48:5:3641:U:C2	48:5:3645:U:C5	2.99	0.51
7:G:34:LYS:O	48:5:4128:A:N3	2.43	0.51
48:5:470:A:C5	48:5:471:A:C8	2.99	0.51
51:9:1588:A:H2'	51:9:1589:A:C8	2.46	0.51
51:9:195:C:C2	51:9:205:G:C2	2.99	0.51
2:B:56:ILE:HG12	2:B:365:LEU:HD22	1.92	0.51
54:CC:192:LEU:HB3	54:CC:227:TRP:HD1	1.74	0.51
4:D:200:MET:HE1	4:D:241:LYS:CE	2.40	0.51
9:I:187:GLU:OE1	9:I:189:ARG:CD	2.58	0.51
48:5:5026:U:C6	60:II:79:ILE:HG13	2.45	0.51
48:5:1959:U:H4'	48:5:1961:G:C5'	2.41	0.51
48:5:2301:G:N1	48:5:2302:C:C4	2.79	0.51
48:5:2505:C:O2	48:5:2505:C:O4'	2.28	0.51
51:9:599:A:H2'	51:9:606:G:N2	2.25	0.51
4:D:122:GLN:O	4:D:248:ARG:NH2	2.43	0.51
48:5:2363:A:C2	48:5:3860:A:C4	2.98	0.51
48:5:4305:G:C2'	48:5:4305:G:N3	2.73	0.51
48:5:671:G:C6	48:5:672:C:C4	2.98	0.51
58:GG:74:ARG:HA	58:GG:96:SER:HA	1.91	0.51
10:J:63:ARG:NH2	50:8:58:G:N7	129.21	0.51
48:5:1835:G:O2'	48:5:1836:G:OP2	2.21	0.51
48:5:1891:A:O2'	48:5:1892:A:O4'	2.25	0.51
48:5:2026:A:H2'	48:5:2027:U:H5'	1.93	0.51
48:5:2297:G:C2	48:5:2338:C:N3	2.79	0.51
48:5:476:G:N2	48:5:679:C:C2	2.79	0.51
48:5:4913:G:O2'	48:5:4914:C:O4'	2.28	0.51
51:9:1139:C:H2'	51:9:1140:G:O4'	2.11	0.51
51:9:1466:G:N1	51:9:1467:C:C4	2.79	0.51
51:9:1500:G:C2	51:9:1501:C:C2	2.98	0.51
51:9:1784:G:N2	51:9:1785:C:C2	2.79	0.51
51:9:305:U:H1'	60:II:55:TYR:CG	2.45	0.51
51:9:412:G:C2	51:9:429:C:C2	2.99	0.51
2:B:378:ARG:HE	22:W:32:LEU:HD21	1.75	0.51
8:H:111:LEU:HD11	8:H:125:ARG:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:70:PRO:O	14:O:72:HIS:CE1	2.64	0.51
48:5:77:U:C4	48:5:335:A:N1	2.76	0.51
48:5:3723:A:C2	48:5:3724:A:C5	2.99	0.51
2:B:252:ALA:HB3	48:5:4457:U:O2	2.10	0.51
50:8:106:G:N2	50:8:107:C:C2	2.79	0.51
51:9:1303:C:O2	51:9:1303:C:O4'	2.24	0.51
48:5:2768:C:O4'	48:5:2768:C:O2	2.26	0.51
48:5:3628:G:C2	48:5:3834:C:C2	2.98	0.51
48:5:3782:C:C2	48:5:3811:G:N2	2.79	0.51
48:5:4093:G:C3'	48:5:4094:G:H5'	2.41	0.51
48:5:5026:U:H3'	60:II:79:ILE:HD11	1.93	0.51
51:9:1735:A:H2'	51:9:1736:G:O4'	2.11	0.51
51:9:211:G:N2	51:9:212:C:C2	2.78	0.51
51:9:379:C:O2	60:II:5:ARG:HD2	2.11	0.51
51:9:88:G:C6	51:9:89:C:C4	2.99	0.51
2:B:340:THR:OG1	2:B:341:LYS:N	2.43	0.51
3:C:334:THR:HG21	6:F:53:TYR:OH	2.11	0.51
67:PP:20:VAL:HG13	67:PP:24:GLN:HG2	1.93	0.51
70:SS:86:ARG:HB2	70:SS:98:VAL:HG23	1.93	0.51
74:WW:81:VAL:HG11	74:WW:86:LEU:HD13	1.92	0.51
25:Z:5:MET:HG2	25:Z:77:TYR:CE1	2.46	0.51
48:5:1358:G:C2'	48:5:1359:G:O4'	2.59	0.51
48:5:1400:G:C6	48:5:1401:C:C4	2.99	0.51
2:B:302:ASN:HB2	2:B:313:SER:HA	1.93	0.51
56:EE:122:LYS:HB3	56:EE:164:LEU:HD21	1.93	0.51
48:5:4303:C:O4'	48:5:4303:C:O2	2.26	0.50
48:5:4758:U:O4'	48:5:4758:U:O2	2.29	0.50
51:9:151:C:O2'	58:GG:132:ARG:NH1	2.43	0.50
51:9:1537:A:C2	51:9:1596:U:N3	2.79	0.50
51:9:56:G:OP1	76:YY:111:LYS:NZ	2.31	0.50
9:I:97:ILE:HD13	9:I:126:VAL:HG11	1.92	0.50
51:9:384:U:O2'	63:LL:135:SER:C	2.50	0.50
21:V:82:ILE:HD12	21:V:104:VAL:HG22	1.93	0.50
23:X:76:ILE:HG21	23:X:112:ALA:HB2	1.91	0.50
47:3:1:G:N1	47:3:2:C:C4	2.80	0.50
48:5:2712:G:N2	48:5:2713:C:C2	2.79	0.50
48:5:4389:C:H2'	48:5:4390:A:H8	1.76	0.50
48:5:4906:C:C2	48:5:4916:G:C2	2.99	0.50
48:5:929:A:H3'	48:5:930:G:C5'	2.40	0.50
55:DD:191:PRO:O	55:DD:193:ASP:N	2.45	0.50
25:Z:15:ALA:HB3	25:Z:79:HIS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3717:A:N1	48:5:3933:G:H1'	2.26	0.50
48:5:4583:C:N4	48:5:4718:G:C6	2.80	0.50
48:5:504:G:C2	48:5:654:C:C2	2.99	0.50
51:9:1666:C:H2'	51:9:1667:U:O4'	2.11	0.50
51:9:1739:C:C2	51:9:1796:G:C2	3.00	0.50
51:9:1207:G:C6	51:9:1837:G:C6	2.99	0.50
51:9:407:G:N3	51:9:407:G:H2'	2.26	0.50
51:9:501:C:C2'	51:9:501:C:O2	2.58	0.50
52:AA:134:LEU:HD21	52:AA:144:THR:HG21	1.93	0.50
46:2:53:G:N2	46:2:62:C:C2	2.79	0.50
48:5:1072:C:O2	48:5:1072:C:C2'	2.60	0.50
48:5:1214:C:H1'	48:5:1215:C:OP2	2.10	0.50
48:5:1265:G:C2'	48:5:1266:G:H5'	2.41	0.50
48:5:2028:C:O2'	48:5:2029:A:O4'	2.29	0.50
48:5:4966:A:C2	48:5:4967:A:C2	2.99	0.50
51:9:1364:U:O4'	51:9:1364:U:O2	2.28	0.50
7:G:95:LEU:HD13	7:G:184:LEU:HD11	1.93	0.50
10:J:156:ARG:NH2	49:7:17:C:OP1	2.44	0.50
14:O:54:TYR:CE1	14:O:145:VAL:HG11	2.47	0.50
51:9:1587:G:N2	71:TT:74:SER:OG	2.45	0.50
48:5:105:A:C2	48:5:336:A:C8	3.00	0.50
48:5:2627:C:O2	48:5:2627:C:O4'	2.30	0.50
48:5:4462:C:C2	48:5:4515:G:C2	3.00	0.50
50:8:125:C:O4'	50:8:125:C:O2	2.29	0.50
51:9:1116:C:O2	51:9:1116:C:O4'	2.28	0.50
51:9:1386:A:HO2'	51:9:1387:G:H5'	1.75	0.50
51:9:155:G:N2	58:GG:56:ASN:OD1	2.45	0.50
51:9:290:U:OP1	56:EE:156:MET:CE	2.60	0.50
51:9:598:G:N2	51:9:639:C:C2	2.79	0.50
2:B:43:LEU:HD13	2:B:196:TRP:CH2	2.46	0.50
12:M:69:ARG:O	12:M:71:LYS:N	2.42	0.50
47:3:31:A:H2'	57:FF:136:ARG:HH22	1.77	0.50
48:5:1171:G:C2	48:5:1191:C:C2	2.99	0.50
48:5:1263:A:C6	48:5:1264:C:C4	3.00	0.50
48:5:2090:U:OP2	48:5:2090:U:O4'	2.30	0.50
48:5:4281:A:C2	48:5:4283:G:C6	2.99	0.50
48:5:93:G:O2'	48:5:94:A:O4'	2.25	0.50
51:9:1622:U:C6	70:SS:120:HIS:CE1	3.00	0.50
51:9:350:C:O2'	51:9:383:G:N1	2.43	0.50
53:BB:150:ILE:O	53:BB:150:ILE:HG23	2.11	0.50
58:GG:5:ILE:HG12	58:GG:111:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:QQ:52:LEU:HD13	68:QQ:56:LEU:HD21	1.94	0.50
48:5:1399:G:H2'	48:5:1400:G:O4'	2.12	0.50
48:5:1983:A:C2	48:5:2010:A:H5''	2.47	0.50
48:5:2123:C:O2'	48:5:2124:G:OP2	2.20	0.50
51:9:1681:U:O2'	51:9:1682:C:C5'	2.60	0.50
51:9:92:A:O4'	56:EE:3:ARG:NH1	2.45	0.50
51:9:970:G:H3'	51:9:971:G:C5'	2.41	0.50
2:B:220:ILE:HG12	2:B:278:THR:HG23	1.93	0.50
56:EE:87:MET:CE	56:EE:236:ILE:HD13	2.42	0.50
63:LL:11:GLN:HB3	63:LL:56:ILE:HD11	1.94	0.50
48:5:1167:C:C2	48:5:1195:G:C2	3.00	0.50
48:5:1235:G:H2'	48:5:1236:C:H5'	1.93	0.50
48:5:1381:U:O2	48:5:1381:U:O4'	2.28	0.50
48:5:1910:G:N2	48:5:1911:C:C2	2.80	0.50
48:5:1998:A:O2'	48:5:1999:A:O4'	2.30	0.50
48:5:4213:A:N6	48:5:4218:U:H3	2.10	0.50
49:7:71:G:C2	49:7:105:C:C2	3.00	0.50
51:9:193:C:C2	51:9:207:G:C2	2.99	0.50
51:9:474:G:N1	51:9:475:C:C4	2.80	0.50
51:9:88:G:C2	51:9:89:C:C2	3.00	0.50
56:EE:131:VAL:HA	56:EE:137:PRO:HA	1.94	0.50
9:I:181:PHE:O	9:I:185:VAL:HG23	2.12	0.50
60:II:76:THR:HG21	60:II:105:ASP:O	2.12	0.50
66:OO:44:VAL:HG11	66:OO:85:CYS:SG	2.52	0.50
48:5:1811:G:N2	48:5:1812:C:C2	2.80	0.50
48:5:2028:C:O2'	48:5:2029:A:C5'	2.60	0.50
48:5:2368:A:N6	48:5:2788:U:O2	2.45	0.50
48:5:2752:G:H2'	48:5:2753:G:O4'	2.12	0.50
48:5:3715:U:O2'	48:5:3716:C:O4'	2.28	0.50
48:5:4094:G:H2'	48:5:4095:G:O4'	2.12	0.50
48:5:5031:G:N2	48:5:5032:C:C2	2.80	0.50
5:E:134:ARG:NH1	5:E:165:SER:O	2.45	0.50
61:JJ:38:ARG:HG2	61:JJ:38:ARG:O	2.12	0.50
17:R:109:TYR:HB3	17:R:115:ILE:HG12	1.94	0.50
70:SS:11:HIS:O	70:SS:12:ILE:CD1	2.52	0.50
48:5:1400:G:C2	48:5:1401:C:C2	3.00	0.49
48:5:166:C:C2	48:5:167:C:H5	2.30	0.49
48:5:1886:G:C2	48:5:1894:C:C2	3.00	0.49
48:5:2311:C:C2	48:5:2328:G:C2	3.00	0.49
48:5:2463:G:N2	48:5:2464:C:C2	2.80	0.49
48:5:975:C:C3'	48:5:976:G:O4'	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:PRO:O	2:B:244:THR:OG1	2.30	0.49
54:CC:107:LEU:HD11	54:CC:129:ALA:HB2	1.93	0.49
71:TT:75:MET:HA	71:TT:78:ILE:HG22	1.93	0.49
48:5:1776:A:C6	48:5:1777:C:C4	2.99	0.49
48:5:1956:A:HO2'	48:5:1957:U:H5'	1.76	0.49
48:5:2588:C:OP1	48:5:2767:U:O2'	2.30	0.49
48:5:1872:G:O2'	48:5:4219:A:N3	2.38	0.49
51:9:182:C:H2'	51:9:184:G:H1'	1.93	0.49
51:9:92:A:C6	51:9:446:G:C6	3.00	0.49
53:BB:137:LEU:HD23	53:BB:215:VAL:HG22	1.94	0.49
5:E:208:LEU:HD12	5:E:208:LEU:O	2.12	0.49
11:L:65:ARG:HG2	11:L:66:TYR:CD2	2.48	0.49
47:3:66:U:H2'	47:3:67:U:O4'	2.11	0.49
48:5:1412:G:N2	48:5:1413:C:C2	2.79	0.49
48:5:2257:C:O2'	48:5:2258:C:O5'	2.25	0.49
48:5:230:G:C2	48:5:239:C:C2	3.01	0.49
51:9:1401:A:C2	51:9:1402:A:N1	2.81	0.49
51:9:887:U:O4'	51:9:887:U:O2	2.29	0.49
1:A:49:ILE:HG22	1:A:58:LEU:HB2	1.94	0.49
56:EE:15:PRO:HD2	56:EE:18:TRP:CZ3	2.47	0.49
56:EE:153:LEU:HD11	58:GG:216:ARG:NE	2.28	0.49
9:I:76:MET:HG3	9:I:87:ILE:HD11	1.93	0.49
17:R:105:LEU:HD12	17:R:138:LEU:HD13	1.94	0.49
48:5:1245:C:C4	48:5:1269:G:O6	2.66	0.49
48:5:2108:G:N2	48:5:2125:C:C2	2.80	0.49
48:5:2336:G:C2	48:5:2337:C:C2	3.01	0.49
48:5:3752:C:H2'	48:5:3777:G:C8	2.47	0.49
48:5:4579:U:O2	48:5:4580:U:C2	2.65	0.49
48:5:93:G:H2'	48:5:94:A:C8	2.48	0.49
48:5:356:G:O2'	50:8:25:G:N3	2.44	0.49
51:9:666:U:H2'	51:9:667:U:C6	2.47	0.49
61:JJ:46:VAL:HG11	61:JJ:106:LEU:HD12	1.94	0.49
13:N:67:ARG:NH1	48:5:2458:C:OP1	2.45	0.49
48:5:1297:U:O4'	48:5:1297:U:P	2.71	0.49
48:5:1613:A:C2	48:5:1630:A:C2	3.00	0.49
48:5:325:U:H2'	48:5:326:C:C6	2.47	0.49
51:9:1408:U:H2'	51:9:1409:A:C8	2.47	0.49
51:9:1481:G:C6	51:9:1482:C:N3	2.80	0.49
51:9:73:C:O4'	51:9:73:C:O2	2.28	0.49
3:C:213:GLU:OE1	3:C:213:GLU:N	2.46	0.49
61:JJ:28:GLU:HB3	61:JJ:40:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:54:GLN:HA	15:P:83:TRP:CD1	2.47	0.49
48:5:1960:A:H4'	48:5:1961:G:OP2	2.11	0.49
48:5:1269:G:C5	48:5:2111:G:C2	3.01	0.49
48:5:2494:U:H2'	48:5:2495:U:O4'	2.12	0.49
48:5:2519:U:C2	48:5:2520:C:C5	3.01	0.49
48:5:300:A:C2	48:5:301:G:C6	3.01	0.49
48:5:4411:G:C2	48:5:4432:C:O2	2.65	0.49
51:9:1511:U:H2'	51:9:1512:C:C6	2.48	0.49
4:D:258:LYS:O	4:D:259:ARG:HG3	2.13	0.49
9:I:46:PHE:CD1	9:I:140:THR:HA	2.48	0.49
9:I:14:ASN:O	9:I:128:ARG:NH2	2.45	0.49
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.47	0.49
48:5:1170:G:C2	48:5:1192:C:C2	3.00	0.49
48:5:2056:G:C8	48:5:2058:G:C8	3.00	0.49
48:5:2557:G:C6	48:5:2558:C:C4	3.01	0.49
48:5:2726:G:C6	48:5:2727:C:N4	2.81	0.49
48:5:3782:C:N3	48:5:3811:G:C2	2.81	0.49
48:5:3626:G:C6	48:5:3836:A:C2	3.01	0.49
4:D:200:MET:HE1	4:D:241:LYS:HG2	1.93	0.49
65:NN:60:VAL:HG23	65:NN:66:VAL:HG21	1.93	0.49
48:5:1301:C:O4'	48:5:1301:C:O2	2.29	0.49
48:5:1726:U:H3	48:5:1836:G:H1	1.61	0.49
48:5:4079:C:C2	48:5:4168:G:C2	3.01	0.49
48:5:4489:G:C6	48:5:4490:C:C4	3.00	0.49
48:5:4574:U:H3'	48:5:4575:G:H5''	1.94	0.49
51:9:1654:G:N2	51:9:1655:C:C2	2.81	0.49
20:U:80:LYS:HD3	20:U:110:TYR:CE2	2.47	0.49
74:WW:90:GLN:HA	74:WW:102:ILE:HD11	1.93	0.49
48:5:1328:G:O2'	48:5:2349:A:OP1	2.31	0.49
48:5:1400:G:H2'	48:5:1401:C:O4'	2.13	0.49
48:5:1754:U:O4'	48:5:1754:U:O2	2.30	0.49
48:5:224:U:O2	48:5:224:U:O4'	2.27	0.49
48:5:384:A:C6	48:5:386:A:C6	3.01	0.49
48:5:4691:A:C2	48:5:4700:A:C4	3.00	0.49
48:5:4735:G:C6	48:5:4736:C:C4	3.01	0.49
48:5:4913:G:HO2'	48:5:4914:C:C1'	2.24	0.49
48:5:4932:U:H2'	48:5:4933:C:O4'	2.13	0.49
48:5:977:C:H2'	48:5:978:G:O4'	2.12	0.49
48:5:986:C:N3	48:5:1068:G:C2	2.81	0.49
47:3:35:U:H1'	51:9:1641:A:P	2.53	0.49
51:9:123:G:C2	51:9:342:C:C2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:635:G:C6	51:9:636:C:C4	3.01	0.49
1:A:107:MET:SD	1:A:113:VAL:HG11	2.53	0.49
1:A:44:ILE:HG22	1:A:87:PHE:CD2	2.48	0.49
5:E:254:LEU:N	5:E:255:PRO:HD2	2.28	0.49
11:L:66:TYR:O	11:L:68:THR:N	2.46	0.49
16:Q:86:ILE:HB	16:Q:105:VAL:HG13	1.95	0.49
47:3:24:G:C6	47:3:25:C:C4	3.01	0.49
48:5:1252:C:C2	48:5:1259:G:C2	3.01	0.49
48:5:2557:G:C2	48:5:2558:C:C2	3.01	0.49
48:5:2730:U:H2'	48:5:2731:C:C6	2.48	0.49
48:5:956:A:H3'	48:5:957:G:C8	2.48	0.49
51:9:1212:G:C2	51:9:1213:C:C2	3.01	0.49
51:9:1315:U:O2	51:9:1315:U:O4'	2.29	0.49
51:9:1406:G:C5	51:9:1407:U:H1'	2.47	0.49
52:AA:42:LYS:HG2	52:AA:48:ILE:HD11	1.95	0.49
2:B:165:HIS:HB3	2:B:180:LEU:HG	1.95	0.49
4:D:195:HIS:CE1	4:D:199:ILE:HD11	2.48	0.49
57:FF:76:MET:HA	57:FF:155:CYS:SG	2.53	0.49
48:5:3724:A:N6	48:5:3725:G:C6	2.81	0.48
48:5:5020:G:H2'	48:5:5021:C:O4'	2.13	0.48
51:9:1411:G:H3'	51:9:1412:C:H4'	1.94	0.48
51:9:1444:U:O2'	51:9:1580:A:N1	2.45	0.48
51:9:958:G:C2	51:9:959:G:C6	3.01	0.48
57:FF:20:PHE:CZ	57:FF:69:VAL:HG11	2.47	0.48
16:Q:11:ARG:NH2	48:5:1690:C:OP2	2.46	0.48
47:3:10:G:N1	47:3:11:C:C4	2.81	0.48
47:3:34:U:O2'	47:3:35:U:O4'	2.31	0.48
47:3:6:G:N1	47:3:7:A:C5	2.81	0.48
48:5:990:C:C4	48:5:1064:G:C2	3.01	0.48
48:5:1279:A:O2'	48:5:1280:C:OP1	2.30	0.48
48:5:1449:C:H2'	48:5:1450:C:O4'	2.12	0.48
48:5:4099:G:C6	48:5:4100:C:C4	3.01	0.48
48:5:4129:G:H2'	48:5:4130:C:O4'	2.14	0.48
51:9:409:C:N3	51:9:432:G:C2	2.81	0.48
51:9:916:A:C5	65:NN:73:ARG:HD3	2.48	0.48
16:Q:186:TYR:CD2	48:5:4307:A:H4'	2.48	0.48
17:R:172:ARG:HH12	51:9:908:A:C5'	1.81	0.48
52:AA:66:VAL:HG11	73:VV:46:PHE:HB2	1.95	0.48
48:5:2027:U:HO2'	48:5:2028:C:H5'	1.77	0.48
48:5:2468:U:O2	48:5:2469:C:C5	2.66	0.48
48:5:4213:A:C2	48:5:4218:U:O4	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:671:G:C2	48:5:672:C:C2	3.01	0.48
48:5:919:C:N4	48:5:920:C:N4	2.61	0.48
51:9:114:G:N7	63:LL:69:ARG:NH1	2.60	0.48
4:D:3:PHE:HB2	48:5:1755:C:C6	2.48	0.48
3:C:303:ARG:O	16:Q:38:ARG:NH1	2.42	0.48
69:RR:91:LEU:HD12	69:RR:92:ASP:N	2.28	0.48
76:YY:113:ARG:O	76:YY:114:MET:CB	2.61	0.48
48:5:100:C:H2'	48:5:101:A:O4'	2.13	0.48
48:5:125:C:O2'	48:5:126:C:OP1	2.22	0.48
48:5:4724:A:C6	48:5:4725:C:C4	3.01	0.48
48:5:505:G:C2	48:5:506:C:C2	3.01	0.48
51:9:17:C:O2'	51:9:1194:A:N1	2.36	0.48
51:9:1212:G:HO2'	51:9:1213:C:C5'	2.24	0.48
48:5:1448:G:N2	48:5:1449:C:C2	2.81	0.48
48:5:2539:C:H2'	48:5:2540:C:C6	2.48	0.48
48:5:4136:G:C6	48:5:4137:C:C4	3.01	0.48
51:9:1380:C:H2'	51:9:1381:G:O4'	2.13	0.48
51:9:1408:U:C4	51:9:1409:A:C6	3.01	0.48
51:9:1617:G:N1	51:9:1620:A:OP2	2.45	0.48
51:9:217:A:C2	51:9:309:G:C6	3.01	0.48
51:9:830:A:C6	51:9:844:U:N3	2.82	0.48
2:B:234:ARG:HA	2:B:272:LYS:HD2	1.95	0.48
64:MM:113:ASP:O	64:MM:115:GLY:N	2.47	0.48
13:N:65:ARG:HG3	13:N:129:PHE:CE1	2.49	0.48
20:U:100:LEU:HD22	20:U:112:LEU:HB3	1.96	0.48
48:5:2336:G:C6	48:5:2337:C:C4	3.02	0.48
48:5:2729:C:H2'	48:5:2730:U:O4'	2.13	0.48
48:5:3586:G:C6	48:5:3587:C:C4	3.02	0.48
48:5:3896:C:O2	48:5:4564:A:N1	2.46	0.48
48:5:4767:C:C2	48:5:4868:G:C2	3.01	0.48
48:5:4989:U:O2	48:5:4989:U:O4'	2.30	0.48
48:5:28:C:C2	48:5:55:G:C2	3.02	0.48
48:5:965:G:H2'	48:5:965:G:N3	2.29	0.48
51:9:1321:G:H2'	51:9:1322:G:O4'	2.14	0.48
7:G:32:PHE:CZ	25:Z:55:ALA:HA	2.48	0.48
61:JJ:45:ARG:O	61:JJ:49:THR:HG23	2.14	0.48
47:3:68:C:H2'	47:3:69:G:C8	2.48	0.48
48:5:1308:C:H2'	48:5:1309:C:C6	2.49	0.48
48:5:1383:G:C5	48:5:1384:C:C4	3.02	0.48
48:5:1910:G:C6	48:5:1911:C:N4	2.82	0.48
48:5:1942:A:N3	48:5:4432:C:O2'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1983:A:C2	48:5:2008:U:O4	2.65	0.48
48:5:2468:U:C4	48:5:2473:A:N6	2.77	0.48
48:5:2496:G:C2	48:5:2497:C:C2	3.02	0.48
48:5:2909:C:C2	48:5:3586:G:C2	3.01	0.48
48:5:2844:A:O2'	48:5:4631:G:H4'	2.14	0.48
51:9:1466:G:C2	51:9:1467:C:C4	3.02	0.48
51:9:629:A:N6	51:9:632:C:C2	2.82	0.48
51:9:841:G:C2	51:9:842:C:C2	3.01	0.48
54:CC:129:ALA:HB2	54:CC:213:LEU:HD11	1.95	0.48
57:FF:68:ILE:HD12	57:FF:112:LEU:HD22	1.94	0.48
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.49	0.48
13:N:124:ASP:OD1	13:N:125:SER:N	2.46	0.48
48:5:2477:A:H2'	48:5:2478:C:C6	2.48	0.48
48:5:3860:A:H61	48:5:4560:C:H5	1.61	0.48
51:9:1235:G:C5'	51:9:1247:C:N4	2.75	0.48
51:9:1771:G:N1	51:9:1772:C:C4	2.82	0.48
51:9:191:A:H3'	51:9:192:C:H5''	1.95	0.48
51:9:322:C:O2	51:9:323:C:C6	2.66	0.48
51:9:516:A:N1	51:9:643:A:O2'	2.44	0.48
51:9:830:A:N6	51:9:844:U:C2	2.81	0.48
52:AA:63:ARG:HG2	52:AA:185:MET:HE1	1.96	0.48
51:9:1333:U:H4'	55:DD:147:ALA:HB2	1.95	0.48
5:E:254:LEU:O	5:E:257:ILE:HG12	2.14	0.48
16:Q:67:ILE:HD12	16:Q:96:PRO:HD2	1.96	0.48
48:5:1699:A:N6	48:5:2094:G:O2'	2.46	0.48
48:5:1878:G:N2	48:5:1879:C:C2	2.81	0.48
48:5:1956:A:C2'	48:5:1957:U:H5'	2.43	0.48
48:5:3714:G:C6	48:5:3715:U:C4	3.02	0.48
48:5:484:U:C4	48:5:486:C:C5	3.02	0.48
48:5:5020:G:C2	48:5:5021:C:C2	3.02	0.48
48:5:80:C:C2	48:5:104:G:C2	3.01	0.48
51:9:1149:A:O2'	51:9:1150:A:H3'	2.14	0.48
4:D:146:LEU:HD11	4:D:159:VAL:HG11	1.94	0.48
67:PP:22:LEU:HA	67:PP:25:LEU:HB2	1.95	0.48
68:QQ:44:PRO:HG2	68:QQ:81:ILE:HD11	1.95	0.48
48:5:984:C:C2	48:5:1070:G:C2	3.01	0.48
48:5:2814:C:C2'	48:5:2814:C:O2	2.62	0.48
48:5:351:C:C2	50:8:25:G:N2	2.82	0.48
48:5:3715:U:H2'	48:5:3716:C:C6	2.48	0.48
51:9:99:A:H2'	51:9:100:U:O4'	2.13	0.48
51:9:506:G:OP1	76:YY:108:LYS:NZ	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3712:A:C2	51:9:970:G:C6	3.02	0.48
2:B:105:VAL:HG11	2:B:150:PHE:CZ	2.49	0.48
9:I:45:GLU:O	9:I:46:PHE:CD1	2.67	0.48
48:5:1075:G:C2	48:5:1076:C:C2	3.02	0.47
48:5:1987:C:C2'	48:5:1987:C:O2	2.61	0.47
48:5:2496:G:C6	48:5:2497:C:C4	3.02	0.47
48:5:505:G:C6	48:5:506:C:C4	3.02	0.47
48:5:508:G:C2	48:5:510:U:C5	3.02	0.47
51:9:185:G:N2	51:9:186:C:C2	2.82	0.47
51:9:491:C:H2'	51:9:492:C:O4'	2.14	0.47
51:9:62:G:O4'	51:9:172:U:N3	2.46	0.47
51:9:830:A:H2'	51:9:831:G:O4'	2.13	0.47
5:E:254:LEU:O	5:E:258:LYS:HG3	2.13	0.47
8:H:39:ASN:O	8:H:40:HIS:HB3	2.14	0.47
48:5:1279:A:H2'	48:5:1280:C:C6	2.49	0.47
48:5:1345:A:H2'	48:5:1346:C:C6	2.48	0.47
48:5:1995:G:C2	48:5:1996:C:C2	3.02	0.47
50:8:139:G:C6	50:8:140:C:C4	3.02	0.47
51:9:1126:G:N2	51:9:1127:C:C2	2.83	0.47
51:9:1537:A:H2'	51:9:1538:C:O4'	2.14	0.47
52:AA:109:THR:O	52:AA:110:ASN:HB2	2.13	0.47
11:L:74:ARG:NH2	48:5:76:A:N7	2.63	0.47
17:R:61:ALA:HB2	48:5:2633:U:H5''	1.96	0.47
48:5:120:A:H2'	48:5:149:A:N6	2.30	0.47
48:5:1958:A:P	48:5:1958:A:H3'	2.54	0.47
48:5:2618:G:N2	48:5:2720:C:C2	2.82	0.47
48:5:279:A:H3'	48:5:279:A:OP1	2.14	0.47
48:5:4152:G:N2	48:5:4153:C:C2	2.82	0.47
48:5:497:G:C2	48:5:657:C:N3	2.82	0.47
48:5:499:G:N3	48:5:499:G:H2'	2.28	0.47
48:5:977:C:H2'	48:5:978:G:H5'	1.96	0.47
51:9:1108:G:C2	51:9:1125:C:C2	3.01	0.47
51:9:1530:U:H2'	51:9:1531:A:O4'	2.14	0.47
51:9:1868:U:N3	52:AA:98:PRO:O	44.39	0.47
2:B:36:ASP:N	2:B:36:ASP:OD1	2.44	0.47
14:O:84:VAL:HG11	14:O:102:LEU:HD22	1.96	0.47
74:WW:89:TRP:CE3	74:WW:93:LEU:HD22	2.49	0.47
47:3:70:G:H4'	48:5:3740:G:O2'	2.15	0.47
48:5:1367:C:H2'	48:5:1367:C:O2	2.14	0.47
48:5:1661:C:C2	48:5:2345:G:N1	2.82	0.47
51:9:1834:A:N3	51:9:1834:A:C2'	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:NH2	48:5:3685:C:OP1	2.47	0.47
4:D:64:ILE:HG13	4:D:105:LEU:HD21	1.95	0.47
5:E:202:VAL:HG12	5:E:256:LYS:HZ1	1.74	0.47
14:O:109:PRO:HB2	14:O:110:PRO:CD	2.43	0.47
48:5:1189:G:C6	48:5:1190:C:C4	3.02	0.47
48:5:1448:G:C6	48:5:1449:C:N4	2.82	0.47
48:5:1468:C:C2	48:5:1498:G:N2	2.82	0.47
48:5:2661:U:HO2'	48:5:2662:G:P	2.37	0.47
48:5:298:G:N2	48:5:299:C:C2	2.83	0.47
48:5:3662:A:N6	48:5:3680:U:N3	2.57	0.47
48:5:4093:G:H3'	48:5:4094:G:H5'	1.95	0.47
48:5:4099:G:C2	48:5:4100:C:C2	3.02	0.47
48:5:4246:G:N2	48:5:4263:C:C2	2.83	0.47
48:5:4378:A:O2'	48:5:4379:A:H2'	2.14	0.47
48:5:4916:G:C2	48:5:4917:C:C2	3.02	0.47
50:8:56:G:C6	50:8:57:C:C4	3.02	0.47
51:9:1537:A:N1	51:9:1596:U:C4	2.83	0.47
51:9:1667:U:H2'	51:9:1668:U:C6	2.49	0.47
2:B:312:LYS:HD2	2:B:370:THR:HG21	1.97	0.47
55:DD:162:ASP:N	55:DD:163:PRO:HD2	2.29	0.47
9:I:184:MET:HE1	9:I:190:LEU:CG	2.45	0.47
14:O:196:LEU:HB3	14:O:202:LEU:HD22	1.97	0.47
66:OO:142:ARG:HG3	66:OO:143:LYS:N	2.30	0.47
67:PP:26:LEU:N	67:PP:28:MET:SD	2.87	0.47
48:5:2097:U:O4'	48:5:2097:U:O2	2.33	0.47
48:5:2297:G:C2	48:5:2338:C:C2	3.03	0.47
48:5:4119:C:O4'	48:5:4119:C:O2	2.30	0.47
48:5:971:U:H2'	48:5:972:C:H5'	1.95	0.47
51:9:1445:U:O4	51:9:1446:A:N6	2.47	0.47
51:9:172:U:O2	51:9:172:U:C2'	2.61	0.47
51:9:1754:G:C6	51:9:1755:C:C4	3.03	0.47
51:9:635:G:C2	51:9:636:C:C2	3.03	0.47
3:C:181:LYS:HD2	48:5:2300:A:N1	2.29	0.47
4:D:76:CYS:SG	4:D:77:ALA:N	2.87	0.47
6:F:211:TRP:CD1	6:F:212:PRO:HD2	2.50	0.47
6:F:49:ARG:NH1	48:5:974:C:O3'	2.48	0.47
9:I:153:ARG:HA	9:I:165:ILE:HD11	1.96	0.47
17:R:11:ALA:HB1	17:R:50:ILE:HD13	1.96	0.47
48:5:1246:G:H2'	48:5:1247:U:O4'	2.14	0.47
48:5:1270:A:H2'	48:5:1271:G:O5'	2.15	0.47
48:5:2089:G:HO2'	48:5:2090:U:P	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:384:A:N6	48:5:386:A:C6	2.83	0.47
48:5:4092:G:C2	48:5:4158:C:C2	3.02	0.47
48:5:1787:A:N3	48:5:4210:U:O2'	2.44	0.47
3:C:290:SER:O	3:C:294:LYS:HG2	2.14	0.47
56:EE:195:ILE:O	56:EE:196:THR:HB	2.15	0.47
58:GG:57:ASP:HA	58:GG:106:LEU:HD23	1.96	0.47
61:JJ:118:GLY:O	61:JJ:120:ALA:N	2.44	0.47
24:Y:52:ASP:OD1	24:Y:52:ASP:N	2.47	0.47
48:5:1357:C:O2'	48:5:1358:G:O4'	2.29	0.47
48:5:1358:G:H2'	48:5:1359:G:C8	2.50	0.47
48:5:2020:U:H2'	48:5:2020:U:O2	2.14	0.47
48:5:2128:G:C6	48:5:2129:C:C4	3.03	0.47
48:5:2459:G:N2	48:5:2462:C:OP2	2.47	0.47
48:5:2586:G:C8	48:5:2770:C:H1'	2.49	0.47
48:5:3938:G:O6	48:5:4172:A:N1	2.48	0.47
48:5:4303:C:O2	48:5:4303:C:O5'	2.32	0.47
48:5:4525:C:H2'	48:5:4526:U:O4'	2.15	0.47
48:5:499:G:C2	48:5:656:C:N3	2.82	0.47
51:9:1115:U:O4'	51:9:1115:U:O2	2.31	0.47
51:9:1541:G:C6	51:9:1542:C:C4	3.03	0.47
52:AA:104:THR:O	52:AA:107:THR:HG23	2.14	0.47
3:C:161:TYR:CD1	3:C:166:GLU:HB3	2.49	0.47
4:D:200:MET:HE1	4:D:241:LYS:HE3	1.96	0.47
5:E:123:SER:O	5:E:126:ARG:HG2	2.15	0.47
5:E:62:LYS:NZ	48:5:978:G:P	2.81	0.47
17:R:44:LEU:HD22	17:R:49:LEU:HD12	1.96	0.47
48:5:2743:A:C2	48:5:2744:A:C4	3.03	0.47
48:5:2907:G:H2'	48:5:2908:U:O4'	2.15	0.47
48:5:4489:G:C2	48:5:4490:C:C2	3.02	0.47
48:5:4730:C:O5'	48:5:4731:G:N2	2.47	0.47
48:5:4919:G:C2	48:5:4920:C:C2	3.02	0.47
3:C:268:ARG:NH2	48:5:655:C:OP2	2.47	0.47
49:7:117:G:C2	49:7:118:C:C2	3.03	0.47
50:8:71:A:C2	50:8:88:A:H1'	2.50	0.47
51:9:1228:A:H2'	51:9:1229:G:C8	2.50	0.47
51:9:322:C:C2'	51:9:323:C:OP2	2.62	0.47
51:9:942:G:N2	66:OO:138:ASP:OD1	2.47	0.47
56:EE:126:VAL:HG13	56:EE:160:ILE:HD11	1.96	0.47
48:5:100:C:O4'	48:5:100:C:O2	2.33	0.47
48:5:1189:G:C2	48:5:1190:C:C2	3.03	0.47
48:5:1240:G:C2	48:5:1241:C:C2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1584:G:C6	48:5:1585:C:C4	3.02	0.47
48:5:1886:G:N2	48:5:1894:C:C2	2.83	0.47
48:5:2089:G:C6	48:5:2262:G:H2'	2.50	0.47
48:5:2468:U:N3	48:5:2473:A:C6	2.83	0.47
14:O:160:ARG:NH2	48:5:4759:C:OP1	2.47	0.47
48:5:4942:C:O3'	48:5:4944:C:P	2.73	0.47
48:5:698:G:N2	48:5:699:C:C2	2.83	0.47
51:9:1129:G:H3'	51:9:1130:G:C8	2.50	0.47
51:9:1141:G:N2	51:9:1147:C:C2	2.83	0.47
51:9:1267:C:C2	51:9:1516:G:C2	3.03	0.47
56:EE:160:ILE:HG21	56:EE:169:ILE:HG22	1.96	0.47
7:G:100:HIS:HA	7:G:103:ARG:HD2	1.95	0.47
8:H:126:VAL:HG11	8:H:161:ILE:HG22	1.97	0.47
51:9:380:G:OP2	60:II:181:GLN:NE2	2.48	0.47
63:LL:126:VAL:HG22	63:LL:142:VAL:HG13	1.97	0.47
48:5:1383:G:C6	48:5:1384:C:C4	3.02	0.47
48:5:1639:U:H3	48:5:1643:A:HO2'	1.58	0.47
48:5:2065:G:C6	48:5:2066:C:C4	3.03	0.47
48:5:2743:A:H2'	48:5:2744:A:C8	2.50	0.47
48:5:967:C:N3	48:5:2254:G:C6	2.82	0.47
51:9:102:A:O2'	51:9:103:A:OP2	2.27	0.47
51:9:1335:G:C6	51:9:1336:C:C4	3.03	0.47
51:9:1500:G:H2'	51:9:1501:C:O4'	2.14	0.47
51:9:1528:G:N1	51:9:1529:C:C4	2.83	0.47
51:9:830:A:N6	51:9:844:U:C4	2.72	0.47
1:A:69:PHE:CD1	11:L:65:ARG:HD3	106.38	0.47
4:D:43:LYS:HB3	4:D:46:THR:CG2	2.45	0.47
5:E:59:TYR:CZ	5:E:64:LEU:HB2	2.49	0.47
14:O:26:GLN:OE1	14:O:31:ARG:NH1	2.48	0.47
66:OO:126:ILE:HG21	66:OO:129:ILE:HD11	1.97	0.47
52:AA:155:ARG:NE	73:VV:61:ARG:O	2.37	0.47
48:5:1221:G:O2'	48:5:1222:A:O5'	2.22	0.46
48:5:1541:C:C2	48:5:1619:G:N2	2.82	0.46
48:5:1732:C:C2	48:5:1798:G:C2	3.03	0.46
48:5:1995:G:C6	48:5:1996:C:C4	3.03	0.46
48:5:2771:G:C6	48:5:2772:C:C4	3.03	0.46
48:5:2858:A:O2'	48:5:2859:G:C8	2.65	0.46
49:7:86:G:C2	49:7:92:C:C2	3.03	0.46
51:9:1139:C:O4'	51:9:1139:C:O2	2.33	0.46
51:9:1406:G:O3'	51:9:1408:U:OP1	2.33	0.46
51:9:1859:A:H2'	51:9:1860:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:LEU:HB3	2:B:241:PRO:HD2	1.96	0.46
56:EE:156:MET:O	56:EE:157:ASN:CB	2.63	0.46
56:EE:31:PRO:HD2	56:EE:38:LEU:HD13	1.97	0.46
15:P:32:THR:HG21	15:P:87:SER:HB3	1.96	0.46
21:V:38:TYR:N	21:V:64:THR:O	2.47	0.46
23:X:52:LEU:HD22	23:X:53:ARG:N	2.30	0.46
45:1:57:ARG:HH22	48:5:3862:A:HO2'	1.57	0.46
48:5:1099:C:H2'	48:5:1100:U:O4'	2.16	0.46
48:5:1957:U:O2'	48:5:1958:A:O4'	2.33	0.46
48:5:199:G:N1	48:5:220:C:C2	2.83	0.46
48:5:2245:G:C2	48:5:2246:C:C2	3.04	0.46
48:5:302:C:N4	48:5:303:C:N4	2.64	0.46
48:5:4461:C:C2	48:5:4516:G:C2	3.03	0.46
48:5:4661:G:C6	48:5:4662:C:C4	3.03	0.46
50:8:56:G:C2	50:8:57:C:C2	3.03	0.46
51:9:125:C:OP2	58:GG:198:ARG:NH1	2.39	0.46
51:9:479:C:H2'	51:9:480:G:O4'	2.16	0.46
51:9:562:U:H2'	51:9:563:G:C8	2.49	0.46
51:9:290:U:OP1	56:EE:156:MET:HE2	2.16	0.46
6:F:98:ARG:HH21	6:F:226:THR:HG22	1.81	0.46
15:P:41:ILE:HD12	15:P:150:LEU:CD1	2.46	0.46
20:U:46:ARG:O	20:U:47:ILE:C	2.53	0.46
75:XX:9:THR:O	75:XX:11:ARG:N	2.48	0.46
48:5:1198:G:H2'	48:5:1199:G:C8	2.49	0.46
13:N:68:ARG:CG	48:5:302:C:OP1	2.63	0.46
48:5:106:A:O2'	48:5:335:A:N3	2.43	0.46
48:5:4537:C:H2'	48:5:4538:G:C8	2.50	0.46
48:5:4740:G:C2	48:5:4741:C:C2	3.04	0.46
48:5:978:G:C6	48:5:979:C:C4	3.04	0.46
50:8:127:U:C4	50:8:128:C:C5	3.03	0.46
48:5:22:G:N1	50:8:35:C:C4	2.83	0.46
51:9:1641:A:OP2	51:9:1641:A:H8	1.99	0.46
51:9:358:C:C2	51:9:405:G:C2	3.03	0.46
2:B:252:ALA:HB1	48:5:4524:G:N3	2.30	0.46
56:EE:65:CYS:SG	56:EE:66:MET:N	2.88	0.46
6:F:41:GLN:CG	48:5:2095:A:N1	2.79	0.46
17:R:119:MET:HG3	17:R:123:LEU:HD22	1.97	0.46
19:T:64:VAL:HG22	19:T:72:VAL:HG11	1.97	0.46
74:WW:52:ILE:HG22	74:WW:61:ILE:HG23	1.96	0.46
48:5:1984:A:N6	48:5:2011:C:O2'	2.48	0.46
48:5:1928:C:C4	48:5:2054:U:O2	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:205:C:C4	48:5:211:G:C6	3.04	0.46
48:5:3766:A:N1	51:9:1827:U:O2'	2.33	0.46
48:5:384:A:C6	48:5:386:A:C5	3.04	0.46
48:5:1591:U:N3	48:5:4555:U:OP1	2.47	0.46
48:5:4587:G:C2	48:5:4716:C:C2	3.04	0.46
48:5:479:G:N2	48:5:480:C:C2	2.83	0.46
48:5:747:A:C2	48:5:749:G:H1'	2.50	0.46
50:8:55:U:N3	50:8:62:A:C2	2.83	0.46
51:9:1835:A:N9	51:9:1863:A:N7	2.63	0.46
51:9:23:G:C6	51:9:24:C:C4	3.03	0.46
1:A:209:HIS:CG	1:A:210:PRO:HD2	2.51	0.46
9:I:87:ILE:HG12	9:I:138:ILE:CG1	2.45	0.46
63:LL:106:HIS:CG	63:LL:106:HIS:O	2.69	0.46
59:HH:145:ARG:HD3	74:WW:51:GLU:HB3	1.97	0.46
56:EE:54:TYR:CD1	76:YY:17:LEU:HD11	2.51	0.46
48:5:1171:G:C6	48:5:1172:C:C4	3.04	0.46
48:5:120:A:C2	48:5:148:C:O2	2.68	0.46
48:5:1270:A:H2'	48:5:1271:G:O4'	2.16	0.46
48:5:1855:G:C6	48:5:1856:C:C4	3.04	0.46
48:5:2046:G:C2	48:5:2047:A:C2	3.03	0.46
48:5:2698:G:C6	48:5:2699:C:C4	3.03	0.46
48:5:3900:G:H5''	48:5:3901:A:H4'	1.97	0.46
48:5:4102:C:C2	48:5:4108:G:C2	3.03	0.46
48:5:4372:U:O2	48:5:4377:G:H1'	2.15	0.46
48:5:4916:G:C6	48:5:4917:C:C4	3.04	0.46
48:5:499:G:C2	48:5:500:G:C8	3.03	0.46
48:5:721:G:C2	48:5:948:C:C2	3.03	0.46
47:3:35:U:C1'	51:9:1641:A:P	3.03	0.46
51:9:1726:G:C6	51:9:1727:G:C5	3.03	0.46
51:9:187:G:C6	51:9:188:C:C4	3.04	0.46
2:B:119:TYR:OH	2:B:129:ALA:N	2.48	0.46
56:EE:199:GLU:HB2	56:EE:207:VAL:HG12	1.97	0.46
48:5:1643:A:H2'	48:5:1644:C:C6	2.50	0.46
48:5:177:G:C6	48:5:178:C:C4	3.03	0.46
48:5:1826:G:C6	48:5:1827:C:C4	3.03	0.46
48:5:1269:G:C8	48:5:2111:G:C6	3.04	0.46
48:5:2128:G:C2	48:5:2129:C:C2	3.03	0.46
48:5:2698:G:C2	48:5:2699:C:C2	3.04	0.46
48:5:2618:G:C2	48:5:2720:C:C2	3.03	0.46
48:5:3597:G:C2	48:5:3598:C:C2	3.03	0.46
2:B:4:ARG:HG3	48:5:4458:C:N4	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:262:GLN:N	48:5:4930:C:OP1	2.47	0.46
48:5:497:G:H3'	48:5:498:C:H5''	1.97	0.46
48:5:654:C:H2'	48:5:654:C:O2	2.15	0.46
51:9:1096:G:OP1	74:WW:22:LYS:NZ	2.46	0.46
51:9:1650:A:C5	51:9:1675:A:C2	3.03	0.46
51:9:1703:C:O2	51:9:1832:A:N1	2.48	0.46
70:SS:66:ARG:HD2	70:SS:70:ILE:HD11	1.97	0.46
71:TT:56:ARG:HD2	71:TT:79:TYR:CD2	2.50	0.46
74:WW:105:THR:HB	74:WW:126:LEU:HD11	1.97	0.46
46:2:30:G:C6	46:2:31:C:C4	3.04	0.46
48:5:1279:A:C4	48:5:1280:C:C4	3.04	0.46
48:5:1280:C:N3	48:5:1282:G:C6	2.83	0.46
48:5:1365:C:O2	48:5:1366:G:C8	2.69	0.46
48:5:1379:C:H4'	48:5:1380:G:C8	2.50	0.46
48:5:177:G:C2	48:5:178:C:C2	3.03	0.46
48:5:2818:C:OP1	48:5:4655:A:H4'	2.15	0.46
48:5:207:G:O4'	48:5:406:C:H5'	2.15	0.46
48:5:4919:G:C6	48:5:4920:C:C4	3.04	0.46
51:9:1401:A:H2'	51:9:1402:A:C8	2.51	0.46
51:9:752:G:N1	51:9:790:C:C4	2.83	0.46
51:9:993:G:C2	51:9:994:C:C2	3.04	0.46
52:AA:159:ILE:O	52:AA:159:ILE:HG23	2.16	0.46
69:RR:36:GLU:HG2	69:RR:47:ARG:HD2	1.98	0.46
18:S:83:ARG:HH21	18:S:83:ARG:CG	2.29	0.46
74:WW:26:LEU:HD11	74:WW:60:LYS:HD3	1.96	0.46
74:WW:53:ILE:HD11	74:WW:62:VAL:HG23	1.98	0.46
48:5:1240:G:C6	48:5:1241:C:C4	3.04	0.46
48:5:199:G:C2	48:5:201:C:N3	2.84	0.46
48:5:3586:G:C2	48:5:3587:C:C2	3.03	0.46
48:5:2847:G:N2	48:5:3842:C:C2	2.84	0.46
48:5:4283:G:N1	48:5:4284:C:C4	2.84	0.46
48:5:746:A:H4'	48:5:747:A:OP1	2.16	0.46
48:5:917:A:C6	48:5:919:C:N4	2.84	0.46
48:5:967:C:OP1	48:5:2254:G:N1	2.48	0.46
51:9:1454:A:P	69:RR:3:ARG:HE	2.39	0.46
51:9:834:C:N4	51:9:841:G:C6	2.84	0.46
51:9:872:A:N6	51:9:914:U:C4	2.83	0.46
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.51	0.46
2:B:156:TYR:CD1	48:5:4909:A:C2'	2.91	0.46
56:EE:126:VAL:CG1	56:EE:160:ILE:HD11	2.46	0.46
47:3:24:G:H2'	47:3:25:C:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:24:G:C2	47:3:25:C:C2	3.03	0.46
47:3:38:A:N3	57:FF:135:ARG:NH2	2.63	0.46
48:5:1416:G:N2	48:5:1417:C:C2	2.84	0.46
48:5:3600:G:C6	48:5:3601:C:C4	3.04	0.46
48:5:4472:G:C6	48:5:4473:A:N7	2.84	0.46
48:5:3900:G:C2	48:5:4562:C:N3	2.84	0.46
51:9:1466:G:C6	51:9:1467:C:N4	2.84	0.46
2:B:29:VAL:CG2	2:B:346:THR:HG21	2.46	0.46
5:E:41:SER:HA	48:5:978:G:H4'	1.96	0.46
47:3:38:A:C2	57:FF:135:ARG:CZ	2.98	0.46
57:FF:99:ILE:HD11	77:ZZ:106:GLN:HE22	1.81	0.46
58:GG:66:GLY:O	58:GG:68:LEU:HD22	2.16	0.46
14:O:12:ARG:O	18:S:171:ARG:NH2	2.49	0.46
67:PP:53:GLN:HE22	67:PP:83:MET:HG3	1.80	0.46
74:WW:27:ILE:HG12	74:WW:61:ILE:HB	1.97	0.46
46:2:54:U:H2'	46:2:55:U:O4'	2.16	0.46
48:5:1613:A:H3'	48:5:1614:C:C5'	2.46	0.46
48:5:2065:G:C2	48:5:2066:C:C2	3.04	0.46
48:5:2065:G:H2'	48:5:2066:C:O4'	2.16	0.46
6:F:41:GLN:HG3	48:5:2095:A:N1	2.31	0.46
48:5:3717:A:O2'	48:5:3718:A:O4'	2.33	0.46
48:5:3729:U:H2'	48:5:3730:U:C6	2.52	0.46
48:5:4136:G:C2	48:5:4137:C:C2	3.04	0.46
48:5:4737:G:C2	48:5:4738:C:C2	3.04	0.46
13:N:169:ARG:NH1	48:5:63:G:OP2	2.43	0.46
48:5:705:G:N2	48:5:706:C:C2	2.84	0.46
48:5:726:G:C6	48:5:727:C:N4	2.84	0.46
48:5:918:G:H2'	48:5:918:G:N3	2.31	0.46
51:9:1102:G:C2	51:9:1103:C:C4	3.04	0.46
51:9:1319:U:H2'	51:9:1320:G:O4'	2.16	0.46
51:9:1563:G:C2	51:9:1564:C:C2	3.04	0.46
1:A:19:HIS:NE2	48:5:1338:G:N2	68.37	0.46
5:E:250:ASP:O	5:E:254:LEU:N	2.46	0.46
12:M:37:LEU:HD23	18:S:100:LEU:HD11	1.98	0.46
48:5:1639:U:H2'	48:5:1639:U:O2	2.16	0.45
48:5:2270:G:C6	48:5:2271:C:C4	3.04	0.45
48:5:181:C:C4	48:5:256:G:N1	2.84	0.45
48:5:2569:G:H2'	48:5:2570:U:O4'	2.15	0.45
48:5:2711:G:H3'	48:5:2712:G:H5''	1.98	0.45
48:5:3690:U:H2'	48:5:3691:G:O4'	2.17	0.45
1:A:207:VAL:HG12	48:5:3919:C:H4'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3941:G:H2'	48:5:3942:A:O4'	2.15	0.45
48:5:5017:G:C2	48:5:5018:C:C2	3.05	0.45
48:5:5017:G:C6	48:5:5018:C:C4	3.04	0.45
48:5:984:C:C2	48:5:1070:G:N2	2.84	0.45
7:G:221:ALA:O	7:G:224:THR:OG1	2.34	0.45
7:G:58:PRO:HD3	23:X:46:PHE:HD2	1.80	0.45
75:XX:57:VAL:HG11	75:XX:115:ILE:HG22	1.97	0.45
46:2:7:G:C6	46:2:49:C:N4	2.84	0.45
47:3:29:A:HO2'	47:3:30:G:P	2.33	0.45
48:5:35:U:O2'	48:5:1525:A:N1	2.46	0.45
48:5:3942:A:H2'	48:5:3943:A:O4'	2.17	0.45
48:5:4423:U:O2	48:5:4423:U:O4'	2.34	0.45
48:5:4773:C:C2	48:5:4863:G:C2	3.04	0.45
48:5:4881:U:O2	48:5:4881:U:O4'	2.34	0.45
48:5:4904:G:N2	48:5:4905:C:C2	2.85	0.45
51:9:1862:G:N2	51:9:1863:A:H2	2.13	0.45
51:9:305:U:O2'	51:9:309:G:O4'	2.28	0.45
51:9:997:A:H2'	51:9:998:A:O4'	2.16	0.45
54:CC:192:LEU:HD23	54:CC:227:TRP:HE1	1.77	0.45
60:II:55:TYR:HB2	60:II:182:CYS:O	2.16	0.45
73:VV:30:ALA:O	73:VV:60:ARG:HD3	2.17	0.45
47:3:67:U:C2'	47:3:68:C:C5'	2.77	0.45
48:5:1826:G:C2	48:5:1827:C:C2	3.04	0.45
48:5:1904:G:N2	48:5:2073:C:C2	2.84	0.45
48:5:2465:C:H2'	48:5:2466:G:C8	2.51	0.45
48:5:77:U:H3	48:5:336:A:N6	2.13	0.45
48:5:4699:U:C4	48:5:4702:G:C6	3.05	0.45
48:5:4883:C:O2'	48:5:4884:G:P	2.74	0.45
48:5:5001:U:H2'	48:5:5002:U:O4'	2.16	0.45
48:5:688:U:H2'	48:5:689:U:C6	2.52	0.45
51:9:1673:U:H2'	51:9:1674:G:O4'	2.16	0.45
51:9:23:G:C2	51:9:24:C:C2	3.04	0.45
51:9:434:G:N3	51:9:473:A:H2	2.13	0.45
51:9:591:U:O4'	51:9:591:U:O2	2.31	0.45
51:9:673:G:C6	51:9:674:C:C4	3.04	0.45
4:D:111:ASN:ND2	4:D:111:ASN:C	2.70	0.45
63:LL:35:ARG:NH2	63:LL:55:TYR:O	2.43	0.45
12:M:119:ARG:NH2	14:O:189:ILE:HD12	2.31	0.45
24:Y:59:ARG:NH2	48:5:200:U:O2'	2.49	0.45
48:5:1098:G:C2	48:5:1099:C:C2	3.05	0.45
48:5:190:G:C2	48:5:252:C:C2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:14:ARG:NH2	48:5:2083:C:OP2	2.49	0.45
48:5:4109:G:C6	48:5:4110:C:C4	3.05	0.45
48:5:4644:G:C6	48:5:4645:C:C4	3.05	0.45
48:5:504:G:O6	48:5:654:C:C4	2.70	0.45
51:9:1294:G:C6	51:9:1295:A:C5	3.04	0.45
51:9:1298:G:O2'	51:9:1299:A:C8	2.69	0.45
51:9:1409:A:C6	51:9:1410:C:C5	3.04	0.45
53:BB:33:VAL:HG21	53:BB:67:PHE:CZ	2.52	0.45
63:LL:76:VAL:HB	63:LL:125:ILE:HD13	1.98	0.45
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	1.97	0.45
73:VV:47:ASN:O	73:VV:49:GLN:N	2.49	0.45
77:ZZ:58:LEU:HD23	77:ZZ:62:VAL:HG21	1.97	0.45
47:3:35:U:O4'	51:9:1641:A:P	2.74	0.45
48:5:1549:G:N2	48:5:1580:C:C2	2.84	0.45
48:5:1925:G:C6	48:5:1926:C:C4	3.05	0.45
48:5:1995:G:C6	48:5:1996:C:N3	2.84	0.45
48:5:2567:G:C2	48:5:2568:C:C2	3.04	0.45
48:5:2395:A:HO2'	48:5:2806:A:H1'	1.77	0.45
48:5:3918:G:C6	48:5:3919:C:C4	3.04	0.45
48:5:5008:C:H2'	48:5:5009:G:O4'	2.16	0.45
48:5:977:C:O2'	48:5:978:G:H5'	2.17	0.45
51:9:1489:A:H4'	51:9:1490:G:OP2	2.15	0.45
51:9:194:C:C2	51:9:206:G:C2	3.05	0.45
51:9:293:C:O2'	51:9:294:U:H3'	2.16	0.45
5:E:124:HIS:NE2	48:5:1282:G:N7	2.65	0.45
9:I:93:PRO:HB2	9:I:125:THR:HB	1.99	0.45
60:II:139:LYS:HD2	60:II:145:ILE:HD12	1.99	0.45
14:O:116:LYS:HD3	18:S:169:THR:HG21	1.98	0.45
48:5:1072:C:O2	48:5:1072:C:H2'	2.17	0.45
48:5:1448:G:C2	48:5:1449:C:C2	3.04	0.45
13:N:179:LYS:O	48:5:298:G:H5'	2.16	0.45
48:5:3727:A:H2'	48:5:3728:A:C8	2.51	0.45
48:5:4473:A:H2'	48:5:4474:A:C8	2.51	0.45
51:9:1274:G:N7	62:KK:43:LEU:HD13	2.32	0.45
51:9:1537:A:N1	51:9:1596:U:O4	2.50	0.45
15:P:41:ILE:HD12	15:P:150:LEU:HD13	1.99	0.45
72:UU:46:LYS:HD3	72:UU:97:ILE:HG23	1.98	0.45
74:WW:8:ALA:HA	74:WW:74:VAL:HG11	1.97	0.45
48:5:179:G:C2	48:5:180:C:C2	3.05	0.45
48:5:199:G:C6	48:5:220:C:N3	2.85	0.45
48:5:2664:G:N2	48:5:2671:C:C2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:351:C:C2	50:8:25:G:C2	3.04	0.45
48:5:1322:A:N6	48:5:4446:U:OP1	2.48	0.45
48:5:488:G:N2	48:5:489:C:C2	2.85	0.45
48:5:5020:G:C6	48:5:5021:C:C4	3.04	0.45
49:7:27:G:C2	49:7:28:C:C2	3.05	0.45
51:9:1041:G:C2	51:9:1075:C:C2	3.04	0.45
51:9:1541:G:C2	51:9:1542:C:C2	3.05	0.45
51:9:1597:C:H4'	51:9:1603:G:C6	2.52	0.45
57:FF:143:PRO:O	57:FF:147:VAL:HG23	2.16	0.45
59:HH:177:TYR:CZ	59:HH:181:THR:HG21	2.51	0.45
61:JJ:94:LEU:HD12	61:JJ:97:ILE:HD12	1.98	0.45
16:Q:17:GLU:HB2	16:Q:18:PRO:HD2	1.98	0.45
70:SS:113:ARG:HG2	70:SS:113:ARG:HH11	1.81	0.45
72:UU:68:THR:HG22	72:UU:69:PRO:O	2.17	0.45
74:WW:82:GLN:O	74:WW:84:LYS:N	2.49	0.45
48:5:994:G:C2	48:5:1050:C:C2	3.04	0.45
48:5:1241:C:C2'	48:5:1242:G:OP1	2.65	0.45
48:5:1855:G:C2	48:5:1856:C:C2	3.04	0.45
48:5:2594:C:C2	48:5:2752:G:C2	3.04	0.45
50:8:94:G:H5'	50:8:94:G:C8	2.52	0.45
51:9:1267:C:HO2'	51:9:1268:C:H5'	1.77	0.45
51:9:1294:G:O2'	51:9:1295:A:O5'	2.29	0.45
51:9:1717:C:C2	51:9:1817:G:C2	3.04	0.45
51:9:1749:G:C2	51:9:1750:C:C2	3.05	0.45
59:HH:115:LYS:O	59:HH:116:ARG:CB	2.65	0.45
9:I:49:CYS:HG	9:I:51:HIS:CD2	2.32	0.45
64:MM:50:CYS:SG	64:MM:51:VAL:N	2.90	0.45
66:OO:62:VAL:HG21	66:OO:73:ALA:HB2	1.98	0.45
71:TT:62:ARG:C	71:TT:62:ARG:HD2	2.37	0.45
48:5:158:A:H5''	48:5:159:C:H2'	1.99	0.45
48:5:1744:U:H2'	48:5:1745:G:O4'	2.17	0.45
48:5:1959:U:H1'	48:5:1961:G:O4'	2.17	0.45
48:5:2898:G:C6	48:5:2899:C:C4	3.05	0.45
48:5:4473:A:C2	48:5:4474:A:C5	3.04	0.45
48:5:4874:A:H3'	48:5:4875:G:C5'	2.47	0.45
48:5:994:G:C2	48:5:995:C:C2	3.05	0.45
51:9:1759:G:C2	51:9:1774:C:C2	3.05	0.45
51:9:751:G:O2'	51:9:752:G:O4'	2.25	0.45
51:9:797:C:O2	51:9:798:G:O2'	2.35	0.45
5:E:157:ARG:HD3	5:E:266:TYR:CZ	2.52	0.45
58:GG:173:ALA:HB1	58:GG:174:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:GG:76:LEU:HD22	58:GG:92:ARG:CG	2.47	0.45
59:HH:15:LYS:N	59:HH:16:PRO:HD2	2.32	0.45
9:I:202:ASN:N	9:I:202:ASN:OD1	2.49	0.45
66:OO:65:ASP:OD1	66:OO:65:ASP:N	2.50	0.45
25:Z:55:ALA:O	25:Z:57:MET:N	2.49	0.45
48:5:1070:G:C6	48:5:1071:C:N4	2.85	0.45
48:5:1947:U:H2'	48:5:1947:U:O2	2.17	0.45
48:5:202:C:C2	48:5:214:G:C2	3.04	0.45
48:5:2245:G:C6	48:5:2246:C:C4	3.05	0.45
48:5:2322:G:C6	48:5:2323:C:C4	3.05	0.45
2:B:249:ARG:NH2	48:5:3845:A:OP2	2.49	0.45
14:O:85:ARG:NH2	48:5:3887:C:OP2	2.43	0.45
48:5:4183:G:N3	48:5:4183:G:H2'	2.32	0.45
48:5:4207:C:C2	48:5:4226:G:N2	2.85	0.45
48:5:751:G:N2	48:5:912:G:C4	2.84	0.45
48:5:994:G:C6	48:5:995:C:C4	3.05	0.45
51:9:1218:C:H6	51:9:1218:C:O5'	2.00	0.45
51:9:1563:G:C6	51:9:1564:C:C4	3.05	0.45
51:9:673:G:C2	51:9:674:C:C2	3.05	0.45
1:A:233:ARG:O	1:A:235:VAL:HB	2.17	0.45
54:CC:112:VAL:HG22	54:CC:123:ARG:O	2.16	0.45
60:II:25:ARG:O	60:II:27:TYR:N	2.50	0.45
18:S:47:PHE:HE1	18:S:125:GLN:HG2	1.81	0.45
23:X:127:LEU:HD12	23:X:127:LEU:C	2.38	0.45
47:3:70:G:O2'	47:3:71:G:O4'	2.22	0.44
48:5:1196:G:C6	48:5:1197:C:C4	3.05	0.44
48:5:1404:G:C6	48:5:1405:C:C4	3.04	0.44
48:5:2122:G:O2'	48:5:2123:C:P	2.74	0.44
48:5:2313:A:O2'	48:5:2314:G:OP1	2.22	0.44
48:5:2517:A:N3	48:5:2539:C:O2'	2.43	0.44
48:5:2559:G:C6	48:5:2560:C:C4	3.04	0.44
48:5:2715:G:C2	48:5:2716:C:C2	3.05	0.44
48:5:278:G:H4'	48:5:279:A:OP2	2.17	0.44
48:5:4731:G:H4'	48:5:4732:G:H5'	1.99	0.44
48:5:973:G:N2	48:5:974:C:C2	2.85	0.44
49:7:111:C:H2'	49:7:112:U:O4'	2.18	0.44
50:8:134:G:C6	50:8:135:C:C4	3.05	0.44
51:9:323:C:H3'	51:9:324:C:C5'	2.47	0.44
51:9:828:G:C6	51:9:829:C:C4	3.05	0.44
51:9:832:G:N2	51:9:843:C:C2	2.85	0.44
1:A:90:CYS:CB	1:A:101:VAL:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:110:ASN:O	52:AA:116:PHE:CD1	2.71	0.44
7:G:159:HIS:CE1	7:G:185:LYS:HE2	2.51	0.44
59:HH:76:GLN:HE22	59:HH:94:PHE:HB2	1.82	0.44
14:O:27:VAL:CG1	14:O:98:ALA:HB1	2.47	0.44
17:R:4:LEU:HD22	17:R:32:ILE:HG22	2.00	0.44
48:5:1196:G:C2	48:5:1197:C:C2	3.05	0.44
48:5:1268:G:C4	48:5:2111:G:N2	2.86	0.44
48:5:1277:G:N1	48:5:1278:C:C4	2.85	0.44
48:5:1823:G:C3'	48:5:1825:A:P	3.05	0.44
48:5:1840:G:C3'	48:5:1842:G:P	3.05	0.44
48:5:2315:G:C2	48:5:2325:C:C2	3.05	0.44
48:5:2376:A:H2'	48:5:2377:C:O4'	2.17	0.44
48:5:2594:C:O2	48:5:2752:G:C2	2.71	0.44
48:5:2682:G:N2	48:5:2683:C:C2	2.85	0.44
48:5:2715:G:C6	48:5:2716:C:C4	3.05	0.44
48:5:3782:C:C2	48:5:3811:G:C2	3.05	0.44
48:5:4109:G:C2	48:5:4110:C:C2	3.06	0.44
48:5:4740:G:C6	48:5:4741:C:C4	3.04	0.44
48:5:978:G:C2	48:5:979:C:C2	3.05	0.44
51:9:1612:G:C2	51:9:1628:C:C2	3.05	0.44
51:9:508:A:H3'	51:9:509:G:H8	1.82	0.44
51:9:697:G:C2	51:9:734:C:C2	3.04	0.44
4:D:146:LEU:HD11	4:D:159:VAL:CG1	2.47	0.44
19:T:80:VAL:O	19:T:82:GLY:N	2.51	0.44
22:W:44:ARG:HH11	22:W:44:ARG:HG2	1.81	0.44
70:SS:8:LYS:HD3	77:ZZ:49:LEU:HD11	2.00	0.44
48:5:1995:G:C5	48:5:1996:C:C4	3.05	0.44
48:5:2609:G:C2	48:5:2731:C:O2	2.70	0.44
48:5:2909:C:O2	48:5:3586:G:C2	2.71	0.44
48:5:4090:G:N2	48:5:4160:C:C2	2.86	0.44
48:5:4451:G:C6	48:5:4522:G:C8	3.05	0.44
48:5:4749:C:O2	48:5:4749:C:O4'	2.32	0.44
48:5:751:G:C2	48:5:752:G:N7	2.84	0.44
49:7:117:G:C6	49:7:118:C:C4	3.05	0.44
49:7:25:G:C6	49:7:26:C:C4	3.06	0.44
51:9:1386:A:H2'	51:9:1387:G:H8	1.82	0.44
51:9:1559:C:C2	51:9:1577:G:C2	3.06	0.44
51:9:200:G:C2	51:9:201:C:C4	3.05	0.44
51:9:834:C:N3	51:9:841:G:N2	2.66	0.44
51:9:917:U:H2'	51:9:918:U:O4'	2.17	0.44
2:B:100:ARG:NH1	48:5:4911:A:OP2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:FF:154:LEU:HA	57:FF:189:ALA:HB2	2.00	0.44
76:YY:7:ILE:HD11	76:YY:40:ILE:HG13	1.99	0.44
48:5:1296:G:C1'	48:5:1297:U:P	3.06	0.44
48:5:192:G:C2	48:5:250:C:C2	3.05	0.44
48:5:4088:C:H2'	48:5:4089:G:C8	2.53	0.44
48:5:4416:G:N1	48:5:4417:C:C4	2.86	0.44
48:5:43:U:C2'	48:5:44:A:O5'	2.66	0.44
48:5:52:G:N1	48:5:53:C:C4	2.86	0.44
48:5:723:A:C2	48:5:724:C:C6	3.06	0.44
51:9:1227:G:C2	51:9:1228:A:C8	3.06	0.44
51:9:1573:G:C6	51:9:1574:C:N3	2.86	0.44
51:9:1552:G:C8	51:9:1578:U:C4	3.05	0.44
51:9:1835:A:C8	51:9:1863:A:C8	3.06	0.44
51:9:594:A:C6	51:9:643:A:C8	3.06	0.44
51:9:841:G:C6	51:9:842:C:C4	3.05	0.44
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.99	0.44
5:E:169:LEU:HD21	5:E:187:GLN:HG3	1.98	0.44
56:EE:15:PRO:HG2	56:EE:18:TRP:CZ2	2.52	0.44
6:F:146:TYR:CE2	6:F:239:GLU:CB	3.01	0.44
8:H:55:LEU:HD22	8:H:77:VAL:HG11	2.00	0.44
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.99	0.44
47:3:35:U:O2'	47:3:36:U:H5'	2.17	0.44
47:3:5:G:N2	47:3:68:C:C2	2.85	0.44
48:5:3600:G:C2	48:5:3601:C:C2	3.06	0.44
48:5:4091:G:N2	48:5:4159:C:C2	2.85	0.44
48:5:4754:G:N2	48:5:4880:C:C2	2.86	0.44
48:5:5038:A:H2'	48:5:5039:U:O4'	2.18	0.44
51:9:1446:A:O2'	51:9:1447:G:H5''	2.18	0.44
51:9:1754:G:C2	51:9:1755:C:C2	3.05	0.44
51:9:1839:U:H2'	51:9:1840:U:C6	2.52	0.44
51:9:374:G:C2	51:9:391:C:C2	3.06	0.44
51:9:480:G:C6	51:9:481:C:N3	2.86	0.44
51:9:666:U:C2	51:9:667:U:C5	3.05	0.44
7:G:51:LEU:HD11	48:5:4086:G:C4	2.53	0.44
64:MM:35:ILE:HD13	64:MM:61:TYR:CE1	2.53	0.44
66:OO:133:THR:O	66:OO:135:ILE:N	2.49	0.44
25:Z:29:ILE:HD12	25:Z:29:ILE:N	2.32	0.44
48:5:1171:G:C2	48:5:1172:C:C2	3.05	0.44
48:5:1430:C:O2	48:5:1455:G:C2	2.70	0.44
48:5:1691:G:C6	48:5:1692:C:C4	3.06	0.44
48:5:1928:C:N4	48:5:2054:U:O2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2288:G:C2	48:5:2290:C:C4	3.05	0.44
48:5:2315:G:C2	48:5:2325:C:O2	2.71	0.44
48:5:2481:G:C6	48:5:2482:C:C4	3.05	0.44
48:5:3882:C:H2'	48:5:3883:U:C6	2.53	0.44
48:5:4129:G:C6	48:5:4130:C:C4	3.05	0.44
48:5:3900:G:C2	48:5:4562:C:C2	3.06	0.44
50:8:10:G:C2	50:8:11:C:C2	3.06	0.44
51:9:126:G:N2	51:9:180:G:O2'	2.49	0.44
51:9:1669:G:C6	51:9:1670:C:C4	3.06	0.44
51:9:31:U:O2'	51:9:595:U:H4'	2.17	0.44
51:9:640:A:H2'	51:9:641:A:C8	2.52	0.44
54:CC:133:TYR:CD1	54:CC:216:MET:HA	2.53	0.44
9:I:47:PRO:HB3	9:I:171:TRP:CE2	2.53	0.44
12:M:116:LYS:HE3	14:O:201:PHE:CE2	2.53	0.44
75:XX:109:GLY:O	75:XX:110:HIS:C	2.56	0.44
48:5:1064:G:C2	48:5:1065:G:C4	3.06	0.44
48:5:125:C:C2	48:5:145:G:C2	3.06	0.44
48:5:1958:A:C4'	48:5:1962:A:O2'	2.63	0.44
48:5:2021:G:C2	48:5:2022:C:C2	3.06	0.44
48:5:2275:G:H5''	48:5:2275:G:H8	1.82	0.44
48:5:3670:C:O2'	48:5:3671:G:O4'	2.36	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
48:5:4408:G:C6	48:5:4409:C:C4	3.06	0.44
48:5:5016:A:N6	48:5:5033:G:O2'	2.50	0.44
48:5:744:G:H2'	48:5:745:G:C8	2.53	0.44
50:8:68:G:H2'	50:8:69:U:O4'	2.17	0.44
51:9:103:A:C6	51:9:356:C:C2	3.06	0.44
51:9:1298:G:O2'	51:9:1299:A:O4'	2.36	0.44
51:9:993:G:C6	51:9:994:C:C4	3.06	0.44
58:GG:7:PHE:CD2	58:GG:10:THR:HG23	2.53	0.44
59:HH:8:ILE:HG21	59:HH:28:LEU:HD13	2.00	0.44
59:HH:66:VAL:HB	59:HH:67:PRO:HD3	2.00	0.44
63:LL:68:ILE:HG21	63:LL:143:LEU:HD21	1.99	0.44
14:O:133:ARG:CZ	48:5:1928:C:C4	3.00	0.44
15:P:18:ARG:HA	15:P:147:GLU:HA	1.99	0.44
67:PP:34:MET:HE2	67:PP:42:ARG:HA	1.99	0.44
51:9:1161:U:O4	75:XX:2:GLY:N	2.50	0.44
25:Z:54:THR:O	25:Z:56:ALA:N	2.51	0.44
48:5:207:G:C6	48:5:208:A:C6	3.05	0.44
48:5:2898:G:C2	48:5:2899:C:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:8:126:C:O2'	50:8:127:U:C5	2.64	0.44
50:8:134:G:C2	50:8:135:C:C2	3.06	0.44
50:8:60:G:O6	50:8:96:C:O2'	2.25	0.44
51:9:1307:U:C3'	51:9:1308:U:H5''	2.46	0.44
51:9:1551:U:O2	51:9:1551:U:O4'	2.35	0.44
51:9:1559:C:C2	51:9:1577:G:N2	2.85	0.44
51:9:1749:G:C6	51:9:1750:C:C4	3.06	0.44
51:9:668:A:N1	51:9:1143:A:C5	2.86	0.44
51:9:752:G:C2	51:9:790:C:N3	2.85	0.44
51:9:832:G:C6	51:9:833:C:C4	3.06	0.44
51:9:1623:A:H5''	70:SS:133:GLY:HA3	2.00	0.44
48:5:1270:A:C5	48:5:1271:G:H1'	2.53	0.44
48:5:1374:G:C6	48:5:1375:C:C4	3.06	0.44
48:5:1404:G:C2	48:5:1405:C:C2	3.06	0.44
48:5:2021:G:C6	48:5:2022:C:C4	3.06	0.44
48:5:2088:A:O2'	48:5:2089:G:P	2.76	0.44
48:5:2270:G:C2	48:5:2271:C:C2	3.06	0.44
48:5:2:G:C2	48:5:3:C:C2	3.06	0.44
48:5:4147:G:C6	48:5:4148:C:C4	3.05	0.44
48:5:4216:G:C2'	48:5:4217:G:H5'	2.48	0.44
48:5:4508:C:N3	48:5:4512:U:H5	2.16	0.44
5:E:132:HIS:CE1	48:5:711:A:H1'	2.53	0.44
48:5:977:C:C3'	48:5:978:G:H5'	2.46	0.44
51:9:1500:G:C6	51:9:1501:C:N3	2.86	0.44
51:9:1345:G:OP1	51:9:1688:C:O2'	2.36	0.44
51:9:187:G:C2	51:9:188:C:C2	3.05	0.44
51:9:696:G:C2	51:9:735:C:C2	3.06	0.44
51:9:964:A:N3	51:9:1054:G:O2'	2.45	0.44
51:9:993:G:OP1	51:9:1131:G:N2	2.40	0.44
52:AA:124:VAL:HG13	52:AA:130:ASP:HB2	1.99	0.44
3:C:28:PHE:HA	3:C:129:ALA:HA	2.00	0.44
60:II:6:ASP:N	60:II:6:ASP:OD1	2.51	0.44
17:R:99:MET:O	17:R:103:ARG:HB2	2.17	0.44
48:5:2612:G:C6	48:5:2613:C:C4	3.05	0.43
48:5:2793:G:H5''	48:5:2794:C:H5''	1.99	0.43
48:5:3861:A:H2'	48:5:3862:A:C8	2.53	0.43
48:5:4713:G:C6	48:5:4714:C:C4	3.05	0.43
48:5:4890:G:C2	48:5:4930:C:C2	3.06	0.43
51:9:1664:A:HO2'	51:9:1665:G:C5'	2.30	0.43
51:9:1777:G:C6	51:9:1778:C:C4	3.06	0.43
51:9:1847:G:C2	51:9:1853:C:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:379:C:N3	60:II:5:ARG:NH1	2.66	0.43
51:9:92:A:H2'	51:9:446:G:N2	2.32	0.43
2:B:154:LYS:CB	2:B:154:LYS:NZ	2.81	0.43
53:BB:189:ILE:HB	53:BB:190:PRO:HD3	1.99	0.43
59:HH:43:LEU:HD22	59:HH:72:PHE:CD2	2.53	0.43
68:QQ:84:ILE:HG13	68:QQ:85:ARG:N	2.32	0.43
69:RR:38:ILE:HD12	69:RR:39:ALA:N	2.33	0.43
19:T:85:LEU:HD13	48:5:4305:G:C2	2.53	0.43
48:5:1280:C:C2	48:5:1282:G:C4	3.06	0.43
48:5:1874:A:C5'	48:5:4218:U:O2	2.66	0.43
48:5:1265:G:OP1	48:5:2115:G:N1	2.51	0.43
48:5:1436:C:O5'	48:5:2119:C:N4	2.51	0.43
48:5:2567:G:C6	48:5:2568:C:C4	3.07	0.43
48:5:2654:C:N3	48:5:2681:G:C2	2.86	0.43
48:5:4139:G:C6	48:5:4140:C:C4	3.06	0.43
48:5:4142:C:C4	48:5:4143:G:N1	2.86	0.43
48:5:4320:G:H2'	48:5:4321:U:O4'	2.18	0.43
48:5:4666:G:C2	48:5:4667:C:C2	3.06	0.43
48:5:4681:A:H2'	48:5:4682:U:O4'	2.18	0.43
48:5:5:A:C6	48:5:6:C:C4	3.07	0.43
51:9:1315:U:C4	51:9:1316:C:C4	3.06	0.43
51:9:1337:C:O2'	72:UU:68:THR:HG23	2.18	0.43
51:9:29:G:C2	51:9:30:C:C2	3.06	0.43
51:9:623:G:N2	51:9:624:C:C2	2.86	0.43
1:A:34:PHE:CD2	48:5:4087:G:C6	3.06	0.43
2:B:56:ILE:CG1	2:B:365:LEU:HD22	2.47	0.43
3:C:262:ASP:O	3:C:271:ALA:O	2.36	0.43
48:5:3610:A:O2'	60:II:89:GLU:OE1	2.19	0.43
2:B:261:ARG:HB2	14:O:64:THR:HG21	2.00	0.43
17:R:99:MET:SD	17:R:99:MET:N	2.91	0.43
47:3:69:G:O2'	47:3:70:G:C8	2.70	0.43
48:5:1090:G:C2	48:5:1091:C:C2	3.06	0.43
48:5:1237:C:O4'	48:5:1237:C:O2	2.33	0.43
48:5:1925:G:C2	48:5:1926:C:C2	3.06	0.43
48:5:254:G:C2	48:5:255:C:C2	3.06	0.43
48:5:2703:G:C2	48:5:2704:C:C2	3.06	0.43
48:5:4482:U:N3	48:5:4483:C:C5	2.86	0.43
48:5:952:G:C6	48:5:953:C:C4	3.06	0.43
51:9:114:G:O6	51:9:351:G:H1'	2.18	0.43
51:9:14:C:O2	51:9:1198:G:C2	2.72	0.43
51:9:1524:G:N2	51:9:1525:C:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1777:G:C2	51:9:1778:C:C2	3.05	0.43
53:BB:125:VAL:HG22	53:BB:169:MET:HG3	2.00	0.43
8:H:117:PHE:CE1	8:H:118:LEU:HD23	2.53	0.43
60:II:182:CYS:SG	60:II:183:GLY:N	2.92	0.43
65:NN:88:LEU:CD2	65:NN:135:LEU:HD11	2.48	0.43
14:O:48:TYR:CE2	48:5:1930:U:C2	3.07	0.43
23:X:119:ILE:HG23	23:X:120:ASP:N	2.33	0.43
48:5:1655:C:H2'	48:5:1656:U:H5''	2.00	0.43
48:5:2457:G:C6	48:5:2458:C:C4	3.06	0.43
48:5:2871:A:H2'	48:5:2872:C:O4'	2.18	0.43
48:5:3590:G:N1	48:5:3591:C:C2	2.86	0.43
51:9:1643:U:H2'	51:9:1644:C:H6	1.83	0.43
56:EE:72:ILE:HD13	56:EE:82:TYR:CD1	2.53	0.43
7:G:30:PRO:HG2	7:G:31:LEU:HD22	2.00	0.43
60:II:38:ILE:HD11	60:II:81:VAL:HG23	2.00	0.43
48:5:1048:G:C6	48:5:1049:C:C4	3.06	0.43
48:5:1270:A:C2'	48:5:1271:G:O5'	2.66	0.43
48:5:1724:G:C4'	48:5:1725:U:OP2	2.63	0.43
48:5:2463:G:C2	48:5:2464:C:C2	3.07	0.43
48:5:2559:G:C2	48:5:2560:C:C2	3.06	0.43
48:5:2612:G:C2	48:5:2613:C:C2	3.06	0.43
48:5:4240:G:C2	48:5:4241:C:C2	3.06	0.43
48:5:4666:G:C6	48:5:4667:C:C4	3.05	0.43
11:L:163:LYS:NZ	48:5:509:A:H5'	2.33	0.43
48:5:476:G:C2	48:5:679:C:C2	3.06	0.43
48:5:76:A:C5	48:5:77:U:C5	3.07	0.43
51:9:1246:A:N3	51:9:1251:A:O2'	2.46	0.43
51:9:1335:G:C2	51:9:1336:C:C2	3.05	0.43
52:AA:33:GLN:HB3	52:AA:154:LEU:HD12	2.01	0.43
53:BB:136:ARG:HG3	53:BB:136:ARG:HH21	1.82	0.43
3:C:86:ARG:HA	3:C:89:GLN:HG3	2.00	0.43
4:D:44:TYR:CD1	48:5:1823:G:H4'	2.54	0.43
8:H:117:PHE:CZ	8:H:118:LEU:HD23	2.54	0.43
60:II:44:HIS:O	60:II:56:ARG:N	2.51	0.43
61:JJ:128:VAL:O	61:JJ:132:GLN:HG3	2.19	0.43
46:2:65:G:N2	46:2:66:C:C2	2.87	0.43
48:5:1048:G:C2	48:5:1049:C:C2	3.05	0.43
48:5:1271:G:H3'	48:5:1272:C:H5'	2.00	0.43
48:5:4250:G:C2	48:5:4259:C:C2	3.06	0.43
48:5:744:G:C2	48:5:921:C:C2	3.06	0.43
51:9:1109:C:C2'	51:9:1109:C:O2	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1121:G:C6	51:9:1122:A:C5	3.06	0.43
52:AA:119:PRO:HG2	52:AA:142:LEU:HD11	2.00	0.43
3:C:342:ARG:HG3	3:C:342:ARG:HH11	1.84	0.43
57:FF:99:ILE:HD13	57:FF:171:GLU:HA	2.00	0.43
47:3:41:U:C4'	57:FF:198:ARG:HD3	2.48	0.43
63:LL:5:GLN:OE1	63:LL:11:GLN:HB2	2.18	0.43
63:LL:77:VAL:HA	63:LL:88:ILE:HG22	2.01	0.43
46:2:35:A:OP2	68:QQ:146:ARG:NH1	2.51	0.43
70:SS:28:PHE:O	70:SS:31:THR:OG1	2.36	0.43
23:X:96:LEU:HG	23:X:140:LEU:HD11	1.99	0.43
47:3:33:U:C5'	57:FF:127:ARG:NH1	2.82	0.43
48:5:1213:G:C6	48:5:1215:C:C4	3.06	0.43
48:5:1358:G:N3	48:5:1359:G:N7	2.66	0.43
48:5:1811:G:C2	48:5:1812:C:C2	3.07	0.43
48:5:2481:G:C2	48:5:2482:C:C2	3.07	0.43
48:5:2816:G:C6	48:5:2817:C:C4	3.06	0.43
48:5:298:G:C2	48:5:299:C:C2	3.07	0.43
48:5:2862:G:N3	48:5:3624:A:H2'	2.34	0.43
48:5:3705:G:C6	48:5:3706:C:C4	3.06	0.43
48:5:4187:G:H2'	48:5:4188:U:O4'	2.19	0.43
48:5:4222:G:C6	48:5:4223:C:C4	3.07	0.43
48:5:4349:C:H3'	48:5:4350:C:C5'	2.48	0.43
48:5:469:C:C2	48:5:470:A:C8	3.07	0.43
48:5:4904:G:C2	48:5:4905:C:C2	3.06	0.43
48:5:642:G:C2	48:5:643:C:C4	3.06	0.43
51:9:1455:A:H2'	51:9:1456:G:H8	1.84	0.43
51:9:29:G:C6	51:9:30:C:C4	3.06	0.43
51:9:839:C:C2'	51:9:839:C:O2	2.65	0.43
2:B:43:LEU:HD13	2:B:196:TRP:HH2	1.82	0.43
3:C:224:ILE:HG22	3:C:227:ILE:HD13	1.99	0.43
54:CC:192:LEU:HD12	54:CC:193:VAL:N	2.33	0.43
7:G:87:LEU:HD11	7:G:91:THR:HG21	2.01	0.43
51:9:65:C:C2	58:GG:174:PRO:HB3	2.54	0.43
58:GG:76:LEU:HD22	58:GG:92:ARG:HG2	2.00	0.43
60:II:25:ARG:HB3	60:II:27:TYR:CE2	2.54	0.43
51:9:522:A:H4'	61:JJ:131:ARG:HH22	1.84	0.43
13:N:180:PHE:O	13:N:182:HIS:N	2.52	0.43
51:9:1492:U:H1'	72:UU:70:CYS:SG	2.58	0.43
48:5:1912:G:C2	48:5:1913:C:C2	3.07	0.43
48:5:199:G:C2	48:5:201:C:C4	3.06	0.43
48:5:2256:C:H1'	48:5:2257:C:OP2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:322:C:O2	48:5:4356:G:C2	2.71	0.43
48:5:4129:G:C2	48:5:4130:C:C2	3.06	0.43
2:B:2:SER:N	48:5:4517:A:OP2	2.52	0.43
48:5:4919:G:N2	48:5:4920:C:C2	2.87	0.43
48:5:744:G:H2'	48:5:745:G:H8	1.83	0.43
51:9:1229:G:C6	51:9:1230:C:C4	3.07	0.43
51:9:1398:G:N1	51:9:1399:C:C4	2.87	0.43
51:9:1728:U:H3'	51:9:1729:U:H5''	2.01	0.43
51:9:911:C:C3'	51:9:912:C:H5'	2.47	0.43
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.59	0.43
9:I:191:ILE:HD12	9:I:200:ILE:HD12	1.56	0.43
16:Q:89:ASP:OD1	16:Q:91:ARG:NH2	2.51	0.43
68:QQ:41:MET:SD	68:QQ:41:MET:N	2.91	0.43
75:XX:84:PHE:HB2	75:XX:118:VAL:HG11	1.99	0.43
47:3:39:U:HO2'	47:3:40:C:H6	1.43	0.43
48:5:1280:C:C4	48:5:1282:G:O6	2.72	0.43
48:5:1374:G:C2	48:5:1375:C:C2	3.07	0.43
48:5:1691:G:C2	48:5:1692:C:C2	3.06	0.43
48:5:1959:U:OP1	48:5:1960:A:O3'	2.37	0.43
48:5:1929:A:C2	48:5:2054:U:O4	2.60	0.43
48:5:258:G:C2	48:5:259:C:C2	3.07	0.43
48:5:2793:G:C6	48:5:2797:C:N4	2.86	0.43
48:5:301:G:C2	48:5:302:C:C2	3.07	0.43
48:5:4274:A:H2'	48:5:4275:G:C8	2.54	0.43
48:5:742:G:C2	48:5:923:C:C2	3.07	0.43
49:7:93:G:C2	49:7:94:C:C2	3.07	0.43
51:9:1097:G:C6	51:9:1098:C:C4	3.07	0.43
51:9:1260:A:C4	51:9:1620:A:N7	2.87	0.43
51:9:1406:G:C4	51:9:1407:U:H1'	2.54	0.43
1:A:103:PRO:HA	1:A:163:ARG:HA	1.99	0.43
56:EE:153:LEU:O	56:EE:155:LYS:HD3	2.19	0.43
57:FF:20:PHE:HZ	57:FF:69:VAL:HG11	1.83	0.43
60:II:79:ILE:HG23	60:II:103:LEU:HB2	1.99	0.43
13:N:50:ARG:NH2	48:5:279:A:OP2	2.51	0.43
15:P:36:ILE:CD1	15:P:48:LEU:HD11	2.49	0.43
21:V:20:LEU:HB2	21:V:55:ALA:O	2.19	0.43
46:2:30:G:N1	46:2:31:C:C2	2.86	0.43
47:3:37:A:N1	57:FF:133:THR:HG23	2.34	0.43
48:5:3891:A:H2'	48:5:3892:U:O4'	2.18	0.43
48:5:4911:A:H3'	48:5:4912:G:H5''	2.01	0.43
48:5:4891:G:C2	48:5:4929:C:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4948:C:H3'	48:5:4949:G:N2	2.33	0.43
50:8:118:C:C2	50:8:133:G:C2	3.06	0.43
51:9:1143:A:H2'	51:9:1144:A:C8	2.54	0.43
51:9:1516:G:O3'	67:PP:122:THR:HG21	2.19	0.43
51:9:841:G:N2	51:9:842:C:C2	2.87	0.43
51:9:910:G:C6	51:9:911:C:C4	3.06	0.43
51:9:981:A:H2'	51:9:982:G:C8	2.54	0.43
56:EE:72:ILE:HD12	56:EE:77:ARG:HB2	2.00	0.43
11:L:19:GLN:HA	11:L:22:VAL:HG23	1.99	0.43
63:LL:106:HIS:O	63:LL:106:HIS:ND1	2.52	0.43
13:N:94:PHE:CE2	13:N:96:ARG:HB2	2.54	0.43
67:PP:20:VAL:HG12	67:PP:25:LEU:HG	2.01	0.43
22:W:44:ARG:CG	22:W:44:ARG:HH11	2.32	0.43
59:HH:145:ARG:HA	74:WW:51:GLU:HB3	2.01	0.43
74:WW:75:ILE:HD11	74:WW:93:LEU:HD11	2.00	0.43
48:5:1075:G:C6	48:5:1076:C:C4	3.08	0.42
1:A:13:GLY:HA2	48:5:1660:U:H3'	71.18	0.42
48:5:1846:G:C2	48:5:1847:C:C2	3.07	0.42
48:5:1959:U:H4'	48:5:1961:G:O4'	2.19	0.42
48:5:2034:G:C6	48:5:2035:C:C4	3.06	0.42
48:5:2076:G:C6	48:5:2077:C:C4	3.07	0.42
48:5:3597:G:C6	48:5:3598:C:C4	3.07	0.42
48:5:702:U:H2'	48:5:703:G:H4'	2.01	0.42
48:5:93:G:O2'	48:5:94:A:O5'	2.37	0.42
50:8:10:G:C6	50:8:11:C:C4	3.07	0.42
50:8:53:G:C6	50:8:54:C:C4	3.07	0.42
51:9:1308:U:H2'	51:9:1309:C:C1'	2.49	0.42
51:9:1568:C:H2'	51:9:1569:A:C8	2.54	0.42
6:F:92:ALA:CB	6:F:127:LEU:HD21	2.49	0.42
66:OO:38:ASN:HA	66:OO:69:SER:OG	2.19	0.42
48:5:1367:C:H1'	48:5:1370:G:C8	2.54	0.42
48:5:1539:G:C6	48:5:1540:C:C4	3.06	0.42
48:5:199:G:C4	48:5:201:C:C5	3.07	0.42
48:5:2358:G:H2'	48:5:2359:U:O4'	2.19	0.42
48:5:405:U:O2'	48:5:407:A:N7	2.39	0.42
48:5:4583:C:N3	48:5:4718:G:C2	2.88	0.42
48:5:4898:G:N2	48:5:4923:C:C2	2.87	0.42
48:5:975:C:H5''	48:5:976:G:OP2	2.20	0.42
48:5:976:G:C6	48:5:977:C:N3	2.87	0.42
51:9:1335:G:N1	51:9:1336:C:C2	2.87	0.42
51:9:1439:A:H2'	51:9:1440:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:35:U:H1'	51:9:1640:A:O3'	2.18	0.42
51:9:1664:A:O2'	51:9:1665:G:H5'	2.20	0.42
51:9:1664:A:O2'	51:9:1665:G:C5'	2.68	0.42
51:9:798:G:O6	51:9:861:A:N7	2.51	0.42
1:A:30:ARG:O	1:A:163:ARG:NH2	2.52	0.42
54:CC:166:ARG:HB3	54:CC:247:THR:HB	2.01	0.42
56:EE:195:ILE:O	56:EE:210:VAL:HA	2.18	0.42
57:FF:179:ASN:HD22	57:FF:179:ASN:N	2.16	0.42
8:H:5:LEU:HD22	8:H:60:TRP:CH2	2.54	0.42
10:J:119:TYR:CB	70:SS:12:ILE:HG21	2.50	0.42
61:JJ:24:ARG:HG2	61:JJ:24:ARG:HH11	1.83	0.42
66:OO:150:ARG:HB3	66:OO:150:ARG:CZ	2.49	0.42
71:TT:28:LEU:O	71:TT:29:LYS:HB2	2.19	0.42
21:V:20:LEU:HD13	21:V:26:ILE:HG21	2.01	0.42
48:5:1584:G:C2	48:5:1585:C:C2	3.08	0.42
48:5:1811:G:C6	48:5:1812:C:C4	3.07	0.42
48:5:208:A:C6	48:5:233:U:C4	3.06	0.42
48:5:4395:U:C6	48:5:4395:U:H5'	2.55	0.42
48:5:504:G:H22	48:5:654:C:H1'	1.84	0.42
48:5:952:G:C2	48:5:953:C:C2	3.07	0.42
49:7:110:G:C2	49:7:111:C:C2	3.06	0.42
51:9:1229:G:C2	51:9:1230:C:C2	3.07	0.42
51:9:1268:C:C2	51:9:1515:G:N2	2.88	0.42
51:9:1454:A:OP1	69:RR:3:ARG:HG2	2.19	0.42
51:9:156:G:H4'	58:GG:108:VAL:HG23	2.00	0.42
51:9:1609:C:H2'	51:9:1610:G:C8	2.53	0.42
51:9:1613:G:N2	51:9:1627:C:C2	2.88	0.42
51:9:833:C:H4'	51:9:834:C:OP1	2.19	0.42
51:9:912:C:H3'	51:9:913:A:C5'	2.49	0.42
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.53	0.42
5:E:59:TYR:CE2	5:E:64:LEU:HD12	2.48	0.42
56:EE:45:ILE:HA	56:EE:61:VAL:HG11	2.01	0.42
8:H:134:CYS:SG	8:H:144:LEU:HD23	2.59	0.42
59:HH:44:ASN:N	59:HH:68:GLN:OE1	2.52	0.42
60:II:156:ALA:O	60:II:158:ILE:N	2.53	0.42
10:J:141:ILE:HD11	49:7:55:A:N3	2.34	0.42
51:9:522:A:C3'	61:JJ:131:ARG:HH22	2.32	0.42
62:KK:64:TRP:O	62:KK:65:ARG:C	2.57	0.42
19:T:40:VAL:HG13	19:T:96:ILE:HG23	2.01	0.42
2:B:378:ARG:NE	22:W:32:LEU:HD21	2.34	0.42
48:5:1431:C:C2	48:5:1454:G:C2	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1431:C:C2	48:5:1454:G:N2	2.87	0.42
48:5:1781:U:C4	48:5:1782:U:C5	3.08	0.42
48:5:2076:G:C2	48:5:2077:C:C2	3.08	0.42
48:5:2606:G:C2	48:5:2607:C:C2	3.07	0.42
48:5:2712:G:N1	48:5:2713:C:C4	2.87	0.42
48:5:3724:A:C6	48:5:3725:G:C5	3.08	0.42
48:5:4152:G:C2	48:5:4153:C:C2	3.08	0.42
48:5:4462:C:C2	48:5:4515:G:N2	2.87	0.42
48:5:4737:G:C6	48:5:4738:C:C4	3.07	0.42
48:5:4920:C:H2'	48:5:4921:C:C6	2.55	0.42
51:9:1236:G:C2	51:9:1237:C:C2	3.07	0.42
51:9:1566:G:N7	71:TT:101:ARG:NH2	2.65	0.42
52:AA:3:GLY:N	73:VV:78:ILE:O	2.52	0.42
5:E:43:ASN:HB3	5:E:58:MET:SD	2.59	0.42
6:F:175:ALA:O	6:F:179:ARG:HB2	2.19	0.42
24:Y:55:VAL:HG13	24:Y:104:VAL:HG13	2.02	0.42
47:3:4:C:O2	47:3:4:C:H2'	2.20	0.42
48:5:1205:G:C2	48:5:1206:C:C2	3.08	0.42
48:5:1466:G:N2	48:5:1467:C:C2	2.88	0.42
48:5:174:C:C2	48:5:263:G:C2	3.07	0.42
48:5:1755:C:C3'	48:5:1756:U:H5''	2.50	0.42
48:5:199:G:C2	48:5:201:C:C2	3.07	0.42
48:5:2468:U:C2	48:5:2473:A:N6	2.85	0.42
48:5:2526:C:N4	48:5:2527:A:N6	2.67	0.42
48:5:2712:G:C2	48:5:2713:C:C2	3.08	0.42
48:5:2609:G:N1	48:5:2731:C:C2	2.88	0.42
48:5:3751:G:HO2'	48:5:3752:C:H5'	1.77	0.42
48:5:3753:G:O2'	48:5:3754:G:H5'	2.20	0.42
48:5:4371:G:C5	48:5:4372:U:C4	3.07	0.42
48:5:4931:G:H2'	48:5:4931:G:N3	2.35	0.42
48:5:5031:G:C6	48:5:5032:C:C4	3.08	0.42
48:5:963:G:H2'	48:5:963:G:N3	2.35	0.42
50:8:139:G:C2	50:8:140:C:C2	3.08	0.42
50:8:31:G:C2	50:8:32:C:C2	3.08	0.42
51:9:1189:A:H2'	51:9:1190:A:C8	2.54	0.42
51:9:1753:C:C2	51:9:1780:G:C2	3.07	0.42
51:9:211:G:C6	51:9:212:C:N4	2.88	0.42
51:9:839:C:O2	51:9:839:C:H2'	2.17	0.42
3:C:86:ARG:HD3	48:5:376:A:OP1	2.19	0.42
55:DD:31:GLU:OE1	55:DD:106:ARG:NH2	2.52	0.42
56:EE:151:ASP:O	56:EE:153:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:126:VAL:HG23	56:EE:157:ASN:H	1.84	0.42
6:F:92:ALA:HB3	6:F:127:LEU:HD21	2.00	0.42
10:J:15:LEU:HD11	10:J:157:ILE:HG23	2.01	0.42
11:L:104:ASN:OD1	11:L:110:LEU:HB2	2.18	0.42
3:C:114:ARG:HB3	13:N:203:TYR:CD1	2.54	0.42
14:O:48:TYR:CE2	14:O:52:LEU:HD11	2.54	0.42
48:5:1075:G:N2	48:5:1076:C:C2	2.88	0.42
48:5:127:G:C2	48:5:128:C:C2	3.07	0.42
48:5:1550:G:C2	48:5:1579:C:O2	2.72	0.42
48:5:1557:C:C2	48:5:1571:G:C2	3.07	0.42
48:5:165:A:H3'	48:5:166:C:H6	1.85	0.42
48:5:1721:G:C6	48:5:1722:C:C4	3.08	0.42
48:5:2294:G:N2	48:5:2295:C:C2	2.87	0.42
48:5:2889:G:C6	48:5:2890:C:C4	3.08	0.42
48:5:4147:G:C2	48:5:4148:C:C2	3.07	0.42
48:5:4326:G:C6	48:5:4327:C:C4	3.08	0.42
48:5:28:C:C2	48:5:55:G:N2	2.88	0.42
51:9:1500:G:C5	51:9:1501:C:C4	3.06	0.42
51:9:1669:G:C2	51:9:1670:C:C2	3.07	0.42
48:5:3712:A:C6	51:9:970:G:C2	3.08	0.42
6:F:92:ALA:HA	6:F:147:PRO:HD3	2.01	0.42
15:P:118:GLN:NE2	48:5:423:G:N3	2.67	0.42
13:N:4:TYR:OH	48:5:151:G:OP2	2.23	0.42
48:5:1757:U:C2	48:5:1758:G:C8	3.07	0.42
48:5:2050:G:C6	48:5:2051:C:C4	3.07	0.42
48:5:2468:U:C4	48:5:2473:A:C6	3.07	0.42
48:5:2542:G:C2	48:5:2775:C:C2	3.07	0.42
48:5:3923:A:H2'	48:5:3924:C:C6	2.55	0.42
48:5:4072:C:H2'	48:5:4073:A:O4'	2.20	0.42
19:T:3:ASN:ND2	48:5:4212:A:N1	2.66	0.42
48:5:479:G:C6	48:5:480:C:C4	3.08	0.42
48:5:5028:G:C2	48:5:5029:C:C2	3.07	0.42
48:5:674:G:C2	48:5:675:C:C2	3.08	0.42
48:5:76:A:C6	48:5:77:U:C5	3.08	0.42
48:5:976:G:OP1	48:5:976:G:C4'	2.68	0.42
51:9:1416:C:O3'	51:9:1417:C:O4'	2.38	0.42
51:9:1604:G:C6	51:9:1605:G:C4	3.07	0.42
51:9:1648:G:C8	68:QQ:125:ARG:HB3	2.54	0.42
51:9:167:G:N2	51:9:168:C:C2	2.88	0.42
51:9:1771:G:C6	51:9:1772:C:N4	2.88	0.42
51:9:1804:U:H2'	51:9:1805:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1847:G:N2	51:9:1853:C:C2	2.88	0.42
51:9:113:G:N2	51:9:293:C:C2	2.88	0.42
51:9:47:G:C2	51:9:48:C:C2	3.08	0.42
51:9:559:G:O2'	51:9:560:A:O4'	2.37	0.42
51:9:799:U:H5''	59:HH:110:THR:HB	2.02	0.42
5:E:116:ASP:N	5:E:116:ASP:OD1	2.52	0.42
61:JJ:120:ALA:O	61:JJ:121:LYS:CB	2.67	0.42
11:L:146:LEU:HB2	11:L:148:THR:HG22	2.01	0.42
24:Y:19:PHE:O	24:Y:26:ARG:NH2	2.52	0.42
48:5:1072:C:H1'	48:5:1073:G:C8	2.54	0.42
48:5:1349:G:C6	48:5:1350:C:C4	3.08	0.42
48:5:179:G:C6	48:5:180:C:C4	3.07	0.42
19:T:109:VAL:HG13	48:5:1803:G:C6	2.54	0.42
48:5:29:G:C2	48:5:30:C:C2	3.08	0.42
48:5:3590:G:C6	48:5:3591:C:C4	3.07	0.42
48:5:3870:C:C2	48:5:3886:G:N2	2.87	0.42
48:5:3868:G:N2	48:5:3900:G:O2'	2.53	0.42
48:5:4212:A:C2	48:5:4218:U:C5	3.07	0.42
48:5:4269:G:C2	48:5:4270:C:C2	3.08	0.42
48:5:691:C:H2'	48:5:692:A:C8	2.55	0.42
48:5:742:G:N2	48:5:923:C:C2	2.88	0.42
48:5:77:U:N3	48:5:335:A:C6	2.86	0.42
48:5:978:G:OP2	48:5:979:C:OP2	2.37	0.42
49:7:93:G:C6	49:7:94:C:C4	3.07	0.42
51:9:999:G:C2	51:9:1000:C:C2	3.08	0.42
51:9:1212:G:O2'	51:9:1213:C:C5'	2.68	0.42
51:9:595:U:H2'	51:9:596:U:C6	2.54	0.42
51:9:949:G:C2	51:9:950:C:C2	3.08	0.42
51:9:978:G:C6	51:9:979:C:C4	3.08	0.42
1:A:196:TRP:CG	1:A:197:PRO:N	2.86	0.42
7:G:63:LEU:HD12	13:N:32:GLN:HB3	2.02	0.42
51:9:163:U:OP1	58:GG:84:TYR:HA	2.20	0.42
60:II:106:SER:HB2	60:II:166:PHE:CD1	2.54	0.42
18:S:95:ARG:HD3	18:S:97:TYR:OH	2.19	0.42
47:3:69:G:O2'	47:3:70:G:O5'	2.37	0.42
48:5:707:C:H42	48:5:1290:G:H1	1.68	0.42
48:5:1359:G:C5	48:5:1360:G:C5	3.07	0.42
48:5:1806:G:C2	48:5:1807:C:C2	3.08	0.42
48:5:1819:G:H5''	48:5:1819:G:C8	2.55	0.42
48:5:2042:A:N3	48:5:4462:C:O2'	2.49	0.42
48:5:196:C:C2	48:5:246:G: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
48:5:2793:G:O6	48:5:2797:C:C5	2.73	0.42
48:5:301:G:C5	48:5:302:C:C4	3.08	0.42
48:5:2831:G:C2	48:5:3855:C:C2	3.08	0.42
48:5:4094:G:H2'	48:5:4095:G:C1'	2.50	0.42
48:5:4595:G:C6	48:5:4596:C:C4	3.08	0.42
50:8:2:G:H2'	50:8:2:G:N3	2.34	0.42
51:9:1089:G:C6	51:9:1090:C:C4	3.08	0.42
51:9:145:G:N1	51:9:146:G:C6	2.88	0.42
51:9:1664:A:O2'	51:9:1665:G:O5'	2.33	0.42
51:9:1686:G:C2	51:9:1687:C:C2	3.07	0.42
51:9:52:G:C6	51:9:53:C:C4	3.07	0.42
51:9:910:G:C2	51:9:911:C:C2	3.08	0.42
51:9:947:G:C2	51:9:948:C:C2	3.08	0.42
5:E:149:LEU:HD11	5:E:191:ILE:HG13	2.01	0.42
57:FF:162:ALA:HB1	57:FF:169:ILE:HD13	2.01	0.42
58:GG:3:LEU:O	58:GG:15:LEU:HA	2.20	0.42
12:M:55:MET:O	18:S:157:ARG:NH2	2.53	0.42
13:N:68:ARG:HG2	48:5:302:C:OP1	2.20	0.42
55:DD:208:VAL:HG21	69:RR:50:ILE:HD11	2.01	0.42
73:VV:32:ILE:O	73:VV:54:ALA:HA	2.19	0.42
75:XX:29:LYS:HD3	75:XX:35:ALA:HB2	2.01	0.42
25:Z:38:TYR:CE1	25:Z:76:ASN:OD1	2.73	0.42
11:L:29:PRO:CB	48:5:1371:A:H2'	2.50	0.42
48:5:1416:G:C2	48:5:1417:C:C2	3.07	0.42
48:5:1448:G:C6	48:5:1449:C:C4	3.08	0.42
48:5:235:A:C2	48:5:238:C:C5	3.08	0.42
48:5:2606:G:C6	48:5:2607:C:C4	3.08	0.42
48:5:3717:A:O2'	48:5:3718:A:O5'	2.38	0.42
48:5:4093:G:C6	48:5:4094:G:N7	2.88	0.42
48:5:4583:C:C2	48:5:4718:G:C2	3.08	0.42
48:5:479:G:C2	48:5:480:C:C2	3.07	0.42
50:8:32:C:H2'	50:8:33:G:O4'	2.20	0.42
50:8:56:G:C4	50:8:62:A:C2	3.08	0.42
51:9:293:C:O2	51:9:293:C:C2'	2.68	0.42
51:9:830:A:C6	51:9:845:G:C4	3.08	0.42
51:9:872:A:N6	51:9:915:G:C4	2.88	0.42
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.50	0.42
3:C:161:TYR:HD1	3:C:166:GLU:OE2	2.02	0.42
54:CC:274:VAL:HG13	54:CC:274:VAL:O	2.20	0.42
4:D:64:ILE:CD1	4:D:109:LEU:HD22	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:DD:115:VAL:HG13	55:DD:138:VAL:HG11	2.01	0.42
5:E:208:LEU:HA	5:E:212:TYR:HD2	1.84	0.42
6:F:164:ILE:HB	6:F:169:ILE:HD12	2.02	0.42
7:G:157:ILE:HG23	7:G:167:VAL:HG11	2.01	0.42
51:9:67:C:OP2	58:GG:132:ARG:NH1	2.53	0.42
58:GG:58:LYS:O	58:GG:59:GLN:HB2	2.20	0.42
14:O:27:VAL:HG13	14:O:98:ALA:HB1	2.01	0.42
47:3:66:U:C4	47:3:67:U:C5	3.08	0.41
47:3:69:G:O2'	47:3:70:G:P	2.78	0.41
48:5:1264:C:C4	48:5:1265:G:N7	2.88	0.41
48:5:1277:G:C2	48:5:1278:C:C2	3.08	0.41
48:5:1358:G:O6	48:5:1379:C:N3	2.52	0.41
48:5:1416:G:C6	48:5:1417:C:C4	3.08	0.41
48:5:1431:C:H2'	48:5:1432:G:O4'	2.20	0.41
48:5:1736:A:C2	48:5:1794:A:C4	3.07	0.41
48:5:1969:G:O2'	48:5:1970:A:C5'	2.66	0.41
48:5:208:A:N6	48:5:233:U:C4	2.88	0.41
48:5:2465:C:H2'	48:5:2466:G:O4'	2.20	0.41
48:5:2623:A:C2	48:5:2624:G:C6	3.08	0.41
48:5:167:C:C2	48:5:269:G:C2	3.08	0.41
48:5:4247:G:C2	48:5:4262:C:C2	3.08	0.41
48:5:4276:G:N2	48:5:4333:C:C2	2.88	0.41
48:5:4713:G:C2	48:5:4714:C:C2	3.07	0.41
51:9:1212:G:O2'	51:9:1213:C:P	2.78	0.41
51:9:1344:A:N6	51:9:1386:A:H5''	2.35	0.41
51:9:1398:G:C6	51:9:1399:C:C4	3.08	0.41
51:9:1485:U:H2'	51:9:1486:A:O4'	2.20	0.41
51:9:194:C:C2	51:9:206:G:N2	2.88	0.41
51:9:52:G:C2	51:9:53:C:C2	3.08	0.41
51:9:912:C:H3'	51:9:913:A:H5''	2.01	0.41
56:EE:126:VAL:HG23	56:EE:156:MET:HA	2.02	0.41
11:L:42:ARG:CG	11:L:45:ARG:HH12	2.34	0.41
5:E:157:ARG:NH2	12:M:106:ASP:OD2	2.53	0.41
68:QQ:42:ILE:N	68:QQ:42:ILE:HD12	2.35	0.41
17:R:4:LEU:HD11	17:R:29:THR:HG23	2.02	0.41
48:5:973:G:N2	48:5:1282:G:HO2'	2.09	0.41
48:5:1379:C:O2	48:5:1379:C:O4'	2.37	0.41
48:5:1484:G:N3	48:5:1484:G:C2'	2.82	0.41
48:5:1484:G:N3	48:5:1484:G:H2'	2.34	0.41
48:5:1573:G:C6	48:5:1574:G:N1	2.89	0.41
48:5:1612:G:N3	48:5:1612:G:C2'	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1615:C:H2'	48:5:1616:U:O4'	2.19	0.41
48:5:2052:G:C2	48:5:2053:C:C2	3.09	0.41
48:5:2463:G:C6	48:5:2464:C:N4	2.89	0.41
48:5:2533:C:C2	48:5:2534:C:C5	3.08	0.41
48:5:2771:G:C2	48:5:2772:C:C2	3.08	0.41
48:5:4586:G:H5''	48:5:4586:G:C8	2.52	0.41
48:5:4904:G:C6	48:5:4905:C:C4	3.07	0.41
48:5:747:A:C2	48:5:918:G:N1	2.88	0.41
6:F:60:HIS:HA	48:5:944:A:C8	2.55	0.41
50:8:128:C:C5	50:8:129:C:C5	3.08	0.41
50:8:46:G:N2	50:8:47:C:C2	2.88	0.41
51:9:1661:A:H2'	51:9:1662:U:O4'	2.20	0.41
51:9:47:G:N2	51:9:48:C:C2	2.88	0.41
1:A:107:MET:SD	1:A:113:VAL:CG1	3.09	0.41
3:C:354:ALA:O	3:C:358:LEU:HG	2.20	0.41
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	2.02	0.41
9:I:49:CYS:SG	9:I:49:CYS:O	2.78	0.41
60:II:165:GLN:O	60:II:169:GLY:N	2.44	0.41
71:TT:6:VAL:HG22	71:TT:65:TYR:CE2	2.54	0.41
25:Z:36:ARG:CD	25:Z:74:VAL:HG11	2.50	0.41
47:3:6:G:C6	47:3:7:A:C5	3.08	0.41
48:5:1098:G:C6	48:5:1099:C:C4	3.08	0.41
48:5:1412:G:C6	48:5:1413:C:C4	3.08	0.41
48:5:1557:C:C2	48:5:1571:G:N2	2.88	0.41
48:5:2050:G:C2	48:5:2051:C:C2	3.08	0.41
48:5:2083:C:H4'	48:5:2084:C:OP2	2.21	0.41
48:5:2468:U:C2	48:5:2469:C:C5	3.08	0.41
48:5:284:G:C2	48:5:304:C:O2	2.73	0.41
1:A:227:ARG:NH2	48:5:3659:G:O2'	2.50	0.41
48:5:3769:C:H2'	48:5:3770:U:O4'	2.20	0.41
48:5:385:A:C2	48:5:386:A:C5	3.08	0.41
48:5:4131:G:C6	48:5:4132:C:C4	3.09	0.41
48:5:4326:G:C2	48:5:4327:C:C2	3.09	0.41
48:5:517:C:C2	48:5:645:G:N2	2.88	0.41
48:5:931:C:C2'	48:5:932:A:O5'	2.68	0.41
48:5:952:G:H2'	48:5:953:C:O4'	2.20	0.41
50:8:60:G:N2	50:8:64:U:C2	2.87	0.41
51:9:1184:G:C6	51:9:1185:C:C4	3.08	0.41
51:9:427:U:O4'	51:9:427:U:O2	2.37	0.41
51:9:664:A:O2'	51:9:670:A:N1	2.39	0.41
1:A:243:THR:HG21	48:5:3748:A:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:VAL:HG21	2:B:196:TRP:CG	2.55	0.41
5:E:174:PRO:O	5:E:177:LEU:N	2.50	0.41
63:LL:15:THR:HG22	63:LL:15:THR:O	2.20	0.41
67:PP:34:MET:CE	67:PP:42:ARG:HA	2.49	0.41
46:2:65:G:C2	46:2:66:C:C2	3.08	0.41
48:5:80:C:C2	48:5:104:G:N2	2.89	0.41
48:5:1234:G:H2'	48:5:1235:G:C8	2.55	0.41
48:5:1268:G:O4'	48:5:2111:G:C5	2.73	0.41
48:5:1329:G:H3'	48:5:1329:G:C8	2.55	0.41
48:5:1466:G:C2	48:5:1467:C:C2	3.09	0.41
48:5:1959:U:O2'	48:5:1960:A:P	2.78	0.41
48:5:2322:G:C2	48:5:2323:C:C2	3.09	0.41
48:5:2703:G:C6	48:5:2704:C:C4	3.08	0.41
48:5:4139:G:C2	48:5:4140:C:C2	3.08	0.41
48:5:4305:G:H2'	48:5:4305:G:N3	2.35	0.41
18:S:173:ASN:HA	48:5:4762:A:H2	1.85	0.41
48:5:4901:G:C2	48:5:4921:C:C2	3.08	0.41
48:5:4901:G:N1	48:5:4921:C:C4	2.88	0.41
48:5:4950:U:O2	48:5:4950:U:O4'	2.38	0.41
48:5:665:C:O2	48:5:665:C:C2'	2.69	0.41
49:7:27:G:C6	49:7:28:C:C4	3.08	0.41
51:9:1323:U:H2'	51:9:1324:G:O4'	2.20	0.41
51:9:1459:G:C6	51:9:1460:C:C4	3.09	0.41
51:9:1654:G:C2	51:9:1655:C:C2	3.08	0.41
51:9:1718:G:C6	51:9:1814:G:C6	3.09	0.41
51:9:1771:G:C2	51:9:1772:C:C4	3.09	0.41
51:9:828:G:C2	51:9:829:C:C2	3.07	0.41
51:9:943:U:H2'	51:9:944:A:O4'	2.20	0.41
3:C:229:LEU:N	3:C:229:LEU:HD22	2.35	0.41
3:C:30:ALA:HB1	3:C:31:PRO:HD2	2.02	0.41
5:E:90:LYS:N	5:E:91:PRO:HD3	2.35	0.41
59:HH:105:THR:OG1	59:HH:108:SER:N	2.52	0.41
10:J:15:LEU:HD21	10:J:157:ILE:HD13	2.02	0.41
13:N:11:TRP:CE3	13:N:44:ARG:NH2	2.89	0.41
14:O:15:LEU:HD11	14:O:129:LEU:HD13	2.01	0.41
66:OO:39:ASP:N	66:OO:69:SER:OG	2.53	0.41
18:S:84:TYR:C	18:S:84:TYR:CD1	2.94	0.41
20:U:21:PHE:CD1	20:U:80:LYS:HG2	2.55	0.41
48:5:1203:G:C2	48:5:1204:C:C2	3.08	0.41
48:5:1275:G:C2	48:5:1276:C:C2	3.08	0.41
12:M:34:ASN:ND2	48:5:1925:G:OP1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2273:G:C2	48:5:2274:C:C2	3.08	0.41
48:5:2478:C:N4	48:5:2479:G:O6	2.54	0.41
48:5:2889:G:C2	48:5:2890:C:C2	3.09	0.41
48:5:4131:G:C2	48:5:4132:C:C2	3.09	0.41
48:5:4182:G:H5'	48:5:4183:G:OP2	2.20	0.41
48:5:4283:G:C6	48:5:4284:C:N4	2.88	0.41
48:5:4492:U:O2'	48:5:4512:U:O2	2.22	0.41
48:5:4966:A:N1	48:5:4967:A:C6	2.88	0.41
48:5:972:C:H2'	48:5:973:G:H8	1.84	0.41
51:9:1134:G:C2	51:9:1135:C:C2	3.08	0.41
51:9:1217:A:H2'	51:9:1218:C:C6	2.56	0.41
51:9:978:G:C2	51:9:979:C:C2	3.09	0.41
52:AA:147:LEU:HD12	52:AA:163:CYS:SG	2.60	0.41
10:J:119:TYR:HB3	70:SS:12:ILE:HG21	2.02	0.41
13:N:198:LEU:HD23	13:N:198:LEU:HA	1.94	0.41
48:5:1075:G:C6	48:5:1076:C:N4	2.88	0.41
48:5:127:G:C6	48:5:128:C:C4	3.08	0.41
48:5:1381:U:H5'	48:5:1382:G:OP2	2.21	0.41
48:5:1424:G:H2'	48:5:1425:G:O4'	2.21	0.41
48:5:1422:G:C2	48:5:1464:C:C2	3.09	0.41
48:5:169:G:C2	48:5:170:C:C2	3.09	0.41
48:5:2052:G:C6	48:5:2053:C:C4	3.08	0.41
48:5:2547:G:C2	48:5:2548:C:C2	3.09	0.41
48:5:4395:U:H6	48:5:4395:U:H5'	1.85	0.41
48:5:4664:A:H2'	48:5:4665:A:O4'	2.21	0.41
48:5:751:G:N2	48:5:752:G:C5	2.89	0.41
51:9:1275:G:HO2'	51:9:1276:A:P	2.43	0.41
51:9:1551:U:C5	51:9:1577:G:C6	3.09	0.41
51:9:1624:U:O4'	51:9:1624:U:O2	2.38	0.41
51:9:1859:A:C2	51:9:1860:A:N1	2.88	0.41
51:9:49:C:N3	51:9:478:G:C6	2.88	0.41
51:9:832:G:C2	51:9:843:C:N3	2.89	0.41
51:9:921:G:C5	74:WW:28:ARG:HD2	2.56	0.41
51:9:958:G:H2'	51:9:959:G:O4'	2.20	0.41
4:D:43:LYS:O	4:D:46:THR:HG22	2.20	0.41
9:I:49:CYS:HB2	9:I:172:GLY:O	2.21	0.41
60:II:102:VAL:HG11	60:II:175:ILE:HD11	2.01	0.41
60:II:60:LEU:HD23	60:II:185:ALA:HB2	2.03	0.41
68:QQ:13:PHE:HA	68:QQ:22:VAL:HA	2.02	0.41
68:QQ:32:ILE:HD11	68:QQ:63:PHE:CD2	2.55	0.41
48:5:116:G:C2	48:5:117:C:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:119:G:H5'	48:5:119:G:C8	2.56	0.41
48:5:1205:G:N1	48:5:1206:C:C4	2.89	0.41
48:5:209:U:C4	48:5:233:U:O4	2.74	0.41
48:5:2267:U:O4'	48:5:2267:U:O2	2.39	0.41
48:5:2311:C:C2	48:5:2328:G:N2	2.89	0.41
48:5:258:G:C6	48:5:259:C:C4	3.08	0.41
48:5:2613:C:N4	48:5:2614:C:N4	2.68	0.41
48:5:307:A:N3	48:5:310:G:O2'	2.41	0.41
48:5:368:C:C2	48:5:374:G:C2	3.09	0.41
48:5:3937:C:H2'	48:5:3938:G:N2	2.35	0.41
48:5:4181:U:O4	48:5:4182:G:C6	2.73	0.41
50:8:49:G:C6	50:8:50:C:C4	3.09	0.41
51:9:1130:G:N2	51:9:1131:G:C8	2.88	0.41
51:9:1220:A:C6	51:9:1221:G:C5	3.08	0.41
51:9:1233:G:C2	51:9:1234:C:C2	3.08	0.41
51:9:1233:G:H2'	51:9:1234:C:H5'	2.02	0.41
51:9:1384:C:O2'	51:9:1385:G:H5'	2.20	0.41
51:9:1473:G:N2	51:9:1475:G:OP2	2.51	0.41
51:9:1537:A:C2	51:9:1538:C:C2	3.09	0.41
51:9:827:A:C5	51:9:828:G:C8	3.09	0.41
51:9:95:G:C6	51:9:96:C:C4	3.09	0.41
52:AA:161:ILE:HG22	52:AA:163:CYS:SG	2.60	0.41
2:B:238:LYS:CE	48:5:3842:C:OP1	2.68	0.41
2:B:36:ASP:OD2	2:B:39:LYS:CE	2.62	0.41
53:BB:171:ILE:HG21	53:BB:197:ILE:HG13	2.03	0.41
54:CC:116:THR:OG1	54:CC:118:ALA:O	2.38	0.41
56:EE:234:PRO:CG	56:EE:238:LEU:HD11	2.51	0.41
56:EE:54:TYR:OH	56:EE:95:THR:HG21	2.21	0.41
8:H:5:LEU:HD13	8:H:60:TRP:CD2	2.56	0.41
15:P:10:ASN:N	15:P:10:ASN:OD1	2.53	0.41
74:WW:3:ARG:HE	74:WW:29:PRO:HG3	1.85	0.41
46:2:40:C:H4'	47:3:36:U:H1'	2.03	0.41
46:2:7:G:C2	46:2:49:C:C2	3.09	0.41
48:5:1090:G:C6	48:5:1091:C:C4	3.08	0.41
48:5:1279:A:C4	48:5:1280:C:N3	2.89	0.41
48:5:1439:C:O2	48:5:1439:C:O4'	2.39	0.41
48:5:1912:G:C6	48:5:1913:C:N4	2.89	0.41
48:5:2058:G:C6	48:5:2059:C:C4	3.09	0.41
48:5:258:G:N2	48:5:259:C:C2	2.89	0.41
48:5:2625:U:C4	48:5:2626:U:C4	3.09	0.41
48:5:2645:G:C2	48:5:2646:C:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4269:G:C6	48:5:4270:C:C4	3.09	0.41
48:5:4473:A:C2	48:5:4474:A:C4	3.09	0.41
48:5:730:G:N2	48:5:939:G:N2	2.69	0.41
48:5:941:C:H2'	48:5:942:G:O4'	2.21	0.41
51:9:1540:G:C2	51:9:1594:A:C2	3.09	0.41
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.48	0.41
51:9:1798:C:H2'	51:9:1799:G:O4'	2.21	0.41
51:9:211:G:C2	51:9:212:C:C2	3.09	0.41
51:9:65:C:O5'	58:GG:174:PRO:HA	2.21	0.41
52:AA:132:GLN:N	52:AA:133:PRO:HD2	2.36	0.41
51:9:688:U:OP2	59:HH:122:LEU:N	2.54	0.41
65:NN:87:ASP:OD2	65:NN:125:LEU:HD11	2.21	0.41
75:XX:82:THR:O	75:XX:118:VAL:HG13	2.21	0.41
46:2:29:C:H2'	46:2:30:G:O4'	2.21	0.41
48:5:1412:G:C2	48:5:1413:C:C2	3.09	0.41
48:5:1721:G:C2	48:5:1722:C:C2	3.09	0.41
48:5:1969:G:HO2'	48:5:1970:A:H5'	1.84	0.41
48:5:2268:A:C4'	48:5:2269:C:H5'	2.49	0.41
48:5:2517:A:N1	48:5:2518:G:C2	2.89	0.41
48:5:254:G:C6	48:5:255:C:C4	3.09	0.41
48:5:4486:C:H2'	48:5:4487:A:O4'	2.21	0.41
48:5:4595:G:C2	48:5:4596:C:C2	3.08	0.41
17:R:58:HIS:HA	48:5:4646:U:OP1	2.21	0.41
48:5:5031:G:C2	48:5:5032:C:C2	3.09	0.41
48:5:937:U:C2'	48:5:937:U:O2	2.69	0.41
48:5:93:G:C2'	48:5:94:A:C8	3.04	0.41
48:5:44:A:O2'	48:5:94:A:N1	2.42	0.41
48:5:971:U:C2'	48:5:972:C:H5'	2.51	0.41
51:9:1293:A:H2'	51:9:1294:G:O4'	2.21	0.41
51:9:1298:G:O2'	51:9:1299:A:O5'	2.38	0.41
51:9:832:G:C2	51:9:833:C:C2	3.09	0.41
51:9:856:C:O2	51:9:856:C:H2'	2.19	0.41
2:B:116:ARG:HB3	2:B:177:LYS:HA	2.03	0.41
3:C:266:THR:HG22	3:C:269:LYS:HB3	2.02	0.41
3:C:76:ILE:HG22	3:C:77:PRO:CD	2.51	0.41
9:I:35:ASP:N	9:I:35:ASP:OD1	2.54	0.41
62:KK:62:PHE:CZ	62:KK:65:ARG:HA	2.56	0.41
66:OO:99:ALA:HB2	66:OO:108:PRO:HA	2.02	0.41
16:Q:41:SER:OG	16:Q:44:ASN:ND2	2.54	0.41
69:RR:126:MET:O	69:RR:127:ASN:ND2	2.54	0.41
70:SS:25:LYS:HA	70:SS:55:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:WW:104:LEU:HB3	74:WW:125:ILE:HA	2.02	0.41
76:YY:62:THR:HA	76:YY:69:THR:HA	2.03	0.41
25:Z:28:ASN:C	25:Z:29:ILE:HD12	2.41	0.41
48:5:2862:G:H2'	48:5:3619:G:O6	2.21	0.41
48:5:369:G:N2	48:5:372:A:OP2	2.50	0.41
48:5:3786:U:O4'	48:5:4537:C:O2'	2.36	0.41
51:9:100:U:H2'	51:9:101:U:O4'	2.21	0.41
51:9:1184:G:C2	51:9:1185:C:C2	3.09	0.41
51:9:1576:G:H2'	51:9:1577:G:O4'	2.20	0.41
51:9:1839:U:C6	51:9:1862:G:N2	2.88	0.41
51:9:1835:A:C8	51:9:1863:A:N7	2.89	0.41
51:9:378:U:H2'	51:9:379:C:O4'	2.21	0.41
51:9:49:C:C2	51:9:478:G:N1	2.89	0.41
51:9:67:C:O2'	58:GG:165:GLU:OE1	2.39	0.41
6:F:168:ARG:HD2	6:F:211:TRP:CD1	2.55	0.41
59:HH:40:LEU:O	59:HH:40:LEU:HD23	2.21	0.41
9:I:184:MET:HB3	9:I:184:MET:HE2	1.78	0.41
67:PP:118:GLU:O	70:SS:120:HIS:N	2.53	0.41
21:V:26:ILE:HG22	21:V:101:ASN:HB3	2.03	0.41
48:5:1506:G:C2	48:5:1507:C:C2	3.09	0.41
48:5:1538:U:O2'	48:5:1629:G:OP1	2.33	0.41
48:5:1970:A:C2	48:5:2016:C:C5	3.09	0.41
17:R:5:ARG:NH2	48:5:2385:U:OP1	2.53	0.41
48:5:3723:A:C2	48:5:3730:U:N3	2.89	0.41
48:5:3752:C:O2'	48:5:3753:G:P	2.78	0.41
48:5:4201:G:C6	48:5:4202:U:C4	3.09	0.41
48:5:4433:G:C2	48:5:4434:C:C2	3.09	0.41
48:5:709:C:H2'	48:5:710:G:O4'	2.20	0.41
48:5:715:G:H1	48:5:953:C:H42	1.68	0.41
48:5:960:A:N6	48:5:1283:G:O6	2.54	0.41
50:8:154:G:C6	50:8:155:C:C4	3.09	0.41
51:9:1212:G:N2	51:9:1213:C:C2	2.89	0.41
51:9:1275:G:O2'	51:9:1276:A:P	2.80	0.41
51:9:821:G:C6	61:JJ:147:PHE:CZ	3.08	0.41
3:C:228:THR:OG1	3:C:248:ARG:NH2	2.54	0.41
4:D:278:ASP:O	4:D:281:ALA:HB3	2.20	0.41
57:FF:127:ARG:HG3	57:FF:127:ARG:HH11	1.86	0.41
59:HH:122:LEU:HD21	59:HH:126:HIS:CE1	2.56	0.41
9:I:187:GLU:O	9:I:188:LYS:HB2	2.21	0.41
18:S:84:TYR:HD1	18:S:84:TYR:C	2.25	0.41
73:VV:9:VAL:HG13	73:VV:10:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:123:LYS:O	25:Z:124:THR:HG23	2.20	0.41
46:2:30:G:C2	46:2:31:C:C2	3.09	0.40
47:3:68:C:N3	47:3:69:G:C5	2.89	0.40
47:3:5:G:C2	47:3:6:G:C5	3.09	0.40
48:5:1176:C:HO2'	48:5:1177:U:C4'	2.29	0.40
48:5:1441:C:N4	48:5:1442:C:N4	2.68	0.40
48:5:1466:G:C6	48:5:1467:C:C4	3.09	0.40
48:5:1550:G:N1	48:5:1551:C:C2	2.89	0.40
48:5:1563:A:C8	51:9:678:U:C4'	2.98	0.40
48:5:1633:G:H5'	48:5:1634:A:OP1	2.20	0.40
48:5:205:C:C2	48:5:211:G:C2	3.09	0.40
48:5:2457:G:C2	48:5:2458:C:C2	3.10	0.40
48:5:2463:G:C6	48:5:2464:C:C4	3.10	0.40
48:5:247:G:C2	48:5:248:C:C2	3.09	0.40
48:5:4277:G:C2	48:5:4278:C:C2	3.09	0.40
48:5:4530:U:H2'	48:5:4531:U:C6	2.55	0.40
50:8:112:G:C6	50:8:113:C:C4	3.09	0.40
51:9:999:G:C6	51:9:1000:C:C4	3.09	0.40
51:9:1137:U:N3	51:9:1148:A:C6	2.89	0.40
51:9:1236:G:C6	51:9:1237:C:C4	3.09	0.40
51:9:86:C:C4	51:9:87:U:C5	3.08	0.40
51:9:95:G:C2	51:9:96:C:C2	3.09	0.40
1:A:117:GLU:OE1	1:A:121:GLY:N	2.52	0.40
4:D:20:PHE:CD1	49:7:10:C:C4	3.10	0.40
6:F:94:VAL:HG13	6:F:142:ILE:HD12	2.04	0.40
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.56	0.40
18:S:54:MET:HE3	18:S:54:MET:HB2	1.92	0.40
47:3:29:A:HO2'	47:3:30:G:C5'	2.23	0.40
48:5:1834:U:H2'	48:5:1834:U:O2	2.20	0.40
48:5:1932:A:H2'	48:5:1933:G:C8	2.57	0.40
48:5:2481:G:N2	48:5:2498:C:C2	2.90	0.40
48:5:2726:G:C2	48:5:2727:C:C2	3.10	0.40
48:5:35:U:H5'	48:5:36:U:OP2	2.21	0.40
48:5:3832:U:H2'	48:5:3833:C:C6	2.57	0.40
48:5:4714:C:C5	48:5:4715:C:C5	3.09	0.40
48:5:4876:U:O4'	48:5:4876:U:O2	2.39	0.40
48:5:518:G:C6	48:5:519:C:C4	3.09	0.40
48:5:695:G:H3'	48:5:696:C:H5'	2.02	0.40
49:7:51:G:C2	49:7:52:C:C2	3.09	0.40
3:C:195:LYS:NZ	50:8:21:C:OP1	2.52	0.40
48:5:22:G:C2	50:8:35:C:C4	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1481:G:H2'	51:9:1482:C:O4'	2.21	0.40
51:9:164:A:H2'	51:9:165:G:C2	2.56	0.40
51:9:1686:G:N2	51:9:1687:C:C2	2.90	0.40
51:9:45:A:N1	51:9:480:G:O2'	2.42	0.40
51:9:600:G:C8	51:9:631:U:C6	3.09	0.40
51:9:834:C:N4	51:9:841:G:N1	2.69	0.40
1:A:200:ARG:NH1	48:5:3690:U:OP2	2.54	0.40
52:AA:157:VAL:HG23	52:AA:157:VAL:O	2.22	0.40
53:BB:87:ILE:O	53:BB:98:THR:HA	2.21	0.40
3:C:27:VAL:HG11	3:C:128:LEU:HD13	2.03	0.40
54:CC:109:ILE:HD11	54:CC:151:ILE:HD11	2.03	0.40
51:9:371:A:OP2	60:II:10:LYS:HB2	2.21	0.40
76:YY:55:ILE:HG12	76:YY:75:ILE:HG23	2.02	0.40
25:Z:38:TYR:CD1	25:Z:76:ASN:OD1	2.74	0.40
25:Z:95:VAL:HG12	25:Z:110:ALA:HA	2.03	0.40
48:5:116:G:C6	48:5:117:C:C4	3.10	0.40
48:5:1359:G:C2'	48:5:1360:G:C8	3.04	0.40
48:5:102:G:C2'	48:5:1381:U:O2'	2.68	0.40
48:5:1356:U:H1'	48:5:1505:C:H1'	2.03	0.40
48:5:1808:C:C2	48:5:1831:G:C2	3.09	0.40
48:5:2301:G:C2	48:5:2302:C:C2	3.09	0.40
48:5:2628:U:C4	48:5:2629:C:C5	3.09	0.40
48:5:3706:C:H2'	48:5:3707:U:O4'	2.22	0.40
48:5:4453:C:H2'	48:5:4454:G:O4'	2.21	0.40
48:5:4495:G:C2	48:5:4506:C:C2	3.09	0.40
48:5:4614:G:C2	48:5:4615:C:C2	3.10	0.40
48:5:4868:G:H3'	48:5:4869:U:H5''	2.03	0.40
48:5:933:G:N1	48:5:939:G:N2	2.69	0.40
49:7:66:G:C6	49:7:67:C:N3	2.89	0.40
50:8:154:G:C2	50:8:155:C:C2	3.09	0.40
50:8:76:C:H2'	50:8:77:A:O4'	2.22	0.40
51:9:1709:G:C6	51:9:1710:C:C4	3.08	0.40
51:9:380:G:OP1	60:II:31:ARG:NE	2.43	0.40
51:9:827:A:C4	51:9:828:G:C8	3.09	0.40
1:A:27:ALA:O	1:A:128:ARG:NH2	2.54	0.40
1:A:66:PRO:HG2	1:A:67:TYR:CE2	2.57	0.40
6:F:118:GLN:HG3	16:Q:3:VAL:HG22	2.03	0.40
7:G:140:VAL:HG13	7:G:200:THR:OG1	2.21	0.40
14:O:14:HIS:CD2	14:O:124:LEU:HD12	2.57	0.40
72:UU:69:PRO:O	72:UU:70:CYS:SG	2.80	0.40
74:WW:89:TRP:HE3	74:WW:93:LEU:HD22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1780:A:N6	48:5:1781:U:C4	2.90	0.40
48:5:303:C:H2'	48:5:304:C:O4'	2.21	0.40
48:5:3680:U:C2'	48:5:3680:U:O2	2.69	0.40
48:5:3918:G:C2	48:5:3919:C:C2	3.10	0.40
48:5:4408:G:C2	48:5:4409:C:C2	3.08	0.40
48:5:4745:G:N2	48:5:4746:C:N4	2.69	0.40
48:5:4900:C:O2'	48:5:4901:G:P	2.80	0.40
48:5:4966:A:C2	48:5:4967:A:C6	3.10	0.40
48:5:940:C:C4	48:5:941:C:C4	3.10	0.40
50:8:115:G:C6	50:8:116:C:C4	3.10	0.40
50:8:31:G:C6	50:8:32:C:C4	3.10	0.40
51:9:999:G:N2	51:9:1000:C:C2	2.89	0.40
51:9:1571:G:C2	51:9:1572:C:C2	3.09	0.40
51:9:480:G:C6	51:9:481:C:C4	3.10	0.40
51:9:636:C:C4	51:9:637:U:C4	3.10	0.40
51:9:752:G:N2	51:9:790:C:C2	2.90	0.40
51:9:751:G:N1	51:9:792:C:C4	2.90	0.40
53:BB:126:ASP:N	53:BB:126:ASP:OD1	2.54	0.40
3:C:143:ARG:N	3:C:179:ASP:OD1	2.54	0.40
6:F:181:LEU:HD11	6:F:209:PHE:HB2	2.02	0.40
10:J:53:ALA:HB2	10:J:68:ILE:CD1	2.51	0.40
61:JJ:102:ILE:HG22	61:JJ:103:GLU:N	2.36	0.40
12:M:116:LYS:HG2	14:O:196:LEU:CD2	2.35	0.40
70:SS:59:LEU:HD23	70:SS:64:VAL:HG12	2.03	0.40
25:Z:73:LYS:HG2	25:Z:75:TYR:CZ	2.56	0.40
46:2:39:G:C2	46:2:40:C:C2	3.09	0.40
47:3:69:G:C2	47:3:70:G:C5	3.09	0.40
48:5:1354:A:N1	48:5:1385:G:O2'	2.45	0.40
1:A:193:ARG:HH12	48:5:3686:G:P	2.44	0.40
48:5:3705:G:C2	48:5:3706:C:C2	3.09	0.40
48:5:3846:C:H4'	48:5:4667:C:O2	2.22	0.40
48:5:990:C:C4	48:5:991:C:C5	3.10	0.40
50:8:103:A:C8	50:8:104:A:C8	3.09	0.40
51:9:1097:G:C2	51:9:1098:C:C2	3.10	0.40
51:9:1129:G:H2'	51:9:1130:G:C1'	2.52	0.40
51:9:1398:G:C2	51:9:1399:C:C2	3.10	0.40
51:9:309:G:C2	51:9:310:C:C2	3.09	0.40
51:9:463:C:H2'	51:9:465:A:C8	2.56	0.40
51:9:475:C:H2'	51:9:476:A:O4'	2.21	0.40
51:9:55:U:H2'	51:9:55:U:O2	2.21	0.40
51:9:592:C:O4'	51:9:592:C:O2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:936:G:C2	51:9:1007:C:C2	3.09	0.40
5:E:174:PRO:O	5:E:176:SER:N	2.55	0.40
5:E:217:GLN:HE22	5:E:233:LYS:HD2	1.85	0.40
6:F:164:ILE:HD12	6:F:169:ILE:HB	2.03	0.40
6:F:147:PRO:HA	6:F:243:ASN:OD1	2.22	0.40
58:GG:102:VAL:CG1	58:GG:109:LEU:HD11	2.52	0.40
59:HH:43:LEU:HD21	59:HH:71:SER:CB	2.51	0.40
10:J:165:TRP:CH2	10:J:170:TYR:HE2	2.39	0.40
13:N:64:ILE:HD11	13:N:102:ALA:HA	2.03	0.40
22:W:9:SER:HA	22:W:52:THR:HG22	2.04	0.40
7:G:58:PRO:CD	23:X:46:PHE:HD2	2.34	0.40
24:Y:24:HIS:CE1	24:Y:25:ILE:HG13	2.57	0.40
77:ZZ:98:LYS:O	77:ZZ:109:TYR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/244 (99%)	209 (86%)	28 (12%)	5 (2%)	8	44
2	B	392/394 (100%)	345 (88%)	42 (11%)	5 (1%)	14	54
3	C	360/362 (99%)	322 (89%)	27 (8%)	11 (3%)	5	36
4	D	290/292 (99%)	262 (90%)	25 (9%)	3 (1%)	18	60
5	E	232/248 (94%)	179 (77%)	36 (16%)	17 (7%)	1	13
6	F	223/225 (99%)	204 (92%)	17 (8%)	2 (1%)	20	63
7	G	239/241 (99%)	203 (85%)	31 (13%)	5 (2%)	8	44
8	H	188/190 (99%)	165 (88%)	20 (11%)	3 (2%)	11	50
9	I	200/213 (94%)	181 (90%)	15 (8%)	4 (2%)	9	45
10	J	167/169 (99%)	147 (88%)	13 (8%)	7 (4%)	3	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	L	208/210 (99%)	180 (86%)	16 (8%)	12 (6%)	2	19
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	25	67
13	N	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
14	O	197/199 (99%)	184 (93%)	12 (6%)	1 (0%)	32	73
15	P	151/153 (99%)	135 (89%)	16 (11%)	0	100	100
16	Q	185/187 (99%)	169 (91%)	14 (8%)	2 (1%)	17	58
17	R	178/180 (99%)	166 (93%)	9 (5%)	3 (2%)	11	49
18	S	173/175 (99%)	157 (91%)	12 (7%)	4 (2%)	7	43
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	9	46
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	3	29
21	V	129/131 (98%)	115 (89%)	13 (10%)	1 (1%)	22	65
22	W	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	11	50
23	X	117/119 (98%)	109 (93%)	6 (5%)	2 (2%)	11	49
24	Y	132/134 (98%)	114 (86%)	17 (13%)	1 (1%)	22	65
25	Z	133/135 (98%)	113 (85%)	13 (10%)	7 (5%)	2	21
26	a	145/147 (99%)	122 (84%)	19 (13%)	4 (3%)	6	38
27	b	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	13	52
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	d	105/107 (98%)	91 (87%)	13 (12%)	1 (1%)	18	60
30	e	126/128 (98%)	115 (91%)	6 (5%)	5 (4%)	3	29
31	f	107/109 (98%)	94 (88%)	8 (8%)	5 (5%)	3	25
32	g	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	20	63
33	h	120/122 (98%)	107 (89%)	9 (8%)	4 (3%)	4	34
34	i	100/102 (98%)	92 (92%)	6 (6%)	2 (2%)	9	45
35	j	84/86 (98%)	70 (83%)	9 (11%)	5 (6%)	2	18
36	k	67/69 (97%)	56 (84%)	7 (10%)	4 (6%)	2	18
37	l	48/50 (96%)	40 (83%)	7 (15%)	1 (2%)	8	44
38	m	50/52 (96%)	44 (88%)	6 (12%)	0	100	100
39	n	21/23 (91%)	21 (100%)	0	0	100	100
40	o	102/104 (98%)	92 (90%)	7 (7%)	3 (3%)	5	37
41	p	89/91 (98%)	80 (90%)	8 (9%)	1 (1%)	17	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	r	123/125 (98%)	102 (83%)	14 (11%)	7 (6%)	2	20
43	s	196/198 (99%)	164 (84%)	22 (11%)	10 (5%)	2	22
44	t	161/163 (99%)	102 (63%)	33 (20%)	26 (16%)	0	2
45	1	13/15 (87%)	11 (85%)	0	2 (15%)	0	3
52	AA	206/208 (99%)	173 (84%)	23 (11%)	10 (5%)	2	23
53	BB	211/213 (99%)	165 (78%)	33 (16%)	13 (6%)	2	18
54	CC	216/218 (99%)	184 (85%)	26 (12%)	6 (3%)	6	38
55	DD	225/227 (99%)	181 (80%)	33 (15%)	11 (5%)	2	23
56	EE	260/262 (99%)	200 (77%)	42 (16%)	18 (7%)	1	15
57	FF	189/191 (99%)	160 (85%)	21 (11%)	8 (4%)	3	28
58	GG	235/237 (99%)	198 (84%)	31 (13%)	6 (3%)	6	39
59	HH	187/189 (99%)	148 (79%)	25 (13%)	14 (8%)	1	13
60	II	204/206 (99%)	168 (82%)	28 (14%)	8 (4%)	3	30
61	JJ	183/185 (99%)	153 (84%)	20 (11%)	10 (6%)	2	20
62	KK	96/98 (98%)	65 (68%)	21 (22%)	10 (10%)	0	7
63	LL	150/152 (99%)	125 (83%)	19 (13%)	6 (4%)	3	29
64	MM	122/124 (98%)	87 (71%)	28 (23%)	7 (6%)	2	20
65	NN	148/150 (99%)	126 (85%)	17 (12%)	5 (3%)	4	34
66	OO	134/136 (98%)	99 (74%)	21 (16%)	14 (10%)	0	7
67	PP	125/127 (98%)	107 (86%)	15 (12%)	3 (2%)	7	42
68	QQ	139/141 (99%)	116 (84%)	18 (13%)	5 (4%)	4	32
69	RR	127/129 (98%)	106 (84%)	15 (12%)	6 (5%)	3	25
70	SS	135/137 (98%)	114 (84%)	16 (12%)	5 (4%)	4	32
71	TT	139/141 (99%)	126 (91%)	10 (7%)	3 (2%)	8	43
72	UU	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	2	19
73	VV	81/83 (98%)	67 (83%)	10 (12%)	4 (5%)	2	23
74	WW	127/129 (98%)	106 (84%)	16 (13%)	5 (4%)	3	30
75	XX	139/141 (99%)	118 (85%)	13 (9%)	8 (6%)	2	19
76	YY	124/126 (98%)	99 (80%)	17 (14%)	8 (6%)	1	16
77	ZZ	73/75 (97%)	59 (81%)	12 (16%)	2 (3%)	6	39
78	aa	96/98 (98%)	73 (76%)	13 (14%)	10 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
79	bb	81/83 (98%)	61 (75%)	16 (20%)	4 (5%)	2	23
80	cc	59/61 (97%)	47 (80%)	10 (17%)	2 (3%)	4	34
81	dd	51/53 (96%)	45 (88%)	3 (6%)	3 (6%)	2	19
82	ee	55/57 (96%)	40 (73%)	12 (22%)	3 (6%)	2	20
83	ff	58/68 (85%)	50 (86%)	6 (10%)	2 (3%)	4	34
84	gg	311/313 (99%)	269 (86%)	33 (11%)	9 (3%)	5	37
86	ii	414/416 (100%)	380 (92%)	26 (6%)	8 (2%)	9	46
87	jj	568/594 (96%)	513 (90%)	41 (7%)	14 (2%)	6	40
All	All	12492/12709 (98%)	10717 (86%)	1333 (11%)	442 (4%)	7	33

All (442) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	TRP
3	C	273	LEU
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	47	PRO
11	L	64	VAL
11	L	67	HIS
17	R	36	ASN
18	S	165	PRO
20	U	47	ILE
25	Z	84	ARG
26	a	90	ALA
29	d	94	GLU
30	e	92	ASN
31	f	80	ASN
33	h	7	ARG
36	k	61	PRO
40	o	32	SER
42	r	86	ALA

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Mol	Chain	Res	Type
43	s	62	ARG
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	186	ARG
53	BB	57	ILE
53	BB	179	ASN
53	BB	191	ASP
55	DD	192	TRP
55	DD	202	LYS
55	DD	223	ILE
56	EE	24	THR
56	EE	76	VAL
56	EE	118	GLU
56	EE	164	LEU
56	EE	196	THR
57	FF	34	SER
57	FF	163	PHE
58	GG	174	PRO
59	HH	18	GLU
59	HH	66	VAL
59	HH	116	ARG
59	HH	159	ASP
60	II	27	TYR
60	II	155	ASN
60	II	157	LYS
61	JJ	4	ALA
61	JJ	22	LYS
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

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Mol	Chain	Res	Type
66	OO	128	ARG
66	OO	140	THR
68	QQ	43	GLU
68	QQ	64	ALA
69	RR	88	VAL
69	RR	93	GLN
71	TT	34	VAL
72	UU	107	GLU
73	VV	41	LYS
73	VV	48	GLY
75	XX	34	THR
75	XX	42	GLY
76	YY	104	ARG
76	YY	114	MET
76	YY	120	THR
77	ZZ	113	THR
78	aa	10	ARG
82	ee	9	VAL
84	gg	254	PRO
84	gg	282	GLU
86	ii	298	THR
87	jj	245	SER
87	jj	455	ILE
1	A	217	GLN
2	B	38	SER
2	B	302	ASN
3	C	73	VAL
3	C	155	GLU
3	C	275	SER
4	D	187	SER
5	E	85	LEU
5	E	92	VAL
5	E	174	PRO
5	E	234	GLU
10	J	116	GLY
10	J	155	HIS
11	L	63	THR
11	L	143	GLU
11	L	172	GLU
17	R	130	ASN
18	S	88	SER
19	T	81	LYS

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Mol	Chain	Res	Type
20	U	98	ASP
23	X	131	ASP
25	Z	34	SER
26	a	76	ASP
30	e	44	ARG
34	i	11	LEU
35	j	36	LYS
35	j	39	TYR
36	k	32	VAL
42	r	67	ARG
42	r	71	ARG
43	s	70	GLU
43	s	106	LYS
43	s	109	ALA
44	t	5	PHE
44	t	26	SER
44	t	39	PRO
44	t	58	ILE
44	t	106	PHE
52	AA	44	ASP
52	AA	45	GLY
53	BB	86	LEU
53	BB	140	VAL
53	BB	153	THR
54	CC	181	PRO
54	CC	190	SER
55	DD	219	PRO
56	EE	40	GLU
56	EE	95	THR
56	EE	153	LEU
56	EE	231	GLY
57	FF	33	ILE
57	FF	80	GLY
58	GG	152	ASP
59	HH	160	LYS
59	HH	190	PRO
60	II	138	ASN
61	JJ	21	GLU
61	JJ	120	ALA
62	KK	3	MET
62	KK	39	ASN
62	KK	63	ALA

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Mol	Chain	Res	Type
63	LL	66	VAL
63	LL	135	SER
64	MM	15	ASN
65	NN	3	ARG
65	NN	28	LEU
65	NN	138	ASN
66	OO	39	ASP
66	OO	104	ARG
66	OO	129	ILE
67	PP	14	LYS
67	PP	75	VAL
69	RR	63	ARG
70	SS	12	ILE
70	SS	92	ASP
71	TT	29	LYS
71	TT	39	LEU
72	UU	50	VAL
74	WW	3	ARG
75	XX	10	ALA
75	XX	110	HIS
76	YY	84	LYS
76	YY	95	GLY
76	YY	127	ALA
77	ZZ	112	ASN
78	aa	8	ASN
78	aa	25	ASN
79	bb	4	ALA
79	bb	82	LYS
80	cc	26	GLN
81	dd	47	ALA
82	ee	43	VAL
84	gg	61	GLY
84	gg	161	SER
86	ii	31	GLY
86	ii	224	LEU
86	ii	315	GLY
86	ii	387	ALA
2	B	18	PRO
3	C	16	GLU
3	C	132	ALA
3	C	248	ARG
5	E	96	LYS

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Mol	Chain	Res	Type
5	E	179	ARG
5	E	232	GLU
6	F	239	GLU
9	I	205	PRO
10	J	11	PRO
10	J	146	ARG
16	Q	14	ARG
17	R	19	LYS
21	V	14	PHE
25	Z	55	ALA
25	Z	124	THR
26	a	92	LYS
30	e	125	PRO
30	e	126	ASN
31	f	37	ASP
31	f	79	GLY
33	h	97	LYS
34	i	3	LEU
37	l	47	THR
42	r	19	LYS
42	r	85	ASN
43	s	69	LEU
43	s	108	PRO
43	s	142	GLY
44	t	54	LYS
44	t	67	ARG
44	t	105	THR
44	t	137	GLN
52	AA	50	ASN
52	AA	191	ARG
53	BB	88	THR
53	BB	206	PRO
54	CC	255	LEU
55	DD	175	VAL
55	DD	200	PRO
55	DD	222	PRO
56	EE	98	ASN
57	FF	119	SER
58	GG	59	GLN
59	HH	107	LYS
60	II	137	LEU
60	II	143	LYS

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Mol	Chain	Res	Type
61	JJ	39	ASN
62	KK	31	LYS
62	KK	65	ARG
62	KK	92	ALA
63	LL	147	LYS
63	LL	149	ALA
64	MM	100	PRO
66	OO	32	HIS
66	OO	64	ALA
67	PP	15	PHE
68	QQ	100	VAL
70	SS	11	HIS
73	VV	21	ASN
73	VV	45	ARG
74	WW	93	LEU
75	XX	6	GLY
76	YY	34	THR
78	aa	9	GLY
78	aa	61	ALA
78	aa	62	TYR
78	aa	64	LEU
78	aa	65	PRO
79	bb	75	GLU
86	ii	28	ARG
87	jj	22	ARG
87	jj	179	ALA
87	jj	421	THR
1	A	180	LEU
2	B	54	THR
5	E	129	PHE
5	E	224	GLN
8	H	101	ILE
11	L	5	ARG
11	L	52	SER
19	T	29	THR
24	Y	83	GLU
25	Z	31	ASP
26	a	98	ALA
30	e	89	LEU
32	g	65	MET
33	h	89	ARG
36	k	29	LYS

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Mol	Chain	Res	Type
41	p	41	PHE
44	t	2	PRO
44	t	18	THR
45	1	57	ARG
52	AA	43	SER
52	AA	102	ARG
52	AA	207	PRO
53	BB	154	SER
54	CC	264	SER
55	DD	191	PRO
56	EE	30	ARG
56	EE	73	ASP
57	FF	132	GLY
59	HH	16	PRO
59	HH	100	ILE
59	HH	111	LYS
59	HH	119	SER
59	HH	122	LEU
61	JJ	138	ARG
61	JJ	147	PHE
63	LL	28	THR
63	LL	32	LYS
66	OO	138	ASP
69	RR	121	GLN
70	SS	7	GLU
72	UU	51	LYS
72	UU	105	SER
72	UU	118	ASP
74	WW	112	ASP
75	XX	53	GLU
75	XX	129	SER
78	aa	15	ARG
78	aa	35	ALA
82	ee	22	GLN
83	ff	85	LYS
83	ff	117	PRO
84	gg	12	LYS
84	gg	190	GLY
84	gg	205	SER
84	gg	296	GLN
86	ii	373	PRO
86	ii	386	GLY

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Mol	Chain	Res	Type
87	jj	285	PHE
1	A	130	SER
2	B	309	LEU
4	D	20	PHE
5	E	218	LEU
5	E	229	PHE
7	G	123	ALA
7	G	125	LYS
10	J	153	ALA
11	L	6	ASN
11	L	103	ARG
16	Q	148	VAL
20	U	27	HIS
25	Z	91	LEU
31	f	107	PRO
33	h	40	ALA
35	j	34	CYS
35	j	61	THR
36	k	21	LYS
40	o	77	CYS
42	r	11	ARG
43	s	34	ASN
44	t	7	PRO
45	l	64	PRO
52	AA	6	ASP
52	AA	36	GLN
53	BB	22	VAL
53	BB	24	PRO
53	BB	208	HIS
54	CC	134	ASN
55	DD	4	GLN
55	DD	199	GLY
56	EE	109	PHE
56	EE	131	VAL
56	EE	152	PRO
57	FF	37	ASP
57	FF	79	HIS
58	GG	54	GLY
58	GG	105	ASN
58	GG	146	ASN
59	HH	6	ALA
60	II	131	PRO

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Mol	Chain	Res	Type
62	KK	90	VAL
64	MM	103	VAL
64	MM	116	LYS
66	OO	54	CYS
68	QQ	35	ASN
69	RR	42	PRO
69	RR	95	ILE
70	SS	59	LEU
74	WW	66	THR
79	bb	38	PRO
80	cc	64	GLU
81	dd	11	PRO
87	jj	47	ILE
1	A	67	TYR
3	C	222	ARG
3	C	309	ILE
10	J	124	GLY
11	L	100	PRO
11	L	169	ILE
14	O	49	ARG
18	S	5	GLY
20	U	67	LYS
22	W	15	PRO
31	f	106	TYR
35	j	60	GLY
40	o	33	LEU
44	t	10	ILE
44	t	19	GLY
44	t	22	VAL
54	CC	261	PHE
56	EE	90	ILE
59	HH	57	ARG
61	JJ	102	ILE
62	KK	32	HIS
62	KK	43	LEU
65	NN	60	VAL
66	OO	24	GLY
66	OO	33	ILE
66	OO	38	ASN
68	QQ	32	ILE
87	jj	24	GLU
87	jj	45	SER

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Mol	Chain	Res	Type
87	jj	402	GLY
3	C	133	LEU
9	I	99	ILE
27	b	21	ILE
43	s	73	PRO
76	YY	126	GLY
87	jj	129	PRO
4	D	125	VAL
9	I	201	PRO
11	L	134	PRO
25	Z	90	PRO
53	BB	93	GLY
55	DD	218	LEU
56	EE	195	ILE
60	II	126	GLY
61	JJ	18	ARG
87	jj	249	VAL
87	jj	432	ILE
3	C	265	GLY
5	E	103	VAL
6	F	230	VAL
7	G	238	GLY
19	T	44	GLY
75	XX	116	PRO
84	gg	163	PRO
87	jj	263	ILE
10	J	174	ILE
12	M	7	VAL
18	S	155	PRO
44	t	3	PRO
44	t	98	ILE
72	UU	52	GLY
74	WW	29	PRO
81	dd	23	VAL
23	X	119	ILE
42	r	69	GLY
44	t	23	GLY
56	EE	107	GLY

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%)	161 (86%)	26 (14%)	4	22
2	B	336/342 (98%)	291 (87%)	45 (13%)	4	23
3	C	302/302 (100%)	260 (86%)	42 (14%)	4	22
4	D	247/247 (100%)	218 (88%)	29 (12%)	6	28
5	E	208/221 (94%)	185 (89%)	23 (11%)	7	31
6	F	194/195 (100%)	165 (85%)	29 (15%)	3	19
7	G	206/206 (100%)	182 (88%)	24 (12%)	6	28
8	H	169/169 (100%)	148 (88%)	21 (12%)	5	26
9	I	174/180 (97%)	153 (88%)	21 (12%)	6	27
10	J	142/142 (100%)	126 (89%)	16 (11%)	7	30
11	L	176/176 (100%)	145 (82%)	31 (18%)	2	11
12	M	117/117 (100%)	102 (87%)	15 (13%)	5	25
13	N	171/171 (100%)	152 (89%)	19 (11%)	7	31
14	O	171/171 (100%)	144 (84%)	27 (16%)	3	17
15	P	134/134 (100%)	120 (90%)	14 (10%)	8	35
16	Q	163/163 (100%)	145 (89%)	18 (11%)	7	32
17	R	159/159 (100%)	140 (88%)	19 (12%)	6	27
18	S	156/156 (100%)	132 (85%)	24 (15%)	3	17
19	T	139/139 (100%)	122 (88%)	17 (12%)	6	27
20	U	89/89 (100%)	82 (92%)	7 (8%)	14	48
21	V	101/101 (100%)	84 (83%)	17 (17%)	2	14
22	W	55/55 (100%)	50 (91%)	5 (9%)	11	41
23	X	107/107 (100%)	97 (91%)	10 (9%)	10	40
24	Y	124/124 (100%)	107 (86%)	17 (14%)	4	22
25	Z	117/117 (100%)	109 (93%)	8 (7%)	18	56
26	a	119/119 (100%)	107 (90%)	12 (10%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	b	62/62 (100%)	57 (92%)	5 (8%)	14	47
28	c	79/79 (100%)	66 (84%)	13 (16%)	2	14
29	d	98/98 (100%)	82 (84%)	16 (16%)	3	15
30	e	114/114 (100%)	99 (87%)	15 (13%)	5	24
31	f	88/88 (100%)	76 (86%)	12 (14%)	4	23
32	g	98/98 (100%)	83 (85%)	15 (15%)	3	18
33	h	109/109 (100%)	97 (89%)	12 (11%)	7	32
34	i	86/86 (100%)	81 (94%)	5 (6%)	23	60
35	j	73/73 (100%)	62 (85%)	11 (15%)	3	19
36	k	64/64 (100%)	56 (88%)	8 (12%)	5	26
37	l	47/47 (100%)	40 (85%)	7 (15%)	3	19
38	m	48/48 (100%)	39 (81%)	9 (19%)	2	9
39	n	22/22 (100%)	18 (82%)	4 (18%)	2	10
40	o	92/92 (100%)	79 (86%)	13 (14%)	4	21
41	p	74/74 (100%)	68 (92%)	6 (8%)	14	47
42	r	109/109 (100%)	88 (81%)	21 (19%)	1	8
43	s	166/166 (100%)	155 (93%)	11 (7%)	19	57
44	t	136/136 (100%)	128 (94%)	8 (6%)	23	60
45	1	13/13 (100%)	12 (92%)	1 (8%)	15	49
52	AA	174/174 (100%)	152 (87%)	22 (13%)	5	26
53	BB	194/194 (100%)	169 (87%)	25 (13%)	5	25
54	CC	183/183 (100%)	155 (85%)	28 (15%)	3	18
55	DD	190/190 (100%)	168 (88%)	22 (12%)	6	29
56	EE	223/223 (100%)	183 (82%)	40 (18%)	2	11
57	FF	161/161 (100%)	126 (78%)	35 (22%)	1	5
58	GG	207/207 (100%)	179 (86%)	28 (14%)	4	23
59	HH	169/169 (100%)	151 (89%)	18 (11%)	8	33
60	II	178/178 (100%)	155 (87%)	23 (13%)	5	25
61	JJ	161/161 (100%)	141 (88%)	20 (12%)	5	26
62	KK	89/89 (100%)	76 (85%)	13 (15%)	3	20
63	LL	136/136 (100%)	110 (81%)	26 (19%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	MM	104/104 (100%)	85 (82%)	19 (18%)	2	10
65	NN	130/130 (100%)	108 (83%)	22 (17%)	2	13
66	OO	106/106 (100%)	81 (76%)	25 (24%)	1	4
67	PP	116/116 (100%)	98 (84%)	18 (16%)	3	17
68	QQ	117/117 (100%)	102 (87%)	15 (13%)	5	25
69	RR	117/117 (100%)	102 (87%)	15 (13%)	5	25
70	SS	119/119 (100%)	100 (84%)	19 (16%)	3	16
71	TT	112/112 (100%)	94 (84%)	18 (16%)	3	16
72	UU	94/94 (100%)	79 (84%)	15 (16%)	3	16
73	VV	67/67 (100%)	61 (91%)	6 (9%)	11	42
74	WW	112/112 (100%)	99 (88%)	13 (12%)	6	29
75	XX	113/113 (100%)	94 (83%)	19 (17%)	2	14
76	YY	108/108 (100%)	88 (82%)	20 (18%)	2	9
77	ZZ	66/66 (100%)	59 (89%)	7 (11%)	8	34
78	aa	85/85 (100%)	77 (91%)	8 (9%)	10	39
79	bb	75/75 (100%)	62 (83%)	13 (17%)	2	12
80	cc	54/54 (100%)	44 (82%)	10 (18%)	2	9
81	dd	47/47 (100%)	40 (85%)	7 (15%)	3	19
82	ee	47/47 (100%)	39 (83%)	8 (17%)	2	13
83	ff	58/61 (95%)	57 (98%)	1 (2%)	66	87
84	gg	272/272 (100%)	250 (92%)	22 (8%)	14	47
86	ii	358/358 (100%)	324 (90%)	34 (10%)	10	39
87	jj	506/522 (97%)	487 (96%)	19 (4%)	38	72
All	All	10889/10934 (100%)	9508 (87%)	1381 (13%)	9	25

All (1381) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	44	ILE
1	A	49	ILE
1	A	64	ARG
1	A	82	ILE
1	A	96	LEU

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Mol	Chain	Res	Type
1	A	97	ASN
1	A	102	LEU
1	A	125	LYS
1	A	128	ARG
1	A	142	GLU
1	A	158	ILE
1	A	163	ARG
1	A	175	ILE
1	A	180	LEU
1	A	193	ARG
1	A	194	ASN
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
1	A	235	VAL
1	A	242	ARG
2	B	4	ARG
2	B	10	ARG
2	B	17	LEU
2	B	19	ARG
2	B	21	ARG
2	B	31	SER
2	B	43	LEU
2	B	56	ILE
2	B	61	ASP
2	B	62	ARG
2	B	66	LYS
2	B	67	VAL
2	B	90	VAL
2	B	97	ARG
2	B	99	LEU
2	B	101	THR
2	B	103	LYS
2	B	115	LYS
2	B	116	ARG
2	B	135	LYS
2	B	138	GLN
2	B	146	LEU

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Mol	Chain	Res	Type
2	B	162	VAL
2	B	167	GLN
2	B	173	LEU
2	B	203	GLN
2	B	213	GLN
2	B	214	ASP
2	B	228	TYR
2	B	244	THR
2	B	248	LEU
2	B	258	HIS
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	381	THR
2	B	383	GLU
3	C	14	LYS
3	C	20	LYS
3	C	44	LEU
3	C	54	VAL
3	C	55	SER
3	C	57	LEU
3	C	66	SER
3	C	71	ARG
3	C	80	ARG
3	C	95	MET
3	C	101	MET
3	C	113	ARG
3	C	114	ARG
3	C	122	TYR
3	C	124	ILE
3	C	144	ILE
3	C	147	VAL
3	C	150	LEU
3	C	155	GLU

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Mol	Chain	Res	Type
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	204	ARG
3	C	208	CYS
3	C	222	ARG
3	C	232	VAL
3	C	237	ILE
3	C	246	VAL
3	C	267	TRP
3	C	281	MET
3	C	284	MET
3	C	287	THR
3	C	294	LYS
3	C	307	LYS
3	C	312	ARG
3	C	333	LYS
3	C	342	ARG
3	C	345	ARG
3	C	348	LYS
4	D	4	VAL
4	D	22	ARG
4	D	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	66	TYR
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	128	ASP
4	D	152	ARG
4	D	179	ARG
4	D	189	GLU
4	D	196	ARG
4	D	202	GLN
4	D	206	ASP

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Mol	Chain	Res	Type
4	D	208	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	279	ARG
4	D	293	ARG
5	E	43	ASN
5	E	46	LEU
5	E	52	ARG
5	E	55	ARG
5	E	58	MET
5	E	101	ARG
5	E	105	LEU
5	E	126	ARG
5	E	134	ARG
5	E	136	LEU
5	E	137	ARG
5	E	148	ILE
5	E	162	LYS
5	E	190	VAL
5	E	197	ILE
5	E	206	LYS
5	E	212	TYR
5	E	230	ASP
5	E	233	LYS
5	E	250	ASP
5	E	254	LEU
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

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Mol	Chain	Res	Type
6	F	90	LYS
6	F	91	LEU
6	F	100	ILE
6	F	101	ASN
6	F	127	LEU
6	F	137	ILE
6	F	154	GLU
6	F	179	ARG
6	F	181	LEU
6	F	189	MET
6	F	190	GLU
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	239	GLU
6	F	248	ARG
6	F	249	MET
7	G	28	VAL
7	G	73	ARG
7	G	75	LYS
7	G	81	ASN
7	G	90	GLN
7	G	95	LEU
7	G	106	THR
7	G	110	LYS
7	G	112	GLN
7	G	131	LYS
7	G	148	GLU
7	G	150	LYS
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	210	GLU
7	G	217	LYS

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Mol	Chain	Res	Type
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	57	VAL
8	H	59	LYS
8	H	66	GLU
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
8	H	183	GLU
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	88	ARG
9	I	116	ARG
9	I	136	MET
9	I	139	ARG
9	I	144	ASN
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	202	ASN

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Mol	Chain	Res	Type
9	I	208	LYS
9	I	212	LEU
10	J	15	LEU
10	J	16	ARG
10	J	33	LEU
10	J	34	THR
10	J	49	VAL
10	J	55	TYR
10	J	72	CYS
10	J	90	ARG
10	J	91	GLU
10	J	110	GLN
10	J	111	GLU
10	J	113	ILE
10	J	146	ARG
10	J	151	ILE
10	J	167	GLN
10	J	168	GLN
11	L	10	LEU
11	L	28	GLN
11	L	35	ARG
11	L	49	ARG
11	L	59	VAL
11	L	61	CYS
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	107	THR
11	L	111	GLN
11	L	113	ASN
11	L	115	GLN
11	L	121	ARG
11	L	123	LYS
11	L	129	ARG
11	L	130	LYS
11	L	143	GLU
11	L	145	LYS
11	L	158	ARG

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Mol	Chain	Res	Type
11	L	162	LYS
11	L	165	LYS
11	L	186	ARG
11	L	190	ARG
11	L	195	ARG
11	L	198	ARG
11	L	201	GLU
12	M	5	ARG
12	M	8	GLU
12	M	25	VAL
12	M	33	GLN
12	M	38	VAL
12	M	48	GLN
12	M	53	LYS
12	M	57	LEU
12	M	61	ILE
12	M	70	GLN
12	M	96	GLU
12	M	105	THR
12	M	118	MET
12	M	119	ARG
12	M	130	LEU
13	N	9	GLU
13	N	17	ASP
13	N	26	ARG
13	N	32	GLN
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	89	VAL
13	N	104	GLU
13	N	108	ARG
13	N	136	ASP
13	N	147	ASP
13	N	174	LEU
13	N	197	THR
13	N	199	GLN
13	N	202	ARG
14	O	5	GLN

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Mol	Chain	Res	Type
14	O	18	ARG
14	O	31	ARG
14	O	36	VAL
14	O	37	ARG
14	O	38	CYS
14	O	42	ASN
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	85	ARG
14	O	103	LYS
14	O	117	ARG
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	7	ASP
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	13	VAL
16	Q	31	LEU

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Mol	Chain	Res	Type
16	Q	37	ARG
16	Q	54	SER
16	Q	63	LEU
16	Q	75	ARG
16	Q	78	LYS
16	Q	85	THR
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	112	ARG
16	Q	140	SER
16	Q	143	ARG
16	Q	187	LYS
17	R	10	LEU
17	R	15	LEU
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	117	ARG
17	R	123	LEU
17	R	133	LYS
17	R	138	LEU
17	R	178	GLN
18	S	2	LYS
18	S	8	ARG
18	S	9	GLU
18	S	17	LEU
18	S	39	VAL
18	S	43	ARG
18	S	67	VAL

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Mol	Chain	Res	Type
18	S	70	LYS
18	S	82	LEU
18	S	83	ARG
18	S	84	TYR
18	S	86	SER
18	S	91	HIS
18	S	95	ARG
18	S	98	ARG
18	S	100	LEU
18	S	102	THR
18	S	125	GLN
18	S	127	MET
18	S	132	ILE
18	S	147	ASP
18	S	149	LYS
18	S	156	HIS
18	S	159	LEU
19	T	5	LYS
19	T	9	ARG
19	T	17	ARG
19	T	33	ILE
19	T	41	ASP
19	T	52	MET
19	T	60	LYS
19	T	81	LYS
19	T	96	ILE
19	T	99	SER
19	T	117	LYS
19	T	118	GLU
19	T	131	GLN
19	T	142	ARG
19	T	144	ASN
19	T	157	GLU
19	T	159	MET
20	U	33	ILE
20	U	46	ARG
20	U	65	ARG
20	U	67	LYS
20	U	80	LYS
20	U	97	ARG
20	U	99	TRP
21	V	15	ARG

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Mol	Chain	Res	Type
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	97	TYR
21	V	99	GLU
21	V	106	VAL
21	V	109	LYS
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	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
24	Y	59	ARG
24	Y	65	GLN
24	Y	72	GLN

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Mol	Chain	Res	Type
24	Y	74	TYR
24	Y	79	VAL
24	Y	87	ARG
24	Y	104	VAL
24	Y	115	ARG
24	Y	126	ARG
25	Z	11	VAL
25	Z	17	ARG
25	Z	57	MET
25	Z	59	LYS
25	Z	67	LYS
25	Z	93	LYS
25	Z	108	ARG
25	Z	112	ARG
26	a	10	LYS
26	a	12	ARG
26	a	39	HIS
26	a	40	HIS
26	a	46	ASP
26	a	47	LYS
26	a	52	TYR
26	a	59	ARG
26	a	63	LEU
26	a	84	GLU
26	a	122	VAL
26	a	132	ARG
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	59	GLU
28	c	61	GLU
28	c	77	ASN
28	c	78	ASN
28	c	81	LEU
28	c	87	LYS
28	c	91	VAL

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Mol	Chain	Res	Type
28	c	94	LEU
28	c	98	ASP
29	d	19	GLU
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	36	VAL
29	d	44	ARG
29	d	48	GLU
29	d	75	LYS
29	d	78	ARG
29	d	79	ASN
29	d	85	ARG
29	d	90	ARG
29	d	94	GLU
29	d	102	LEU
29	d	107	THR
29	d	116	ASN
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	24	GLN
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	91	CYS
30	e	104	SER
30	e	106	LYS
30	e	107	ASN
30	e	113	GLU
31	f	16	ARG
31	f	33	VAL
31	f	36	ARG
31	f	38	GLU
31	f	40	GLU
31	f	46	ARG
31	f	52	LYS
31	f	56	ASN
31	f	69	VAL

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Mol	Chain	Res	Type
31	f	84	VAL
31	f	100	ARG
31	f	101	ILE
32	g	5	LEU
32	g	6	THR
32	g	11	LEU
32	g	14	ASN
32	g	15	THR
32	g	21	ARG
32	g	32	TYR
32	g	54	ARG
32	g	60	ARG
32	g	64	LEU
32	g	66	ARG
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	46	LYS
33	h	65	GLN
33	h	67	GLU
33	h	88	THR
33	h	89	ARG
33	h	97	LYS
33	h	104	THR
33	h	117	ARG
33	h	121	VAL
33	h	122	LYS
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
35	j	20	ARG
35	j	25	LYS
35	j	29	LEU
35	j	33	THR

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Mol	Chain	Res	Type
35	j	61	THR
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	37	ARG
36	k	39	SER
36	k	57	LYS
36	k	69	LEU
36	k	70	LYS
37	l	8	ARG
37	l	16	LYS
37	l	17	GLN
37	l	21	ARG
37	l	36	ARG
37	l	46	ARG
37	l	49	LEU
38	m	79	GLU
38	m	82	LEU
38	m	85	LEU
38	m	88	LYS
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	13	LEU
39	n	21	ARG
40	o	17	LYS
40	o	24	THR
40	o	26	TYR
40	o	31	ASP
40	o	33	LEU
40	o	36	GLN
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	96	ASP
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	17	LEU
42	r	18	ILE
42	r	20	ARG
42	r	21	ASN
42	r	24	THR
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	41	ASN
42	r	60	VAL
42	r	67	ARG
42	r	70	GLN
42	r	71	ARG
42	r	80	THR
42	r	103	HIS
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	133	GLU
43	s	146	LYS
43	s	149	ARG
43	s	174	LEU
43	s	185	PHE
43	s	191	GLN
44	t	1	MET

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Mol	Chain	Res	Type
44	t	14	TYR
44	t	40	LYS
44	t	95	GLN
44	t	104	ILE
44	t	106	PHE
44	t	114	ARG
44	t	123	ARG
45	1	63	SER
52	AA	8	LEU
52	AA	9	GLN
52	AA	14	ASP
52	AA	23	THR
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	111	GLN
52	AA	113	GLN
52	AA	131	HIS
52	AA	136	GLU
52	AA	142	LEU
52	AA	150	THR
52	AA	158	ASP
52	AA	178	LEU
52	AA	200	ASP
53	BB	27	LYS
53	BB	38	MET
53	BB	43	ASN
53	BB	47	THR
53	BB	51	ARG
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

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Mol	Chain	Res	Type
53	BB	126	ASP
53	BB	134	LEU
53	BB	136	ARG
53	BB	139	CYS
53	BB	142	PHE
53	BB	143	THR
53	BB	150	ILE
53	BB	151	ARG
53	BB	157	GLN
53	BB	163	GLN
53	BB	169	MET
53	BB	212	VAL
53	BB	213	ARG
54	CC	66	LEU
54	CC	78	LEU
54	CC	79	GLU
54	CC	107	LEU
54	CC	110	MET
54	CC	114	LYS
54	CC	120	GLN
54	CC	121	ARG
54	CC	137	VAL
54	CC	152	ARG
54	CC	166	ARG
54	CC	167	ARG
54	CC	182	CYS
54	CC	183	LYS
54	CC	192	LEU
54	CC	202	THR
54	CC	208	PRO
54	CC	227	TRP
54	CC	230	THR
54	CC	233	LEU
54	CC	240	THR
54	CC	247	THR
54	CC	248	TYR
54	CC	251	LEU
54	CC	254	ASP
54	CC	257	LYS
54	CC	262	THR
54	CC	275	LYS
55	DD	9	ARG

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Mol	Chain	Res	Type
55	DD	22	ASN
55	DD	31	GLU
55	DD	40	ARG
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	113	LEU
55	DD	117	ARG
55	DD	120	TYR
55	DD	142	LEU
55	DD	154	ASP
55	DD	156	LEU
55	DD	167	TYR
55	DD	176	LEU
55	DD	190	LEU
55	DD	212	GLU
55	DD	221	THR
56	EE	3	ARG
56	EE	12	VAL
56	EE	17	HIS
56	EE	24	THR
56	EE	32	SER
56	EE	33	THR
56	EE	38	LEU
56	EE	42	LEU
56	EE	49	ARG
56	EE	53	LYS
56	EE	54	TYR
56	EE	59	ASP
56	EE	65	CYS
56	EE	66	MET
56	EE	67	GLN
56	EE	73	ASP
56	EE	92	ILE
56	EE	95	THR
56	EE	100	ARG
56	EE	105	THR
56	EE	123	LEU

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Mol	Chain	Res	Type
56	EE	130	PHE
56	EE	148	ARG
56	EE	165	GLU
56	EE	169	ILE
56	EE	171	ASP
56	EE	174	LYS
56	EE	176	ASP
56	EE	181	CYS
56	EE	182	MET
56	EE	198	ARG
56	EE	205	PHE
56	EE	207	VAL
56	EE	220	THR
56	EE	222	LEU
56	EE	225	ILE
56	EE	240	ARG
56	EE	244	ILE
56	EE	250	GLU
56	EE	259	LYS
57	FF	35	LEU
57	FF	36	GLN
57	FF	43	GLU
57	FF	47	LYS
57	FF	63	LYS
57	FF	73	THR
57	FF	76	MET
57	FF	78	MET
57	FF	79	HIS
57	FF	88	MET
57	FF	89	THR
57	FF	91	ARG
57	FF	93	VAL
57	FF	95	HIS
57	FF	103	LEU
57	FF	106	GLU
57	FF	118	ASN
57	FF	125	SER
57	FF	126	THR
57	FF	130	ARG
57	FF	136	ARG
57	FF	141	VAL
57	FF	145	ARG

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Mol	Chain	Res	Type
57	FF	149	GLN
57	FF	152	TRP
57	FF	160	GLU
57	FF	168	THR
57	FF	171	GLU
57	FF	173	LEU
57	FF	179	ASN
57	FF	187	SER
57	FF	190	ILE
57	FF	194	ASP
57	FF	203	ASN
57	FF	204	ARG
58	GG	14	LYS
58	GG	15	LEU
58	GG	30	LYS
58	GG	50	VAL
58	GG	56	ASN
58	GG	58	LYS
58	GG	64	LYS
58	GG	68	LEU
58	GG	76	LEU
58	GG	120	ASP
58	GG	121	ILE
58	GG	128	THR
58	GG	132	ARG
58	GG	136	LYS
58	GG	137	ARG
58	GG	143	LYS
58	GG	164	LYS
58	GG	172	LYS
58	GG	178	ARG
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	196	LYS
58	GG	208	GLU
58	GG	216	ARG
58	GG	224	ARG
58	GG	227	GLN
58	GG	235	SER
59	HH	7	LYS
59	HH	34	SER

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Mol	Chain	Res	Type
59	HH	35	ASP
59	HH	36	LEU
59	HH	72	PHE
59	HH	74	LYS
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	121	THR
59	HH	145	ARG
59	HH	148	LEU
59	HH	153	LEU
59	HH	172	THR
60	II	12	ARG
60	II	21	TYR
60	II	23	LYS
60	II	52	ASN
60	II	70	GLU
60	II	74	ARG
60	II	76	THR
60	II	82	VAL
60	II	86	SER
60	II	88	ASN
60	II	96	LEU
60	II	100	CYS
60	II	111	GLN
60	II	115	SER
60	II	123	ARG
60	II	130	THR
60	II	140	LYS
60	II	153	LYS
60	II	162	LEU
60	II	168	GLN
60	II	196	GLU
60	II	203	LYS
60	II	206	LYS
61	JJ	21	GLU
61	JJ	29	LEU
61	JJ	39	ASN

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Mol	Chain	Res	Type
61	JJ	42	GLU
61	JJ	45	ARG
61	JJ	65	GLU
61	JJ	69	ARG
61	JJ	86	VAL
61	JJ	101	LYS
61	JJ	110	LEU
61	JJ	116	LYS
61	JJ	127	ARG
61	JJ	131	ARG
61	JJ	133	ARG
61	JJ	135	ILE
61	JJ	136	ARG
61	JJ	138	ARG
61	JJ	162	ARG
61	JJ	172	ARG
61	JJ	176	LYS
62	KK	1	MET
62	KK	2	LEU
62	KK	13	GLU
62	KK	16	PHE
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	89	ILE
63	LL	8	ARG
63	LL	16	ILE
63	LL	18	GLN
63	LL	22	ARG
63	LL	31	GLU
63	LL	40	ILE
63	LL	56	ILE
63	LL	66	VAL
63	LL	67	SER
63	LL	69	ARG
63	LL	74	SER
63	LL	76	VAL

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Mol	Chain	Res	Type
63	LL	78	THR
63	LL	85	THR
63	LL	90	ARG
63	LL	91	ASP
63	LL	97	ARG
63	LL	106	HIS
63	LL	109	MET
63	LL	111	VAL
63	LL	114	SER
63	LL	121	GLN
63	LL	126	VAL
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	36	ARG
64	MM	45	ARG
64	MM	48	HIS
64	MM	60	MET
64	MM	73	GLN
64	MM	74	ILE
64	MM	77	ILE
64	MM	78	LYS
64	MM	83	LYS
64	MM	88	TRP
64	MM	96	ARG
64	MM	101	ARG
64	MM	114	TYR
64	MM	127	TYR
65	NN	5	HIS
65	NN	13	GLN
65	NN	25	TRP
65	NN	27	LYS
65	NN	52	VAL
65	NN	57	SER
65	NN	64	ARG
65	NN	70	LYS
65	NN	75	LEU

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Mol	Chain	Res	Type
65	NN	76	LYS
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	94	LYS
65	NN	102	LEU
65	NN	107	LYS
65	NN	110	ASP
65	NN	114	ARG
65	NN	120	SER
65	NN	121	ARG
65	NN	125	LEU
65	NN	142	GLU
66	OO	34	PHE
66	OO	38	ASN
66	OO	39	ASP
66	OO	50	LYS
66	OO	51	GLU
66	OO	53	ILE
66	OO	61	LYS
66	OO	65	ASP
66	OO	69	SER
66	OO	80	ASP
66	OO	81	VAL
66	OO	85	CYS
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
66	OO	131	ASP
66	OO	133	THR
66	OO	137	SER
66	OO	142	ARG
66	OO	146	ARG
66	OO	151	LEU
67	PP	5	GLU
67	PP	7	LYS
67	PP	10	ARG
67	PP	17	TYR

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Mol	Chain	Res	Type
67	PP	21	ASP
67	PP	28	MET
67	PP	29	SER
67	PP	30	TYR
67	PP	37	TYR
67	PP	40	ARG
67	PP	43	ARG
67	PP	44	ARG
67	PP	52	LYS
67	PP	65	LYS
67	PP	88	GLU
67	PP	100	LYS
67	PP	107	ILE
67	PP	121	ILE
68	QQ	20	THR
68	QQ	26	LYS
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	73	LYS
68	QQ	85	ARG
68	QQ	89	SER
68	QQ	90	LYS
68	QQ	97	GLN
68	QQ	119	LEU
68	QQ	126	ARG
68	QQ	131	LYS
68	QQ	140	ARG
68	QQ	145	TYR
68	QQ	146	ARG
69	RR	43	SER
69	RR	47	ARG
69	RR	58	MET
69	RR	77	GLU
69	RR	78	ARG
69	RR	79	GLU
69	RR	82	ASP
69	RR	87	GLU
69	RR	88	VAL
69	RR	99	ASP
69	RR	101	ASP
69	RR	109	LEU
69	RR	118	GLN

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Mol	Chain	Res	Type
69	RR	121	GLN
69	RR	127	ASN
70	SS	7	GLU
70	SS	8	LYS
70	SS	10	GLN
70	SS	14	ARG
70	SS	17	ASN
70	SS	34	LYS
70	SS	52	LEU
70	SS	59	LEU
70	SS	63	GLU
70	SS	78	LYS
70	SS	81	ASP
70	SS	82	TRP
70	SS	86	ARG
70	SS	113	ARG
70	SS	115	LYS
70	SS	118	ARG
70	SS	131	VAL
70	SS	134	GLN
70	SS	136	THR
71	TT	4	VAL
71	TT	8	ASP
71	TT	28	LEU
71	TT	35	ASP
71	TT	37	VAL
71	TT	39	LEU
71	TT	62	ARG
71	TT	67	ARG
71	TT	74	SER
71	TT	84	ARG
71	TT	92	PHE
71	TT	93	SER
71	TT	102	ARG
71	TT	108	GLU
71	TT	121	ARG
71	TT	123	LEU
71	TT	124	THR
71	TT	128	GLN
72	UU	31	SER
72	UU	33	GLU
72	UU	36	CYS

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Mol	Chain	Res	Type
72	UU	48	LEU
72	UU	49	LYS
72	UU	51	LYS
72	UU	55	ARG
72	UU	56	MET
72	UU	62	ARG
72	UU	68	THR
72	UU	81	GLN
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	31	SER
73	VV	38	GLU
73	VV	40	ASP
73	VV	74	LYS
74	WW	3	ARG
74	WW	22	LYS
74	WW	23	ARG
74	WW	25	VAL
74	WW	36	ARG
74	WW	74	VAL
74	WW	80	ASP
74	WW	83	LEU
74	WW	103	VAL
74	WW	104	LEU
74	WW	110	ILE
74	WW	111	MET
74	WW	117	ARG
75	XX	3	LYS
75	XX	4	CYS
75	XX	5	ARG
75	XX	9	THR
75	XX	12	LYS
75	XX	14	ARG
75	XX	29	LYS
75	XX	37	LYS
75	XX	61	GLN
75	XX	67	ARG
75	XX	68	LYS

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Mol	Chain	Res	Type
75	XX	71	ARG
75	XX	98	ASP
75	XX	105	PHE
75	XX	112	VAL
75	XX	115	ILE
75	XX	123	VAL
75	XX	128	VAL
75	XX	130	LEU
76	YY	7	ILE
76	YY	10	ARG
76	YY	14	THR
76	YY	16	ARG
76	YY	20	ARG
76	YY	32	LYS
76	YY	40	ILE
76	YY	44	LEU
76	YY	46	LYS
76	YY	61	ARG
76	YY	62	THR
76	YY	69	THR
76	YY	72	PHE
76	YY	74	MET
76	YY	87	PRO
76	YY	98	GLU
76	YY	99	LYS
76	YY	100	LYS
76	YY	107	ARG
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	110	THR
77	ZZ	114	LYS
78	aa	19	GLN
78	aa	23	CYS
78	aa	26	CYS
78	aa	33	ASP
78	aa	41	ILE
78	aa	51	ARG
78	aa	52	ASP

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Mol	Chain	Res	Type
78	aa	94	ASP
79	bb	3	LEU
79	bb	17	ARG
79	bb	27	SER
79	bb	36	LYS
79	bb	37	CYS
79	bb	44	THR
79	bb	51	GLN
79	bb	60	SER
79	bb	63	LEU
79	bb	72	ARG
79	bb	81	ARG
79	bb	83	GLN
79	bb	84	HIS
80	cc	31	ARG
80	cc	34	PHE
80	cc	35	MET
80	cc	58	LEU
80	cc	60	GLU
80	cc	61	SER
80	cc	62	GLU
80	cc	63	ARG
80	cc	67	ARG
80	cc	68	LEU
81	dd	5	GLN
81	dd	6	LEU
81	dd	16	GLN
81	dd	26	ASN
81	dd	27	ARG
81	dd	39	CYS
81	dd	54	LYS
82	ee	15	GLN
82	ee	18	LYS
82	ee	24	LYS
82	ee	34	ARG
82	ee	36	MET
82	ee	41	ARG
82	ee	43	VAL
82	ee	52	LYS
83	ff	81	THR
84	gg	20	GLN
84	gg	29	ASP

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Mol	Chain	Res	Type
84	gg	36	ARG
84	gg	44	LYS
84	gg	47	ARG
84	gg	49	GLU
84	gg	63	SER
84	gg	64	HIS
84	gg	65	PHE
84	gg	93	THR
84	gg	99	ARG
84	gg	100	ARG
84	gg	107	ASP
84	gg	143	GLN
84	gg	156	PHE
84	gg	172	LYS
84	gg	186	THR
84	gg	234	ASP
84	gg	282	GLU
84	gg	289	LEU
84	gg	298	LEU
84	gg	306	LEU
86	ii	45	ILE
86	ii	61	ASN
86	ii	65	ARG
86	ii	67	ASN
86	ii	80	GLN
86	ii	82	LEU
86	ii	86	ASN
86	ii	103	GLU
86	ii	111	ASN
86	ii	112	ILE
86	ii	128	ASP
86	ii	136	LEU
86	ii	139	LEU
86	ii	164	ASN
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

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Mol	Chain	Res	Type
86	ii	231	ASP
86	ii	232	PHE
86	ii	241	MET
86	ii	246	LEU
86	ii	255	ASP
86	ii	300	LYS
86	ii	333	LEU
86	ii	339	GLU
86	ii	340	GLU
86	ii	361	GLU
86	ii	368	LEU
86	ii	415	TYR
87	jj	52	GLU
87	jj	75	LEU
87	jj	90	ASN
87	jj	106	LEU
87	jj	131	LEU
87	jj	161	GLU
87	jj	248	ASP
87	jj	250	LYS
87	jj	289	LEU
87	jj	296	TYR
87	jj	320	GLU
87	jj	374	ILE
87	jj	399	ASP
87	jj	411	TYR
87	jj	455	ILE
87	jj	486	ASP
87	jj	494	SER
87	jj	567	ARG
87	jj	574	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	217	GLN
7	G	29	ASN
42	r	103	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	20 (27%)	0
47	3	72/75 (96%)	36 (50%)	0
48	5	3643/3662 (99%)	1179 (32%)	0
49	7	119/120 (99%)	19 (15%)	0
50	8	155/156 (99%)	52 (33%)	0
51	9	1709/1719 (99%)	608 (35%)	0
85	hh	11/12 (91%)	7 (63%)	0
All	All	5783/5820 (99%)	1921 (33%)	0

All (1921) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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(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	2	C
47	3	5	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	34	U
47	3	35	U
47	3	38	A
47	3	39	U
47	3	41	U
47	3	42	G
47	3	47	U
47	3	48	C
47	3	49	C
47	3	58	A
47	3	60	U
47	3	61	C
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	21	G
48	5	25	A
48	5	30	C
48	5	39	A
48	5	42	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

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Mol	Chain	Res	Type
48	5	59	A
48	5	64	A
48	5	65	A
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	95	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	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
48	5	174	C
48	5	175	C

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Mol	Chain	Res	Type
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	209	U
48	5	210	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	253	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	286	U
48	5	296	A
48	5	297	U
48	5	300	A

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Mol	Chain	Res	Type
48	5	306	A
48	5	309	C
48	5	315	G
48	5	316	U
48	5	319	A
48	5	321	U
48	5	322	C
48	5	326	C
48	5	328	A
48	5	334	A
48	5	337	U
48	5	340	C
48	5	347	A
48	5	349	A
48	5	350	C
48	5	353	A
48	5	357	U
48	5	361	C
48	5	362	A
48	5	363	A
48	5	385	A
48	5	386	A
48	5	387	G
48	5	399	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	424	U
48	5	429	A
48	5	431	G
48	5	432	U
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

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Mol	Chain	Res	Type
48	5	454	U
48	5	455	C
48	5	458	C
48	5	465	G
48	5	467	U
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	501	C
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	682	G
48	5	684	G
48	5	685	C
48	5	686	A
48	5	690	C
48	5	694	C
48	5	695	G

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Mol	Chain	Res	Type
48	5	696	C
48	5	697	G
48	5	701	G
48	5	703	G
48	5	707	C
48	5	718	C
48	5	721	G
48	5	722	G
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	756	G
48	5	911	U
48	5	914	U
48	5	915	A
48	5	917	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

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Mol	Chain	Res	Type
48	5	942	G
48	5	943	A
48	5	944	A
48	5	945	U
48	5	946	C
48	5	947	C
48	5	957	G
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	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

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Mol	Chain	Res	Type
48	5	1177	U
48	5	1181	C
48	5	1182	C
48	5	1183	C
48	5	1193	C
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	1234	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	1279	A
48	5	1280	C
48	5	1281	G

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Mol	Chain	Res	Type
48	5	1285	U
48	5	1286	C
48	5	1287	G
48	5	1288	G
48	5	1289	C
48	5	1293	G
48	5	1294	A
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

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Mol	Chain	Res	Type
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
48	5	1418	C
48	5	1420	A
48	5	1421	G
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	1449	C
48	5	1455	G
48	5	1456	C
48	5	1457	G
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	1504	G
48	5	1514	U
48	5	1516	G

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Mol	Chain	Res	Type
48	5	1518	A
48	5	1523	A
48	5	1524	A
48	5	1533	A
48	5	1534	A
48	5	1547	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1568	C
48	5	1578	U
48	5	1582	U
48	5	1586	G
48	5	1591	U
48	5	1592	G
48	5	1596	U
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1614	C
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	1655	C
48	5	1656	U
48	5	1661	C
48	5	1670	G
48	5	1676	C
48	5	1677	U
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

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Mol	Chain	Res	Type
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	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	1803	G
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

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Mol	Chain	Res	Type
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1847	C
48	5	1848	C
48	5	1855	G
48	5	1867	A
48	5	1869	G
48	5	1882	U
48	5	1885	G
48	5	1886	G
48	5	1889	U
48	5	1892	A
48	5	1897	A
48	5	1899	G
48	5	1900	C
48	5	1910	G
48	5	1918	U
48	5	1919	G
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
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	1960	A
48	5	1961	G
48	5	1964	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

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Mol	Chain	Res	Type
48	5	1981	G
48	5	1983	A
48	5	1984	A
48	5	1985	G
48	5	1986	U
48	5	1987	C
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	2046	G
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

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Mol	Chain	Res	Type
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
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	2103	G
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	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

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Mol	Chain	Res	Type
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
48	5	2260	C
48	5	2261	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	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	2324	C
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	2382	A
48	5	2383	C
48	5	2395	A

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Mol	Chain	Res	Type
48	5	2396	A
48	5	2399	G
48	5	2417	A
48	5	2422	C
48	5	2424	G
48	5	2425	U
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	2447	U
48	5	2450	G
48	5	2458	C
48	5	2469	C
48	5	2471	G
48	5	2473	A
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	2512	A
48	5	2513	A
48	5	2514	G
48	5	2519	U
48	5	2521	G
48	5	2527	A
48	5	2530	U
48	5	2536	A
48	5	2537	A

Continued on next page...

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Mol	Chain	Res	Type
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
48	5	2571	C
48	5	2575	U
48	5	2577	C
48	5	2583	C
48	5	2587	A
48	5	2588	C
48	5	2589	C
48	5	2591	A
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	2647	A
48	5	2653	C
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	2679	G
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2688	G
48	5	2695	A
48	5	2696	A
48	5	2704	C
48	5	2708	U

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Mol	Chain	Res	Type
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	2724	G
48	5	2725	A
48	5	2726	G
48	5	2733	C
48	5	2740	U
48	5	2743	A
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	2794	C
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	2835	A
48	5	2838	G

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Mol	Chain	Res	Type
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
48	5	2910	G
48	5	3594	C
48	5	3595	U
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	3630	A
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3662	A
48	5	3668	C
48	5	3670	C
48	5	3671	G
48	5	3673	C
48	5	3674	G
48	5	3680	U
48	5	3682	A
48	5	3689	G
48	5	3692	A
48	5	3696	C
48	5	3698	G
48	5	3702	A
48	5	3709	U
48	5	3710	G

Continued on next page...

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Mol	Chain	Res	Type
48	5	3711	A
48	5	3712	A
48	5	3717	A
48	5	3718	A
48	5	3722	G
48	5	3728	A
48	5	3729	U
48	5	3737	A
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3752	C
48	5	3753	G
48	5	3755	G
48	5	3756	A
48	5	3759	A
48	5	3760	A
48	5	3764	U
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	3783	A
48	5	3784	A
48	5	3786	U
48	5	3788	C
48	5	3798	U
48	5	3799	A
48	5	3802	U
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3813	A
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3831	U
48	5	3836	A

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Mol	Chain	Res	Type
48	5	3838	U
48	5	3839	G
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	3889	G
48	5	3897	G
48	5	3900	G
48	5	3901	A
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	3924	C
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	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4087	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

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Mol	Chain	Res	Type
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
48	5	4127	A
48	5	4134	C
48	5	4143	G
48	5	4144	C
48	5	4145	C
48	5	4155	C
48	5	4161	G
48	5	4162	C
48	5	4163	U
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	4219	A
48	5	4225	G
48	5	4226	G
48	5	4229	U
48	5	4232	U

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Mol	Chain	Res	Type
48	5	4233	A
48	5	4238	G
48	5	4241	C
48	5	4251	A
48	5	4254	G
48	5	4258	C
48	5	4265	U
48	5	4266	G
48	5	4267	G
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4282	A
48	5	4291	G
48	5	4297	G
48	5	4302	U
48	5	4303	C
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4307	A
48	5	4311	A
48	5	4312	U
48	5	4313	A
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4329	G
48	5	4330	G
48	5	4331	G
48	5	4332	C
48	5	4335	C
48	5	4336	A
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	4368	G
48	5	4372	U

Continued on next page...

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Mol	Chain	Res	Type
48	5	4373	G
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	4396	A
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	4430	G
48	5	4433	G
48	5	4438	U
48	5	4439	U
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	4454	G
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	4484	A
48	5	4488	A
48	5	4491	G
48	5	4495	G
48	5	4500	U

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Mol	Chain	Res	Type
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	4535	A
48	5	4548	A
48	5	4549	G
48	5	4550	G
48	5	4557	U
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
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4591	U
48	5	4606	G
48	5	4618	G
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

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Mol	Chain	Res	Type
48	5	4694	G
48	5	4695	C
48	5	4700	A
48	5	4701	A
48	5	4702	G
48	5	4709	U
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
48	5	4749	C
48	5	4750	G
48	5	4753	U
48	5	4754	G
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

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Mol	Chain	Res	Type
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
48	5	4931	G
48	5	4932	U
48	5	4934	A
48	5	4935	C
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	4959	U
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4975	G
48	5	4976	U
48	5	4985	U
48	5	4988	U
48	5	4989	U

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Mol	Chain	Res	Type
48	5	4990	C
48	5	4991	U
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
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	51	G
49	7	53	U
49	7	54	A
49	7	64	G
49	7	74	A
49	7	76	U
49	7	97	G
49	7	99	G

Continued on next page...

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Mol	Chain	Res	Type
49	7	100	A
49	7	106	G
49	7	110	G
49	7	111	C
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	52	A
50	8	55	U
50	8	57	C
50	8	59	A
50	8	62	A
50	8	63	U
50	8	74	U
50	8	75	G
50	8	79	G
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	99	U
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

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Mol	Chain	Res	Type
50	8	113	C
50	8	114	G
50	8	115	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	2	A
51	9	3	C
51	9	4	C
51	9	6	G
51	9	9	U
51	9	10	G
51	9	11	A
51	9	17	C
51	9	19	A
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
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	61	A
51	9	63	U
51	9	65	C
51	9	66	G

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Mol	Chain	Res	Type
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	93	U
51	9	95	G
51	9	99	A
51	9	100	U
51	9	103	A
51	9	109	U
51	9	110	U
51	9	111	A
51	9	113	G
51	9	114	G
51	9	115	U
51	9	116	U
51	9	119	U
51	9	124	U
51	9	126	G
51	9	140	C
51	9	141	A
51	9	142	C
51	9	147	A
51	9	150	A
51	9	155	G
51	9	158	A
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

Continued on next page...

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Mol	Chain	Res	Type
51	9	173	A
51	9	180	G
51	9	183	G
51	9	184	G
51	9	185	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	215	G
51	9	216	C
51	9	225	G
51	9	289	G
51	9	291	G
51	9	292	A
51	9	293	C
51	9	294	U
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	320	G
51	9	321	C
51	9	322	C
51	9	323	C
51	9	324	C
51	9	326	C
51	9	327	G
51	9	328	U
51	9	338	G
51	9	339	A

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Mol	Chain	Res	Type
51	9	343	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	370	G
51	9	373	G
51	9	385	G
51	9	386	C
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	428	U
51	9	432	G
51	9	435	A
51	9	438	G
51	9	441	C
51	9	447	A
51	9	448	A
51	9	449	A
51	9	450	C
51	9	457	C
51	9	459	C
51	9	460	A
51	9	464	A
51	9	465	A
51	9	466	G
51	9	467	G
51	9	469	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	482	G
51	9	483	C

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Mol	Chain	Res	Type
51	9	487	U
51	9	488	U
51	9	489	A
51	9	492	C
51	9	493	A
51	9	503	C
51	9	508	A
51	9	511	U
51	9	512	A
51	9	523	A
51	9	525	A
51	9	528	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	562	U
51	9	563	G
51	9	568	C
51	9	576	A
51	9	577	U
51	9	579	C
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U

Continued on next page...

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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	596	U
51	9	597	G
51	9	598	G
51	9	603	C
51	9	604	A
51	9	605	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	609	U
51	9	613	G
51	9	614	C
51	9	620	G
51	9	621	C
51	9	623	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	631	U
51	9	632	C
51	9	643	A
51	9	644	G
51	9	654	A
51	9	658	U
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	671	A
51	9	672	A
51	9	673	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	698	G
51	9	731	G

Continued on next page...

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Mol	Chain	Res	Type
51	9	735	C
51	9	737	G
51	9	738	C
51	9	747	U
51	9	748	C
51	9	749	U
51	9	752	G
51	9	753	C
51	9	788	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	859	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	875	A
51	9	877	C
51	9	878	G

Continued on next page...

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Mol	Chain	Res	Type
51	9	879	C
51	9	880	G
51	9	887	U
51	9	888	U
51	9	890	U
51	9	892	U
51	9	893	U
51	9	901	G
51	9	902	G
51	9	903	A
51	9	909	G
51	9	910	G
51	9	912	C
51	9	913	A
51	9	914	U
51	9	917	U
51	9	919	A
51	9	920	A
51	9	921	G
51	9	922	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	938	A
51	9	943	U
51	9	956	G
51	9	958	G
51	9	971	G
51	9	978	G
51	9	985	G
51	9	990	A
51	9	992	A
51	9	996	A
51	9	999	G
51	9	1002	U
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

Continued on next page...

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Mol	Chain	Res	Type
51	9	1045	U
51	9	1049	A
51	9	1058	A
51	9	1060	A
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1096	G
51	9	1099	G
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	1117	C
51	9	1118	C
51	9	1120	U
51	9	1121	G
51	9	1126	G
51	9	1131	G
51	9	1133	A
51	9	1137	U
51	9	1138	C
51	9	1139	C
51	9	1143	A
51	9	1144	A
51	9	1146	C
51	9	1148	A
51	9	1149	A
51	9	1150	A
51	9	1153	C
51	9	1154	U
51	9	1161	U
51	9	1165	G
51	9	1166	G
51	9	1170	A
51	9	1181	A
51	9	1195	A
51	9	1207	G

Continued on next page...

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Mol	Chain	Res	Type
51	9	1208	A
51	9	1209	A
51	9	1211	G
51	9	1212	G
51	9	1213	C
51	9	1215	C
51	9	1221	G
51	9	1224	G
51	9	1227	G
51	9	1240	A
51	9	1242	U
51	9	1243	U
51	9	1244	U
51	9	1247	C
51	9	1248	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	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	1283	C
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1288	U
51	9	1289	U
51	9	1291	A
51	9	1292	C
51	9	1293	A

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Mol	Chain	Res	Type
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	1308	U
51	9	1309	C
51	9	1310	U
51	9	1312	G
51	9	1314	U
51	9	1315	U
51	9	1316	C
51	9	1322	G
51	9	1330	G
51	9	1331	C
51	9	1342	U
51	9	1343	U
51	9	1345	G
51	9	1347	U
51	9	1348	G
51	9	1364	U
51	9	1371	U
51	9	1372	U
51	9	1378	A
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	1401	A
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

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Mol	Chain	Res	Type
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
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	1450	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	1489	A
51	9	1490	G
51	9	1494	U
51	9	1495	G
51	9	1496	U
51	9	1498	A
51	9	1499	U

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Mol	Chain	Res	Type
51	9	1500	G
51	9	1507	G
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1523	C
51	9	1525	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	1548	G
51	9	1552	G
51	9	1553	C
51	9	1554	C
51	9	1555	U
51	9	1556	A
51	9	1558	C
51	9	1560	U
51	9	1563	G
51	9	1564	C
51	9	1565	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	1594	A
51	9	1595	U
51	9	1596	U
51	9	1599	U
51	9	1600	G
51	9	1601	A

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Mol	Chain	Res	Type
51	9	1603	G
51	9	1604	G
51	9	1606	G
51	9	1618	C
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1624	U
51	9	1625	U
51	9	1630	A
51	9	1632	G
51	9	1633	A
51	9	1637	A
51	9	1638	G
51	9	1639	G
51	9	1641	A
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
51	9	1681	U
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1688	C
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1706	G
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	1739	C
51	9	1742	C

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Mol	Chain	Res	Type
51	9	1745	A
51	9	1746	U
51	9	1750	C
51	9	1753	C
51	9	1756	C
51	9	1757	G
51	9	1758	G
51	9	1783	C
51	9	1786	U
51	9	1789	G
51	9	1800	A
51	9	1802	C
51	9	1809	A
51	9	1812	U
51	9	1813	A
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1827	U
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1837	G
51	9	1838	U
51	9	1839	U
51	9	1849	G
51	9	1850	A
51	9	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1867	U
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G
85	hh	49	U
85	hh	50	A
85	hh	52	G

There are no RNA pucker outliers to report.

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	-	25,29,29	1.08	2 (8%)	24,45,45	1.79	2 (8%)
91	ADP	jj	603	-	25,29,29	1.08	2 (8%)	24,45,45	1.81	2 (8%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	602	ADP	C2-N3	2.07	1.35	1.32
91	jj	603	ADP	C2-N3	2.16	1.35	1.32
91	jj	602	ADP	C5-C4	3.28	1.47	1.40
91	jj	603	ADP	C5-C4	3.34	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	jj	602	ADP	N3-C2-N1	-6.96	122.80	128.86
91	jj	603	ADP	N3-C2-N1	-6.95	122.81	128.86
91	jj	603	ADP	C4-C5-N7	-3.07	106.45	109.41
91	jj	602	ADP	C4-C5-N7	-3.07	106.45	109.41

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.