Full wwPDB EM Validation Report

Mar 25, 2026 – 12:10 PM UTC

PDB ID	:	3JAI / pdb_00003jai
EMDB ID	:	EMD-3040
Title	:	Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UGA stop codon
Authors	:	Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.
Deposited on	:	2015-06-10
Resolution	:	3.65 Å(reported)
Based on initial models	:	1DT9, 4V51, 3BK7, 3J92, 3J7P

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

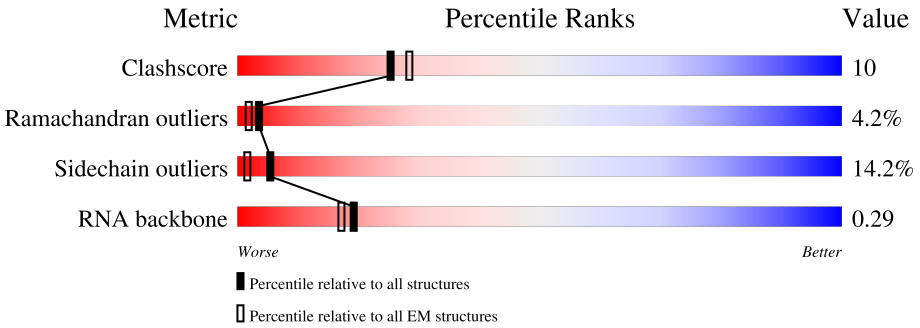
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

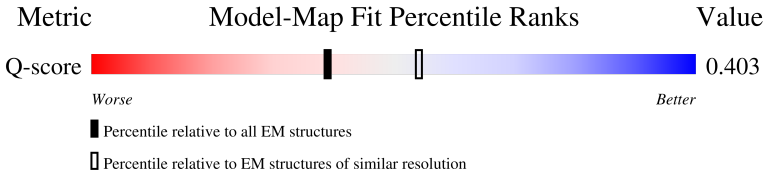
1 Overall quality at a glance

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

The reported resolution of this entry is 3.65 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9087 (3.33 - 4.33)

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

Mol	Chain	Length	Quality of chain
1	A	244	61% 33% 6%
2	B	394	65% 27% 6%
3	C	361	66% 27% 7%

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Mol	Chain	Length	Quality of chain
4	D	292	76% 22%
5	E	248	9% 55% 29% 11% 5%
6	F	225	63% 32% 5%
7	G	241	9% 66% 29%
8	H	190	68% 29%
9	I	213	59% 31% 5%
10	J	169	74% 21%
11	L	210	61% 31% 6%
12	M	138	65% 32%
13	N	203	66% 29% 5%
14	O	199	64% 28% 8%
15	P	153	71% 24% 6%
16	Q	187	70% 28%
17	R	180	72% 23%
18	S	175	65% 30%
19	T	159	75% 22%
20	U	99	73% 23%
21	V	131	74% 21% 5%
22	W	63	73% 24%
23	X	119	70% 28%
24	Y	134	75% 16% 7%
25	Z	135	62% 30% 7%
26	a	147	76% 18% 5%
27	b	75	13% 76% 15% 9%
28	c	94	63% 32% 5%

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Mol	Chain	Length	Quality of chain
29	d	107	69% 21% 9%
30	e	128	54% 42%
31	f	109	56% 36% 8%
32	g	114	72% 24%
33	h	122	75% 17% 7%
34	i	102	74% 25%
35	j	86	63% 30% 6%
36	k	69	77% 19%
37	l	50	66% 32%
38	m	52	63% 33%
39	n	23	78% 22%
40	o	104	71% 21% 7%
41	p	91	63% 31% 7%
42	r	125	56% 33% 10%
43	s	198	49% 78% 21%
44	t	163	35% 73% 24%
45	1	15	73% 20% 7%
46	2	76	45% 45% 8%
47	3	75	15% 39% 41% 15% 5%
48	5	3662	6% 35% 43% 19%
49	7	120	60% 29% 11%
50	8	156	44% 37% 19%
51	9	1719	6% 37% 42% 18%
52	AA	208	62% 30% 7%
53	BB	213	62% 31% 6%

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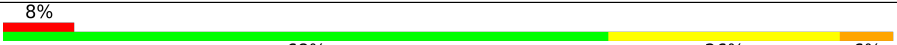
Mol	Chain	Length	Quality of chain
54	CC	218	
55	DD	227	
56	EE	262	
57	FF	191	
58	GG	237	
59	HH	189	
60	II	206	
61	JJ	185	
62	KK	98	
63	LL	152	
64	MM	124	
65	NN	150	
66	OO	136	
67	PP	127	
68	QQ	141	
69	RR	129	
70	SS	137	
71	TT	141	
72	UU	104	
73	VV	83	
74	WW	129	
75	XX	141	
76	YY	126	
77	ZZ	75	
78	aa	98	

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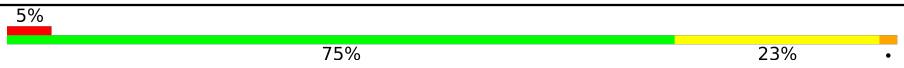
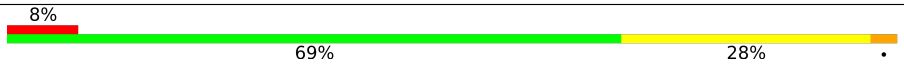
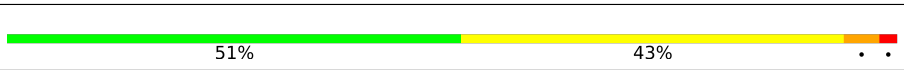
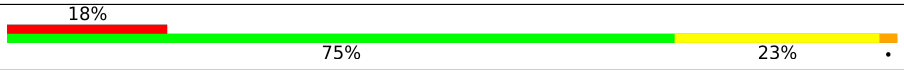
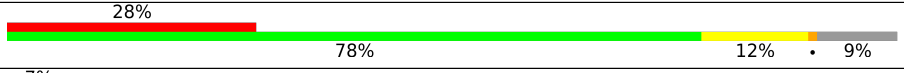
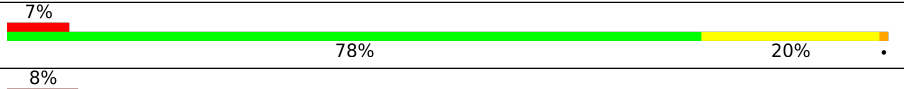
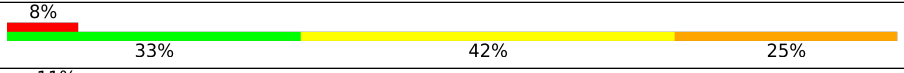
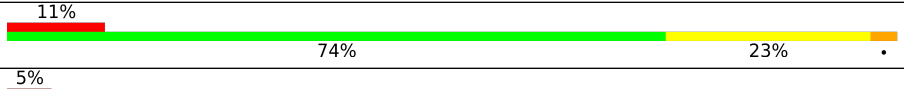
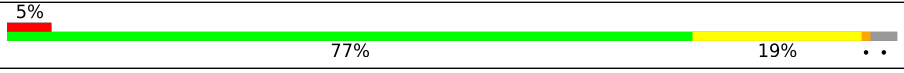
Mol	Chain	Length	Quality of chain
79	bb	83	
80	cc	61	
81	dd	53	
82	ee	57	
83	ff	68	
84	gg	313	
85	hh	12	
86	ii	416	
87	jj	594	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
89	ZN	ff	200	-	-	X	-
89	ZN	m	201	-	-	X	-
90	SF4	jj	600	-	-	X	-
90	SF4	jj	601	-	-	X	-

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 226453 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	361	Total	C	N	O	S	0	0
			2875	1808	576	477	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	361	LYS	-	expression tag	UNP G1SVW5
C	362	SER	-	expression tag	UNP G1SVW5

- 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 eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called peptide.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	218	Total	C	N	O	S	0	0
			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	577	Total	C	N	O	S	0	0
			4551	2910	780	830	31		

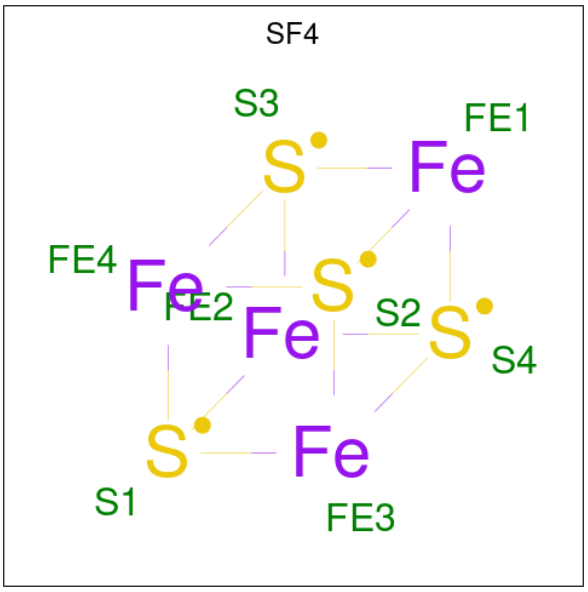
- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
88	C	1	Total Mg 1 1	0
88	I	1	Total Mg 1 1	0
88	P	1	Total Mg 1 1	0
88	V	1	Total Mg 1 1	0
88	g	1	Total Mg 1 1	0
88	5	147	Total Mg 147 147	0
88	7	5	Total Mg 5 5	0
88	8	2	Total Mg 2 2	0
88	9	35	Total Mg 35 35	0
88	hh	1	Total Mg 1 1	0

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

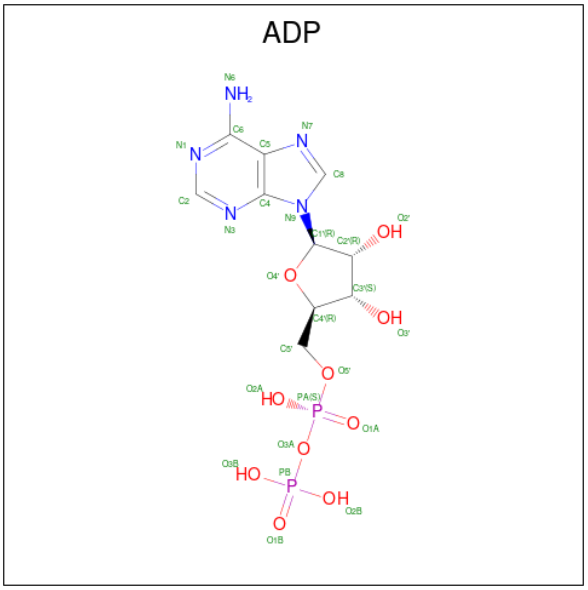
Mol	Chain	Residues	Atoms	AltConf
89	g	1	Total Zn 1 1	0
89	j	1	Total Zn 1 1	0
89	m	1	Total Zn 1 1	0
89	o	1	Total Zn 1 1	0
89	p	1	Total Zn 1 1	0
89	aa	1	Total Zn 1 1	0
89	dd	1	Total Zn 1 1	0
89	ff	1	Total Zn 1 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
90	jj	1	Total	Fe	S	0
			8	4	4	
90	jj	1	Total	Fe	S	0
			8	4	4	

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



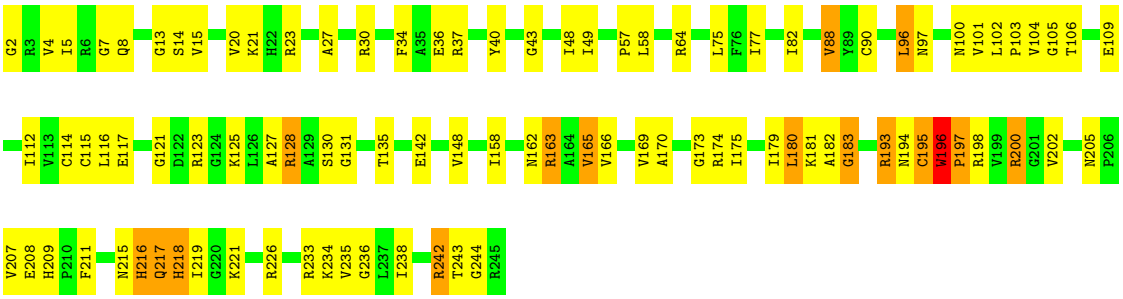
Mol	Chain	Residues	Atoms					AltConf
91	jj	1	Total	C	N	O	P	0
			27	10	5	10	2	
91	jj	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

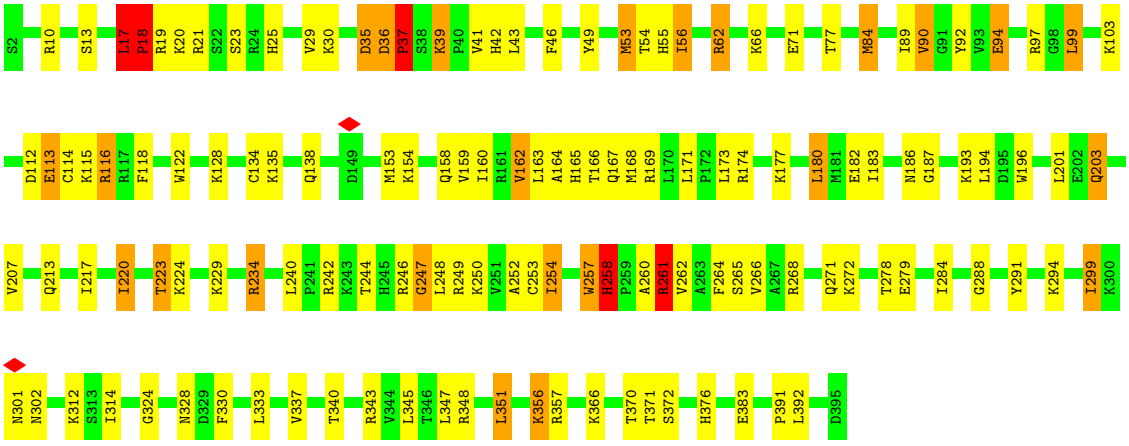
• Molecule 1: uL2

Chain A:



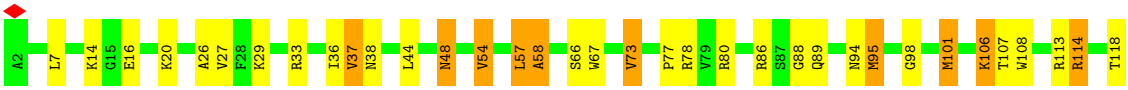
• Molecule 2: uL3

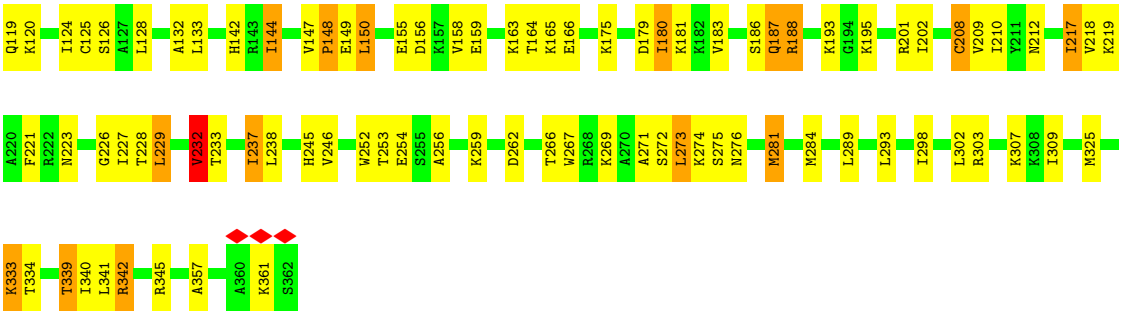
Chain B:



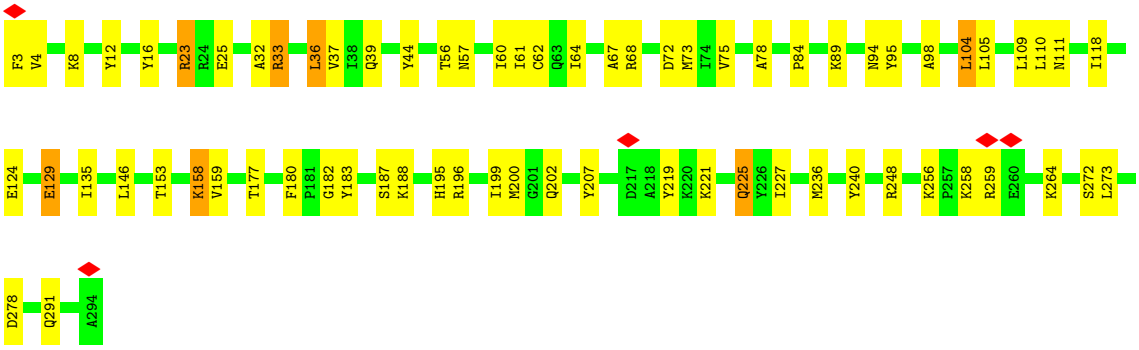
• Molecule 3: uL4

Chain C:

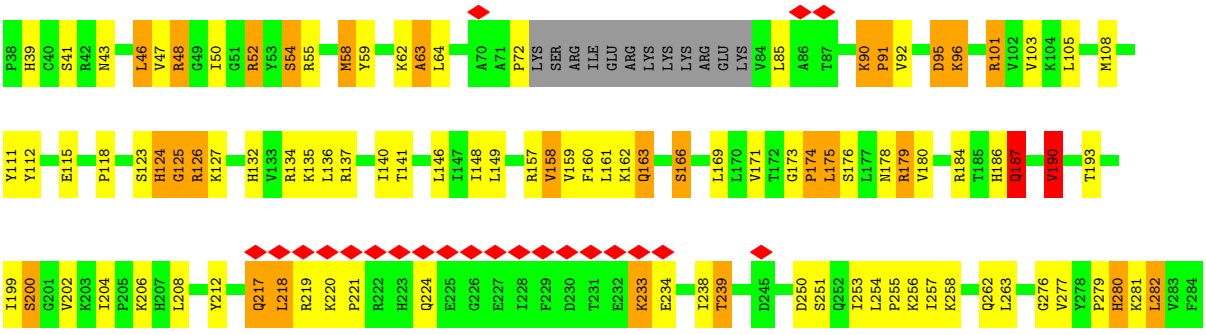




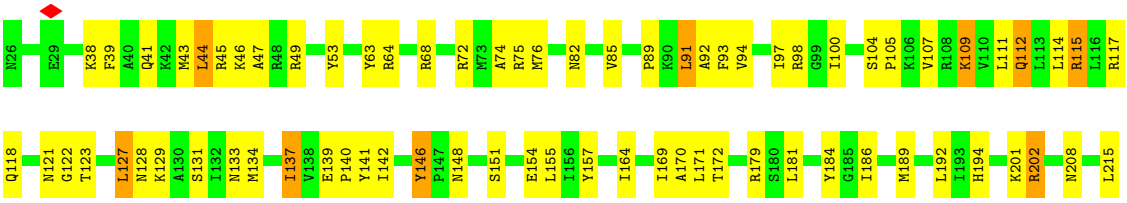
• Molecule 4: uL18

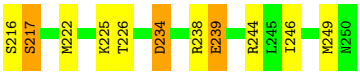


• Molecule 5: eL6



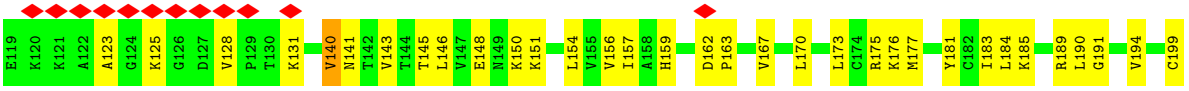
• Molecule 6: uL30

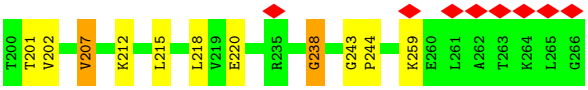




• Molecule 7: eL8

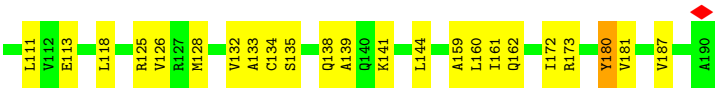
Chain G:





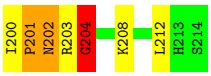
• Molecule 8: uL6

Chain H:



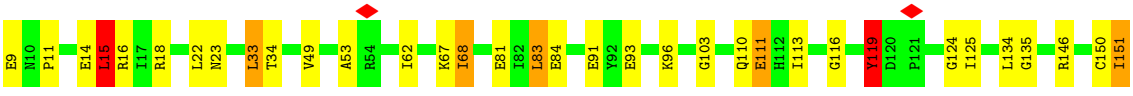
• Molecule 9: uL16

Chain I:



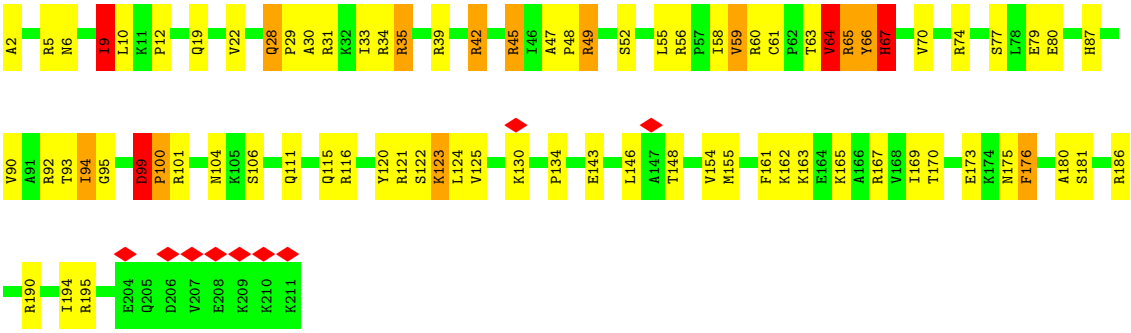
• Molecule 10: uL5

Chain J:



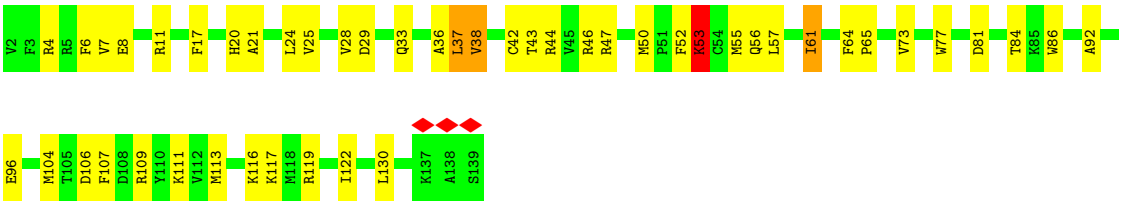
• Molecule 11: eL13

Chain L:



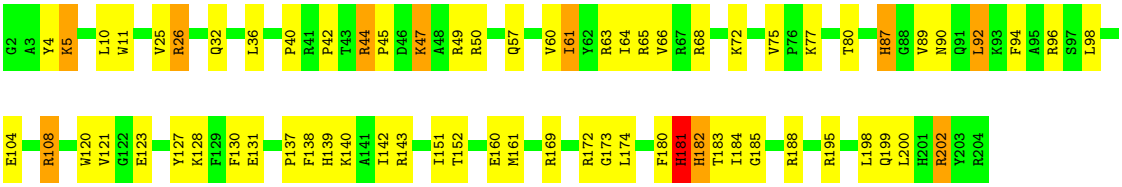
• Molecule 12: eL14

Chain M:



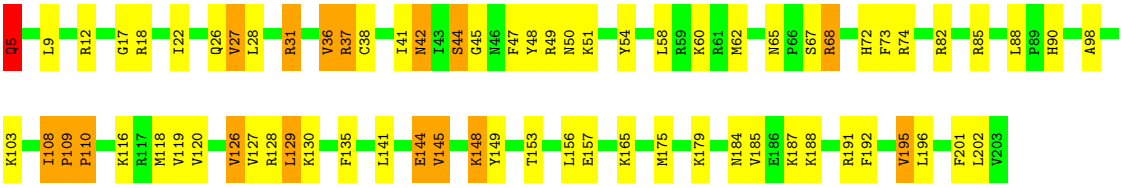
• Molecule 13: eL15

Chain N:



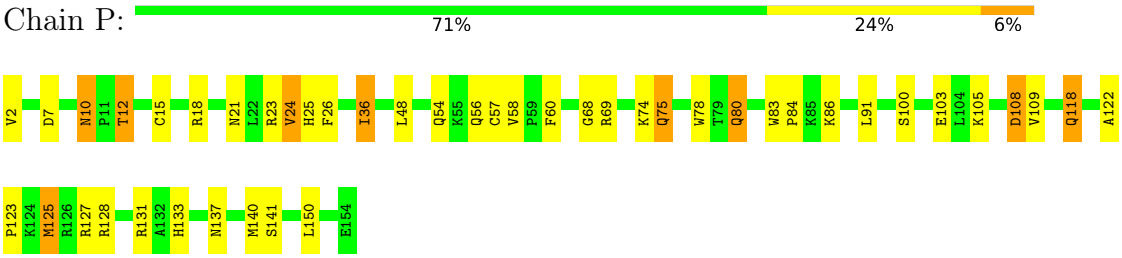
• Molecule 14: uL13

Chain O:



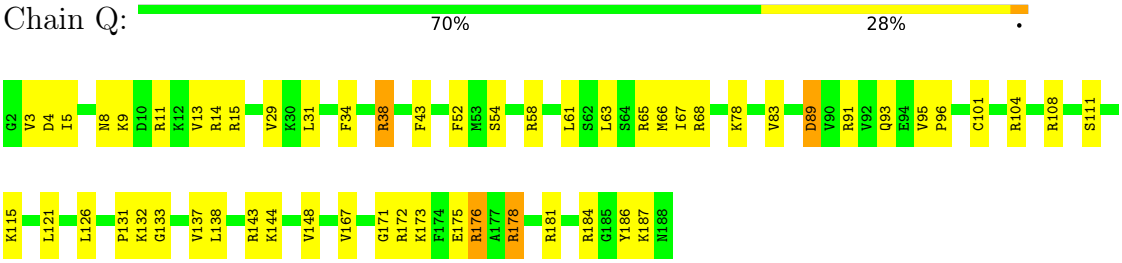
• Molecule 15: uL22

Chain P:



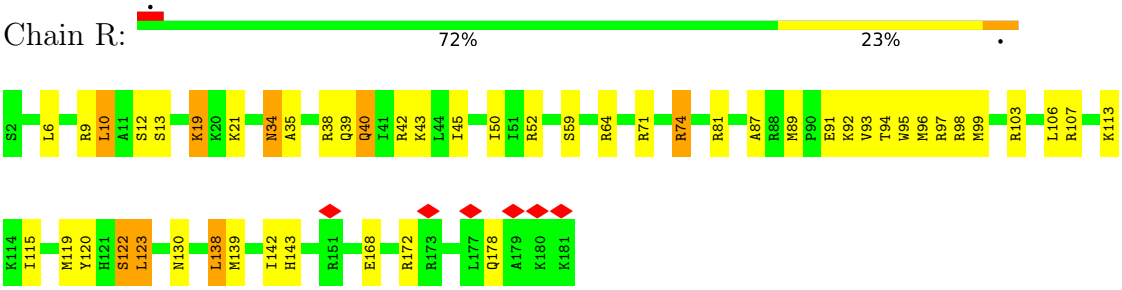
• Molecule 16: eL18

Chain Q:



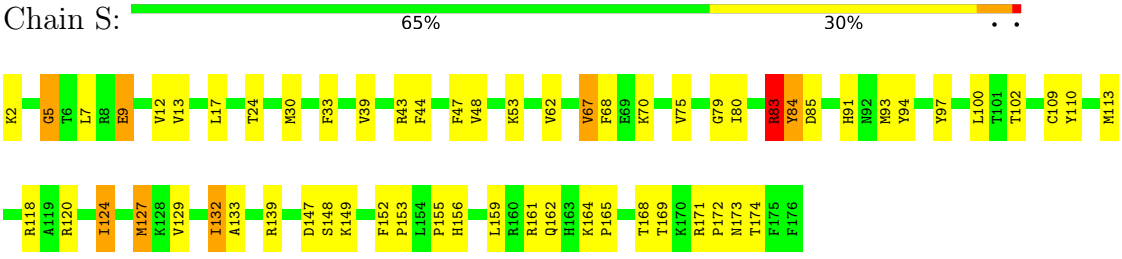
• Molecule 17: eL19

Chain R:



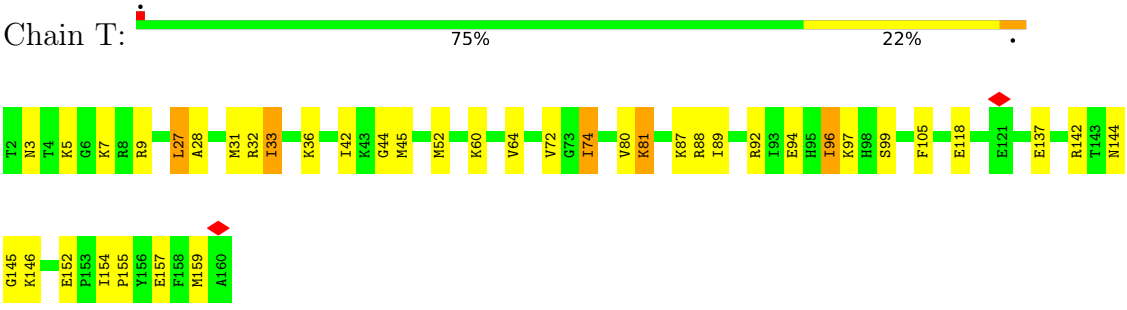
• Molecule 18: eL20

Chain S:



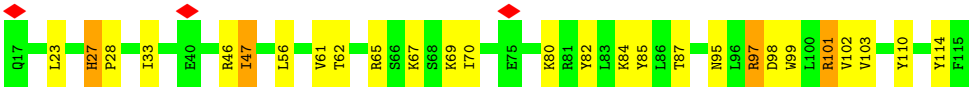
• Molecule 19: eL21

Chain T:



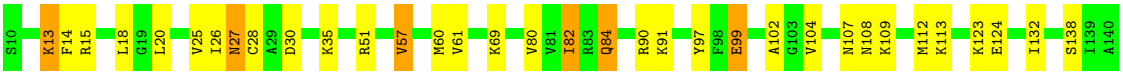
• Molecule 20: eL22

Chain U:



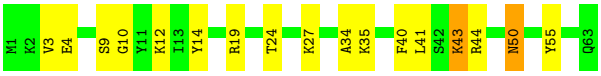
• Molecule 21: uL14

Chain V:



• Molecule 22: eL24

Chain W:

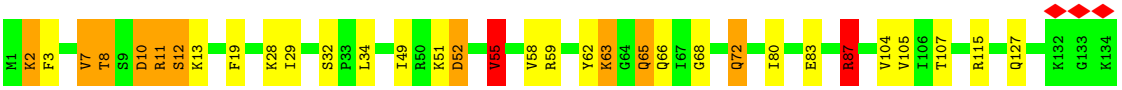


• Molecule 23: uL23

Chain X:

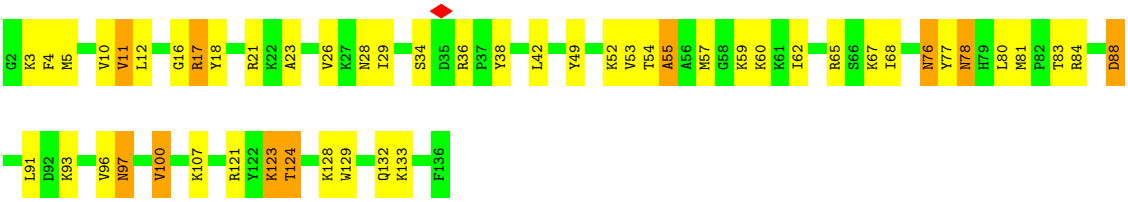
• Molecule 24: uL24

Chain Y:



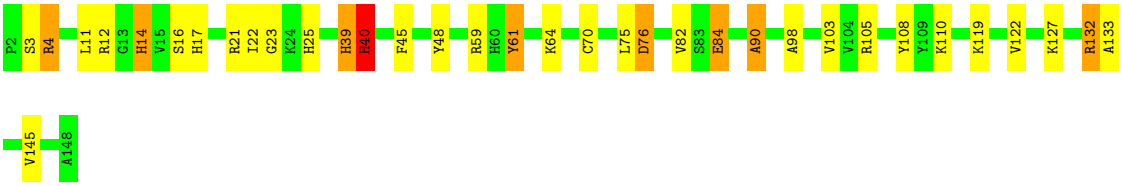
• Molecule 25: eL27

Chain Z:



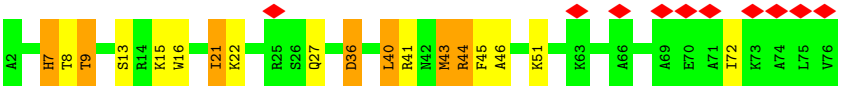
• Molecule 26: uL15

Chain a:



• Molecule 27: eL29

Chain b:



• Molecule 28: eL30

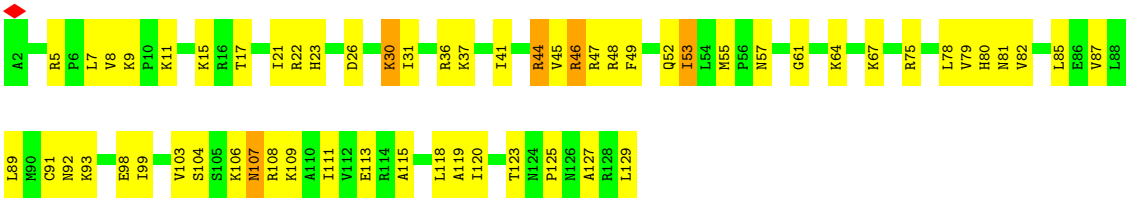
Chain c:

• Molecule 29: eL31

Chain d:

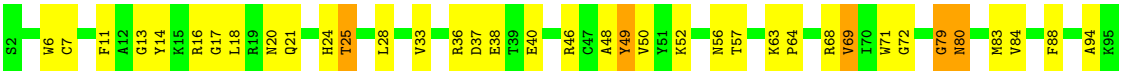
• Molecule 30: eL32

Chain e:



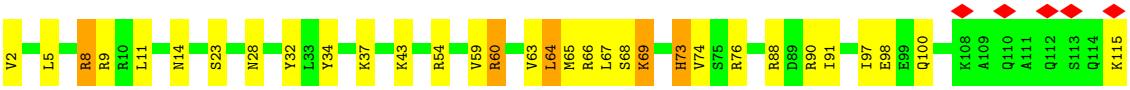
• Molecule 31: eL33

Chain f:



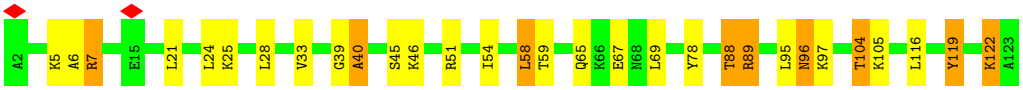
• Molecule 32: eL34

Chain g:



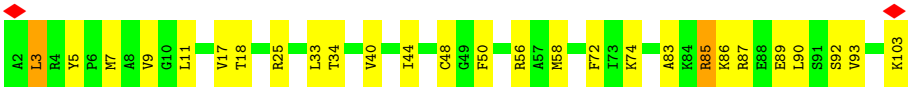
• Molecule 33: uL29

Chain h:



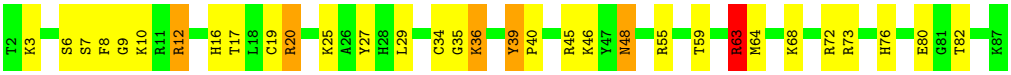
• Molecule 34: eL36

Chain i:



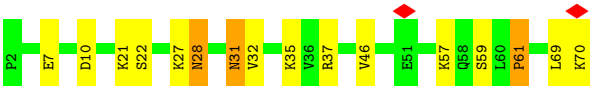
• Molecule 35: eL37

Chain j:



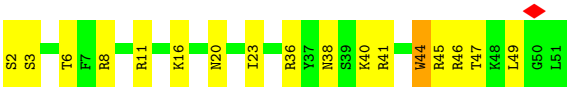
• Molecule 36: eL38

Chain k:



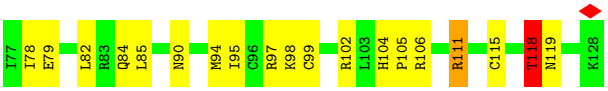
• Molecule 37: eL39

Chain l:



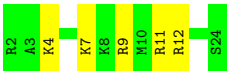
• Molecule 38: eL40

Chain m:



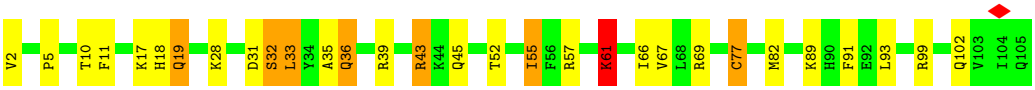
• Molecule 39: eL41

Chain n:



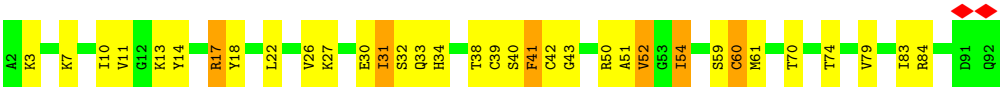
• Molecule 40: eL42

Chain o:



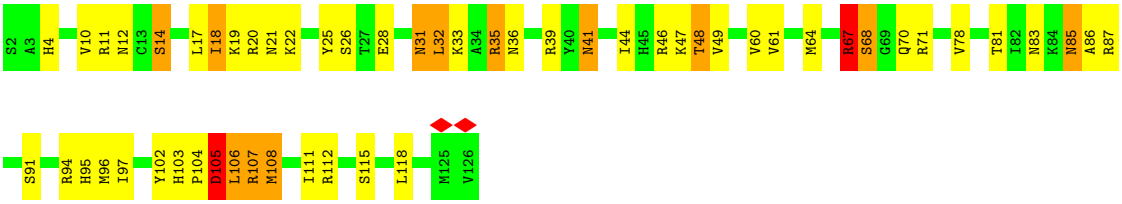
• Molecule 41: eL43

Chain p:



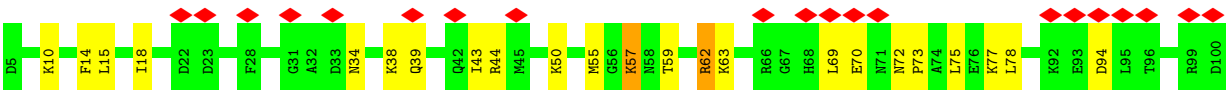
• Molecule 42: eL28

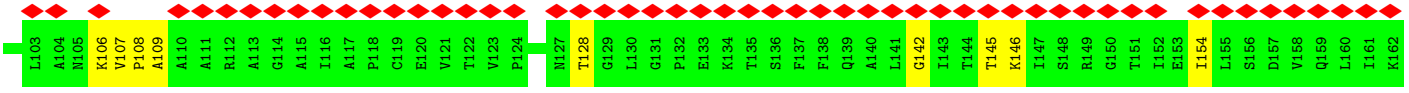
Chain r:

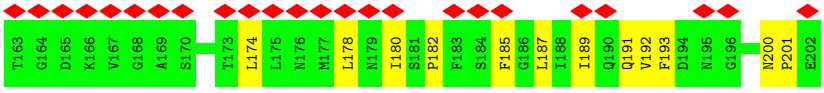


• Molecule 43: uL10

Chain s:

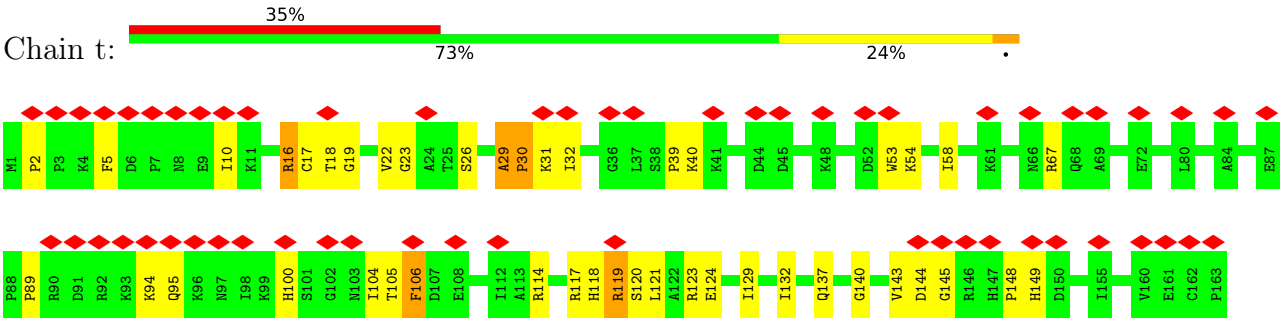






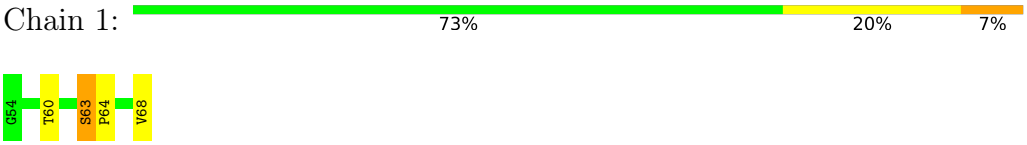
• Molecule 44: uL11

Chain t:



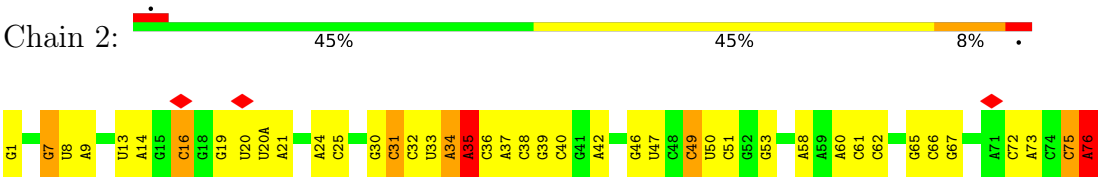
• Molecule 45: peptide

Chain 1:



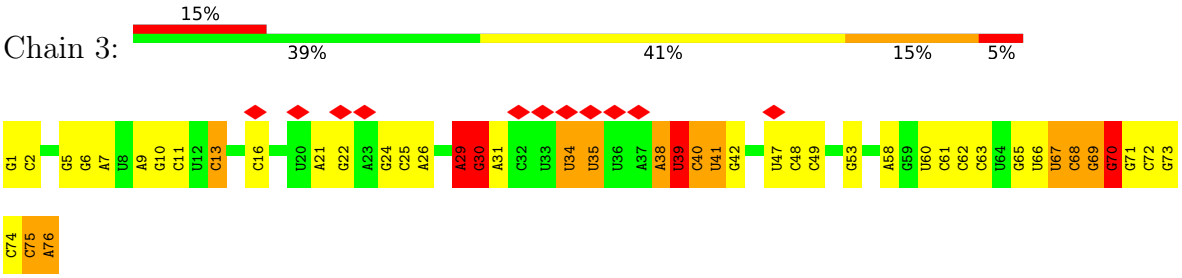
• Molecule 46: tRNA(Val)

Chain 2:



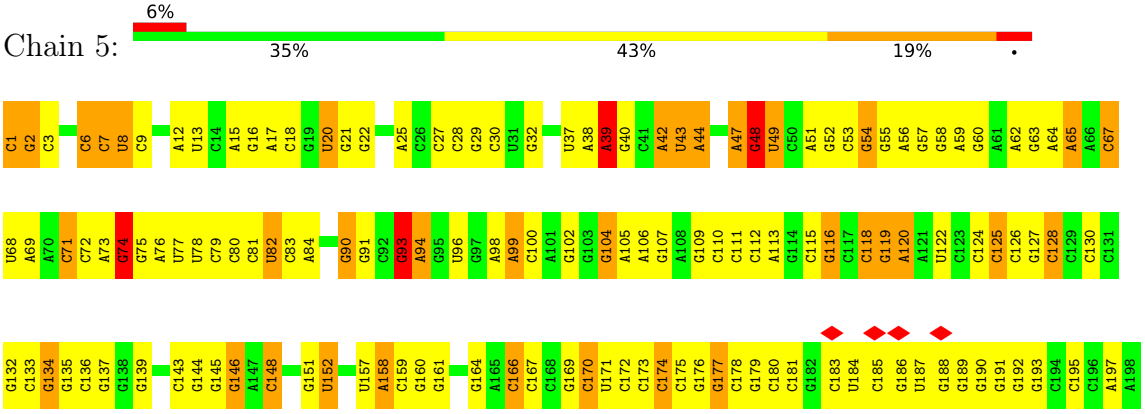
• Molecule 47: tRNA(Lys)

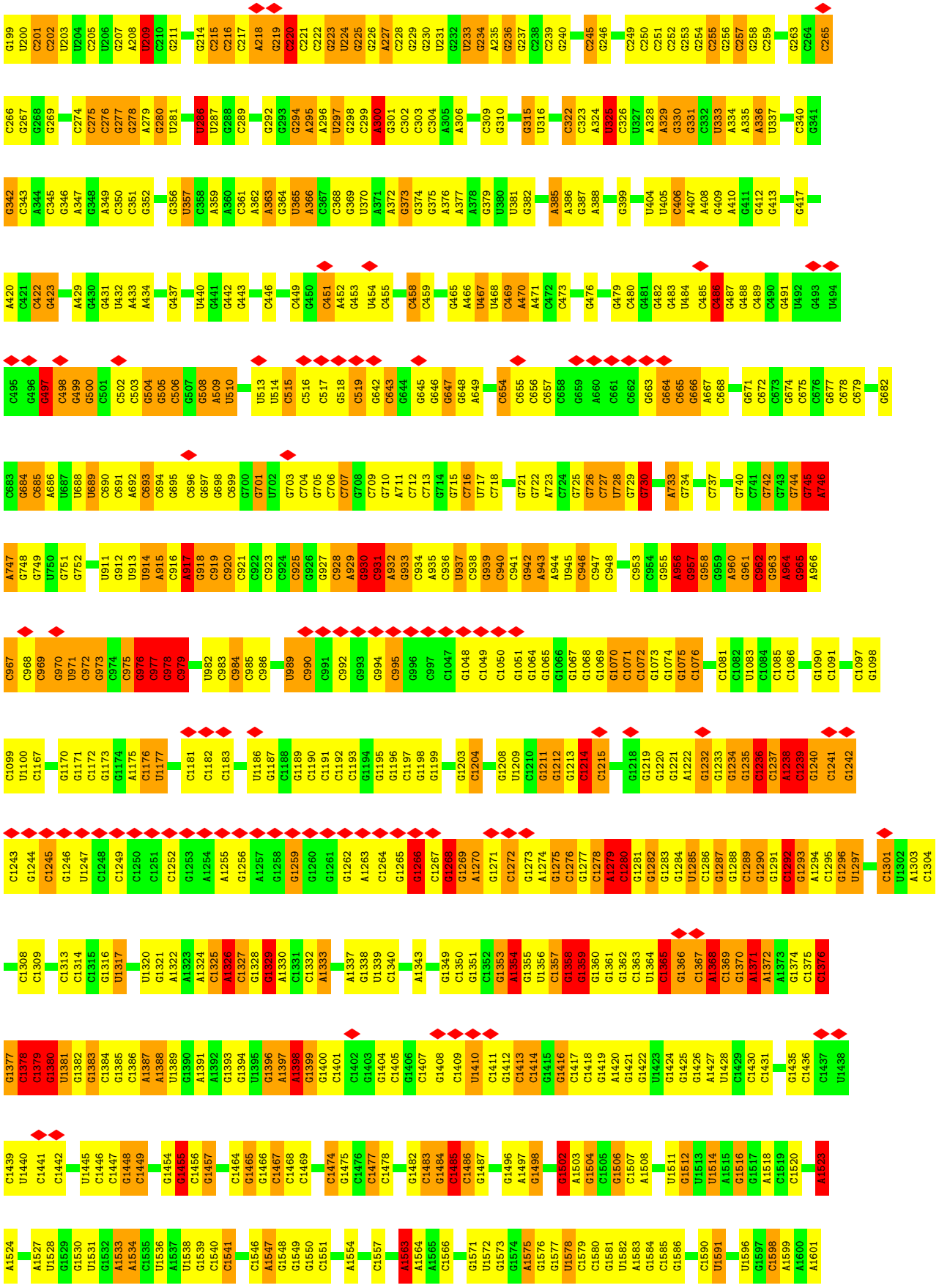
Chain 3:

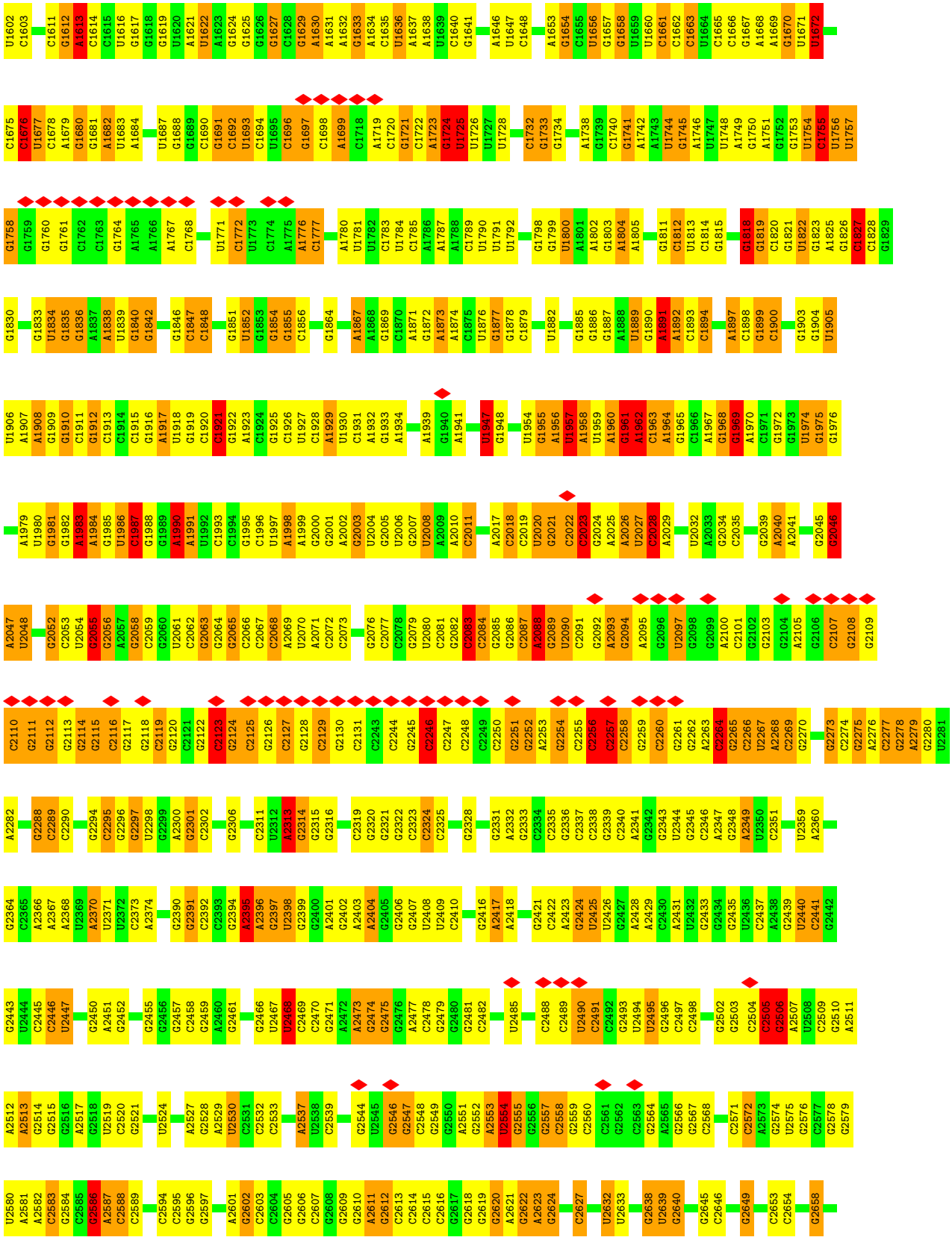


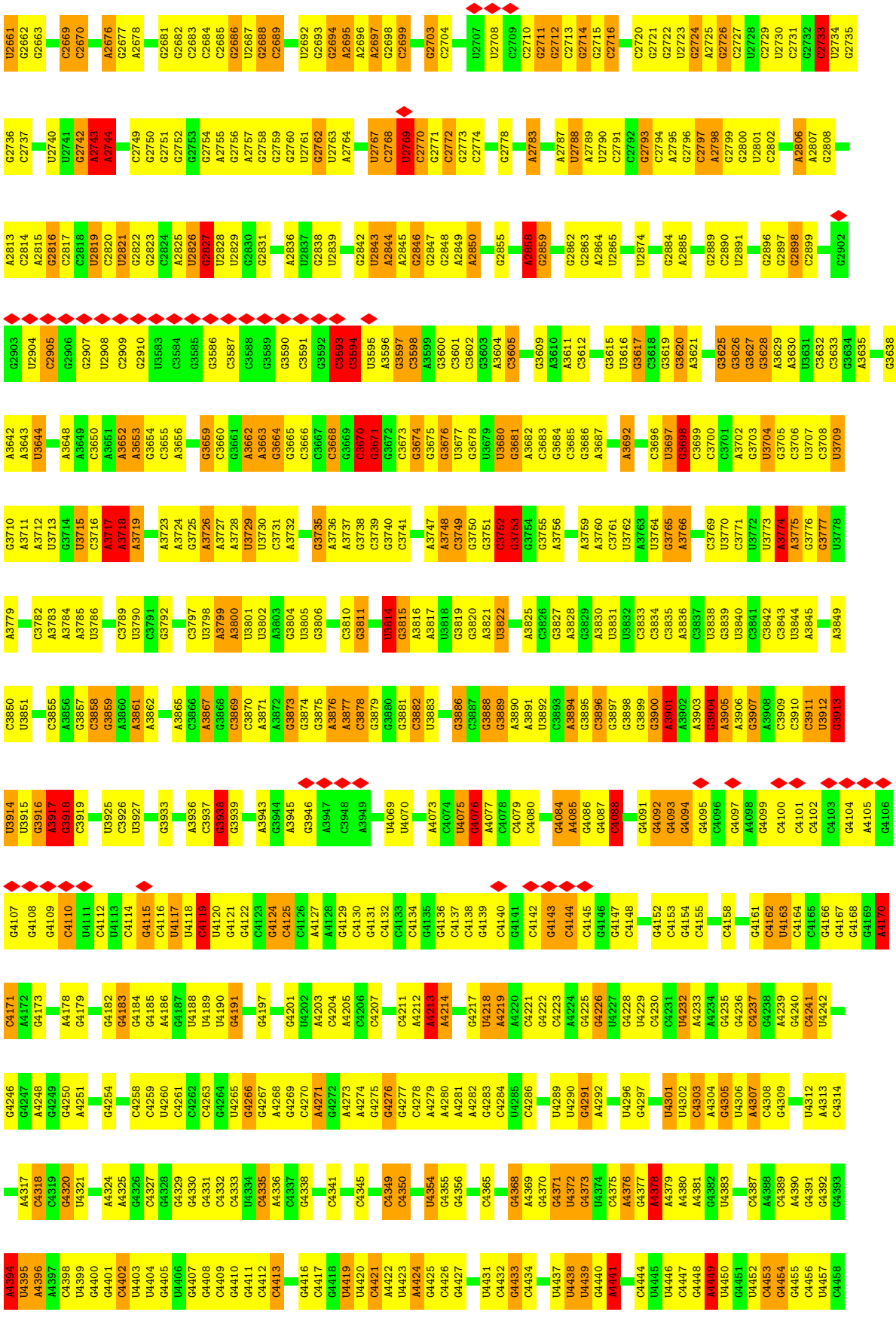
• Molecule 48: 28S ribosomal RNA

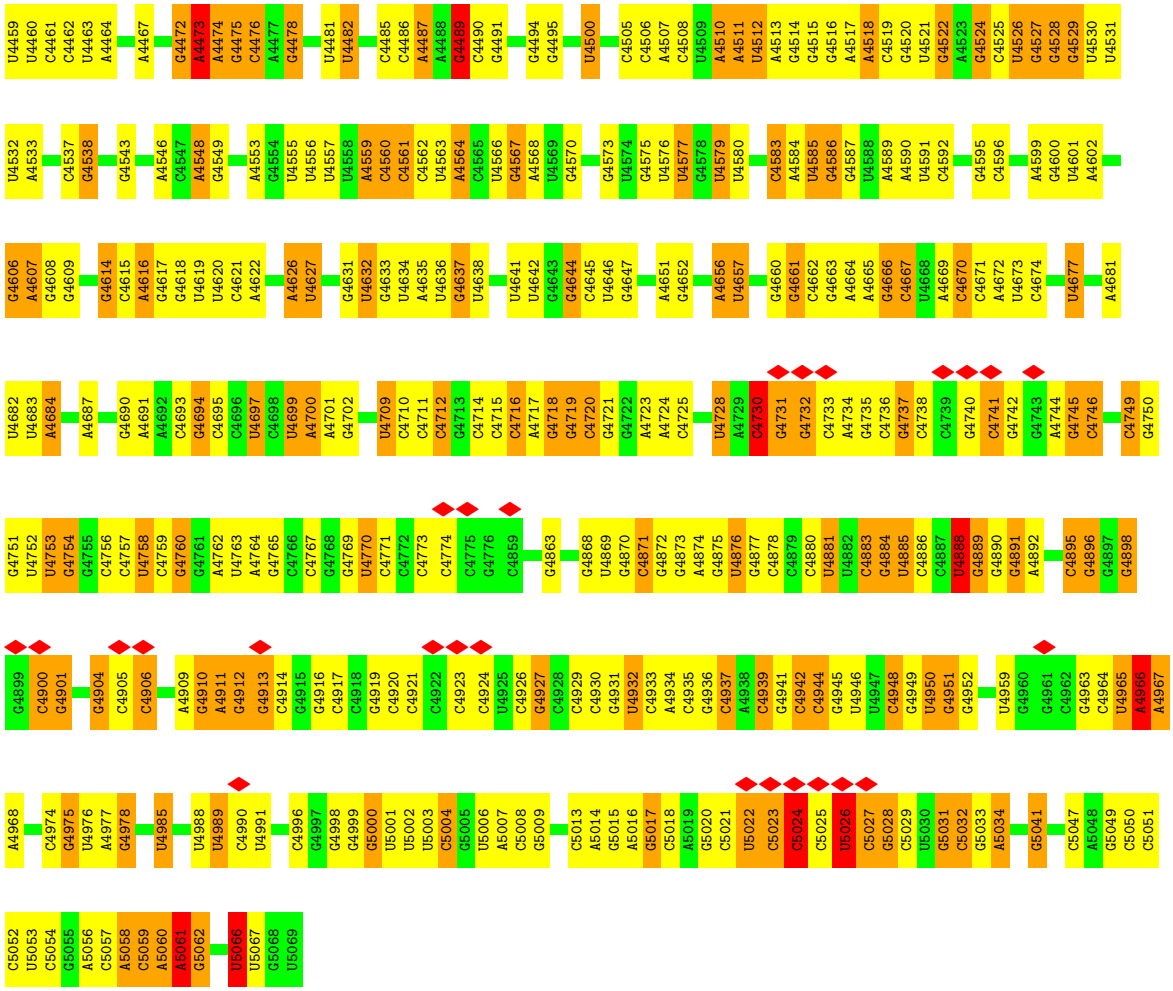
Chain 5:





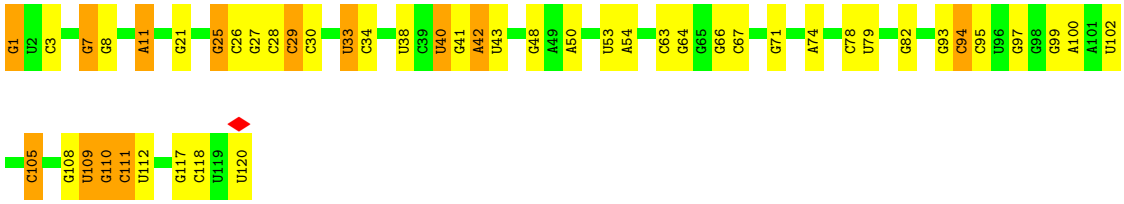






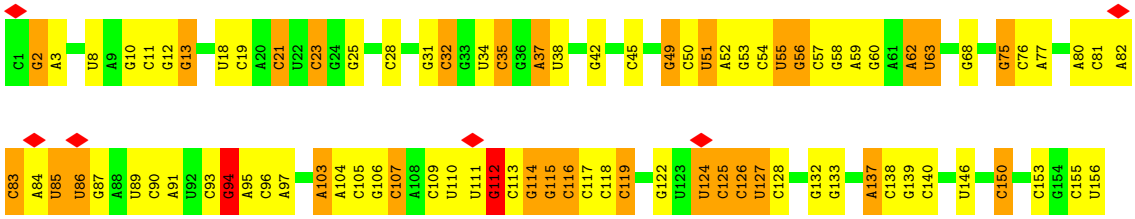
• Molecule 49: 5S ribosomal RNA

Chain 7:



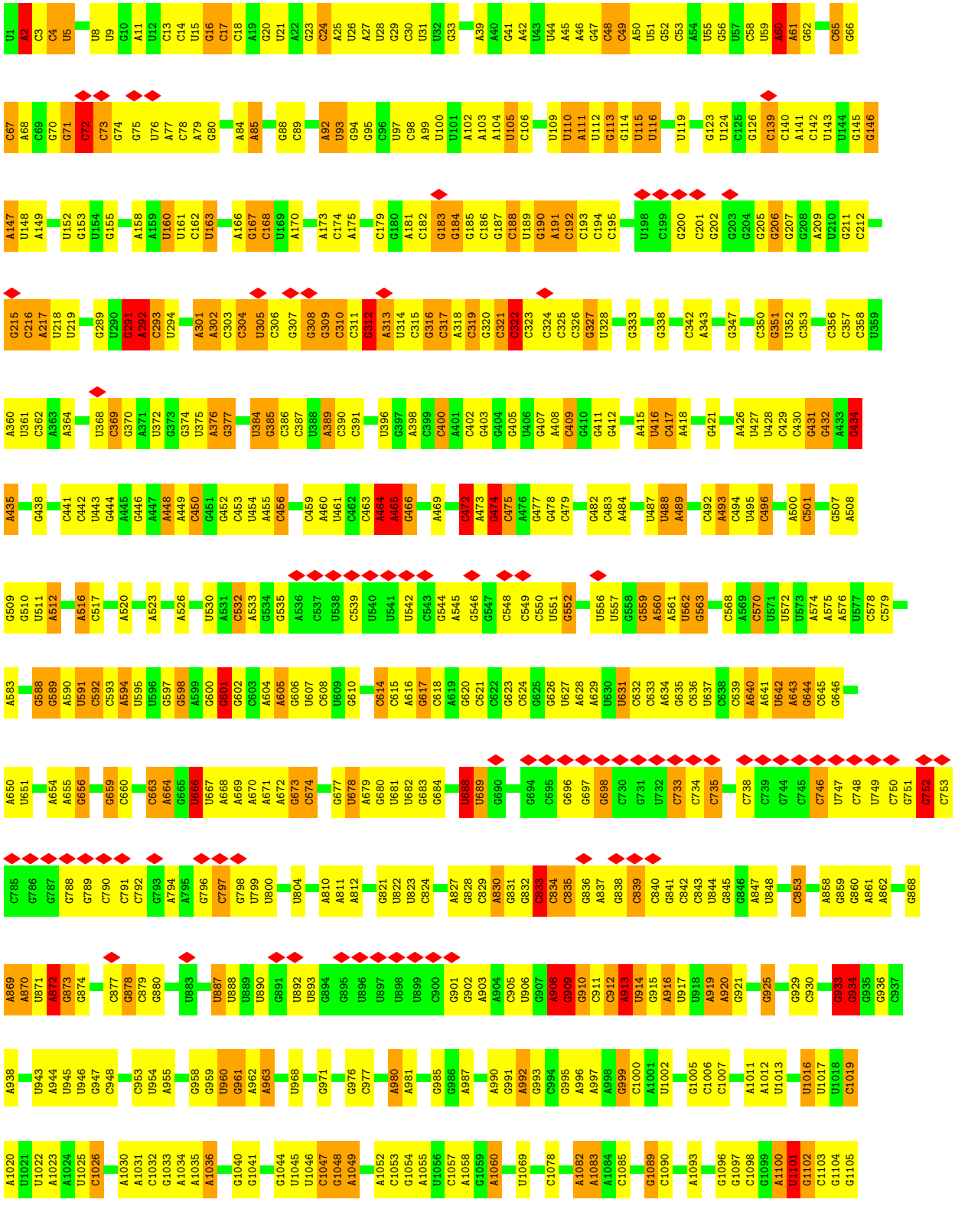
• Molecule 50: 5.8S ribosomal RNA

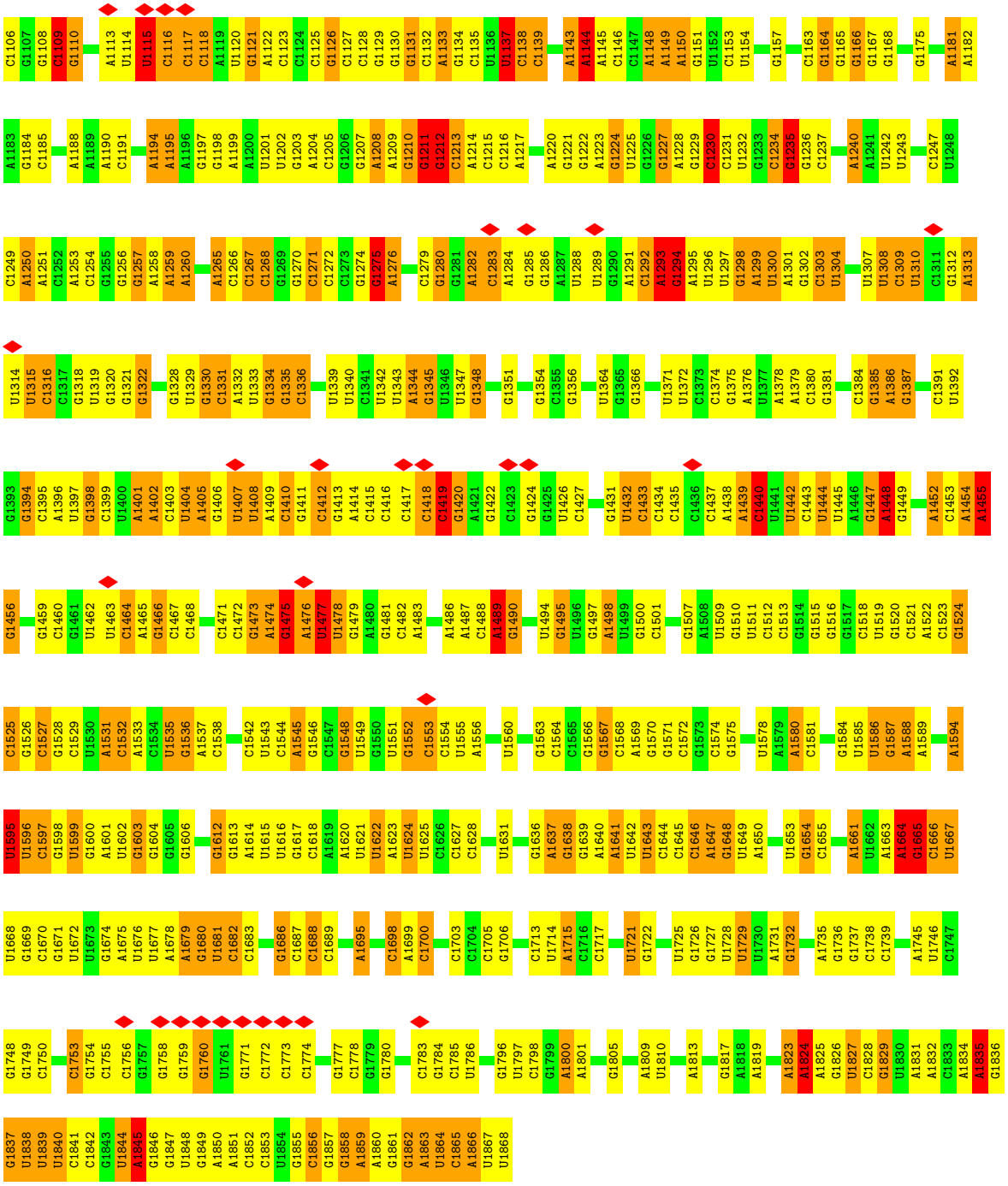
Chain 8:



• Molecule 51: 18S ribosomal RNA

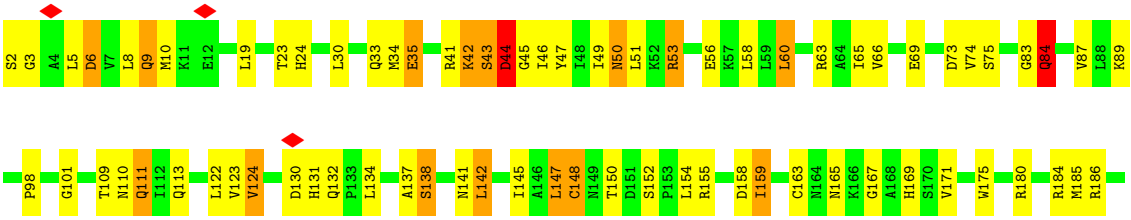
Chain 9:

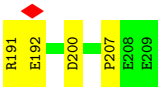




• Molecule 52: uS2

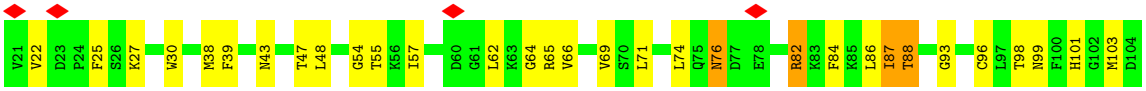
Chain AA:





• Molecule 53: eS1

Chain BB:

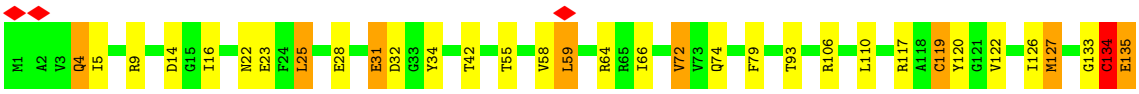


• Molecule 54: uS5

Chain CC:

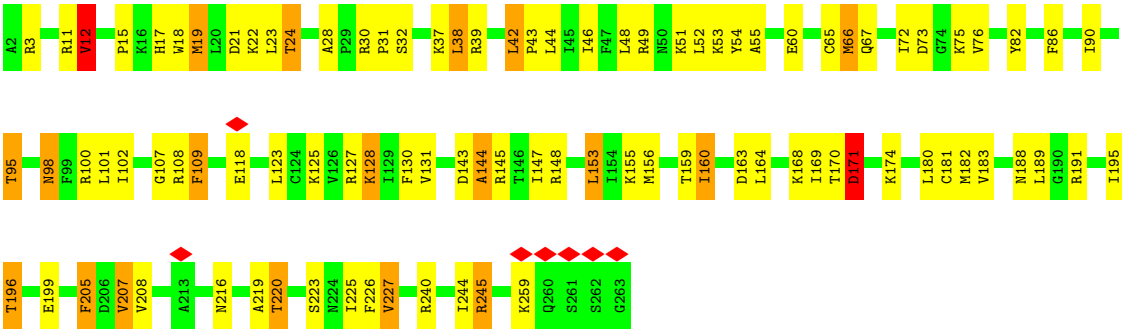
• Molecule 55: uS3

Chain DD:



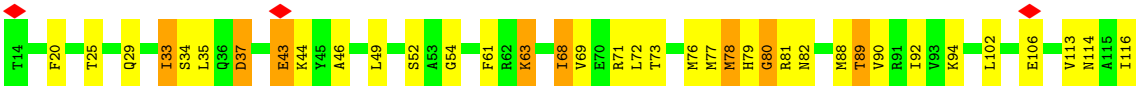
• Molecule 56: eS4

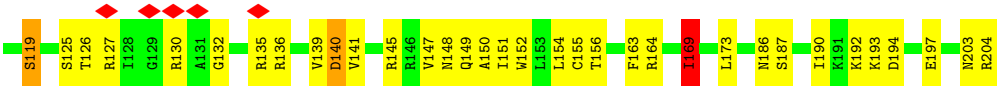
Chain EE:



• Molecule 57: uS7

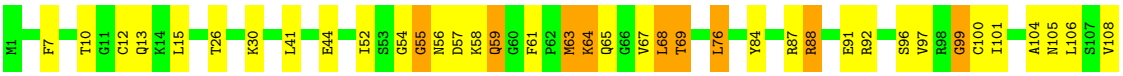
Chain FF:

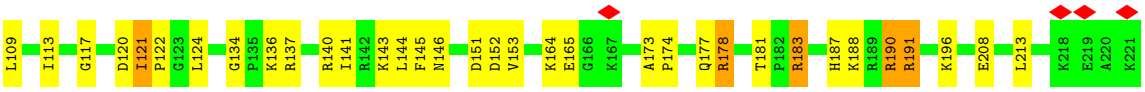


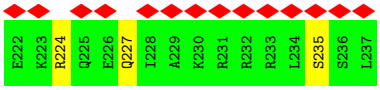


• Molecule 58: eS6

Chain GG:

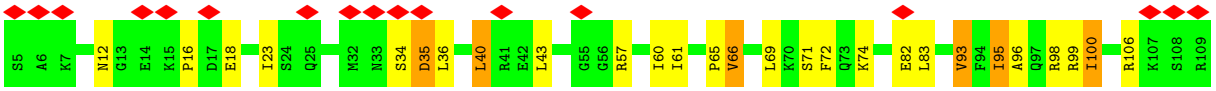


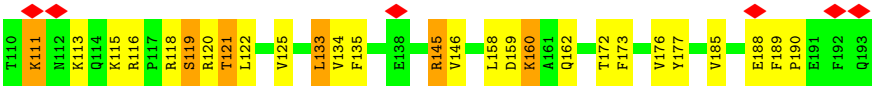




• Molecule 59: eS7

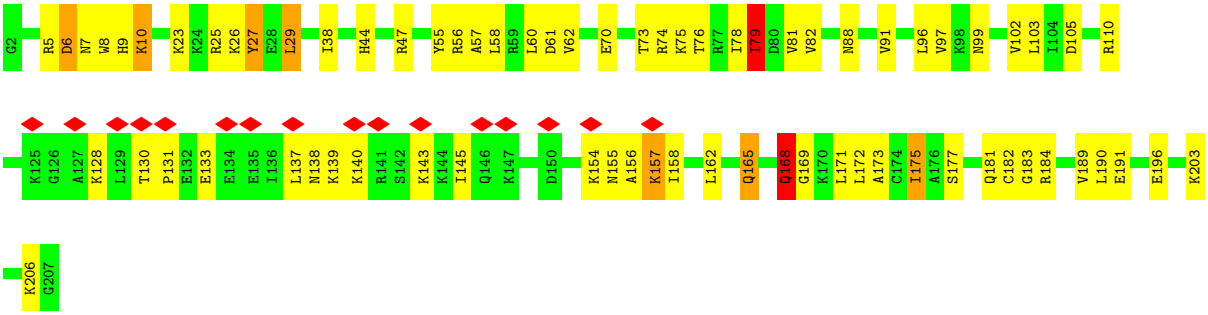
Chain HH:



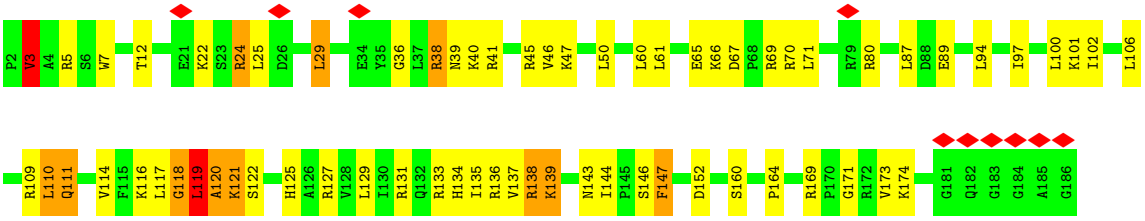


• Molecule 60: eS8

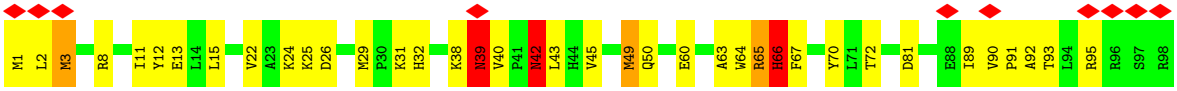
Chain II:



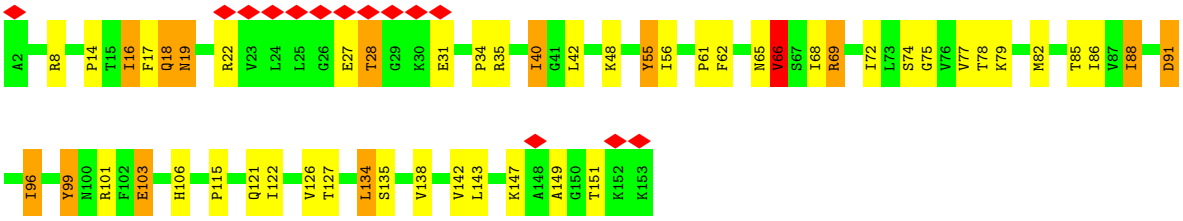
• Molecule 61: uS4



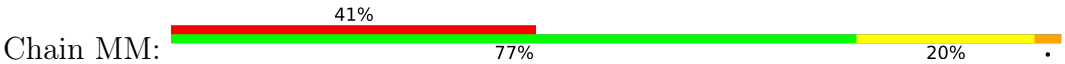
• Molecule 62: eS10

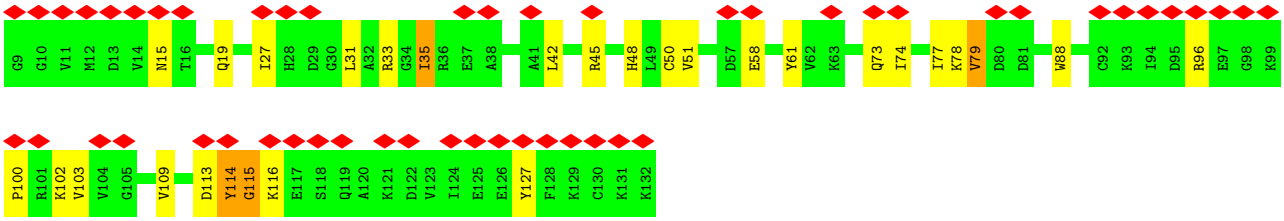


• Molecule 63: uS17



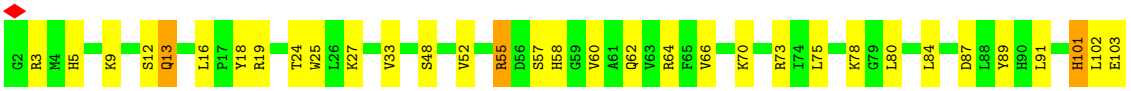
• Molecule 64: eS12





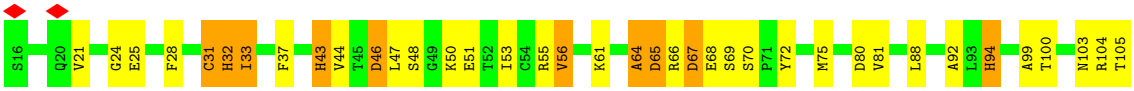
• Molecule 65: uS15

Chain NN:



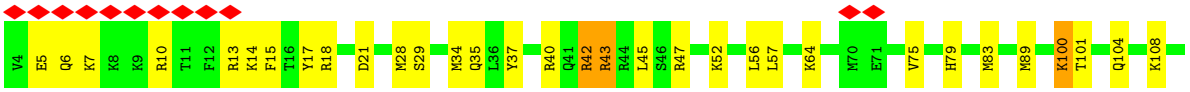
• Molecule 66: uS11

Chain OO:



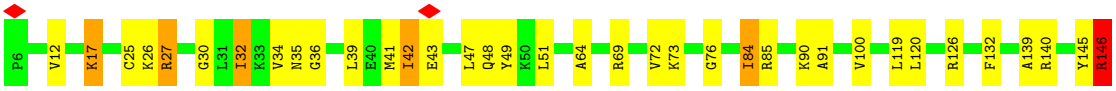
• Molecule 67: uS19

Chain PP:



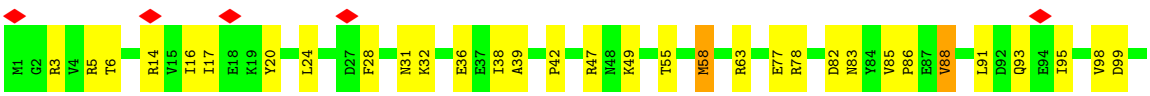
• Molecule 68: uS9

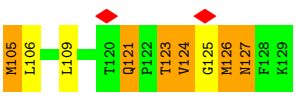
Chain QQ:



• Molecule 69: eS17

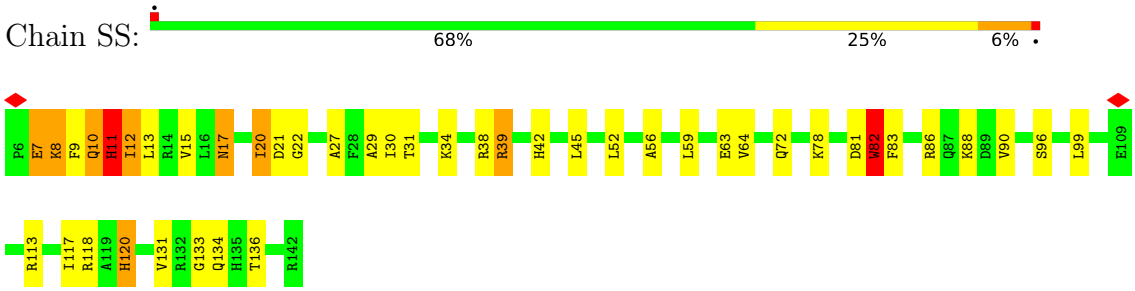
Chain RR:





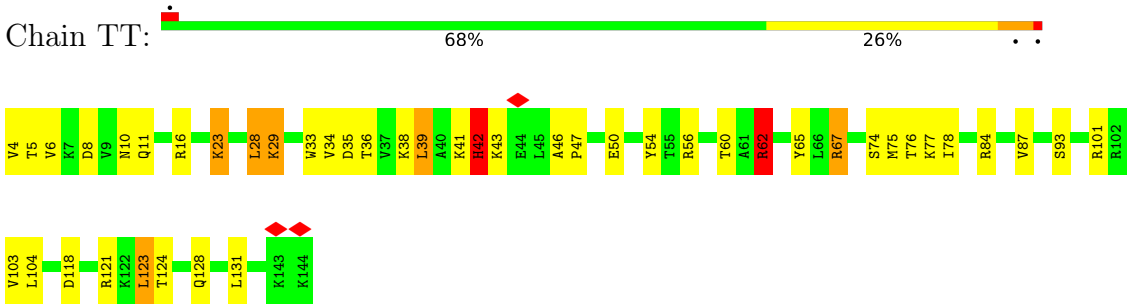
• Molecule 70: uS13

Chain SS:



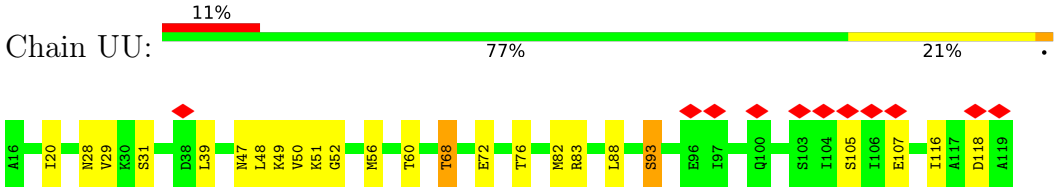
• Molecule 71: eS19

Chain TT:



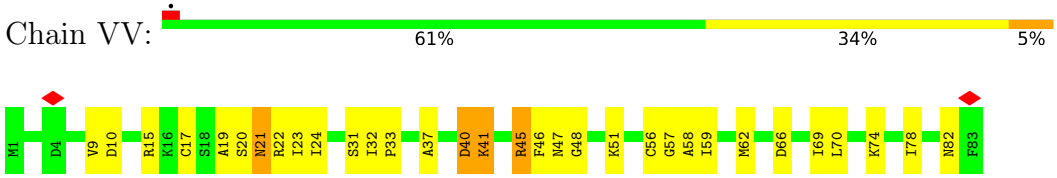
• Molecule 72: uS10

Chain UU:



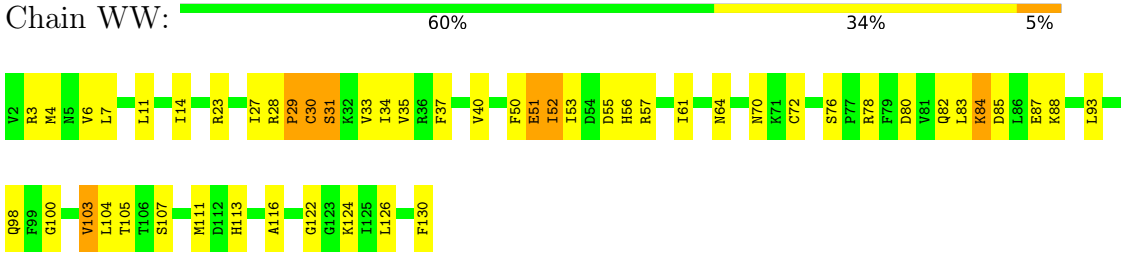
• Molecule 73: eS21

Chain VV:



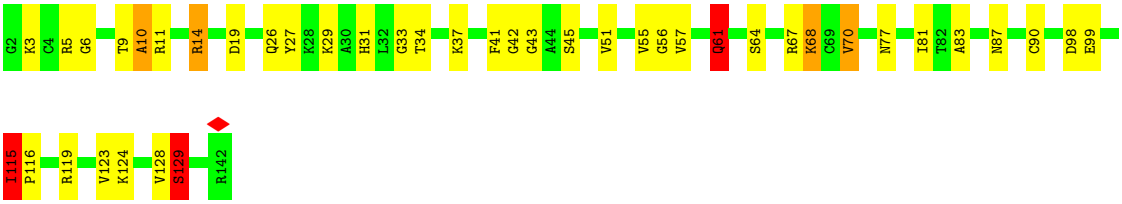
• Molecule 74: uS8

Chain WW:

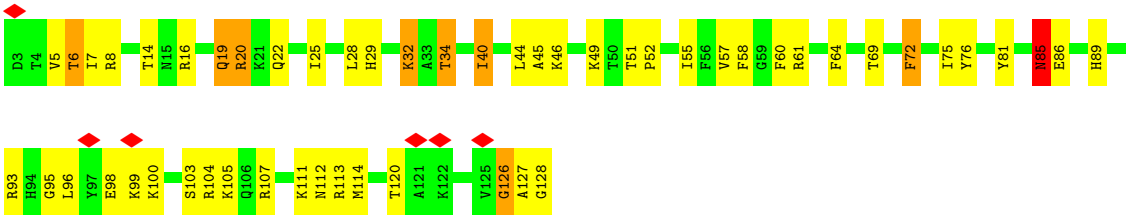


• Molecule 75: uS12

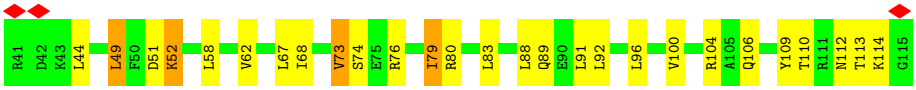
Chain XX:



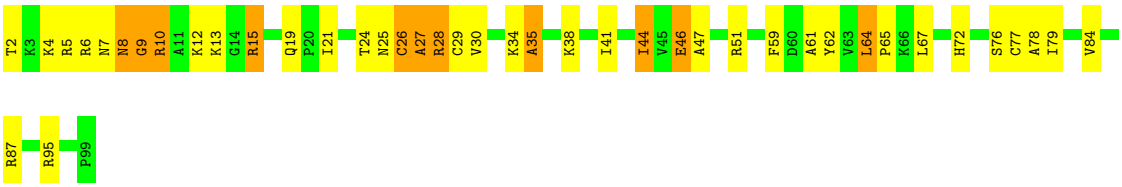
• Molecule 76: eS24



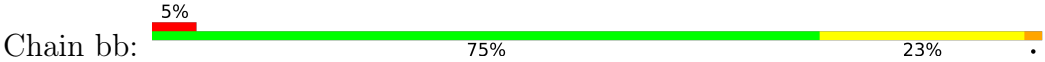
• Molecule 77: eS25

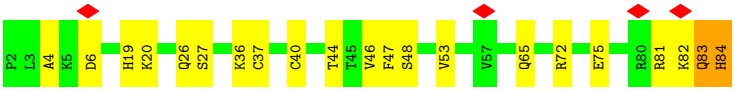


• Molecule 78: eS26

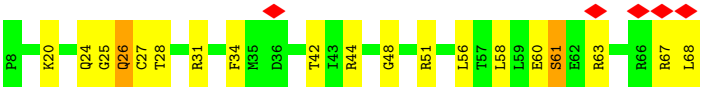


• Molecule 79: eS27



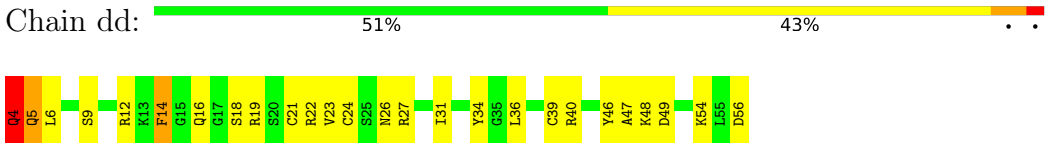


• Molecule 80: eS28



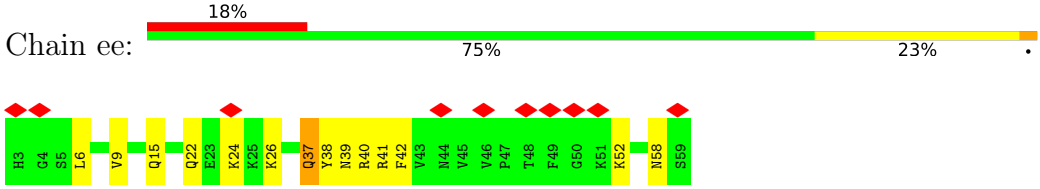
• Molecule 81: uS14

Chain dd:



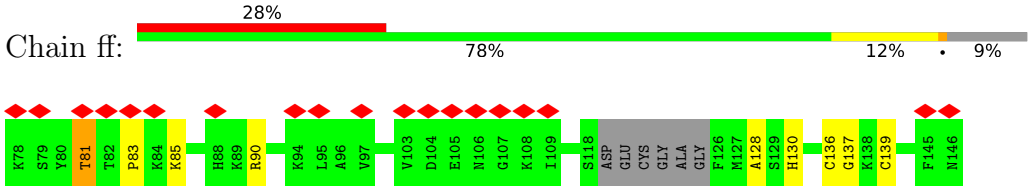
• Molecule 82: eS30

Chain ee:



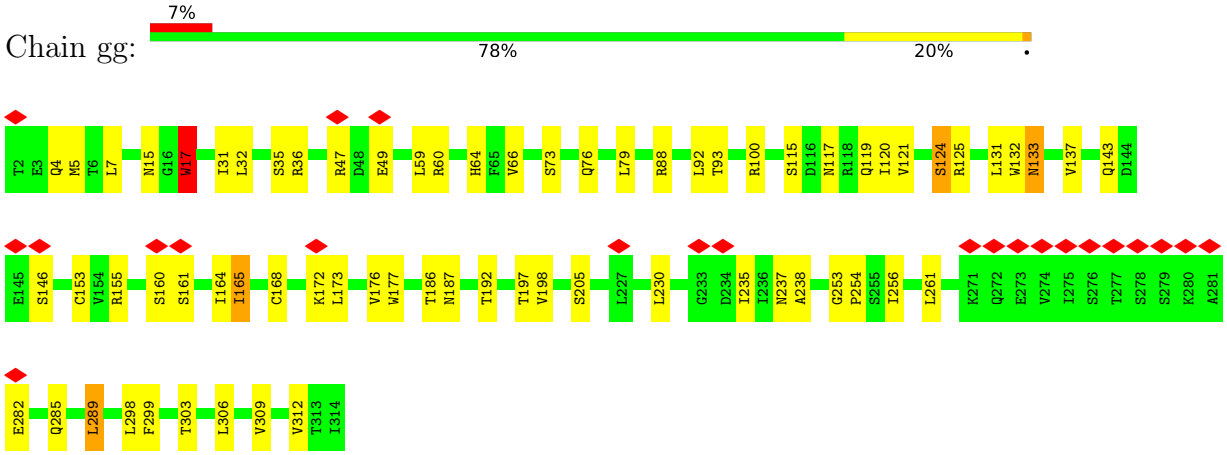
• Molecule 83: eS31

Chain ff:



• Molecule 84: RACK1

Chain gg:

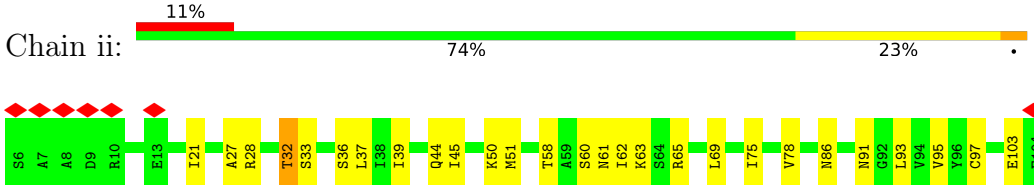


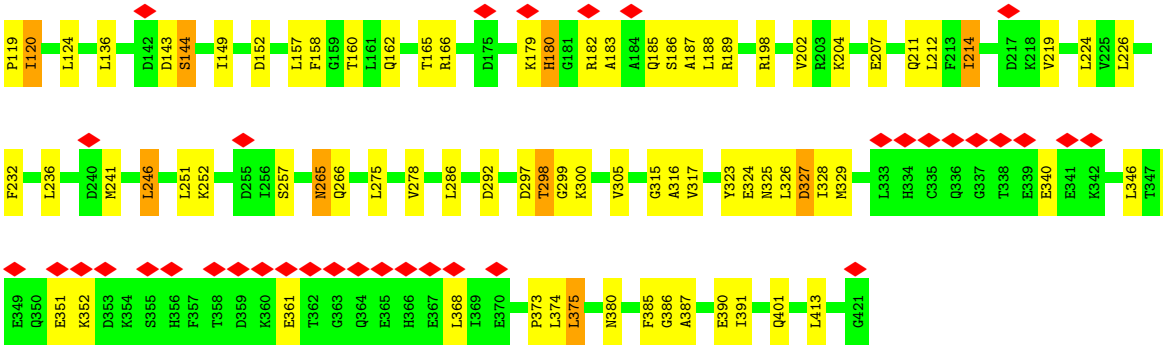
• Molecule 85: mRNA

Chain hh:

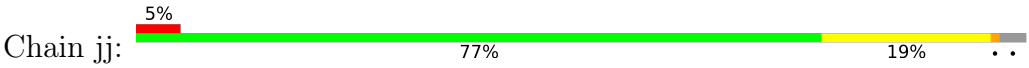
• Molecule 86: eRF1

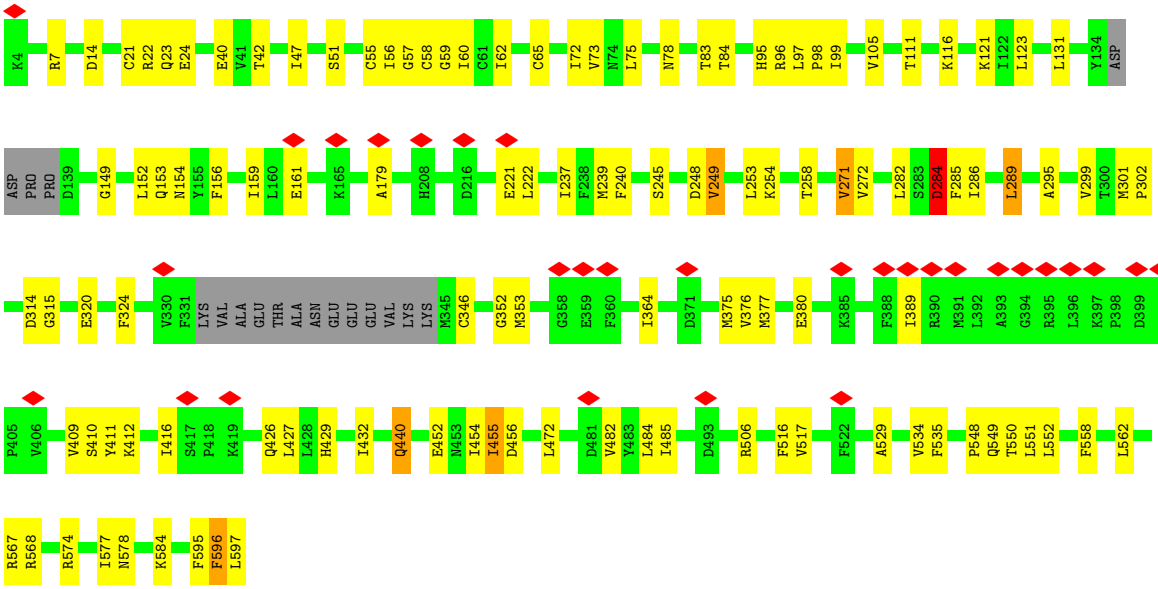
Chain ii:





• Molecule 87: ABCE1





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	22058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.719	Depositor
Minimum map value	-0.488	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3399999, 1.3399999, 1.3399999	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, SF4, MG, 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.93	2/1906 (0.1%)	1.05	4/2556 (0.2%)
2	B	0.82	5/3216 (0.2%)	1.05	11/4311 (0.3%)
3	C	0.87	5/2929 (0.2%)	1.07	11/3935 (0.3%)
4	D	0.65	1/2432 (0.0%)	0.95	0/3257
5	E	0.77	5/1936 (0.3%)	1.08	9/2600 (0.3%)
6	F	0.87	4/1905 (0.2%)	1.02	2/2539 (0.1%)
7	G	0.79	3/1967 (0.2%)	1.03	8/2647 (0.3%)
8	H	0.70	1/1535 (0.1%)	0.95	0/2063
9	I	0.73	2/1693 (0.1%)	0.99	4/2260 (0.2%)
10	J	0.62	1/1376 (0.1%)	0.90	1/1841 (0.1%)
11	L	0.82	2/1734 (0.1%)	1.00	4/2317 (0.2%)
12	M	0.75	1/1158 (0.1%)	0.98	2/1547 (0.1%)
13	N	0.92	1/1746 (0.1%)	1.14	4/2338 (0.2%)
14	O	0.87	2/1671 (0.1%)	1.11	8/2234 (0.4%)
15	P	0.91	3/1268 (0.2%)	1.06	4/1701 (0.2%)
16	Q	0.84	1/1530 (0.1%)	1.04	2/2041 (0.1%)
17	R	0.75	1/1524 (0.1%)	0.96	0/2013
18	S	0.85	1/1493 (0.1%)	1.02	4/2002 (0.2%)
19	T	0.71	0/1326	0.95	2/1770 (0.1%)
20	U	0.63	1/822 (0.1%)	0.86	0/1103
21	V	0.81	0/993	1.01	1/1332 (0.1%)
22	W	0.73	0/541	0.96	2/720 (0.3%)
23	X	0.74	0/993	0.96	1/1334 (0.1%)
24	Y	0.75	0/1132	1.02	5/1504 (0.3%)
25	Z	0.79	3/1130 (0.3%)	1.04	2/1507 (0.1%)
26	a	0.86	0/1191	1.07	2/1590 (0.1%)
27	b	0.75	1/619 (0.2%)	0.97	0/818
28	c	0.74	1/742 (0.1%)	1.03	1/996 (0.1%)
29	d	0.79	0/903	1.04	1/1216 (0.1%)
30	e	0.81	0/1071	1.05	2/1429 (0.1%)
31	f	0.94	3/895 (0.3%)	1.13	6/1198 (0.5%)
32	g	0.79	1/916 (0.1%)	0.97	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	h	0.70	1/1021 (0.1%)	1.01	0/1348
34	i	0.70	0/841	0.95	0/1112
35	j	1.02	3/720 (0.4%)	1.20	5/952 (0.5%)
36	k	0.69	1/575 (0.2%)	1.01	3/761 (0.4%)
37	l	0.85	0/454	1.00	1/599 (0.2%)
38	m	0.73	0/435	1.04	1/575 (0.2%)
39	n	0.77	0/223	0.96	0/284
40	o	0.78	1/864 (0.1%)	0.96	1/1140 (0.1%)
41	p	0.77	0/718	1.07	3/953 (0.3%)
42	r	0.90	3/1017 (0.3%)	1.13	2/1364 (0.1%)
43	s	0.60	1/1547 (0.1%)	0.81	3/2088 (0.1%)
44	t	0.65	1/1257 (0.1%)	0.99	5/1697 (0.3%)
45	1	0.86	0/129	1.18	2/173 (1.2%)
46	2	0.40	0/1805	0.84	5/2809 (0.2%)
47	3	0.44	0/1777	0.92	11/2763 (0.4%)
48	5	0.51	4/87790 (0.0%)	1.01	557/136937 (0.4%)
49	7	0.48	0/2858	0.87	4/4455 (0.1%)
50	8	0.50	0/3701	0.94	11/5766 (0.2%)
51	9	0.47	2/41013 (0.0%)	0.95	164/63919 (0.3%)
52	AA	0.71	3/1679 (0.2%)	0.99	2/2283 (0.1%)
53	BB	0.71	2/1756 (0.1%)	1.02	6/2350 (0.3%)
54	CC	0.70	1/1730 (0.1%)	1.02	4/2344 (0.2%)
55	DD	0.63	1/1792 (0.1%)	0.93	1/2412 (0.0%)
56	EE	0.66	0/2115	1.05	3/2843 (0.1%)
57	FF	0.71	2/1531 (0.1%)	1.01	5/2059 (0.2%)
58	GG	0.67	3/1946 (0.2%)	0.92	2/2590 (0.1%)
59	HH	0.63	1/1544 (0.1%)	0.94	1/2068 (0.0%)
60	II	0.72	0/1715	0.98	4/2287 (0.2%)
61	JJ	0.71	2/1550 (0.1%)	1.03	0/2069
62	KK	0.73	2/851 (0.2%)	1.02	3/1147 (0.3%)
63	LL	0.77	1/1259 (0.1%)	1.02	4/1684 (0.2%)
64	MM	0.69	2/968 (0.2%)	0.92	0/1296
65	NN	0.75	3/1232 (0.2%)	1.05	4/1656 (0.2%)
66	OO	0.83	3/1029 (0.3%)	1.15	7/1380 (0.5%)
67	PP	0.69	3/1079 (0.3%)	1.00	4/1437 (0.3%)
68	QQ	0.68	1/1142 (0.1%)	0.93	1/1528 (0.1%)
69	RR	0.66	1/1060 (0.1%)	0.93	0/1421
70	SS	0.65	1/1157 (0.1%)	0.97	2/1548 (0.1%)
71	TT	0.68	1/1120 (0.1%)	1.03	2/1499 (0.1%)
72	UU	0.66	1/831 (0.1%)	0.93	1/1115 (0.1%)
73	VV	0.71	1/645 (0.2%)	1.01	0/865
74	WW	0.82	3/1051 (0.3%)	1.04	4/1406 (0.3%)
75	XX	0.81	3/1116 (0.3%)	1.08	3/1490 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	YY	0.69	3/1040 (0.3%)	0.95	2/1382 (0.1%)
77	ZZ	0.67	1/604 (0.2%)	0.99	1/810 (0.1%)
78	aa	0.75	0/794	1.06	1/1065 (0.1%)
79	bb	0.57	0/665	0.86	1/891 (0.1%)
80	cc	0.74	1/478 (0.2%)	0.99	0/640
81	dd	0.77	1/455 (0.2%)	0.98	0/603
82	ee	0.75	1/462 (0.2%)	0.93	0/607
83	ff	0.53	0/531	0.70	0/703
84	gg	0.61	4/2493 (0.2%)	0.84	4/3394 (0.1%)
85	hh	0.48	0/287	0.94	1/445 (0.2%)
86	ii	0.62	5/3333 (0.2%)	0.94	6/4483 (0.1%)
87	jj	0.57	2/4633 (0.0%)	0.92	3/6249 (0.0%)
All	All	0.61	127/242711 (0.1%)	0.99	963/355683 (0.3%)

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	2
2	B	0	6
3	C	0	5
4	D	0	1
5	E	0	4
7	G	0	1
9	I	0	4
11	L	0	1
14	O	0	3
18	S	0	2
19	T	0	1
21	V	0	1
23	X	0	1
24	Y	0	1
26	a	0	2
31	f	0	1
33	h	0	1
36	k	0	1
38	m	0	1
42	r	0	1
51	9	0	3
52	AA	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	BB	0	3
55	DD	0	1
56	EE	0	2
57	FF	0	1
59	HH	0	1
61	JJ	0	1
63	LL	0	2
66	OO	0	2
68	QQ	0	1
70	SS	0	3
71	TT	0	1
72	UU	0	2
73	VV	0	1
74	WW	0	1
75	XX	0	1
76	YY	0	1
78	aa	0	2
86	ii	0	3
87	jj	0	2
All	All	0	76

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	957	G	O3'-P	7.88	1.73	1.61
48	5	3859	G	O3'-P	-6.46	1.51	1.61
48	5	1847	C	O3'-P	-6.28	1.51	1.61
7	G	29	ASN	C-N	6.22	1.39	1.33
35	j	48	ASN	CG-OD1	6.13	1.35	1.23
1	A	205	ASN	CG-OD1	5.85	1.34	1.23
3	C	38	ASN	CG-OD1	5.83	1.34	1.23
48	5	956	A	O3'-P	5.78	1.69	1.61
74	WW	64	ASN	CG-OD1	5.70	1.34	1.23
6	F	133	ASN	CG-OD1	5.69	1.34	1.23
61	JJ	143	ASN	CG-OD1	5.68	1.34	1.23
31	f	20	ASN	CG-OD1	5.64	1.34	1.23
54	CC	113	GLN	CD-OE1	5.63	1.34	1.23
75	XX	77	ASN	CG-OD1	5.63	1.34	1.23
57	FF	114	ASN	CG-OD1	5.62	1.34	1.23
18	S	162	GLN	CD-OE1	5.61	1.34	1.23
52	AA	132	GLN	CD-OE1	5.58	1.34	1.23
53	BB	76	ASN	CG-OD1	5.55	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	27	GLN	CD-OE1	5.53	1.34	1.23
76	YY	85	ASN	CG-OD1	5.51	1.34	1.23
58	GG	65	GLN	CD-OE1	5.51	1.34	1.23
65	NN	5	HIS	CD2-NE2	-5.51	1.31	1.37
67	PP	35	GLN	CD-OE1	5.50	1.33	1.23
15	P	56	GLN	CD-OE1	5.49	1.33	1.23
17	R	34	ASN	CG-OD1	5.48	1.33	1.23
3	C	142	HIS	ND1-CE1	5.47	1.38	1.32
3	C	48	ASN	CG-OD1	5.47	1.33	1.23
13	N	182	HIS	ND1-CE1	5.47	1.38	1.32
14	O	184	ASN	CG-OD1	5.46	1.33	1.23
57	FF	186	ASN	CG-OD1	5.44	1.33	1.23
66	OO	94	HIS	ND1-CE1	5.44	1.38	1.32
8	H	42	ASN	CG-OD1	5.43	1.33	1.23
86	ii	180	HIS	CD2-NE2	-5.43	1.31	1.37
64	MM	73	GLN	CD-OE1	5.43	1.33	1.23
12	M	20	HIS	ND1-CE1	5.42	1.38	1.32
2	B	301	ASN	CG-OD1	5.41	1.33	1.23
63	LL	18	GLN	CD-OE1	5.40	1.33	1.23
74	WW	70	ASN	CG-OD1	5.40	1.33	1.23
14	O	5	GLN	CD-OE1	5.40	1.33	1.23
76	YY	19	GLN	CD-OE1	5.39	1.33	1.23
16	Q	8	ASN	CG-OD1	5.39	1.33	1.23
82	ee	37	GLN	CD-OE1	5.39	1.33	1.23
7	G	94	GLN	CD-OE1	5.38	1.33	1.23
25	Z	97	ASN	CG-OD1	5.37	1.33	1.23
66	OO	113	GLN	CD-OE1	5.37	1.33	1.23
7	G	85	GLN	CD-OE1	5.36	1.33	1.23
65	NN	62	GLN	CD-OE1	5.36	1.33	1.23
58	GG	177	GLN	CD-OE1	5.36	1.33	1.23
76	YY	89	HIS	ND1-CE1	5.36	1.38	1.32
36	k	31	ASN	CG-OD1	5.36	1.33	1.23
52	AA	9	GLN	CD-OE1	5.36	1.33	1.23
66	OO	43	HIS	ND1-CE1	5.36	1.38	1.32
87	jj	23	GLN	CD-OE1	5.35	1.33	1.23
43	s	39	GLN	CD-OE1	5.35	1.33	1.23
5	E	187	GLN	CD-OE1	5.34	1.33	1.23
86	ii	180	HIS	ND1-CE1	5.34	1.37	1.32
62	KK	39	ASN	CG-OD1	5.33	1.33	1.23
6	F	112	GLN	CD-OE1	5.31	1.33	1.23
25	Z	76	ASN	CG-OD1	5.31	1.33	1.23
32	g	28	ASN	CG-OD1	5.30	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DD	4	GLN	CD-OE1	5.29	1.33	1.23
59	HH	12	ASN	CG-OD1	5.29	1.33	1.23
2	B	25	HIS	ND1-CE1	5.29	1.37	1.32
15	P	75	GLN	CD-OE1	5.29	1.33	1.23
64	MM	19	GLN	CD-OE1	5.29	1.33	1.23
58	GG	59	GLN	CD-OE1	5.29	1.33	1.23
44	t	100	HIS	ND1-CE1	5.28	1.37	1.32
81	dd	4	GLN	CD-OE1	5.28	1.33	1.23
40	o	19	GLN	CD-OE1	5.28	1.33	1.23
80	cc	26	GLN	CD-OE1	5.28	1.33	1.23
11	L	87	HIS	ND1-CE1	5.26	1.37	1.32
35	j	76	HIS	ND1-CE1	5.26	1.37	1.32
65	NN	58	HIS	ND1-CE1	5.26	1.37	1.32
69	RR	83	ASN	CG-OD1	5.26	1.33	1.23
10	J	23	ASN	CG-OD1	5.25	1.33	1.23
68	QQ	48	GLN	CD-OE1	5.24	1.33	1.23
15	P	133	HIS	ND1-CE1	5.24	1.37	1.32
86	ii	111	ASN	CG-OD1	5.23	1.33	1.23
67	PP	79	HIS	ND1-CE1	5.22	1.37	1.32
86	ii	266	GLN	CD-OE1	5.21	1.33	1.23
67	PP	128	HIS	ND1-CE1	5.20	1.37	1.32
52	AA	169	HIS	ND1-CE1	5.20	1.37	1.32
84	gg	237	ASN	CG-OD1	5.20	1.33	1.23
31	f	56	ASN	CG-OD1	5.19	1.33	1.23
9	I	123	GLN	CD-OE1	5.19	1.33	1.23
70	SS	120	HIS	CD2-NE2	-5.18	1.32	1.37
71	TT	11	GLN	CD-OE1	5.18	1.33	1.23
3	C	212	ASN	CG-OD1	5.17	1.33	1.23
72	UU	28	ASN	CG-OD1	5.17	1.33	1.23
33	h	96	ASN	CG-OD1	5.16	1.33	1.23
75	XX	31	HIS	ND1-CE1	5.16	1.37	1.32
11	L	19	GLN	CD-OE1	5.16	1.33	1.23
84	gg	133	ASN	CG-OD1	5.16	1.33	1.23
86	ii	380	ASN	CG-OD1	5.16	1.33	1.23
2	B	203	GLN	CD-OE1	5.15	1.33	1.23
9	I	59	GLN	CD-OE1	5.15	1.33	1.23
74	WW	113	HIS	ND1-CE1	5.14	1.37	1.32
6	F	82	ASN	CG-OD1	5.14	1.33	1.23
2	B	138	GLN	CD-OE1	5.13	1.33	1.23
42	r	41	ASN	CG-OD1	5.11	1.33	1.23
73	VV	47	ASN	CG-OD1	5.11	1.33	1.23
84	gg	187	ASN	CG-OD1	5.10	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	r	4	HIS	ND1-CE1	5.10	1.37	1.32
28	c	51	ASN	CG-ND2	-5.08	1.22	1.33
51	9	677	G	O3'-P	-5.08	1.53	1.61
35	j	16	HIS	CD2-NE2	-5.07	1.32	1.37
87	jj	440	GLN	CD-OE1	5.07	1.33	1.23
20	U	95	ASN	CG-OD1	5.07	1.33	1.23
5	E	163	GLN	CD-OE1	5.05	1.33	1.23
6	F	194	HIS	ND1-CE1	5.05	1.37	1.32
1	A	216	HIS	CD2-NE2	-5.04	1.32	1.37
84	gg	15	ASN	CG-OD1	5.04	1.33	1.23
51	9	1473	G	O3'-P	5.04	1.68	1.61
62	KK	66	HIS	ND1-CE1	5.04	1.37	1.32
31	f	16	ARG	CA-C	-5.03	1.46	1.52
2	B	328	ASN	CG-OD1	5.03	1.33	1.23
75	XX	61	GLN	CD-OE1	5.03	1.33	1.23
77	ZZ	106	GLN	CD-OE1	5.03	1.33	1.23
4	D	225	GLN	CD-OE1	5.02	1.33	1.23
25	Z	76	ASN	CG-ND2	-5.01	1.22	1.33
53	BB	148	ASN	CG-OD1	5.01	1.33	1.23
42	r	4	HIS	CD2-NE2	-5.01	1.32	1.37
5	E	280	HIS	ND1-CE1	5.01	1.37	1.32
3	C	94	ASN	CG-OD1	5.00	1.33	1.23
5	E	39	HIS	ND1-CE1	5.00	1.37	1.32
61	JJ	111	GLN	CD-OE1	5.00	1.33	1.23
5	E	39	HIS	CD2-NE2	-5.00	1.32	1.37

All (963) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	1965	G	P-O3'-C3'	15.99	144.18	120.20
48	5	4975	G	C2'-C3'-O3'	15.61	132.91	109.50
48	5	1358	G	C4'-C3'-O3'	14.12	134.18	113.00
48	5	2022	C	C4'-C3'-O3'	13.60	133.40	113.00
48	5	1847	C	C4'-C3'-O3'	-12.98	93.53	113.00
48	5	385	A	C4'-C3'-O3'	12.82	128.63	109.40
48	5	47	A	C4'-C3'-O3'	12.58	128.27	109.40
51	9	1835	A	C2'-C3'-O3'	12.52	128.28	109.50
48	5	1357	C	C4'-C3'-O3'	12.50	131.75	113.00
48	5	2046	G	C2'-C3'-O3'	12.02	127.53	109.50
48	5	4548	A	C2'-C3'-O3'	11.99	127.49	109.50
48	5	1357	C	C2'-C3'-O3'	-11.95	95.78	113.70
2	B	261	ARG	N-CA-C	-11.81	92.20	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	3888	G	C2'-C3'-O3'	11.55	131.03	113.70
48	5	276	C	C4'-C3'-O3'	-11.11	96.34	113.00
51	9	1844	U	C4'-C3'-O3'	-11.08	96.38	113.00
48	5	2858	A	C4'-C3'-O3'	11.04	129.56	113.00
51	9	1212	G	C2'-C3'-O3'	-10.95	97.28	113.70
48	5	1239	C	C2'-C3'-O3'	10.82	125.73	109.50
48	5	2067	C	C4'-C3'-O3'	-10.68	96.98	113.00
48	5	2695	A	C2'-C3'-O3'	10.64	125.45	109.50
48	5	3718	A	C4'-C3'-O3'	10.63	128.94	113.00
48	5	1961	G	C4'-C3'-O3'	10.60	128.89	113.00
51	9	1235	G	C4'-C3'-O3'	10.36	128.53	113.00
51	9	312	G	C2'-C3'-O3'	10.30	124.95	109.50
48	5	1477	C	C2'-C3'-O3'	10.29	129.14	113.70
48	5	3753	G	N9-C1'-C2'	-10.23	96.66	112.00
48	5	118	C	C4'-C3'-O3'	-10.18	97.74	113.00
14	O	110	PRO	N-CA-C	10.06	122.97	110.70
48	5	1282	G	C1'-C2'-O2'	10.06	123.49	108.40
51	9	1212	G	C4'-C3'-O3'	10.06	128.08	113.00
48	5	3697	U	C2'-C3'-O3'	10.00	128.70	113.70
48	5	1398	A	C2'-C3'-O3'	9.96	124.43	109.50
48	5	1365	C	C4'-C3'-O3'	9.92	124.28	109.40
51	9	1235	G	N9-C1'-C2'	-9.82	97.27	112.00
48	5	1292	C	C2'-C3'-O3'	9.72	128.28	113.70
48	5	5061	A	C2'-C3'-O3'	9.63	123.94	109.50
48	5	1280	C	C2'-C3'-O3'	9.61	123.92	109.50
48	5	3859	G	C4'-C3'-O3'	-9.58	98.63	113.00
51	9	1394	G	C2'-C3'-O3'	9.49	127.94	113.70
48	5	4951	G	C2'-C3'-O3'	9.45	123.67	109.50
48	5	1393	G	C4'-C3'-O3'	-9.42	98.87	113.00
47	3	70	G	N9-C1'-C2'	-9.37	97.94	112.00
51	9	1109	C	C1'-C2'-O2'	9.30	125.76	111.80
48	5	406	C	C2'-C3'-O3'	9.20	127.50	113.70
48	5	7	C	C4'-C3'-O3'	-9.17	99.24	113.00
48	5	1211	G	C2'-C3'-O3'	9.10	127.36	113.70
48	5	2769	U	C4'-C3'-O3'	8.97	122.86	109.40
51	9	72	C	C4'-C3'-O3'	8.97	122.86	109.40
51	9	870	A	C4'-C3'-O3'	8.96	122.85	109.40
48	5	3858	C	C4'-C3'-O3'	-8.95	99.57	113.00
48	5	4666	G	C4'-C3'-O3'	-8.91	99.64	113.00
48	5	2068	C	C4'-C3'-O3'	8.90	122.75	109.40
48	5	2398	U	C4'-C3'-O3'	8.89	122.74	109.40
48	5	2123	C	C2'-C3'-O3'	8.87	122.81	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	2021	G	C1'-C2'-O2'	-8.81	95.18	108.40
48	5	1455	G	C2'-C3'-O3'	8.81	126.91	113.70
48	5	2083	C	C4'-C3'-O3'	8.71	126.07	113.00
48	5	957	G	C2'-C3'-O3'	8.68	122.52	109.50
48	5	2116	C	C2'-C3'-O3'	8.65	122.48	109.50
51	9	1212	G	N9-C1'-C2'	-8.65	99.03	112.00
48	5	3619	G	C4'-C3'-O3'	-8.63	100.05	113.00
48	5	4084	G	C2'-C3'-O3'	8.62	122.42	109.50
48	5	3718	A	N9-C1'-C2'	-8.61	99.09	112.00
51	9	588	G	C2'-C3'-O3'	8.59	122.38	109.50
48	5	1969	G	C4'-C3'-O3'	8.57	125.86	113.00
51	9	1455	A	N9-C1'-C2'	-8.55	99.18	112.00
51	9	1535	U	C4'-C3'-O3'	-8.55	96.58	109.40
48	5	1693	U	C4'-C3'-O3'	-8.50	100.25	113.00
3	C	232	VAL	CB-CA-C	-8.45	100.98	112.04
48	5	4517	A	C4'-C3'-O3'	-8.44	100.34	113.00
48	5	1343	A	C4'-C3'-O3'	-8.39	100.41	113.00
48	5	4948	C	C2'-C3'-O3'	8.36	126.24	113.70
26	a	61	TYR	N-CA-C	8.36	120.39	111.28
51	9	1647	A	C2'-C3'-O3'	8.25	121.87	109.50
48	5	1292	C	C4'-C3'-O3'	-8.24	100.64	113.00
48	5	5024	C	C2'-C3'-O3'	8.19	121.78	109.50
48	5	1667	G	C4'-C3'-O3'	-8.16	100.76	113.00
48	5	4266	G	C2'-C3'-O3'	-8.15	101.47	113.70
48	5	1969	G	N9-C1'-C2'	-8.15	99.77	112.00
48	5	928	C	C2'-C3'-O3'	-8.12	101.51	113.70
50	8	94	G	C2'-C3'-O3'	8.10	121.66	109.50
51	9	112	U	C2'-C3'-O3'	-8.08	101.58	113.70
48	5	3625	G	C2'-C3'-O3'	8.01	125.72	113.70
48	5	2027	U	C4'-C3'-O3'	7.99	124.98	113.00
48	5	125	C	C2'-C3'-O3'	7.99	125.68	113.70
48	5	4325	A	C4'-C3'-O3'	-7.91	101.14	113.00
87	jj	14	ASP	N-CA-C	7.91	119.98	111.36
48	5	1974	U	C4'-C3'-O3'	7.84	121.16	109.40
51	9	110	U	C2'-C3'-O3'	7.83	125.44	113.70
51	9	111	A	C4'-C3'-O3'	-7.82	101.27	113.00
48	5	4335	C	C4'-C3'-O3'	-7.81	101.28	113.00
48	5	1893	C	C4'-C3'-O3'	-7.80	101.29	113.00
48	5	4730	C	C4'-C3'-O3'	7.80	121.10	109.40
48	5	2093	A	C2'-C3'-O3'	7.78	121.18	109.50
48	5	1410	U	C2'-C3'-O3'	7.78	121.17	109.50
51	9	327	G	C2'-C3'-O3'	7.78	121.16	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	917	A	C4'-C3'-O3'	7.76	121.04	109.40
51	9	909	G	C2'-C3'-O3'	-7.75	102.08	113.70
48	5	2256	C	C2'-C3'-O3'	7.74	121.11	109.50
51	9	909	G	N9-C1'-C2'	-7.74	100.40	112.00
48	5	1957	U	C3'-C2'-O2'	7.73	122.30	110.70
48	5	90	G	C4'-C3'-O3'	-7.69	101.46	113.00
48	5	3896	C	C2'-C3'-O3'	-7.65	102.23	113.70
51	9	1448	A	C2'-C3'-O3'	-7.64	102.23	113.70
48	5	5060	A	C2'-C3'-O3'	7.63	125.15	113.70
48	5	1380	G	C4'-C3'-O3'	7.62	124.42	113.00
48	5	1724	G	C4'-C3'-O3'	7.61	120.81	109.40
87	jj	121	LYS	CD-CE-NZ	-7.60	87.57	111.90
48	5	4975	G	C4'-C3'-O3'	-7.59	98.01	109.40
48	5	39	A	C1'-C2'-O2'	-7.59	100.42	111.80
31	f	83	MET	N-CA-C	-7.59	100.31	110.55
48	5	372	A	C4'-C3'-O3'	-7.58	101.64	113.00
48	5	1627	G	C2'-C3'-O3'	-7.56	102.36	113.70
51	9	1664	A	C4'-C3'-O3'	7.56	120.74	109.40
51	9	688	U	C2'-C3'-O3'	7.54	120.81	109.50
48	5	4375	C	C4'-C3'-O3'	-7.53	101.70	113.00
48	5	3670	C	C4'-C3'-O3'	7.53	124.29	113.00
48	5	90	G	C2'-C3'-O3'	7.51	124.96	113.70
47	3	39	U	C2'-C3'-O3'	-7.50	102.45	113.70
48	5	2506	G	C4'-C3'-O3'	7.48	120.62	109.40
86	ii	180	HIS	CB-CG-CD2	-7.48	121.47	131.20
51	9	1473	G	C4'-C3'-O3'	7.47	124.21	113.00
48	5	2632	U	N1-C1'-C2'	7.45	123.17	112.00
51	9	1419	C	C2'-C3'-O3'	7.43	124.84	113.70
16	Q	187	LYS	N-CA-C	7.42	120.49	108.76
51	9	980	A	C4'-C3'-O3'	-7.42	101.86	113.00
48	5	3800	A	C2'-C3'-O3'	-7.41	102.59	113.70
48	5	3659	G	C4'-C3'-O3'	-7.40	101.90	113.00
51	9	1109	C	C2'-C3'-O3'	7.39	120.58	109.50
48	5	4670	C	C2'-C3'-O3'	-7.39	102.62	113.70
51	9	183	G	C4'-C3'-O3'	7.39	120.48	109.40
48	5	1266	G	C2'-C3'-O3'	7.36	124.74	113.70
48	5	2321	G	C2'-C3'-O3'	-7.36	102.66	113.70
48	5	4076	G	C1'-C2'-O2'	-7.36	100.77	111.80
47	3	70	G	C4'-C3'-O3'	7.36	124.03	113.00
48	5	1755	C	C2'-C3'-O3'	7.33	120.49	109.50
48	5	2022	C	C2'-C3'-O3'	-7.32	102.72	113.70
48	5	47	A	C2'-C3'-O3'	-7.31	98.53	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	1961	G	N9-C1'-C2'	-7.28	101.08	112.00
48	5	215	C	C2'-C3'-O3'	7.27	124.60	113.70
48	5	275	C	C2'-C3'-O3'	7.26	124.59	113.70
48	5	5027	C	C2'-C3'-O3'	7.26	120.39	109.50
48	5	2027	U	N1-C1'-C2'	-7.25	101.13	112.00
70	SS	120	HIS	CB-CG-CD2	-7.24	121.79	131.20
48	5	3806	G	C4'-C3'-O3'	-7.23	102.16	113.00
9	I	204	GLY	CA-C-N	-7.23	112.53	119.76
9	I	204	GLY	C-N-CA	-7.23	112.53	119.76
51	9	322	C	N1-C1'-C2'	-7.22	101.17	112.00
48	5	2724	G	C4'-C3'-O3'	7.21	120.22	109.40
51	9	666	U	N1-C1'-C2'	7.18	122.77	112.00
48	5	654	C	C2'-C3'-O3'	-7.16	102.95	113.70
74	WW	113	HIS	CB-CG-CD2	-7.16	121.89	131.20
51	9	1824	A	C2'-C3'-O3'	7.16	124.44	113.70
2	B	258	HIS	N-CA-C	7.13	125.58	109.81
48	5	1236	C	C2'-C3'-O3'	7.13	124.39	113.70
48	5	4528	G	C2'-C3'-O3'	7.13	124.39	113.70
56	EE	147	ILE	N-CA-C	-7.13	102.28	110.05
48	5	4170	A	C2'-C3'-O3'	7.12	120.18	109.50
48	5	956	A	C4'-C3'-O3'	7.11	120.06	109.40
48	5	3671	G	C4'-C3'-O3'	-7.10	102.35	113.00
48	5	1268	G	C4'-C3'-O3'	7.08	120.02	109.40
51	9	604	A	C4'-C3'-O3'	-7.08	102.39	113.00
51	9	797	C	C4'-C3'-O3'	7.08	120.01	109.40
48	5	4543	G	C4'-C3'-O3'	-7.07	102.39	113.00
48	5	1563	A	C3'-C2'-O2'	7.06	121.29	110.70
48	5	1804	A	C4'-C3'-O3'	7.06	119.99	109.40
48	5	93	G	C2'-C3'-O3'	-7.06	103.11	113.70
48	5	3709	U	C4'-C3'-O3'	7.05	119.97	109.40
11	L	9	ILE	N-CA-C	-7.05	99.48	109.63
76	YY	89	HIS	CB-CG-CD2	-7.05	122.04	131.20
48	5	1506	G	C2'-C3'-O3'	-7.03	103.16	113.70
48	5	4585	U	C4'-C3'-O3'	-7.02	102.47	113.00
48	5	2028	C	C2'-C3'-O3'	-7.01	103.18	113.70
51	9	1535	U	C2'-C3'-O3'	7.00	120.00	109.50
51	9	454	U	C4'-C3'-O3'	-7.00	102.50	113.00
48	5	1957	U	C1'-C2'-O2'	-7.00	97.91	108.40
48	5	1927	U	C4'-C3'-O3'	-6.98	102.53	113.00
48	5	1814	C	C4'-C3'-O3'	-6.98	102.54	113.00
5	E	39	HIS	CB-CG-CD2	-6.97	122.13	131.20
13	N	182	HIS	CB-CG-CD2	-6.97	122.14	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	3718	A	C2'-C3'-O3'	-6.96	103.27	113.70
44	t	100	HIS	CB-CG-CD2	-6.95	122.17	131.20
51	9	605	A	C4'-C3'-O3'	-6.94	102.59	113.00
48	5	325	U	C4'-C3'-O3'	-6.93	102.61	113.00
48	5	1380	G	C1'-C2'-O2'	-6.90	98.05	108.40
48	5	4974	C	C4'-C3'-O3'	-6.89	102.67	113.00
48	5	2858	A	C1'-C2'-O2'	-6.88	98.07	108.40
75	XX	31	HIS	CB-CG-CD2	-6.86	122.28	131.20
51	9	1489	A	C4'-C3'-O3'	6.85	123.28	113.00
55	DD	134	CYS	N-CA-C	6.85	119.27	108.79
48	5	1279	A	C2'-C3'-O3'	6.85	119.78	109.50
48	5	1672	U	N1-C1'-C2'	6.85	122.27	112.00
1	A	216	HIS	CB-CG-CD2	-6.83	122.32	131.20
48	5	1696	C	C2'-C3'-O3'	6.81	119.72	109.50
12	M	20	HIS	CB-CG-CD2	-6.81	122.35	131.20
51	9	1022	U	C4'-C3'-O3'	-6.81	102.79	113.00
47	3	29	A	C2'-C3'-O3'	-6.80	103.49	113.70
24	Y	58	VAL	CB-CA-C	-6.79	104.78	111.30
45	1	63	SER	CA-C-N	6.79	128.32	119.84
45	1	63	SER	C-N-CA	6.79	128.32	119.84
63	LL	99	TYR	N-CA-C	-6.79	97.67	108.73
48	5	3901	A	C4'-C3'-O3'	-6.77	102.85	113.00
48	5	4378	A	C2'-C3'-O3'	6.76	119.64	109.50
48	5	2107	C	C2'-C3'-O3'	6.76	119.63	109.50
48	5	4885	U	C2'-C3'-O3'	6.76	123.84	113.70
48	5	1485	C	C2'-C3'-O3'	6.75	119.63	109.50
48	5	3888	G	C4'-C3'-O3'	-6.74	102.89	113.00
48	5	3753	G	C4'-C3'-O3'	6.74	123.11	113.00
67	PP	128	HIS	CB-CG-CD2	-6.74	122.44	131.20
51	9	1115	U	C4'-C3'-O3'	6.74	119.51	109.40
36	k	61	PRO	N-CA-C	6.74	118.92	110.70
25	Z	54	THR	N-CA-C	6.73	122.92	113.56
50	8	45	C	C4'-C3'-O3'	-6.73	102.90	113.00
48	5	2474	G	C2'-C3'-O3'	6.72	123.79	113.70
48	5	333	U	C2'-C3'-O3'	-6.72	103.62	113.70
51	9	860	G	C2'-C3'-O3'	-6.72	103.61	113.70
11	L	87	HIS	CB-CG-CD2	-6.72	122.47	131.20
48	5	2404	A	C1'-C2'-O2'	6.72	118.48	108.40
48	5	4211	C	C4'-C3'-O3'	-6.70	102.95	113.00
51	9	872	A	C2'-C3'-O3'	6.70	119.55	109.50
77	ZZ	49	LEU	N-CA-C	6.70	119.25	109.07
13	N	181	HIS	CB-CG-CD2	-6.69	122.50	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	77	PRO	CA-C-N	6.68	127.22	119.47
7	G	77	PRO	C-N-CA	6.68	127.22	119.47
48	5	4553	A	C4'-C3'-O3'	-6.68	102.98	113.00
65	NN	58	HIS	CB-CG-CD2	-6.68	122.51	131.20
51	9	933	G	C2'-C3'-O3'	-6.68	103.69	113.70
24	Y	87	ARG	NE-CZ-NH2	6.67	125.21	119.20
7	G	57	TRP	CA-C-N	6.67	128.18	119.84
7	G	57	TRP	C-N-CA	6.67	128.18	119.84
35	j	16	HIS	CB-CG-CD2	-6.67	122.53	131.20
14	O	109	PRO	CA-C-N	6.66	127.24	120.38
14	O	109	PRO	C-N-CA	6.66	127.24	120.38
51	9	1026	C	C4'-C3'-O3'	-6.66	103.00	113.00
71	TT	42	HIS	CB-CA-C	-6.66	99.78	110.84
48	5	4115	G	C4'-C3'-O3'	6.66	119.38	109.40
60	II	44	HIS	CB-CG-CD2	-6.66	122.55	131.20
48	5	4699	U	C4'-C3'-O3'	6.65	119.38	109.40
66	OO	43	HIS	CB-CG-CD2	-6.64	122.56	131.20
72	UU	93	SER	N-CA-C	6.64	114.19	108.22
50	8	124	U	C4'-C3'-O3'	6.63	119.35	109.40
21	V	13	LYS	N-CA-C	6.63	118.58	111.36
44	t	140	GLY	N-CA-C	6.62	122.08	113.27
42	r	4	HIS	CB-CG-CD2	-6.60	122.62	131.20
48	5	1232	G	C2'-C3'-O3'	6.60	119.40	109.50
48	5	4577	U	C1'-C2'-O2'	6.60	118.30	108.40
48	5	286	U	N1-C1'-C2'	6.60	121.90	112.00
48	5	1648	C	C4'-C3'-O3'	-6.60	103.10	113.00
48	5	3903	A	C4'-C3'-O3'	-6.60	103.11	113.00
48	5	5059	C	C2'-C3'-O3'	6.59	123.59	113.70
15	P	133	HIS	CB-CG-CD2	-6.59	122.63	131.20
48	5	1728	U	C4'-C3'-O3'	-6.59	103.11	113.00
48	5	4888	U	C2'-C3'-O3'	6.59	119.38	109.50
48	5	1908	A	C4'-C3'-O3'	-6.59	103.12	113.00
48	5	1848	C	C4'-C3'-O3'	-6.58	103.13	113.00
48	5	3894	A	C2'-C3'-O3'	-6.58	103.84	113.70
51	9	913	A	C4'-C3'-O3'	-6.57	99.54	109.40
65	NN	5	HIS	CB-CG-CD2	-6.57	122.66	131.20
54	CC	113	GLN	N-CA-C	6.56	119.15	108.26
48	5	2714	G	C4'-C3'-O3'	-6.56	103.17	113.00
2	B	25	HIS	CB-CG-CD2	-6.55	122.68	131.20
48	5	965	G	C2'-C3'-O3'	6.55	119.33	109.50
48	5	1657	G	C2'-C3'-O3'	-6.55	103.87	113.70
50	8	150	C	C2'-C3'-O3'	-6.55	103.87	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	4489	G	C4'-C3'-O3'	-6.55	103.17	113.00
48	5	1838	A	C4'-C3'-O3'	-6.55	103.18	113.00
5	E	217	GLN	N-CA-C	6.54	118.45	110.41
46	2	35	A	C4'-C3'-O3'	-6.54	103.20	113.00
6	F	194	HIS	CB-CG-CD2	-6.53	122.71	131.20
48	5	2554	U	C4'-C3'-O3'	6.53	122.79	113.00
51	9	1293	A	C2'-C3'-O3'	-6.53	103.91	113.70
48	5	1	C	C4'-C3'-O3'	6.52	119.18	109.40
5	E	280	HIS	CB-CG-CD2	-6.52	122.72	131.20
51	9	1235	G	C2'-C3'-O3'	-6.52	103.92	113.70
48	5	1633	G	C4'-C3'-O3'	6.52	122.78	113.00
48	5	962	C	C2'-C3'-O3'	6.51	119.27	109.50
63	LL	106	HIS	CB-CG-CD2	-6.48	122.78	131.20
15	P	125	MET	N-CA-C	-6.47	102.18	110.53
48	5	4301	U	C4'-C3'-O3'	-6.47	103.29	113.00
48	5	1818	G	C2'-C3'-O3'	6.47	123.40	113.70
51	9	292	A	O4'-C4'-C3'	-6.46	99.64	106.10
48	5	4375	C	C2'-C3'-O3'	-6.46	104.01	113.70
51	9	677	G	C4'-C3'-O3'	-6.46	103.31	113.00
48	5	2663	G	C4'-C3'-O3'	-6.46	103.31	113.00
48	5	4394	A	C4'-C3'-O3'	6.46	119.09	109.40
48	5	3899	G	C4'-C3'-O3'	-6.46	103.32	113.00
51	9	1858	G	C3'-C2'-O2'	6.46	120.39	110.70
5	E	72	PRO	N-CA-CB	6.45	110.09	103.00
48	5	2028	C	N1-C1'-C2'	-6.44	102.34	112.00
48	5	1633	G	C3'-C2'-O2'	6.44	120.36	110.70
48	5	385	A	C2'-C3'-O3'	-6.44	99.85	109.50
48	5	1921	C	C2'-C3'-O3'	6.43	119.14	109.50
51	9	465	A	C4'-C3'-O3'	6.43	119.04	109.40
46	2	34	A	C4'-C3'-O3'	6.40	119.01	109.40
50	8	93	C	C4'-C3'-O3'	-6.40	103.41	113.00
48	5	4467	A	C1'-C2'-O2'	6.39	117.98	108.40
5	E	90	LYS	CA-C-N	6.38	127.82	119.84
5	E	90	LYS	C-N-CA	6.38	127.82	119.84
3	C	340	ILE	CB-CA-C	-6.38	105.38	111.44
51	9	1637	A	C2'-C3'-O3'	6.37	119.05	109.50
3	C	142	HIS	CB-CG-CD2	-6.37	122.92	131.20
48	5	4701	A	C1'-C2'-O2'	6.37	117.95	108.40
48	5	4965	U	C4'-C3'-O3'	-6.37	103.45	113.00
48	5	1800	U	C4'-C3'-O3'	-6.36	103.46	113.00
66	OO	94	HIS	CB-CG-CD2	-6.36	122.93	131.20
47	3	38	A	C4'-C3'-O3'	6.36	122.54	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	2743	A	C4'-C3'-O3'	-6.35	103.47	113.00
48	5	2678	A	C4'-C3'-O3'	-6.35	103.47	113.00
86	ii	180	HIS	CB-CG-ND1	6.35	132.22	122.70
48	5	4616	A	C4'-C3'-O3'	-6.34	103.49	113.00
3	C	340	ILE	N-CA-C	-6.33	106.11	111.56
7	G	45	ILE	N-CA-C	6.33	122.50	109.34
48	5	2699	C	C4'-C3'-O3'	-6.33	103.51	113.00
48	5	4900	C	C2'-C3'-O3'	6.32	118.98	109.50
51	9	1477	U	C2'-C3'-O3'	6.32	118.98	109.50
51	9	1047	C	C1'-C2'-O2'	6.32	117.88	108.40
48	5	1527	A	C4'-C3'-O3'	-6.31	103.53	113.00
62	KK	66	HIS	CB-CG-CD2	-6.31	123.00	131.20
48	5	2027	U	C2'-C3'-O3'	-6.31	104.24	113.70
48	5	4487	A	C4'-C3'-O3'	-6.30	103.55	113.00
48	5	1741	G	C4'-C3'-O3'	6.30	118.84	109.40
48	5	2742	G	C4'-C3'-O3'	-6.29	103.56	113.00
48	5	84	A	C2'-C3'-O3'	-6.29	100.06	109.50
48	5	1692	C	C4'-C3'-O3'	-6.28	103.58	113.00
48	5	1629	G	C2'-C3'-O3'	-6.27	104.30	113.70
41	p	17	ARG	N-CA-C	6.26	118.38	110.24
48	5	3913	G	C4'-C3'-O3'	6.26	118.79	109.40
51	9	640	A	C4'-C3'-O3'	-6.26	103.61	113.00
48	5	1740	C	C3'-C2'-O2'	6.25	120.08	110.70
85	hh	42	C	C2'-C3'-O3'	6.25	118.88	109.50
48	5	4345	C	C4'-C3'-O3'	-6.25	103.63	113.00
48	5	1697	G	C4'-C3'-O3'	6.24	118.76	109.40
48	5	2615	C	C4'-C3'-O3'	-6.23	103.66	113.00
48	5	2733	C	C4'-C3'-O3'	-6.23	103.66	113.00
48	5	4638	U	C4'-C3'-O3'	-6.23	103.66	113.00
48	5	977	C	C4'-C3'-O3'	-6.22	103.66	113.00
48	5	746	A	C4'-C3'-O3'	6.22	118.73	109.40
48	5	3726	A	C2'-C3'-O3'	-6.22	104.37	113.70
58	GG	187	HIS	CB-CG-CD2	-6.22	123.11	131.20
48	5	4217	G	C1'-C2'-O2'	6.21	117.72	108.40
48	5	2423	A	C4'-C3'-O3'	-6.20	103.69	113.00
70	SS	120	HIS	CB-CG-ND1	6.20	132.01	122.70
37	l	6	THR	N-CA-C	-6.20	100.81	110.42
76	YY	89	HIS	CB-CG-ND1	6.20	132.00	122.70
51	9	833	C	C4'-C3'-O3'	6.19	122.29	113.00
41	p	11	VAL	N-CA-C	6.19	117.42	111.91
16	Q	176	ARG	N-CA-C	6.19	120.07	111.90
48	5	2065	G	C4'-C3'-O3'	-6.18	103.73	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	3749	C	C2'-C3'-O3'	-6.17	104.44	113.70
48	5	977	C	C2'-C3'-O3'	6.16	122.94	113.70
48	5	4144	C	C4'-C3'-O3'	6.15	118.63	109.40
48	5	497	G	C2'-C3'-O3'	-6.15	104.48	113.70
48	5	1990	A	C2'-C3'-O3'	6.14	122.92	113.70
67	PP	79	HIS	CB-CG-CD2	-6.14	123.21	131.20
48	5	1891	A	C2'-C3'-O3'	6.14	118.71	109.50
44	t	100	HIS	CB-CG-ND1	6.14	131.90	122.70
48	5	231	U	C4'-C3'-O3'	-6.13	103.80	113.00
48	5	2452	G	C4'-C3'-O3'	-6.13	103.80	113.00
48	5	2067	C	C2'-C3'-O3'	6.13	122.89	113.70
22	W	14	TYR	CA-C-N	6.13	127.50	119.84
22	W	14	TYR	C-N-CA	6.13	127.50	119.84
54	CC	184	VAL	CB-CA-C	-6.13	103.37	111.70
52	AA	169	HIS	CB-CG-CD2	-6.12	123.24	131.20
51	9	1448	A	N9-C1'-C2'	-6.12	102.82	112.00
48	5	1912	G	C4'-C3'-O3'	-6.11	103.83	113.00
51	9	1220	A	C4'-C3'-O3'	-6.11	103.83	113.00
48	5	3738	G	C4'-C3'-O3'	-6.11	103.84	113.00
48	5	67	C	C1'-C2'-O2'	6.10	117.55	108.40
74	WW	113	HIS	CB-CG-ND1	6.10	131.85	122.70
48	5	1799	G	C4'-C3'-O3'	-6.10	103.85	113.00
51	9	61	A	C4'-C3'-O3'	-6.08	103.88	113.00
5	E	39	HIS	CB-CG-ND1	6.08	131.82	122.70
48	5	4324	A	C4'-C3'-O3'	-6.08	103.88	113.00
18	S	79	GLY	N-CA-C	-6.08	104.43	112.82
50	8	21	C	C4'-C3'-O3'	-6.08	103.88	113.00
48	5	2858	A	N9-C1'-C2'	-6.08	102.89	112.00
48	5	2396	A	C2'-C3'-O3'	-6.07	100.39	109.50
50	8	56	G	C1'-C2'-O2'	6.07	117.51	108.40
48	5	1630	A	C4'-C3'-O3'	-6.07	103.90	113.00
48	5	2441	C	C2'-C3'-O3'	-6.07	104.60	113.70
51	9	1385	G	C4'-C3'-O3'	6.06	122.09	113.00
51	9	431	G	C4'-C3'-O3'	-6.05	103.92	113.00
51	9	1049	A	C2'-C3'-O3'	-6.05	104.62	113.70
51	9	1144	A	N9-C1'-C2'	6.05	121.07	112.00
53	BB	150	ILE	N-CA-CB	-6.04	105.14	112.33
48	5	1238	A	C2'-C3'-O3'	6.04	122.76	113.70
48	5	1238	A	C3'-C2'-O2'	6.04	119.76	110.70
3	C	98	GLY	N-CA-C	-6.04	98.86	113.18
48	5	366	A	C1'-C2'-O2'	6.04	117.46	108.40
49	7	29	C	C4'-C3'-O3'	-6.04	103.94	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	4341	C	C1'-C2'-O2'	6.04	117.45	108.40
48	5	2791	C	C4'-C3'-O3'	-6.03	103.95	113.00
48	5	4485	C	C4'-C3'-O3'	-6.03	103.95	113.00
51	9	110	U	C3'-C2'-O2'	6.03	119.75	110.70
51	9	465	A	C2'-C3'-O3'	6.03	118.54	109.50
48	5	1636	U	C4'-C3'-O3'	-6.02	103.97	113.00
48	5	2298	U	C1'-C2'-O2'	6.02	117.43	108.40
48	5	1383	G	C4'-C3'-O3'	-6.02	103.97	113.00
48	5	3627	G	C1'-C2'-O2'	6.02	117.43	108.40
48	5	964	A	O4'-C1'-C2'	-6.01	101.59	107.60
48	5	2021	G	C4'-C3'-O3'	6.00	122.00	113.00
48	5	1903	G	C1'-C2'-O2'	6.00	117.39	108.40
48	5	1329	G	C2'-C3'-O3'	6.00	122.69	113.70
46	2	1	G	C5'-C4'-C3'	5.99	124.99	116.00
2	B	17	LEU	N-CA-C	5.99	123.04	109.81
48	5	5041	G	C2'-C3'-O3'	-5.99	104.72	113.70
51	9	1418	C	C4'-C3'-O3'	5.98	118.38	109.40
51	9	452	G	C4'-C3'-O3'	-5.98	104.03	113.00
48	5	2359	U	C2'-C3'-O3'	-5.98	104.73	113.70
48	5	3869	C	C3'-C2'-O2'	5.98	119.67	110.70
2	B	37	PRO	CA-N-CD	-5.98	103.63	112.00
48	5	2586	G	N9-C1'-C2'	5.98	122.96	114.00
48	5	1353	G	C4'-C3'-O3'	-5.97	104.04	113.00
48	5	3797	C	C4'-C3'-O3'	-5.97	104.05	113.00
48	5	3918	G	C1'-C2'-O2'	5.96	117.35	108.40
48	5	3790	U	C4'-C3'-O3'	5.96	118.34	109.40
48	5	3911	C	C4'-C3'-O3'	-5.96	104.06	113.00
48	5	4966	A	N9-C1'-C2'	5.96	120.94	112.00
13	N	182	HIS	CB-CG-ND1	5.96	131.63	122.70
67	PP	128	HIS	CB-CG-ND1	5.95	131.63	122.70
48	5	1326	A	C2'-C3'-O3'	-5.95	104.78	113.70
51	9	1646	C	C3'-C2'-O2'	5.94	119.61	110.70
48	5	71	C	C4'-C3'-O3'	-5.94	104.09	113.00
51	9	908	A	N9-C1'-C2'	-5.93	103.10	112.00
47	3	38	A	N9-C1'-C2'	-5.93	103.10	112.00
48	5	195	C	C4'-C3'-O3'	-5.93	104.10	113.00
60	II	79	ILE	CB-CA-C	5.93	119.69	111.92
48	5	7	C	C2'-C3'-O3'	5.92	122.58	113.70
48	5	3774	A	C4'-C3'-O3'	-5.92	104.13	113.00
48	5	2296	G	C4'-C3'-O3'	-5.91	104.13	113.00
51	9	1647	A	C4'-C3'-O3'	5.90	118.25	109.40
44	t	29	ALA	CA-C-N	5.89	127.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	t	29	ALA	C-N-CA	5.89	127.20	119.84
48	5	2297	G	C4'-C3'-O3'	-5.89	104.17	113.00
48	5	2692	U	C1'-C2'-O2'	5.88	117.23	108.40
48	5	2816	G	C1'-C2'-O2'	5.88	117.22	108.40
2	B	25	HIS	CB-CG-ND1	5.88	131.51	122.70
35	j	76	HIS	CB-CG-CD2	-5.88	123.56	131.20
48	5	4454	G	C1'-C2'-O2'	5.87	117.21	108.40
7	G	140	VAL	CB-CA-C	-5.87	104.35	112.04
48	5	1214	C	C2'-C3'-O3'	5.87	118.31	109.50
48	5	4514	G	C4'-C3'-O3'	-5.87	104.20	113.00
48	5	48	G	C3'-C2'-O2'	5.86	123.39	114.60
51	9	477	G	C1'-C2'-O2'	5.86	117.20	108.40
48	5	4236	G	C4'-C3'-O3'	-5.86	104.21	113.00
51	9	678	U	C1'-C2'-O2'	5.86	117.19	108.40
51	9	1519	U	C2'-C3'-O3'	5.86	118.28	109.50
48	5	369	G	C1'-C2'-O2'	5.86	117.18	108.40
68	QQ	146	ARG	NE-CZ-NH2	5.85	124.47	119.20
48	5	3698	G	C2'-C3'-O3'	-5.84	104.94	113.70
35	j	16	HIS	CB-CG-ND1	5.84	131.46	122.70
48	5	1852	U	C4'-C3'-O3'	-5.84	104.25	113.00
75	XX	31	HIS	CB-CG-ND1	5.83	131.44	122.70
1	A	216	HIS	CB-CG-ND1	5.82	131.43	122.70
57	FF	43	GLU	N-CA-C	-5.82	98.40	110.80
13	N	181	HIS	CB-CG-ND1	5.82	131.43	122.70
51	9	1595	U	N1-C1'-C2'	5.82	120.73	112.00
30	e	103	VAL	CB-CA-C	-5.82	103.08	111.34
51	9	160	U	C2'-C3'-O3'	5.82	118.22	109.50
48	5	2395	A	C2'-C3'-O3'	5.81	118.22	109.50
51	9	417	C	C4'-C3'-O3'	-5.81	104.29	113.00
51	9	1856	C	C4'-C3'-O3'	-5.80	104.29	113.00
48	5	3643	A	C1'-C2'-O2'	-5.80	103.10	111.80
48	5	726	G	C4'-C3'-O3'	-5.80	104.30	113.00
48	5	3865	A	C1'-C2'-O2'	5.79	117.09	108.40
47	3	38	A	C2'-C3'-O3'	-5.79	105.01	113.70
56	EE	128	LYS	N-CA-C	5.79	117.34	108.42
11	L	99	ASP	N-CA-C	-5.79	102.86	110.39
5	E	280	HIS	CB-CG-ND1	5.79	131.38	122.70
51	9	1532	C	C4'-C3'-O3'	-5.79	104.32	113.00
48	5	2404	A	C2'-C3'-O3'	-5.78	105.03	113.70
48	5	2836	A	C1'-C2'-O2'	5.78	117.07	108.40
51	9	1859	A	C4'-C3'-O3'	-5.78	104.34	113.00
51	9	633	C	C4'-C3'-O3'	-5.77	104.34	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	3	30	G	C4'-C3'-O3'	5.77	121.65	113.00
48	5	2063	G	C4'-C3'-O3'	-5.77	104.35	113.00
48	5	1474	C	C2'-C3'-O3'	5.76	122.34	113.70
48	5	1962	A	N9-C1'-C2'	-5.76	103.36	112.00
74	WW	76	SER	N-CA-C	-5.76	101.62	110.32
63	LL	106	HIS	CB-CG-ND1	5.76	131.34	122.70
48	5	116	G	C4'-C3'-O3'	-5.75	104.37	113.00
48	5	2251	G	C4'-C3'-O3'	5.75	118.02	109.40
48	5	2661	U	C2'-C3'-O3'	5.74	118.12	109.50
51	9	1234	C	C2'-C3'-O3'	5.74	122.31	113.70
48	5	2396	A	C4'-C3'-O3'	5.73	118.00	109.40
51	9	474	G	C4'-C3'-O3'	-5.73	104.40	113.00
66	OO	94	HIS	CB-CG-ND1	5.73	131.30	122.70
48	5	3739	C	C4'-C3'-O3'	-5.73	104.40	113.00
54	CC	207	ALA	CA-C-N	5.73	125.20	119.24
54	CC	207	ALA	C-N-CA	5.73	125.20	119.24
48	5	1327	C	C1'-C2'-O2'	5.73	116.99	108.40
15	P	133	HIS	CB-CG-ND1	5.72	131.29	122.70
48	5	38	A	C4'-C3'-O3'	-5.72	104.41	113.00
48	5	1465	G	C2'-C3'-O3'	5.72	122.29	113.70
48	5	2021	G	N9-C1'-C2'	-5.71	103.43	112.00
48	5	497	G	C4'-C3'-O3'	5.71	121.56	113.00
78	aa	47	ALA	N-CA-C	5.71	119.76	112.34
48	5	2649	G	C4'-C3'-O3'	-5.70	104.44	113.00
48	5	3779	A	C1'-C2'-O2'	5.70	116.96	108.40
48	5	4526	U	C4'-C3'-O3'	-5.70	104.44	113.00
87	jj	286	ILE	N-CA-C	5.70	116.96	108.46
12	M	20	HIS	CB-CG-ND1	5.70	131.25	122.70
48	5	1214	C	C4'-C3'-O3'	5.70	117.95	109.40
19	T	27	LEU	N-CA-C	5.70	117.49	111.28
48	5	976	G	C3'-C2'-O2'	5.70	119.24	110.70
48	5	1380	G	N9-C1'-C2'	5.70	120.54	112.00
48	5	4656	A	C4'-C3'-O3'	5.69	117.94	109.40
48	5	2023	C	C4'-C3'-O3'	-5.69	104.46	113.00
48	5	1682	A	C4'-C3'-O3'	-5.69	104.47	113.00
48	5	3593	C	C4'-C3'-O3'	5.69	117.94	109.40
51	9	1643	U	C4'-C3'-O3'	-5.69	104.47	113.00
46	2	34	A	C1'-C2'-O2'	-5.69	103.27	111.80
48	5	3891	A	C1'-C2'-O2'	5.69	116.93	108.40
48	5	375	G	C1'-C2'-O2'	5.68	116.92	108.40
65	NN	58	HIS	CB-CG-ND1	5.68	131.22	122.70
14	O	110	PRO	CA-C-N	-5.68	113.90	119.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	O	110	PRO	C-N-CA	-5.68	113.90	119.64
48	5	1622	U	C4'-C3'-O3'	-5.68	104.49	113.00
51	9	301	A	C2'-C3'-O3'	-5.68	105.18	113.70
14	O	90	HIS	N-CA-C	5.67	119.68	112.87
7	G	29	ASN	CA-C-N	-5.67	114.03	120.89
7	G	29	ASN	C-N-CA	-5.67	114.03	120.89
48	5	3917	A	C3'-C2'-O2'	5.67	119.20	110.70
48	5	3844	U	C1'-C2'-O2'	5.66	116.89	108.40
48	5	964	A	C4'-C3'-O3'	5.66	121.49	113.00
48	5	2813	A	C1'-C2'-O2'	5.66	116.89	108.40
51	9	752	G	C4'-C3'-O3'	5.66	117.89	109.40
38	m	118	THR	N-CA-C	5.66	117.90	111.11
48	5	5066	U	N1-C1'-C2'	5.66	120.48	112.00
48	5	4684	A	C1'-C2'-O2'	5.65	116.88	108.40
51	9	501	C	N1-C1'-C2'	5.65	120.48	112.00
48	5	102	G	C3'-C2'-O2'	-5.65	102.22	110.70
48	5	323	C	C4'-C3'-O3'	-5.65	104.53	113.00
48	5	2068	C	C2'-C3'-O3'	5.65	117.97	109.50
9	I	97	ILE	CB-CA-C	5.65	117.45	110.73
51	9	1060	A	N9-C1'-C2'	5.65	122.47	114.00
48	5	2468	U	C4'-C3'-O3'	5.64	117.86	109.40
48	5	265	C	C4'-C3'-O3'	5.64	117.86	109.40
48	5	2505	C	C4'-C3'-O3'	5.64	117.86	109.40
48	5	975	C	C2'-C3'-O3'	-5.64	105.24	113.70
48	5	4248	A	C1'-C2'-O2'	5.63	116.85	108.40
48	5	1890	G	C1'-C2'-O2'	-5.63	103.35	111.80
60	II	44	HIS	CB-CG-ND1	5.63	131.15	122.70
48	5	1457	G	C4'-C3'-O3'	-5.63	104.56	113.00
48	5	1575	A	C4'-C3'-O3'	-5.63	104.56	113.00
51	9	434	G	C4'-C3'-O3'	5.63	121.44	113.00
48	5	930	G	C4'-C3'-O3'	5.63	117.84	109.40
48	5	134	G	C4'-C3'-O3'	5.62	117.83	109.40
51	9	1211	G	N9-C1'-C2'	-5.62	103.56	112.00
11	L	87	HIS	CB-CG-ND1	5.62	131.13	122.70
48	5	931	C	C3'-C2'-O2'	5.62	119.13	110.70
48	5	1961	G	C2'-C3'-O3'	-5.62	105.27	113.70
48	5	2055	G	C2'-C3'-O3'	-5.62	101.07	109.50
48	5	3904	G	C2'-C3'-O3'	5.62	117.93	109.50
48	5	4365	C	C4'-C3'-O3'	-5.62	104.57	113.00
51	9	1275	G	C4'-C3'-O3'	-5.62	104.57	113.00
51	9	1665	G	C1'-C2'-O2'	-5.62	103.37	111.80
48	5	1905	U	C4'-C3'-O3'	-5.61	104.58	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	450	C	C2'-C3'-O3'	-5.61	105.28	113.70
66	OO	37	PHE	N-CA-C	-5.61	101.74	110.10
42	r	4	HIS	CB-CG-ND1	5.61	131.11	122.70
48	5	4579	U	N1-C1'-C2'	5.60	120.40	112.00
50	8	146	U	C3'-C2'-O2'	5.60	119.10	110.70
48	5	4307	A	C4'-C3'-O3'	-5.59	104.61	113.00
66	OO	43	HIS	CB-CG-ND1	5.59	131.09	122.70
48	5	1289	C	C4'-C3'-O3'	-5.59	104.61	113.00
51	9	1137	U	C3'-C2'-O2'	5.59	119.09	110.70
6	F	194	HIS	CB-CG-ND1	5.59	131.09	122.70
48	5	4505	C	C3'-C2'-O2'	5.59	119.09	110.70
51	9	319	C	C4'-C3'-O3'	-5.59	104.61	113.00
51	9	1335	G	C3'-C2'-O2'	5.59	119.08	110.70
48	5	4998	G	C4'-C3'-O3'	-5.58	104.63	113.00
48	5	1613	A	C4'-C3'-O3'	5.58	117.77	109.40
48	5	4560	C	C1'-C2'-O2'	-5.58	103.43	111.80
19	T	33	ILE	N-CA-C	5.58	115.92	108.11
48	5	1359	G	N9-C1'-C2'	5.58	120.36	112.00
48	5	4538	G	C4'-C3'-O3'	-5.57	104.64	113.00
51	9	1234	C	N1-C1'-C2'	-5.57	103.64	112.00
48	5	54	G	C4'-C3'-O3'	-5.57	104.65	113.00
48	5	684	G	C2'-C3'-O3'	5.57	122.05	113.70
48	5	1358	G	O4'-C1'-C2'	-5.56	102.04	107.60
48	5	1598	C	C2'-C3'-O3'	-5.56	105.36	113.70
3	C	237	ILE	N-CA-C	-5.56	105.43	110.82
23	X	96	LEU	N-CA-C	-5.55	101.69	109.69
51	9	1188	A	C1'-C2'-O2'	5.55	116.73	108.40
51	9	602	G	C1'-C2'-O2'	5.55	116.72	108.40
48	5	2827	G	C2'-C3'-O3'	-5.54	101.19	109.50
51	9	315	C	C2'-C3'-O3'	-5.54	105.39	113.70
51	9	472	C	C2'-C3'-O3'	5.54	122.02	113.70
43	s	200	ASN	CA-C-N	5.54	126.77	119.84
43	s	200	ASN	C-N-CA	5.54	126.77	119.84
48	5	74	G	C4'-C3'-O3'	-5.54	104.69	113.00
48	5	2273	G	C4'-C3'-O3'	-5.54	104.69	113.00
48	5	5004	C	C4'-C3'-O3'	-5.54	104.69	113.00
48	5	408	A	C2'-C3'-O3'	-5.54	105.39	113.70
48	5	4683	U	C4'-C3'-O3'	-5.54	104.69	113.00
48	5	2264	C	C4'-C3'-O3'	-5.52	104.72	113.00
48	5	2649	G	C2'-C3'-O3'	5.52	121.98	113.70
48	5	1541	C	C4'-C3'-O3'	-5.52	104.72	113.00
48	5	2446	C	C2'-C3'-O3'	-5.52	105.43	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	97	U	C4'-C3'-O3'	-5.51	104.73	113.00
71	TT	62	ARG	NE-CZ-NH2	5.51	124.16	119.20
1	A	200	ARG	N-CA-CB	5.50	118.37	110.06
3	C	67	TRP	N-CA-C	-5.50	102.25	110.23
48	5	1378	C	O5'-C5'-C4'	5.50	119.75	111.50
48	5	4561	C	C1'-C2'-O2'	5.50	116.65	108.40
3	C	142	HIS	CB-CG-ND1	5.50	130.95	122.70
48	5	4716	C	C1'-C2'-O2'	5.50	116.65	108.40
53	BB	215	VAL	N-CA-C	-5.50	99.88	108.95
48	5	2313	A	C3'-C2'-O2'	5.49	118.93	110.70
48	5	1630	A	C1'-C2'-O2'	5.49	116.63	108.40
51	9	215	G	C2'-C3'-O3'	5.49	117.73	109.50
51	9	1048	G	C2'-C3'-O3'	-5.49	105.47	113.70
35	j	63	ARG	CG-CD-NE	5.49	124.07	112.00
51	9	1845	A	C4'-C3'-O3'	-5.48	104.77	113.00
51	9	1101	U	C4'-C3'-O3'	-5.48	104.78	113.00
48	5	1887	G	C4'-C3'-O3'	-5.48	104.78	113.00
51	9	317	C	C4'-C3'-O3'	-5.48	104.79	113.00
65	NN	5	HIS	CB-CG-ND1	5.48	130.91	122.70
48	5	3875	G	C1'-C2'-O2'	5.47	116.61	108.40
48	5	684	G	C4'-C3'-O3'	-5.47	104.80	113.00
48	5	1603	C	C1'-C2'-O2'	5.47	116.60	108.40
62	KK	66	HIS	CB-CG-ND1	5.47	130.90	122.70
48	5	2581	A	C4'-C3'-O3'	-5.46	104.80	113.00
48	5	3697	U	C3'-C2'-O2'	5.46	118.89	110.70
84	gg	235	ILE	N-CA-C	5.46	116.46	109.30
86	ii	180	HIS	N-CA-C	5.46	118.46	109.72
48	5	486	C	C2'-C3'-O3'	5.46	121.89	113.70
48	5	4614	G	C4'-C3'-O3'	-5.46	104.81	113.00
48	5	236	G	C4'-C3'-O3'	-5.45	104.82	113.00
48	5	3801	U	C4'-C3'-O3'	-5.45	104.82	113.00
48	5	664	G	C4'-C3'-O3'	5.45	117.58	109.40
48	5	1329	G	C4'-C3'-O3'	5.45	121.18	113.00
48	5	2836	A	C4'-C3'-O3'	-5.45	104.83	113.00
51	9	1336	C	C4'-C3'-O3'	-5.45	104.83	113.00
48	5	1317	U	C3'-C2'-O2'	5.45	118.87	110.70
48	5	1889	U	C1'-C2'-O2'	5.45	116.57	108.40
10	J	119	TYR	CA-CB-CG	5.44	123.70	113.90
48	5	1376	C	C4'-C3'-O3'	5.44	117.56	109.40
48	5	2257	C	C4'-C3'-O3'	5.44	117.56	109.40
48	5	1371	A	O4'-C1'-C2'	-5.44	102.16	107.60
3	C	180	ILE	N-CA-C	-5.44	105.03	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	594	A	C4'-C3'-O3'	5.44	117.56	109.40
48	5	1877	G	C4'-C3'-O3'	-5.43	104.85	113.00
48	5	4376	A	C2'-C3'-O3'	-5.43	105.55	113.70
14	O	108	ILE	CA-C-N	5.43	125.97	120.38
14	O	108	ILE	C-N-CA	5.43	125.97	120.38
63	LL	96	ILE	N-CA-C	-5.43	100.66	108.53
48	5	2546	G	C3'-C2'-O2'	5.43	118.84	110.70
2	B	71	GLU	N-CA-C	-5.42	102.85	110.50
51	9	432	G	C2'-C3'-O3'	-5.42	105.56	113.70
48	5	3873	G	C1'-C2'-O2'	5.42	116.53	108.40
48	5	1512	G	C4'-C3'-O3'	-5.42	104.87	113.00
48	5	3752	C	C2'-C3'-O3'	-5.42	105.58	113.70
48	5	4119	C	C2'-C3'-O3'	5.42	121.83	113.70
48	5	3936	A	C4'-C3'-O3'	-5.41	104.88	113.00
48	5	4978	G	C4'-C3'-O3'	-5.41	104.88	113.00
29	d	25	TYR	N-CA-C	-5.41	100.51	108.79
48	5	3800	A	C4'-C3'-O3'	-5.41	104.89	113.00
51	9	13	C	C1'-C2'-O2'	5.41	116.52	108.40
47	3	30	G	N9-C1'-C2'	-5.41	103.89	112.00
48	5	274	C	C4'-C3'-O3'	-5.41	104.89	113.00
48	5	1621	A	C1'-C2'-O2'	5.41	116.51	108.40
48	5	2797	C	N1-C1'-C2'	-5.41	105.89	114.00
48	5	4665	A	C4'-C3'-O3'	-5.40	104.90	113.00
51	9	1837	G	C2'-C3'-O3'	-5.40	105.60	113.70
53	BB	205	TYR	CA-C-N	5.39	126.58	119.84
53	BB	205	TYR	C-N-CA	5.39	126.58	119.84
48	5	5033	G	C4'-C3'-O3'	-5.39	104.91	113.00
48	5	2530	U	C1'-C2'-O2'	-5.39	103.72	111.80
51	9	2	A	C4'-C3'-O3'	5.39	117.48	109.40
48	5	300	A	N9-C1'-C2'	5.38	120.08	112.00
48	5	362	A	C3'-C2'-O2'	5.38	118.77	110.70
48	5	3833	C	C3'-C2'-O2'	5.38	118.77	110.70
51	9	1473	G	O4'-C1'-C2'	-5.38	102.22	107.60
48	5	3867	A	C2'-C3'-O3'	-5.38	105.63	113.70
48	5	4327	C	C4'-C3'-O3'	-5.38	104.93	113.00
51	9	1600	G	C4'-C3'-O3'	-5.38	104.93	113.00
48	5	1987	C	O4'-C1'-C2'	-5.38	102.22	107.60
48	5	2744	A	C1'-C2'-O2'	5.38	116.46	108.40
48	5	406	C	C3'-C2'-O2'	5.37	118.76	110.70
48	5	3769	C	C1'-C2'-O2'	5.37	116.46	108.40
51	9	456	C	C4'-C3'-O3'	-5.37	104.94	113.00
66	OO	109	GLY	CA-C-N	5.37	125.19	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	OO	109	GLY	C-N-CA	5.37	125.19	119.28
48	5	82	U	C1'-C2'-O2'	5.37	116.46	108.40
31	f	49	TYR	N-CA-C	-5.37	101.22	109.76
31	f	80	ASN	N-CA-C	5.37	122.23	110.80
46	2	76	A	C3'-C2'-O2'	5.37	118.75	110.70
48	5	1523	A	C4'-C3'-O3'	-5.37	104.95	113.00
48	5	4237	C	C4'-C3'-O3'	-5.37	104.95	113.00
86	ii	257	SER	N-CA-C	-5.37	103.61	110.53
48	5	3717	A	C3'-C2'-O2'	5.36	118.75	110.70
51	9	646	G	C4'-C3'-O3'	-5.36	104.95	113.00
67	PP	79	HIS	CB-CG-ND1	5.36	130.75	122.70
26	a	23	GLY	N-CA-C	-5.36	104.86	112.37
48	5	289	C	C4'-C3'-O3'	-5.36	104.96	113.00
48	5	1663	C	C4'-C3'-O3'	-5.36	104.96	113.00
51	9	105	U	C3'-C2'-O2'	5.36	118.74	110.70
48	5	1573	G	C4'-C3'-O3'	-5.36	104.97	113.00
48	5	3670	C	C3'-C2'-O2'	5.36	118.73	110.70
48	5	4427	G	C4'-C3'-O3'	-5.36	104.97	113.00
51	9	291	G	O4'-C4'-C3'	-5.36	100.74	106.10
48	5	979	C	C2'-C3'-O3'	5.35	121.73	113.70
51	9	631	U	C2'-C3'-O3'	5.35	117.53	109.50
51	9	389	A	C4'-C3'-O3'	-5.35	104.97	113.00
51	9	1330	G	C4'-C3'-O3'	-5.35	101.38	109.40
48	5	42	A	C1'-C2'-O2'	-5.35	103.78	111.80
48	5	1871	A	C3'-C2'-O2'	5.35	118.72	110.70
48	5	4473	A	N9-C1'-C2'	5.35	120.02	112.00
48	5	2279	A	C3'-C2'-O2'	5.35	118.72	110.70
48	5	4392	G	C3'-C2'-O2'	5.35	118.72	110.70
48	5	717	U	C4'-C3'-O3'	-5.34	104.99	113.00
48	5	3815	G	C4'-C3'-O3'	-5.34	104.99	113.00
48	5	6	C	C3'-C2'-O2'	5.34	118.71	110.70
48	5	4753	U	C1'-C2'-O2'	5.34	116.40	108.40
28	c	14	ILE	N-CA-C	-5.33	105.30	110.42
48	5	4383	U	C4'-C3'-O3'	-5.33	105.00	113.00
48	5	989	U	C3'-C2'-O2'	5.33	118.69	110.70
48	5	2119	C	C2'-C3'-O3'	5.33	117.50	109.50
48	5	3674	G	C4'-C3'-O3'	-5.33	105.00	113.00
49	7	1	G	C5'-C4'-C3'	5.33	123.99	116.00
48	5	1947	U	C2'-C3'-O3'	-5.32	105.71	113.70
48	5	2793	G	C4'-C3'-O3'	-5.32	105.02	113.00
48	5	4888	U	C4'-C3'-O3'	5.32	117.38	109.40
48	5	329	A	C4'-C3'-O3'	-5.32	105.03	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	2884	G	C2'-C3'-O3'	5.32	121.67	113.70
51	9	322	C	C2'-C3'-O3'	-5.31	105.73	113.70
48	5	1379	C	O4'-C1'-C2'	-5.31	100.49	105.80
48	5	1599	A	C2'-C3'-O3'	-5.31	105.73	113.70
48	5	4474	A	C3'-C2'-O2'	5.31	118.66	110.70
53	BB	87	ILE	N-CA-C	5.31	115.77	108.12
51	9	1294	G	N9-C1'-C2'	-5.31	104.04	112.00
51	9	139	C	C4'-C3'-O3'	5.30	120.95	113.00
56	EE	28	ALA	N-CA-C	-5.30	102.31	110.58
48	5	4228	G	C4'-C3'-O3'	-5.30	101.45	109.40
30	e	104	SER	N-CA-C	5.30	118.32	110.48
48	5	4394	A	C1'-C2'-O2'	-5.30	103.85	111.80
50	8	19	C	C4'-C3'-O3'	-5.29	105.06	113.00
48	5	4186	A	C4'-C3'-O3'	-5.29	105.06	113.00
36	k	59	SER	N-CA-C	5.29	119.48	113.19
48	5	1354	A	C2'-C3'-O3'	-5.29	101.57	109.50
48	5	3633	C	C4'-C3'-O3'	-5.29	105.07	113.00
48	5	4719	G	C4'-C3'-O3'	5.29	120.93	113.00
48	5	2320	G	C4'-C3'-O3'	-5.28	105.08	113.00
48	5	2246	C	C2'-C3'-O3'	5.28	121.62	113.70
48	5	2275	G	C4'-C3'-O3'	-5.28	105.08	113.00
48	5	3938	G	C2'-C3'-O3'	-5.28	101.58	109.50
48	5	693	C	C2'-C3'-O3'	5.28	121.61	113.70
48	5	4186	A	C1'-C2'-O2'	5.28	116.31	108.40
49	7	1	G	C5'-C4'-O4'	5.28	117.71	109.80
57	FF	68	ILE	CB-CA-C	-5.28	103.98	112.16
51	9	146	G	C2'-C3'-O3'	5.27	117.41	109.50
51	9	1448	A	C4'-C3'-O3'	5.27	120.91	113.00
48	5	3816	A	C4'-C3'-O3'	-5.27	105.10	113.00
59	HH	133	LEU	N-CA-C	5.27	117.77	111.71
48	5	209	U	C4'-C3'-O3'	5.27	117.30	109.40
48	5	508	G	C4'-C3'-O3'	-5.26	105.10	113.00
51	9	369	C	C4'-C3'-O3'	5.26	117.30	109.40
48	5	3678	G	C2'-C3'-O3'	-5.26	101.61	109.50
47	3	30	G	C2'-C3'-O3'	-5.26	105.81	113.70
48	5	2349	A	C4'-C3'-O3'	-5.26	105.11	113.00
48	5	3652	A	C1'-C2'-O2'	5.26	116.29	108.40
48	5	1725	U	C1'-C2'-O2'	5.26	116.29	108.40
51	9	919	A	C4'-C3'-O3'	5.26	117.29	109.40
48	5	2528	G	N9-C1'-C2'	5.26	119.89	112.00
48	5	1738	A	C3'-C2'-O2'	5.26	118.58	110.70
51	9	507	G	C2'-C3'-O3'	5.26	117.38	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	9	1698	C	C4'-C3'-O3'	-5.25	101.52	109.40
48	5	3861	A	C1'-C2'-O2'	5.25	116.28	108.40
60	II	91	VAL	CB-CA-C	-5.25	104.97	112.22
51	9	1475	G	C4'-C3'-O3'	5.25	117.28	109.40
48	5	4632	U	C1'-C2'-O2'	5.25	116.28	108.40
51	9	532	C	C2'-C3'-O3'	5.25	121.57	113.70
51	9	601	G	C1'-C2'-O2'	5.25	116.27	108.40
51	9	934	G	C1'-C2'-O2'	5.25	116.27	108.40
51	9	1535	U	N1-C1'-C2'	5.25	121.87	114.00
2	B	18	PRO	N-CA-C	-5.25	101.66	112.47
48	5	1965	G	OP1-P-O3'	5.25	123.74	108.00
48	5	2028	C	C4'-C3'-O3'	5.24	120.87	113.00
51	9	376	A	C1'-C2'-O2'	5.24	116.26	108.40
58	GG	187	HIS	CB-CG-ND1	5.24	130.56	122.70
48	5	4656	A	C2'-C3'-O3'	5.24	117.36	109.50
48	5	3700	C	C1'-C2'-O2'	5.24	116.25	108.40
51	9	1313	A	C4'-C3'-O3'	5.24	117.25	109.40
48	5	3652	A	C2'-C3'-O3'	-5.23	105.86	113.70
48	5	2260	C	C3'-C2'-O2'	5.23	118.54	110.70
48	5	237	G	C4'-C3'-O3'	-5.22	105.16	113.00
48	5	4657	U	C2'-C3'-O3'	-5.22	101.66	109.50
51	9	1036	A	C1'-C2'-O2'	5.22	116.24	108.40
48	5	3692	A	C1'-C2'-O2'	5.22	116.23	108.40
51	9	1230	C	C4'-C3'-O3'	-5.22	105.17	113.00
48	5	2455	G	C3'-C2'-O2'	5.22	118.53	110.70
48	5	1691	G	C1'-C2'-O2'	5.22	116.23	108.40
48	5	3594	C	N1-C1'-C2'	5.22	119.83	112.00
48	5	2843	U	C4'-C3'-O3'	-5.22	105.17	113.00
48	5	4441	A	C4'-C3'-O3'	-5.22	105.18	113.00
52	AA	169	HIS	CB-CG-ND1	5.22	130.53	122.70
53	BB	127	VAL	N-CA-C	5.21	115.23	108.35
48	5	99	A	C3'-C2'-O2'	5.21	118.52	110.70
48	5	4677	U	C2'-C3'-O3'	5.21	117.31	109.50
24	Y	72	GLN	N-CA-C	5.21	116.99	108.76
48	5	223	G	C4'-C3'-O3'	-5.20	105.19	113.00
48	5	4318	C	C4'-C3'-O3'	-5.20	105.19	113.00
86	ii	202	VAL	CB-CA-C	-5.20	105.12	112.14
48	5	1333	A	C4'-C3'-O3'	-5.20	105.20	113.00
48	5	4438	U	C1'-C2'-O2'	5.20	116.19	108.40
1	A	7	GLY	N-CA-C	-5.19	100.87	113.18
48	5	1827	C	C2'-C3'-O3'	-5.19	105.91	113.70
48	5	4553	A	C1'-C2'-O2'	5.19	116.19	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	S	83	ARG	CG-CD-NE	5.19	123.41	112.00
48	5	1321	G	C1'-C2'-O2'	5.19	116.18	108.40
48	5	4320	G	C3'-C2'-O2'	5.18	118.48	110.70
51	9	291	G	C4'-C3'-O3'	5.18	117.18	109.40
51	9	1440	C	C4'-C3'-O3'	-5.18	105.22	113.00
48	5	2039	G	C4'-C3'-O3'	-5.18	105.23	113.00
48	5	2266	C	C2'-C3'-O3'	5.18	117.27	109.50
48	5	2114	G	C2'-C3'-O3'	-5.18	105.93	113.70
43	s	72	ASN	N-CA-C	5.18	116.35	109.93
51	9	4	C	C4'-C3'-O3'	-5.18	105.23	113.00
51	9	1524	G	C3'-C2'-O2'	5.17	118.46	110.70
48	5	2445	C	C4'-C3'-O3'	-5.17	105.24	113.00
51	9	663	C	C4'-C3'-O3'	-5.17	105.24	113.00
41	p	7	LYS	N-CA-C	5.17	116.51	110.41
48	5	2466	G	C4'-C3'-O3'	-5.17	105.25	113.00
48	5	2425	U	C2'-C3'-O3'	-5.17	101.75	109.50
48	5	4213	A	C4'-C3'-O3'	-5.17	105.25	113.00
50	8	18	U	C4'-C3'-O3'	-5.17	105.25	113.00
48	5	1496	G	C2'-C3'-O3'	-5.17	105.95	113.70
48	5	4232	U	C4'-C3'-O3'	5.16	117.14	109.40
48	5	4564	A	C1'-C2'-O2'	5.16	116.14	108.40
48	5	4669	A	C4'-C3'-O3'	-5.16	105.26	113.00
48	5	486	C	C3'-C2'-O2'	5.16	118.44	110.70
48	5	3676	G	C4'-C3'-O3'	-5.16	105.26	113.00
48	5	3886	G	C3'-C2'-O2'	5.16	118.44	110.70
86	ii	316	ALA	N-CA-C	5.16	116.58	110.19
47	3	39	U	N1-C1'-C2'	-5.15	104.27	112.00
48	5	420	A	C1'-C2'-O2'	5.15	116.13	108.40
51	9	60	A	C4'-C3'-O3'	-5.15	105.27	113.00
48	5	4449	A	C4'-C3'-O3'	5.15	117.13	109.40
48	5	4522	G	C3'-C2'-O2'	5.15	118.42	110.70
3	C	150	LEU	CA-C-N	-5.15	113.40	119.84
3	C	150	LEU	C-N-CA	-5.15	113.40	119.84
48	5	3604	A	C2'-C3'-O3'	-5.15	105.98	113.70
18	S	83	ARG	NE-CZ-NH2	5.14	123.83	119.20
48	5	2822	G	C2'-C3'-O3'	-5.14	105.98	113.70
48	5	4413	C	C4'-C3'-O3'	-5.14	105.28	113.00
48	5	1915	C	C2'-C3'-O3'	-5.14	101.79	109.50
48	5	2397	G	C2'-C3'-O3'	-5.14	101.79	109.50
48	5	2821	U	C1'-C2'-O2'	5.14	116.11	108.40
31	f	96	ALA	N-CA-C	5.14	116.88	111.28
2	B	62	ARG	CB-CA-C	5.14	115.57	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	1427	A	C4'-C3'-O3'	-5.14	105.30	113.00
48	5	3735	G	C4'-C3'-O3'	-5.14	105.30	113.00
48	5	3814	U	C2'-C3'-O3'	-5.14	106.00	113.70
57	FF	44	LYS	N-CA-C	-5.14	106.70	113.12
15	P	24	VAL	CB-CA-C	-5.13	102.91	110.82
51	9	1845	A	C2'-C3'-O3'	5.13	121.40	113.70
18	S	124	ILE	N-CA-C	5.13	116.35	108.71
48	5	745	G	C3'-C2'-O2'	5.13	118.39	110.70
48	5	216	C	C3'-C2'-O2'	5.13	118.39	110.70
51	9	308	G	C2'-C3'-O3'	-5.13	106.01	113.70
5	E	159	VAL	N-CA-C	5.13	115.23	107.80
48	5	15	A	C3'-C2'-O2'	5.13	118.39	110.70
51	9	1597	C	C4'-C3'-O3'	-5.13	105.31	113.00
48	5	134	G	C2'-C3'-O3'	5.12	117.19	109.50
48	5	4239	A	C1'-C2'-O2'	5.12	116.09	108.40
48	5	3825	A	C1'-C2'-O2'	5.12	116.09	108.40
48	5	1732	C	C4'-C3'-O3'	-5.12	105.32	113.00
48	5	2845	A	C1'-C2'-O2'	5.12	116.08	108.40
84	gg	17	TRP	CA-CB-CG	5.12	123.33	113.60
51	9	1385	G	N9-C1'-C2'	-5.12	104.32	112.00
48	5	1502	G	C4'-C3'-O3'	-5.12	105.32	113.00
9	I	37	GLY	N-CA-C	-5.12	105.89	111.21
48	5	1368	A	C3'-C2'-O2'	5.12	118.37	110.70
48	5	5026	U	N1-C1'-C2'	5.12	119.67	112.00
79	bb	65	GLN	N-CA-C	-5.12	103.20	109.65
48	5	5022	U	C3'-C2'-O2'	5.11	118.37	110.70
35	j	76	HIS	CB-CG-ND1	5.11	130.37	122.70
48	5	1582	U	C1'-C2'-O2'	5.11	116.07	108.40
48	5	1676	C	C3'-C2'-O2'	5.11	118.36	110.70
48	5	342	G	C4'-C3'-O3'	-5.10	105.35	113.00
48	5	2278	G	C2'-C3'-O3'	5.10	117.16	109.50
48	5	4494	G	C1'-C2'-O2'	5.10	116.05	108.40
51	9	1631	U	C4'-C3'-O3'	-5.10	105.35	113.00
48	5	1965	G	OP2-P-O3'	-5.10	92.70	108.00
48	5	1983	A	C2'-C3'-O3'	-5.10	101.85	109.50
48	5	4088	C	C4'-C3'-O3'	-5.10	105.35	113.00
51	9	109	U	C4'-C3'-O3'	-5.10	105.35	113.00
51	9	746	C	C3'-C2'-O2'	5.10	118.35	110.70
48	5	1502	G	C2'-C3'-O3'	-5.09	106.06	113.70
2	B	220	ILE	N-CA-C	-5.09	100.87	108.46
51	9	319	C	C2'-C3'-O3'	5.09	121.34	113.70
48	5	2610	G	C3'-C2'-O2'	5.09	118.34	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	5	2783	A	C4'-C3'-O3'	-5.09	105.37	113.00
48	5	451	C	C2'-C3'-O3'	5.09	117.13	109.50
48	5	1916	G	C2'-C3'-O3'	-5.08	106.08	113.70
48	5	1487	G	C3'-C2'-O2'	5.08	118.32	110.70
48	5	3619	G	C2'-C3'-O3'	5.08	121.32	113.70
24	Y	29	ILE	CB-CA-C	-5.08	105.21	112.22
48	5	1280	C	C3'-C2'-O2'	-5.08	106.98	114.60
57	FF	169	ILE	N-CA-C	-5.08	104.95	110.23
48	5	957	G	P-O3'-C3'	5.07	127.81	120.20
51	9	21	U	C4'-C3'-O3'	-5.07	105.39	113.00
2	B	162	VAL	N-CA-C	-5.07	101.18	108.89
48	5	4213	A	N9-C1'-C2'	5.07	119.61	112.00
50	8	112	G	C3'-C2'-O2'	5.07	118.31	110.70
48	5	3639	U	C4'-C3'-O3'	-5.07	105.40	113.00
36	k	28	ASN	N-CA-C	5.07	117.54	111.71
48	5	730	G	C1'-C2'-O2'	5.07	116.00	108.40
48	5	4637	G	C4'-C3'-O3'	-5.07	105.40	113.00
48	5	1428	U	C4'-C3'-O3'	-5.07	105.40	113.00
48	5	2819	U	C4'-C3'-O3'	-5.07	105.40	113.00
84	gg	124	SER	N-CA-C	5.07	115.73	108.74
51	9	1859	A	N9-C1'-C2'	5.06	119.60	112.00
74	WW	55	ASP	N-CA-C	-5.06	103.71	110.55
40	o	61	LYS	N-CA-C	5.06	117.85	109.85
48	5	37	U	C1'-C2'-O2'	5.06	116.00	108.40
48	5	3704	U	C3'-C2'-O2'	5.06	118.30	110.70
48	5	3715	U	C4'-C3'-O3'	5.06	120.59	113.00
51	9	24	C	C4'-C3'-O3'	-5.06	105.41	113.00
48	5	4521	U	C4'-C3'-O3'	-5.06	105.41	113.00
84	gg	17	TRP	N-CA-CB	5.06	117.59	110.36
48	5	4881	U	C4'-C3'-O3'	-5.06	105.42	113.00
48	5	373	G	C4'-C3'-O3'	-5.05	105.42	113.00
48	5	2533	C	C3'-C2'-O2'	5.05	118.27	110.70
48	5	4881	U	C3'-C2'-O2'	5.05	118.27	110.70
48	5	2885	A	C1'-C2'-O2'	5.04	115.96	108.40
48	5	4402	C	C4'-C3'-O3'	-5.04	105.43	113.00
25	Z	123	LYS	N-CA-C	-5.04	103.40	110.50
48	5	1290	G	C4'-C3'-O3'	-5.04	105.44	113.00
48	5	57	G	C4'-C3'-O3'	-5.04	105.44	113.00
48	5	4425	G	C1'-C2'-O2'	5.04	115.95	108.40
51	9	1688	C	C4'-C3'-O3'	-5.03	105.45	113.00
75	XX	115	ILE	N-CA-CB	5.03	118.25	111.21
48	5	2845	A	C4'-C3'-O3'	-5.03	105.45	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	7	105	C	C4'-C3'-O3'	-5.03	105.45	113.00
62	KK	42	ASN	N-CA-C	-5.03	102.84	110.28
48	5	2844	A	C3'-C2'-O2'	5.03	118.24	110.70
48	5	4191	G	C1'-C2'-O2'	5.03	115.94	108.40
48	5	4627	U	C1'-C2'-O2'	5.03	115.94	108.40
51	9	464	A	C2'-C3'-O3'	5.03	117.04	109.50
48	5	4278	C	C1'-C2'-O2'	-5.02	100.86	108.40
48	5	48	G	C2'-C3'-O3'	5.02	117.03	109.50
51	9	1495	G	C4'-C3'-O3'	-5.02	105.47	113.00
51	9	453	C	C3'-C2'-O2'	5.02	118.22	110.70
48	5	3789	C	C4'-C3'-O3'	-5.02	105.48	113.00
48	5	4201	G	C4'-C3'-O3'	-5.01	105.48	113.00
48	5	220	C	C4'-C3'-O3'	-5.01	105.48	113.00
48	5	1744	U	C1'-C2'-O2'	5.01	115.92	108.40
51	9	1294	G	C4'-C3'-O3'	5.01	120.52	113.00
24	Y	55	VAL	N-CA-C	5.01	114.47	108.06
48	5	1396	G	C4'-C3'-O3'	-5.01	105.48	113.00
48	5	2088	A	C1'-C2'-O2'	-5.01	104.28	111.80
51	9	472	C	C4'-C3'-O3'	-5.00	105.49	113.00
31	f	63	LYS	CA-C-N	5.00	126.09	119.84
31	f	63	LYS	C-N-CA	5.00	126.09	119.84
48	5	346	G	C1'-C2'-O2'	5.00	115.90	108.40
48	5	978	G	O4'-C4'-C3'	-5.00	99.00	104.00
48	5	2324	C	C4'-C3'-O3'	-5.00	105.50	113.00
51	9	1019	C	C4'-C3'-O3'	-5.00	105.50	113.00
57	FF	78	MET	N-CA-C	5.00	116.67	109.07

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	9	1212	G	Sidechain
51	9	1235	G	Sidechain
51	9	909	G	Sidechain
1	A	195	CYS	Peptide
1	A	196	TRP	Peptide
52	AA	42	LYS	Peptide
52	AA	73	ASP	Peptide
2	B	17	LEU	Peptide
2	B	257	TRP	Peptide
2	B	35	ASP	Peptide
2	B	351	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	B	36	ASP	Peptide
2	B	37	PRO	Peptide
53	BB	106	THR	Peptide
53	BB	150	ILE	Peptide
53	BB	211	PHE	Peptide
3	C	149	GLU	Peptide
3	C	245	HIS	Peptide
3	C	339	THR	Peptide
3	C	48	ASN	Peptide
3	C	73	VAL	Peptide
4	D	36	LEU	Peptide
55	DD	201	LYS	Peptide
5	E	123	SER	Peptide
5	E	125	GLY	Peptide
5	E	126	ARG	Peptide
5	E	149	LEU	Peptide
56	EE	205	PHE	Peptide
56	EE	66	MET	Peptide
57	FF	43	GLU	Peptide
7	G	27	VAL	Peptide
59	HH	111	LYS	Peptide
9	I	167	ILE	Peptide
9	I	168	SER	Peptide
9	I	203	ARG	Peptide
9	I	204	GLY	Peptide
61	JJ	38	ARG	Peptide
11	L	66	TYR	Peptide
63	LL	115	PRO	Peptide
63	LL	134	LEU	Peptide
14	O	148	LYS	Peptide
14	O	191	ARG	Peptide
14	O	68	ARG	Peptide
66	OO	103	ASN	Peptide
66	OO	145	GLY	Peptide
68	QQ	42	ILE	Peptide
18	S	164	LYS	Peptide
18	S	5	GLY	Peptide
70	SS	11	HIS	Peptide
70	SS	88	LYS	Peptide
70	SS	9	PHE	Peptide
19	T	32	ARG	Peptide
71	TT	42	HIS	Peptide

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Mol	Chain	Res	Type	Group
72	UU	68	THR	Peptide
72	UU	72	GLU	Peptide
21	V	97	TYR	Peptide
73	VV	32	ILE	Peptide
74	WW	27	ILE	Peptide
23	X	126	THR	Peptide
75	XX	98	ASP	Peptide
24	Y	7	VAL	Peptide
76	YY	32	LYS	Peptide
26	a	14	HIS	Peptide
26	a	90	ALA	Peptide
78	aa	46	GLU	Peptide
78	aa	9	GLY	Peptide
31	f	105	LEU	Peptide
33	h	95	LEU	Peptide
86	ii	323	TYR	Peptide
86	ii	325	ASN	Peptide
86	ii	326	LEU	Peptide
87	jj	284	ASP	Peptide
87	jj	596	PHE	Peptide
36	k	28	ASN	Peptide
38	m	111	ARG	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	51	0
2	B	3148	0	3267	75	0
3	C	2875	0	3049	71	0
4	D	2386	0	2419	35	0
5	E	1898	0	2035	75	0
6	F	1870	0	1994	49	0
7	G	1934	0	2087	43	0
8	H	1516	0	1597	31	0
9	I	1655	0	1704	63	0
10	J	1353	0	1386	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	1703	0	1820	68	0
12	M	1137	0	1211	34	0
13	N	1701	0	1749	47	0
14	O	1638	0	1777	40	0
15	P	1242	0	1269	16	0
16	Q	1506	0	1623	22	0
17	R	1508	0	1664	31	0
18	S	1454	0	1496	35	0
19	T	1298	0	1366	12	0
20	U	808	0	831	10	0
21	V	979	0	1039	12	0
22	W	528	0	541	7	0
23	X	976	0	1053	23	0
24	Y	1115	0	1205	13	0
25	Z	1107	0	1182	23	0
26	a	1162	0	1209	20	0
27	b	609	0	650	9	0
28	c	732	0	769	18	0
29	d	888	0	930	15	0
30	e	1053	0	1147	29	0
31	f	876	0	912	29	0
32	g	906	0	998	14	0
33	h	1013	0	1147	30	0
34	i	830	0	916	12	0
35	j	705	0	738	16	0
36	k	569	0	637	3	0
37	l	444	0	483	6	0
38	m	429	0	467	10	0
39	n	222	0	264	6	0
40	o	851	0	922	12	0
41	p	708	0	756	18	0
42	r	1001	0	1060	58	0
43	s	1523	0	1577	30	0
44	t	1238	0	1295	10	0
45	1	125	0	117	2	0
46	2	1616	0	824	23	0
47	3	1593	0	811	47	0
48	5	78486	0	39663	1657	0
49	7	2558	0	1296	31	0
50	8	3314	0	1683	58	0
51	9	36680	0	18530	739	0
52	AA	1642	0	1646	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	BB	1729	0	1803	32	0
54	CC	1692	0	1780	46	0
55	DD	1764	0	1863	27	0
56	EE	2073	0	2175	47	0
57	FF	1509	0	1563	29	0
58	GG	1923	0	2089	32	0
59	HH	1521	0	1616	27	0
60	II	1686	0	1772	34	0
61	JJ	1525	0	1640	32	0
62	KK	827	0	854	14	0
63	LL	1238	0	1315	21	0
64	MM	958	0	993	4	0
65	NN	1208	0	1294	13	0
66	OO	1016	0	1039	29	0
67	PP	1060	0	1120	14	0
68	QQ	1124	0	1193	12	0
69	RR	1047	0	1103	16	0
70	SS	1139	0	1191	16	0
71	TT	1102	0	1142	21	0
72	UU	821	0	883	2	0
73	VV	636	0	634	14	0
74	WW	1034	0	1080	22	0
75	XX	1098	0	1167	11	0
76	YY	1023	0	1090	19	0
77	ZZ	598	0	656	9	0
78	aa	781	0	829	23	0
79	bb	651	0	672	7	0
80	cc	475	0	497	7	0
81	dd	445	0	439	13	0
82	ee	457	0	502	5	0
83	ff	520	0	536	13	0
84	gg	2436	0	2393	20	0
85	hh	257	0	129	3	0
86	ii	3280	0	3326	42	0
87	jj	4551	0	4687	75	0
88	5	147	0	0	0	0
88	7	5	0	0	0	0
88	8	2	0	0	0	0
88	9	35	0	0	0	0
88	C	1	0	0	0	0
88	I	1	0	0	0	0
88	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
89	dd	1	0	0	0	0
89	ff	1	0	0	2	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	2	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	16	0	0	7	0
91	jj	54	0	24	0	0
All	All	226453	0	169859	4093	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 10.

All (4093) 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)
9:I:191:ILE:HD12	9:I:200:ILE:CD1	1.25	1.59
9:I:191:ILE:CD1	9:I:200:ILE:HD12	1.17	1.55
87:jj:568:ARG:CD	87:jj:597:LEU:O	1.66	1.42
5:E:279:PRO:HG2	31:f:7:CYS:SG	1.60	1.41
42:r:103:HIS:ND1	42:r:106:LEU:CD2	1.85	1.38
9:I:191:ILE:CD1	9:I:200:ILE:CD1	1.90	1.34
48:5:1968:G:H1	48:5:2018:C:N4	1.21	1.34
42:r:64:MET:HE1	42:r:102:TYR:CD1	1.64	1.33
48:5:976:G:H2'	48:5:977:C:O4'	1.21	1.31
51:9:1137:U:O4	51:9:1148:A:N1	1.64	1.29
48:5:2022:C:C5	48:5:2023:C:C6	2.19	1.29
87:jj:568:ARG:HD2	87:jj:597:LEU:O	1.15	1.29
51:9:1309:C:OP1	83:ff:128:ALA:HB1	1.22	1.26
5:E:279:PRO:CG	31:f:7:CYS:SG	2.21	1.25
43:s:59:THR:HG23	48:5:1961:G:OP2	1.20	1.24
5:E:126:ARG:NH2	48:5:1285:U:OP1	1.71	1.22
48:5:2468:U:O4	48:5:2473:A:N1	1.70	1.22
78:aa:26:CYS:SG	89:aa:201:ZN:ZN	1.27	1.20
7:G:86:VAL:CG1	7:G:185:LYS:HG2	1.71	1.19
51:9:872:A:N1	51:9:914:U:O4	1.77	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:568:ARG:NH1	87:jj:597:LEU:C	2.03	1.17
9:I:51:HIS:O	9:I:53:VAL:HG23	1.48	1.14
48:5:1278:C:H3'	48:5:1279:A:H4'	1.29	1.13
48:5:1968:G:N1	48:5:2018:C:N4	1.97	1.13
42:r:103:HIS:CE1	42:r:106:LEU:CD2	2.32	1.12
43:s:14:PHE:CE2	48:5:1960:A:C2	2.38	1.12
48:5:1960:A:C3'	48:5:1961:G:H5"	1.79	1.12
51:9:1137:U:C4	51:9:1148:A:N1	2.18	1.11
9:I:87:ILE:HG12	9:I:138:ILE:HG12	1.32	1.11
9:I:191:ILE:HD11	9:I:200:ILE:HD12	1.13	1.11
11:L:49:ARG:HG2	33:h:119:TYR:HE1	1.14	1.10
42:r:103:HIS:ND1	42:r:106:LEU:HD23	1.51	1.10
48:5:2022:C:C5	48:5:2023:C:C5	2.40	1.09
4:D:200:MET:HA	4:D:200:MET:HE3	1.35	1.08
7:G:86:VAL:HG11	7:G:185:LYS:CG	1.84	1.08
9:I:191:ILE:HD12	9:I:200:ILE:HD11	1.26	1.08
48:5:2367:A:N1	48:5:2788:U:O4	1.87	1.08
48:5:4213:A:N1	48:5:4218:U:O4	1.86	1.08
51:9:1307:U:H2'	51:9:1308:U:H5"	1.30	1.08
42:r:46:ARG:NH2	48:5:666:G:N7	2.00	1.08
46:2:35:A:OP2	68:QQ:146:ARG:NH1	1.87	1.07
51:9:1309:C:P	83:ff:128:ALA:HB1	1.94	1.07
48:5:1960:A:C4'	48:5:1961:G:H5"	1.85	1.06
43:s:14:PHE:HE2	48:5:1960:A:C2	1.72	1.06
11:L:49:ARG:CG	33:h:119:TYR:CE1	2.37	1.06
2:B:163:LEU:CD2	2:B:182:GLU:HG2	1.85	1.05
48:5:2409:U:C4	48:5:2783:A:N1	2.25	1.04
48:5:2409:U:O4	48:5:2783:A:N1	1.90	1.04
43:s:14:PHE:CE2	48:5:1960:A:H2	1.75	1.03
48:5:1279:A:H3'	48:5:1280:C:H5"	1.36	1.03
48:5:2022:C:C6	48:5:2023:C:C6	2.47	1.03
11:L:170:THR:HG23	11:L:173:GLU:H	1.18	1.03
48:5:1960:A:H3'	48:5:1961:G:H5"	1.39	1.03
48:5:2022:C:H2'	48:5:2023:C:C4'	1.88	1.03
5:E:279:PRO:CD	31:f:7:CYS:SG	2.47	1.03
11:L:49:ARG:HG2	33:h:119:TYR:CE1	1.94	1.03
51:9:1309:C:P	83:ff:128:ALA:CB	2.47	1.03
9:I:149:VAL:HG22	9:I:167:ILE:HD11	1.33	1.02
11:L:49:ARG:HG3	33:h:119:TYR:CD1	1.94	1.02
51:9:830:A:N1	51:9:844:U:O4	1.92	1.02
48:5:1929:A:N1	48:5:2054:U:O4	1.93	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:46:ARG:NH2	48:5:666:G:C5	2.27	1.01
43:s:59:THR:CG2	48:5:1961:G:OP2	2.07	1.01
51:9:1137:U:O4	51:9:1148:A:C2	2.15	1.00
51:9:830:A:N6	51:9:844:U:N3	2.09	0.99
9:I:149:VAL:CG2	9:I:167:ILE:HD11	1.93	0.99
42:r:103:HIS:CE1	42:r:106:LEU:HD21	1.96	0.99
42:r:64:MET:HE1	42:r:102:TYR:CE1	1.98	0.98
47:3:67:U:C2'	47:3:68:C:H5'	1.92	0.98
2:B:163:LEU:HD23	2:B:182:GLU:HG2	1.46	0.98
48:5:976:G:C2'	48:5:977:C:O4'	2.12	0.96
5:E:59:TYR:CD2	5:E:64:LEU:HD12	2.00	0.96
9:I:82:LYS:HE3	48:5:1990:A:OP1	1.64	0.96
48:5:3914:U:H3	48:5:4378:A:H61	1.06	0.96
51:9:872:A:N1	51:9:914:U:C4	2.34	0.96
48:5:48:G:O2'	48:5:49:U:OP2	1.82	0.95
11:L:49:ARG:HG3	33:h:119:TYR:CE1	2.01	0.95
48:5:1279:A:C3'	48:5:1280:C:H5"	1.97	0.95
42:r:64:MET:CE	42:r:102:TYR:CD1	2.49	0.94
87:jj:65:CYS:HG	90:jj:601:SF4:FE3	0.63	0.94
51:9:1309:C:OP1	83:ff:128:ALA:CB	2.13	0.94
7:G:29:ASN:HD21	7:G:31:LEU:HD23	1.34	0.94
48:5:1957:U:O2'	48:5:1958:A:O4'	1.87	0.93
5:E:126:ARG:HH21	48:5:1285:U:P	1.91	0.93
7:G:86:VAL:HG11	7:G:185:LYS:HG2	0.93	0.92
51:9:1385:G:C2'	51:9:1386:A:H5'	2.00	0.92
87:jj:568:ARG:HH11	87:jj:597:LEU:C	1.72	0.92
42:r:46:ARG:NH2	48:5:666:G:C8	2.37	0.92
48:5:4633:G:O2'	48:5:4635:A:OP2	1.88	0.91
87:jj:98:PRO:HG2	87:jj:123:LEU:HD11	1.50	0.91
48:5:1983:A:N1	48:5:2008:U:C4	2.39	0.91
48:5:2468:U:N3	48:5:2473:A:N6	2.17	0.91
51:9:1235:G:H2'	51:9:1236:G:H8	1.34	0.90
38:m:99:CYS:HG	89:m:201:ZN:ZN	0.62	0.90
48:5:1968:G:H1	48:5:2018:C:H41	1.15	0.89
48:5:2638:G:N2	48:5:2697:A:N1	2.20	0.89
83:ff:139:CYS:HG	89:ff:200:ZN:ZN	0.55	0.89
51:9:1109:C:O2'	51:9:1110:G:O5'	1.91	0.89
87:jj:58:CYS:HG	90:jj:600:SF4:FE4	0.61	0.89
11:L:56:ARG:O	11:L:116:ARG:NH2	2.06	0.89
48:5:957:G:H1'	48:5:958:G:OP2	1.71	0.88
42:r:103:HIS:ND1	42:r:106:LEU:HD22	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:745:G:H2'	48:5:746:A:O4'	1.74	0.87
2:B:163:LEU:HD21	2:B:182:GLU:HG2	1.57	0.87
38:m:99:CYS:SG	89:m:201:ZN:ZN	1.62	0.87
5:E:279:PRO:HG2	31:f:7:CYS:HG	1.02	0.87
7:G:29:ASN:ND2	7:G:31:LEU:HD23	1.89	0.87
51:9:1109:C:O2	51:9:1109:C:H2'	1.73	0.86
48:5:1968:G:N2	48:5:2018:C:H42	1.73	0.86
51:9:1144:A:H2'	51:9:1145:A:C8	2.09	0.86
83:ff:139:CYS:SG	89:ff:200:ZN:ZN	1.63	0.86
51:9:1235:G:H2'	51:9:1236:G:C8	2.09	0.86
87:jj:55:CYS:HG	90:jj:600:SF4:FE2	0.63	0.85
48:5:1960:A:H3'	48:5:1961:G:C5'	2.06	0.85
54:CC:204:ILE:HD11	54:CC:215:LEU:CD2	2.06	0.85
9:I:49:CYS:SG	9:I:51:HIS:NE2	2.49	0.85
48:5:2395:A:O2'	48:5:2806:A:H1'	1.75	0.85
2:B:163:LEU:CD2	2:B:182:GLU:CG	2.54	0.84
11:L:116:ARG:NH1	11:L:155:MET:O	2.10	0.84
48:5:1958:A:N1	48:5:2026:A:C6	2.45	0.84
86:ii:78:VAL:HG23	86:ii:95:VAL:HG11	1.60	0.84
9:I:49:CYS:HA	9:I:138:ILE:O	1.77	0.84
48:5:1279:A:H3'	48:5:1280:C:C5'	2.08	0.84
43:s:14:PHE:CE2	48:5:1960:A:N3	2.45	0.84
14:O:22:ILE:HD13	14:O:120:VAL:HG11	1.57	0.83
11:L:170:THR:CG2	11:L:173:GLU:HB2	2.08	0.83
3:C:114:ARG:HB2	3:C:114:ARG:CZ	2.07	0.83
47:3:67:U:C3'	47:3:68:C:H5'	2.07	0.83
48:5:1929:A:H61	48:5:2054:U:H3	1.25	0.83
45:1:68:VAL:C	46:2:76:A:O2'	2.22	0.83
47:3:67:U:H2'	47:3:68:C:H5'	1.60	0.83
12:M:81:ASP:OD1	12:M:84:THR:HG23	1.77	0.82
51:9:1307:U:C2'	51:9:1308:U:H5"	2.08	0.82
87:jj:568:ARG:HD3	87:jj:597:LEU:O	1.79	0.82
17:R:168:GLU:O	17:R:172:ARG:HG2	1.79	0.82
48:5:77:U:O4	48:5:335:A:N1	2.12	0.82
87:jj:568:ARG:NH1	87:jj:597:LEU:O	2.11	0.82
11:L:95:GLY:HA3	33:h:119:TYR:HE2	1.43	0.82
42:r:64:MET:CE	42:r:102:TYR:CE1	2.62	0.81
51:9:1102:G:N2	51:9:1103:C:C2	2.47	0.81
21:V:28:CYS:SG	21:V:30:ASP:OD1	2.38	0.81
87:jj:21:CYS:HG	90:jj:601:SF4:FE2	0.53	0.81
5:E:126:ARG:NH1	48:5:712:C:O2'	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:157:ARG:O	5:E:178:ASN:ND2	2.13	0.81
48:5:1755:C:O2'	48:5:1756:U:O5'	1.99	0.81
48:5:1840:G:H3'	48:5:1842:G:P	2.21	0.81
48:5:919:C:N4	48:5:920:C:C4	2.49	0.81
51:9:1309:C:O5'	83:ff:128:ALA:HB2	1.79	0.81
9:I:49:CYS:HB2	9:I:51:HIS:CE1	2.15	0.81
48:5:1278:C:C3'	48:5:1279:A:H4'	2.09	0.81
9:I:51:HIS:O	9:I:53:VAL:CG2	2.28	0.81
48:5:2022:C:H5	48:5:2023:C:C5	1.97	0.81
5:E:124:HIS:O	48:5:1282:G:O6	1.99	0.80
5:E:238:ILE:O	5:E:239:THR:OG1	1.98	0.80
48:5:1957:U:H2'	48:5:1958:A:H8	1.46	0.80
53:BB:172:MET:HE3	53:BB:212:VAL:HG12	1.63	0.80
87:jj:21:CYS:SG	90:jj:601:SF4:FE2	1.70	0.80
48:5:3723:A:H2'	48:5:3724:A:C8	2.17	0.80
43:s:57:LYS:NZ	48:5:1961:G:P	2.54	0.80
47:3:29:A:O2'	47:3:30:G:O5'	1.98	0.80
48:5:4723:A:H2'	48:5:4724:A:C8	2.16	0.79
5:E:251:SER:O	5:E:255:PRO:HD3	1.82	0.79
48:5:2022:C:H2'	48:5:2023:C:O4'	1.81	0.79
48:5:3914:U:H3	48:5:4378:A:N6	1.80	0.79
5:E:254:LEU:O	5:E:254:LEU:HD23	1.83	0.79
48:5:976:G:H4'	48:5:976:G:OP1	1.82	0.79
28:c:83:THR:O	65:NN:151:ALA:O	2.01	0.78
48:5:1960:A:C3'	48:5:1961:G:C5'	2.60	0.78
48:5:1280:C:C4	48:5:1282:G:C6	2.72	0.78
47:3:29:A:HO2'	47:3:30:G:P	2.06	0.78
54:CC:199:PRO:O	54:CC:202:THR:OG1	2.02	0.78
70:SS:11:HIS:O	70:SS:12:ILE:HD12	1.83	0.78
48:5:2758:G:O2'	48:5:2764:A:N3	2.17	0.78
51:9:1385:G:H2'	51:9:1386:A:H5'	1.65	0.78
48:5:1823:G:O3'	48:5:1825:A:P	2.42	0.77
51:9:1137:U:O4	51:9:1148:A:C6	2.37	0.77
42:r:103:HIS:CE1	42:r:106:LEU:HD22	2.17	0.77
11:L:170:THR:HG23	11:L:173:GLU:N	1.96	0.77
48:5:482:G:H2'	48:5:483:G:C8	2.19	0.77
87:jj:568:ARG:NE	87:jj:597:LEU:O	2.16	0.77
51:9:1598:G:H3'	77:ZZ:80:ARG:HD2	1.67	0.77
51:9:1681:U:O2'	51:9:1682:C:O4'	2.03	0.77
42:r:104:PRO:O	42:r:105:ASP:C	2.28	0.77
48:5:504:G:N1	48:5:654:C:C2	2.53	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:62:LYS:HE3	48:5:978:G:OP2	1.85	0.77
38:m:115:CYS:SG	38:m:118:THR:OG1	2.42	0.77
48:5:2468:U:C4	48:5:2473:A:N1	2.52	0.77
51:9:1614:A:OP2	67:PP:42:ARG:NH1	2.18	0.76
51:9:1680:G:O2'	51:9:1681:U:H5'	1.84	0.76
2:B:163:LEU:HD21	2:B:182:GLU:CG	2.14	0.76
42:r:17:LEU:HD21	42:r:19:LYS:HG3	1.66	0.76
48:5:1960:A:C5'	48:5:1961:G:H5"	2.16	0.76
48:5:1983:A:N1	48:5:2008:U:O4	2.18	0.76
4:D:200:MET:HA	4:D:200:MET:CE	2.13	0.76
51:9:1407:U:H2'	51:9:1408:U:C5	2.21	0.76
54:CC:204:ILE:CD1	54:CC:215:LEU:HD21	2.15	0.76
48:5:2773:G:N2	48:5:2774:C:C2	2.54	0.76
51:9:1416:C:H2'	51:9:1417:C:C2	2.21	0.76
51:9:322:C:O2'	51:9:323:C:O5'	2.03	0.76
51:9:1420:G:HO2'	71:TT:4:VAL:N	1.84	0.75
30:e:85:LEU:HD22	30:e:120:ILE:HD13	1.68	0.75
86:ii:39:ILE:HD12	86:ii:93:LEU:HD23	1.67	0.75
47:3:38:A:O2'	47:3:39:U:H5'	1.86	0.75
48:5:2468:U:H3	48:5:2473:A:N6	1.81	0.75
51:9:1144:A:C2	51:9:1145:A:C2	2.75	0.75
19:T:64:VAL:HG13	19:T:72:VAL:HG13	1.68	0.75
51:9:911:C:C2'	51:9:912:C:H5'	2.16	0.75
56:EE:52:LEU:HB3	56:EE:54:TYR:CD1	2.20	0.75
3:C:271:ALA:O	3:C:272:SER:OG	2.01	0.75
9:I:49:CYS:HG	9:I:51:HIS:HE2	1.30	0.75
48:5:504:G:C2	48:5:654:C:O2	2.39	0.75
51:9:1267:C:O2'	51:9:1268:C:H5'	1.87	0.74
54:CC:73:VAL:O	54:CC:73:VAL:HG12	1.87	0.74
14:O:5:GLN:N	14:O:5:GLN:HE21	1.84	0.74
51:9:872:A:C2	51:9:914:U:O4	2.40	0.74
48:5:2826:U:H4'	48:5:2827:G:H5'	1.69	0.74
51:9:1386:A:H2'	51:9:1387:G:C8	2.23	0.74
51:9:872:A:C6	51:9:914:U:O4	2.40	0.74
48:5:2022:C:C3'	48:5:2023:C:H5"	2.17	0.74
4:D:95:TYR:HH	4:D:195:HIS:HE2	1.33	0.74
8:H:27:VAL:HG12	8:H:84:VAL:HG21	1.67	0.74
43:s:14:PHE:CZ	48:5:1960:A:N3	2.55	0.74
49:7:30:C:C2	49:7:48:G:N2	2.55	0.74
11:L:42:ARG:HE	11:L:45:ARG:NH1	1.86	0.73
48:5:2769:U:C2	48:5:2770:C:C5	2.75	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1307:U:H2'	51:9:1308:U:C5'	2.16	0.73
51:9:309:G:N2	51:9:310:C:C2	2.57	0.73
48:5:1835:G:O2'	48:5:1836:G:OP2	2.04	0.73
48:5:2084:C:H3'	48:5:2085:G:C5'	2.18	0.73
87:jj:568:ARG:CZ	87:jj:597:LEU:C	2.61	0.73
48:5:977:C:C2'	48:5:978:G:H5'	2.18	0.73
47:3:35:U:C1'	51:9:1641:A:OP1	2.36	0.73
51:9:945:U:H2'	51:9:946:U:C6	2.24	0.73
11:L:163:LYS:HE2	48:5:509:A:H4'	1.69	0.73
86:ii:91:ASN:HA	86:ii:119:PRO:HA	1.70	0.72
38:m:115:CYS:HG	38:m:118:THR:HG1	1.34	0.72
11:L:100:PRO:O	34:i:25:ARG:NH2	2.22	0.72
13:N:202:ARG:NH2	48:5:1372:A:OP1	2.21	0.72
51:9:872:A:C6	51:9:914:U:C4	2.77	0.72
51:9:1408:U:H2'	51:9:1409:A:C8	2.24	0.72
13:N:181:HIS:CD2	48:5:99:A:H4'	2.24	0.72
48:5:2288:G:N2	48:5:2290:C:C2	2.57	0.72
7:G:86:VAL:HG21	7:G:185:LYS:HE3	1.70	0.72
51:9:1385:G:O2'	51:9:1386:A:H5'	1.89	0.72
51:9:1386:A:H2'	51:9:1387:G:H8	1.54	0.72
18:S:53:LYS:NZ	49:7:74:A:O2'	2.22	0.72
46:2:35:A:OP2	68:QQ:146:ARG:CZ	2.37	0.72
51:9:1447:G:O2'	51:9:1448:A:H5'	1.89	0.72
11:L:42:ARG:HE	11:L:45:ARG:HH12	1.37	0.72
48:5:4371:G:O2'	48:5:4372:U:OP2	2.07	0.72
48:5:1213:G:C6	48:5:1215:C:C2	2.78	0.72
48:5:1359:G:H2'	48:5:1360:G:C8	2.24	0.72
48:5:977:C:C2	48:5:978:G:C8	2.78	0.72
48:5:1176:C:O2'	48:5:1177:U:O4'	2.08	0.72
51:9:1374:C:O2'	51:9:1464:C:O2	2.07	0.72
4:D:33:ARG:NH2	49:7:7:G:O3'	2.23	0.72
48:5:2517:A:N3	48:5:2539:C:O2'	2.22	0.72
51:9:830:A:N6	51:9:844:U:H3	1.86	0.72
51:9:1102:G:C2	51:9:1130:G:N2	2.58	0.72
51:9:1406:G:H3'	51:9:1407:U:H4'	1.71	0.72
78:aa:30:VAL:HG11	78:aa:35:ALA:HB2	1.72	0.72
42:r:64:MET:HE1	42:r:102:TYR:CG	2.24	0.71
46:2:38:C:O2'	51:9:1058:A:OP1	2.08	0.71
87:jj:568:ARG:CZ	87:jj:597:LEU:O	2.38	0.71
48:5:1968:G:H22	48:5:2018:C:H42	1.38	0.71
48:5:181:C:N3	48:5:256:G:C2	2.59	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1724:G:H4'	48:5:1725:U:OP2	1.90	0.71
48:5:2022:C:C4	48:5:2023:C:C2	2.79	0.71
48:5:2022:C:H3'	48:5:2023:C:H5"	1.72	0.71
51:9:1407:U:H2'	51:9:1408:U:C6	2.25	0.71
81:dd:21:CYS:SG	81:dd:23:VAL:N	2.62	0.71
87:jj:249:VAL:HG11	87:jj:562:LEU:HD13	1.72	0.71
4:D:200:MET:HE3	4:D:200:MET:CA	2.15	0.71
8:H:19:SER:OG	8:H:26:ILE:HG13	1.91	0.71
30:e:91:CYS:O	30:e:93:LYS:N	2.24	0.71
48:5:1929:A:N6	48:5:2054:U:H3	1.88	0.71
51:9:751:G:C2	51:9:792:C:N3	2.58	0.71
87:jj:7:ARG:CZ	87:jj:56:ILE:O	2.39	0.71
48:5:516:C:C2	48:5:646:G:N2	2.59	0.71
48:5:2409:U:C4	48:5:2783:A:C2	2.78	0.71
48:5:4461:C:O2	48:5:4516:G:C2	2.44	0.71
16:Q:65:ARG:NH1	48:5:1502:G:OP1	2.24	0.71
54:CC:204:ILE:HD11	54:CC:215:LEU:HD21	1.69	0.71
48:5:4579:U:O2	48:5:4580:U:C2	2.44	0.70
48:5:4901:G:N2	48:5:4921:C:C2	2.59	0.70
51:9:1454:A:OP1	69:RR:3:ARG:NE	2.24	0.70
6:F:171:LEU:HB2	6:F:189:MET:HE1	1.74	0.70
48:5:2022:C:H2'	48:5:2023:C:H4'	1.73	0.70
48:5:5024:C:H2'	60:II:168:GLN:HG3	1.72	0.70
51:9:17:C:O2'	51:9:1194:A:N1	2.21	0.70
54:CC:204:ILE:HD11	54:CC:215:LEU:HD23	1.71	0.70
5:E:279:PRO:HD2	31:f:7:CYS:SG	2.30	0.70
43:s:10:LYS:NZ	48:5:1961:G:OP1	2.24	0.70
48:5:499:G:N2	48:5:656:C:C2	2.60	0.70
56:EE:52:LEU:HB3	56:EE:54:TYR:HD1	1.52	0.70
48:5:2089:G:O2'	48:5:2090:U:OP2	2.08	0.70
48:5:4453:C:C2	48:5:4529:G:C2	2.80	0.70
87:jj:568:ARG:CZ	87:jj:597:LEU:HA	2.21	0.70
48:5:499:G:C2	48:5:656:C:C2	2.80	0.70
48:5:4892:A:N1	48:5:4927:G:O6	2.25	0.70
9:I:51:HIS:ND1	9:I:137:SER:HB2	2.07	0.70
51:9:1011:A:H2'	51:9:1012:A:O4'	1.91	0.70
6:F:164:ILE:HB	6:F:169:ILE:HD12	1.73	0.69
48:5:2367:A:N6	48:5:2798:A:O4'	2.25	0.69
48:5:3751:G:C2'	48:5:3752:C:H5'	2.22	0.69
86:ii:324:GLU:HB3	86:ii:391:ILE:HG23	1.74	0.69
13:N:160:GLU:OE1	13:N:160:GLU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1102:G:N1	51:9:1103:C:C4	2.61	0.69
53:BB:39:PHE:CE2	53:BB:74:LEU:HD23	2.27	0.69
39:n:4:LYS:CE	51:9:1844:U:O4	2.39	0.69
48:5:1682:A:C2	48:5:1683:U:C2	2.81	0.69
48:5:1958:A:C6	48:5:2026:A:C6	2.80	0.69
86:ii:375:LEU:HD12	86:ii:375:LEU:O	1.93	0.69
11:L:170:THR:HG22	11:L:173:GLU:HB2	1.74	0.69
48:5:1378:C:H3'	48:5:1379:C:H5'	1.74	0.69
48:5:1929:A:N7	48:5:1932:A:H1'	2.08	0.69
48:5:2022:C:H2'	48:5:2023:C:C5'	2.22	0.69
25:Z:52:LYS:O	25:Z:65:ARG:NH2	2.25	0.69
43:s:57:LYS:HZ3	48:5:1961:G:P	2.14	0.69
9:I:87:ILE:HG12	9:I:138:ILE:CG1	2.19	0.69
48:5:1367:C:N3	48:5:1369:C:OP2	2.26	0.69
48:5:1962:A:OP1	48:5:2020:U:OP2	2.11	0.68
63:LL:103:GLU:OE1	75:XX:14:ARG:NH2	2.26	0.68
12:M:81:ASP:OD1	12:M:84:THR:CG2	2.42	0.68
11:L:74:ARG:NH2	48:5:76:A:N7	2.41	0.68
41:p:39:CYS:O	41:p:41:PHE:N	2.26	0.68
48:5:4291:G:H5"	48:5:4291:G:N3	2.09	0.68
1:A:180:LEU:HD21	41:p:26:VAL:HG21	1.76	0.68
14:O:18:ARG:NH1	48:5:2053:C:O3'	2.27	0.68
48:5:1367:C:C2	48:5:1370:G:H2'	2.28	0.68
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.76	0.68
48:5:642:G:N2	48:5:643:C:C2	2.62	0.68
48:5:2367:A:N6	48:5:2788:U:N3	2.42	0.68
51:9:1308:U:H2'	51:9:1309:C:O4'	1.94	0.68
10:J:83:LEU:HD12	10:J:170:TYR:OH	1.92	0.68
48:5:4473:A:C2	48:5:4474:A:C5	2.82	0.68
2:B:163:LEU:HD23	2:B:182:GLU:CG	2.18	0.67
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.26	0.67
42:r:64:MET:CE	42:r:102:TYR:CG	2.76	0.67
48:5:2367:A:N6	48:5:2788:U:H3	1.93	0.67
48:5:199:G:C6	48:5:201:C:N4	2.62	0.67
48:5:1379:C:H4'	48:5:1380:G:O4'	1.92	0.67
51:9:980:A:H2'	51:9:981:A:C8	2.30	0.67
36:k:35:LYS:NZ	48:5:2693:G:OP1	2.28	0.67
48:5:1956:A:H2'	48:5:1957:U:H5'	1.77	0.67
51:9:1190:A:H2'	51:9:1191:C:O4'	1.95	0.67
59:HH:172:THR:O	59:HH:176:VAL:HG23	1.95	0.67
31:f:24:HIS:C	31:f:25:THR:HG1	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3751:G:O2'	48:5:3775:A:N6	2.28	0.67
68:QQ:146:ARG:HH21	68:QQ:146:ARG:HG3	1.59	0.67
48:5:3724:A:N6	48:5:3725:G:C6	2.63	0.67
48:5:4942:C:O3'	48:5:4944:C:P	2.53	0.67
57:FF:20:PHE:O	57:FF:94:LYS:NZ	2.27	0.67
5:E:257:ILE:HG22	5:E:263:LEU:HD23	1.77	0.67
26:a:12:ARG:NH1	48:5:1660:U:C4	2.63	0.67
47:3:39:U:O2'	47:3:40:C:H6	1.78	0.67
48:5:504:G:C6	48:5:654:C:N3	2.63	0.67
48:5:4481:U:H2'	48:5:4482:U:C6	2.29	0.67
47:3:35:U:H1'	51:9:1641:A:OP1	1.94	0.66
48:5:1984:A:N6	48:5:2011:C:O2'	2.28	0.66
48:5:2022:C:C4	48:5:2023:C:C6	2.83	0.66
48:5:2905:C:C2	48:5:3590:G:N2	2.63	0.66
51:9:1344:A:N6	51:9:1386:A:H5"	2.09	0.66
48:5:1378:C:H3'	48:5:1379:C:C5'	2.25	0.66
48:5:2793:G:C6	48:5:2797:C:C4	2.83	0.66
74:WW:111:MET:HE3	74:WW:116:ALA:HA	1.76	0.66
12:M:38:VAL:HG21	12:M:55:MET:HE1	1.76	0.66
48:5:1958:A:C6	48:5:2026:A:N1	2.63	0.66
51:9:1406:G:C3'	51:9:1407:U:H4'	2.25	0.66
52:AA:19:LEU:HD11	69:RR:106:LEU:HD11	1.78	0.66
4:D:199:ILE:HG22	4:D:200:MET:SD	2.36	0.66
37:l:2:SER:N	48:5:2406:G:N7	2.43	0.66
48:5:2409:U:O4	48:5:2783:A:C6	2.48	0.66
51:9:1842:C:C2	51:9:1858:G:C2	2.84	0.66
87:jj:597:LEU:C	87:jj:597:LEU:HD12	2.20	0.66
9:I:181:PHE:O	9:I:185:VAL:HG23	1.95	0.66
48:5:1268:G:H4'	48:5:1269:G:OP1	1.96	0.66
48:5:4213:A:H61	48:5:4218:U:H3	1.43	0.66
87:jj:389:ILE:HG12	87:jj:484:LEU:HD22	1.77	0.66
13:N:161:MET:HE2	48:5:54:G:O2'	1.96	0.66
48:5:1960:A:H4'	48:5:1961:G:H5"	1.77	0.66
48:5:22:G:N2	50:8:35:C:C2	2.64	0.66
48:5:4462:C:C2	48:5:4515:G:C2	2.84	0.66
60:II:38:ILE:HD11	60:II:81:VAL:HG23	1.77	0.66
61:JJ:118:GLY:O	61:JJ:120:ALA:N	2.29	0.66
74:WW:11:LEU:HD22	74:WW:72:CYS:SG	2.36	0.66
11:L:95:GLY:HA3	33:h:119:TYR:CE2	2.30	0.66
51:9:1664:A:O2'	51:9:1665:G:O5'	2.14	0.66
55:DD:134:CYS:SG	55:DD:135:GLU:N	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:ii:327:ASP:O	86:ii:329:MET:HG3	1.97	0.66
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.76	0.65
21:V:57:VAL:HG23	21:V:84:GLN:HG2	1.77	0.65
51:9:1679:A:O2'	51:9:1680:G:OP2	2.09	0.65
2:B:39:LYS:NZ	2:B:39:LYS:HB3	2.11	0.65
47:3:76:A:N6	48:5:4371:G:N7	2.45	0.65
48:5:2554:U:H4'	48:5:2555:G:OP1	1.96	0.65
48:5:3656:A:O4'	48:5:3747:A:C2	2.48	0.65
51:9:1012:A:C2	51:9:1013:U:C2	2.84	0.65
51:9:1309:C:O5'	83:ff:128:ALA:CB	2.42	0.65
54:CC:118:ALA:O	54:CC:119:ALA:HB3	1.95	0.65
48:5:1279:A:C2'	48:5:1280:C:H5"	2.26	0.65
51:9:434:G:H2'	51:9:435:A:C8	2.31	0.65
48:5:497:G:N2	48:5:657:C:C2	2.64	0.65
87:jj:65:CYS:SG	90:jj:601:SF4:FE3	1.80	0.65
3:C:209:VAL:HB	3:C:229:LEU:HD13	1.77	0.65
48:5:976:G:H2'	48:5:977:C:C1'	2.24	0.65
42:r:49:VAL:HG22	42:r:64:MET:SD	2.37	0.65
48:5:1957:U:C2'	48:5:1958:A:H8	2.10	0.65
48:5:2022:C:C4	48:5:2023:C:N1	2.65	0.65
3:C:341:LEU:HD21	5:E:46:LEU:HD21	1.78	0.65
8:H:98:HIS:CD2	87:jj:440:GLN:HG2	2.31	0.65
48:5:106:A:H1'	48:5:336:A:C8	2.32	0.65
48:5:917:A:C2	48:5:919:C:C5	2.84	0.64
48:5:1074:G:N2	48:5:1075:G:C2	2.66	0.64
51:9:1265:A:N3	51:9:1265:A:H2'	2.10	0.64
5:E:124:HIS:ND1	5:E:124:HIS:C	2.55	0.64
9:I:149:VAL:CG2	9:I:167:ILE:CD1	2.74	0.64
51:9:14:C:OP2	54:CC:232:THR:HG21	1.97	0.64
51:9:200:G:N2	51:9:201:C:C2	2.65	0.64
11:L:163:LYS:CE	48:5:509:A:H4'	2.27	0.64
48:5:300:A:C2	48:5:301:G:C5	2.86	0.64
9:I:187:GLU:O	9:I:188:LYS:HB2	1.97	0.64
48:5:1081:C:C2	48:5:1220:G:C2	2.85	0.64
48:5:2022:C:N4	48:5:2023:C:N3	2.46	0.64
48:5:4473:A:C2	48:5:4482:U:N3	2.65	0.64
54:CC:75:ILE:HG23	54:CC:80:GLU:OE1	1.97	0.64
48:5:1280:C:H3'	48:5:1281:G:H5"	1.80	0.64
86:ii:78:VAL:HB	86:ii:97:CYS:SG	2.37	0.64
24:Y:49:ILE:HD13	24:Y:80:ILE:HD13	1.79	0.64
48:5:222:C:H2'	48:5:223:G:O4'	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1186:U:H2'	48:5:1187:G:O4'	1.98	0.64
48:5:1468:C:C2	48:5:1498:G:N2	2.66	0.64
48:5:1975:G:O4'	48:5:1984:A:H1'	1.97	0.64
48:5:2256:C:O2	48:5:2256:C:H2'	1.96	0.64
48:5:4462:C:C2	48:5:4515:G:N2	2.65	0.64
48:5:4939:C:O3'	48:5:4941:G:P	2.55	0.64
56:EE:160:ILE:HG21	56:EE:169:ILE:HG22	1.80	0.64
30:e:108:ARG:NH2	30:e:127:ALA:HB3	2.12	0.64
47:3:39:U:HO2'	47:3:40:C:H6	1.45	0.64
48:5:93:G:H2'	48:5:94:A:C8	2.33	0.64
48:5:1958:A:N6	48:5:2026:A:N6	2.45	0.64
51:9:1102:G:C2	51:9:1103:C:C4	2.86	0.64
5:E:108:MET:SD	42:r:94:ARG:NH1	2.70	0.64
9:I:47:PRO:O	9:I:48:LEU:HB2	1.97	0.64
14:O:37:ARG:NH2	48:5:4760:G:OP2	2.31	0.64
29:d:79:ASN:OD1	29:d:79:ASN:N	2.31	0.64
48:5:2768:C:O5'	48:5:2769:U:H5'	1.98	0.64
50:8:60:G:O6	50:8:96:C:O2'	2.16	0.64
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.79	0.64
60:II:182:CYS:SG	60:II:183:GLY:N	2.71	0.64
48:5:2088:A:O2'	48:5:2089:G:P	2.56	0.64
51:9:908:A:O2'	51:9:909:G:O5'	2.12	0.64
51:9:200:G:N1	51:9:201:C:C4	2.66	0.63
51:9:640:A:H2'	51:9:641:A:C8	2.32	0.63
48:5:1358:G:C6	48:5:1379:C:N3	2.66	0.63
58:GG:188:LYS:HA	58:GG:191:ARG:HD3	1.80	0.63
78:aa:8:ASN:O	78:aa:10:ARG:N	2.31	0.63
7:G:29:ASN:OD1	7:G:30:PRO:HD2	1.99	0.63
35:j:59:THR:O	50:8:42:G:OP1	2.15	0.63
48:5:111:C:C2	48:5:331:G:C2	2.86	0.63
48:5:1840:G:C3'	48:5:1842:G:P	2.85	0.63
51:9:1204:A:O2'	51:9:1700:C:OP2	2.15	0.63
5:E:254:LEU:HD23	5:E:254:LEU:C	2.24	0.63
15:P:36:ILE:HD11	15:P:48:LEU:HD11	1.81	0.63
48:5:933:G:C2	48:5:940:C:C6	2.86	0.63
3:C:233:THR:HG22	3:C:259:LYS:HZ2	1.62	0.63
13:N:195:ARG:NH2	48:5:98:A:O3'	2.31	0.63
48:5:1404:G:C2	48:5:1414:C:C2	2.86	0.63
48:5:1550:G:C2	48:5:1579:C:C2	2.85	0.63
48:5:2288:G:N1	48:5:2290:C:C4	2.66	0.63
51:9:911:C:H2'	51:9:912:C:H5'	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:529:ALA:HB3	87:jj:551:LEU:HD12	1.81	0.63
4:D:219:TYR:CE2	4:D:227:ILE:HD11	2.34	0.63
11:L:9:ILE:HD11	26:a:45:PHE:CZ	2.34	0.63
48:5:1999:A:H1'	48:5:2017:A:N1	2.13	0.63
54:CC:100:ALA:O	54:CC:102:LEU:N	2.32	0.63
5:E:202:VAL:HG13	5:E:256:LYS:NZ	2.14	0.63
8:H:93:ARG:HD3	38:m:82:LEU:HD21	1.81	0.63
32:g:64:LEU:HB3	48:5:2749:C:H4'	1.80	0.63
48:5:1957:U:H2'	48:5:1958:A:C8	2.33	0.63
48:5:2258:C:O2	48:5:2258:C:H2'	1.98	0.63
87:jj:595:PHE:CE2	87:jj:596:PHE:O	2.52	0.63
11:L:161:PHE:CD1	26:a:105:ARG:HD2	2.33	0.63
48:5:956:A:H4'	48:5:957:G:OP2	1.98	0.63
51:9:152:U:H2'	51:9:153:G:O4'	1.99	0.63
51:9:1129:G:H3'	51:9:1130:G:H8	1.64	0.63
2:B:312:LYS:HD2	2:B:370:THR:HG21	1.81	0.63
40:o:61:LYS:NZ	48:5:4338:G:N7	2.47	0.63
48:5:181:C:C2	48:5:256:G:N2	2.67	0.63
48:5:2773:G:N1	48:5:2774:C:C4	2.66	0.63
51:9:309:G:N1	51:9:310:C:C4	2.67	0.63
55:DD:126:ILE:HD11	55:DD:134:CYS:SG	2.38	0.63
60:II:162:LEU:HD11	60:II:191:GLU:HG2	1.81	0.63
10:J:62:ILE:HB	10:J:68:ILE:HD11	1.81	0.62
51:9:751:G:N2	51:9:792:C:C2	2.67	0.62
51:9:1408:U:C4	51:9:1409:A:N6	2.67	0.62
51:9:1839:U:H2'	51:9:1840:U:C6	2.34	0.62
48:5:2547:G:N2	48:5:2548:C:C2	2.66	0.62
54:CC:204:ILE:CD1	54:CC:215:LEU:CD2	2.74	0.62
56:EE:55:ALA:HB1	56:EE:60:GLU:HB2	1.81	0.62
48:5:3717:A:O2'	48:5:3718:A:O4'	2.16	0.62
51:9:1228:A:H2'	51:9:1229:G:C8	2.34	0.62
51:9:1339:U:H2'	51:9:1340:U:O4'	1.99	0.62
7:G:86:VAL:HG12	7:G:87:LEU:N	2.15	0.62
48:5:51:A:N3	48:5:1528:U:O2'	2.31	0.62
48:5:1074:G:C2	48:5:1238:A:C2	2.87	0.62
48:5:1956:A:C2'	48:5:1957:U:H5'	2.29	0.62
48:5:5000:G:C2	48:5:5051:C:C2	2.87	0.62
54:CC:94:ILE:HG21	54:CC:159:LYS:HB3	1.80	0.62
87:jj:353:MET:HB2	87:jj:364:ILE:HD12	1.81	0.62
13:N:195:ARG:HH21	48:5:99:A:P	2.22	0.62
48:5:22:G:C2	50:8:35:C:N3	2.67	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1279:A:C2	48:5:1280:C:C2	2.87	0.62
51:9:1771:G:N2	51:9:1772:C:C2	2.67	0.62
57:FF:76:MET:HA	57:FF:155:CYS:SG	2.40	0.62
69:RR:126:MET:O	69:RR:127:ASN:ND2	2.32	0.62
5:E:62:LYS:HE2	48:5:979:C:OP2	1.98	0.62
47:3:1:G:N2	47:3:2:C:C2	2.68	0.62
48:5:1328:G:O2'	48:5:2349:A:OP1	2.18	0.62
48:5:1958:A:C2	48:5:2026:A:C2	2.88	0.62
51:9:1401:A:C2	51:9:1402:A:C6	2.87	0.62
46:2:53:G:C2	46:2:62:C:C2	2.88	0.62
48:5:4510:A:O2'	48:5:4511:A:O4'	2.16	0.62
57:FF:71:ARG:NH1	57:FF:148:ASN:OD1	2.30	0.62
59:HH:43:LEU:HD22	59:HH:72:PHE:CD2	2.35	0.62
87:jj:240:PHE:HB2	87:jj:271:VAL:HG23	1.81	0.62
48:5:112:C:C2	48:5:330:G:C2	2.88	0.62
48:5:1264:C:H2'	48:5:1265:G:O4'	2.00	0.62
53:BB:125:VAL:HG11	53:BB:173:THR:HG23	1.80	0.62
5:E:174:PRO:O	5:E:176:SER:N	2.33	0.62
48:5:723:A:C2	48:5:943:A:N1	2.68	0.62
48:5:1958:A:N6	48:5:2026:A:H61	1.97	0.62
48:5:1968:G:H22	48:5:2018:C:N4	1.97	0.62
48:5:2023:C:H4'	48:5:2023:C:OP1	1.99	0.62
49:7:30:C:N3	49:7:48:G:C2	2.68	0.62
51:9:1235:G:H5'	51:9:1247:C:H42	1.64	0.62
56:EE:100:ARG:HD2	56:EE:102:ILE:HD11	1.81	0.62
40:o:39:ARG:NH1	48:5:295:A:OP2	2.33	0.62
47:3:39:U:O2'	47:3:40:C:C6	2.52	0.62
48:5:1358:G:H8	48:5:1358:G:H3'	1.63	0.62
51:9:1616:U:O4	67:PP:40:ARG:NH1	2.31	0.62
11:L:170:THR:HG23	11:L:173:GLU:HB2	1.82	0.61
48:5:1279:A:H2'	48:5:1280:C:C6	2.35	0.61
48:5:1957:U:O2'	48:5:1958:A:H5'	2.00	0.61
48:5:1957:U:C2'	48:5:1958:A:C8	2.83	0.61
50:8:118:C:C2	50:8:133:G:C2	2.88	0.61
48:5:3752:C:O2'	48:5:3753:G:OP2	2.15	0.61
61:JJ:29:LEU:HD11	82:ee:37:GLN:HG2	1.82	0.61
10:J:53:ALA:HB2	10:J:68:ILE:HD12	1.81	0.61
48:5:707:C:H42	48:5:1290:G:H1	1.48	0.61
1:A:13:GLY:O	1:A:15:VAL:N	2.32	0.61
48:5:1213:G:N1	48:5:1215:C:C2	2.69	0.61
48:5:1984:A:N7	48:5:2011:C:H4'	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:5066:U:H2'	48:5:5067:U:C6	2.35	0.61
51:9:322:C:HO2'	51:9:323:C:P	2.24	0.61
51:9:1589:A:N3	51:9:1653:U:O2'	2.33	0.61
5:E:125:GLY:O	5:E:127:LYS:HG3	2.00	0.61
9:I:191:ILE:HD12	9:I:200:ILE:HD12	0.86	0.61
42:r:103:HIS:ND1	42:r:106:LEU:HD21	1.97	0.61
48:5:1999:A:O2'	48:5:2000:G:O4'	2.18	0.61
48:5:3751:G:O2'	48:5:3752:C:H5'	2.01	0.61
48:5:960:A:N6	48:5:1283:G:O6	2.33	0.61
48:5:1991:A:N6	48:5:2003:G:OP1	2.34	0.61
13:N:180:PHE:O	13:N:182:HIS:N	2.33	0.61
42:r:104:PRO:O	42:r:106:LEU:N	2.33	0.61
48:5:515:C:C2	48:5:647:G:C2	2.89	0.61
48:5:5061:A:O2'	48:5:5062:G:OP2	2.08	0.61
5:E:54:SER:OG	5:E:55:ARG:N	2.33	0.61
13:N:10:LEU:HD12	34:i:48:CYS:SG	2.40	0.61
48:5:977:C:C4	48:5:978:G:N7	2.69	0.61
55:DD:31:GLU:OE1	55:DD:106:ARG:NH2	2.34	0.61
86:ii:324:GLU:CB	86:ii:391:ILE:HG23	2.31	0.61
48:5:504:G:C6	48:5:654:C:C2	2.89	0.61
51:9:830:A:N1	51:9:844:U:C4	2.67	0.61
78:aa:78:ALA:HB1	78:aa:84:VAL:HG22	1.82	0.61
14:O:26:GLN:OE1	14:O:31:ARG:NH1	2.33	0.61
42:r:17:LEU:HD23	42:r:18:ILE:N	2.16	0.61
48:5:1280:C:HO2'	48:5:1282:G:H8	1.46	0.61
51:9:1681:U:O2'	51:9:1682:C:O5'	2.18	0.61
87:jj:412:LYS:HD2	87:jj:485:ILE:HG23	1.82	0.61
43:s:57:LYS:NZ	48:5:1961:G:OP1	2.32	0.60
51:9:1613:G:C2	51:9:1627:C:C2	2.88	0.60
64:MM:50:CYS:SG	64:MM:51:VAL:N	2.74	0.60
4:D:129:GLU:HG3	4:D:177:THR:HG21	1.83	0.60
28:c:32:LYS:HD2	48:5:2658:G:O6	2.01	0.60
28:c:82:GLY:HA2	28:c:91:VAL:CG1	2.31	0.60
28:c:82:GLY:HA2	28:c:91:VAL:HG13	1.83	0.60
48:5:1899:G:N2	48:5:1900:C:C2	2.69	0.60
48:5:2022:C:C3'	48:5:2023:C:C5'	2.79	0.60
48:5:2814:C:O2	48:5:2814:C:C2'	2.49	0.60
51:9:195:C:C2	51:9:205:G:N2	2.70	0.60
51:9:1102:G:N2	51:9:1130:G:N2	2.48	0.60
5:E:217:GLN:NE2	5:E:233:LYS:HD2	2.16	0.60
42:r:64:MET:HE3	42:r:102:TYR:CZ	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4600:G:OP1	87:jj:506:ARG:NH1	2.34	0.60
51:9:163:U:OP2	58:GG:87:ARG:NH2	2.35	0.60
51:9:1409:A:N6	51:9:1410:C:C4	2.69	0.60
86:ii:21:ILE:HD11	86:ii:136:LEU:HB3	1.83	0.60
6:F:91:LEU:HD22	6:F:92:ALA:N	2.17	0.60
11:L:167:ARG:NH1	11:L:173:GLU:OE1	2.34	0.60
26:a:61:TYR:N	48:5:4354:U:O4	2.33	0.60
42:r:48:THR:N	42:r:102:TYR:OH	2.31	0.60
48:5:4901:G:C2	48:5:4921:C:N3	2.70	0.60
67:PP:34:MET:HE2	67:PP:34:MET:HA	1.83	0.60
16:Q:43:PHE:CE2	16:Q:138:LEU:HD12	2.37	0.60
43:s:14:PHE:HE2	48:5:1960:A:N3	1.91	0.60
48:5:2108:G:C6	48:5:2125:C:N4	2.69	0.60
48:5:4281:A:C2	48:5:4283:G:C6	2.90	0.60
51:9:1298:G:O2'	51:9:1299:A:C8	2.50	0.60
56:EE:102:ILE:HG23	56:EE:182:MET:HE1	1.82	0.60
65:NN:55:ARG:HD2	79:bb:47:PHE:CD2	2.36	0.60
76:YY:85:ASN:HD22	76:YY:85:ASN:H	1.49	0.60
29:d:23:ARG:HD3	29:d:57:MET:HE1	1.83	0.60
48:5:1983:A:C6	48:5:2008:U:O4	2.55	0.60
48:5:1987:C:O2	48:5:1987:C:H2'	2.00	0.60
48:5:4714:C:C5	48:5:4715:C:C5	2.89	0.60
51:9:488:U:O2	51:9:488:U:H2'	2.01	0.60
2:B:39:LYS:HB3	2:B:39:LYS:HZ3	1.66	0.60
48:5:2089:G:H2'	48:5:2089:G:N3	2.16	0.60
48:5:1358:G:H3'	48:5:1358:G:C8	2.36	0.60
48:5:1360:G:C6	48:5:1361:G:C5	2.90	0.60
48:5:2022:C:N4	48:5:2023:C:C2	2.70	0.60
86:ii:327:ASP:HB3	86:ii:348:PRO:HG3	1.83	0.60
43:s:43:ILE:HD13	43:s:187:LEU:HD21	1.84	0.60
43:s:57:LYS:HZ1	48:5:1961:G:P	2.22	0.60
48:5:986:C:C2	48:5:1068:G:N2	2.69	0.60
48:5:1358:G:O2'	48:5:1359:G:O4'	2.18	0.60
9:I:49:CYS:SG	9:I:51:HIS:CE1	2.95	0.60
51:9:909:G:HO2'	51:9:910:G:H8	1.48	0.60
48:5:3668:C:C2	48:5:3675:G:C2	2.90	0.59
48:5:4411:G:C2	48:5:4432:C:C2	2.90	0.59
51:9:50:A:C2	51:9:488:U:O4	2.55	0.59
48:5:1983:A:C2	48:5:2008:U:C4	2.89	0.59
48:5:2446:C:C2	48:5:2515:G:C2	2.90	0.59
1:A:179:ILE:HB	48:5:3653:A:H4'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:150:CYS:SG	10:J:151:ILE:N	2.71	0.59
25:Z:11:VAL:HG11	25:Z:80:LEU:HD13	1.84	0.59
48:5:2408:U:C2	48:5:2409:U:O4	2.55	0.59
51:9:834:C:N3	51:9:841:G:C2	2.71	0.59
4:D:3:PHE:HB2	48:5:1755:C:C6	2.37	0.59
8:H:19:SER:OG	8:H:26:ILE:CG1	2.50	0.59
13:N:138:PHE:CZ	48:5:18:C:H1'	2.38	0.59
28:c:38:ILE:HD11	28:c:46:VAL:HG21	1.84	0.59
42:r:10:VAL:O	42:r:12:ASN:N	2.35	0.59
49:7:30:C:C2	49:7:48:G:C2	2.91	0.59
51:9:1398:G:N2	51:9:1399:C:C2	2.70	0.59
52:AA:24:HIS:HB3	52:AA:51:LEU:HD11	1.84	0.59
62:KK:15:LEU:HD22	62:KK:49:MET:HE1	1.83	0.59
3:C:357:ALA:O	3:C:361:LYS:HG3	2.03	0.59
9:I:49:CYS:CB	9:I:51:HIS:CE1	2.86	0.59
18:S:93:MET:SD	18:S:113:MET:HE1	2.43	0.59
48:5:2090:U:P	48:5:2090:U:O4'	2.60	0.59
48:5:2616:C:C2	48:5:2722:G:C2	2.90	0.59
48:5:4757:C:O2	48:5:4757:C:O4'	2.20	0.59
51:9:291:G:O5'	51:9:291:G:C8	2.55	0.59
2:B:261:ARG:HE	48:5:3870:C:H4'	1.68	0.59
9:I:184:MET:HE2	9:I:189:ARG:HD2	1.84	0.59
47:3:68:C:O2'	47:3:69:G:O4'	2.19	0.59
51:9:598:G:N2	51:9:639:C:C2	2.71	0.59
51:9:1528:G:N2	51:9:1529:C:C2	2.71	0.59
59:HH:61:ILE:HD13	59:HH:93:VAL:HG13	1.83	0.59
87:jj:485:ILE:HD12	87:jj:517:VAL:HG22	1.84	0.59
3:C:158:VAL:HG12	3:C:217:ILE:HD12	1.83	0.59
8:H:99:PHE:HA	87:jj:440:GLN:NE2	2.16	0.59
35:j:17:THR:HG22	35:j:29:LEU:HD21	1.84	0.59
48:5:1297:U:OP2	48:5:1297:U:O4'	2.21	0.59
48:5:1928:C:C4	48:5:2054:U:O2	2.56	0.59
48:5:1958:A:C6	48:5:2026:A:N6	2.71	0.59
48:5:2688:G:N2	48:5:2689:C:C2	2.71	0.59
50:8:56:G:C4	50:8:62:A:C2	2.90	0.59
51:9:15:U:H2'	51:9:16:G:O4'	2.03	0.59
51:9:1298:G:O2'	51:9:1299:A:O5'	2.20	0.59
59:HH:23:ILE:HD11	59:HH:60:ILE:HD13	1.84	0.59
86:ii:327:ASP:OD1	86:ii:327:ASP:N	2.35	0.59
10:J:83:LEU:HD12	10:J:170:TYR:CZ	2.37	0.59
47:3:10:G:N2	47:3:11:C:C2	2.71	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:841:G:N2	51:9:842:C:C2	2.71	0.59
51:9:872:A:N6	51:9:914:U:C5	2.71	0.59
48:5:77:U:N3	48:5:335:A:N6	2.51	0.59
48:5:1277:G:N2	48:5:1278:C:C2	2.70	0.59
49:7:82:G:C2	49:7:95:C:C2	2.91	0.59
51:9:211:G:N2	51:9:212:C:C2	2.71	0.59
42:r:17:LEU:HD23	42:r:17:LEU:C	2.28	0.59
48:5:1541:C:C2	48:5:1619:G:C2	2.90	0.59
48:5:2294:G:N2	48:5:2295:C:C2	2.70	0.59
51:9:115:U:H2'	51:9:116:U:C6	2.37	0.59
51:9:1835:A:C4	51:9:1863:A:N7	2.70	0.59
61:JJ:97:ILE:O	61:JJ:100:LEU:HB2	2.02	0.59
23:X:52:LEU:HD22	23:X:53:ARG:N	2.18	0.58
33:h:119:TYR:N	33:h:119:TYR:HD1	2.01	0.58
48:5:642:G:N1	48:5:643:C:C4	2.70	0.58
48:5:2089:G:HO2'	48:5:2090:U:P	2.25	0.58
48:5:4419:U:OP1	48:5:4421:C:N4	2.36	0.58
53:BB:62:LEU:HA	53:BB:65:ARG:HE	1.68	0.58
86:ii:119:PRO:HB2	86:ii:165:THR:HG21	1.84	0.58
30:e:30:LYS:NZ	48:5:2347:A:N3	2.51	0.58
32:g:9:ARG:HG3	32:g:34:TYR:CE2	2.39	0.58
48:5:1550:G:N1	48:5:1551:C:C2	2.71	0.58
48:5:2793:G:C5	48:5:2797:C:N4	2.71	0.58
51:9:1201:U:H2'	51:9:1202:U:C6	2.38	0.58
51:9:1235:G:O2'	51:9:1236:G:O4'	2.13	0.58
19:T:27:LEU:O	19:T:28:ALA:C	2.46	0.58
9:I:92:HIS:HB2	9:I:94:PHE:CE2	2.39	0.58
14:O:156:LEU:HD13	48:5:4910:G:C4	2.39	0.58
31:f:49:TYR:O	31:f:69:VAL:HB	2.03	0.58
51:9:1455:A:O2'	51:9:1456:G:O5'	2.21	0.58
48:5:2693:G:C6	48:5:2694:G:N1	2.71	0.58
48:5:3612:C:H1'	48:5:5016:A:C8	2.38	0.58
51:9:1717:C:C2	51:9:1817:G:N2	2.72	0.58
30:e:36:ARG:NH1	48:5:2322:G:OP1	2.36	0.58
48:5:106:A:H2'	48:5:107:G:O4'	2.04	0.58
48:5:181:C:N4	48:5:256:G:C6	2.71	0.58
48:5:685:C:O2	48:5:685:C:C2'	2.52	0.58
48:5:2729:C:H2'	48:5:2730:U:O4'	2.04	0.58
48:5:4213:A:N1	48:5:4218:U:C4	2.70	0.58
51:9:316:G:N2	51:9:317:C:C2	2.72	0.58
51:9:1695:A:N1	51:9:1832:A:O2'	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:NN:124:ARG:O	65:NN:125:LEU:C	2.46	0.58
9:I:4:ARG:NH2	9:I:9:TYR:OH	2.37	0.58
9:I:191:ILE:CD1	9:I:200:ILE:HD11	2.00	0.58
44:t:121:LEU:HD22	44:t:132:ILE:HD13	1.85	0.58
47:3:53:G:C2	47:3:62:C:C2	2.90	0.58
48:5:1485:C:O2	48:5:1485:C:O4'	2.19	0.58
51:9:1100:A:C2	51:9:1101:U:C2	2.91	0.58
76:YY:55:ILE:HG12	76:YY:75:ILE:HG23	1.85	0.58
11:L:31:ARG:HD2	48:5:337:U:OP1	2.03	0.58
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.34	0.58
42:r:47:LYS:HG2	42:r:102:TYR:CE2	2.38	0.58
48:5:199:G:C2	48:5:220:C:O2	2.57	0.58
48:5:1550:G:C2	48:5:1579:C:O2	2.57	0.58
48:5:1958:A:N3	48:5:2026:A:C2	2.72	0.58
48:5:3684:G:C6	48:5:3685:C:N4	2.72	0.58
9:I:49:CYS:HG	9:I:51:HIS:CD2	2.19	0.58
12:M:42:CYS:HG	12:M:77:TRP:CG	2.22	0.58
17:R:115:ILE:HG22	17:R:119:MET:HE3	1.85	0.58
48:5:1378:C:OP1	48:5:1379:C:H3'	2.04	0.58
48:5:4189:U:H2'	48:5:4190:U:O4'	2.04	0.58
51:9:409:C:C2	51:9:432:G:N2	2.72	0.58
51:9:1406:G:H2'	51:9:1407:U:O3'	2.03	0.58
51:9:1566:G:N7	71:TT:101:ARG:NH2	2.52	0.58
87:jj:254:LYS:O	87:jj:258:THR:HG23	2.04	0.58
35:j:80:GLU:O	35:j:82:THR:HG23	2.04	0.58
42:r:85:ASN:O	42:r:87:ARG:N	2.37	0.58
48:5:665:C:O2	48:5:665:C:H2'	2.03	0.58
48:5:1662:C:H2'	48:5:1663:C:C6	2.39	0.58
48:5:1874:A:H5'	48:5:4218:U:O2	2.03	0.58
48:5:4395:U:H6	48:5:4395:U:H5'	1.68	0.58
13:N:104:GLU:OE2	13:N:161:MET:HE1	2.03	0.57
18:S:9:GLU:HB3	18:S:67:VAL:HG13	1.86	0.57
48:5:2468:U:O4	48:5:2473:A:C2	2.53	0.57
48:5:4462:C:N3	48:5:4515:G:C2	2.72	0.57
51:9:446:G:OP2	60:II:47:ARG:NH1	2.37	0.57
52:AA:111:GLN:HB3	54:CC:63:VAL:CG1	2.34	0.57
61:JJ:46:VAL:HG21	61:JJ:106:LEU:HD11	1.86	0.57
1:A:196:TRP:CG	1:A:197:PRO:N	2.72	0.57
5:E:135:LYS:O	5:E:163:GLN:NE2	2.37	0.57
26:a:21:ARG:NH1	48:5:1317:U:OP1	2.36	0.57
30:e:36:ARG:NH2	48:5:1661:C:OP1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4207:C:C2	48:5:4226:G:C2	2.92	0.57
48:5:4754:G:C2	48:5:4880:C:C2	2.93	0.57
51:9:1235:G:C5'	51:9:1247:C:H42	2.17	0.57
71:TT:33:TRP:O	71:TT:35:ASP:N	2.36	0.57
86:ii:149:ILE:HB	86:ii:226:LEU:HD23	1.85	0.57
87:jj:7:ARG:HD3	87:jj:57:GLY:HA3	1.86	0.57
19:T:74:ILE:HD13	19:T:96:ILE:HD11	1.85	0.57
48:5:3627:G:N2	48:5:3835:C:C2	2.72	0.57
51:9:944:A:C5	51:9:945:U:C5	2.93	0.57
1:A:196:TRP:O	1:A:197:PRO:C	2.47	0.57
44:t:129:ILE:HA	44:t:132:ILE:HD12	1.86	0.57
48:5:127:G:N2	48:5:128:C:C2	2.72	0.57
48:5:2557:G:C2	48:5:2571:C:C2	2.92	0.57
51:9:1526:G:N2	51:9:1527:C:C2	2.72	0.57
61:JJ:94:LEU:HD12	61:JJ:97:ILE:HD12	1.86	0.57
47:3:39:U:O4'	57:FF:135:ARG:NH2	2.38	0.57
48:5:2084:C:H3'	48:5:2085:G:H5'	1.85	0.57
48:5:2623:A:C2	48:5:2624:G:C5	2.92	0.57
51:9:291:G:H4'	51:9:292:A:OP1	2.04	0.57
51:9:833:C:H4'	51:9:834:C:OP1	2.05	0.57
87:jj:568:ARG:CZ	87:jj:597:LEU:CA	2.82	0.57
2:B:21:ARG:HD3	2:B:271:GLN:OE1	2.05	0.57
16:Q:11:ARG:NH2	48:5:1690:C:OP2	2.38	0.57
48:5:2022:C:C5	48:5:2023:C:N1	2.71	0.57
48:5:2654:C:C2	48:5:2681:G:N2	2.73	0.57
48:5:4723:A:C2	48:5:4724:A:C5	2.92	0.57
50:8:83:C:H4'	50:8:85:U:O2	2.04	0.57
51:9:412:G:N2	51:9:429:C:C2	2.72	0.57
68:QQ:12:VAL:HG21	68:QQ:91:ALA:HA	1.86	0.57
8:H:72:THR:HG1	48:5:4690:G:HO2'	1.51	0.57
48:5:516:C:N3	48:5:646:G:C2	2.73	0.57
48:5:1929:A:C8	48:5:1932:A:H1'	2.39	0.57
48:5:1962:A:OP1	48:5:2020:U:P	2.63	0.57
48:5:4691:A:C2	48:5:4700:A:C4	2.92	0.57
48:5:4709:U:C4	48:5:4710:C:C4	2.93	0.57
6:F:115:ARG:HH21	6:F:208:ASN:HA	1.69	0.57
11:L:65:ARG:HG2	11:L:66:TYR:CE2	2.39	0.57
46:2:53:G:N2	46:2:62:C:C2	2.73	0.57
48:5:245:C:O4'	48:5:245:C:O2	2.22	0.57
48:5:1213:G:C2	48:5:1215:C:O2	2.58	0.57
48:5:1278:C:C6	48:5:1279:A:H1'	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1297:U:O4'	48:5:1297:U:P	2.63	0.57
48:5:1354:A:H2'	48:5:1502:G:N1	2.20	0.57
48:5:1886:G:N2	48:5:1894:C:C2	2.72	0.57
48:5:5028:G:C6	48:5:5029:C:N4	2.72	0.57
51:9:1108:G:C2	51:9:1125:C:C2	2.92	0.57
66:OO:105:THR:O	66:OO:106:LYS:C	2.48	0.57
71:TT:65:TYR:HA	71:TT:123:LEU:HD22	1.86	0.57
1:A:4:VAL:HG12	1:A:8:GLN:HB2	1.86	0.57
30:e:44:ARG:HE	30:e:52:GLN:CD	2.12	0.57
48:5:466:A:C2	48:5:467:U:C4	2.92	0.57
48:5:2408:U:C1'	48:5:2409:U:C5	2.88	0.57
48:5:2588:C:OP1	48:5:2767:U:O2'	2.23	0.57
48:5:4441:A:C8	48:5:4441:A:H5"	2.40	0.57
51:9:1760:G:C2	51:9:1773:C:C2	2.92	0.57
87:jj:375:MET:HE1	87:jj:548:PRO:HB3	1.86	0.57
1:A:131:GLY:HA3	48:5:3683:C:C4	2.39	0.57
3:C:253:THR:O	3:C:254:GLU:C	2.46	0.57
33:h:7:ARG:HG3	50:8:86:U:C5	2.40	0.57
48:5:937:U:H2'	48:5:937:U:O2	2.05	0.57
48:5:1279:A:C4	48:5:1280:C:C4	2.92	0.57
48:5:2022:C:C6	48:5:2023:C:H6	2.17	0.57
48:5:3766:A:N1	51:9:1827:U:O2'	2.33	0.57
51:9:1784:G:N2	51:9:1785:C:C2	2.73	0.57
51:9:1857:G:OP2	66:OO:146:ARG:NH1	2.38	0.57
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	1.87	0.57
66:OO:75:MET:SD	80:cc:63:ARG:NH2	2.78	0.57
12:M:116:LYS:HB3	14:O:196:LEU:HD21	1.86	0.56
14:O:27:VAL:CG1	14:O:98:ALA:HB1	2.35	0.56
26:a:132:ARG:NH1	48:5:1468:C:OP1	2.37	0.56
48:5:1468:C:C2	48:5:1498:G:C2	2.93	0.56
51:9:358:C:C2	51:9:405:G:C2	2.93	0.56
60:II:61:ASP:O	60:II:78:ILE:N	2.37	0.56
9:I:191:ILE:HD11	9:I:200:ILE:CD1	1.95	0.56
48:5:976:G:C6	48:5:977:C:C4	2.92	0.56
48:5:1268:G:C2	48:5:1270:A:C8	2.93	0.56
48:5:1358:G:C8	48:5:1358:G:C3'	2.88	0.56
48:5:2547:G:N1	48:5:2548:C:C4	2.73	0.56
56:EE:191:ARG:HD3	56:EE:245:ARG:HB3	1.87	0.56
75:XX:57:VAL:HG11	75:XX:115:ILE:HG22	1.87	0.56
9:I:202:ASN:HB3	49:7:63:C:N3	2.21	0.56
11:L:175:ASN:O	11:L:176:PHE:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:57:ASN:O	48:5:2319:C:H1'	2.05	0.56
44:t:30:PRO:O	44:t:32:ILE:N	2.38	0.56
48:5:723:A:H2	48:5:943:A:N1	2.03	0.56
48:5:1723:A:N1	48:5:1838:A:C2	2.73	0.56
48:5:3765:G:O2'	48:5:3766:A:N7	2.34	0.56
48:5:4075:U:O2'	48:5:4076:G:P	2.63	0.56
51:9:1717:C:C2	51:9:1817:G:C2	2.93	0.56
56:EE:19:MET:SD	56:EE:108:ARG:HD2	2.45	0.56
2:B:174:ARG:NH1	48:5:4985:U:O2	2.39	0.56
24:Y:10:ASP:O	24:Y:11:ARG:C	2.48	0.56
48:5:4461:C:N3	48:5:4516:G:C6	2.74	0.56
48:5:4967:A:C2	48:5:4968:A:C4	2.94	0.56
51:9:1860:A:OP2	78:aa:10:ARG:NH2	2.39	0.56
3:C:262:ASP:O	3:C:271:ALA:O	2.23	0.56
42:r:47:LYS:HB3	42:r:102:TYR:CZ	2.40	0.56
48:5:3726:A:H2'	48:5:3727:A:C8	2.41	0.56
51:9:322:C:O2'	51:9:323:C:P	2.63	0.56
86:ii:328:ILE:HG22	86:ii:374:LEU:HD12	1.88	0.56
2:B:116:ARG:HD2	2:B:122:TRP:CD2	2.41	0.56
3:C:66:SER:HA	3:C:77:PRO:HA	1.88	0.56
11:L:94:ILE:C	33:h:119:TYR:CE2	2.84	0.56
14:O:36:VAL:HG11	14:O:108:ILE:HD12	1.88	0.56
17:R:92:LYS:NZ	48:5:2606:G:O3'	2.38	0.56
18:S:9:GLU:HG2	18:S:33:PHE:CE1	2.40	0.56
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.39	0.56
30:e:37:LYS:NZ	30:e:55:MET:HE3	2.21	0.56
48:5:2256:C:O2	48:5:2256:C:C2'	2.53	0.56
48:5:4508:C:N3	48:5:4512:U:H5	2.02	0.56
51:9:639:C:H2'	51:9:640:A:C8	2.41	0.56
51:9:1303:C:O2	51:9:1303:C:O4'	2.23	0.56
48:5:1447:C:H2'	48:5:1448:G:O4'	2.05	0.56
48:5:1929:A:N1	48:5:2054:U:C4	2.71	0.56
48:5:2367:A:N1	48:5:2788:U:C4	2.70	0.56
48:5:3594:C:O2	48:5:3594:C:H2'	2.03	0.56
51:9:912:C:H3'	51:9:913:A:H5"	1.88	0.56
51:9:1674:G:N7	68:QQ:17:LYS:NZ	2.54	0.56
3:C:271:ALA:C	3:C:272:SER:HG	2.06	0.56
29:d:85:ARG:NH2	29:d:117:LEU:HD12	2.19	0.56
48:5:2027:U:O2'	48:5:2028:C:H5'	2.06	0.56
48:5:4101:C:C2	48:5:4109:G:C2	2.94	0.56
51:9:1727:G:H2'	51:9:1728:U:O4'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:JJ:39:ASN:OD1	61:JJ:41:ARG:HB3	2.06	0.56
61:JJ:110:LEU:HD22	61:JJ:114:VAL:HG23	1.86	0.56
12:M:53:LYS:NZ	48:5:1921:C:O2'	2.39	0.56
17:R:6:LEU:HD13	17:R:10:LEU:HD23	1.88	0.56
25:Z:16:GLY:O	25:Z:18:TYR:N	2.39	0.56
48:5:77:U:H3	48:5:336:A:N6	2.03	0.56
48:5:976:G:C2	48:5:977:C:C2	2.94	0.56
48:5:977:C:H2'	48:5:978:G:O4'	2.05	0.56
48:5:1280:C:C2	48:5:1282:G:C4	2.94	0.56
48:5:1726:U:H3	48:5:1836:G:H1	1.54	0.56
48:5:1960:A:H5"	48:5:1961:G:H5"	1.86	0.56
48:5:2258:C:O2	48:5:2258:C:C2'	2.54	0.56
48:5:4601:U:OP2	48:5:4609:G:N1	2.36	0.56
51:9:291:G:N2	51:9:293:C:OP2	2.33	0.56
51:9:474:G:N2	51:9:475:C:C2	2.74	0.56
51:9:872:A:N6	51:9:914:U:C4	2.74	0.56
51:9:1019:C:H2'	51:9:1020:A:O4'	2.05	0.56
1:A:40:TYR:CE1	48:5:4117:U:C4	2.94	0.56
48:5:685:C:O2	48:5:685:C:H2'	2.06	0.56
48:5:1213:G:O6	48:5:1215:C:C4	2.59	0.56
48:5:1404:G:N2	48:5:1414:C:C2	2.74	0.56
48:5:3685:C:H2'	48:5:3686:G:O4'	2.06	0.56
53:BB:217:MET:HE2	53:BB:220:LYS:HG3	1.88	0.56
55:DD:206:ASP:N	55:DD:206:ASP:OD1	2.39	0.56
5:E:254:LEU:HD21	5:E:258:LYS:CE	2.35	0.55
9:I:3:ARG:NH2	48:5:4431:U:OP2	2.39	0.55
9:I:82:LYS:HE3	48:5:1990:A:P	2.46	0.55
40:o:43:ARG:NH2	48:5:294:G:OP2	2.39	0.55
48:5:3870:C:C2	48:5:3886:G:C2	2.94	0.55
51:9:853:C:O4'	51:9:853:C:O2	2.24	0.55
3:C:228:THR:C	3:C:229:LEU:HD22	2.32	0.55
3:C:229:LEU:HD22	3:C:229:LEU:N	2.21	0.55
4:D:200:MET:O	4:D:240:TYR:HD2	1.89	0.55
14:O:72:HIS:N	48:5:4586:G:OP1	2.39	0.55
48:5:3945:A:H4'	53:BB:54:GLY:HA2	1.89	0.55
48:5:4579:U:H2'	48:5:4580:U:C6	2.41	0.55
51:9:415:A:H2'	51:9:416:U:O4'	2.06	0.55
51:9:1537:A:C2	51:9:1538:C:C2	2.94	0.55
76:YY:85:ASN:H	76:YY:85:ASN:ND2	2.04	0.55
33:h:119:TYR:CD1	33:h:119:TYR:N	2.73	0.55
35:j:27:TYR:HA	35:j:34:CYS:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2:65:G:N2	46:2:66:C:C2	2.74	0.55
48:5:1358:G:H2'	48:5:1359:G:O4'	2.07	0.55
48:5:4589:A:N1	48:5:4621:C:O2'	2.30	0.55
51:9:17:C:H2'	51:9:18:C:C6	2.42	0.55
30:e:108:ARG:HH22	30:e:127:ALA:HB3	1.69	0.55
35:j:19:CYS:SG	35:j:20:ARG:N	2.79	0.55
39:n:11:ARG:HH22	51:9:1844:U:P	2.29	0.55
47:3:35:U:O4'	51:9:1641:A:P	2.64	0.55
48:5:977:C:O2'	48:5:978:G:H5'	2.07	0.55
48:5:1872:G:O2'	48:5:4219:A:N3	2.29	0.55
51:9:830:A:H2'	51:9:831:G:O4'	2.06	0.55
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.89	0.55
48:5:917:A:C6	48:5:919:C:N4	2.74	0.55
48:5:1958:A:C5	48:5:2026:A:N1	2.75	0.55
48:5:1960:A:C4'	48:5:1961:G:C5'	2.74	0.55
48:5:4587:G:C2	48:5:4716:C:C2	2.95	0.55
50:8:139:G:C6	50:8:140:C:C4	2.95	0.55
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.42	0.55
51:9:830:A:N6	51:9:844:U:C2	2.73	0.55
9:I:35:ASP:N	9:I:35:ASP:OD1	2.40	0.55
21:V:20:LEU:HD22	21:V:26:ILE:CG2	2.37	0.55
48:5:1834:U:O2	48:5:1834:U:H2'	2.06	0.55
48:5:2391:G:N2	48:5:2392:C:C2	2.74	0.55
48:5:2827:G:N3	48:5:2827:G:H2'	2.22	0.55
51:9:1144:A:HO2'	51:9:1199:A:HO2'	1.50	0.55
18:S:13:VAL:HG23	18:S:62:VAL:HB	1.87	0.55
48:5:22:G:C2	50:8:35:C:C2	2.94	0.55
48:5:2315:G:C2	48:5:2325:C:O2	2.59	0.55
48:5:3748:A:H2'	48:5:3749:C:C6	2.41	0.55
48:5:4281:A:C2	48:5:4283:G:C5	2.94	0.55
61:JJ:125:HIS:CE1	61:JJ:129:LEU:HD21	2.42	0.55
70:SS:8:LYS:HD3	77:ZZ:49:LEU:HD11	1.88	0.55
11:L:170:THR:HG23	11:L:173:GLU:CB	2.37	0.55
22:W:40:PHE:HD1	22:W:41:LEU:HD22	1.72	0.55
24:Y:2:LYS:C	24:Y:3:PHE:CD1	2.85	0.55
25:Z:49:TYR:CE2	25:Z:133:LYS:HA	2.42	0.55
48:5:962:C:OP2	48:5:2264:C:N3	2.39	0.55
48:5:973:G:N2	48:5:1282:G:HO2'	2.05	0.55
48:5:1534:A:C8	48:5:1637:A:N1	2.75	0.55
48:5:2123:C:O2'	48:5:2124:G:OP2	2.17	0.55
48:5:2494:U:H2'	48:5:2495:U:O4'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:48:LYS:HB3	23:X:42:THR:HG23	1.88	0.55
32:g:59:VAL:HG21	32:g:63:VAL:HG11	1.89	0.55
40:o:55:ILE:HD12	40:o:57:ARG:NH2	2.22	0.55
47:3:35:U:H1'	51:9:1641:A:P	2.46	0.55
48:5:960:A:H5'	48:5:961:G:OP2	2.07	0.55
51:9:832:G:N2	51:9:843:C:C2	2.74	0.55
51:9:1403:C:O2	51:9:1403:C:C2'	2.54	0.55
51:9:1760:G:N2	51:9:1773:C:C2	2.75	0.55
74:WW:82:GLN:O	74:WW:84:LYS:N	2.40	0.55
76:YY:5:VAL:O	76:YY:28:LEU:O	2.25	0.55
2:B:53:MET:HE3	48:5:4626:A:H5'	1.89	0.55
4:D:64:ILE:HD12	4:D:109:LEU:HD22	1.89	0.55
10:J:119:TYR:CD2	70:SS:12:ILE:HG21	2.42	0.55
16:Q:78:LYS:HG2	16:Q:137:VAL:HG23	1.88	0.55
48:5:1266:G:H5"	48:5:2112:G:C2	2.41	0.55
51:9:1292:C:H3'	51:9:1293:A:H5"	1.88	0.55
51:9:1454:A:OP1	69:RR:3:ARG:HG2	2.06	0.55
51:9:1597:C:H4'	51:9:1603:G:C6	2.42	0.55
60:II:182:CYS:SG	60:II:184:ARG:N	2.79	0.55
66:OO:64:ALA:O	66:OO:66:ARG:N	2.40	0.55
48:5:1249:C:C2	48:5:1262:G:C2	2.95	0.54
48:5:2065:G:H2'	48:5:2066:C:O4'	2.07	0.54
48:5:3663:A:H4'	48:5:3664:G:OP2	2.06	0.54
48:5:4724:A:C6	48:5:4725:C:C4	2.94	0.54
51:9:1108:G:N2	51:9:1125:C:C2	2.75	0.54
51:9:1411:G:H3'	51:9:1412:C:H4'	1.88	0.54
12:M:37:LEU:HD11	12:M:47:ARG:HD2	1.89	0.54
14:O:44:SER:HB3	14:O:129:LEU:HD11	1.89	0.54
42:r:97:ILE:HD13	42:r:107:ARG:HA	1.89	0.54
48:5:3876:A:O2'	48:5:3877:A:P	2.64	0.54
76:YY:40:ILE:HG21	76:YY:57:VAL:HG11	1.87	0.54
14:O:126:VAL:O	14:O:126:VAL:HG22	2.08	0.54
23:X:127:LEU:HD12	23:X:127:LEU:C	2.32	0.54
25:Z:78:ASN:OD1	25:Z:78:ASN:N	2.40	0.54
27:b:8:THR:OG1	27:b:9:THR:N	2.40	0.54
29:d:22:THR:HG22	29:d:89:SER:HB3	1.90	0.54
35:j:63:ARG:NH2	50:8:58:G:N7	2.55	0.54
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.54
48:5:2022:C:H3'	48:5:2023:C:C5'	2.37	0.54
48:5:2313:A:O2'	48:5:2314:G:OP1	2.15	0.54
48:5:4495:G:N2	48:5:4506:C:C2	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1537:A:H2'	51:9:1538:C:O4'	2.08	0.54
5:E:52:ARG:NE	5:E:52:ARG:O	2.37	0.54
11:L:63:THR:O	11:L:65:ARG:N	2.40	0.54
28:c:29:LEU:HD23	28:c:94:LEU:HB2	1.90	0.54
35:j:72:ARG:NH2	50:8:94:G:OP2	2.40	0.54
48:5:746:A:H4'	48:5:747:A:OP1	2.07	0.54
48:5:1269:G:C6	48:5:2111:G:N2	2.75	0.54
48:5:4250:G:C2	48:5:4259:C:C2	2.95	0.54
48:5:4283:G:N2	48:5:4284:C:C2	2.74	0.54
48:5:4730:C:O2	48:5:4730:C:O4'	2.25	0.54
51:9:1401:A:C2	51:9:1402:A:N1	2.76	0.54
69:RR:17:ILE:HG23	69:RR:58:MET:HE1	1.89	0.54
1:A:117:GLU:OE1	1:A:121:GLY:N	2.41	0.54
5:E:62:LYS:CE	48:5:978:G:OP2	2.54	0.54
7:G:32:PHE:CZ	25:Z:55:ALA:HA	2.42	0.54
29:d:26:THR:HG23	48:5:4996:C:H4'	1.89	0.54
48:5:100:C:O4'	48:5:100:C:O2	2.24	0.54
48:5:286:U:H2'	48:5:287:U:C6	2.43	0.54
48:5:1268:G:C4	48:5:2111:G:N2	2.76	0.54
48:5:2409:U:C5	48:5:2783:A:C2	2.96	0.54
48:5:3593:C:H4'	48:5:3594:C:OP2	2.07	0.54
51:9:1118:C:O2	51:9:1118:C:O4'	2.24	0.54
54:CC:83:LEU:HD23	54:CC:84:PHE:CE2	2.43	0.54
57:FF:139:VAL:HG21	80:cc:27:CYS:SG	2.48	0.54
77:ZZ:68:ILE:HB	77:ZZ:109:TYR:HB2	1.90	0.54
85:hh:47:U:H2'	85:hh:48:U:C6	2.42	0.54
86:ii:166:ARG:NH2	86:ii:265:ASN:HB3	2.22	0.54
18:S:169:THR:OG1	48:5:4876:U:C2	2.61	0.54
48:5:3782:C:N3	48:5:3811:G:C2	2.76	0.54
51:9:113:G:C2	51:9:293:C:C2	2.95	0.54
51:9:167:G:C6	51:9:168:C:C5	2.96	0.54
51:9:216:C:O2	51:9:216:C:O4'	2.26	0.54
51:9:1117:C:O2	51:9:1117:C:O4'	2.25	0.54
51:9:1705:C:O5'	51:9:1705:C:H6	1.91	0.54
52:AA:123:VAL:HG13	52:AA:145:ILE:HB	1.89	0.54
55:DD:142:LEU:HD13	55:DD:182:LEU:HD11	1.90	0.54
5:E:95:ASP:OD1	5:E:96:LYS:N	2.37	0.54
48:5:1380:G:O2'	48:5:1381:U:O2	2.17	0.54
48:5:1483:C:O4'	48:5:1483:C:O2	2.25	0.54
48:5:1929:A:H3'	48:5:1929:A:N3	2.23	0.54
48:5:2301:G:N2	48:5:2302:C:C2	2.76	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3642:A:OP1	48:5:3644:U:OP1	2.26	0.54
48:5:4524:G:OP2	48:5:4524:G:H4'	2.06	0.54
48:5:4714:C:C6	48:5:4715:C:C5	2.96	0.54
50:8:56:G:C2	50:8:57:C:C2	2.96	0.54
51:9:615:C:H2'	51:9:616:A:O4'	2.07	0.54
78:aa:30:VAL:CG1	78:aa:35:ALA:HB2	2.37	0.54
87:jj:58:CYS:SG	90:jj:600:SF4:FE4	1.80	0.54
7:G:157:ILE:HG23	7:G:167:VAL:HG11	1.88	0.54
36:k:37:ARG:NH2	48:5:2537:A:OP2	2.41	0.54
48:5:43:U:H2'	48:5:44:A:O5'	2.07	0.54
48:5:4454:G:O2'	48:5:4500:U:O2'	2.19	0.54
49:7:111:C:H2'	49:7:112:U:O4'	2.07	0.54
51:9:145:G:N1	51:9:146:G:C6	2.76	0.54
51:9:1406:G:C4	51:9:1407:U:H1'	2.43	0.54
11:L:99:ASP:OD1	11:L:101:ARG:N	2.41	0.54
16:Q:67:ILE:HD12	16:Q:96:PRO:HD2	1.89	0.54
16:Q:186:TYR:CD2	48:5:4307:A:H4'	2.42	0.54
18:S:84:TYR:CD1	18:S:84:TYR:C	2.86	0.54
42:r:31:ASN:HD21	42:r:35:ARG:N	2.06	0.54
48:5:1755:C:O2'	48:5:1755:C:O2	2.16	0.54
48:5:3680:U:O2	48:5:3680:U:H2'	2.06	0.54
48:5:3782:C:C2	48:5:3811:G:N2	2.76	0.54
49:7:108:G:C6	49:7:109:U:C4	2.96	0.54
51:9:1650:A:C5	51:9:1675:A:C2	2.95	0.54
56:EE:49:ARG:HB3	56:EE:55:ALA:HB3	1.89	0.54
56:EE:102:ILE:CG2	56:EE:182:MET:HE1	2.38	0.54
57:FF:25:THR:HG21	57:FF:46:ALA:HB3	1.89	0.54
57:FF:61:PHE:CE2	80:cc:51:ARG:HD2	2.43	0.54
32:g:8:ARG:HH22	48:5:2521:G:P	2.30	0.54
40:o:18:HIS:HD1	48:5:4318:C:HO2'	1.56	0.54
47:3:35:U:C1'	51:9:1641:A:P	2.96	0.54
48:5:32:G:N1	48:5:48:G:O2'	2.38	0.54
48:5:516:C:C2	48:5:646:G:C2	2.95	0.54
48:5:747:A:C5	48:5:916:C:N4	2.76	0.54
48:5:2020:U:O2	48:5:2020:U:H2'	2.08	0.54
48:5:3911:C:H2'	48:5:3912:U:C6	2.42	0.54
51:9:872:A:N6	51:9:915:G:C4	2.76	0.54
51:9:1401:A:H2'	51:9:1402:A:C8	2.43	0.54
51:9:1542:C:H5"	71:TT:62:ARG:NH1	2.23	0.54
54:CC:233:LEU:C	54:CC:233:LEU:HD12	2.32	0.54
5:E:112:TYR:CE2	42:r:108:MET:HE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:184:TYR:HB3	6:F:202:ARG:HG2	1.90	0.53
14:O:192:PHE:O	14:O:195:VAL:N	2.41	0.53
48:5:940:C:H2'	48:5:941:C:O4'	2.08	0.53
48:5:1296:G:H1'	48:5:1297:U:P	2.48	0.53
48:5:1979:A:N1	48:5:1983:A:H5'	2.22	0.53
48:5:4489:G:N2	48:5:4592:C:OP1	2.41	0.53
50:8:76:C:H2'	50:8:77:A:O4'	2.07	0.53
51:9:217:A:C2	51:9:309:G:N1	2.76	0.53
51:9:1384:C:H2'	51:9:1385:G:O4'	2.08	0.53
55:DD:158:ILE:HG23	55:DD:189:MET:HE1	1.90	0.53
56:EE:199:GLU:HB2	56:EE:207:VAL:HG12	1.89	0.53
6:F:94:VAL:HG13	6:F:142:ILE:HD12	1.90	0.53
19:T:154:ILE:HD12	19:T:154:ILE:O	2.08	0.53
48:5:975:C:C3'	48:5:976:G:O4'	2.57	0.53
48:5:1332:C:H2'	48:5:1333:A:C8	2.43	0.53
48:5:2614:C:O2	48:5:2726:G:C2	2.60	0.53
51:9:698:G:N1	51:9:733:C:C2	2.76	0.53
51:9:1137:U:C4	51:9:1148:A:C6	2.94	0.53
57:FF:102:LEU:HD11	77:ZZ:100:VAL:HG21	1.90	0.53
1:A:96:LEU:CD2	1:A:166:VAL:HG21	2.39	0.53
3:C:186:SER:O	3:C:188:ARG:HD2	2.09	0.53
11:L:65:ARG:HG2	11:L:66:TYR:CD2	2.43	0.53
27:b:15:LYS:NZ	48:5:1670:G:OP1	2.24	0.53
41:p:39:CYS:SG	41:p:41:PHE:HB2	2.49	0.53
48:5:1308:C:H2'	48:5:1309:C:C6	2.43	0.53
48:5:1430:C:C2	48:5:1455:G:C2	2.96	0.53
48:5:1998:A:O2'	48:5:1999:A:O4'	2.26	0.53
48:5:2368:A:N6	48:5:2788:U:O2	2.41	0.53
48:5:2394:G:O2'	48:5:2819:U:O4	2.24	0.53
48:5:2743:A:C2	48:5:2744:A:C4	2.96	0.53
2:B:252:ALA:HB3	48:5:4457:U:O2	2.07	0.53
8:H:134:CYS:SG	8:H:135:SER:N	2.81	0.53
48:5:965:G:H2'	48:5:965:G:N3	2.23	0.53
48:5:3916:G:C2	48:5:3917:A:C4	2.97	0.53
48:5:4138:C:C2	48:5:4147:G:C2	2.96	0.53
48:5:5023:C:O2	48:5:5023:C:O4'	2.23	0.53
51:9:71:G:O2'	51:9:72:C:OP1	2.22	0.53
51:9:1856:C:H2'	51:9:1857:G:C8	2.44	0.53
61:JJ:146:SER:O	61:JJ:147:PHE:C	2.51	0.53
4:D:258:LYS:O	4:D:259:ARG:HG3	2.08	0.53
7:G:86:VAL:CG1	7:G:87:LEU:N	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:92:ARG:NH2	48:5:4313:A:OP1	2.41	0.53
48:5:181:C:C2	48:5:256:G:C2	2.97	0.53
48:5:286:U:O2	48:5:287:U:C2	2.61	0.53
48:5:294:G:H3'	48:5:294:G:N3	2.23	0.53
48:5:497:G:C2	48:5:657:C:C2	2.96	0.53
48:5:705:G:N2	48:5:706:C:C2	2.76	0.53
48:5:1241:C:N4	48:5:1270:A:O2'	2.41	0.53
48:5:3765:G:O2'	48:5:3766:A:C8	2.57	0.53
51:9:73:C:O2	51:9:73:C:O4'	2.27	0.53
51:9:641:A:OP1	61:JJ:40:LYS:HE2	2.07	0.53
53:BB:48:LEU:C	53:BB:48:LEU:HD12	2.34	0.53
1:A:130:SER:OG	1:A:131:GLY:N	2.42	0.53
3:C:266:THR:HG22	3:C:269:LYS:HB3	1.91	0.53
18:S:120:ARG:HD2	48:5:2061:U:OP1	2.07	0.53
29:d:78:ARG:HG2	29:d:78:ARG:HH11	1.72	0.53
48:5:2408:U:O4'	48:5:2409:U:C5	2.60	0.53
48:5:4413:C:O4'	48:5:4413:C:O2	2.24	0.53
51:9:1520:G:N3	51:9:1520:G:H2'	2.23	0.53
52:AA:87:VAL:HG12	52:AA:175:TRP:CZ2	2.44	0.53
6:F:115:ARG:NH2	6:F:208:ASN:HA	2.24	0.53
11:L:146:LEU:HB2	11:L:148:THR:HG22	1.90	0.53
27:b:45:PHE:CD1	48:5:1815:G:N7	2.77	0.53
31:f:50:VAL:HG22	31:f:69:VAL:CG1	2.39	0.53
48:5:721:G:C2	48:5:948:C:C2	2.96	0.53
48:5:946:C:C2	48:5:947:C:C5	2.96	0.53
48:5:1969:G:O2'	48:5:1970:A:H5'	2.08	0.53
48:5:2505:C:O2	48:5:2505:C:O4'	2.26	0.53
48:5:2622:G:C6	48:5:2623:A:N7	2.77	0.53
48:5:4524:G:N2	48:5:4525:C:C2	2.77	0.53
48:5:4635:A:C2	48:5:4664:A:C5	2.97	0.53
51:9:1737:G:C5	51:9:1738:C:C5	2.97	0.53
54:CC:66:LEU:HD12	54:CC:93:ILE:HD13	1.90	0.53
43:s:10:LYS:HE2	48:5:1961:G:OP1	2.08	0.53
48:5:158:A:C6	48:5:277:G:C5	2.97	0.53
48:5:1677:U:H4'	48:5:1680:G:N1	2.24	0.53
48:5:2905:C:C2	48:5:3590:G:C2	2.97	0.53
51:9:50:A:N1	51:9:488:U:O4	2.42	0.53
51:9:356:C:H3'	51:9:356:C:O2	2.09	0.53
51:9:398:A:C8	51:9:398:A:H5'	2.44	0.53
51:9:1545:A:H2'	51:9:1546:G:C8	2.44	0.53
53:BB:139:CYS:N	53:BB:172:MET:HE1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:FF:73:THR:HG21	57:FF:90:VAL:HG22	1.91	0.53
59:HH:43:LEU:HD21	59:HH:71:SER:HB3	1.91	0.53
69:RR:126:MET:HA	69:RR:126:MET:HE3	1.91	0.53
2:B:337:VAL:HG21	2:B:345:LEU:HD21	1.90	0.53
3:C:195:LYS:NZ	50:8:21:C:OP1	2.42	0.53
4:D:95:TYR:OH	4:D:195:HIS:NE2	2.34	0.53
5:E:251:SER:O	5:E:255:PRO:CD	2.55	0.53
6:F:85:VAL:HG22	18:S:62:VAL:HA	1.91	0.53
13:N:172:ARG:HG2	48:5:29:G:H5"	1.91	0.53
27:b:40:LEU:O	27:b:41:ARG:C	2.52	0.53
42:r:22:LYS:HA	48:5:2289:C:O2	2.09	0.53
43:s:10:LYS:CE	48:5:1961:G:OP1	2.56	0.53
48:5:919:C:C4	48:5:920:C:C5	2.97	0.53
48:5:1279:A:C5	48:5:1280:C:C4	2.97	0.53
48:5:1412:G:N2	48:5:1413:C:C2	2.76	0.53
48:5:4888:U:O2'	48:5:4889:G:O5'	2.27	0.53
51:9:88:G:C6	51:9:89:C:C4	2.97	0.53
51:9:312:G:O2'	51:9:313:A:OP1	2.16	0.53
51:9:1144:A:C2	51:9:1145:A:N1	2.76	0.53
51:9:1386:A:OP1	51:9:1483:A:N3	2.42	0.53
51:9:1594:A:C6	51:9:1595:U:C5	2.97	0.53
58:GG:141:ILE:HG21	58:GG:153:VAL:HG13	1.91	0.53
12:M:38:VAL:CG2	12:M:55:MET:HE1	2.38	0.53
15:P:15:CYS:SG	15:P:150:LEU:HB2	2.49	0.53
28:c:34:THR:OG1	28:c:95:ALA:HB2	2.08	0.53
31:f:57:THR:HG21	31:f:68:ARG:HG2	1.89	0.53
48:5:1516:G:C6	48:5:1518:A:C4	2.96	0.53
48:5:1987:C:O2	48:5:1987:C:C2'	2.57	0.53
48:5:4583:C:N4	48:5:4718:G:C6	2.77	0.53
51:9:113:G:N2	51:9:293:C:C2	2.77	0.53
51:9:873:G:C6	51:9:914:U:C5	2.97	0.53
51:9:1229:G:H2'	51:9:1230:C:O4'	2.08	0.53
51:9:1406:G:C5	51:9:1407:U:H1'	2.43	0.53
51:9:1661:A:C8	81:dd:14:PHE:HD2	2.26	0.53
51:9:1835:A:N9	51:9:1863:A:N7	2.56	0.53
55:DD:162:ASP:O	55:DD:163:PRO:C	2.52	0.53
59:HH:145:ARG:HA	74:WW:51:GLU:HB2	1.91	0.53
87:jj:116:LYS:CE	87:jj:272:VAL:HG11	2.39	0.53
11:L:95:GLY:CA	33:h:119:TYR:HE2	2.19	0.52
48:5:929:A:H3'	48:5:930:G:C5'	2.39	0.52
48:5:1523:A:C5	48:5:1653:A:C2	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4966:A:C2	48:5:4967:A:C2	2.97	0.52
51:9:464:A:H4'	51:9:465:A:OP2	2.07	0.52
51:9:1489:A:H4'	51:9:1490:G:OP2	2.09	0.52
51:9:1500:G:C2	51:9:1501:C:C2	2.97	0.52
51:9:1644:C:H2'	51:9:1645:C:O4'	2.09	0.52
53:BB:190:PRO:O	53:BB:192:SER:N	2.42	0.52
7:G:102:TYR:CE2	7:G:207:VAL:HG12	2.44	0.52
9:I:45:GLU:O	9:I:46:PHE:CD1	2.63	0.52
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.89	0.52
17:R:71:ARG:NH1	48:5:3605:C:OP2	2.38	0.52
26:a:75:LEU:O	26:a:76:ASP:C	2.52	0.52
48:5:978:G:H2'	48:5:979:C:O4'	2.09	0.52
48:5:1886:G:C2	48:5:1894:C:N3	2.76	0.52
48:5:2424:G:C2	48:5:2426:U:O2	2.62	0.52
51:9:1599:U:O2	51:9:1599:U:O4'	2.26	0.52
51:9:1828:C:H2'	51:9:1829:G:O4'	2.09	0.52
51:9:1834:A:N3	51:9:1834:A:H2'	2.25	0.52
55:DD:16:ILE:HD11	81:dd:36:LEU:HD23	1.91	0.52
68:QQ:34:VAL:HG21	68:QQ:84:ILE:HD12	1.91	0.52
81:dd:4:GLN:HG3	81:dd:5:GLN:N	2.24	0.52
1:A:181:LYS:HD2	48:5:1577:G:C4	2.44	0.52
5:E:62:LYS:O	5:E:63:ALA:HB3	2.09	0.52
14:O:109:PRO:HB2	14:O:110:PRO:CD	2.39	0.52
48:5:8:U:H2'	48:5:9:C:O4'	2.10	0.52
48:5:301:G:C6	48:5:302:C:C4	2.97	0.52
48:5:4895:C:H1'	48:5:4896:G:C8	2.45	0.52
51:9:501:C:O2	51:9:501:C:C2'	2.57	0.52
51:9:911:C:O2'	51:9:912:C:H5'	2.09	0.52
87:jj:289:LEU:HD21	87:jj:299:VAL:HG22	1.91	0.52
8:H:98:HIS:CD2	87:jj:440:GLN:CG	2.92	0.52
13:N:161:MET:HA	13:N:161:MET:HE3	1.91	0.52
14:O:36:VAL:CG1	14:O:108:ILE:HD12	2.40	0.52
48:5:726:G:N2	48:5:940:C:N3	2.58	0.52
48:5:1072:C:O2	48:5:1072:C:C2'	2.58	0.52
48:5:1279:A:H2'	48:5:1280:C:H5"	1.92	0.52
48:5:1982:G:O2'	48:5:2010:A:H4'	2.10	0.52
48:5:2654:C:C2	48:5:2681:G:C2	2.98	0.52
48:5:3878:C:N4	48:5:4518:A:C4	2.77	0.52
48:5:4723:A:C2	48:5:4724:A:C6	2.97	0.52
51:9:50:A:N1	51:9:488:U:C4	2.77	0.52
51:9:688:U:O2	59:HH:122:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1293:A:H2'	51:9:1294:G:O4'	2.09	0.52
53:BB:169:MET:SD	53:BB:169:MET:N	2.82	0.52
56:EE:183:VAL:HG11	56:EE:220:THR:HG21	1.92	0.52
81:dd:6:LEU:HA	81:dd:9:SER:HB2	1.91	0.52
82:ee:41:ARG:HB2	82:ee:42:PHE:CD2	2.44	0.52
3:C:180:ILE:HD11	3:C:227:ILE:HD11	1.91	0.52
9:I:17:TYR:CE2	9:I:23:CYS:SG	3.00	0.52
31:f:100:ARG:NH1	48:5:4752:U:OP1	2.42	0.52
47:3:70:G:H2'	47:3:71:G:C8	2.44	0.52
48:5:2280:G:O5'	48:5:2280:G:H8	1.92	0.52
48:5:3717:A:N1	48:5:3933:G:H1'	2.25	0.52
48:5:4411:G:C2	48:5:4432:C:O2	2.62	0.52
48:5:4769:G:H2'	48:5:4770:U:O4'	2.09	0.52
51:9:195:C:C2	51:9:205:G:C2	2.98	0.52
51:9:309:G:C2	51:9:310:C:C4	2.98	0.52
51:9:832:G:C2	51:9:843:C:C2	2.98	0.52
51:9:958:G:H2'	51:9:959:G:O4'	2.10	0.52
51:9:1149:A:O2'	51:9:1150:A:H3'	2.09	0.52
51:9:1526:G:N1	51:9:1527:C:C4	2.78	0.52
56:EE:38:LEU:C	56:EE:38:LEU:HD12	2.35	0.52
2:B:247:GLY:HA3	2:B:250:LYS:HD2	1.91	0.52
11:L:122:SER:OG	11:L:123:LYS:N	2.42	0.52
48:5:80:C:C2	48:5:104:G:C2	2.97	0.52
48:5:199:G:C2	48:5:201:C:C4	2.98	0.52
48:5:1757:U:H2'	48:5:1758:G:O4'	2.09	0.52
48:5:2579:G:H5"	48:5:2580:U:OP2	2.09	0.52
51:9:2:A:H3'	54:CC:205:VAL:HG11	1.92	0.52
51:9:1431:G:C4	51:9:1432:U:H1'	2.45	0.52
86:ii:328:ILE:O	86:ii:374:LEU:HB2	2.09	0.52
2:B:94:GLU:HB2	2:B:158:GLN:HG3	1.90	0.52
18:S:44:PHE:CZ	18:S:48:VAL:HG21	2.45	0.52
42:r:107:ARG:HD2	42:r:111:ILE:HD12	1.92	0.52
47:3:5:G:N2	47:3:68:C:C2	2.78	0.52
48:5:931:C:O2'	48:5:932:A:P	2.67	0.52
48:5:1301:C:O2	48:5:1301:C:O4'	2.28	0.52
48:5:1422:G:C2	48:5:1464:C:C2	2.98	0.52
48:5:3594:C:O2	48:5:3594:C:C2'	2.57	0.52
48:5:3724:A:C6	48:5:3725:G:C5	2.98	0.52
48:5:4260:U:H2'	48:5:4261:C:C6	2.45	0.52
49:7:42:A:C5	49:7:43:U:C5	2.97	0.52
73:VV:57:GLY:O	73:VV:58:ALA:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:ii:298:THR:OG1	86:ii:299:GLY:N	2.43	0.52
12:M:104:MET:SD	12:M:109:ARG:HA	2.49	0.52
18:S:84:TYR:C	18:S:84:TYR:HD1	2.18	0.52
42:r:67:ARG:O	42:r:68:SER:C	2.52	0.52
48:5:698:G:N2	48:5:699:C:C2	2.78	0.52
48:5:1367:C:O2	48:5:1367:C:H2'	2.09	0.52
48:5:1693:U:H2'	48:5:1694:C:O4'	2.10	0.52
48:5:1910:G:N2	48:5:1911:C:C2	2.78	0.52
48:5:4399:U:H2'	48:5:4400:G:O4'	2.10	0.52
51:9:664:A:H1'	51:9:1164:G:N2	2.25	0.52
51:9:1666:C:H2'	51:9:1667:U:O4'	2.10	0.52
2:B:164:ALA:HB3	2:B:183:ILE:HD11	1.92	0.52
10:J:153:ALA:O	10:J:155:HIS:N	2.42	0.52
12:M:11:ARG:HA	12:M:61:ILE:HG22	1.91	0.52
37:l:20:ASN:O	37:l:41:ARG:NE	2.43	0.52
42:r:32:LEU:HD11	42:r:106:LEU:HD12	1.92	0.52
48:5:1236:C:O2'	48:5:1237:C:O5'	2.25	0.52
48:5:1541:C:C2	48:5:1619:G:N2	2.78	0.52
48:5:1819:G:H5"	48:5:1819:G:C8	2.45	0.52
48:5:1840:G:O3'	48:5:1842:G:P	2.68	0.52
48:5:4094:G:H2'	48:5:4095:G:O4'	2.10	0.52
51:9:303:C:H2'	51:9:304:C:O4'	2.10	0.52
51:9:1405:A:H2'	51:9:1406:G:O4'	2.10	0.52
54:CC:168:GLY:N	54:CC:179:THR:O	2.40	0.52
61:JJ:24:ARG:HG2	61:JJ:24:ARG:HH11	1.75	0.52
68:QQ:39:LEU:HA	68:QQ:42:ILE:HD13	1.92	0.52
86:ii:327:ASP:CB	86:ii:348:PRO:HG3	2.40	0.52
2:B:41:VAL:HA	2:B:187:GLY:HA3	1.92	0.52
3:C:302:LEU:HD22	16:Q:38:ARG:HB2	1.91	0.52
6:F:146:TYR:CE2	6:F:239:GLU:HB3	2.45	0.52
43:s:57:LYS:HE2	48:5:1961:G:OP2	2.09	0.52
46:2:16:C:O4'	46:2:16:C:O2	2.26	0.52
48:5:671:G:C6	48:5:672:C:C4	2.98	0.52
48:5:1339:U:H2'	48:5:1340:C:C6	2.44	0.52
48:5:1958:A:C4	48:5:2026:A:C2	2.98	0.52
48:5:4966:A:H2'	48:5:4967:A:O4'	2.10	0.52
51:9:960:U:H1'	51:9:963:A:N7	2.25	0.52
51:9:1234:C:H6	51:9:1234:C:H5"	1.75	0.52
51:9:1553:C:O2	51:9:1553:C:O4'	2.25	0.52
54:CC:188:CYS:SG	54:CC:235:ASN:OD1	2.68	0.52
60:II:139:LYS:HD2	60:II:145:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:558:PHE:CZ	87:jj:562:LEU:HD11	2.44	0.52
2:B:39:LYS:NZ	2:B:39:LYS:CB	2.73	0.51
8:H:162:GLN:HG3	8:H:180:TYR:HA	1.91	0.51
15:P:118:GLN:NE2	48:5:423:G:N3	2.58	0.51
48:5:1277:G:N1	48:5:1278:C:C4	2.78	0.51
48:5:1322:A:N6	48:5:4446:U:OP1	2.43	0.51
48:5:2127:C:H2'	48:5:2128:G:C8	2.45	0.51
48:5:2490:U:O2'	48:5:2491:C:O4'	2.23	0.51
51:9:752:G:C6	51:9:790:C:N4	2.78	0.51
57:FF:35:LEU:HD23	57:FF:147:VAL:HG22	1.92	0.51
60:II:76:THR:HG21	60:II:105:ASP:O	2.09	0.51
87:jj:482:VAL:HG13	87:jj:516:PHE:CD1	2.45	0.51
5:E:202:VAL:HG13	5:E:256:LYS:HZ1	1.73	0.51
7:G:31:LEU:HB3	25:Z:53:VAL:HG11	1.92	0.51
9:I:47:PRO:HB3	9:I:171:TRP:CE2	2.45	0.51
48:5:2669:C:H2'	48:5:2670:C:O4'	2.10	0.51
48:5:4735:G:C2	48:5:4736:C:C2	2.99	0.51
50:8:137:A:H2'	50:8:138:C:C6	2.46	0.51
51:9:751:G:C6	51:9:792:C:N4	2.78	0.51
51:9:1466:G:N2	51:9:1467:C:C2	2.78	0.51
51:9:1646:C:N3	51:9:1678:A:C8	2.78	0.51
51:9:1834:A:N3	51:9:1834:A:C2'	2.73	0.51
51:9:1864:U:OP2	78:aa:4:LYS:NZ	2.43	0.51
71:TT:23:LYS:HA	71:TT:54:TYR:CE1	2.45	0.51
3:C:57:LEU:O	3:C:58:ALA:C	2.52	0.51
7:G:140:VAL:HG23	7:G:141:ASN:N	2.25	0.51
48:5:751:G:C2	48:5:752:G:N7	2.78	0.51
48:5:1958:A:C2	48:5:2026:A:N1	2.79	0.51
50:8:103:A:C8	50:8:104:A:C8	2.98	0.51
51:9:1857:G:H3'	66:OO:146:ARG:HH22	1.73	0.51
53:BB:110:MET:HE1	53:BB:140:VAL:HG21	1.91	0.51
71:TT:5:THR:HG1	71:TT:65:TYR:HH	1.59	0.51
3:C:95:MET:SD	3:C:95:MET:N	2.80	0.51
7:G:184:LEU:HD12	7:G:190:LEU:CD1	2.40	0.51
9:I:51:HIS:ND1	9:I:137:SER:CB	2.73	0.51
30:e:89:LEU:HD13	30:e:118:LEU:HD22	1.92	0.51
48:5:48:G:HO2'	48:5:49:U:P	2.21	0.51
48:5:190:G:C2	48:5:252:C:C2	2.98	0.51
51:9:592:C:O2	51:9:592:C:O4'	2.27	0.51
51:9:623:G:N2	51:9:624:C:C2	2.78	0.51
51:9:913:A:OP1	59:HH:99:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:RR:38:ILE:HD12	69:RR:39:ALA:N	2.26	0.51
10:J:18:ARG:HG3	10:J:135:GLY:HA3	1.91	0.51
15:P:131:ARG:HD2	15:P:137:ASN:ND2	2.26	0.51
48:5:919:C:N4	48:5:920:C:C5	2.78	0.51
48:5:1285:U:C4	48:5:1286:C:C4	2.98	0.51
48:5:2022:C:C2'	48:5:2023:C:C5'	2.87	0.51
48:5:2108:G:N1	48:5:2125:C:C4	2.79	0.51
51:9:193:C:C2	51:9:207:G:C2	2.99	0.51
51:9:217:A:C2	51:9:218:U:C6	2.99	0.51
51:9:830:A:C6	51:9:844:U:N3	2.78	0.51
51:9:1109:C:O2	51:9:1109:C:C2'	2.49	0.51
51:9:1231:C:H2'	51:9:1232:U:O4'	2.09	0.51
51:9:1379:A:H2'	51:9:1380:C:C6	2.45	0.51
1:A:211:PHE:CG	1:A:219:ILE:HG23	2.45	0.51
2:B:18:PRO:O	2:B:20:LYS:N	2.43	0.51
8:H:72:THR:OG1	48:5:4690:G:O2'	2.23	0.51
39:n:12:ARG:NH1	51:9:1848:U:O4	2.44	0.51
42:r:32:LEU:O	42:r:33:LYS:HB3	2.10	0.51
48:5:721:G:N2	48:5:948:C:C2	2.78	0.51
48:5:1167:C:C2	48:5:1195:G:C2	2.99	0.51
48:5:4758:U:O2	48:5:4758:U:O4'	2.25	0.51
51:9:751:G:O2'	51:9:752:G:O4'	2.25	0.51
51:9:823:U:O2	51:9:823:U:O4'	2.28	0.51
51:9:1308:U:O3'	83:ff:128:ALA:CB	2.58	0.51
51:9:1616:U:OP2	67:PP:43:ARG:NH2	2.43	0.51
58:GG:44:GLU:HB3	58:GG:121:ILE:HD11	1.92	0.51
58:GG:57:ASP:HA	58:GG:106:LEU:HD23	1.91	0.51
66:OO:139:SER:OG	66:OO:140:THR:N	2.43	0.51
1:A:103:PRO:O	1:A:106:THR:OG1	2.26	0.51
19:T:42:ILE:HD13	19:T:89:ILE:HD11	1.93	0.51
30:e:81:ASN:HA	30:e:111:ILE:HD11	1.93	0.51
48:5:363:A:C8	48:5:365:U:C2	2.98	0.51
48:5:1214:C:H1'	48:5:1215:C:OP2	2.10	0.51
48:5:1280:C:O2'	48:5:1282:G:C8	2.61	0.51
48:5:1367:C:H3'	48:5:1368:A:H5"	1.93	0.51
48:5:1958:A:C2	48:5:2026:A:C6	2.98	0.51
48:5:2276:A:H2'	48:5:2277:C:O4'	2.11	0.51
51:9:398:A:H5"	51:9:400:C:O4'	2.10	0.51
51:9:913:A:N3	59:HH:66:VAL:HG11	2.26	0.51
87:jj:96:ARG:HD2	87:jj:299:VAL:O	2.10	0.51
87:jj:568:ARG:NH1	87:jj:597:LEU:CA	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:HIS:O	2:B:260:ALA:N	2.44	0.51
43:s:57:LYS:HE2	43:s:59:THR:HG23	1.93	0.51
48:5:32:G:H1	48:5:48:G:HO2'	1.57	0.51
48:5:105:A:C2	48:5:336:A:C8	2.98	0.51
48:5:1280:C:C2	48:5:1282:G:C5	2.99	0.51
48:5:2022:C:C2'	48:5:2023:C:H5"	2.40	0.51
48:5:2084:C:H3'	48:5:2085:G:H5"	1.91	0.51
48:5:3878:C:N4	48:5:4518:A:O4'	2.42	0.51
48:5:4080:C:C2	48:5:4167:G:C2	2.99	0.51
48:5:4476:C:O2'	48:5:4478:G:OP2	2.27	0.51
51:9:1309:C:O2'	51:9:1310:U:O5'	2.27	0.51
58:GG:68:LEU:O	58:GG:69:THR:O	2.29	0.51
65:NN:135:LEU:HD22	65:NN:139:TRP:CG	2.46	0.51
71:TT:60:THR:HG23	71:TT:75:MET:HE2	1.92	0.51
2:B:42:HIS:CE1	2:B:186:ASN:O	2.64	0.51
2:B:49:TYR:CE2	2:B:168:MET:HE1	2.46	0.51
33:h:88:THR:O	33:h:89:ARG:C	2.54	0.51
40:o:35:ALA:O	40:o:36:GLN:C	2.54	0.51
48:5:199:G:N1	48:5:220:C:C2	2.79	0.51
48:5:230:G:N2	48:5:239:C:C2	2.79	0.51
48:5:956:A:H3'	48:5:957:G:C8	2.45	0.51
48:5:2021:G:O2'	48:5:2022:C:H5'	2.11	0.51
48:5:2481:G:C2	48:5:2498:C:C2	2.99	0.51
48:5:2684:C:H2'	48:5:2685:C:O4'	2.10	0.51
48:5:4681:A:H2'	48:5:4682:U:O4'	2.11	0.51
52:AA:47:TYR:HB2	52:AA:150:THR:HG21	1.93	0.51
54:CC:118:ALA:O	54:CC:119:ALA:CB	2.57	0.51
58:GG:61:PHE:CE2	58:GG:96:SER:HB3	2.46	0.51
68:QQ:51:LEU:HD22	68:QQ:84:ILE:HD11	1.92	0.51
86:ii:75:ILE:HA	86:ii:78:VAL:HG12	1.92	0.51
7:G:99:ALA:O	7:G:102:TYR:N	2.43	0.51
14:O:42:ASN:N	14:O:42:ASN:OD1	2.43	0.51
38:m:95:ILE:HD13	38:m:102:ARG:HA	1.93	0.51
48:5:1928:C:N4	48:5:2054:U:O2	2.43	0.51
48:5:4891:G:C2	48:5:4929:C:C2	2.99	0.51
51:9:52:G:C6	51:9:53:C:C4	2.99	0.51
51:9:384:U:O4	60:II:5:ARG:NH2	2.44	0.51
51:9:688:U:O2	59:HH:122:LEU:HG	2.11	0.51
51:9:1282:A:H3'	51:9:1283:C:C5'	2.40	0.51
51:9:1315:U:O2	51:9:1315:U:O4'	2.28	0.51
51:9:1500:G:C6	51:9:1501:C:C4	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1654:G:N2	51:9:1655:C:C2	2.79	0.51
57:FF:140:ASP:OD1	57:FF:140:ASP:N	2.44	0.51
3:C:86:ARG:HA	3:C:89:GLN:HG3	1.92	0.50
11:L:59:VAL:HG13	48:5:74:G:H5'	1.93	0.50
18:S:127:MET:HE1	19:T:155:PRO:HA	1.92	0.50
40:o:45:GLN:OE1	40:o:52:THR:OG1	2.20	0.50
46:2:39:G:N2	46:2:40:C:C2	2.79	0.50
48:5:279:A:O2'	48:5:280:G:OP2	2.25	0.50
48:5:919:C:N4	48:5:920:C:N4	2.59	0.50
48:5:2076:G:C6	48:5:2077:C:C4	3.00	0.50
48:5:4495:G:C2	48:5:4506:C:C2	2.99	0.50
51:9:834:C:N4	51:9:841:G:C6	2.79	0.50
51:9:1100:A:C6	51:9:1101:U:C4	2.99	0.50
51:9:1432:U:N3	51:9:1433:C:C5	2.80	0.50
51:9:1809:A:C6	51:9:1810:U:C4	2.99	0.50
52:AA:53:ARG:HD3	73:VV:82:ASN:HB3	1.93	0.50
66:OO:31:CYS:HB2	66:OO:44:VAL:HG22	1.92	0.50
84:gg:124:SER:OG	84:gg:125:ARG:N	2.44	0.50
86:ii:251:LEU:HD11	86:ii:278:VAL:CG2	2.41	0.50
7:G:86:VAL:HG21	7:G:185:LYS:CE	2.40	0.50
9:I:87:ILE:HG22	9:I:88:ARG:N	2.26	0.50
11:L:60:ARG:HD3	11:L:67:HIS:O	2.10	0.50
23:X:80:PRO:CD	33:h:33:VAL:HG22	2.40	0.50
42:r:104:PRO:O	42:r:107:ARG:N	2.45	0.50
48:5:470:A:C5	48:5:471:A:C8	2.99	0.50
48:5:1723:A:N1	48:5:1838:A:N1	2.59	0.50
48:5:1771:U:H2'	48:5:1772:C:O4'	2.11	0.50
48:5:2108:G:C2	48:5:2125:C:N3	2.79	0.50
48:5:2773:G:C2	48:5:2774:C:C4	2.99	0.50
48:5:3752:C:H2'	48:5:3777:G:C8	2.47	0.50
62:KK:39:ASN:O	62:KK:40:VAL:C	2.55	0.50
5:E:47:VAL:O	5:E:48:ARG:C	2.55	0.50
6:F:63:TYR:O	6:F:64:ARG:C	2.54	0.50
48:5:1365:C:H4'	48:5:1366:G:OP1	2.11	0.50
48:5:4452:U:O2'	86:ii:185:GLN:HG3	2.12	0.50
48:5:4473:A:C2	48:5:4474:A:C4	3.00	0.50
48:5:4473:A:N1	48:5:4474:A:C6	2.80	0.50
48:5:4583:C:N3	48:5:4718:G:C2	2.80	0.50
48:5:4591:U:H2'	48:5:4592:C:C6	2.46	0.50
51:9:1439:A:H2'	51:9:1440:C:O4'	2.11	0.50
51:9:1442:U:N3	51:9:1443:C:C5	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
72:UU:60:THR:HG22	72:UU:83:ARG:HG2	1.94	0.50
2:B:260:ALA:C	2:B:261:ARG:HD3	2.36	0.50
5:E:276:GLY:C	5:E:277:VAL:HG23	2.36	0.50
9:I:49:CYS:HG	9:I:51:HIS:CE1	2.23	0.50
23:X:105:ASN:OD1	23:X:108:GLN:HG3	2.11	0.50
35:j:12:ARG:NH1	48:5:2801:U:O2'	2.45	0.50
42:r:61:VAL:HG12	42:r:81:THR:HA	1.92	0.50
47:3:39:U:O2'	47:3:40:C:O5'	2.29	0.50
48:5:211:G:H4'	48:5:234:G:C8	2.47	0.50
48:5:730:G:C2	48:5:939:G:N2	2.79	0.50
48:5:1724:G:C4'	48:5:1725:U:OP2	2.57	0.50
48:5:4532:U:H2'	48:5:4533:A:O4'	2.11	0.50
51:9:887:U:O2	51:9:887:U:O4'	2.28	0.50
51:9:1129:G:H3'	51:9:1130:G:C8	2.46	0.50
51:9:1568:C:H2'	51:9:1569:A:C8	2.46	0.50
51:9:1624:U:O2	51:9:1624:U:O4'	2.29	0.50
5:E:127:LYS:O	5:E:132:HIS:CD2	2.64	0.50
48:5:1362:G:N2	48:5:1363:C:C2	2.80	0.50
48:5:1563:A:C8	48:5:1563:A:O5'	2.65	0.50
48:5:1907:A:H2'	48:5:1908:A:C8	2.46	0.50
48:5:2685:C:H3'	48:5:2686:G:H5"	1.93	0.50
51:9:305:U:O2'	51:9:309:G:O4'	2.26	0.50
51:9:639:C:H2'	51:9:640:A:H8	1.77	0.50
51:9:1537:A:H2'	51:9:1538:C:C6	2.47	0.50
51:9:1667:U:H2'	51:9:1668:U:C6	2.46	0.50
51:9:1705:C:H2'	51:9:1706:G:C8	2.47	0.50
62:KK:24:LYS:O	62:KK:26:ASP:N	2.45	0.50
86:ii:375:LEU:HD12	86:ii:375:LEU:C	2.36	0.50
87:jj:99:ILE:HD12	87:jj:99:ILE:N	2.27	0.50
87:jj:284:ASP:N	87:jj:284:ASP:OD1	2.44	0.50
2:B:160:ILE:HD13	2:B:194:LEU:HD13	1.93	0.50
6:F:114:LEU:O	6:F:123:THR:HG21	2.12	0.50
13:N:90:ASN:O	13:N:92:LEU:N	2.44	0.50
35:j:39:TYR:CG	35:j:40:PRO:N	2.78	0.50
44:t:94:LYS:HA	44:t:95:GLN:C	2.37	0.50
48:5:230:G:C2	48:5:239:C:C2	2.99	0.50
48:5:986:C:C2	48:5:1068:G:C2	3.00	0.50
48:5:1358:G:C2'	48:5:1359:G:O4'	2.59	0.50
48:5:3652:A:C2	48:5:3653:A:N1	2.80	0.50
48:5:4423:U:O2	48:5:4423:U:O4'	2.29	0.50
48:5:5015:G:O2'	48:5:5034:A:N6	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:909:G:O2'	51:9:910:G:O5'	2.29	0.50
51:9:1863:A:H1'	78:aa:79:ILE:HD13	1.93	0.50
57:FF:71:ARG:HB3	57:FF:151:ILE:HD13	1.94	0.50
58:GG:121:ILE:HG23	58:GG:122:PRO:HD2	1.94	0.50
66:OO:146:ARG:HA	78:aa:29:CYS:HB2	1.92	0.50
76:YY:58:PHE:CZ	76:YY:72:PHE:HB3	2.47	0.50
10:J:83:LEU:CD1	10:J:170:TYR:CZ	2.95	0.50
11:L:55:LEU:HD22	11:L:120:TYR:CG	2.46	0.50
11:L:90:VAL:O	11:L:93:THR:OG1	2.23	0.50
11:L:94:ILE:O	33:h:119:TYR:CE2	2.65	0.50
11:L:175:ASN:O	11:L:176:PHE:C	2.54	0.50
26:a:25:HIS:CG	48:5:1338:G:H22	2.29	0.50
33:h:6:ALA:O	33:h:7:ARG:C	2.55	0.50
39:n:4:LYS:HE2	51:9:1844:U:O4	2.12	0.50
43:s:10:LYS:NZ	48:5:1961:G:P	2.85	0.50
48:5:973:G:N2	48:5:1282:G:O2'	2.44	0.50
48:5:1235:G:H2'	48:5:1236:C:H5'	1.93	0.50
48:5:1557:C:C2	48:5:1571:G:N2	2.79	0.50
48:5:1908:A:H2'	48:5:1909:G:O4'	2.12	0.50
48:5:1960:A:H4'	48:5:1961:G:C5'	2.41	0.50
51:9:1398:G:N1	51:9:1399:C:C4	2.79	0.50
51:9:1528:G:C2	51:9:1529:C:C4	3.00	0.50
66:OO:21:VAL:HG23	66:OO:25:GLU:HB2	1.93	0.50
70:SS:27:ALA:HB1	70:SS:42:HIS:CE1	2.47	0.50
5:E:199:ILE:O	5:E:256:LYS:NZ	2.44	0.50
7:G:58:PRO:CD	23:X:46:PHE:CD2	2.94	0.50
7:G:100:HIS:HA	7:G:103:ARG:HD2	1.94	0.50
8:H:132:VAL:HG12	8:H:133:ALA:N	2.26	0.50
12:M:122:ILE:HG22	14:O:185:VAL:HG11	1.92	0.50
24:Y:87:ARG:HH21	24:Y:87:ARG:HG3	1.77	0.50
48:5:40:G:H1'	48:5:3914:U:N3	2.27	0.50
48:5:199:G:C6	48:5:220:C:N3	2.79	0.50
48:5:1371:A:N6	50:8:28:C:O2'	2.45	0.50
48:5:1378:C:OP1	48:5:1379:C:C3'	2.60	0.50
48:5:2726:G:C6	48:5:2727:C:N4	2.79	0.50
48:5:4767:C:C2	48:5:4868:G:C2	3.00	0.50
50:8:139:G:C2	50:8:140:C:C2	3.00	0.50
51:9:316:G:N1	51:9:317:C:C4	2.79	0.50
51:9:562:U:H2'	51:9:563:G:C8	2.47	0.50
51:9:659:G:H2'	51:9:659:G:N3	2.27	0.50
51:9:1650:A:C6	51:9:1675:A:C2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1839:U:O4	78:aa:28:ARG:NH2	2.44	0.50
66:OO:145:GLY:O	66:OO:147:ARG:N	2.43	0.50
68:QQ:34:VAL:O	68:QQ:36:GLY:N	2.45	0.50
1:A:37:ARG:NH1	48:5:4088:C:OP1	2.45	0.50
2:B:30:LYS:NZ	48:5:4717:A:OP2	2.35	0.50
6:F:215:LEU:O	48:5:2073:C:H5'	2.12	0.50
10:J:14:GLU:O	10:J:15:LEU:C	2.55	0.50
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.60	0.50
28:c:85:CYS:SG	28:c:94:LEU:HD22	2.51	0.50
37:l:38:ASN:O	37:l:40:LYS:N	2.40	0.50
48:5:181:C:C4	48:5:256:G:N1	2.80	0.50
48:5:707:C:N4	48:5:1290:G:H1	2.10	0.50
48:5:1431:C:C2	48:5:1454:G:N2	2.80	0.50
48:5:1823:G:C3'	48:5:1825:A:P	3.00	0.50
51:9:219:U:H1'	60:II:184:ARG:HD2	1.94	0.50
51:9:516:A:C6	51:9:644:G:N7	2.80	0.50
51:9:570:C:O2	76:YY:34:THR:HB	2.12	0.50
51:9:688:U:H4'	51:9:689:U:O5'	2.12	0.50
51:9:1144:A:C2'	51:9:1145:A:C8	2.90	0.50
51:9:1698:C:O2	51:9:1698:C:O4'	2.29	0.50
52:AA:111:GLN:HB3	54:CC:63:VAL:HG12	1.94	0.50
53:BB:88:THR:HG22	53:BB:96:CYS:HB3	1.92	0.50
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.47	0.50
86:ii:324:GLU:HB3	86:ii:391:ILE:CG2	2.41	0.50
3:C:342:ARG:HG3	3:C:342:ARG:HH11	1.77	0.49
6:F:216:SER:OG	6:F:217:SER:N	2.43	0.49
9:I:12:CYS:HB2	9:I:57:TYR:CE2	2.47	0.49
10:J:93:GLU:HB3	10:J:173:ILE:HD11	1.93	0.49
26:a:70:CYS:SG	26:a:110:LYS:HB2	2.52	0.49
29:d:33:ILE:O	29:d:36:VAL:HG22	2.12	0.49
42:r:47:LYS:CG	42:r:102:TYR:CE2	2.94	0.49
48:5:27:C:O2'	48:5:60:G:N3	2.44	0.49
48:5:1962:A:C2'	48:5:1963:C:O5'	2.60	0.49
48:5:2110:C:C6	48:5:2110:C:OP1	2.65	0.49
48:5:2586:G:O2'	48:5:2587:A:C8	2.64	0.49
48:5:2618:G:C2	48:5:2720:C:C2	3.00	0.49
51:9:448:A:H5"	60:II:25:ARG:HA	1.94	0.49
51:9:1143:A:H2'	51:9:1144:A:O4'	2.12	0.49
51:9:1518:C:O2	51:9:1518:C:O5'	2.30	0.49
59:HH:177:TYR:CD2	59:HH:185:VAL:HG21	2.47	0.49
67:PP:57:LEU:HD11	67:PP:89:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:O	1:A:183:GLY:C	2.54	0.49
6:F:157:TYR:CE1	6:F:189:MET:HG2	2.47	0.49
9:I:153:ARG:HA	9:I:165:ILE:HD11	1.94	0.49
34:i:74:LYS:HA	34:i:83:ALA:HB2	1.94	0.49
34:i:89:GLU:O	34:i:92:SER:OG	2.26	0.49
42:r:106:LEU:O	42:r:108:MET:N	2.45	0.49
48:5:504:G:C2	48:5:654:C:C2	2.99	0.49
48:5:963:G:H2'	48:5:963:G:N3	2.27	0.49
48:5:1086:C:C2	48:5:1212:G:C2	3.00	0.49
48:5:1400:G:C6	48:5:1401:C:C4	3.01	0.49
48:5:1897:A:H3'	48:5:1897:A:N3	2.27	0.49
48:5:1957:U:HO2'	48:5:1958:A:C1'	2.24	0.49
48:5:3627:G:C2	48:5:3835:C:N3	2.80	0.49
51:9:488:U:H3'	51:9:489:A:H5'	1.92	0.49
72:UU:20:ILE:HD12	72:UU:116:ILE:HA	1.93	0.49
74:WW:85:ASP:O	74:WW:88:LYS:N	2.45	0.49
84:gg:254:PRO:HA	84:gg:285:GLN:HA	1.94	0.49
87:jj:595:PHE:CD2	87:jj:596:PHE:O	2.65	0.49
5:E:140:ILE:HD13	5:E:169:LEU:HD11	1.93	0.49
5:E:238:ILE:C	5:E:239:THR:HG1	2.16	0.49
23:X:45:THR:HG22	48:5:4085:A:OP1	2.12	0.49
32:g:54:ARG:NH2	48:5:2653:C:OP1	2.45	0.49
43:s:10:LYS:HZ1	48:5:1961:G:P	2.35	0.49
47:3:24:G:C6	47:3:25:C:C4	3.01	0.49
48:5:130:C:C2	48:5:139:G:N2	2.81	0.49
48:5:300:A:C2	48:5:301:G:C6	3.00	0.49
48:5:1263:A:C6	48:5:1264:C:C4	3.00	0.49
48:5:1557:C:C2	48:5:1571:G:C2	3.00	0.49
48:5:1613:A:H3'	48:5:1614:C:H5'	1.94	0.49
48:5:4507:A:H2'	48:5:4508:C:C6	2.47	0.49
49:7:25:G:C6	49:7:26:C:C4	3.00	0.49
49:7:66:G:C2	49:7:67:C:C2	3.00	0.49
50:8:125:C:O2	50:8:125:C:O4'	2.29	0.49
51:9:598:G:C2	51:9:639:C:C2	3.00	0.49
51:9:1012:A:H2'	51:9:1013:U:O4'	2.12	0.49
51:9:1648:G:O2'	51:9:1674:G:O6	2.31	0.49
60:II:171:LEU:HD13	60:II:189:VAL:HG11	1.94	0.49
61:JJ:22:LYS:HA	61:JJ:25:LEU:HD12	1.94	0.49
1:A:193:ARG:O	1:A:195:CYS:N	2.45	0.49
1:A:207:VAL:HG23	1:A:208:GLU:HG3	1.94	0.49
8:H:44:GLU:HB3	8:H:58:ASP:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:19:LYS:HG2	48:5:2823:G:OP1	2.12	0.49
30:e:82:VAL:HG22	30:e:111:ILE:HA	1.94	0.49
40:o:10:THR:OG1	40:o:11:PHE:N	2.44	0.49
48:5:120:A:C2	48:5:148:C:O2	2.64	0.49
48:5:2267:U:O4'	48:5:2267:U:O2	2.26	0.49
48:5:2524:U:H5"	48:5:2711:G:C2	2.47	0.49
51:9:191:A:H3'	51:9:192:C:H5"	1.94	0.49
51:9:292:A:C4	51:9:292:A:O5'	2.65	0.49
51:9:559:G:O2'	51:9:560:A:O5'	2.29	0.49
51:9:650:A:H2'	51:9:651:U:O4'	2.12	0.49
51:9:1537:A:C2	51:9:1596:U:N3	2.81	0.49
51:9:1546:G:N2	51:9:1670:C:O2	2.41	0.49
56:EE:22:LYS:HB3	56:EE:23:LEU:HD12	1.95	0.49
5:E:254:LEU:C	5:E:254:LEU:CD2	2.86	0.49
6:F:92:ALA:HB3	6:F:127:LEU:HD21	1.94	0.49
6:F:118:GLN:HB2	6:F:121:ASN:ND2	2.27	0.49
7:G:156:VAL:HG11	7:G:184:LEU:HG	1.95	0.49
13:N:137:PRO:O	13:N:152:THR:HG22	2.12	0.49
18:S:67:VAL:HA	48:5:728:U:O4	2.12	0.49
18:S:109:CYS:O	18:S:110:TYR:C	2.54	0.49
48:5:505:G:C6	48:5:506:C:C4	3.00	0.49
48:5:1268:G:C4	48:5:2111:G:C2	3.00	0.49
48:5:1370:G:H4'	48:5:1371:A:H4'	1.95	0.49
48:5:1886:G:C2	48:5:1894:C:C2	3.01	0.49
48:5:3869:C:O5'	48:5:3869:C:H6	1.95	0.49
48:5:3912:U:O2'	48:5:3913:G:H5'	2.12	0.49
51:9:389:A:H2'	51:9:390:C:C6	2.47	0.49
51:9:635:G:C6	51:9:636:C:C4	3.01	0.49
51:9:1408:U:O4	51:9:1409:A:N6	2.45	0.49
54:CC:249:SER:C	73:VV:23:ILE:HD11	2.37	0.49
56:EE:86:PHE:HE2	56:EE:226:PHE:CD2	2.31	0.49
56:EE:160:ILE:HG21	56:EE:169:ILE:CG2	2.42	0.49
87:jj:116:LYS:HE3	87:jj:272:VAL:HG11	1.93	0.49
2:B:242:ARG:NH2	48:5:1591:U:OP2	2.45	0.49
13:N:40:PRO:HG3	48:5:8:U:H5"	1.94	0.49
23:X:46:PHE:CD1	23:X:46:PHE:C	2.89	0.49
47:3:76:A:N7	48:5:4371:G:C6	2.80	0.49
51:9:50:A:C2	51:9:51:U:C1'	2.95	0.49
51:9:1260:A:C4	51:9:1620:A:N7	2.80	0.49
51:9:1549:U:OP1	81:dd:34:TYR:OH	2.25	0.49
51:9:1617:G:N7	67:PP:43:ARG:NH1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1771:G:N1	51:9:1772:C:C4	2.81	0.49
73:VV:20:SER:HB3	73:VV:59:ILE:HD11	1.93	0.49
2:B:89:ILE:CD1	2:B:153:MET:HE1	2.43	0.49
15:P:10:ASN:N	15:P:10:ASN:OD1	2.46	0.49
48:5:1398:A:O2'	48:5:1399:G:OP2	2.28	0.49
48:5:1484:G:H2'	48:5:1484:G:N3	2.27	0.49
48:5:1665:C:H2'	48:5:1666:C:C6	2.47	0.49
49:7:66:G:C6	49:7:67:C:C4	3.00	0.49
51:9:55:U:O2	51:9:55:U:C2'	2.61	0.49
51:9:925:G:N2	65:NN:48:SER:OG	2.45	0.49
51:9:1045:U:H2'	51:9:1046:U:O4'	2.13	0.49
51:9:1444:U:H2'	51:9:1445:U:C6	2.47	0.49
51:9:1613:G:N2	51:9:1627:C:C2	2.81	0.49
54:CC:201:GLY:O	54:CC:202:THR:C	2.55	0.49
75:XX:56:GLY:HA2	82:ee:6:LEU:HD21	1.94	0.49
14:O:12:ARG:O	18:S:171:ARG:NH2	2.45	0.49
14:O:28:LEU:HD11	14:O:88:LEU:HD23	1.95	0.49
16:Q:175:GLU:O	16:Q:176:ARG:HG2	2.12	0.49
28:c:22:MET:HE1	28:c:27:TYR:CD2	2.48	0.49
41:p:31:ILE:HG22	41:p:32:SER:N	2.26	0.49
47:3:5:G:N2	47:3:6:G:C4	2.80	0.49
47:3:38:A:N3	57:FF:135:ARG:NH2	2.60	0.49
48:5:81:C:H2'	48:5:82:U:O4'	2.13	0.49
48:5:190:G:C2	48:5:252:C:O2	2.66	0.49
48:5:1617:G:H1'	48:5:2513:A:N6	2.28	0.49
48:5:2552:G:C6	48:5:2553:A:C6	3.00	0.49
48:5:3665:G:H2'	48:5:3666:C:O4'	2.13	0.49
51:9:71:G:H3'	51:9:72:C:H5"	1.94	0.49
51:9:501:C:O2	51:9:501:C:H2'	2.12	0.49
51:9:688:U:OP2	59:HH:122:LEU:N	2.44	0.49
51:9:1474:A:H2'	51:9:1475:G:H5"	1.95	0.49
87:jj:73:VAL:HG21	87:jj:295:ALA:HB1	1.95	0.49
3:C:26:ALA:O	3:C:27:VAL:C	2.56	0.49
9:I:80:CYS:HB2	9:I:144:ASN:HD21	1.78	0.49
42:r:95:HIS:O	42:r:96:MET:C	2.55	0.49
48:5:67:C:H2'	48:5:68:U:O4'	2.13	0.49
48:5:969:C:O2'	48:5:970:G:N3	2.38	0.49
48:5:1213:G:C6	48:5:1215:C:N3	2.81	0.49
48:5:1400:G:C2	48:5:1401:C:C2	3.00	0.49
48:5:1822:U:O2	48:5:1822:U:O4'	2.31	0.49
48:5:2058:G:N2	48:5:2059:C:C2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2555:G:O6	48:5:2572:C:N4	2.46	0.49
48:5:2909:C:C2	48:5:3586:G:C2	3.00	0.49
48:5:3910:C:H2'	48:5:3911:C:C6	2.48	0.49
48:5:4459:U:H2'	48:5:4460:U:C6	2.47	0.49
48:5:4773:C:C2	48:5:4863:G:C2	3.01	0.49
51:9:52:G:C2	51:9:53:C:C2	3.01	0.49
51:9:1308:U:H2'	51:9:1309:C:C1'	2.43	0.49
51:9:1364:U:O2	51:9:1364:U:O4'	2.28	0.49
61:JJ:29:LEU:HD22	82:ee:38:TYR:HB2	1.95	0.49
13:N:68:ARG:HD2	13:N:128:LYS:HG3	1.95	0.49
25:Z:36:ARG:HG2	25:Z:38:TYR:CE1	2.48	0.49
40:o:61:LYS:HB3	48:5:4373:G:O6	2.13	0.49
47:3:39:U:O2'	47:3:40:C:C5'	2.61	0.49
48:5:197:A:N1	48:5:225:G:O2'	2.39	0.49
48:5:671:G:C2	48:5:672:C:C2	3.01	0.49
48:5:1754:U:O2	48:5:1754:U:O4'	2.29	0.49
48:5:2459:G:H2'	48:5:2461:G:OP2	2.12	0.49
48:5:2521:G:H5'	48:5:2640:G:H1'	1.95	0.49
48:5:2864:A:H2'	48:5:2865:U:C6	2.47	0.49
48:5:3771:C:O2	48:5:3771:C:O4'	2.31	0.49
48:5:4320:G:H2'	48:5:4321:U:O4'	2.13	0.49
51:9:1865:C:OP2	78:aa:5:ARG:NH1	2.46	0.49
52:AA:42:LYS:C	52:AA:43:SER:O	2.55	0.49
54:CC:133:TYR:CD1	54:CC:216:MET:HA	2.48	0.49
55:DD:167:TYR:CE2	55:DD:204:LEU:HG	2.48	0.49
56:EE:208:VAL:HB	56:EE:225:ILE:CD1	2.43	0.49
60:II:6:ASP:OD1	60:II:6:ASP:N	2.45	0.49
61:JJ:117:LEU:O	61:JJ:119:LEU:HB2	2.13	0.49
70:SS:15:VAL:HB	70:SS:20:ILE:HD11	1.95	0.49
87:jj:58:CYS:SG	87:jj:59:GLY:N	2.86	0.49
1:A:2:GLY:N	48:5:4185:G:OP1	2.46	0.48
2:B:252:ALA:HB1	48:5:4524:G:N3	2.28	0.48
17:R:35:ALA:HA	17:R:40:GLN:HG2	1.95	0.48
31:f:13:GLY:HA2	31:f:97:ILE:CD1	2.43	0.48
48:5:166:C:O5'	48:5:166:C:H6	1.96	0.48
48:5:1398:A:H1'	48:5:1399:G:C8	2.48	0.48
48:5:3698:G:N2	48:5:3699:C:C2	2.81	0.48
48:5:4424:A:N7	48:5:4475:G:C6	2.81	0.48
48:5:4931:G:H2'	48:5:4931:G:N3	2.28	0.48
51:9:463:C:O2'	51:9:466:G:O6	2.26	0.48
51:9:987:A:C2	53:BB:114:VAL:HG21	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:65:ILE:HG23	52:AA:74:VAL:HG21	1.93	0.48
14:O:45:GLY:O	14:O:135:PHE:HA	2.13	0.48
23:X:155:ILE:O	23:X:156:ILE:HB	2.13	0.48
31:f:50:VAL:HG22	31:f:69:VAL:HG11	1.95	0.48
48:5:2021:G:O2'	48:5:2022:C:O4'	2.29	0.48
48:5:4749:C:O2	48:5:4749:C:O4'	2.31	0.48
51:9:1116:C:O2	51:9:1116:C:O4'	2.30	0.48
54:CC:124:PHE:O	54:CC:143:CYS:HA	2.13	0.48
86:ii:251:LEU:HD21	86:ii:278:VAL:HG21	1.93	0.48
11:L:99:ASP:OD1	11:L:99:ASP:C	2.55	0.48
48:5:1198:G:H2'	48:5:1199:G:C8	2.47	0.48
48:5:1252:C:C2	48:5:1259:G:C2	3.01	0.48
48:5:1776:A:C6	48:5:1777:C:C4	3.01	0.48
48:5:2268:A:H4'	48:5:2269:C:H5'	1.95	0.48
51:9:14:C:O2	51:9:1198:G:C2	2.66	0.48
51:9:145:G:N7	58:GG:178:ARG:NH1	2.53	0.48
51:9:495:U:C4	51:9:496:C:C4	3.02	0.48
52:AA:124:VAL:HG13	52:AA:130:ASP:HB2	1.94	0.48
53:BB:134:LEU:HD22	53:BB:218:LEU:HD12	1.94	0.48
56:EE:15:PRO:HD2	56:EE:18:TRP:CE3	2.48	0.48
58:GG:7:PHE:HB2	58:GG:113:ILE:HD12	1.95	0.48
78:aa:76:SER:OG	78:aa:77:CYS:N	2.45	0.48
3:C:114:ARG:CZ	48:5:1358:G:H5"	2.42	0.48
4:D:78:ALA:HB1	4:D:104:LEU:HD13	1.94	0.48
43:s:189:ILE:HD11	43:s:192:VAL:HG22	1.95	0.48
48:5:169:G:N1	48:5:170:C:C4	2.82	0.48
48:5:707:C:C2	48:5:1291:G:C2	3.00	0.48
48:5:1867:A:N6	48:5:4441:A:O2'	2.44	0.48
48:5:4079:C:C2	48:5:4168:G:C2	3.01	0.48
48:5:4152:G:N2	48:5:4153:C:C2	2.81	0.48
48:5:4735:G:C6	48:5:4736:C:C4	3.01	0.48
51:9:211:G:N1	51:9:212:C:C4	2.82	0.48
51:9:409:C:C2	51:9:432:G:C2	3.01	0.48
51:9:1144:A:C2	51:9:1145:A:C6	3.01	0.48
51:9:1471:C:H2'	51:9:1472:C:C6	2.49	0.48
52:AA:33:GLN:HB3	52:AA:154:LEU:HD12	1.95	0.48
8:H:23:ARG:NH2	8:H:39:ASN:HA	2.28	0.48
12:M:17:PHE:HA	12:M:21:ALA:HB2	1.94	0.48
13:N:173:GLY:O	13:N:183:THR:HG21	2.13	0.48
15:P:57:CYS:SG	15:P:58:VAL:N	2.87	0.48
18:S:12:VAL:HG11	18:S:44:PHE:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:17:THR:HG21	48:5:1301:C:O2'	2.13	0.48
48:5:229:G:C2	48:5:240:G:C2	3.02	0.48
48:5:1958:A:N1	48:5:2026:A:N1	2.61	0.48
48:5:2639:U:O2'	48:5:2694:G:N1	2.34	0.48
48:5:3705:G:C6	48:5:3706:C:C4	3.01	0.48
51:9:1130:G:C2	51:9:1131:G:C8	3.02	0.48
54:CC:263:LYS:O	54:CC:264:SER:HB3	2.14	0.48
56:EE:31:PRO:HD3	56:EE:38:LEU:HD13	1.94	0.48
59:HH:135:PHE:CD1	59:HH:135:PHE:C	2.91	0.48
71:TT:38:LYS:O	71:TT:39:LEU:HB2	2.12	0.48
76:YY:20:ARG:HB3	76:YY:76:TYR:CD1	2.48	0.48
87:jj:315:GLY:HA2	87:jj:324:PHE:CZ	2.48	0.48
4:D:8:LYS:HG2	4:D:12:TYR:CE2	2.48	0.48
18:S:147:ASP:OD1	18:S:148:SER:N	2.46	0.48
48:5:82:U:H2'	48:5:83:C:O4'	2.12	0.48
48:5:298:G:N2	48:5:299:C:C2	2.81	0.48
48:5:356:G:OP1	48:5:2343:G:N1	2.41	0.48
48:5:977:C:N3	48:5:978:G:N7	2.62	0.48
48:5:2814:C:O2	48:5:2814:C:H2'	2.12	0.48
48:5:3783:A:C8	48:5:3792:G:C6	3.02	0.48
48:5:4308:C:H2'	48:5:4309:G:O4'	2.13	0.48
51:9:65:C:N4	58:GG:134:GLY:O	2.40	0.48
51:9:292:A:O2'	51:9:293:C:OP2	2.31	0.48
51:9:868:G:C2	59:HH:115:LYS:HA	2.49	0.48
51:9:1149:A:C6	51:9:1151:G:C4	3.01	0.48
51:9:1208:A:H4'	51:9:1835:A:N7	2.29	0.48
51:9:1308:U:O3'	83:ff:128:ALA:HB3	2.14	0.48
51:9:1476:A:C8	69:RR:3:ARG:HB2	2.48	0.48
60:II:165:GLN:O	60:II:169:GLY:N	2.47	0.48
61:JJ:136:ARG:HD3	61:JJ:160:SER:HA	1.96	0.48
4:D:56:THR:HG23	49:7:27:G:OP2	2.14	0.48
15:P:54:GLN:HA	15:P:83:TRP:CD1	2.48	0.48
18:S:173:ASN:HA	48:5:4762:A:H2	1.78	0.48
20:U:28:PRO:HA	20:U:114:TYR:OH	2.14	0.48
21:V:13:LYS:O	21:V:14:PHE:HB2	2.14	0.48
48:5:199:G:C2	48:5:201:C:N3	2.82	0.48
48:5:499:G:H2'	48:5:499:G:N3	2.28	0.48
48:5:931:C:HO2'	48:5:932:A:P	2.36	0.48
48:5:1279:A:C3'	48:5:1280:C:C5'	2.77	0.48
48:5:1672:U:C5	48:5:1684:A:N1	2.82	0.48
49:7:30:C:C4	49:7:48:G:N1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:402:C:H2'	51:9:403:G:O4'	2.13	0.48
51:9:574:A:H2'	51:9:575:A:C8	2.49	0.48
51:9:1109:C:HO2'	51:9:1110:G:C5'	2.16	0.48
52:AA:50:ASN:HB3	52:AA:53:ARG:HB2	1.96	0.48
55:DD:142:LEU:CD1	55:DD:182:LEU:HD11	2.42	0.48
55:DD:161:GLY:O	55:DD:164:VAL:HG12	2.14	0.48
56:EE:128:LYS:HA	56:EE:156:MET:SD	2.53	0.48
58:GG:144:LEU:HD23	58:GG:145:PHE:CE2	2.48	0.48
62:KK:29:MET:HE3	62:KK:42:ASN:HB2	1.94	0.48
2:B:249:ARG:NH2	48:5:3845:A:OP2	2.47	0.48
5:E:59:TYR:CZ	5:E:64:LEU:HB2	2.48	0.48
8:H:39:ASN:O	8:H:40:HIS:HB3	2.14	0.48
8:H:74:CYS:SG	8:H:75:SER:N	2.85	0.48
11:L:55:LEU:HD12	11:L:154:VAL:HG13	1.96	0.48
28:c:77:ASN:OD1	28:c:78:ASN:N	2.47	0.48
46:2:35:A:H2'	46:2:36:C:O4'	2.13	0.48
48:5:3909:C:C5	48:5:3910:C:C5	3.02	0.48
48:5:4119:C:O2	48:5:4119:C:O4'	2.32	0.48
48:5:4213:A:N6	48:5:4218:U:H3	2.09	0.48
49:7:93:G:C6	49:7:94:C:C4	3.02	0.48
51:9:1229:G:C2	51:9:1230:C:C2	3.02	0.48
51:9:1528:G:C6	51:9:1529:C:N4	2.82	0.48
51:9:1735:A:H2'	51:9:1736:G:O4'	2.12	0.48
87:jj:389:ILE:HG23	87:jj:484:LEU:HD13	1.95	0.48
87:jj:597:LEU:C	87:jj:597:LEU:CD1	2.86	0.48
9:I:82:LYS:CE	48:5:1990:A:OP1	2.52	0.48
12:M:43:THR:O	12:M:44:ARG:HB2	2.14	0.48
21:V:82:ILE:HD12	21:V:104:VAL:HG22	1.95	0.48
25:Z:16:GLY:O	25:Z:17:ARG:C	2.56	0.48
48:5:233:U:H3'	48:5:234:G:H5'	1.96	0.48
48:5:1690:C:H2'	48:5:1691:G:O4'	2.13	0.48
48:5:2557:G:C6	48:5:2558:C:C4	3.02	0.48
48:5:3873:G:H2'	48:5:3874:G:C8	2.49	0.48
51:9:361:U:C2	51:9:1175:G:N3	2.82	0.48
51:9:1334:G:C4	51:9:1498:A:C2	3.02	0.48
51:9:1416:C:H2'	51:9:1417:C:N1	2.28	0.48
51:9:1681:U:HO2'	51:9:1682:C:H6	1.61	0.48
71:TT:4:VAL:O	71:TT:4:VAL:HG23	2.12	0.48
31:f:11:PHE:CZ	31:f:97:ILE:HD13	2.49	0.48
48:5:422:C:C2	50:8:13:G:C2	3.02	0.48
48:5:2046:G:H1'	48:5:2047:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2065:G:C2	48:5:2066:C:C2	3.02	0.48
48:5:2477:A:H2'	48:5:2478:C:C6	2.49	0.48
48:5:2831:G:C2	48:5:3855:C:C2	3.02	0.48
48:5:4906:C:C2	48:5:4916:G:C2	3.01	0.48
51:9:443:U:O4	51:9:444:G:C6	2.65	0.48
51:9:832:G:C2	51:9:843:C:N3	2.82	0.48
55:DD:191:PRO:O	55:DD:193:ASP:N	2.46	0.48
6:F:44:LEU:O	6:F:45:ARG:C	2.57	0.47
7:G:156:VAL:CG1	7:G:184:LEU:HG	2.44	0.47
14:O:118:MET:HE2	14:O:118:MET:HA	1.95	0.47
48:5:1751:A:C2	48:5:1780:A:C2	3.01	0.47
48:5:2370:A:N1	48:5:2390:G:O2'	2.39	0.47
48:5:2768:C:O2	48:5:2768:C:O4'	2.29	0.47
48:5:4099:G:C6	48:5:4100:C:C4	3.01	0.47
48:5:5003:U:H2'	48:5:5004:C:O4'	2.14	0.47
51:9:589:G:C4	51:9:591:U:C5	3.02	0.47
53:BB:30:TRP:CH2	53:BB:48:LEU:HD23	2.48	0.47
77:ZZ:73:VAL:HG21	77:ZZ:88:LEU:HD21	1.96	0.47
84:gg:165:ILE:HG13	84:gg:177:TRP:HB2	1.95	0.47
1:A:96:LEU:HD13	41:p:83:ILE:HG23	1.96	0.47
6:F:107:VAL:CG1	6:F:111:LEU:HD12	2.44	0.47
6:F:109:LYS:O	6:F:112:GLN:HG2	2.14	0.47
20:U:80:LYS:HD3	20:U:110:TYR:CE2	2.49	0.47
25:Z:53:VAL:CG2	25:Z:62:ILE:HG23	2.44	0.47
48:5:978:G:C6	48:5:979:C:C4	3.02	0.47
48:5:1075:G:C2	48:5:1076:C:C2	3.02	0.47
48:5:1379:C:O2	48:5:1379:C:O4'	2.32	0.47
48:5:2863:G:C6	48:5:2864:A:C6	3.03	0.47
48:5:4136:G:C6	48:5:4137:C:C4	3.02	0.47
51:9:49:C:O2	51:9:478:G:C2	2.67	0.47
51:9:301:A:N3	60:II:73:THR:HG21	2.29	0.47
51:9:427:U:O2	51:9:427:U:O4'	2.32	0.47
51:9:680:G:C6	51:9:681:U:C4	3.02	0.47
51:9:834:C:H3'	51:9:835:C:C4'	2.44	0.47
51:9:1102:G:N2	51:9:1103:C:N3	2.62	0.47
51:9:1578:U:C5	55:DD:5:ILE:HA	2.48	0.47
52:AA:41:ARG:HD3	52:AA:47:TYR:CZ	2.49	0.47
53:BB:82:ARG:HD2	53:BB:103:MET:HE3	1.95	0.47
57:FF:20:PHE:CZ	57:FF:69:VAL:HG11	2.50	0.47
60:II:103:LEU:HA	60:II:171:LEU:O	2.14	0.47
5:E:173:GLY:O	5:E:174:PRO:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:62:MET:HA	48:5:2045:G:C5	2.49	0.47
17:R:42:ARG:HA	17:R:45:ILE:HD12	1.97	0.47
18:S:174:THR:HG21	48:5:4762:A:O2'	2.14	0.47
28:c:52:CYS:HA	28:c:92:CYS:SG	2.54	0.47
35:j:17:THR:CG2	35:j:29:LEU:HD21	2.45	0.47
46:2:34:A:O2'	46:2:35:A:O4'	2.32	0.47
48:5:115:C:O2	48:5:115:C:O4'	2.29	0.47
48:5:368:C:C2	48:5:374:G:C2	3.02	0.47
48:5:1067:G:H2'	48:5:1068:G:O4'	2.14	0.47
48:5:1170:G:C2	48:5:1192:C:C2	3.02	0.47
48:5:2097:U:O2	48:5:2097:U:O4'	2.32	0.47
48:5:2108:G:N2	48:5:2125:C:C2	2.82	0.47
48:5:3907:G:C2	48:5:3909:C:C4	3.02	0.47
48:5:4093:G:C3'	48:5:4094:G:H5'	2.44	0.47
48:5:4389:C:H2'	48:5:4390:A:C8	2.49	0.47
48:5:4441:A:H5"	48:5:4441:A:H8	1.79	0.47
51:9:916:A:C5	65:NN:73:ARG:HD3	2.49	0.47
51:9:947:G:H2'	51:9:948:C:O4'	2.14	0.47
51:9:1551:U:H2'	51:9:1552:G:C8	2.50	0.47
51:9:1672:U:O3'	68:QQ:76:GLY:HA3	2.15	0.47
52:AA:87:VAL:HG12	52:AA:175:TRP:CE2	2.49	0.47
52:AA:122:LEU:HG	52:AA:142:LEU:HD22	1.95	0.47
59:HH:158:LEU:HD12	59:HH:189:PHE:CZ	2.49	0.47
66:OO:67:ASP:N	66:OO:67:ASP:OD1	2.47	0.47
87:jj:7:ARG:NH1	87:jj:56:ILE:O	2.46	0.47
2:B:41:VAL:HG21	2:B:196:TRP:CG	2.50	0.47
3:C:164:THR:HG21	48:5:223:G:H2'	1.95	0.47
5:E:186:HIS:O	5:E:187:GLN:C	2.57	0.47
6:F:93:PHE:CD2	6:F:246:ILE:HD11	2.49	0.47
7:G:159:HIS:CE1	7:G:185:LYS:HE2	2.48	0.47
11:L:94:ILE:O	33:h:119:TYR:CD2	2.67	0.47
17:R:59:SER:N	48:5:4646:U:OP1	2.47	0.47
25:Z:5:MET:HG2	25:Z:77:TYR:CE1	2.50	0.47
31:f:6:TRP:CD2	31:f:102:ARG:HG2	2.49	0.47
33:h:21:LEU:HD11	33:h:54:ILE:HG23	1.96	0.47
41:p:13:LYS:HG3	41:p:14:TYR:N	2.30	0.47
48:5:357:U:C2	48:5:359:A:N7	2.82	0.47
48:5:677:G:N2	48:5:678:C:C2	2.82	0.47
48:5:1325:C:O2	48:5:1325:C:O5'	2.32	0.47
48:5:1383:G:C6	48:5:1384:C:C4	3.02	0.47
48:5:2609:G:C2	48:5:2731:C:O2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:39:A:C2	51:9:517:C:C6	3.01	0.47
51:9:643:A:P	61:JJ:38:ARG:NH2	2.87	0.47
55:DD:23:GLU:HG2	62:KK:64:TRP:CD1	2.50	0.47
75:XX:9:THR:O	75:XX:10:ALA:C	2.57	0.47
7:G:51:LEU:O	7:G:52:THR:C	2.57	0.47
8:H:98:HIS:NE2	87:jj:440:GLN:HG2	2.29	0.47
13:N:66:VAL:HG11	13:N:98:LEU:HB3	1.95	0.47
15:P:125:MET:HG2	15:P:141:SER:HB3	1.97	0.47
24:Y:19:PHE:CD2	50:8:23:C:C5	3.03	0.47
48:5:256:G:N2	48:5:257:C:C2	2.83	0.47
48:5:1846:G:H2'	48:5:1847:C:C6	2.50	0.47
48:5:1855:G:C6	48:5:1856:C:C4	3.03	0.47
48:5:2632:U:H2'	48:5:2633:U:C6	2.50	0.47
48:5:2715:G:C2	48:5:2716:C:C2	3.03	0.47
48:5:3586:G:C6	48:5:3587:C:C4	3.03	0.47
48:5:3662:A:H61	48:5:3680:U:H3	1.61	0.47
48:5:4075:U:O2'	48:5:4076:G:H2'	2.14	0.47
48:5:4644:G:C6	48:5:4645:C:C4	3.03	0.47
50:8:106:G:N2	50:8:107:C:C2	2.82	0.47
51:9:55:U:O2	51:9:55:U:H2'	2.14	0.47
51:9:552:G:OP1	82:ee:39:ASN:ND2	2.48	0.47
51:9:908:A:H8	51:9:908:A:OP2	1.98	0.47
51:9:1115:U:O2	51:9:1115:U:O4'	2.32	0.47
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.47	0.47
54:CC:180:VAL:HG22	54:CC:219:ILE:HD13	1.95	0.47
56:EE:183:VAL:CG1	56:EE:220:THR:HG21	2.44	0.47
60:II:156:ALA:O	60:II:157:LYS:C	2.58	0.47
62:KK:15:LEU:HD22	62:KK:49:MET:CE	2.44	0.47
79:bb:19:HIS:O	79:bb:20:LYS:C	2.57	0.47
3:C:44:LEU:HD11	3:C:120:LYS:HD3	1.97	0.47
7:G:86:VAL:CG1	7:G:87:LEU:H	2.28	0.47
13:N:169:ARG:NH1	48:5:63:G:OP2	2.47	0.47
34:i:56:ARG:HD3	34:i:72:PHE:CZ	2.49	0.47
41:p:50:ARG:HD2	41:p:54:ILE:HD11	1.97	0.47
47:3:1:G:N1	47:3:2:C:C4	2.83	0.47
48:5:1359:G:H2'	48:5:1360:G:H8	1.75	0.47
48:5:2846:G:H2'	48:5:2847:G:O4'	2.15	0.47
48:5:5026:U:H3'	60:II:79:ILE:HD12	1.97	0.47
50:8:119:C:C2	50:8:132:G:C2	3.03	0.47
51:9:1452:A:H4'	51:9:1453:C:O4'	2.15	0.47
51:9:1669:G:N2	51:9:1670:C:C2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:156:MET:HE3	56:EE:156:MET:HB3	1.81	0.47
60:II:57:ALA:O	60:II:58:LEU:HD23	2.14	0.47
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	1.97	0.47
77:ZZ:58:LEU:HD23	77:ZZ:62:VAL:HG21	1.97	0.47
2:B:248:LEU:HD12	2:B:248:LEU:C	2.40	0.47
5:E:146:LEU:HD13	5:E:190:VAL:CG1	2.45	0.47
8:H:172:ILE:HD12	38:m:90:ASN:HB3	1.96	0.47
14:O:126:VAL:HG13	14:O:127:VAL:HG23	1.95	0.47
17:R:122:SER:O	17:R:123:LEU:C	2.58	0.47
18:S:30:MET:HE1	18:S:47:PHE:CB	2.44	0.47
19:T:3:ASN:OD1	19:T:9:ARG:NH1	2.48	0.47
23:X:43:SER:OG	23:X:44:PRO:HD2	2.15	0.47
26:a:3:SER:O	26:a:4:ARG:C	2.56	0.47
33:h:119:TYR:HD1	33:h:119:TYR:H	1.60	0.47
42:r:32:LEU:O	42:r:33:LYS:CB	2.61	0.47
43:s:128:THR:HG22	43:s:178:LEU:HD21	1.96	0.47
48:5:207:G:H2'	48:5:208:A:C8	2.50	0.47
48:5:479:G:N2	48:5:480:C:C2	2.83	0.47
48:5:499:G:C2	48:5:656:C:N3	2.82	0.47
48:5:698:G:N1	48:5:699:C:C4	2.83	0.47
48:5:751:G:N2	48:5:912:G:C4	2.83	0.47
48:5:990:C:C4	48:5:1064:G:C2	3.03	0.47
48:5:1359:G:H2'	48:5:1360:G:O4'	2.15	0.47
48:5:1724:G:H2'	48:5:1724:G:N3	2.30	0.47
48:5:1854:G:N2	48:5:4394:A:O4'	2.47	0.47
48:5:1910:G:C6	48:5:1911:C:N4	2.83	0.47
48:5:2301:G:N1	48:5:2302:C:C4	2.82	0.47
48:5:2315:G:C2	48:5:2325:C:C2	3.01	0.47
48:5:2402:G:C2	48:5:2403:A:C8	3.02	0.47
48:5:2519:U:C2	48:5:2520:C:C5	3.02	0.47
48:5:2750:G:H2'	48:5:2751:G:O4'	2.14	0.47
48:5:3900:G:N2	48:5:4562:C:C2	2.83	0.47
48:5:4075:U:O2'	48:5:4076:G:OP1	2.33	0.47
48:5:4102:C:C2	48:5:4108:G:C2	3.02	0.47
51:9:750:C:O2	51:9:750:C:H2'	2.13	0.47
51:9:853:C:O2	51:9:853:C:O5'	2.32	0.47
51:9:993:G:N7	78:aa:15:ARG:NH1	2.63	0.47
51:9:1054:G:H2'	51:9:1055:A:O4'	2.13	0.47
51:9:1210:G:C5'	51:9:1211:G:OP2	2.62	0.47
51:9:1409:A:C6	51:9:1410:C:C5	3.03	0.47
52:AA:3:GLY:N	73:VV:78:ILE:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:43:SER:OG	52:AA:44:ASP:N	2.47	0.47
53:BB:71:LEU:O	53:BB:74:LEU:N	2.47	0.47
53:BB:121:ILE:HG21	53:BB:164:ILE:CG2	2.43	0.47
54:CC:66:LEU:HD11	54:CC:81:ILE:HD11	1.97	0.47
58:GG:76:LEU:HD22	58:GG:92:ARG:CG	2.45	0.47
59:HH:133:LEU:HD21	59:HH:176:VAL:HG11	1.97	0.47
63:LL:91:ASP:OD1	63:LL:91:ASP:N	2.48	0.47
78:aa:24:THR:OG1	78:aa:72:HIS:O	2.32	0.47
79:bb:46:VAL:HG12	79:bb:47:PHE:N	2.29	0.47
3:C:125:CYS:O	3:C:126:SER:C	2.58	0.47
3:C:183:VAL:HG21	3:C:226:GLY:HA3	1.97	0.47
4:D:180:PHE:HB3	4:D:195:HIS:CD2	2.49	0.47
16:Q:101:CYS:SG	16:Q:121:LEU:HB2	2.55	0.47
26:a:103:VAL:CG1	26:a:108:TYR:HB2	2.45	0.47
30:e:7:LEU:HB2	30:e:93:LYS:HB3	1.97	0.47
47:3:10:G:N1	47:3:11:C:C4	2.83	0.47
47:3:24:G:C2	47:3:25:C:C2	3.02	0.47
48:5:1072:C:O2	48:5:1072:C:H2'	2.15	0.47
48:5:1234:G:H2'	48:5:1235:G:C8	2.50	0.47
48:5:1399:G:H2'	48:5:1400:G:O4'	2.15	0.47
48:5:2557:G:C2	48:5:2558:C:C2	3.03	0.47
48:5:2609:G:N1	48:5:2731:C:C2	2.83	0.47
48:5:4291:G:N3	48:5:4291:G:C5'	2.77	0.47
48:5:4631:G:H2'	48:5:4632:U:O4'	2.15	0.47
48:5:4989:U:O2	48:5:4989:U:O4'	2.30	0.47
50:8:53:G:C2	50:8:54:C:C2	3.03	0.47
51:9:680:G:C5	51:9:681:U:C5	3.03	0.47
51:9:696:G:C2	51:9:735:C:C2	3.03	0.47
51:9:1265:A:N3	51:9:1265:A:C2'	2.78	0.47
51:9:1735:A:C4	51:9:1800:A:C2	3.03	0.47
65:NN:18:TYR:O	65:NN:19:ARG:C	2.58	0.47
66:OO:43:HIS:HA	66:OO:55:ARG:HA	1.96	0.47
87:jj:484:LEU:C	87:jj:485:ILE:HG13	2.40	0.47
2:B:391:PRO:C	2:B:392:LEU:HD22	2.39	0.47
3:C:293:LEU:HD22	16:Q:34:PHE:CE2	2.49	0.47
6:F:98:ARG:HG2	6:F:141:TYR:HA	1.96	0.47
8:H:92:MET:HB3	8:H:181:VAL:HA	1.97	0.47
12:M:42:CYS:HG	12:M:77:TRP:CD1	2.32	0.47
48:5:505:G:C2	48:5:506:C:C2	3.02	0.47
48:5:962:C:P	48:5:2264:C:N3	2.88	0.47
48:5:1072:C:H1'	48:5:1073:G:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1171:G:C2	48:5:1191:C:C2	3.02	0.47
48:5:1448:G:N2	48:5:1449:C:C2	2.82	0.47
48:5:1539:G:C6	48:5:1540:C:C4	3.02	0.47
48:5:1733:G:N3	48:5:4214:A:H2'	2.30	0.47
48:5:1846:G:C2	48:5:1847:C:C2	3.03	0.47
48:5:1904:G:C2	48:5:2073:C:C2	3.03	0.47
48:5:2496:G:C2	48:5:2497:C:C2	3.03	0.47
48:5:3900:G:H5"	48:5:3901:A:H4'	1.96	0.47
48:5:4099:G:C2	48:5:4100:C:C2	3.03	0.47
51:9:635:G:C2	51:9:636:C:C2	3.02	0.47
51:9:823:U:C5	76:YY:64:PHE:CE2	3.03	0.47
56:EE:31:PRO:CD	56:EE:38:LEU:HD13	2.45	0.47
63:LL:16:ILE:HD13	63:LL:16:ILE:H	1.79	0.47
86:ii:91:ASN:CA	86:ii:119:PRO:HA	2.42	0.47
2:B:46:PHE:CE1	2:B:84:MET:HG3	2.50	0.47
2:B:163:LEU:CD2	2:B:182:GLU:HG3	2.40	0.47
9:I:76:MET:HB3	9:I:85:PHE:CE2	2.50	0.47
12:M:64:PHE:CE2	12:M:73:VAL:HG23	2.50	0.47
21:V:80:VAL:HG11	21:V:132:ILE:HD13	1.97	0.47
29:d:46:LEU:HD22	48:5:2373:C:H5'	1.96	0.47
37:l:44:TRP:CH2	37:l:45:ARG:HD3	2.50	0.47
46:2:30:G:C6	46:2:31:C:C4	3.03	0.47
48:5:224:U:O2	48:5:224:U:O4'	2.31	0.47
48:5:1416:G:N2	48:5:1417:C:C2	2.83	0.47
48:5:1912:G:N2	48:5:1913:C:C2	2.83	0.47
48:5:1962:A:O2'	48:5:1963:C:O5'	2.31	0.47
48:5:1995:G:C2	48:5:1996:C:C2	3.03	0.47
48:5:2367:A:C8	48:5:2798:A:C6	3.03	0.47
48:5:2898:G:C6	48:5:2899:C:C4	3.03	0.47
48:5:4767:C:C2	48:5:4868:G:N2	2.83	0.47
48:5:4916:G:C2	48:5:4917:C:C2	3.03	0.47
48:5:5006:U:H4'	48:5:5007:A:H5'	1.96	0.47
49:7:29:C:O2'	49:7:50:A:N1	2.47	0.47
50:8:53:G:H2'	50:8:54:C:O4'	2.15	0.47
51:9:682:U:O2'	74:WW:4:MET:SD	2.64	0.47
51:9:1134:G:N2	51:9:1135:C:C2	2.82	0.47
51:9:1407:U:C2'	51:9:1408:U:C6	2.96	0.47
51:9:1528:G:N1	51:9:1529:C:C4	2.83	0.47
58:GG:12:CYS:SG	58:GG:13:GLN:N	2.88	0.47
71:TT:104:LEU:HD13	71:TT:121:ARG:HE	1.80	0.47
81:dd:46:TYR:O	81:dd:47:ALA:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.96	0.46
2:B:271:GLN:NE2	48:5:4978:G:OP1	2.41	0.46
6:F:117:ARG:NH1	16:Q:4:ASP:O	2.44	0.46
20:U:46:ARG:O	20:U:47:ILE:C	2.59	0.46
48:5:279:A:OP1	48:5:279:A:H3'	2.15	0.46
48:5:1846:G:H2'	48:5:1847:C:H6	1.80	0.46
48:5:1934:A:N1	48:5:2048:U:C4	2.83	0.46
48:5:4242:U:N3	48:5:4281:A:C2	2.79	0.46
48:5:4728:U:O2	48:5:4728:U:H2'	2.16	0.46
48:5:4932:U:H2'	48:5:4933:C:O4'	2.14	0.46
51:9:88:G:C2	51:9:89:C:C2	3.03	0.46
51:9:697:G:C2	51:9:734:C:C2	3.03	0.46
51:9:1109:C:C2'	51:9:1110:G:O5'	2.62	0.46
51:9:1398:G:C2	51:9:1399:C:C6	3.03	0.46
73:VV:20:SER:O	73:VV:22:ARG:N	2.48	0.46
74:WW:100:GLY:HA2	74:WW:130:PHE:HB3	1.97	0.46
76:YY:45:ALA:O	76:YY:49:LYS:N	2.48	0.46
86:ii:226:LEU:HD22	86:ii:236:LEU:HD23	1.97	0.46
86:ii:317:VAL:HG12	86:ii:413:LEU:HD22	1.97	0.46
1:A:112:ILE:HG13	41:p:79:VAL:HG13	1.97	0.46
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.96	0.46
2:B:234:ARG:HA	2:B:272:LYS:HD2	1.96	0.46
3:C:66:SER:CA	3:C:77:PRO:HA	2.45	0.46
9:I:45:GLU:O	9:I:46:PHE:CG	2.68	0.46
12:M:24:LEU:HB2	12:M:43:THR:HG21	1.97	0.46
26:a:22:ILE:HD12	26:a:22:ILE:N	2.30	0.46
48:5:1878:G:N2	48:5:1879:C:C2	2.83	0.46
48:5:1941:A:N6	48:5:2040:A:C4	2.83	0.46
48:5:2391:G:N1	48:5:2392:C:C4	2.83	0.46
48:5:2898:G:C2	48:5:2899:C:C2	3.03	0.46
48:5:4093:G:H3'	48:5:4094:G:H5'	1.97	0.46
48:5:4883:C:O2'	48:5:4884:G:P	2.73	0.46
51:9:67:C:O2'	58:GG:165:GLU:OE1	2.31	0.46
51:9:123:G:C2	51:9:342:C:C2	3.04	0.46
51:9:1109:C:C2	51:9:1110:G:C8	3.03	0.46
51:9:1234:C:H2'	51:9:1235:G:C8	2.50	0.46
51:9:1328:G:H2'	51:9:1329:U:O4'	2.15	0.46
51:9:1500:G:H2'	51:9:1501:C:O4'	2.15	0.46
51:9:1754:G:C6	51:9:1755:C:C4	3.03	0.46
57:FF:119:SER:O	57:FF:193:LYS:HB2	2.16	0.46
60:II:156:ALA:O	60:II:158:ILE:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:O	1:A:163:ARG:NH2	2.49	0.46
2:B:92:TYR:HB2	2:B:159:VAL:HB	1.98	0.46
2:B:257:TRP:HB3	48:5:4518:A:OP1	2.15	0.46
2:B:261:ARG:HD3	2:B:261:ARG:N	2.29	0.46
3:C:54:VAL:HG21	3:C:101:MET:CE	2.45	0.46
6:F:107:VAL:HG12	6:F:111:LEU:HD12	1.97	0.46
9:I:60:LEU:HD13	9:I:159:PHE:CD1	2.51	0.46
9:I:87:ILE:CG2	9:I:88:ARG:N	2.77	0.46
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.50	0.46
24:Y:52:ASP:OD1	24:Y:52:ASP:N	2.45	0.46
33:h:104:THR:O	33:h:105:LYS:C	2.58	0.46
48:5:322:C:O2	48:5:4356:G:C2	2.68	0.46
48:5:1189:G:C6	48:5:1190:C:C4	3.03	0.46
48:5:2586:G:C8	48:5:2770:C:H1’	2.51	0.46
48:5:4919:G:C2	48:5:4920:C:C2	3.03	0.46
49:7:71:G:C2	49:7:105:C:C2	3.04	0.46
50:8:10:G:C2	50:8:11:C:C2	3.03	0.46
50:8:75:G:N2	50:8:76:C:C2	2.83	0.46
50:8:139:G:N1	50:8:140:C:C2	2.84	0.46
51:9:163:U:OP1	58:GG:84:TYR:HA	2.15	0.46
51:9:194:C:C2	51:9:206:G:C2	3.04	0.46
51:9:321:C:O2’	51:9:322:C:H5’	2.15	0.46
51:9:920:A:OP1	74:WW:57:ARG:NH1	2.49	0.46
51:9:1304:U:OP2	83:ff:90:ARG:NH2	2.48	0.46
51:9:1416:C:O3’	51:9:1417:C:O4’	2.33	0.46
51:9:1535:U:O2	51:9:1535:U:C2’	2.63	0.46
53:BB:87:ILE:O	53:BB:98:THR:HA	2.14	0.46
55:DD:74:GLN:HA	55:DD:79:PHE:HB2	1.96	0.46
56:EE:143:ASP:O	56:EE:144:ALA:HB3	2.13	0.46
12:M:56:GLN:HB2	48:5:4871:C:N3	2.30	0.46
13:N:45:PRO:O	13:N:49:ARG:HG3	2.15	0.46
13:N:120:TRP:NE1	13:N:123:GLU:OE1	2.35	0.46
21:V:104:VAL:HB	21:V:112:MET:HE3	1.97	0.46
31:f:48:ALA:HB2	31:f:71:TRP:CZ3	2.50	0.46
46:2:50:U:H2’	46:2:51:C:C6	2.50	0.46
47:3:76:A:C2	48:5:4370:G:C4	3.04	0.46
48:5:497:G:H3’	48:5:498:C:H5”	1.97	0.46
48:5:1590:C:H5”	48:5:1591:U:O5’	2.16	0.46
48:5:1699:A:N6	48:5:2094:G:O2’	2.48	0.46
48:5:2065:G:C6	48:5:2066:C:C4	3.03	0.46
48:5:2586:G:C8	48:5:2587:A:C5	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3703:G:C6	48:5:3704:U:C4	3.03	0.46
51:9:166:A:C2	51:9:167:G:C8	3.03	0.46
51:9:488:U:O2	51:9:488:U:C2'	2.63	0.46
51:9:909:G:O2'	51:9:910:G:H8	1.97	0.46
51:9:1224:G:C6	51:9:1225:U:C4	3.04	0.46
51:9:1839:U:O2	51:9:1840:U:C2	2.68	0.46
63:LL:75:GLY:HA3	63:LL:88:ILE:HD12	1.97	0.46
66:OO:123:GLY:O	66:OO:124:MET:C	2.58	0.46
67:PP:56:LEU:HG	67:PP:83:MET:HE1	1.97	0.46
1:A:27:ALA:N	48:5:3680:U:OP1	2.48	0.46
3:C:36:ILE:O	3:C:37:VAL:C	2.58	0.46
4:D:146:LEU:HD11	4:D:159:VAL:HG11	1.97	0.46
8:H:95:VAL:HG12	38:m:78:ILE:HD11	1.96	0.46
9:I:61:SER:HA	9:I:126:VAL:HG23	1.97	0.46
9:I:139:ARG:NH1	9:I:195:CYS:SG	2.89	0.46
11:L:170:THR:CG2	11:L:173:GLU:CB	2.86	0.46
24:Y:62:TYR:O	24:Y:63:LYS:C	2.58	0.46
30:e:5:ARG:NH2	48:5:704:C:OP2	2.48	0.46
48:5:20:U:H2'	50:8:37:A:H61	1.81	0.46
48:5:967:C:N3	48:5:2254:G:C6	2.83	0.46
48:5:2022:C:N4	48:5:2023:C:C4	2.82	0.46
48:5:2090:U:OP2	48:5:2090:U:O4'	2.34	0.46
48:5:2597:G:C2	48:5:2749:C:C2	3.03	0.46
48:5:2793:G:C6	48:5:2797:C:N4	2.84	0.46
48:5:3909:C:O2	48:5:4396:A:N1	2.49	0.46
48:5:4274:A:H2'	48:5:4275:G:C8	2.50	0.46
51:9:5:U:C2	51:9:20:G:N2	2.83	0.46
57:FF:149:GLN:O	57:FF:150:ALA:C	2.58	0.46
63:LL:40:ILE:HD11	63:LL:68:ILE:HG13	1.98	0.46
65:NN:55:ARG:HD2	79:bb:47:PHE:CE2	2.50	0.46
84:gg:5:MET:HE2	84:gg:5:MET:N	2.30	0.46
87:jj:152:LEU:HD12	87:jj:156:PHE:CE2	2.50	0.46
1:A:49:ILE:CG2	1:A:58:LEU:HB2	2.46	0.46
2:B:35:ASP:OD1	2:B:35:ASP:N	2.49	0.46
5:E:179:ARG:NE	48:5:4937:C:OP1	2.44	0.46
5:E:254:LEU:O	5:E:257:ILE:HG13	2.15	0.46
7:G:43:GLN:O	7:G:45:ILE:N	2.49	0.46
13:N:121:VAL:CG1	13:N:131:GLU:HG3	2.46	0.46
30:e:31:ILE:HD11	48:5:2347:A:C4	2.50	0.46
42:r:106:LEU:O	42:r:107:ARG:C	2.58	0.46
46:2:37:A:C2	85:hh:46:G:C6	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:931:C:O2'	48:5:932:A:OP1	2.29	0.46
48:5:1171:G:C6	48:5:1172:C:C4	3.04	0.46
48:5:1280:C:C4	48:5:1282:G:N1	2.84	0.46
48:5:1682:A:C2	48:5:1683:U:N1	2.84	0.46
48:5:1791:U:C5	48:5:1792:U:C6	3.04	0.46
48:5:2311:C:C2	48:5:2328:G:C2	3.03	0.46
48:5:2468:U:N3	48:5:2473:A:C6	2.79	0.46
48:5:2468:U:C4	48:5:2473:A:N6	2.82	0.46
48:5:2606:G:C6	48:5:2607:C:C4	3.04	0.46
48:5:2698:G:C6	48:5:2699:C:C4	3.04	0.46
48:5:2715:G:C6	48:5:2716:C:C4	3.04	0.46
48:5:3861:A:H2'	48:5:3862:A:C8	2.50	0.46
48:5:4305:G:C2'	48:5:4305:G:N3	2.78	0.46
48:5:4559:A:H3'	48:5:4559:A:C8	2.51	0.46
51:9:92:A:H4'	51:9:93:U:OP2	2.14	0.46
51:9:302:A:H1'	60:II:73:THR:HG23	1.97	0.46
51:9:384:U:O2'	63:LL:135:SER:C	2.58	0.46
51:9:878:G:C6	51:9:909:G:C6	3.04	0.46
51:9:1048:G:N2	51:9:1069:U:C5	2.83	0.46
51:9:1474:A:H2'	51:9:1475:G:C5'	2.45	0.46
51:9:1481:G:C6	51:9:1482:C:N3	2.84	0.46
61:JJ:120:ALA:O	61:JJ:121:LYS:CB	2.63	0.46
62:KK:8:ARG:NH1	62:KK:12:TYR:OH	2.49	0.46
3:C:266:THR:OG1	3:C:267:TRP:N	2.47	0.46
13:N:108:ARG:NH2	48:5:54:G:O2'	2.49	0.46
17:R:123:LEU:HD21	17:R:142:ILE:HG12	1.98	0.46
42:r:46:ARG:NH2	48:5:666:G:C4	2.81	0.46
48:5:69:A:N1	48:5:324:A:O2'	2.41	0.46
48:5:733:A:H2'	48:5:734:G:O4'	2.16	0.46
48:5:1448:G:C6	48:5:1449:C:N4	2.84	0.46
48:5:1995:G:C6	48:5:1996:C:N3	2.84	0.46
48:5:2698:G:H2'	48:5:2699:C:O4'	2.16	0.46
48:5:3889:G:C4	48:5:4720:C:C4	3.04	0.46
48:5:4240:G:C6	48:5:4241:C:C4	3.04	0.46
48:5:4432:C:H2'	48:5:4433:G:O4'	2.15	0.46
51:9:999:G:C6	51:9:1000:C:C4	3.03	0.46
51:9:1129:G:C3'	51:9:1130:G:H8	2.27	0.46
51:9:1839:U:C6	51:9:1862:G:N2	2.84	0.46
58:GG:58:LYS:O	58:GG:59:GLN:HB2	2.15	0.46
66:OO:151:LEU:C	66:OO:151:LEU:HD22	2.41	0.46
67:PP:18:ARG:HG2	70:SS:90:VAL:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:XX:41:PHE:O	75:XX:43:GLY:N	2.49	0.46
3:C:218:VAL:HG22	3:C:229:LEU:HG	1.97	0.46
11:L:22:VAL:CG1	13:N:200:LEU:HD12	2.46	0.46
12:M:116:LYS:O	12:M:117:LYS:C	2.58	0.46
32:g:37:LYS:HB2	32:g:60:ARG:HD3	1.97	0.46
32:g:90:ARG:O	32:g:91:ILE:C	2.59	0.46
41:p:33:GLN:HG3	41:p:34:HIS:CD2	2.50	0.46
48:5:725:G:H2'	48:5:726:G:C8	2.51	0.46
48:5:977:C:C3'	48:5:978:G:H5'	2.45	0.46
48:5:1550:G:C6	48:5:1551:C:C4	3.04	0.46
48:5:1661:C:C2	48:5:2345:G:N1	2.84	0.46
48:5:1789:C:H2'	48:5:1790:U:H6	1.79	0.46
48:5:2446:C:H2'	48:5:2447:U:C6	2.51	0.46
48:5:2496:G:C6	48:5:2497:C:C4	3.04	0.46
48:5:2567:G:C2	48:5:2568:C:C2	3.04	0.46
48:5:3904:G:H4'	48:5:3905:A:OP1	2.14	0.46
48:5:3918:G:C6	48:5:3919:C:C4	3.04	0.46
48:5:4092:G:N2	48:5:4158:C:C2	2.83	0.46
48:5:4666:G:H2'	48:5:4667:C:C6	2.50	0.46
48:5:4904:G:N2	48:5:4905:C:C2	2.84	0.46
48:5:4977:A:H2'	48:5:4978:G:O4'	2.16	0.46
48:5:5057:C:H2'	48:5:5058:A:C8	2.51	0.46
51:9:182:C:H2'	51:9:184:G:H1'	1.97	0.46
51:9:511:U:H2'	51:9:512:A:C8	2.51	0.46
51:9:623:G:N1	51:9:624:C:C4	2.84	0.46
51:9:1512:C:H2'	51:9:1513:C:C6	2.51	0.46
51:9:1784:G:N1	51:9:1785:C:C4	2.84	0.46
51:9:1865:C:OP1	78:aa:87:ARG:NH2	2.48	0.46
56:EE:52:LEU:O	56:EE:54:TYR:N	2.49	0.46
76:YY:85:ASN:ND2	76:YY:85:ASN:N	2.63	0.46
81:dd:31:ILE:HD11	81:dd:40:ARG:HA	1.97	0.46
83:ff:81:THR:HG22	83:ff:83:PRO:HD2	1.98	0.46
87:jj:58:CYS:SG	87:jj:60:ILE:N	2.89	0.46
3:C:54:VAL:HG21	3:C:101:MET:HE2	1.98	0.46
6:F:44:LEU:O	6:F:47:ALA:N	2.49	0.46
13:N:181:HIS:NE2	48:5:99:A:H4'	2.30	0.46
46:2:32:C:C5	46:2:33:U:C5	3.03	0.46
48:5:281:U:O2'	48:5:329:A:H1'	2.16	0.46
48:5:1376:C:H4'	48:5:1377:G:OP1	2.16	0.46
48:5:1379:C:H4'	48:5:1380:G:C8	2.51	0.46
48:5:1584:G:C6	48:5:1585:C:C4	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2026:A:C2'	48:5:2027:U:H5'	2.46	0.46
48:5:2245:G:C2	48:5:2246:C:C2	3.04	0.46
48:5:4576:U:C4	48:5:4577:U:C4	3.04	0.46
48:5:4916:G:C6	48:5:4917:C:C4	3.04	0.46
50:8:94:G:C8	50:8:94:G:H5'	2.51	0.46
51:9:16:G:C2	51:9:17:C:N3	2.84	0.46
51:9:614:C:C2	51:9:626:G:C2	3.03	0.46
51:9:1089:G:C6	51:9:1090:C:C4	3.04	0.46
51:9:1259:A:H3'	51:9:1259:A:N3	2.30	0.46
51:9:1859:A:C2	51:9:1860:A:C6	3.04	0.46
59:HH:121:THR:O	59:HH:122:LEU:C	2.59	0.46
60:II:61:ASP:OD1	60:II:62:VAL:N	2.48	0.46
65:NN:122:ILE:HG21	65:NN:141:TYR:CD2	2.50	0.46
74:WW:30:CYS:SG	74:WW:31:SER:N	2.89	0.46
87:jj:98:PRO:CG	87:jj:123:LEU:HD11	2.33	0.46
4:D:56:THR:HG21	49:7:26:C:H5"	1.97	0.46
5:E:146:LEU:HD13	5:E:190:VAL:HG11	1.98	0.46
32:g:37:LYS:HB2	32:g:60:ARG:CD	2.46	0.46
48:5:177:G:C2	48:5:178:C:C2	3.03	0.46
48:5:177:G:C6	48:5:178:C:C4	3.04	0.46
48:5:940:C:C4	48:5:941:C:C4	3.04	0.46
48:5:1270:A:H2'	48:5:1271:G:O4'	2.16	0.46
48:5:1721:G:C6	48:5:1722:C:C4	3.04	0.46
48:5:1990:A:H3'	48:5:1991:A:H5"	1.98	0.46
48:5:2021:G:C2	48:5:2022:C:C2	3.04	0.46
48:5:2045:G:O6	48:5:3870:C:O2'	2.28	0.46
48:5:2627:C:O4'	48:5:2627:C:O2	2.33	0.46
48:5:4740:G:C2	48:5:4741:C:C2	3.04	0.46
51:9:1236:G:C6	51:9:1237:C:C4	3.04	0.46
51:9:1331:C:C2	51:9:1489:A:C5	3.04	0.46
78:aa:26:CYS:O	78:aa:27:ALA:HB3	2.16	0.46
80:cc:61:SER:O	80:cc:61:SER:OG	2.30	0.46
1:A:116:LEU:CD2	1:A:148:VAL:HG11	2.47	0.45
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.56	0.45
3:C:186:SER:O	3:C:187:GLN:C	2.59	0.45
3:C:208:CYS:HG	3:C:228:THR:HG1	1.56	0.45
5:E:127:LYS:O	5:E:132:HIS:NE2	2.49	0.45
6:F:139:GLU:N	6:F:140:PRO:HD2	2.31	0.45
6:F:234:ASP:O	6:F:238:ARG:NH2	2.49	0.45
17:R:172:ARG:NE	17:R:172:ARG:HA	2.31	0.45
41:p:22:LEU:O	41:p:26:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:994:G:C2	48:5:1050:C:C2	3.04	0.45
48:5:1196:G:C6	48:5:1197:C:C4	3.04	0.45
48:5:1240:G:C6	48:5:1241:C:C4	3.04	0.45
48:5:1550:G:C2	48:5:1551:C:C2	3.04	0.45
48:5:2909:C:O2	48:5:3586:G:C2	2.69	0.45
48:5:3680:U:O2	48:5:3680:U:C2'	2.64	0.45
48:5:4619:U:H2'	48:5:4620:U:O4'	2.15	0.45
48:5:4737:G:C2	48:5:4738:C:C2	3.04	0.45
48:5:4911:A:H3'	48:5:4912:G:C5'	2.46	0.45
51:9:834:C:C2	51:9:841:G:N2	2.84	0.45
51:9:1122:A:N3	53:BB:146:ARG:NH1	2.62	0.45
51:9:1276:A:N6	51:9:1321:G:O2'	2.45	0.45
51:9:1845:A:C2	51:9:1855:G:C6	3.04	0.45
52:AA:60:LEU:HD13	52:AA:159:ILE:HD11	1.97	0.45
58:GG:68:LEU:HA	58:GG:101:ILE:HD13	1.98	0.45
58:GG:121:ILE:HG22	58:GG:124:LEU:HB3	1.97	0.45
87:jj:454:ILE:O	87:jj:456:ASP:N	2.50	0.45
1:A:236:GLY:N	48:5:3687:A:O2'	2.50	0.45
3:C:181:LYS:HD3	48:5:218:A:C8	2.51	0.45
3:C:233:THR:HG22	3:C:259:LYS:NZ	2.31	0.45
5:E:161:LEU:HD22	5:E:204:ILE:HD13	1.98	0.45
12:M:50:MET:HE3	12:M:55:MET:HB3	1.98	0.45
14:O:148:LYS:HB2	14:O:149:TYR:CD2	2.52	0.45
40:o:66:ILE:HD13	40:o:91:PHE:CE2	2.50	0.45
48:5:28:C:C2	48:5:55:G:N2	2.84	0.45
48:5:43:U:C2'	48:5:44:A:O5'	2.63	0.45
48:5:691:C:H2'	48:5:692:A:C8	2.51	0.45
48:5:984:C:C2	48:5:1070:G:N2	2.85	0.45
48:5:1381:U:O2	48:5:1381:U:O4'	2.33	0.45
48:5:1448:G:C2	48:5:1449:C:C2	3.04	0.45
48:5:2336:G:C2	48:5:2337:C:C2	3.04	0.45
48:5:2559:G:C6	48:5:2560:C:C4	3.04	0.45
48:5:2619:G:H5'	48:5:2620:G:OP2	2.16	0.45
48:5:2736:G:N2	48:5:2737:C:C2	2.84	0.45
48:5:5001:U:H2'	48:5:5002:U:O4'	2.16	0.45
50:8:53:G:C6	50:8:54:C:C4	3.04	0.45
51:9:872:A:C6	51:9:915:G:C5	3.04	0.45
51:9:1455:A:H2'	51:9:1456:G:H8	1.80	0.45
51:9:1643:U:H2'	51:9:1644:C:C6	2.51	0.45
51:9:1859:A:H2'	51:9:1860:A:C8	2.50	0.45
59:HH:100:ILE:CG1	59:HH:125:VAL:HG11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:bb:53:VAL:HG23	79:bb:53:VAL:O	2.16	0.45
84:gg:17:TRP:HB3	84:gg:303:THR:HA	1.97	0.45
3:C:334:THR:HG21	6:F:53:TYR:OH	2.16	0.45
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.98	0.45
14:O:58:LEU:HD23	14:O:72:HIS:CD2	2.50	0.45
16:Q:15:ARG:HD2	16:Q:52:PHE:O	2.16	0.45
23:X:93:ASN:OD1	48:5:2532:C:O2'	2.34	0.45
48:5:227:A:C6	48:5:228:C:C2	3.04	0.45
48:5:1203:G:N2	48:5:1204:C:C2	2.84	0.45
48:5:1549:G:C2	48:5:1580:C:C2	3.04	0.45
48:5:1905:U:H2'	48:5:1906:U:O4'	2.16	0.45
48:5:1925:G:C6	48:5:1926:C:C4	3.05	0.45
48:5:2457:G:C6	48:5:2458:C:C4	3.04	0.45
48:5:3894:A:H2'	48:5:3895:G:O4'	2.17	0.45
48:5:4661:G:C6	48:5:4662:C:C4	3.04	0.45
48:5:4730:C:O5'	48:5:4731:G:N2	2.50	0.45
48:5:4977:A:C2	48:5:4978:G:C4	3.04	0.45
48:5:5026:U:C6	60:II:79:ILE:HD11	2.51	0.45
51:9:561:A:OP1	61:JJ:171:GLY:N	2.50	0.45
51:9:953:C:H2'	51:9:954:U:O4'	2.17	0.45
51:9:1102:G:C2	51:9:1103:C:C5	3.04	0.45
51:9:1166:G:O2'	51:9:1195:A:N1	2.44	0.45
51:9:1243:U:O4	51:9:1257:G:N2	2.43	0.45
55:DD:163:PRO:HA	55:DD:166:TYR:CZ	2.52	0.45
60:II:25:ARG:O	60:II:27:TYR:N	2.49	0.45
63:LL:17:PHE:CZ	63:LL:19:ASN:HB2	2.50	0.45
63:LL:99:TYR:O	63:LL:101:ARG:N	2.49	0.45
87:jj:99:ILE:HD13	87:jj:302:PRO:CG	2.46	0.45
1:A:125:LYS:HG3	48:5:3681:G:C6	2.50	0.45
2:B:112:ASP:O	2:B:113:GLU:C	2.59	0.45
7:G:190:LEU:HD23	7:G:199:CYS:O	2.17	0.45
11:L:95:GLY:CA	33:h:119:TYR:CE2	2.97	0.45
25:Z:11:VAL:N	25:Z:23:ALA:O	2.50	0.45
26:a:75:LEU:HD11	26:a:133:ALA:HA	1.98	0.45
39:n:7:LYS:NZ	51:9:1844:U:OP2	2.48	0.45
48:5:209:U:C4	48:5:233:U:O4	2.69	0.45
48:5:303:C:H2'	48:5:304:C:O4'	2.16	0.45
48:5:499:G:C2	48:5:500:G:C8	3.04	0.45
48:5:508:G:C2	48:5:510:U:C5	3.04	0.45
48:5:746:A:O2'	48:5:747:A:O5'	2.30	0.45
48:5:1891:A:O2'	48:5:1892:A:O4'	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2366:A:H1'	48:5:3851:U:O5'	2.17	0.45
48:5:2439:G:H2'	48:5:2440:U:H5'	1.97	0.45
48:5:2606:G:C2	48:5:2607:C:C2	3.05	0.45
48:5:2612:G:C6	48:5:2613:C:C4	3.05	0.45
48:5:3586:G:C2	48:5:3587:C:C2	3.04	0.45
48:5:3626:G:C6	48:5:3836:A:C2	3.05	0.45
48:5:4283:G:N1	48:5:4284:C:C4	2.85	0.45
51:9:980:A:C2	51:9:981:A:C6	3.05	0.45
51:9:1204:A:H2'	51:9:1205:C:O4'	2.16	0.45
51:9:1664:A:O2'	51:9:1665:G:C5'	2.65	0.45
54:CC:102:LEU:HG	54:CC:130:ILE:HD11	1.97	0.45
55:DD:219:PRO:HB3	84:gg:192:THR:HG22	1.97	0.45
58:GG:7:PHE:CD2	58:GG:10:THR:HG23	2.52	0.45
59:HH:96:ALA:HB3	59:HH:98:ARG:NH1	2.32	0.45
76:YY:76:TYR:OH	76:YY:86:GLU:HG2	2.16	0.45
20:U:80:LYS:HD3	20:U:110:TYR:CZ	2.51	0.45
25:Z:28:ASN:HB2	25:Z:77:TYR:OH	2.16	0.45
26:a:11:LEU:HD12	26:a:17:HIS:CE1	2.51	0.45
35:j:39:TYR:CD1	35:j:39:TYR:C	2.88	0.45
42:r:107:ARG:HH11	42:r:107:ARG:HG3	1.81	0.45
48:5:76:A:C6	48:5:77:U:C5	3.03	0.45
48:5:1189:G:C2	48:5:1190:C:C2	3.04	0.45
48:5:1332:C:H2'	48:5:1333:A:H8	1.81	0.45
48:5:2478:C:N4	48:5:2479:G:O6	2.49	0.45
48:5:2602:G:C6	48:5:2603:C:C4	3.04	0.45
48:5:2800:G:C6	48:5:2801:U:C4	3.04	0.45
48:5:3877:A:N3	48:5:4401:G:O2'	2.39	0.45
48:5:4109:G:C6	48:5:4110:C:C4	3.05	0.45
48:5:4461:C:C2	48:5:4516:G:C2	3.04	0.45
48:5:4562:C:C4	48:5:4563:U:C4	3.04	0.45
51:9:60:A:H2'	51:9:61:A:C8	2.51	0.45
51:9:1005:G:C6	51:9:1006:C:C4	3.05	0.45
51:9:1035:A:H2'	51:9:1036:A:O4'	2.16	0.45
51:9:1190:A:N3	51:9:1714:U:O2'	2.49	0.45
51:9:1271:C:C5	51:9:1272:C:C5	3.04	0.45
51:9:1391:C:H2'	51:9:1392:U:O4'	2.15	0.45
54:CC:194:ARG:HD3	54:CC:196:ILE:HD11	1.99	0.45
55:DD:127:MET:HE1	55:DD:133:GLY:HA2	1.98	0.45
1:A:173:GLY:O	1:A:174:ARG:C	2.59	0.45
2:B:77:THR:HG21	2:B:337:VAL:HG22	1.97	0.45
2:B:234:ARG:NH2	48:5:4566:U:O2'	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:158:VAL:HG21	5:E:180:VAL:HG11	1.97	0.45
9:I:49:CYS:HB2	9:I:51:HIS:HE1	1.78	0.45
17:R:138:LEU:O	17:R:139:MET:C	2.59	0.45
20:U:56:LEU:HB3	20:U:61:VAL:HG22	1.99	0.45
22:W:9:SER:OG	22:W:10:GLY:N	2.50	0.45
33:h:58:LEU:HB3	50:8:60:G:C8	2.51	0.45
43:s:180:ILE:HG22	43:s:182:PRO:HD3	1.98	0.45
48:5:202:C:C2	48:5:214:G:C2	3.05	0.45
48:5:222:C:C2	48:5:236:G:N2	2.85	0.45
48:5:957:G:N2	48:5:958:G:N7	2.57	0.45
48:5:994:G:C6	48:5:995:C:C4	3.04	0.45
48:5:1240:G:C2	48:5:1241:C:C2	3.04	0.45
48:5:3629:A:H4’	51:9:1721:U:O2	2.17	0.45
48:5:4919:G:C6	48:5:4920:C:C4	3.05	0.45
50:8:31:G:C6	50:8:32:C:C4	3.05	0.45
51:9:385:G:N3	51:9:385:G:H2’	2.32	0.45
51:9:455:A:H2’	51:9:456:C:C6	2.51	0.45
51:9:1535:U:O2	51:9:1535:U:H2’	2.17	0.45
62:KK:66:HIS:O	62:KK:67:PHE:HB2	2.17	0.45
70:SS:117:ILE:HG22	70:SS:117:ILE:O	2.15	0.45
86:ii:157:LEU:HD23	86:ii:158:PHE:N	2.31	0.45
1:A:20:VAL:HG12	1:A:23:ARG:HD2	1.98	0.45
3:C:106:LYS:HG2	3:C:108:TRP:CZ2	2.52	0.45
4:D:64:ILE:HG22	4:D:75:VAL:HG12	1.99	0.45
4:D:118:ILE:CG2	4:D:135:ILE:HD12	2.46	0.45
9:I:184:MET:CE	9:I:189:ARG:HD2	2.47	0.45
12:M:64:PHE:HB2	12:M:65:PRO:HD2	1.97	0.45
17:R:172:ARG:N	17:R:172:ARG:HD2	2.32	0.45
25:Z:88:ASP:OD1	25:Z:88:ASP:N	2.50	0.45
31:f:28:LEU:HG	31:f:101:ILE:HD11	1.99	0.45
42:r:103:HIS:HE1	42:r:106:LEU:HD21	1.65	0.45
48:5:497:G:C2	48:5:657:C:N3	2.85	0.45
48:5:956:A:H3’	48:5:957:G:C4	2.51	0.45
48:5:1196:G:C2	48:5:1197:C:C2	3.04	0.45
48:5:1238:A:O2’	48:5:1239:C:O5’	2.24	0.45
48:5:2458:C:H2’	48:5:2459:G:O4’	2.17	0.45
48:5:2771:G:C6	48:5:2772:C:C4	3.04	0.45
48:5:3905:A:C2	48:5:4449:A:C6	3.05	0.45
48:5:4158:C:O2	48:5:4158:C:H2’	2.17	0.45
50:8:56:G:C6	50:8:57:C:C4	3.04	0.45
51:9:123:G:N2	51:9:342:C:C2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:190:G:O2'	51:9:209:A:N6	2.49	0.45
51:9:1031:A:C6	51:9:1032:C:C4	3.05	0.45
51:9:1212:G:O2'	51:9:1213:C:O4'	2.27	0.45
51:9:1321:G:H2'	51:9:1322:G:O4'	2.17	0.45
51:9:1335:G:C6	51:9:1336:C:C4	3.05	0.45
51:9:1344:A:N3	51:9:1345:G:H1'	2.31	0.45
51:9:1759:G:C2	51:9:1774:C:C2	3.05	0.45
52:AA:34:MET:O	52:AA:35:GLU:C	2.59	0.45
54:CC:63:VAL:HG12	54:CC:63:VAL:O	2.16	0.45
84:gg:153:CYS:SG	84:gg:155:ARG:NH1	2.90	0.45
1:A:90:CYS:CB	1:A:101:VAL:HG13	2.46	0.45
2:B:54:THR:OG1	2:B:55:HIS:N	2.50	0.45
2:B:92:TYR:HB3	2:B:99:LEU:HD13	1.99	0.45
3:C:119:GLN:O	3:C:120:LYS:C	2.60	0.45
5:E:160:PHE:CD1	5:E:169:LEU:HD13	2.52	0.45
6:F:225:LYS:HE3	48:5:1907:A:H4'	1.98	0.45
10:J:119:TYR:HB3	70:SS:12:ILE:HD13	1.98	0.45
11:L:146:LEU:HD12	11:L:148:THR:HG22	1.98	0.45
29:d:65:ASP:OD1	29:d:66:THR:N	2.50	0.45
32:g:68:SER:O	32:g:69:LYS:C	2.60	0.45
32:g:73:HIS:ND1	48:5:2751:G:OP1	2.50	0.45
48:5:6:C:O2'	48:5:7:C:H5'	2.17	0.45
48:5:931:C:C2'	48:5:932:A:O5'	2.64	0.45
48:5:1358:G:N3	48:5:1359:G:N7	2.64	0.45
48:5:1635:C:O2'	48:5:1636:U:H5'	2.17	0.45
48:5:2080:U:H2'	48:5:2081:C:C6	2.52	0.45
48:5:2128:G:C2	48:5:2129:C:C2	3.05	0.45
48:5:3751:G:H2'	48:5:3752:C:H5'	1.98	0.45
48:5:4188:U:C2	48:5:4189:U:C5	3.05	0.45
48:5:4476:C:O2	48:5:4476:C:O4'	2.32	0.45
48:5:4579:U:H2'	48:5:4580:U:O4'	2.16	0.45
48:5:4595:G:C6	48:5:4596:C:C4	3.05	0.45
51:9:102:A:C5	51:9:357:C:C4	3.04	0.45
51:9:1838:U:O2	66:OO:150:ARG:HD2	2.17	0.45
52:AA:83:GLY:O	52:AA:84:GLN:C	2.60	0.45
56:EE:11:ARG:O	56:EE:12:VAL:HG12	2.16	0.45
59:HH:61:ILE:CD1	59:HH:93:VAL:HG13	2.45	0.45
69:RR:124:VAL:HB	69:RR:126:MET:HE1	1.98	0.45
84:gg:35:SER:O	84:gg:66:VAL:N	2.46	0.45
84:gg:120:ILE:O	84:gg:132:TRP:N	2.46	0.45
2:B:224:LYS:HG3	2:B:340:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:181:TYR:CD1	7:G:181:TYR:C	2.95	0.45
8:H:98:HIS:CE1	48:5:4602:A:H5"	2.51	0.45
11:L:6:ASN:HB2	26:a:48:TYR:CE1	2.52	0.45
11:L:64:VAL:HA	11:L:67:HIS:CD2	2.51	0.45
15:P:26:PHE:CD1	15:P:26:PHE:C	2.95	0.45
17:R:91:GLU:O	17:R:92:LYS:C	2.58	0.45
24:Y:8:THR:O	48:5:347:A:OP1	2.34	0.45
24:Y:65:GLN:N	24:Y:66:GLN:OE1	2.47	0.45
25:Z:28:ASN:C	25:Z:29:ILE:HD12	2.41	0.45
26:a:4:ARG:NH2	48:5:2341:A:OP2	2.39	0.45
34:i:50:PHE:HZ	34:i:93:VAL:HG21	1.82	0.45
46:2:7:G:C6	46:2:49:C:N4	2.85	0.45
48:5:351:C:C2	50:8:25:G:C2	3.05	0.45
48:5:2128:G:C6	48:5:2129:C:C4	3.05	0.45
48:5:2557:G:N1	48:5:2558:C:C2	2.85	0.45
48:5:3628:G:C2	48:5:3834:C:C2	3.05	0.45
48:5:3715:U:H2'	48:5:3716:C:C6	2.52	0.45
48:5:4537:C:H2'	48:5:4538:G:C8	2.52	0.45
51:9:561:A:OP2	61:JJ:173:VAL:HB	2.17	0.45
51:9:1444:U:O2'	51:9:1580:A:N1	2.50	0.45
53:BB:62:LEU:HD11	53:BB:96:CYS:SG	2.57	0.45
56:EE:52:LEU:HB3	56:EE:54:TYR:CE1	2.52	0.45
56:EE:208:VAL:CG1	56:EE:225:ILE:HD13	2.46	0.45
58:GG:104:ALA:O	58:GG:106:LEU:N	2.49	0.45
61:JJ:110:LEU:O	61:JJ:114:VAL:N	2.49	0.45
69:RR:28:PHE:CE2	69:RR:32:LYS:HD3	2.52	0.45
1:A:216:HIS:O	1:A:218:HIS:N	2.50	0.45
3:C:188:ARG:NH1	3:C:202:ILE:HD12	2.32	0.45
4:D:207:TYR:CE1	49:7:33:U:C6	3.05	0.45
6:F:104:SER:OG	6:F:105:PRO:HD2	2.17	0.45
7:G:191:GLY:O	7:G:194:VAL:O	2.35	0.45
14:O:109:PRO:HB2	14:O:110:PRO:HD2	1.99	0.45
15:P:2:VAL:HG21	15:P:18:ARG:NH1	2.32	0.45
40:o:31:ASP:O	40:o:33:LEU:N	2.49	0.45
47:3:13:C:N3	47:3:22:G:O6	2.50	0.45
48:5:132:G:C2	48:5:133:C:H1'	2.52	0.45
48:5:167:C:C2	48:5:269:G:N2	2.85	0.45
48:5:976:G:C6	48:5:977:C:N3	2.85	0.45
48:5:1213:G:C6	48:5:1215:C:C4	3.05	0.45
48:5:1329:G:C8	48:5:1329:G:H3'	2.51	0.45
48:5:1349:G:C6	48:5:1350:C:C4	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1520:C:C2	48:5:1658:G:N2	2.85	0.45
48:5:2409:U:O4	48:5:2783:A:C2	2.64	0.45
48:5:4136:G:C2	48:5:4137:C:C2	3.05	0.45
48:5:4587:G:N2	48:5:4716:C:C2	2.85	0.45
50:8:10:G:C6	50:8:11:C:C4	3.04	0.45
51:9:99:A:H2'	51:9:100:U:O4'	2.17	0.45
51:9:185:G:N2	51:9:186:C:C2	2.85	0.45
51:9:1681:U:H2'	51:9:1682:C:C6	2.52	0.45
53:BB:120:MET:HE2	53:BB:122:GLU:CG	2.47	0.45
55:DD:59:LEU:HB2	55:DD:66:ILE:HD12	1.99	0.45
56:EE:37:LYS:O	56:EE:38:LEU:C	2.60	0.45
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	1.98	0.45
73:VV:40:ASP:O	73:VV:41:LYS:CB	2.65	0.45
74:WW:28:ARG:N	74:WW:29:PRO:CD	2.80	0.45
74:WW:37:PHE:CZ	74:WW:103:VAL:HG11	2.52	0.45
1:A:169:VAL:HG12	1:A:170:ALA:N	2.31	0.44
2:B:55:HIS:O	2:B:56:ILE:HD12	2.17	0.44
4:D:68:ARG:HG3	4:D:73:MET:HE3	1.99	0.44
6:F:170:ALA:O	6:F:172:THR:HG23	2.17	0.44
6:F:171:LEU:CB	6:F:189:MET:HE1	2.43	0.44
13:N:172:ARG:NH1	48:5:62:A:OP1	2.50	0.44
17:R:95:TRP:O	17:R:96:MET:C	2.57	0.44
27:b:43:MET:O	27:b:44:ARG:C	2.59	0.44
31:f:50:VAL:HG13	31:f:69:VAL:HG12	1.99	0.44
38:m:94:MET:HG2	38:m:105:PRO:HA	1.98	0.44
48:5:169:G:N2	48:5:170:C:C2	2.85	0.44
48:5:1246:G:H2'	48:5:1247:U:O4'	2.17	0.44
48:5:1278:C:H2'	48:5:1279:A:O3'	2.16	0.44
48:5:1646:A:H2'	48:5:1647:U:C6	2.52	0.44
48:5:2816:G:C6	48:5:2817:C:C4	3.06	0.44
48:5:2889:G:C6	48:5:2890:C:C4	3.05	0.44
48:5:3662:A:N7	48:5:3681:G:C2	2.85	0.44
48:5:4473:A:N1	48:5:4482:U:O4	2.49	0.44
48:5:4740:G:C6	48:5:4741:C:C4	3.05	0.44
51:9:832:G:C6	51:9:833:C:C4	3.06	0.44
51:9:1105:G:C2	51:9:1128:C:C2	3.06	0.44
51:9:1134:G:C2	51:9:1135:C:C2	3.06	0.44
51:9:1236:G:C2	51:9:1237:C:C2	3.05	0.44
51:9:1299:A:O2'	51:9:1300:U:H3'	2.18	0.44
51:9:1571:G:C2	51:9:1572:C:C2	3.05	0.44
53:BB:25:PHE:CD1	66:OO:88:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:HH:133:LEU:HD21	59:HH:176:VAL:CG1	2.46	0.44
61:JJ:47:LYS:HG3	61:JJ:102:ILE:HD11	1.99	0.44
61:JJ:137:VAL:O	61:JJ:139:LYS:N	2.50	0.44
81:dd:21:CYS:SG	81:dd:22:ARG:N	2.90	0.44
85:hh:49:U:O2	86:ii:62:ILE:HA	2.17	0.44
1:A:88:VAL:HG12	1:A:88:VAL:O	2.16	0.44
4:D:32:ALA:O	4:D:33:ARG:C	2.60	0.44
6:F:128:ASN:O	6:F:129:LYS:C	2.60	0.44
14:O:74:ARG:NH2	48:5:4712:C:OP1	2.51	0.44
28:c:45:LEU:HD23	28:c:96:ILE:HD12	1.99	0.44
33:h:24:LEU:O	33:h:25:LYS:C	2.59	0.44
41:p:31:ILE:O	41:p:32:SER:C	2.59	0.44
48:5:209:U:N3	48:5:233:U:C4	2.85	0.44
48:5:994:G:C2	48:5:995:C:C2	3.05	0.44
48:5:1381:U:C5	48:5:1382:G:H1’	2.52	0.44
48:5:1995:G:C6	48:5:1996:C:C4	3.06	0.44
48:5:2294:G:N1	48:5:2295:C:C4	2.85	0.44
48:5:2481:G:C6	48:5:2482:C:C4	3.05	0.44
48:5:2567:G:C6	48:5:2568:C:C4	3.06	0.44
48:5:2602:G:C2	48:5:2603:C:C2	3.05	0.44
48:5:4094:G:H2’	48:5:4095:G:C1’	2.47	0.44
48:5:4109:G:C2	48:5:4110:C:C2	3.06	0.44
48:5:4277:G:O2’	48:5:4282:A:N1	2.47	0.44
48:5:4407:G:C4	48:5:4408:G:C8	3.04	0.44
48:5:4666:G:C2	48:5:4667:C:C2	3.05	0.44
48:5:5017:G:C2	48:5:5018:C:C2	3.06	0.44
51:9:642:U:H4’	51:9:643:A:OP1	2.17	0.44
51:9:869:A:N3	51:9:915:G:H1’	2.32	0.44
51:9:1409:A:N6	51:9:1410:C:C5	2.86	0.44
51:9:1551:U:O2	51:9:1551:U:O4’	2.32	0.44
51:9:1728:U:C4	51:9:1729:U:C5	3.05	0.44
51:9:1749:G:C6	51:9:1750:C:C4	3.06	0.44
52:AA:66:VAL:HG11	73:VV:46:PHE:HB2	1.99	0.44
53:BB:71:LEU:HD21	53:BB:84:PHE:CE1	2.53	0.44
61:JJ:66:LYS:HA	61:JJ:71:LEU:HD11	1.98	0.44
63:LL:142:VAL:C	63:LL:143:LEU:HD12	2.42	0.44
74:WW:31:SER:OG	74:WW:33:VAL:N	2.48	0.44
75:XX:124:LYS:HA	75:XX:129:SER:HA	1.98	0.44
1:A:218:HIS:ND1	1:A:218:HIS:C	2.75	0.44
3:C:128:LEU:HD22	3:C:252:TRP:CH2	2.52	0.44
5:E:280:HIS:CD2	31:f:38:GLU:CG	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:94:VAL:O	6:F:122:GLY:HA2	2.17	0.44
14:O:38:CYS:O	14:O:41:ILE:N	2.42	0.44
18:S:68:PHE:CD2	48:5:728:U:C4	3.05	0.44
24:Y:10:ASP:O	24:Y:12:SER:N	2.50	0.44
30:e:87:VAL:HG11	42:r:25:TYR:CD2	2.52	0.44
42:r:64:MET:HE3	42:r:102:TYR:CE2	2.52	0.44
43:s:78:LEU:HD11	43:s:193:PHE:CD1	2.52	0.44
46:2:75:C:H2'	46:2:76:A:O4'	2.18	0.44
48:5:707:C:O2	48:5:1291:G:C2	2.70	0.44
48:5:956:A:H3'	48:5:957:G:C5	2.52	0.44
48:5:967:C:OP1	48:5:2254:G:N1	2.48	0.44
48:5:986:C:N3	48:5:1068:G:C2	2.86	0.44
48:5:1358:G:N2	48:5:1359:G:O6	2.50	0.44
48:5:1404:G:C6	48:5:1405:C:C4	3.05	0.44
48:5:1876:U:H2'	48:5:1877:G:O4'	2.16	0.44
48:5:1954:U:H2'	48:5:1955:G:O4'	2.16	0.44
48:5:2245:G:C6	48:5:2246:C:C4	3.06	0.44
48:5:2439:G:C4	48:5:2440:U:C5	3.05	0.44
48:5:4276:G:C2	48:5:4333:C:C2	3.05	0.44
50:8:62:A:H4'	50:8:63:U:O5'	2.17	0.44
51:9:666:U:C2	51:9:667:U:C5	3.05	0.44
51:9:828:G:C6	51:9:829:C:C4	3.06	0.44
51:9:830:A:N6	51:9:844:U:C4	2.73	0.44
51:9:934:G:H2'	51:9:934:G:N3	2.33	0.44
51:9:1294:G:C6	51:9:1295:A:C5	3.06	0.44
51:9:1516:G:O3'	67:PP:122:THR:HG21	2.17	0.44
51:9:1542:C:C5'	71:TT:62:ARG:NH1	2.81	0.44
51:9:1686:G:N2	51:9:1687:C:C2	2.85	0.44
51:9:1731:A:H2'	51:9:1732:G:H8	1.82	0.44
51:9:1749:G:C2	51:9:1750:C:C2	3.05	0.44
54:CC:69:LEU:HG	54:CC:273:LEU:HD21	1.99	0.44
63:LL:14:PRO:O	63:LL:16:ILE:HD13	2.17	0.44
63:LL:35:ARG:NH2	63:LL:55:TYR:O	2.41	0.44
86:ii:328:ILE:CG2	86:ii:374:LEU:HD12	2.47	0.44
5:E:280:HIS:CD2	31:f:38:GLU:HG3	2.52	0.44
11:L:58:ILE:HG23	11:L:70:VAL:CG1	2.47	0.44
14:O:185:VAL:HG13	14:O:188:LYS:HG2	1.99	0.44
29:d:41:ARG:O	29:d:42:ALA:C	2.60	0.44
43:s:75:LEU:HA	43:s:78:LEU:HD12	2.00	0.44
48:5:709:C:H2'	48:5:710:G:O4'	2.17	0.44
48:5:1241:C:C2'	48:5:1242:G:OP1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1818:G:O2'	48:5:1819:G:OP1	2.28	0.44
48:5:1957:U:O2'	48:5:1958:A:C8	2.70	0.44
48:5:4246:G:C2	48:5:4263:C:C2	3.05	0.44
48:5:4371:G:C5	48:5:4372:U:C4	3.06	0.44
51:9:1415:C:H2'	51:9:1416:C:O4'	2.17	0.44
53:BB:25:PHE:CG	66:OO:88:LEU:HD21	2.52	0.44
69:RR:126:MET:N	69:RR:126:MET:SD	2.90	0.44
76:YY:113:ARG:O	76:YY:114:MET:HB2	2.18	0.44
78:aa:44:ILE:HG13	78:aa:67:LEU:HD12	1.98	0.44
87:jj:152:LEU:HD12	87:jj:156:PHE:HE2	1.81	0.44
1:A:8:GLN:NE2	48:5:3668:C:OP1	2.49	0.44
5:E:90:LYS:N	5:E:91:PRO:HD3	2.33	0.44
5:E:279:PRO:HA	5:E:282:LEU:CD2	2.48	0.44
12:M:81:ASP:CG	12:M:84:THR:CG2	2.90	0.44
18:S:168:THR:OG1	18:S:169:THR:N	2.49	0.44
23:X:76:ILE:HG23	23:X:77:ILE:HG13	2.00	0.44
31:f:28:LEU:N	31:f:28:LEU:CD1	2.81	0.44
48:5:76:A:C5	48:5:77:U:C5	3.05	0.44
48:5:113:A:C2	48:5:278:G:C4	3.04	0.44
48:5:351:C:C2	50:8:25:G:N2	2.86	0.44
48:5:726:G:H1	48:5:940:C:N4	2.15	0.44
48:5:1098:G:C2	48:5:1099:C:C2	3.06	0.44
48:5:1171:G:C2	48:5:1172:C:C2	3.05	0.44
48:5:1237:C:O2	48:5:1237:C:O4'	2.35	0.44
48:5:1656:U:H6	48:5:1656:U:H5'	1.82	0.44
48:5:2367:A:C8	48:5:2798:A:C5	3.05	0.44
48:5:2905:C:N3	48:5:3590:G:C2	2.85	0.44
48:5:3937:C:H2'	48:5:3938:G:N2	2.33	0.44
48:5:4076:G:OP2	48:5:4163:U:N3	2.50	0.44
48:5:4289:U:H2'	48:5:4290:U:C6	2.52	0.44
48:5:5020:G:O6	48:5:5028:G:O6	2.35	0.44
51:9:396:U:OP2	63:LL:79:LYS:NZ	2.43	0.44
51:9:455:A:O2'	51:9:1735:A:N3	2.43	0.44
51:9:616:A:N7	51:9:617:G:C8	2.85	0.44
51:9:1148:A:H4'	51:9:1149:A:O4'	2.17	0.44
51:9:1275:G:O2'	51:9:1276:A:OP2	2.35	0.44
51:9:1298:G:O2'	51:9:1299:A:P	2.75	0.44
51:9:1587:G:O2'	71:TT:67:ARG:NH2	2.43	0.44
51:9:1753:C:C2	51:9:1780:G:C2	3.05	0.44
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.81	0.44
87:jj:484:LEU:HD23	87:jj:516:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:LYS:HD3	48:5:4717:A:H4'	1.98	0.44
2:B:324:GLY:HA2	48:5:5051:C:O3'	2.17	0.44
3:C:218:VAL:O	3:C:218:VAL:HG12	2.16	0.44
3:C:221:PHE:HB3	3:C:227:ILE:HG21	1.99	0.44
3:C:333:LYS:HE2	5:E:50:ILE:HA	2.00	0.44
4:D:182:GLY:O	4:D:183:TYR:C	2.61	0.44
7:G:159:HIS:ND1	7:G:185:LYS:HA	2.33	0.44
13:N:42:PRO:CA	13:N:61:ILE:HD12	2.47	0.44
18:S:97:TYR:CZ	18:S:109:CYS:HA	2.52	0.44
19:T:105:PHE:CD1	48:5:1802:A:H4'	2.53	0.44
25:Z:10:VAL:HG11	25:Z:129:TRP:HZ3	1.82	0.44
31:f:94:ALA:HA	31:f:97:ILE:HG12	2.00	0.44
48:5:939:G:H2'	48:5:939:G:N3	2.33	0.44
48:5:985:C:C2	48:5:1069:G:C2	3.06	0.44
48:5:1400:G:H2'	48:5:1401:C:O4'	2.16	0.44
48:5:2586:G:H8	48:5:2770:C:H1'	1.82	0.44
48:5:2586:G:N7	48:5:2587:A:C6	2.86	0.44
48:5:2594:C:C2	48:5:2752:G:C2	3.06	0.44
48:5:4583:C:C4	48:5:4718:G:C6	3.05	0.44
51:9:167:G:N1	51:9:168:C:C4	2.86	0.44
51:9:1512:C:H2'	51:9:1513:C:H6	1.82	0.44
51:9:1866:A:N1	78:aa:87:ARG:HD2	2.32	0.44
52:AA:145:ILE:HD13	52:AA:159:ILE:CG2	2.48	0.44
55:DD:119:CYS:O	55:DD:120:TYR:C	2.60	0.44
56:EE:163:ASP:O	56:EE:164:LEU:HB2	2.17	0.44
17:R:21:LYS:NZ	48:5:2821:U:OP1	2.46	0.44
30:e:85:LEU:HD11	30:e:115:ALA:HB2	1.98	0.44
41:p:60:CYS:O	41:p:61:MET:HB2	2.17	0.44
48:5:28:C:C2	48:5:55:G:C2	3.06	0.44
48:5:978:G:C2	48:5:979:C:C2	3.06	0.44
48:5:1349:G:C6	48:5:1508:A:N1	2.86	0.44
48:5:1360:G:N1	48:5:1361:G:C4	2.86	0.44
48:5:1873:A:C2	48:5:1874:A:C8	3.06	0.44
48:5:2076:G:C2	48:5:2077:C:C2	3.04	0.44
48:5:2306:G:N3	48:5:2331:G:C2	2.86	0.44
48:5:2559:G:C2	48:5:2560:C:C2	3.06	0.44
48:5:2715:G:N3	48:5:2715:G:H2'	2.31	0.44
48:5:3882:C:H2'	48:5:3883:U:C6	2.52	0.44
48:5:4489:G:C6	48:5:4490:C:C4	3.05	0.44
48:5:4745:G:N2	48:5:4746:C:N4	2.66	0.44
48:5:5017:G:C6	48:5:5018:C:C4	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:8:55:U:O4	50:8:62:A:N1	2.50	0.44
50:8:115:G:C2	50:8:116:C:C2	3.06	0.44
51:9:105:U:C5	51:9:106:C:C5	3.06	0.44
51:9:200:G:C2	51:9:201:C:C4	3.06	0.44
51:9:666:U:H2'	51:9:667:U:C6	2.53	0.44
51:9:832:G:C2	51:9:833:C:C2	3.06	0.44
51:9:1089:G:C2	51:9:1090:C:C2	3.05	0.44
51:9:1459:G:C2	51:9:1468:C:C2	3.05	0.44
51:9:1511:U:H2'	51:9:1512:C:C6	2.53	0.44
51:9:1847:G:N2	51:9:1853:C:C2	2.86	0.44
65:NN:33:VAL:HG21	65:NN:66:VAL:HG11	2.00	0.44
66:OO:94:HIS:HA	66:OO:127:GLY:O	2.18	0.44
2:B:165:HIS:ND1	2:B:166:THR:O	2.50	0.44
3:C:293:LEU:HD13	48:5:2088:A:H2'	2.00	0.44
13:N:60:VAL:HG12	13:N:61:ILE:N	2.33	0.44
33:h:78:TYR:CZ	48:5:16:G:H4'	2.53	0.44
44:t:16:ARG:HG3	44:t:17:CYS:N	2.32	0.44
48:5:469:C:C2	48:5:470:A:C8	3.06	0.44
48:5:1367:C:O2	48:5:1370:G:H2'	2.17	0.44
48:5:1387:A:O4'	48:5:1397:A:N6	2.51	0.44
48:5:1622:U:O2'	48:5:1627:G:H4'	2.18	0.44
48:5:1635:C:C2'	48:5:1636:U:H5'	2.47	0.44
48:5:1981:G:O2'	48:5:1982:G:O4'	2.36	0.44
48:5:2021:G:C6	48:5:2022:C:C4	3.06	0.44
48:5:2468:U:C4	48:5:2473:A:C6	3.06	0.44
48:5:2682:G:N2	48:5:2683:C:C2	2.86	0.44
48:5:3627:G:C2	48:5:3835:C:C2	3.06	0.44
48:5:3804:G:C6	48:5:3805:U:C4	3.06	0.44
48:5:3870:C:C2	48:5:3886:G:N2	2.86	0.44
48:5:4412:C:H2'	48:5:4413:C:O2	2.16	0.44
48:5:4416:G:N2	48:5:4417:C:C2	2.86	0.44
49:7:25:G:C2	49:7:26:C:C2	3.05	0.44
51:9:16:G:C6	51:9:17:C:N4	2.86	0.44
51:9:510:G:OP1	61:JJ:3:VAL:HA	2.18	0.44
51:9:578:C:H2'	51:9:579:C:O4'	2.18	0.44
51:9:1126:G:N2	51:9:1127:C:C2	2.86	0.44
51:9:1145:A:C5	51:9:1146:C:H1'	2.52	0.44
51:9:1166:G:C6	51:9:1167:G:N7	2.86	0.44
51:9:1374:C:H2'	51:9:1375:G:O4'	2.18	0.44
51:9:1407:U:C2'	51:9:1407:U:O2	2.65	0.44
86:ii:32:THR:OG1	86:ii:33:SER:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:194:ILE:O	11:L:195:ARG:C	2.60	0.44
12:M:6:PHE:O	12:M:11:ARG:HD2	2.17	0.44
23:X:72:ASP:O	23:X:76:ILE:HG22	2.18	0.44
41:p:42:CYS:SG	41:p:43:GLY:N	2.90	0.44
48:5:1286:C:H2'	48:5:1287:G:C8	2.53	0.44
48:5:1374:G:C6	48:5:1375:C:C4	3.06	0.44
48:5:1899:G:N1	48:5:1900:C:C4	2.86	0.44
48:5:1956:A:C3'	48:5:1957:U:H5'	2.48	0.44
48:5:2034:G:C6	48:5:2035:C:C4	3.06	0.44
48:5:2336:G:C6	48:5:2337:C:C4	3.06	0.44
48:5:2578:G:C6	48:5:2584:G:C6	3.06	0.44
48:5:3724:A:C6	48:5:3725:G:C6	3.06	0.44
50:8:127:U:C4	50:8:128:C:C5	3.05	0.44
50:8:155:C:H2'	50:8:156:U:O4'	2.18	0.44
51:9:216:C:C5	51:9:217:A:C8	3.05	0.44
51:9:1616:U:H2'	51:9:1617:G:O4'	2.18	0.44
62:KK:38:LYS:O	62:KK:40:VAL:N	2.51	0.44
87:jj:426:GLN:HA	87:jj:429:HIS:CD2	2.53	0.44
2:B:249:ARG:C	2:B:250:LYS:HG3	2.43	0.43
3:C:267:TRP:CD1	3:C:281:MET:HE1	2.53	0.43
5:E:101:ARG:HG2	48:5:470:A:N1	2.33	0.43
5:E:254:LEU:CD2	5:E:258:LYS:HD2	2.48	0.43
7:G:184:LEU:HD12	7:G:190:LEU:HD13	1.99	0.43
11:L:49:ARG:CG	33:h:119:TYR:CD1	2.72	0.43
17:R:172:ARG:HG3	17:R:172:ARG:HH21	1.83	0.43
23:X:53:ARG:NH1	48:5:2475:G:N7	2.65	0.43
29:d:36:VAL:HG23	29:d:41:ARG:HG2	2.00	0.43
48:5:176:G:H2'	48:5:177:G:O4'	2.18	0.43
48:5:325:U:H2'	48:5:326:C:C6	2.53	0.43
48:5:730:G:N2	48:5:939:G:N2	2.66	0.43
48:5:1404:G:C2	48:5:1405:C:C2	3.06	0.43
48:5:2473:A:C6	48:5:2506:G:N7	2.86	0.43
48:5:2688:G:N1	48:5:2689:C:C4	2.86	0.43
48:5:2698:G:C2	48:5:2699:C:C2	3.06	0.43
48:5:3648:A:H1'	48:5:3785:A:N6	2.32	0.43
48:5:3811:G:C4	48:5:3814:U:C5	3.06	0.43
48:5:4395:U:H5'	48:5:4395:U:C6	2.51	0.43
50:8:126:C:O2'	50:8:127:U:C5	2.69	0.43
51:9:187:G:C6	51:9:188:C:C4	3.05	0.43
51:9:823:U:O2	51:9:823:U:O5'	2.35	0.43
51:9:1398:G:C6	51:9:1399:C:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1500:G:C5	51:9:1501:C:C4	3.06	0.43
51:9:1777:G:C6	51:9:1778:C:C4	3.06	0.43
60:II:55:TYR:HB2	60:II:182:CYS:O	2.18	0.43
66:OO:56:VAL:CG1	66:OO:81:VAL:HG23	2.48	0.43
74:WW:34:ILE:O	74:WW:35:VAL:C	2.60	0.43
77:ZZ:51:ASP:OD1	77:ZZ:51:ASP:N	2.49	0.43
84:gg:5:MET:HE1	84:gg:312:VAL:HG22	1.99	0.43
1:A:208:GLU:HG2	48:5:1629:G:H1	1.82	0.43
2:B:114:CYS:SG	2:B:165:HIS:CD2	3.12	0.43
3:C:298:ILE:HG12	16:Q:131:PRO:HB3	1.99	0.43
4:D:95:TYR:O	4:D:98:ALA:HB3	2.18	0.43
6:F:89:PRO:HG3	6:F:146:TYR:CE1	2.53	0.43
9:I:93:PRO:HB2	9:I:125:THR:HB	1.99	0.43
15:P:131:ARG:CD	15:P:137:ASN:ND2	2.81	0.43
17:R:96:MET:O	17:R:97:ARG:C	2.61	0.43
21:V:20:LEU:HD13	21:V:26:ILE:HG21	2.00	0.43
28:c:22:MET:SD	28:c:27:TYR:CE2	3.11	0.43
41:p:22:LEU:HD23	41:p:22:LEU:HA	1.87	0.43
47:3:35:U:O4’	51:9:1641:A:OP1	2.35	0.43
48:5:1270:A:H2’	48:5:1271:G:O5’	2.18	0.43
48:5:1533:A:H1’	48:5:1536:U:O4	2.18	0.43
48:5:1744:U:H2’	48:5:1745:G:O4’	2.18	0.43
48:5:1947:U:O2	48:5:1947:U:H2’	2.17	0.43
48:5:2769:U:OP1	48:5:2770:C:OP1	2.36	0.43
48:5:3597:G:C2	48:5:3598:C:C2	3.06	0.43
48:5:3705:G:C2	48:5:3706:C:C2	3.06	0.43
48:5:3723:A:C2	48:5:3724:A:C6	3.06	0.43
48:5:3727:A:H2’	48:5:3728:A:C8	2.53	0.43
48:5:4139:G:C6	48:5:4140:C:C4	3.06	0.43
48:5:4178:A:H2’	48:5:4179:G:C8	2.53	0.43
48:5:4919:G:N2	48:5:4920:C:C2	2.86	0.43
48:5:4950:U:O2	48:5:4950:U:O4’	2.36	0.43
51:9:1222:G:H2’	51:9:1223:A:C8	2.52	0.43
51:9:1240:A:C4	67:PP:100:LYS:HG2	2.54	0.43
51:9:1500:G:C6	51:9:1501:C:N3	2.86	0.43
51:9:1536:G:H2’	51:9:1537:A:H8	1.83	0.43
51:9:1777:G:C2	51:9:1778:C:C2	3.05	0.43
58:GG:64:LYS:HG2	58:GG:97:VAL:HG21	1.99	0.43
61:JJ:60:LEU:HD22	61:JJ:70:ARG:HA	2.00	0.43
64:MM:35:ILE:HD13	64:MM:61:TYR:CE1	2.53	0.43
66:OO:31:CYS:HA	66:OO:44:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:WW:53:ILE:HD12	74:WW:53:ILE:N	2.33	0.43
2:B:89:ILE:HD13	2:B:153:MET:HE1	2.00	0.43
7:G:58:PRO:CD	23:X:46:PHE:HD2	2.31	0.43
7:G:86:VAL:CG1	7:G:185:LYS:CG	2.66	0.43
9:I:184:MET:HE2	9:I:189:ARG:HB2	2.00	0.43
11:L:2:ALA:N	48:5:1514:U:OP1	2.51	0.43
14:O:201:PHE:CD1	14:O:201:PHE:N	2.84	0.43
30:e:15:LYS:NZ	30:e:61:GLY:O	2.46	0.43
35:j:7:SER:C	35:j:9:GLY:N	2.74	0.43
47:3:41:U:H2'	47:3:42:G:C8	2.53	0.43
47:3:66:U:C4	47:3:67:U:C5	3.05	0.43
48:5:77:U:C4	48:5:335:A:N1	2.85	0.43
48:5:964:A:N1	48:5:2252:G:N7	2.66	0.43
48:5:2008:U:C2	48:5:2010:A:OP2	2.72	0.43
48:5:2733:C:H2'	48:5:2734:U:O4'	2.18	0.43
48:5:2793:G:C2	48:5:2799:G:C6	3.06	0.43
48:5:3729:U:H2'	48:5:3730:U:C6	2.53	0.43
48:5:4230:C:H1'	48:5:4271:A:C2	2.53	0.43
48:5:5000:G:N2	48:5:5051:C:C2	2.87	0.43
51:9:841:G:C2	51:9:842:C:C2	3.05	0.43
51:9:841:G:N1	51:9:842:C:C4	2.86	0.43
51:9:944:A:C6	51:9:945:U:C5	3.06	0.43
51:9:996:A:H2'	51:9:997:A:O4'	2.18	0.43
51:9:1057:C:O2	51:9:1057:C:O4'	2.35	0.43
51:9:1249:C:N4	51:9:1250:A:C6	2.86	0.43
51:9:1268:C:C2	51:9:1515:G:N2	2.86	0.43
51:9:1865:C:C2	78:aa:5:ARG:HG2	2.53	0.43
52:AA:167:GLY:O	52:AA:171:VAL:HG23	2.18	0.43
54:CC:65:LYS:HG3	54:CC:273:LEU:HD22	2.00	0.43
63:LL:27:GLU:O	63:LL:28:THR:HG22	2.18	0.43
63:LL:135:SER:OG	63:LL:138:VAL:HG23	2.19	0.43
66:OO:44:VAL:HB	66:OO:53:ILE:O	2.17	0.43
7:G:65:ARG:O	7:G:68:ALA:N	2.50	0.43
11:L:146:LEU:HB2	11:L:148:THR:CG2	2.48	0.43
14:O:51:LYS:N	14:O:141:LEU:HD11	2.33	0.43
17:R:91:GLU:O	17:R:94:THR:N	2.51	0.43
20:U:87:THR:HG23	20:U:102:VAL:HG21	1.99	0.43
43:s:145:THR:HG22	43:s:154:ILE:HG13	2.01	0.43
48:5:199:G:N2	48:5:201:C:C2	2.86	0.43
48:5:504:G:O6	48:5:654:C:C4	2.72	0.43
48:5:677:G:C2	48:5:678:C:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:726:G:C6	48:5:727:C:N4	2.87	0.43
48:5:1090:G:C2	48:5:1091:C:C2	3.06	0.43
48:5:1245:C:C4	48:5:1269:G:O6	2.72	0.43
48:5:1506:G:C2	48:5:1507:C:C2	3.06	0.43
48:5:1826:G:C2	48:5:1827:C:C2	3.07	0.43
48:5:2622:G:C5	48:5:2623:A:N7	2.86	0.43
48:5:3857:G:C6	48:5:3858:C:C4	3.06	0.43
51:9:115:U:H2'	51:9:116:U:H6	1.81	0.43
51:9:302:A:O2'	60:II:73:THR:O	2.21	0.43
51:9:1221:G:C2	51:9:1222:G:C5	3.06	0.43
51:9:1571:G:C6	51:9:1572:C:C4	3.06	0.43
51:9:1737:G:C6	51:9:1738:C:C4	3.06	0.43
54:CC:130:ILE:HG22	54:CC:158:ALA:HB1	1.99	0.43
54:CC:137:VAL:HG13	54:CC:217:ALA:HA	2.01	0.43
54:CC:244:ILE:HA	54:CC:247:THR:HG23	2.00	0.43
55:DD:198:ILE:O	55:DD:199:GLY:O	2.36	0.43
73:VV:15:ARG:NH2	73:VV:24:ILE:HG21	2.34	0.43
1:A:48:ILE:HD11	1:A:82:ILE:HG22	1.99	0.43
4:D:16:TYR:O	49:7:11:A:N6	2.51	0.43
10:J:166:PHE:CE2	10:J:172:GLY:HA3	2.54	0.43
13:N:94:PHE:CE2	13:N:96:ARG:HB2	2.53	0.43
14:O:17:GLY:HA3	48:5:2052:G:O3'	2.18	0.43
32:g:68:SER:HA	48:5:2769:U:OP1	2.18	0.43
40:o:32:SER:OG	40:o:35:ALA:N	2.51	0.43
45:1:68:VAL:O	46:2:76:A:O2'	2.37	0.43
48:5:179:G:C2	48:5:180:C:C2	3.06	0.43
48:5:665:C:O2	48:5:665:C:C2'	2.66	0.43
48:5:688:U:H2'	48:5:689:U:C6	2.53	0.43
48:5:701:G:N3	48:5:701:G:H2'	2.33	0.43
48:5:1048:G:C2	48:5:1049:C:C2	3.06	0.43
48:5:1584:G:C2	48:5:1585:C:C2	3.07	0.43
48:5:1672:U:C6	48:5:1684:A:C2	3.06	0.43
48:5:1757:U:C2	48:5:1758:G:C8	3.06	0.43
48:5:1995:G:C5	48:5:1996:C:C4	3.06	0.43
48:5:2863:G:C6	48:5:2864:A:C5	3.07	0.43
48:5:3783:A:N7	48:5:3792:G:C6	2.86	0.43
48:5:3822:U:O2	48:5:3822:U:H2'	2.18	0.43
48:5:3904:G:HO2'	48:5:3905:A:P	2.41	0.43
48:5:4402:C:C5	48:5:4403:U:C5	3.06	0.43
48:5:4455:G:C6	48:5:4456:C:C4	3.07	0.43
48:5:4904:G:C2	48:5:4905:C:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:23:G:C6	51:9:24:C:C4	3.06	0.43
51:9:1103:C:C2	51:9:1104:G:C8	3.07	0.43
51:9:1296:U:C4	51:9:1297:U:C4	3.07	0.43
51:9:1650:A:C5	51:9:1675:A:N1	2.87	0.43
51:9:1754:G:C2	51:9:1755:C:C2	3.05	0.43
55:DD:25:LEU:HB3	55:DD:34:TYR:CE1	2.53	0.43
56:EE:72:ILE:HD13	56:EE:82:TYR:CD1	2.53	0.43
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	1.99	0.43
71:TT:42:HIS:HB2	71:TT:43:LYS:HG2	1.99	0.43
74:WW:50:PHE:CD1	74:WW:50:PHE:C	2.97	0.43
76:YY:5:VAL:HG23	76:YY:6:THR:N	2.33	0.43
76:YY:103:SER:O	76:YY:105:LYS:N	2.52	0.43
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.48	0.43
7:G:30:PRO:CG	25:Z:124:THR:C	2.91	0.43
8:H:4:ILE:HD11	18:S:152:PHE:CD2	2.54	0.43
11:L:28:GLN:HG2	11:L:29:PRO:HD3	2.01	0.43
11:L:77:SER:OG	11:L:80:GLU:HG3	2.18	0.43
26:a:145:VAL:HG13	34:i:5:TYR:CZ	2.53	0.43
43:s:10:LYS:NZ	48:5:1960:A:O3'	2.50	0.43
47:3:34:U:H1'	51:9:1642:U:OP2	2.17	0.43
48:5:179:G:N2	48:5:180:C:C2	2.87	0.43
48:5:1962:A:HO2'	48:5:1963:C:C5'	2.30	0.43
48:5:3600:G:C2	48:5:3601:C:C2	3.07	0.43
48:5:4966:A:H2'	48:5:4967:A:C8	2.53	0.43
51:9:211:G:C6	51:9:212:C:N4	2.87	0.43
51:9:412:G:C2	51:9:429:C:C2	3.06	0.43
51:9:929:G:N1	51:9:930:C:C2	2.86	0.43
51:9:1132:C:C5	51:9:1133:A:C8	3.07	0.43
61:JJ:46:VAL:HG21	61:JJ:106:LEU:CD1	2.49	0.43
71:TT:46:ALA:HB1	71:TT:47:PRO:CD	2.49	0.43
73:VV:24:ILE:HG12	73:VV:56:CYS:HA	2.00	0.43
78:aa:34:LYS:O	78:aa:35:ALA:HB3	2.18	0.43
3:C:237:ILE:O	3:C:238:LEU:C	2.62	0.43
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.54	0.43
12:M:107:PHE:CZ	12:M:111:LYS:HE2	2.53	0.43
13:N:57:GLN:HB3	13:N:139:HIS:CE1	2.54	0.43
16:Q:61:LEU:HD22	16:Q:66:MET:HB2	2.01	0.43
47:3:75:C:O2'	47:3:76:A:OP2	2.24	0.43
48:5:39:A:C4	48:5:1654:G:C6	3.07	0.43
48:5:1378:C:H5'	48:5:1379:C:H3'	2.00	0.43
48:5:2021:G:O2'	48:5:2022:C:C5'	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2602:G:H2'	48:5:2603:C:O4'	2.18	0.43
48:5:2612:G:C2	48:5:2613:C:C2	3.06	0.43
48:5:3600:G:C6	48:5:3601:C:C4	3.07	0.43
48:5:3878:C:C4	48:5:4518:A:C4	3.06	0.43
48:5:4911:A:C3'	48:5:4912:G:H5"	2.49	0.43
51:9:94:G:C5	51:9:95:G:C8	3.06	0.43
51:9:1584:G:C6	51:9:1586:U:C2	3.07	0.43
51:9:1669:G:C2	51:9:1670:C:C2	3.06	0.43
51:9:1771:G:C2	51:9:1772:C:C4	3.07	0.43
51:9:1842:C:C2	51:9:1858:G:N2	2.87	0.43
59:HH:146:VAL:HG21	74:WW:50:PHE:CE1	2.54	0.43
84:gg:164:ILE:CG2	84:gg:176:VAL:HG13	2.49	0.43
2:B:220:ILE:HG12	2:B:278:THR:HG23	2.00	0.43
5:E:254:LEU:N	5:E:255:PRO:CD	2.81	0.43
6:F:91:LEU:HD22	6:F:91:LEU:C	2.44	0.43
8:H:104:VAL:HG13	8:H:113:GLU:HB2	2.00	0.43
12:M:81:ASP:CG	12:M:84:THR:OG1	2.62	0.43
13:N:25:VAL:O	13:N:26:ARG:C	2.60	0.43
18:S:30:MET:HE1	18:S:47:PHE:HB3	2.01	0.43
18:S:132:ILE:HG22	18:S:133:ALA:O	2.18	0.43
22:W:50:ASN:HA	22:W:55:TYR:CG	2.54	0.43
47:3:39:U:O2'	47:3:40:C:O4'	2.37	0.43
48:5:258:G:C2	48:5:259:C:C2	3.07	0.43
48:5:674:G:C2	48:5:675:C:C2	3.07	0.43
48:5:933:G:C2	48:5:939:G:N2	2.87	0.43
48:5:1358:G:H2'	48:5:1359:G:H8	1.84	0.43
48:5:1547:A:H3'	48:5:1548:G:H8	1.82	0.43
48:5:2843:U:O2'	48:5:4632:U:OP1	2.32	0.43
48:5:3740:G:C5	48:5:3741:C:C5	3.07	0.43
48:5:3777:G:N2	48:5:3815:G:H2'	2.34	0.43
48:5:4439:U:H2'	48:5:4440:G:O4'	2.19	0.43
48:5:4901:G:C2	48:5:4921:C:C2	3.06	0.43
48:5:4999:G:H2'	48:5:4999:G:N3	2.34	0.43
48:5:4999:G:N2	48:5:5052:C:C2	2.87	0.43
48:5:5020:G:C2	48:5:5021:C:C2	3.06	0.43
49:7:38:U:C2	49:7:40:U:OP2	2.72	0.43
49:7:93:G:C2	49:7:94:C:C2	3.07	0.43
51:9:351:G:C6	51:9:352:U:C5	3.07	0.43
51:9:1137:U:O2'	51:9:1138:C:OP1	2.30	0.43
51:9:1347:U:H2'	51:9:1348:G:C8	2.53	0.43
51:9:1587:G:N3	51:9:1587:G:H2'	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1731:A:H2'	51:9:1732:G:C8	2.54	0.43
52:AA:3:GLY:O	52:AA:5:LEU:N	2.51	0.43
52:AA:30:LEU:HB2	52:AA:47:TYR:CE2	2.53	0.43
57:FF:154:LEU:HD12	57:FF:155:CYS:N	2.34	0.43
74:WW:6:VAL:HG13	74:WW:29:PRO:HG2	2.01	0.43
78:aa:6:ARG:O	78:aa:7:ASN:C	2.61	0.43
81:dd:21:CYS:SG	81:dd:24:CYS:N	2.90	0.43
2:B:13:SER:HB2	48:5:4622:A:H4'	1.99	0.43
3:C:210:ILE:CG2	3:C:232:VAL:HG13	2.49	0.43
8:H:34:LEU:HD12	8:H:84:VAL:HG23	2.01	0.43
17:R:38:ARG:NH2	48:5:2527:A:OP2	2.41	0.43
23:X:76:ILE:HG21	23:X:112:ALA:CB	2.48	0.43
31:f:17:GLY:O	31:f:18:LEU:C	2.60	0.43
41:p:17:ARG:NH2	48:5:1577:G:OP1	2.52	0.43
42:r:47:LYS:HD2	42:r:102:TYR:CD2	2.54	0.43
43:s:15:LEU:HA	43:s:18:ILE:HG22	2.00	0.43
47:3:38:A:C2	57:FF:135:ARG:NH1	2.86	0.43
48:5:52:G:N2	48:5:53:C:C2	2.87	0.43
48:5:674:G:N2	48:5:675:C:C2	2.87	0.43
48:5:1563:A:C8	51:9:678:U:H4'	2.54	0.43
48:5:1811:G:C2	48:5:1812:C:C2	3.07	0.43
48:5:4080:C:C2	48:5:4167:G:N2	2.86	0.43
48:5:4303:C:O2	48:5:4303:C:O4'	2.33	0.43
51:9:913:A:H2'	59:HH:120:ARG:NH2	2.34	0.43
51:9:1144:A:O2'	51:9:1199:A:O2'	2.25	0.43
51:9:1224:G:C4	51:9:1225:U:C5	3.06	0.43
51:9:1466:G:C6	51:9:1467:C:N4	2.87	0.43
51:9:1615:U:H3'	67:PP:43:ARG:NH2	2.33	0.43
51:9:1771:G:C6	51:9:1772:C:N4	2.87	0.43
71:TT:75:MET:HA	71:TT:78:ILE:HG22	2.00	0.43
74:WW:52:ILE:HG22	74:WW:61:ILE:HG23	2.01	0.43
76:YY:126:GLY:O	76:YY:128:GLY:N	2.51	0.43
8:H:126:VAL:HG11	8:H:161:ILE:HG22	2.01	0.43
8:H:138:GLN:O	8:H:139:ALA:HB3	2.18	0.43
20:U:84:LYS:HA	20:U:87:THR:HG22	2.00	0.43
22:W:34:ALA:O	22:W:35:LYS:C	2.62	0.43
43:s:14:PHE:HZ	48:5:1960:A:N3	2.12	0.43
48:5:79:C:H2'	48:5:80:C:C6	2.54	0.43
48:5:174:C:C2	48:5:263:G:C2	3.06	0.43
48:5:192:G:H2'	48:5:193:G:O4'	2.18	0.43
48:5:254:G:C2	48:5:255:C:C2	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1546:C:N3	48:5:1612:G:O6	2.52	0.43
48:5:1668:A:C4	48:5:2282:A:C2	3.07	0.43
48:5:1912:G:C2	48:5:1913:C:C2	3.07	0.43
48:5:1964:A:N1	48:5:4694:G:C5	2.87	0.43
48:5:2273:G:C6	48:5:2274:C:C4	3.06	0.43
48:5:2306:G:C2	48:5:2331:G:C4	3.07	0.43
48:5:2457:G:C2	48:5:2458:C:C2	3.07	0.43
48:5:2595:C:H2'	48:5:2596:G:O4'	2.19	0.43
48:5:2620:G:C6	48:5:2621:A:C5	3.06	0.43
48:5:3717:A:OP2	48:5:3735:G:N2	2.49	0.43
48:5:4240:G:C2	48:5:4241:C:C2	3.06	0.43
48:5:4489:G:C2	48:5:4490:C:C2	3.06	0.43
48:5:4898:G:N2	48:5:4923:C:C2	2.87	0.43
51:9:666:U:C5	51:9:1150:A:C4	3.07	0.43
51:9:1567:G:H1'	70:SS:82:TRP:CH2	2.52	0.43
54:CC:127:PHE:CZ	54:CC:234:GLY:HA3	2.54	0.43
56:EE:39:ARG:HE	56:EE:39:ARG:HA	1.84	0.43
63:LL:103:GLU:OE2	75:XX:11:ARG:NH1	2.52	0.43
65:NN:107:LYS:O	65:NN:109:LYS:N	2.51	0.43
84:gg:256:ILE:HG21	84:gg:289:LEU:CD1	2.49	0.43
5:E:217:GLN:NE2	5:E:233:LYS:CD	2.82	0.42
5:E:257:ILE:HG22	5:E:263:LEU:CD2	2.47	0.42
6:F:97:ILE:HB	6:F:222:MET:HE1	2.01	0.42
9:I:79:SER:HB2	9:I:147:HIS:ND1	2.33	0.42
11:L:125:VAL:O	11:L:125:VAL:HG12	2.19	0.42
17:R:9:ARG:O	17:R:10:LEU:C	2.61	0.42
18:S:84:TYR:CZ	18:S:93:MET:HE3	2.54	0.42
48:5:29:G:C6	48:5:54:G:C6	3.07	0.42
48:5:80:C:C2	48:5:104:G:N2	2.87	0.42
48:5:302:C:N4	48:5:303:C:N4	2.66	0.42
48:5:642:G:C2	48:5:643:C:C4	3.07	0.42
48:5:1048:G:C6	48:5:1049:C:C4	3.07	0.42
48:5:1090:G:C6	48:5:1091:C:C4	3.07	0.42
48:5:1277:G:C2	48:5:1278:C:C2	3.07	0.42
48:5:2470:C:O2	48:5:2470:C:O4'	2.37	0.42
48:5:2907:G:H2'	48:5:2908:U:O4'	2.19	0.42
48:5:3617:G:O2'	48:5:3620:G:N7	2.52	0.42
49:7:110:G:H2'	49:7:111:C:C6	2.54	0.42
51:9:442:C:H2'	51:9:443:U:O4'	2.19	0.42
51:9:520:A:H5"	61:JJ:12:THR:HG23	2.00	0.42
51:9:614:C:N4	51:9:626:G:C6	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1622:U:C6	70:SS:120:HIS:CE1	3.07	0.42
51:9:1845:A:C2	51:9:1855:G:C5	3.07	0.42
55:DD:204:LEU:HD23	55:DD:205:PRO:CD	2.49	0.42
57:FF:76:MET:O	57:FF:78:MET:N	2.52	0.42
64:MM:51:VAL:HG13	64:MM:109:VAL:HG22	2.00	0.42
84:gg:4:GLN:C	84:gg:5:MET:HE2	2.44	0.42
86:ii:329:MET:HG2	86:ii:373:PRO:HA	2.00	0.42
87:jj:62:ILE:HD11	87:jj:72:ILE:HB	2.01	0.42
87:jj:376:VAL:HG21	87:jj:529:ALA:HB2	2.01	0.42
2:B:49:TYR:CE1	2:B:171:LEU:HD11	2.54	0.42
4:D:67:ALA:HA	4:D:72:ASP:HA	2.00	0.42
6:F:146:TYR:CE2	6:F:239:GLU:CB	3.02	0.42
11:L:22:VAL:HG13	13:N:200:LEU:HD12	2.00	0.42
11:L:106:SER:HB2	34:i:17:VAL:CG1	2.49	0.42
17:R:168:GLU:O	17:R:172:ARG:CG	2.60	0.42
23:X:60:TYR:CD1	33:h:78:TYR:HB3	2.54	0.42
48:5:366:A:C2	48:5:376:A:C4	3.07	0.42
48:5:1388:A:C6	48:5:1389:U:N3	2.88	0.42
48:5:1676:C:N4	48:5:4378:A:C8	2.87	0.42
48:5:1986:U:H2'	48:5:2007:G:O6	2.19	0.42
48:5:2773:G:C2	48:5:2774:C:C5	3.07	0.42
48:5:3590:G:N1	48:5:3591:C:C2	2.87	0.42
48:5:4911:A:H3'	48:5:4912:G:H5"	2.01	0.42
48:5:5028:G:C2	48:5:5029:C:N3	2.88	0.42
50:8:89:U:H2'	50:8:90:C:C6	2.54	0.42
51:9:293:C:O2'	51:9:294:U:H3'	2.19	0.42
51:9:376:A:H2'	51:9:377:G:O4'	2.20	0.42
51:9:673:G:C2	51:9:674:C:C2	3.07	0.42
51:9:936:G:C2	51:9:1007:C:C2	3.07	0.42
51:9:1235:G:C5'	51:9:1247:C:N4	2.81	0.42
56:EE:125:LYS:HB2	56:EE:226:PHE:HD1	1.83	0.42
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.99	0.42
76:YY:25:ILE:HD11	76:YY:44:LEU:HD21	2.01	0.42
83:ff:136:CYS:SG	83:ff:137:GLY:N	2.91	0.42
86:ii:224:LEU:HG	86:ii:246:LEU:CD2	2.49	0.42
87:jj:21:CYS:O	87:jj:22:ARG:HG2	2.19	0.42
2:B:115:LYS:HA	2:B:118:PHE:HD1	1.84	0.42
3:C:120:LYS:HD2	48:5:1374:G:OP1	2.18	0.42
12:M:113:MET:SD	12:M:113:MET:C	3.02	0.42
13:N:11:TRP:CE3	13:N:44:ARG:NH2	2.88	0.42
13:N:49:ARG:NH2	48:5:152:U:OP2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:108:ARG:NH2	48:5:54:G:O3'	2.50	0.42
15:P:108:ASP:O	15:P:109:VAL:C	2.63	0.42
18:S:91:HIS:NE2	48:5:2032:U:O2'	2.49	0.42
23:X:52:LEU:HD22	23:X:53:ARG:H	1.85	0.42
31:f:14:TYR:HD2	31:f:21:GLN:CD	2.26	0.42
31:f:96:ALA:O	31:f:97:ILE:C	2.61	0.42
48:5:209:U:C4	48:5:233:U:C4	3.07	0.42
48:5:2306:G:N2	48:5:2331:G:C4	2.88	0.42
48:5:2410:C:C2	48:5:2435:G:N2	2.87	0.42
48:5:2551:A:N6	48:5:2552:G:C6	2.87	0.42
48:5:4269:G:C2	48:5:4270:C:C2	3.07	0.42
48:5:4269:G:C6	48:5:4270:C:C4	3.08	0.42
50:8:49:G:C2	50:8:50:C:C2	3.08	0.42
51:9:905:C:H2'	51:9:906:U:O4'	2.19	0.42
51:9:1034:A:C5	51:9:1082:A:C5	3.07	0.42
51:9:1227:G:C2	51:9:1638:G:C2	3.07	0.42
53:BB:47:THR:HG22	53:BB:48:LEU:N	2.34	0.42
59:HH:118:ARG:O	59:HH:119:SER:C	2.62	0.42
67:PP:108:LYS:O	67:PP:111:MET:HB2	2.19	0.42
71:TT:28:LEU:O	71:TT:29:LYS:HB2	2.20	0.42
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	2.01	0.42
77:ZZ:74:SER:HA	77:ZZ:79:ILE:HG22	2.01	0.42
3:C:132:ALA:O	3:C:133:LEU:HB2	2.19	0.42
3:C:163:LYS:N	3:C:166:GLU:OE1	2.50	0.42
6:F:74:ALA:O	6:F:75:ARG:C	2.62	0.42
6:F:148:ASN:HB3	6:F:151:SER:H	1.84	0.42
6:F:215:LEU:HD13	6:F:249:MET:HE3	2.01	0.42
9:I:199:TYR:CE2	9:I:201:PRO:HB3	2.55	0.42
11:L:163:LYS:NZ	48:5:509:A:H5'	2.34	0.42
13:N:63:ARG:HA	13:N:130:PHE:O	2.20	0.42
16:Q:178:ARG:HA	16:Q:184:ARG:O	2.20	0.42
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	2.01	0.42
27:b:13:SER:HA	27:b:16:TRP:CE3	2.54	0.42
38:m:104:HIS:CD2	48:5:4697:U:H4'	2.54	0.42
48:5:124:C:C2	48:5:146:G:C2	3.08	0.42
48:5:181:C:C4	48:5:256:G:C2	3.08	0.42
48:5:315:G:H2'	48:5:315:G:N3	2.34	0.42
48:5:1359:G:C5	48:5:1360:G:C5	3.07	0.42
48:5:1511:U:C2	48:5:1512:G:C8	3.07	0.42
48:5:1851:G:H2'	48:5:1852:U:O4'	2.19	0.42
48:5:2055:G:H3'	48:5:2056:G:H5"	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2082:G:C6	48:5:2083:C:C4	3.07	0.42
48:5:2088:A:HO2'	48:5:2089:G:P	2.41	0.42
48:5:2339:G:N2	48:5:2340:C:C2	2.87	0.42
48:5:2889:G:C6	48:5:2890:C:N3	2.88	0.42
48:5:4207:C:C2	48:5:4226:G:N2	2.88	0.42
51:9:572:U:H5'	76:YY:60:PHE:O	2.18	0.42
51:9:976:G:C6	51:9:977:C:C4	3.08	0.42
51:9:1105:G:C6	51:9:1106:C:C4	3.07	0.42
51:9:1797:U:H2'	51:9:1798:C:C6	2.54	0.42
63:LL:126:VAL:CG2	63:LL:142:VAL:HG13	2.50	0.42
69:RR:36:GLU:HG2	69:RR:47:ARG:HD2	2.01	0.42
70:SS:30:ILE:CD1	70:SS:45:LEU:HD21	2.50	0.42
87:jj:529:ALA:HB3	87:jj:551:LEU:CD1	2.48	0.42
2:B:29:VAL:HG13	2:B:348:ARG:HD3	2.02	0.42
2:B:229:LYS:HG3	2:B:272:LYS:HD3	1.99	0.42
2:B:291:TYR:CE1	2:B:299:ILE:HG13	2.54	0.42
3:C:233:THR:CG2	3:C:259:LYS:NZ	2.82	0.42
11:L:180:ALA:O	11:L:181:SER:C	2.61	0.42
12:M:52:PHE:O	12:M:53:LYS:C	2.62	0.42
29:d:36:VAL:HG23	29:d:41:ARG:CG	2.49	0.42
33:h:39:GLY:O	33:h:40:ALA:HB2	2.19	0.42
46:2:65:G:C2	46:2:66:C:C2	3.08	0.42
47:3:35:U:H1'	51:9:1640:A:O3'	2.18	0.42
48:5:2:G:C2	48:5:3:C:C2	3.07	0.42
48:5:22:G:N1	50:8:35:C:C4	2.87	0.42
48:5:458:C:H2'	48:5:459:C:O4'	2.19	0.42
48:5:937:U:O2	48:5:937:U:C2'	2.68	0.42
48:5:1064:G:C2	48:5:1065:G:C4	3.07	0.42
48:5:1356:U:N3	48:5:1357:C:C4	2.88	0.42
48:5:1681:G:C2	48:5:1682:A:C8	3.08	0.42
48:5:2297:G:C2	48:5:2338:C:N3	2.88	0.42
48:5:2767:U:C4	48:5:2769:U:O4	2.73	0.42
48:5:3717:A:O2'	48:5:3718:A:C5'	2.68	0.42
48:5:3737:A:O5'	48:5:3737:A:H8	2.02	0.42
48:5:4408:G:N2	48:5:4409:C:C2	2.87	0.42
48:5:4737:G:C6	48:5:4738:C:C4	3.07	0.42
50:8:115:G:N2	50:8:116:C:C2	2.87	0.42
51:9:618:C:OP1	75:XX:87:ASN:N	2.47	0.42
51:9:1417:C:O2'	51:9:1419:C:OP1	2.34	0.42
51:9:1726:G:C6	51:9:1727:G:C5	3.08	0.42
55:DD:72:VAL:HG22	62:KK:22:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:FF:145:ARG:HB2	80:cc:48:GLY:HA3	2.01	0.42
58:GG:88:ARG:HB3	58:GG:91:GLU:HB2	2.02	0.42
73:VV:37:ALA:HB1	73:VV:46:PHE:CD1	2.54	0.42
87:jj:482:VAL:HG13	87:jj:516:PHE:CE1	2.53	0.42
5:E:276:GLY:O	5:E:277:VAL:CG2	2.67	0.42
5:E:276:GLY:O	5:E:277:VAL:HG23	2.20	0.42
6:F:93:PHE:CE1	6:F:155:LEU:HD13	2.55	0.42
12:M:7:VAL:N	18:S:152:PHE:O	2.49	0.42
14:O:47:PHE:O	14:O:50:ASN:N	2.53	0.42
17:R:93:VAL:O	17:R:94:THR:C	2.61	0.42
25:Z:100:VAL:HG13	25:Z:107:LYS:HA	2.02	0.42
26:a:39:HIS:O	26:a:40:HIS:ND1	2.53	0.42
35:j:35:GLY:O	35:j:36:LYS:HB2	2.20	0.42
48:5:127:G:C2	48:5:128:C:C2	3.07	0.42
48:5:404:U:H2'	48:5:405:U:O4'	2.20	0.42
48:5:725:G:H2'	48:5:726:G:H8	1.84	0.42
48:5:947:C:H2'	48:5:948:C:H6	1.84	0.42
48:5:1660:U:O4'	48:5:2346:C:O4'	2.37	0.42
48:5:2451:A:C2	48:5:2509:C:C2	3.07	0.42
48:5:2524:U:H5"	48:5:2711:G:N2	2.34	0.42
48:5:3670:C:O2'	48:5:3671:G:C5'	2.67	0.42
48:5:3684:G:C2	48:5:3685:C:N3	2.88	0.42
48:5:3911:C:H2'	48:5:3912:U:H6	1.84	0.42
48:5:4901:G:N1	48:5:4921:C:C4	2.87	0.42
49:7:27:G:C2	49:7:28:C:C2	3.08	0.42
50:8:68:G:C2	50:8:91:A:C2	3.07	0.42
50:8:112:G:N2	50:8:113:C:C2	2.87	0.42
50:8:113:C:H2'	50:8:114:G:O4'	2.20	0.42
51:9:474:G:N1	51:9:475:C:C4	2.88	0.42
51:9:644:G:C6	51:9:645:C:N4	2.88	0.42
51:9:1121:G:C5	51:9:1122:A:N7	2.88	0.42
51:9:1139:C:O2	51:9:1139:C:OP1	2.37	0.42
51:9:1417:C:O2	51:9:1419:C:H5'	2.19	0.42
57:FF:61:PHE:CZ	80:cc:51:ARG:HD2	2.54	0.42
60:II:38:ILE:HG12	60:II:96:LEU:HD11	2.02	0.42
62:KK:64:TRP:O	62:KK:65:ARG:C	2.63	0.42
3:C:119:GLN:HG2	48:5:1351:G:O4'	2.19	0.42
6:F:98:ARG:HH21	6:F:226:THR:HA	1.84	0.42
7:G:57:TRP:O	7:G:62:ARG:NH2	2.48	0.42
13:N:185:GLY:O	48:5:78:U:OP1	2.37	0.42
16:Q:89:ASP:HA	48:5:1502:G:O6	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:64:VAL:HG13	19:T:72:VAL:CG1	2.42	0.42
24:Y:10:ASP:O	24:Y:13:LYS:N	2.53	0.42
25:Z:12:LEU:HB2	25:Z:81:MET:HB3	2.01	0.42
29:d:33:ILE:HD11	29:d:41:ARG:HB3	2.02	0.42
43:s:55:MET:HB2	48:5:1998:A:C8	2.55	0.42
48:5:169:G:C2	48:5:170:C:C2	3.07	0.42
48:5:1075:G:C6	48:5:1076:C:C4	3.08	0.42
48:5:1213:G:C2	48:5:1215:C:C2	3.08	0.42
48:5:1277:G:C6	48:5:1278:C:N4	2.88	0.42
48:5:1468:C:N3	48:5:1498:G:C2	2.87	0.42
48:5:2481:G:C2	48:5:2482:C:C2	3.08	0.42
48:5:2703:G:C6	48:5:2704:C:C4	3.08	0.42
48:5:2711:G:H3'	48:5:2712:G:H5"	2.02	0.42
48:5:4433:G:N2	48:5:4434:C:C2	2.88	0.42
48:5:4526:U:C5	48:5:4527:G:C6	3.07	0.42
48:5:4644:G:C2	48:5:4645:C:C2	3.08	0.42
48:5:4731:G:H4'	48:5:4732:G:H5'	2.02	0.42
48:5:4881:U:O2	48:5:4881:U:O4'	2.37	0.42
51:9:14:C:C2	51:9:1198:G:N1	2.88	0.42
51:9:113:G:N2	51:9:293:C:O4'	2.52	0.42
51:9:187:G:C2	51:9:188:C:C2	3.07	0.42
51:9:211:G:C2	51:9:212:C:C4	3.08	0.42
51:9:441:C:H2'	51:9:442:C:C6	2.55	0.42
51:9:1229:G:C6	51:9:1230:C:C4	3.08	0.42
51:9:1612:G:N2	51:9:1628:C:C2	2.88	0.42
51:9:1840:U:C4	51:9:1841:C:C4	3.07	0.42
53:BB:139:CYS:O	53:BB:140:VAL:HB	2.20	0.42
63:LL:77:VAL:HG22	63:LL:86:ILE:HD12	2.01	0.42
69:RR:20:TYR:CE2	69:RR:38:ILE:HB	2.55	0.42
71:TT:38:LYS:O	71:TT:39:LEU:CB	2.67	0.42
73:VV:17:CYS:SG	73:VV:20:SER:N	2.93	0.42
87:jj:240:PHE:CB	87:jj:271:VAL:HG23	2.50	0.42
2:B:116:ARG:HB3	2:B:177:LYS:HG3	2.01	0.42
18:S:80:ILE:HG13	18:S:129:VAL:HG22	2.01	0.42
26:a:145:VAL:HG13	34:i:5:TYR:CE1	2.55	0.42
31:f:6:TRP:CE3	31:f:102:ARG:HG2	2.55	0.42
44:t:143:VAL:O	44:t:145:GLY:N	2.52	0.42
48:5:301:G:C2	48:5:302:C:C2	3.08	0.42
48:5:484:U:C4	48:5:486:C:C5	3.08	0.42
48:5:705:G:N1	48:5:706:C:C4	2.88	0.42
48:5:1271:G:H3'	48:5:1272:C:H5'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1412:G:N1	48:5:1413:C:C4	2.88	0.42
48:5:1466:G:C6	48:5:1467:C:C4	3.08	0.42
48:5:1733:G:C4	48:5:4214:A:C2	3.08	0.42
48:5:1967:A:H2'	48:5:1968:G:H5'	2.01	0.42
48:5:2579:G:C2	48:5:2583:C:C2	3.07	0.42
48:5:2703:G:C2	48:5:2704:C:C2	3.07	0.42
48:5:2769:U:H1'	48:5:2770:C:C6	2.53	0.42
50:8:115:G:C6	50:8:116:C:C4	3.08	0.42
51:9:318:A:OP2	58:GG:183:ARG:NH2	2.52	0.42
51:9:1097:G:C6	51:9:1098:C:C4	3.08	0.42
51:9:1315:U:C4	51:9:1316:C:C4	3.08	0.42
51:9:1823:A:H2'	51:9:1824:A:H5'	2.01	0.42
52:AA:180:ARG:HD2	52:AA:184:ARG:CZ	2.49	0.42
54:CC:113:GLN:HB3	54:CC:122:THR:HA	2.00	0.42
56:EE:43:PRO:O	56:EE:46:ILE:N	2.51	0.42
56:EE:195:ILE:O	56:EE:196:THR:CB	2.67	0.42
56:EE:244:ILE:O	56:EE:245:ARG:HB3	2.20	0.42
64:MM:113:ASP:O	64:MM:115:GLY:N	2.52	0.42
73:VV:20:SER:C	73:VV:22:ARG:N	2.77	0.42
87:jj:83:THR:HG22	87:jj:95:HIS:CE1	2.55	0.42
8:H:86:LEU:O	8:H:187:VAL:HB	2.20	0.42
8:H:159:ALA:O	8:H:160:LEU:C	2.62	0.42
9:I:180:GLU:O	9:I:184:MET:HG3	2.20	0.42
10:J:103:GLY:O	10:J:134:LEU:HD12	2.19	0.42
15:P:60:PHE:O	15:P:78:TRP:NE1	2.53	0.42
15:P:74:LYS:O	15:P:75:GLN:C	2.62	0.42
20:U:27:HIS:N	20:U:28:PRO:HD2	2.35	0.42
28:c:82:GLY:CA	28:c:91:VAL:HG13	2.49	0.42
35:j:55:ARG:NH2	48:5:364:G:O6	2.48	0.42
37:l:41:ARG:NH1	48:5:2431:A:OP1	2.53	0.42
46:2:24:A:C6	46:2:25:C:C4	3.07	0.42
48:5:744:G:C2	48:5:921:C:C2	3.07	0.42
48:5:1580:C:C5	48:5:1581:G:N7	2.88	0.42
48:5:1721:G:C2	48:5:1722:C:C2	3.08	0.42
48:5:1912:G:C6	48:5:1913:C:N4	2.88	0.42
48:5:3621:A:N7	48:5:4642:U:O2'	2.40	0.42
48:5:4495:G:C2	48:5:4506:C:N3	2.87	0.42
48:5:4673:U:H2'	48:5:4674:C:C6	2.55	0.42
48:5:4754:G:N2	48:5:4880:C:C2	2.88	0.42
48:5:5031:G:N2	48:5:5032:C:C2	2.87	0.42
50:8:112:G:C6	50:8:113:C:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:50:A:C2	51:9:51:U:H1'	2.55	0.42
51:9:145:G:N1	51:9:146:G:O6	2.53	0.42
51:9:1279:C:C4	51:9:1280:G:N7	2.88	0.42
52:AA:147:LEU:HD13	52:AA:163:CYS:SG	2.60	0.42
56:EE:102:ILE:HG23	56:EE:182:MET:CE	2.47	0.42
56:EE:188:ASN:ND2	56:EE:219:ALA:O	2.53	0.42
59:HH:40:LEU:O	59:HH:40:LEU:HD23	2.20	0.42
66:OO:32:HIS:O	66:OO:33:ILE:HB	2.20	0.42
1:A:104:VAL:O	1:A:105:GLY:C	2.63	0.42
5:E:199:ILE:O	5:E:200:SER:C	2.62	0.42
10:J:111:GLU:CB	10:J:125:ILE:HG21	2.50	0.42
46:2:7:G:C2	46:2:49:C:C2	3.08	0.42
48:5:44:A:O2'	48:5:94:A:N1	2.48	0.42
48:5:77:U:H3	48:5:336:A:H62	1.68	0.42
48:5:381:U:O4	48:5:382:G:C6	2.73	0.42
48:5:517:C:C2	48:5:645:G:N2	2.87	0.42
48:5:744:G:C2	48:5:745:G:C5	3.07	0.42
48:5:1431:C:C2	48:5:1454:G:C2	3.08	0.42
48:5:1550:G:N3	48:5:1579:C:O2	2.53	0.42
48:5:1732:C:C2	48:5:1798:G:C2	3.08	0.42
48:5:1846:G:C6	48:5:1847:C:C4	3.08	0.42
48:5:1957:U:O2'	48:5:1958:A:C5'	2.67	0.42
48:5:2771:G:C2	48:5:2772:C:C2	3.08	0.42
48:5:3654:G:C5	48:5:3655:C:C5	3.08	0.42
50:8:31:G:C2	50:8:32:C:C2	3.08	0.42
51:9:352:U:H2'	51:9:353:C:C6	2.55	0.42
51:9:910:G:C6	51:9:911:C:C4	3.08	0.42
51:9:1025:U:H2'	51:9:1026:C:O4'	2.20	0.42
51:9:1366:G:C2	51:9:1374:C:C2	3.08	0.42
56:EE:38:LEU:HD12	56:EE:38:LEU:O	2.19	0.42
58:GG:55:GLY:N	58:GG:63:MET:SD	2.93	0.42
63:LL:99:TYR:N	63:LL:99:TYR:CD1	2.88	0.42
66:OO:99:ALA:HB2	66:OO:108:PRO:HA	2.02	0.42
86:ii:324:GLU:CB	86:ii:391:ILE:CG2	2.98	0.42
2:B:217:ILE:HG21	2:B:284:ILE:HD11	2.02	0.41
3:C:302:LEU:HD22	16:Q:38:ARG:CB	2.49	0.41
3:C:333:LYS:NZ	48:5:976:G:OP1	2.52	0.41
8:H:144:LEU:HD22	8:H:161:ILE:CD1	2.50	0.41
9:I:204:GLY:O	49:7:63:C:H6	2.03	0.41
11:L:39:ARG:NH2	48:5:1362:G:OP1	2.53	0.41
13:N:65:ARG:HD3	13:N:127:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:82:TYR:O	20:U:85:TYR:HB3	2.20	0.41
28:c:48:LEU:HD23	28:c:93:THR:HG23	2.03	0.41
48:5:710:G:H2'	48:5:711:A:C8	2.55	0.41
48:5:1383:G:C2	48:5:1384:C:C2	3.08	0.41
48:5:1416:G:C6	48:5:1417:C:C4	3.08	0.41
48:5:1448:G:C6	48:5:1449:C:C4	3.08	0.41
48:5:1826:G:C6	48:5:1827:C:C4	3.07	0.41
48:5:2288:G:C2	48:5:2290:C:C4	3.08	0.41
48:5:2322:G:N2	48:5:2323:C:C2	2.88	0.41
48:5:4124:G:O2'	48:5:4125:C:OP1	2.37	0.41
48:5:4139:G:C2	48:5:4140:C:C2	3.08	0.41
48:5:4303:C:O2	48:5:4303:C:O5'	2.37	0.41
48:5:4389:C:H2'	48:5:4390:A:H8	1.84	0.41
48:5:4453:C:C2	48:5:4529:G:N2	2.88	0.41
48:5:4651:A:H2'	48:5:4652:G:O4'	2.20	0.41
50:8:50:C:H3'	50:8:51:U:C5'	2.50	0.41
51:9:173:A:C5	51:9:174:C:C5	3.08	0.41
51:9:305:U:C6	60:II:182:CYS:O	2.73	0.41
51:9:1203:G:H2'	51:9:1204:A:C8	2.55	0.41
51:9:1380:C:H2'	51:9:1381:G:O4'	2.20	0.41
51:9:1588:A:H2'	51:9:1589:A:C8	2.55	0.41
51:9:1784:G:C6	51:9:1785:C:N4	2.87	0.41
54:CC:210:PRO:HA	54:CC:240:THR:HG21	2.01	0.41
58:GG:173:ALA:HB1	58:GG:174:PRO:HD2	2.01	0.41
65:NN:89:TYR:CD1	65:NN:89:TYR:C	2.98	0.41
86:ii:214:ILE:HA	86:ii:219:VAL:HA	2.01	0.41
86:ii:346:LEU:HD23	86:ii:351:GLU:HA	2.02	0.41
1:A:20:VAL:O	1:A:21:LYS:C	2.62	0.41
3:C:147:VAL:HG13	3:C:148:PRO:HD2	2.02	0.41
3:C:210:ILE:HG21	3:C:232:VAL:HG13	2.01	0.41
4:D:56:THR:O	4:D:57:ASN:C	2.63	0.41
8:H:43:VAL:C	48:5:4763:U:O2	2.63	0.41
13:N:5:LYS:HG2	34:i:40:VAL:HG21	2.02	0.41
24:Y:66:GLN:OE1	24:Y:66:GLN:N	2.53	0.41
25:Z:4:PHE:HE1	28:c:39:ARG:HA	1.84	0.41
25:Z:128:LYS:O	25:Z:132:GLN:HG3	2.21	0.41
30:e:46:ARG:HA	30:e:55:MET:SD	2.60	0.41
30:e:67:LYS:O	30:e:75:ARG:NH1	2.53	0.41
47:3:6:G:N1	47:3:7:A:C5	2.88	0.41
48:5:7:C:H2'	48:5:8:U:C6	2.55	0.41
48:5:39:A:C5	48:5:1654:G:C6	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:469:C:H2'	48:5:470:A:O4'	2.20	0.41
48:5:715:G:H1	48:5:953:C:H42	1.67	0.41
48:5:1048:G:N2	48:5:1049:C:C2	2.88	0.41
48:5:2086:G:C2	48:5:2087:C:C2	3.08	0.41
48:5:2676:A:C2	48:5:2677:G:H1'	2.55	0.41
48:5:2712:G:N2	48:5:2713:C:C2	2.88	0.41
48:5:3670:C:O2'	48:5:3671:G:O5'	2.38	0.41
48:5:3820:G:C6	48:5:3821:A:C5	3.08	0.41
48:5:4595:G:C2	48:5:4596:C:C2	3.08	0.41
51:9:47:G:C2	51:9:48:C:C2	3.08	0.41
51:9:374:G:C2	51:9:391:C:C2	3.07	0.41
51:9:478:G:N2	51:9:479:C:C2	2.89	0.41
51:9:483:C:N4	51:9:484:A:N1	2.67	0.41
51:9:1134:G:C6	51:9:1135:C:C4	3.07	0.41
51:9:1184:G:C6	51:9:1185:C:C4	3.09	0.41
51:9:1292:C:H3'	51:9:1293:A:C5'	2.50	0.41
55:DD:192:TRP:HB3	55:DD:196:GLY:HA3	2.01	0.41
60:II:102:VAL:HG11	60:II:175:ILE:HD11	2.01	0.41
70:SS:20:ILE:HG22	70:SS:29:ALA:HB1	2.01	0.41
70:SS:113:ARG:HH11	70:SS:113:ARG:HG2	1.85	0.41
71:TT:76:THR:OG1	71:TT:77:LYS:N	2.53	0.41
75:XX:26:GLN:O	75:XX:27:TYR:C	2.63	0.41
84:gg:73:SER:HB3	84:gg:117:ASN:HD21	1.84	0.41
2:B:36:ASP:OD1	2:B:36:ASP:N	2.43	0.41
4:D:158:LYS:O	4:D:159:VAL:C	2.63	0.41
5:E:127:LYS:HB2	5:E:127:LYS:HE3	1.81	0.41
5:E:157:ARG:NH2	12:M:106:ASP:OD2	2.54	0.41
5:E:184:ARG:NE	48:5:4941:G:OP1	2.46	0.41
7:G:38:ASN:OD1	7:G:43:GLN:NE2	2.54	0.41
9:I:46:PHE:CD1	9:I:140:THR:HA	2.55	0.41
18:S:118:ARG:HE	48:5:2035:C:H5'	1.86	0.41
21:V:27:ASN:O	21:V:102:ALA:HA	2.20	0.41
41:p:51:ALA:O	41:p:52:VAL:C	2.63	0.41
48:5:1085:C:C2	48:5:1213:G:N1	2.88	0.41
48:5:1416:G:C2	48:5:1417:C:C2	3.07	0.41
48:5:1484:G:C2	48:5:1486:C:C4	3.09	0.41
48:5:1756:U:H5'	48:5:1757:U:OP2	2.19	0.41
48:5:2256:C:H1'	48:5:2257:C:OP2	2.21	0.41
48:5:2898:G:C2	48:5:3602:C:C2	3.09	0.41
48:5:3648:A:C4	48:5:3785:A:C6	3.08	0.41
48:5:3723:A:C2	48:5:3730:U:N3	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4246:G:N2	48:5:4263:C:C2	2.89	0.41
48:5:4566:U:H2'	48:5:4567:G:O4'	2.20	0.41
48:5:4904:G:C6	48:5:4905:C:C4	3.07	0.41
50:8:139:G:C6	50:8:140:C:N3	2.88	0.41
51:9:217:A:N3	51:9:309:G:C2	2.88	0.41
51:9:1137:U:N3	51:9:1148:A:N6	2.68	0.41
51:9:1478:U:H2'	51:9:1479:G:O4'	2.20	0.41
51:9:1531:A:H2'	51:9:1532:C:C6	2.55	0.41
51:9:1650:A:C4	51:9:1675:A:C6	3.08	0.41
51:9:1686:G:C6	51:9:1687:C:C4	3.08	0.41
52:AA:63:ARG:CG	52:AA:185:MET:HE1	2.50	0.41
66:OO:72:TYR:CE1	80:cc:63:ARG:NH1	2.88	0.41
79:bb:83:GLN:OE1	79:bb:84:HIS:N	2.54	0.41
86:ii:183:ALA:O	86:ii:187:ALA:HB2	2.20	0.41
86:ii:204:LYS:HA	86:ii:207:GLU:HG2	2.02	0.41
2:B:223:THR:O	2:B:343:ARG:NH1	2.54	0.41
3:C:274:LYS:O	3:C:276:ASN:N	2.53	0.41
14:O:65:ASN:HB3	14:O:68:ARG:HD2	2.02	0.41
17:R:120:TYR:CD1	17:R:120:TYR:C	2.99	0.41
19:T:87:LYS:NZ	48:5:4301:U:P	2.94	0.41
31:f:11:PHE:CE2	31:f:97:ILE:HD13	2.54	0.41
31:f:50:VAL:HG21	31:f:102:ARG:HD2	2.02	0.41
37:l:49:LEU:HD23	48:5:2407:G:OP1	2.20	0.41
48:5:233:U:C3'	48:5:234:G:C5'	2.98	0.41
48:5:504:G:N2	48:5:654:C:H1'	2.35	0.41
48:5:1549:G:N2	48:5:1580:C:C2	2.88	0.41
48:5:1669:A:N1	48:5:1670:G:C6	2.89	0.41
48:5:1907:A:C5	48:5:1908:A:C6	3.09	0.41
48:5:2027:U:O2'	48:5:2028:C:C5'	2.69	0.41
48:5:3918:G:C2	48:5:3919:C:C2	3.08	0.41
48:5:4170:A:H4'	48:5:4171:C:O5'	2.20	0.41
48:5:4633:G:O3'	48:5:4634:U:H3'	2.21	0.41
48:5:4661:G:C2	48:5:4662:C:C2	3.09	0.41
48:5:4966:A:N1	48:5:4967:A:C6	2.88	0.41
51:9:16:G:H2'	51:9:17:C:C6	2.55	0.41
51:9:1031:A:C5	51:9:1032:C:C5	3.08	0.41
51:9:1046:U:H2'	51:9:1047:C:O4'	2.19	0.41
51:9:1398:G:O2'	84:gg:88:ARG:NH2	2.53	0.41
51:9:1552:G:C8	51:9:1578:U:C4	3.09	0.41
51:9:1563:G:C2	51:9:1564:C:C2	3.08	0.41
51:9:1739:C:C2	51:9:1796:G:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:AA:111:GLN:CB	54:CC:63:VAL:HG11	2.50	0.41
53:BB:121:ILE:HD12	53:BB:207:LEU:HD21	2.02	0.41
56:EE:19:MET:HG3	56:EE:51:LYS:NZ	2.35	0.41
57:FF:33:ILE:O	57:FF:33:ILE:HG23	2.20	0.41
57:FF:73:THR:HG22	57:FF:89:THR:CG2	2.50	0.41
60:II:102:VAL:N	60:II:173:ALA:O	2.52	0.41
84:gg:168:CYS:SG	84:gg:198:VAL:HG23	2.60	0.41
87:jj:105:VAL:N	87:jj:284:ASP:OD1	2.53	0.41
1:A:114:CYS:SG	1:A:165:VAL:HG22	2.61	0.41
2:B:21:ARG:NH2	48:5:4568:A:O3'	2.53	0.41
3:C:293:LEU:HD23	3:C:293:LEU:HA	1.88	0.41
9:I:137:SER:OG	9:I:173:PHE:CE1	2.70	0.41
14:O:48:TYR:CD1	48:5:1930:U:C6	3.08	0.41
20:U:101:ARG:HD2	20:U:103:VAL:HG23	2.02	0.41
21:V:99:GLU:HB3	22:W:24:THR:HG23	2.02	0.41
31:f:79:GLY:HA3	48:5:1917:A:H4'	2.01	0.41
33:h:45:SER:O	33:h:46:LYS:C	2.63	0.41
42:r:108:MET:SD	42:r:112:ARG:NH2	2.93	0.41
48:5:179:G:C6	48:5:180:C:C4	3.08	0.41
48:5:256:G:C2	48:5:257:C:C2	3.08	0.41
48:5:751:G:N2	48:5:752:G:C5	2.89	0.41
48:5:971:U:H2'	48:5:972:C:H5"	2.02	0.41
48:5:1098:G:C6	48:5:1099:C:C4	3.08	0.41
48:5:2006:U:H2'	48:5:2007:G:O4'	2.20	0.41
48:5:2089:G:O2'	48:5:2090:U:P	2.74	0.41
51:9:493:A:C2	51:9:494:C:C6	3.09	0.41
51:9:1097:G:C2	51:9:1098:C:C2	3.08	0.41
51:9:1319:U:H2'	51:9:1320:G:O4'	2.20	0.41
51:9:1354:G:H2'	51:9:1356:G:N7	2.36	0.41
51:9:1447:G:H2'	51:9:1448:A:C8	2.56	0.41
53:BB:87:ILE:HD13	53:BB:101:HIS:CD2	2.55	0.41
53:BB:139:CYS:SG	53:BB:140:VAL:N	2.92	0.41
63:LL:126:VAL:HG23	63:LL:142:VAL:HG13	2.02	0.41
86:ii:286:LEU:HD21	86:ii:390:GLU:HG3	2.02	0.41
2:B:254:ILE:CG2	2:B:266:VAL:HG11	2.51	0.41
7:G:143:VAL:O	7:G:146:LEU:N	2.53	0.41
9:I:145:LYS:HE3	9:I:167:ILE:HG21	2.03	0.41
12:M:42:CYS:HG	12:M:77:TRP:HB3	1.85	0.41
15:P:68:GLY:O	15:P:80:GLN:HA	2.21	0.41
21:V:107:ASN:O	21:V:108:ASN:C	2.63	0.41
31:f:72:GLY:HA2	31:f:88:PHE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:91:SER:O	42:r:95:HIS:ND1	2.54	0.41
48:5:286:U:C2	48:5:287:U:C4	3.09	0.41
48:5:342:G:N2	48:5:343:C:C2	2.89	0.41
48:5:370:U:C6	48:5:1637:A:C2	3.08	0.41
48:5:381:U:C4	48:5:382:G:C5	3.09	0.41
48:5:914:U:C4	48:5:915:A:C5	3.09	0.41
48:5:1269:G:C5	48:5:2111:G:C2	3.08	0.41
48:5:1326:A:H2'	48:5:1327:C:C6	2.56	0.41
48:5:1721:G:N2	48:5:1722:C:C2	2.88	0.41
48:5:2684:C:H2'	48:5:2685:C:C6	2.56	0.41
48:5:3702:A:C6	48:5:3774:A:C6	3.08	0.41
48:5:3896:C:O2	48:5:4564:A:N1	2.53	0.41
48:5:4129:G:C6	48:5:4130:C:C4	3.08	0.41
48:5:4183:G:H2'	48:5:4183:G:N3	2.35	0.41
48:5:5028:G:H2'	48:5:5029:C:C6	2.55	0.41
49:7:110:G:C2	49:7:111:C:C2	3.08	0.41
51:9:23:G:C2	51:9:24:C:C2	3.09	0.41
51:9:959:G:O6	66:OO:68:GLU:OE2	2.38	0.41
51:9:1137:U:H3	51:9:1148:A:N6	2.17	0.41
51:9:1669:G:C6	51:9:1670:C:C4	3.08	0.41
54:CC:183:LYS:HD3	54:CC:196:ILE:HG23	2.01	0.41
56:EE:127:ARG:O	56:EE:156:MET:SD	2.79	0.41
58:GG:108:VAL:CG1	58:GG:109:LEU:N	2.83	0.41
65:NN:101:HIS:CD2	65:NN:101:HIS:C	2.98	0.41
67:PP:13:ARG:O	67:PP:15:PHE:N	2.54	0.41
70:SS:22:GLY:HA2	70:SS:56:ALA:HB3	2.02	0.41
73:VV:17:CYS:SG	73:VV:19:ALA:HB3	2.59	0.41
77:ZZ:91:LEU:HD23	77:ZZ:96:LEU:HD12	2.02	0.41
86:ii:21:ILE:HD11	86:ii:136:LEU:CB	2.49	0.41
5:E:254:LEU:HD21	5:E:258:LYS:HE3	2.03	0.41
6:F:134:MET:HA	6:F:137:ILE:HG22	2.03	0.41
12:M:28:VAL:HB	12:M:37:LEU:HD13	2.02	0.41
13:N:4:TYR:OH	48:5:151:G:OP2	2.28	0.41
13:N:181:HIS:O	13:N:184:ILE:HB	2.20	0.41
17:R:12:SER:OG	17:R:13:SER:N	2.54	0.41
23:X:80:PRO:HD2	33:h:33:VAL:HG22	2.02	0.41
27:b:46:ALA:HB1	48:5:1813:U:O2	2.21	0.41
30:e:23:HIS:HB2	30:e:53:ILE:HD11	2.03	0.41
30:e:53:ILE:HA	48:5:437:G:H4'	2.02	0.41
46:2:39:G:C6	46:2:40:C:N4	2.89	0.41
48:5:119:G:C8	48:5:119:G:H5"	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:342:G:C6	48:5:343:C:N4	2.89	0.41
48:5:476:G:C2	48:5:679:C:C2	3.09	0.41
48:5:504:G:H22	48:5:654:C:H1'	1.85	0.41
48:5:742:G:C2	48:5:923:C:C2	3.09	0.41
48:5:914:U:C4	48:5:915:A:C4	3.09	0.41
48:5:1265:G:OP1	48:5:2115:G:N1	2.53	0.41
48:5:1275:G:N2	48:5:1276:C:C2	2.89	0.41
48:5:1277:G:C2	48:5:1278:C:C4	3.09	0.41
48:5:1322:A:C6	48:5:1326:A:C8	3.09	0.41
48:5:1388:A:C5	48:5:1389:U:C4	3.09	0.41
48:5:1424:G:H2'	48:5:1425:G:O4'	2.21	0.41
48:5:1539:G:C2	48:5:1540:C:C2	3.09	0.41
48:5:2557:G:C2	48:5:2571:C:O2	2.73	0.41
48:5:2574:G:O6	48:5:2762:G:O6	2.39	0.41
48:5:3611:A:C6	48:5:3612:C:C4	3.09	0.41
48:5:3632:C:C2	48:5:3830:A:C2	3.09	0.41
48:5:3676:G:C6	48:5:3677:U:C4	3.09	0.41
48:5:3707:U:H2'	48:5:3708:C:C6	2.56	0.41
48:5:4152:G:C6	48:5:4153:C:N4	2.88	0.41
48:5:4473:A:C2	48:5:4474:A:C6	3.08	0.41
51:9:455:A:C6	51:9:456:C:N4	2.88	0.41
51:9:1078:C:O2	51:9:1078:C:H2'	2.21	0.41
51:9:1181:A:H2'	51:9:1182:A:O4'	2.21	0.41
51:9:1459:G:C6	51:9:1460:C:C4	3.09	0.41
56:EE:52:LEU:O	56:EE:54:TYR:CD1	2.73	0.41
74:WW:105:THR:N	74:WW:124:LYS:O	2.46	0.41
84:gg:197:THR:HG21	84:gg:238:ALA:HA	2.02	0.41
87:jj:377:MET:HB3	87:jj:535:PHE:HE2	1.85	0.41
3:C:78:ARG:HB3	3:C:88:GLY:HA2	2.01	0.41
3:C:180:ILE:O	3:C:183:VAL:N	2.54	0.41
3:C:341:LEU:CD2	5:E:46:LEU:HD21	2.49	0.41
4:D:272:SER:O	4:D:273:LEU:C	2.63	0.41
5:E:132:HIS:CE1	48:5:711:A:H1'	2.56	0.41
9:I:182:GLU:OE2	9:I:182:GLU:HA	2.20	0.41
10:J:175:LEU:HD12	10:J:176:PRO:O	2.21	0.41
16:Q:171:GLY:O	16:Q:173:LYS:N	2.54	0.41
17:R:142:ILE:O	17:R:143:HIS:C	2.61	0.41
21:V:25:VAL:HG22	48:5:2848:G:OP1	2.20	0.41
30:e:45:VAL:HG12	30:e:55:MET:SD	2.61	0.41
41:p:26:VAL:O	41:p:27:LYS:C	2.64	0.41
44:t:117:ARG:O	44:t:119:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:373:G:H2'	48:5:374:G:O4'	2.21	0.41
48:5:433:A:C2	48:5:434:A:C4	3.08	0.41
48:5:674:G:C6	48:5:675:C:C4	3.08	0.41
48:5:1359:G:C2'	48:5:1360:G:C8	3.01	0.41
48:5:1385:G:C6	48:5:1386:C:C4	3.08	0.41
48:5:1964:A:C2	48:5:4694:G:C4	3.08	0.41
48:5:1967:A:C2'	48:5:1968:G:H5'	2.51	0.41
48:5:2297:G:N2	48:5:2338:C:C2	2.89	0.41
48:5:2395:A:O2'	48:5:2806:A:C1'	2.60	0.41
48:5:4222:G:C6	48:5:4223:C:C4	3.09	0.41
48:5:4709:U:C2	48:5:4710:C:C6	3.09	0.41
48:5:4711:C:H2'	48:5:4712:C:O4'	2.21	0.41
48:5:4920:C:H2'	48:5:4921:C:C6	2.56	0.41
48:5:4946:U:O2	48:5:4946:U:H2'	2.19	0.41
48:5:5028:G:C2	48:5:5029:C:C2	3.09	0.41
50:8:13:G:N3	50:8:13:G:H2'	2.35	0.41
51:9:333:G:N7	58:GG:190:ARG:NH1	2.68	0.41
51:9:374:G:H2'	51:9:375:U:C6	2.56	0.41
51:9:1005:G:C2	51:9:1006:C:C2	3.08	0.41
51:9:1102:G:N1	51:9:1103:C:N4	2.68	0.41
51:9:1307:U:C3'	51:9:1308:U:H5"	2.49	0.41
51:9:1411:G:H3'	51:9:1412:C:C4'	2.50	0.41
52:AA:6:ASP:OD1	52:AA:6:ASP:N	2.53	0.41
54:CC:161:SER:O	54:CC:162:ILE:C	2.62	0.41
62:KK:40:VAL:HG13	62:KK:40:VAL:O	2.20	0.41
69:RR:85:VAL:HG12	69:RR:86:PRO:O	2.20	0.41
75:XX:81:ILE:HG22	75:XX:83:ALA:N	2.36	0.41
84:gg:133:ASN:HD22	84:gg:137:VAL:HB	1.86	0.41
87:jj:116:LYS:HE2	87:jj:272:VAL:HG11	2.02	0.41
1:A:43:GLY:O	1:A:88:VAL:N	2.54	0.41
2:B:264:PHE:CD1	2:B:265:SER:N	2.89	0.41
3:C:33:ARG:NH1	48:5:1350:C:O3'	2.50	0.41
6:F:39:PHE:CD1	48:5:2123:C:H3'	2.56	0.41
6:F:181:LEU:HD23	6:F:186:ILE:HG21	2.03	0.41
6:F:244:ARG:NH1	48:5:942:G:OP2	2.54	0.41
11:L:30:ALA:HA	11:L:33:ILE:HD12	2.02	0.41
11:L:34:ARG:O	11:L:35:ARG:C	2.62	0.41
11:L:101:ARG:NH1	48:5:65:A:OP2	2.53	0.41
13:N:68:ARG:CG	48:5:302:C:OP1	2.69	0.41
13:N:140:LYS:HA	13:N:143:ARG:HB2	2.03	0.41
14:O:144:GLU:OE2	48:5:4681:A:O2'	2.26	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:83:ARG:HH21	18:S:83:ARG:CG	2.34	0.41
18:S:173:ASN:HA	48:5:4762:A:C2	2.56	0.41
23:X:53:ARG:NH1	48:5:2475:G:C8	2.89	0.41
25:Z:4:PHE:CD2	28:c:66:LEU:HB3	2.56	0.41
26:a:40:HIS:HB2	48:5:1675:C:O2	2.20	0.41
27:b:7:HIS:CG	27:b:8:THR:N	2.88	0.41
32:g:97:ILE:O	32:g:98:GLU:C	2.63	0.41
34:i:58:MET:SD	34:i:90:LEU:HD22	2.60	0.41
34:i:85:ARG:HG3	34:i:85:ARG:HH11	1.86	0.41
36:k:7:GLU:HB2	36:k:10:ASP:HB2	2.03	0.41
41:p:26:VAL:HG12	41:p:30:GLU:HB2	2.02	0.41
42:r:14:SER:OG	42:r:17:LEU:N	2.52	0.41
42:r:35:ARG:NH1	48:5:2265:G:OP1	2.54	0.41
46:2:30:G:C2	46:2:31:C:C2	3.09	0.41
48:5:2:G:C6	48:5:3:C:C4	3.09	0.41
48:5:124:C:C2	48:5:146:G:N2	2.89	0.41
48:5:193:G:C2	48:5:249:C:C2	3.09	0.41
48:5:518:G:C6	48:5:519:C:C4	3.09	0.41
48:5:918:G:H2'	48:5:918:G:N3	2.36	0.41
48:5:1203:G:C2	48:5:1204:C:C2	3.08	0.41
48:5:1268:G:C2	48:5:2111:G:N2	2.89	0.41
48:5:1277:G:C6	48:5:1278:C:C4	3.09	0.41
48:5:1279:A:C5	48:5:1280:C:N4	2.89	0.41
48:5:1412:G:C6	48:5:1413:C:C4	3.09	0.41
48:5:1612:G:H2'	48:5:1612:G:N3	2.35	0.41
48:5:1934:A:C2	48:5:2048:U:N3	2.89	0.41
48:5:2417:A:C4	48:5:2418:A:C8	3.08	0.41
48:5:2609:G:C2	48:5:2731:C:C2	3.08	0.41
48:5:2712:G:C2	48:5:2713:C:C2	3.09	0.41
48:5:3597:G:C6	48:5:3598:C:C4	3.09	0.41
48:5:3799:A:C6	48:5:3800:A:C6	3.09	0.41
48:5:3849:A:O2'	48:5:3850:C:H5'	2.21	0.41
48:5:4147:G:C6	48:5:4148:C:C4	3.08	0.41
48:5:4606:G:C2'	48:5:4607:A:O5'	2.69	0.41
49:7:110:G:C6	49:7:111:C:N4	2.88	0.41
50:8:2:G:N3	50:8:2:G:H2'	2.36	0.41
51:9:27:A:H2'	51:9:28:U:O4'	2.21	0.41
51:9:147:A:H2'	51:9:148:U:C6	2.56	0.41
51:9:411:G:N2	51:9:430:C:C2	2.89	0.41
51:9:526:A:O2'	61:JJ:125:HIS:ND1	2.50	0.41
51:9:591:U:O2	51:9:591:U:O4'	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:673:G:C6	51:9:674:C:C4	3.08	0.41
51:9:804:U:O3'	74:WW:122:GLY:HA3	2.20	0.41
51:9:828:G:C2	51:9:829:C:C2	3.09	0.41
51:9:839:C:O2	51:9:839:C:C2'	2.69	0.41
51:9:909:G:H2'	51:9:910:G:C8	2.56	0.41
51:9:995:G:N2	51:9:999:G:C4	2.89	0.41
51:9:1405:A:C6	51:9:1406:G:C5	3.09	0.41
51:9:1535:U:C2	57:FF:82:ASN:ND2	2.88	0.41
51:9:1548:G:O6	51:9:1584:G:O6	2.39	0.41
51:9:1649:U:N3	51:9:1675:A:C2	2.89	0.41
52:AA:148:CYS:HB3	52:AA:152:SER:CB	2.51	0.41
53:BB:64:GLY:N	53:BB:88:THR:OG1	2.52	0.41
53:BB:171:ILE:HD13	53:BB:197:ILE:HA	2.03	0.41
70:SS:31:THR:HG21	70:SS:38:ARG:HG3	2.03	0.41
70:SS:39:ARG:NH1	71:TT:36:THR:O	2.54	0.41
76:YY:19:GLN:HG2	76:YY:81:TYR:CD2	2.56	0.41
84:gg:31:ILE:HD13	84:gg:299:PHE:CD2	2.56	0.41
87:jj:84:THR:HG21	87:jj:97:LEU:HG	2.03	0.41
3:C:253:THR:O	3:C:256:ALA:N	2.53	0.41
3:C:325:MET:HE1	6:F:157:TYR:CZ	2.55	0.41
7:G:81:ASN:OD1	7:G:238:GLY:N	2.54	0.41
13:N:137:PRO:HD2	13:N:138:PHE:CE1	2.56	0.41
17:R:6:LEU:HD22	17:R:10:LEU:CD2	2.50	0.41
22:W:3:VAL:HG21	22:W:12:LYS:HD2	2.02	0.41
24:Y:55:VAL:N	24:Y:68:GLY:O	2.53	0.41
30:e:99:ILE:HG21	30:e:108:ARG:HD2	2.02	0.41
30:e:107:ASN:OD1	30:e:107:ASN:N	2.53	0.41
44:t:17:CYS:SG	44:t:18:THR:N	2.94	0.41
44:t:123:ARG:CD	44:t:129:ILE:HD11	2.51	0.41
47:3:75:C:O2'	47:3:76:A:P	2.78	0.41
48:5:111:C:C2	48:5:331:G:N2	2.89	0.41
48:5:127:G:C6	48:5:128:C:C4	3.09	0.41
48:5:479:G:C2	48:5:480:C:C2	3.09	0.41
48:5:647:G:C5	48:5:648:G:C8	3.08	0.41
48:5:1075:G:H2'	48:5:1076:C:C6	2.56	0.41
48:5:1855:G:C2	48:5:1856:C:C2	3.08	0.41
48:5:2028:C:O2'	48:5:2029:A:O4'	2.37	0.41
48:5:2316:G:C2	48:5:2324:C:C2	3.08	0.41
48:5:2858:A:O2'	48:5:2859:G:O5'	2.38	0.41
48:5:4281:A:O2'	48:5:4282:A:O5'	2.38	0.41
48:5:4614:G:N2	48:5:4615:C:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:170:A:OP2	58:GG:140:ARG:NE	2.54	0.41
51:9:185:G:C2	51:9:186:C:C2	3.08	0.41
51:9:933:G:N7	51:9:992:A:N1	2.69	0.41
51:9:976:G:C2	51:9:977:C:C2	3.09	0.41
51:9:1083:A:N7	51:9:1841:C:O2'	2.47	0.41
51:9:1145:A:C6	51:9:1146:C:H1'	2.56	0.41
51:9:1476:A:H3'	51:9:1477:U:C5'	2.51	0.41
51:9:1524:G:N2	51:9:1525:C:C2	2.89	0.41
51:9:1650:A:H5"	68:QQ:139:ALA:HB2	2.02	0.41
51:9:1678:A:H2'	51:9:1679:A:C8	2.55	0.41
51:9:1686:G:C2	51:9:1687:C:C2	3.08	0.41
54:CC:185:THR:OG1	54:CC:186:GLY:N	2.54	0.41
60:II:6:ASP:O	60:II:9:HIS:ND1	2.52	0.41
66:OO:46:ASP:O	66:OO:47:LEU:C	2.63	0.41
74:WW:7:LEU:C	74:WW:7:LEU:HD13	2.46	0.41
78:aa:64:LEU:HD23	78:aa:65:PRO:HD3	2.02	0.41
86:ii:143:ASP:O	86:ii:144:SER:C	2.64	0.41
1:A:34:PHE:CD2	48:5:4087:G:C6	3.09	0.40
2:B:356:LYS:O	2:B:357:ARG:C	2.63	0.40
3:C:223:ASN:HD22	3:C:223:ASN:HA	1.68	0.40
5:E:41:SER:CB	48:5:978:G:H5"	2.51	0.40
7:G:95:LEU:HD21	7:G:156:VAL:HG21	2.03	0.40
8:H:60:TRP:CE3	18:S:153:PRO:HD2	2.56	0.40
13:N:36:LEU:O	13:N:36:LEU:HD23	2.21	0.40
23:X:79:PHE:HB2	23:X:80:PRO:HD2	2.03	0.40
29:d:30:HIS:CG	29:d:82:TYR:CD1	3.09	0.40
33:h:5:LYS:O	33:h:6:ALA:C	2.63	0.40
35:j:34:CYS:SG	35:j:36:LYS:HB3	2.60	0.40
48:5:256:G:C6	48:5:257:C:C4	3.09	0.40
48:5:458:C:C4	48:5:459:C:C4	3.10	0.40
48:5:715:G:C6	48:5:716:C:C4	3.09	0.40
48:5:912:G:C6	48:5:913:U:C5	3.09	0.40
48:5:975:C:H3'	48:5:976:G:O4'	2.21	0.40
48:5:1099:C:H2'	48:5:1100:U:O4'	2.22	0.40
48:5:1270:A:C2'	48:5:1271:G:O5'	2.69	0.40
48:5:1292:C:C2	48:5:1293:G:C8	3.09	0.40
48:5:1630:A:N1	48:5:3638:G:O2'	2.45	0.40
48:5:1676:C:H2'	48:5:3914:U:C4	2.56	0.40
48:5:2611:A:H2'	48:5:2612:G:C8	2.56	0.40
48:5:2645:G:C2	48:5:2646:C:C2	3.09	0.40
48:5:2759:G:O2'	48:5:2762:G:N2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4472:G:H3'	48:5:4473:A:H5'	2.01	0.40
51:9:309:G:C2	51:9:310:C:C2	3.09	0.40
51:9:561:A:O2'	61:JJ:134:HIS:NE2	2.48	0.40
51:9:751:G:N1	51:9:792:C:C4	2.89	0.40
51:9:1309:C:HO2'	51:9:1310:U:P	2.43	0.40
52:AA:49:ILE:O	69:RR:105:MET:HE1	2.21	0.40
56:EE:107:GLY:HA3	56:EE:189:LEU:HD23	2.03	0.40
57:FF:49:LEU:HD21	68:QQ:49:TYR:HB2	2.02	0.40
66:OO:128:ARG:CZ	78:aa:59:PHE:CZ	3.04	0.40
67:PP:15:PHE:CE2	67:PP:17:TYR:HB2	2.56	0.40
81:dd:14:PHE:N	81:dd:14:PHE:CD1	2.90	0.40
1:A:97:ASN:OD1	1:A:97:ASN:N	2.54	0.40
1:A:215:ASN:ND2	48:5:4546:A:N7	2.69	0.40
1:A:242:ARG:CD	1:A:243:THR:N	2.84	0.40
2:B:41:VAL:HG11	2:B:193:LYS:HA	2.03	0.40
3:C:144:ILE:O	3:C:144:ILE:HD13	2.22	0.40
4:D:118:ILE:HG23	4:D:135:ILE:HD12	2.02	0.40
6:F:100:ILE:HD11	16:Q:4:ASP:HB3	2.02	0.40
9:I:98:ARG:NH1	48:5:1864:G:OP1	2.52	0.40
10:J:33:LEU:CD1	10:J:67:LYS:HB3	2.50	0.40
12:M:81:ASP:OD2	12:M:84:THR:HG21	2.22	0.40
13:N:47:LYS:HA	13:N:50:ARG:HH11	1.87	0.40
14:O:54:TYR:OH	14:O:73:PHE:O	2.35	0.40
17:R:87:ALA:HB2	48:5:1549:G:H4'	2.03	0.40
27:b:45:PHE:CG	48:5:1815:G:C8	3.09	0.40
30:e:26:ASP:OD1	30:e:26:ASP:N	2.52	0.40
42:r:105:ASP:OD1	42:r:105:ASP:N	2.53	0.40
47:3:5:G:C2	47:3:68:C:N3	2.89	0.40
48:5:192:G:C2	48:5:250:C:C2	3.10	0.40
48:5:297:U:C2	48:5:298:G:C8	3.08	0.40
48:5:713:C:H42	48:5:955:G:H1	1.68	0.40
48:5:933:G:N1	48:5:939:G:N2	2.68	0.40
48:5:1279:A:O3'	48:5:1279:A:OP1	2.38	0.40
48:5:1387:A:N1	48:5:1396:G:O2'	2.51	0.40
48:5:1550:G:C6	48:5:1579:C:N3	2.90	0.40
48:5:1687:U:H2'	48:5:1688:G:O4'	2.21	0.40
48:5:1932:A:O2'	48:5:1933:G:H5'	2.22	0.40
48:5:2076:G:C6	48:5:2077:C:N3	2.89	0.40
48:5:3675:G:C2	48:5:3676:G:N7	2.90	0.40
48:5:3752:C:O2'	48:5:3753:G:P	2.79	0.40
48:5:4142:C:C4	48:5:4143:G:N1	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4222:G:N2	48:5:4223:C:C2	2.89	0.40
48:5:4368:G:C6	48:5:4369:A:C5	3.09	0.40
48:5:4615:C:O2'	48:5:4616:A:H5'	2.20	0.40
48:5:4723:A:C2	48:5:4724:A:C4	3.09	0.40
51:9:50:A:C4	87:jj:149:GLY:O	2.74	0.40
51:9:84:A:H2'	51:9:85:A:O4'	2.21	0.40
51:9:428:U:C6	61:JJ:7:TRP:CH2	3.09	0.40
51:9:824:C:C6	61:JJ:144:ILE:HD12	2.57	0.40
51:9:1016:U:OP2	79:bb:20:LYS:NZ	2.51	0.40
56:EE:159:THR:HG23	56:EE:227:VAL:HG22	2.03	0.40
57:FF:127:ARG:O	57:FF:127:ARG:HD2	2.21	0.40
62:KK:64:TRP:CE3	81:dd:23:VAL:HG22	2.55	0.40
66:OO:28:PHE:CE1	66:OO:92:ALA:HB1	2.56	0.40
87:jj:99:ILE:HD13	87:jj:302:PRO:HG3	2.02	0.40
2:B:288:GLY:HA3	2:B:330:PHE:CE1	2.56	0.40
6:F:181:LEU:HB3	6:F:186:ILE:HB	2.03	0.40
12:M:86:TRP:CE2	12:M:92:ALA:HB2	2.57	0.40
14:O:108:ILE:HG22	14:O:157:GLU:OE1	2.21	0.40
15:P:122:ALA:HB1	15:P:123:PRO:CD	2.51	0.40
17:R:95:TRP:CE2	48:5:1572:U:H4'	2.55	0.40
18:S:94:TYR:O	18:S:139:ARG:NH1	2.50	0.40
22:W:50:ASN:OD1	22:W:50:ASN:N	2.53	0.40
35:j:12:ARG:HD2	48:5:2404:A:H1'	2.03	0.40
42:r:41:ASN:HB3	42:r:44:ILE:HD12	2.04	0.40
48:5:191:G:C2	48:5:251:C:C2	3.09	0.40
48:5:322:C:N3	48:5:4356:G:C6	2.88	0.40
48:5:488:G:C6	48:5:489:C:C4	3.08	0.40
48:5:751:G:N2	48:5:912:G:N3	2.70	0.40
48:5:947:C:H2'	48:5:948:C:C6	2.56	0.40
48:5:1203:G:C6	48:5:1204:C:C4	3.09	0.40
48:5:1280:C:C5	48:5:1282:G:C6	3.09	0.40
48:5:1374:G:C2	48:5:1375:C:C2	3.09	0.40
48:5:2509:C:O2'	48:5:2510:G:H5'	2.20	0.40
48:5:2889:G:C2	48:5:2890:C:C2	3.09	0.40
48:5:3718:A:H2'	48:5:3719:A:C8	2.56	0.40
48:5:3731:C:H2'	48:5:3732:A:O4'	2.22	0.40
48:5:4131:G:C2	48:5:4132:C:C2	3.10	0.40
48:5:4147:G:C2	48:5:4148:C:C2	3.10	0.40
48:5:4154:G:C2	48:5:4155:C:C2	3.09	0.40
48:5:4371:G:HO2'	48:5:4372:U:P	2.39	0.40
48:5:4486:C:H2'	48:5:4487:A:O4'	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4562:C:H2'	48:5:4563:U:O4'	2.21	0.40
49:7:110:G:N2	49:7:111:C:C2	2.89	0.40
51:9:448:A:N6	60:II:29:LEU:HD13	2.36	0.40
51:9:472:C:H4'	51:9:474:G:OP1	2.22	0.40
51:9:961:G:C6	51:9:962:A:C5	3.09	0.40
51:9:1126:G:C6	51:9:1127:C:C4	3.09	0.40
51:9:1387:G:N1	55:DD:206:ASP:OD2	2.49	0.40
51:9:1403:C:O2	51:9:1403:C:O2'	2.37	0.40
51:9:1404:U:O4'	51:9:1581:C:O2	2.39	0.40
51:9:1676:U:H2'	51:9:1677:U:O4'	2.22	0.40
51:9:1715:A:C2	51:9:1819:A:C2	3.10	0.40
54:CC:169:TYR:CE1	54:CC:177:PRO:HA	2.56	0.40
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	2.02	0.40
56:EE:170:THR:C	56:EE:171:ASP:CG	2.90	0.40
57:FF:73:THR:O	57:FF:89:THR:HG21	2.21	0.40
57:FF:79:HIS:O	57:FF:80:GLY:C	2.64	0.40
57:FF:92:ILE:HD13	57:FF:169:ILE:HG21	2.02	0.40
58:GG:52:ILE:HD11	58:GG:109:LEU:CD2	2.51	0.40
58:GG:67:VAL:HG23	58:GG:99:GLY:HA2	2.04	0.40
63:LL:40:ILE:HG21	63:LL:62:PHE:CE1	2.56	0.40
1:A:77:ILE:HD12	1:A:115:CYS:SG	2.62	0.40
4:D:258:LYS:O	4:D:259:ARG:CG	2.69	0.40
5:E:43:ASN:HB3	5:E:58:MET:HE1	2.03	0.40
5:E:280:HIS:CD2	5:E:281:LYS:N	2.89	0.40
7:G:86:VAL:HG13	7:G:183:ILE:O	2.22	0.40
10:J:53:ALA:HB2	10:J:68:ILE:CD1	2.49	0.40
11:L:65:ARG:NH1	48:5:1382:G:OP1	2.54	0.40
11:L:94:ILE:HG22	11:L:124:LEU:HD11	2.04	0.40
16:Q:181:ARG:NH1	48:5:1391:A:OP2	2.55	0.40
23:X:76:ILE:HG21	23:X:112:ALA:HB2	2.02	0.40
28:c:50:ASN:C	28:c:50:ASN:ND2	2.80	0.40
30:e:87:VAL:CG1	42:r:25:TYR:CG	3.05	0.40
32:g:76:ARG:NH2	48:5:2583:C:OP2	2.46	0.40
39:n:4:LYS:HE3	51:9:1844:U:O4	2.18	0.40
44:t:123:ARG:NE	44:t:129:ILE:HD11	2.37	0.40
47:3:68:C:C2'	47:3:69:G:O4'	2.69	0.40
48:5:376:A:H2'	48:5:377:A:O4'	2.21	0.40
48:5:442:G:H2'	48:5:443:G:O4'	2.22	0.40
48:5:677:G:C6	48:5:678:C:C4	3.09	0.40
48:5:963:G:N3	48:5:963:G:C2'	2.83	0.40
48:5:1356:U:C4	48:5:1357:C:N4	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1383:G:C5	48:5:1384:C:C4	3.10	0.40
48:5:1504:G:O5’	48:5:1504:G:H8	2.04	0.40
48:5:1748:U:H2’	48:5:1749:A:O4’	2.22	0.40
48:5:3909:C:C4	48:5:3910:C:C5	3.10	0.40
48:5:4129:G:C2	48:5:4130:C:C2	3.08	0.40
48:5:4303:C:H2’	48:5:4305:G:C8	2.56	0.40
48:5:4349:C:H3’	48:5:4350:C:H5’	2.04	0.40
48:5:4583:C:C4	48:5:4718:G:N1	2.89	0.40
48:5:4765:G:N1	48:5:4870:G:C8	2.90	0.40
48:5:4967:A:C2	48:5:4968:A:C5	3.10	0.40
48:5:5008:C:H2’	48:5:5009:G:O4’	2.21	0.40
49:7:117:G:C2	49:7:118:C:C2	3.10	0.40
51:9:29:G:C6	51:9:30:C:C4	3.09	0.40
51:9:431:G:H2’	51:9:432:G:O4’	2.22	0.40
51:9:483:C:N4	51:9:484:A:C6	2.90	0.40
51:9:656:G:O2’	54:CC:227:TRP:CE3	2.74	0.40
51:9:841:G:C6	51:9:842:C:C4	3.10	0.40
66:OO:151:LEU:HD22	66:OO:151:LEU:OXT	2.21	0.40
74:WW:105:THR:CG2	74:WW:126:LEU:HD21	2.52	0.40
86:ii:50:LYS:O	86:ii:51:MET:C	2.64	0.40
1:A:217:GLN:NE2	48:5:3650:C:OP1	2.54	0.40
7:G:86:VAL:HG22	7:G:183:ILE:HG22	2.03	0.40
7:G:243:GLY:O	7:G:244:PRO:C	2.64	0.40
13:N:121:VAL:HG11	13:N:131:GLU:HG3	2.03	0.40
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.57	0.40
16:Q:43:PHE:CD1	16:Q:133:GLY:HA3	2.57	0.40
23:X:53:ARG:NH1	48:5:2475:G:C5	2.90	0.40
29:d:32:ARG:HB3	29:d:48:GLU:HG2	2.04	0.40
32:g:76:ARG:NH1	48:5:2582:A:OP1	2.55	0.40
42:r:104:PRO:C	42:r:106:LEU:N	2.78	0.40
47:3:34:U:O2	51:9:1641:A:H5”	2.22	0.40
48:5:219:G:OP1	48:5:219:G:H4’	2.22	0.40
48:5:258:G:N2	48:5:259:C:C2	2.90	0.40
48:5:298:G:C2	48:5:299:C:C2	3.10	0.40
48:5:740:G:C2	48:5:925:C:C2	3.09	0.40
48:5:964:A:H2’	48:5:965:G:OP1	2.22	0.40
48:5:1070:G:C6	48:5:1071:C:N4	2.89	0.40
48:5:1412:G:C2	48:5:1413:C:C2	3.09	0.40
48:5:1448:G:C2	48:5:2097:U:C4	3.10	0.40
48:5:1576:G:C4	48:5:1578:U:C6	3.10	0.40
48:5:1783:C:H2’	48:5:1784:U:O4’	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2468:U:C2	48:5:2473:A:N6	2.88	0.40
48:5:2616:C:C2	48:5:2722:G:N2	2.89	0.40
48:5:2771:G:H2'	48:5:2772:C:O4'	2.21	0.40
48:5:2849:A:O4'	48:5:2850:A:C2	2.75	0.40
48:5:3804:G:C5	48:5:3805:U:C5	3.09	0.40
48:5:4162:C:O2	48:5:4162:C:O4'	2.37	0.40
48:5:4410:G:C2	48:5:4411:G:C8	3.09	0.40
48:5:4913:G:HO2'	48:5:4914:C:C1'	2.35	0.40
51:9:113:G:N2	51:9:292:A:H1'	2.37	0.40
51:9:387:C:OP2	60:II:10:LYS:HE3	2.22	0.40
51:9:600:G:C2'	51:9:601:G:O5'	2.69	0.40
56:EE:42:LEU:HD12	56:EE:109:PHE:CB	2.51	0.40
81:dd:18:SER:OG	81:dd:19:ARG:N	2.55	0.40
84:gg:32:LEU:HD13	84:gg:92:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	242/244 (99%)	199 (82%)	34 (14%)	9 (4%)	2 19
2	B	392/394 (100%)	338 (86%)	44 (11%)	10 (3%)	4 24
3	C	359/361 (99%)	302 (84%)	48 (13%)	9 (2%)	4 25
4	D	290/292 (99%)	255 (88%)	31 (11%)	4 (1%)	9 34
5	E	232/248 (94%)	172 (74%)	37 (16%)	23 (10%)	0 5
6	F	223/225 (99%)	204 (92%)	18 (8%)	1 (0%)	30 58
7	G	239/241 (99%)	205 (86%)	26 (11%)	8 (3%)	3 21
8	H	188/190 (99%)	161 (86%)	25 (13%)	2 (1%)	11 39
9	I	200/213 (94%)	178 (89%)	17 (8%)	5 (2%)	4 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	J	167/169 (99%)	141 (84%)	18 (11%)	8 (5%)	2 14
11	L	208/210 (99%)	174 (84%)	25 (12%)	9 (4%)	2 16
12	M	136/138 (99%)	123 (90%)	12 (9%)	1 (1%)	18 48
13	N	201/203 (99%)	167 (83%)	32 (16%)	2 (1%)	12 41
14	O	197/199 (99%)	176 (89%)	20 (10%)	1 (0%)	24 55
15	P	151/153 (99%)	134 (89%)	13 (9%)	4 (3%)	4 24
16	Q	185/187 (99%)	161 (87%)	20 (11%)	4 (2%)	5 27
17	R	178/180 (99%)	151 (85%)	25 (14%)	2 (1%)	11 39
18	S	173/175 (99%)	151 (87%)	18 (10%)	4 (2%)	5 26
19	T	157/159 (99%)	137 (87%)	17 (11%)	3 (2%)	6 30
20	U	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	2 17
21	V	129/131 (98%)	110 (85%)	19 (15%)	0	100 100
22	W	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	7 32
23	X	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	7 31
24	Y	132/134 (98%)	114 (86%)	13 (10%)	5 (4%)	2 18
25	Z	133/135 (98%)	113 (85%)	14 (10%)	6 (4%)	2 15
26	a	145/147 (99%)	114 (79%)	24 (17%)	7 (5%)	2 14
27	b	73/75 (97%)	65 (89%)	5 (7%)	3 (4%)	2 17
28	c	92/94 (98%)	87 (95%)	5 (5%)	0	100 100
29	d	105/107 (98%)	86 (82%)	17 (16%)	2 (2%)	6 30
30	e	126/128 (98%)	110 (87%)	12 (10%)	4 (3%)	3 21
31	f	107/109 (98%)	88 (82%)	12 (11%)	7 (6%)	1 11
32	g	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	6 30
33	h	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3 21
34	i	100/102 (98%)	87 (87%)	11 (11%)	2 (2%)	6 29
35	j	84/86 (98%)	73 (87%)	8 (10%)	3 (4%)	2 19
36	k	67/69 (97%)	53 (79%)	10 (15%)	4 (6%)	1 12
37	l	48/50 (96%)	41 (85%)	5 (10%)	2 (4%)	2 16
38	m	50/52 (96%)	43 (86%)	7 (14%)	0	100 100
39	n	21/23 (91%)	21 (100%)	0	0	100 100
40	o	102/104 (98%)	79 (78%)	19 (19%)	4 (4%)	2 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	p	89/91 (98%)	75 (84%)	9 (10%)	5 (6%)	1 13
42	r	123/125 (98%)	104 (85%)	10 (8%)	9 (7%)	1 8
43	s	196/198 (99%)	163 (83%)	21 (11%)	12 (6%)	1 11
44	t	161/163 (99%)	100 (62%)	36 (22%)	25 (16%)	0 2
45	1	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1 7
52	AA	206/208 (99%)	153 (74%)	37 (18%)	16 (8%)	1 7
53	BB	211/213 (99%)	165 (78%)	34 (16%)	12 (6%)	1 12
54	CC	216/218 (99%)	184 (85%)	22 (10%)	10 (5%)	2 15
55	DD	225/227 (99%)	184 (82%)	30 (13%)	11 (5%)	1 14
56	EE	260/262 (99%)	197 (76%)	43 (16%)	20 (8%)	1 7
57	FF	189/191 (99%)	156 (82%)	22 (12%)	11 (6%)	1 12
58	GG	235/237 (99%)	198 (84%)	29 (12%)	8 (3%)	3 21
59	HH	187/189 (99%)	144 (77%)	30 (16%)	13 (7%)	1 9
60	II	204/206 (99%)	169 (83%)	25 (12%)	10 (5%)	1 14
61	JJ	183/185 (99%)	152 (83%)	19 (10%)	12 (7%)	1 10
62	KK	96/98 (98%)	65 (68%)	20 (21%)	11 (12%)	0 3
63	LL	150/152 (99%)	125 (83%)	16 (11%)	9 (6%)	1 12
64	MM	122/124 (98%)	87 (71%)	25 (20%)	10 (8%)	0 6
65	NN	148/150 (99%)	121 (82%)	21 (14%)	6 (4%)	2 17
66	OO	134/136 (98%)	96 (72%)	24 (18%)	14 (10%)	0 4
67	PP	125/127 (98%)	102 (82%)	20 (16%)	3 (2%)	4 25
68	QQ	139/141 (99%)	115 (83%)	14 (10%)	10 (7%)	1 9
69	RR	127/129 (98%)	100 (79%)	18 (14%)	9 (7%)	1 9
70	SS	135/137 (98%)	110 (82%)	15 (11%)	10 (7%)	1 8
71	TT	139/141 (99%)	127 (91%)	9 (6%)	3 (2%)	5 27
72	UU	102/104 (98%)	84 (82%)	12 (12%)	6 (6%)	1 12
73	VV	81/83 (98%)	65 (80%)	9 (11%)	7 (9%)	0 6
74	WW	127/129 (98%)	101 (80%)	21 (16%)	5 (4%)	2 18
75	XX	139/141 (99%)	122 (88%)	8 (6%)	9 (6%)	1 11
76	YY	124/126 (98%)	100 (81%)	15 (12%)	9 (7%)	1 8
77	ZZ	73/75 (97%)	58 (80%)	11 (15%)	4 (6%)	1 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
78	aa	96/98 (98%)	76 (79%)	8 (8%)	12 (12%)	0 3
79	bb	81/83 (98%)	59 (73%)	16 (20%)	6 (7%)	1 8
80	cc	59/61 (97%)	47 (80%)	11 (19%)	1 (2%)	7 31
81	dd	51/53 (96%)	40 (78%)	11 (22%)	0	100 100
82	ee	55/57 (96%)	39 (71%)	14 (26%)	2 (4%)	2 19
83	ff	58/68 (85%)	49 (84%)	8 (14%)	1 (2%)	7 31
84	gg	311/313 (99%)	263 (85%)	40 (13%)	8 (3%)	4 24
86	ii	414/416 (100%)	378 (91%)	25 (6%)	11 (3%)	4 24
87	jj	569/594 (96%)	501 (88%)	54 (10%)	14 (2%)	4 25
All	All	12492/12708 (98%)	10443 (84%)	1523 (12%)	526 (4%)	3 16

All (526) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	196	TRP
1	A	197	PRO
2	B	37	PRO
2	B	302	ASN
3	C	73	VAL
3	C	217	ILE
5	E	91	PRO
5	E	96	LYS
5	E	118	PRO
5	E	174	PRO
5	E	175	LEU
5	E	200	SER
5	E	221	PRO
6	F	239	GLU
7	G	44	ASP
7	G	45	ILE
7	G	128	VAL
8	H	40	HIS
9	I	47	PRO
9	I	48	LEU
10	J	11	PRO
11	L	64	VAL
11	L	67	HIS
11	L	176	PHE

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Mol	Chain	Res	Type
13	N	87	HIS
18	S	155	PRO
18	S	165	PRO
24	Y	51	LYS
25	Z	34	SER
25	Z	84	ARG
25	Z	91	LEU
26	a	90	ALA
29	d	94	GLU
30	e	44	ARG
30	e	92	ASN
31	f	79	GLY
31	f	80	ASN
32	g	69	LYS
33	h	7	ARG
33	h	122	LYS
35	j	36	LYS
36	k	61	PRO
41	p	40	SER
42	r	11	ARG
42	r	86	ALA
42	r	105	ASP
42	r	107	ARG
43	s	62	ARG
43	s	201	PRO
44	t	29	ALA
44	t	30	PRO
44	t	31	LYS
44	t	89	PRO
44	t	106	PHE
44	t	137	GLN
44	t	144	ASP
44	t	149	HIS
45	1	64	PRO
52	AA	43	SER
52	AA	138	SER
53	BB	57	ILE
53	BB	140	VAL
53	BB	179	ASN
53	BB	191	ASP
54	CC	255	LEU
55	DD	199	GLY

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Mol	Chain	Res	Type
55	DD	202	LYS
56	EE	12	VAL
56	EE	118	GLU
56	EE	168	LYS
56	EE	223	SER
57	FF	163	PHE
58	GG	105	ASN
59	HH	18	GLU
59	HH	66	VAL
60	II	27	TYR
60	II	157	LYS
61	JJ	119	LEU
61	JJ	121	LYS
62	KK	63	ALA
62	KK	93	THR
62	KK	95	ARG
63	LL	66	VAL
64	MM	79	VAL
64	MM	102	LYS
64	MM	114	TYR
66	OO	56	VAL
66	OO	65	ASP
66	OO	138	ASP
66	OO	140	THR
67	PP	14	LYS
68	QQ	43	GLU
69	RR	88	VAL
69	RR	93	GLN
70	SS	81	ASP
70	SS	133	GLY
71	TT	29	LYS
71	TT	34	VAL
72	UU	107	GLU
73	VV	41	LYS
74	WW	29	PRO
75	XX	34	THR
76	YY	104	ARG
77	ZZ	104	ARG
77	ZZ	113	THR
79	bb	82	LYS
82	ee	9	VAL
84	gg	161	SER

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Mol	Chain	Res	Type
84	gg	282	GLU
86	ii	27	ALA
86	ii	32	THR
86	ii	120	ILE
86	ii	298	THR
87	jj	237	ILE
87	jj	245	SER
87	jj	455	ILE
1	A	217	GLN
2	B	18	PRO
2	B	247	GLY
3	C	273	LEU
3	C	275	SER
4	D	187	SER
5	E	54	SER
5	E	85	LEU
5	E	92	VAL
5	E	95	ASP
7	G	85	GLN
10	J	91	GLU
10	J	124	GLY
10	J	155	HIS
11	L	143	GLU
12	M	53	LYS
13	N	181	HIS
16	Q	14	ARG
16	Q	148	VAL
16	Q	178	ARG
17	R	19	LYS
17	R	130	ASN
19	T	44	GLY
20	U	98	ASP
24	Y	11	ARG
24	Y	83	GLU
25	Z	17	ARG
25	Z	124	THR
26	a	76	ASP
33	h	40	ALA
41	p	10	ILE
42	r	20	ARG
42	r	67	ARG
42	r	71	ARG

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Mol	Chain	Res	Type
43	s	34	ASN
43	s	70	GLU
43	s	106	LYS
43	s	109	ALA
43	s	142	GLY
44	t	19	GLY
44	t	22	VAL
44	t	39	PRO
44	t	53	TRP
44	t	54	LYS
44	t	58	ILE
44	t	67	ARG
52	AA	44	ASP
52	AA	45	GLY
52	AA	186	ARG
53	BB	86	LEU
53	BB	93	GLY
53	BB	190	PRO
53	BB	206	PRO
54	CC	101	ALA
54	CC	119	ALA
55	DD	191	PRO
55	DD	219	PRO
56	EE	24	THR
56	EE	53	LYS
56	EE	95	THR
56	EE	101	LEU
56	EE	171	ASP
56	EE	196	THR
56	EE	216	ASN
57	FF	52	SER
57	FF	54	GLY
57	FF	77	MET
57	FF	80	GLY
58	GG	54	GLY
58	GG	69	THR
59	HH	159	ASP
59	HH	190	PRO
60	II	8	TRP
60	II	138	ASN
60	II	154	LYS
60	II	155	ASN

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Mol	Chain	Res	Type
61	JJ	3	VAL
61	JJ	118	GLY
61	JJ	120	ALA
62	KK	3	MET
63	LL	55	TYR
63	LL	149	ALA
65	NN	24	THR
65	NN	138	ASN
66	OO	24	GLY
66	OO	48	SER
66	OO	106	LYS
67	PP	75	VAL
68	QQ	64	ALA
68	QQ	100	VAL
69	RR	123	THR
70	SS	11	HIS
70	SS	12	ILE
70	SS	82	TRP
71	TT	39	LEU
72	UU	50	VAL
72	UU	52	GLY
73	VV	21	ASN
73	VV	31	SER
73	VV	48	GLY
74	WW	30	CYS
74	WW	83	LEU
74	WW	107	SER
75	XX	6	GLY
76	YY	95	GLY
76	YY	120	THR
76	YY	127	ALA
78	aa	9	GLY
78	aa	25	ASN
78	aa	28	ARG
78	aa	46	GLU
79	bb	4	ALA
79	bb	6	ASP
79	bb	26	GLN
84	gg	160	SER
84	gg	253	GLY
86	ii	144	SER
86	ii	305	VAL

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Mol	Chain	Res	Type
86	ii	315	GLY
86	ii	387	ALA
87	jj	24	GLU
87	jj	179	ALA
87	jj	249	VAL
87	jj	550	THR
1	A	194	ASN
3	C	16	GLU
5	E	63	ALA
5	E	166	SER
5	E	179	ARG
5	E	187	GLN
5	E	234	GLU
9	I	99	ILE
9	I	201	PRO
10	J	15	LEU
10	J	116	GLY
10	J	154	LYS
16	Q	172	ARG
19	T	81	LYS
20	U	97	ARG
22	W	43	LYS
23	X	131	ASP
24	Y	63	LYS
26	a	40	HIS
26	a	84	GLU
26	a	119	LYS
27	b	7	HIS
29	d	60	PRO
32	g	67	LEU
37	l	44	TRP
40	o	32	SER
40	o	77	CYS
41	p	18	TYR
41	p	41	PHE
42	r	68	SER
42	r	85	ASN
43	s	69	LEU
43	s	108	PRO
44	t	5	PHE
44	t	26	SER
44	t	105	THR

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Mol	Chain	Res	Type
44	t	118	HIS
44	t	119	ARG
52	AA	6	ASP
52	AA	84	GLN
52	AA	191	ARG
52	AA	207	PRO
54	CC	190	SER
55	DD	143	ARG
56	EE	98	ASN
56	EE	153	LEU
57	FF	34	SER
57	FF	37	ASP
57	FF	63	LYS
58	GG	152	ASP
59	HH	57	ARG
59	HH	160	LYS
60	II	137	LEU
60	II	168	GLN
61	JJ	5	ARG
61	JJ	138	ARG
61	JJ	147	PHE
62	KK	25	LYS
62	KK	31	LYS
62	KK	39	ASN
62	KK	92	ALA
63	LL	19	ASN
63	LL	147	LYS
64	MM	100	PRO
65	NN	3	ARG
66	OO	64	ALA
66	OO	129	ILE
67	PP	121	ILE
68	QQ	17	LYS
68	QQ	35	ASN
68	QQ	132	PHE
70	SS	7	GLU
72	UU	51	LYS
74	WW	93	LEU
75	XX	10	ALA
75	XX	116	PRO
77	ZZ	52	LYS
78	aa	13	LYS

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Mol	Chain	Res	Type
78	aa	62	TYR
79	bb	48	SER
84	gg	60	ARG
84	gg	76	GLN
86	ii	386	GLY
87	jj	285	PHE
1	A	127	ALA
2	B	372	SER
2	B	376	HIS
5	E	103	VAL
5	E	218	LEU
5	E	224	GLN
9	I	46	PHE
11	L	5	ARG
14	O	126	VAL
15	P	12	THR
15	P	108	ASP
23	X	73	HIS
25	Z	55	ALA
30	e	119	ALA
30	e	125	PRO
31	f	25	THR
31	f	37	ASP
34	i	3	LEU
35	j	39	TYR
36	k	22	SER
36	k	32	VAL
40	o	5	PRO
40	o	99	ARG
41	p	31	ILE
43	s	63	LYS
44	t	148	PRO
52	AA	35	GLU
52	AA	165	ASN
53	BB	88	THR
53	BB	106	THR
55	DD	214	LYS
55	DD	223	ILE
56	EE	30	ARG
56	EE	73	ASP
56	EE	131	VAL
58	GG	146	ASN

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Mol	Chain	Res	Type
59	HH	16	PRO
59	HH	111	LYS
60	II	143	LYS
61	JJ	133	ARG
62	KK	32	HIS
63	LL	69	ARG
63	LL	151	THR
64	MM	116	LYS
65	NN	13	GLN
65	NN	108	ASP
66	OO	32	HIS
66	OO	128	ARG
68	QQ	145	TYR
69	RR	63	ARG
69	RR	121	GLN
70	SS	10	GLN
70	SS	83	PHE
72	UU	105	SER
73	VV	45	ARG
75	XX	42	GLY
76	YY	34	THR
78	aa	8	ASN
78	aa	15	ARG
78	aa	64	LEU
79	bb	75	GLU
82	ee	22	GLN
83	ff	85	LYS
84	gg	146	SER
84	gg	205	SER
86	ii	28	ARG
87	jj	47	ILE
87	jj	346	CYS
87	jj	452	GLU
1	A	244	GLY
2	B	113	GLU
2	B	169	ARG
2	B	254	ILE
3	C	58	ALA
3	C	187	GLN
3	C	309	ILE
4	D	44	TYR
4	D	158	LYS

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Mol	Chain	Res	Type
4	D	188	LYS
7	G	123	ALA
11	L	134	PRO
15	P	21	ASN
20	U	27	HIS
20	U	47	ILE
26	a	4	ARG
31	f	97	ILE
31	f	107	PRO
33	h	89	ARG
34	i	11	LEU
36	k	21	LYS
37	l	47	THR
43	s	57	LYS
43	s	73	PRO
44	t	120	SER
52	AA	98	PRO
52	AA	110	ASN
52	AA	137	ALA
53	BB	22	VAL
53	BB	76	ASN
54	CC	202	THR
54	CC	261	PHE
54	CC	274	VAL
55	DD	4	GLN
55	DD	93	THR
55	DD	200	PRO
56	EE	76	VAL
56	EE	109	PHE
56	EE	144	ALA
57	FF	119	SER
58	GG	55	GLY
58	GG	117	GLY
59	HH	113	LYS
60	II	131	PRO
61	JJ	122	SER
62	KK	90	VAL
63	LL	28	THR
63	LL	34	PRO
64	MM	15	ASN
64	MM	103	VAL
66	OO	104	ARG

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Mol	Chain	Res	Type
68	QQ	27	ARG
69	RR	95	ILE
72	UU	118	ASP
73	VV	33	PRO
75	XX	68	LYS
75	XX	129	SER
76	YY	52	PRO
76	YY	126	GLY
78	aa	27	ALA
78	aa	35	ALA
78	aa	61	ALA
86	ii	385	PHE
5	E	48	ARG
5	E	239	THR
7	G	125	LYS
11	L	169	ILE
24	Y	10	ASP
26	a	98	ALA
31	f	106	TYR
35	j	8	PHE
52	AA	10	MET
54	CC	181	PRO
57	FF	33	ILE
57	FF	132	GLY
59	HH	35	ASP
59	HH	65	PRO
59	HH	100	ILE
64	MM	58	GLU
64	MM	96	ARG
66	OO	33	ILE
68	QQ	32	ILE
70	SS	17	ASN
70	SS	39	ARG
73	VV	10	ASP
77	ZZ	112	ASN
2	B	90	VAL
7	G	238	GLY
8	H	104	VAL
18	S	5	GLY
19	T	145	GLY
44	t	2	PRO
44	t	10	ILE

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Mol	Chain	Res	Type
52	AA	101	GLY
54	CC	264	SER
65	NN	150	VAL
68	QQ	30	GLY
69	RR	42	PRO
76	YY	51	THR
18	S	172	PRO
27	b	36	ASP
44	t	23	GLY
56	EE	90	ILE
59	HH	116	ARG
61	JJ	164	PRO
66	OO	144	GLY
75	XX	61	GLN
1	A	183	GLY
3	C	148	PRO
11	L	100	PRO
58	GG	99	GLY
61	JJ	36	GLY
69	RR	125	GLY
75	XX	33	GLY
80	cc	25	GLY
87	jj	352	GLY
1	A	57	PRO
5	E	190	VAL
7	G	163	PRO
10	J	174	ILE
11	L	12	PRO
27	b	21	ILE
54	CC	111	PRO
55	DD	218	LEU
62	KK	91	PRO
64	MM	115	GLY
69	RR	124	VAL
87	jj	432	ILE
5	E	220	LYS
15	P	84	PRO
76	YY	29	HIS
87	jj	42	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	157 (84%)	30 (16%)	2	14
2	B	336/342 (98%)	285 (85%)	51 (15%)	3	15
3	C	301/301 (100%)	259 (86%)	42 (14%)	3	17
4	D	247/247 (100%)	219 (89%)	28 (11%)	5	24
5	E	208/221 (94%)	178 (86%)	30 (14%)	3	16
6	F	194/195 (100%)	171 (88%)	23 (12%)	5	22
7	G	206/206 (100%)	173 (84%)	33 (16%)	2	14
8	H	169/169 (100%)	144 (85%)	25 (15%)	3	16
9	I	174/180 (97%)	155 (89%)	19 (11%)	6	25
10	J	142/142 (100%)	124 (87%)	18 (13%)	4	20
11	L	176/176 (100%)	149 (85%)	27 (15%)	3	14
12	M	117/117 (100%)	103 (88%)	14 (12%)	5	22
13	N	171/171 (100%)	149 (87%)	22 (13%)	4	19
14	O	171/171 (100%)	143 (84%)	28 (16%)	2	13
15	P	134/134 (100%)	116 (87%)	18 (13%)	4	19
16	Q	163/163 (100%)	139 (85%)	24 (15%)	3	16
17	R	159/159 (100%)	138 (87%)	21 (13%)	4	19
18	S	156/156 (100%)	134 (86%)	22 (14%)	3	17
19	T	139/139 (100%)	115 (83%)	24 (17%)	2	12
20	U	89/89 (100%)	79 (89%)	10 (11%)	6	24
21	V	101/101 (100%)	82 (81%)	19 (19%)	1	9
22	W	55/55 (100%)	49 (89%)	6 (11%)	6	25
23	X	107/107 (100%)	92 (86%)	15 (14%)	3	17
24	Y	124/124 (100%)	106 (86%)	18 (14%)	3	16
25	Z	117/117 (100%)	97 (83%)	20 (17%)	2	12
26	a	119/119 (100%)	108 (91%)	11 (9%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	b	62/62 (100%)	53 (86%)	9 (14%)	3 16
28	c	79/79 (100%)	65 (82%)	14 (18%)	2 11
29	d	98/98 (100%)	78 (80%)	20 (20%)	1 7
30	e	114/114 (100%)	91 (80%)	23 (20%)	1 8
31	f	88/88 (100%)	75 (85%)	13 (15%)	3 16
32	g	98/98 (100%)	81 (83%)	17 (17%)	2 12
33	h	109/109 (100%)	95 (87%)	14 (13%)	4 20
34	i	86/86 (100%)	75 (87%)	11 (13%)	4 20
35	j	73/73 (100%)	60 (82%)	13 (18%)	2 11
36	k	64/64 (100%)	58 (91%)	6 (9%)	8 30
37	l	47/47 (100%)	40 (85%)	7 (15%)	3 15
38	m	48/48 (100%)	39 (81%)	9 (19%)	1 9
39	n	22/22 (100%)	21 (96%)	1 (4%)	24 48
40	o	92/92 (100%)	76 (83%)	16 (17%)	2 11
41	p	74/74 (100%)	65 (88%)	9 (12%)	5 21
42	r	109/109 (100%)	89 (82%)	20 (18%)	2 10
43	s	166/166 (100%)	155 (93%)	11 (7%)	15 40
44	t	136/136 (100%)	130 (96%)	6 (4%)	25 49
45	1	13/13 (100%)	11 (85%)	2 (15%)	2 14
52	AA	174/174 (100%)	143 (82%)	31 (18%)	2 11
53	BB	194/194 (100%)	163 (84%)	31 (16%)	2 14
54	CC	183/183 (100%)	164 (90%)	19 (10%)	7 27
55	DD	190/190 (100%)	154 (81%)	36 (19%)	1 9
56	EE	223/223 (100%)	189 (85%)	34 (15%)	3 15
57	FF	161/161 (100%)	132 (82%)	29 (18%)	2 11
58	GG	207/207 (100%)	178 (86%)	29 (14%)	3 17
59	HH	169/169 (100%)	152 (90%)	17 (10%)	7 28
60	II	178/178 (100%)	147 (83%)	31 (17%)	2 11
61	JJ	161/161 (100%)	135 (84%)	26 (16%)	2 13
62	KK	89/89 (100%)	74 (83%)	15 (17%)	2 12
63	LL	136/136 (100%)	111 (82%)	25 (18%)	1 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
64	MM	104/104 (100%)	90 (86%)	14 (14%)	4 18
65	NN	130/130 (100%)	104 (80%)	26 (20%)	1 8
66	OO	106/106 (100%)	88 (83%)	18 (17%)	2 12
67	PP	116/116 (100%)	98 (84%)	18 (16%)	2 14
68	QQ	117/117 (100%)	100 (86%)	17 (14%)	3 16
69	RR	117/117 (100%)	97 (83%)	20 (17%)	2 12
70	SS	119/119 (100%)	97 (82%)	22 (18%)	1 10
71	TT	112/112 (100%)	91 (81%)	21 (19%)	1 9
72	UU	94/94 (100%)	82 (87%)	12 (13%)	4 20
73	VV	67/67 (100%)	57 (85%)	10 (15%)	3 15
74	WW	112/112 (100%)	97 (87%)	15 (13%)	4 19
75	XX	113/113 (100%)	93 (82%)	20 (18%)	2 11
76	YY	108/108 (100%)	86 (80%)	22 (20%)	1 7
77	ZZ	66/66 (100%)	55 (83%)	11 (17%)	2 13
78	aa	85/85 (100%)	74 (87%)	11 (13%)	4 19
79	bb	75/75 (100%)	66 (88%)	9 (12%)	5 22
80	cc	54/54 (100%)	40 (74%)	14 (26%)	0 4
81	dd	47/47 (100%)	35 (74%)	12 (26%)	0 4
82	ee	47/47 (100%)	41 (87%)	6 (13%)	4 20
83	ff	58/61 (95%)	56 (97%)	2 (3%)	32 53
84	gg	272/272 (100%)	247 (91%)	25 (9%)	8 30
86	ii	358/358 (100%)	314 (88%)	44 (12%)	4 21
87	jj	507/522 (97%)	469 (92%)	38 (8%)	12 37
All	All	10889/10933 (100%)	9340 (86%)	1549 (14%)	5 17

All (1549) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	36	GLU
1	A	64	ARG
1	A	75	LEU
1	A	88	VAL
1	A	96	LEU

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Mol	Chain	Res	Type
1	A	100	ASN
1	A	102	LEU
1	A	109	GLU
1	A	123	ARG
1	A	128	ARG
1	A	135	THR
1	A	142	GLU
1	A	158	ILE
1	A	162	ASN
1	A	163	ARG
1	A	165	VAL
1	A	175	ILE
1	A	180	LEU
1	A	193	ARG
1	A	198	ARG
1	A	200	ARG
1	A	202	VAL
1	A	209	HIS
1	A	218	HIS
1	A	221	LYS
1	A	226	ARG
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	19	ARG
2	B	23	SER
2	B	37	PRO
2	B	39	LYS
2	B	43	LEU
2	B	53	MET
2	B	56	ILE
2	B	62	ARG
2	B	66	LYS
2	B	84	MET
2	B	90	VAL
2	B	94	GLU
2	B	97	ARG
2	B	99	LEU
2	B	103	LYS
2	B	116	ARG

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Mol	Chain	Res	Type
2	B	128	LYS
2	B	134	CYS
2	B	135	LYS
2	B	154	LYS
2	B	162	VAL
2	B	167	GLN
2	B	173	LEU
2	B	180	LEU
2	B	201	LEU
2	B	203	GLN
2	B	207	VAL
2	B	213	GLN
2	B	223	THR
2	B	234	ARG
2	B	240	LEU
2	B	244	THR
2	B	246	ARG
2	B	253	CYS
2	B	258	HIS
2	B	261	ARG
2	B	262	VAL
2	B	268	ARG
2	B	279	GLU
2	B	294	LYS
2	B	299	ILE
2	B	314	ILE
2	B	333	LEU
2	B	347	LEU
2	B	351	LEU
2	B	356	LYS
2	B	366	LYS
2	B	371	THR
2	B	383	GLU
3	C	7	LEU
3	C	14	LYS
3	C	20	LYS
3	C	29	LYS
3	C	37	VAL
3	C	54	VAL
3	C	57	LEU
3	C	80	ARG
3	C	95	MET

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Mol	Chain	Res	Type
3	C	101	MET
3	C	106	LYS
3	C	107	THR
3	C	113	ARG
3	C	114	ARG
3	C	118	THR
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	155	GLU
3	C	156	ASP
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	201	ARG
3	C	208	CYS
3	C	219	LYS
3	C	229	LEU
3	C	232	VAL
3	C	246	VAL
3	C	273	LEU
3	C	281	MET
3	C	284	MET
3	C	289	LEU
3	C	303	ARG
3	C	307	LYS
3	C	333	LYS
3	C	339	THR
3	C	342	ARG
3	C	345	ARG
4	D	4	VAL
4	D	23	ARG
4	D	25	GLU
4	D	33	ARG
4	D	36	LEU
4	D	37	VAL
4	D	39	GLN
4	D	60	ILE
4	D	61	ILE

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Mol	Chain	Res	Type
4	D	84	PRO
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	129	GLU
4	D	153	THR
4	D	196	ARG
4	D	202	GLN
4	D	221	LYS
4	D	225	GLN
4	D	236	MET
4	D	248	ARG
4	D	256	LYS
4	D	264	LYS
4	D	278	ASP
4	D	291	GLN
5	E	46	LEU
5	E	52	ARG
5	E	58	MET
5	E	101	ARG
5	E	105	LEU
5	E	111	TYR
5	E	115	GLU
5	E	124	HIS
5	E	134	ARG
5	E	136	LEU
5	E	137	ARG
5	E	141	THR
5	E	148	ILE
5	E	158	VAL
5	E	162	LYS
5	E	166	SER
5	E	171	VAL
5	E	175	LEU
5	E	190	VAL
5	E	193	THR
5	E	206	LYS
5	E	208	LEU
5	E	212	TYR

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Mol	Chain	Res	Type
5	E	218	LEU
5	E	219	ARG
5	E	233	LYS
5	E	250	ASP
5	E	253	ILE
5	E	262	GLN
5	E	282	LEU
6	F	38	LYS
6	F	41	GLN
6	F	43	MET
6	F	44	LEU
6	F	46	LYS
6	F	49	ARG
6	F	68	ARG
6	F	72	ARG
6	F	76	MET
6	F	91	LEU
6	F	109	LYS
6	F	115	ARG
6	F	127	LEU
6	F	131	SER
6	F	137	ILE
6	F	146	TYR
6	F	154	GLU
6	F	179	ARG
6	F	192	LEU
6	F	201	LYS
6	F	202	ARG
6	F	217	SER
6	F	234	ASP
7	G	28	VAL
7	G	31	LEU
7	G	46	GLN
7	G	55	VAL
7	G	59	ARG
7	G	62	ARG
7	G	75	LYS
7	G	81	ASN
7	G	90	GLN
7	G	106	THR
7	G	110	LYS
7	G	112	GLN

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Mol	Chain	Res	Type
7	G	131	LYS
7	G	145	THR
7	G	148	GLU
7	G	150	LYS
7	G	151	LYS
7	G	154	LEU
7	G	162	ASP
7	G	170	LEU
7	G	173	LEU
7	G	175	ARG
7	G	176	LYS
7	G	177	MET
7	G	189	ARG
7	G	201	THR
7	G	202	VAL
7	G	207	VAL
7	G	212	LYS
7	G	215	LEU
7	G	218	LEU
7	G	220	GLU
7	G	259	LYS
8	H	1	MET
8	H	18	ILE
8	H	20	LEU
8	H	26	ILE
8	H	36	ARG
8	H	41	ILE
8	H	52	LYS
8	H	57	VAL
8	H	59	LYS
8	H	65	LYS
8	H	74	CYS
8	H	78	GLN
8	H	80	MET
8	H	82	LYS
8	H	92	MET
8	H	94	SER
8	H	104	VAL
8	H	105	ILE
8	H	111	LEU
8	H	118	LEU
8	H	125	ARG

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Mol	Chain	Res	Type
8	H	128	MET
8	H	141	LYS
8	H	173	ARG
8	H	180	TYR
9	I	13	LYS
9	I	35	ASP
9	I	36	LEU
9	I	39	LYS
9	I	48	LEU
9	I	55	ASP
9	I	76	MET
9	I	99	ILE
9	I	100	ASN
9	I	116	ARG
9	I	144	ASN
9	I	146	GLU
9	I	148	VAL
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	202	ASN
9	I	208	LYS
9	I	212	LEU
10	J	9	GLU
10	J	15	LEU
10	J	16	ARG
10	J	22	LEU
10	J	33	LEU
10	J	34	THR
10	J	49	VAL
10	J	68	ILE
10	J	81	GLU
10	J	83	LEU
10	J	84	GLU
10	J	96	LYS
10	J	110	GLN
10	J	111	GLU
10	J	113	ILE
10	J	119	TYR
10	J	146	ARG
10	J	151	ILE
11	L	9	ILE

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Mol	Chain	Res	Type
11	L	10	LEU
11	L	28	GLN
11	L	35	ARG
11	L	42	ARG
11	L	45	ARG
11	L	49	ARG
11	L	52	SER
11	L	59	VAL
11	L	61	CYS
11	L	64	VAL
11	L	65	ARG
11	L	67	HIS
11	L	79	GLU
11	L	92	ARG
11	L	94	ILE
11	L	99	ASP
11	L	104	ASN
11	L	111	GLN
11	L	115	GLN
11	L	121	ARG
11	L	123	LYS
11	L	130	LYS
11	L	162	LYS
11	L	165	LYS
11	L	186	ARG
11	L	190	ARG
12	M	4	ARG
12	M	8	GLU
12	M	25	VAL
12	M	29	ASP
12	M	33	GLN
12	M	37	LEU
12	M	38	VAL
12	M	46	ARG
12	M	53	LYS
12	M	57	LEU
12	M	61	ILE
12	M	96	GLU
12	M	119	ARG
12	M	130	LEU
13	N	5	LYS
13	N	26	ARG

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Mol	Chain	Res	Type
13	N	32	GLN
13	N	44	ARG
13	N	47	LYS
13	N	61	ILE
13	N	64	ILE
13	N	72	LYS
13	N	75	VAL
13	N	77	LYS
13	N	80	THR
13	N	87	HIS
13	N	89	VAL
13	N	92	LEU
13	N	108	ARG
13	N	142	ILE
13	N	151	ILE
13	N	174	LEU
13	N	188	ARG
13	N	198	LEU
13	N	199	GLN
13	N	202	ARG
14	O	5	GLN
14	O	9	LEU
14	O	27	VAL
14	O	31	ARG
14	O	36	VAL
14	O	37	ARG
14	O	42	ASN
14	O	44	SER
14	O	49	ARG
14	O	60	LYS
14	O	67	SER
14	O	82	ARG
14	O	85	ARG
14	O	103	LYS
14	O	116	LYS
14	O	119	VAL
14	O	128	ARG
14	O	129	LEU
14	O	130	LYS
14	O	144	GLU
14	O	145	VAL
14	O	153	THR

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Mol	Chain	Res	Type
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	187	LYS
14	O	195	VAL
14	O	202	LEU
15	P	7	ASP
15	P	10	ASN
15	P	12	THR
15	P	23	ARG
15	P	24	VAL
15	P	25	HIS
15	P	36	ILE
15	P	69	ARG
15	P	80	GLN
15	P	86	LYS
15	P	91	LEU
15	P	100	SER
15	P	103	GLU
15	P	105	LYS
15	P	118	GLN
15	P	127	ARG
15	P	128	ARG
15	P	140	MET
16	Q	3	VAL
16	Q	5	ILE
16	Q	9	LYS
16	Q	13	VAL
16	Q	29	VAL
16	Q	31	LEU
16	Q	38	ARG
16	Q	54	SER
16	Q	58	ARG
16	Q	63	LEU
16	Q	68	ARG
16	Q	83	VAL
16	Q	89	ASP
16	Q	91	ARG
16	Q	93	GLN
16	Q	95	VAL
16	Q	108	ARG
16	Q	111	SER

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Mol	Chain	Res	Type
16	Q	115	LYS
16	Q	126	LEU
16	Q	132	LYS
16	Q	143	ARG
16	Q	144	LYS
16	Q	167	VAL
17	R	10	LEU
17	R	34	ASN
17	R	39	GLN
17	R	40	GLN
17	R	43	LYS
17	R	50	ILE
17	R	52	ARG
17	R	64	ARG
17	R	74	ARG
17	R	81	ARG
17	R	89	MET
17	R	98	ARG
17	R	99	MET
17	R	103	ARG
17	R	106	LEU
17	R	107	ARG
17	R	113	LYS
17	R	122	SER
17	R	123	LEU
17	R	138	LEU
17	R	178	GLN
18	S	2	LYS
18	S	7	LEU
18	S	9	GLU
18	S	17	LEU
18	S	24	THR
18	S	39	VAL
18	S	43	ARG
18	S	67	VAL
18	S	70	LYS
18	S	75	VAL
18	S	83	ARG
18	S	84	TYR
18	S	85	ASP
18	S	100	LEU
18	S	102	THR

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Mol	Chain	Res	Type
18	S	124	ILE
18	S	127	MET
18	S	132	ILE
18	S	149	LYS
18	S	156	HIS
18	S	159	LEU
18	S	161	ARG
19	T	5	LYS
19	T	7	LYS
19	T	31	MET
19	T	33	ILE
19	T	36	LYS
19	T	45	MET
19	T	52	MET
19	T	60	LYS
19	T	74	ILE
19	T	80	VAL
19	T	81	LYS
19	T	88	ARG
19	T	94	GLU
19	T	96	ILE
19	T	97	LYS
19	T	99	SER
19	T	118	GLU
19	T	137	GLU
19	T	142	ARG
19	T	144	ASN
19	T	146	LYS
19	T	152	GLU
19	T	157	GLU
19	T	159	MET
20	U	23	LEU
20	U	33	ILE
20	U	62	THR
20	U	65	ARG
20	U	67	LYS
20	U	69	LYS
20	U	70	ILE
20	U	97	ARG
20	U	99	TRP
20	U	101	ARG
21	V	15	ARG

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Mol	Chain	Res	Type
21	V	18	LEU
21	V	27	ASN
21	V	35	LYS
21	V	51	ARG
21	V	57	VAL
21	V	60	MET
21	V	61	VAL
21	V	69	LYS
21	V	82	ILE
21	V	84	GLN
21	V	90	ARG
21	V	91	LYS
21	V	99	GLU
21	V	109	LYS
21	V	113	LYS
21	V	123	LYS
21	V	124	GLU
21	V	138	SER
22	W	4	GLU
22	W	19	ARG
22	W	27	LYS
22	W	43	LYS
22	W	44	ARG
22	W	50	ASN
23	X	39	LYS
23	X	41	ARG
23	X	50	LYS
23	X	52	LEU
23	X	53	ARG
23	X	59	LYS
23	X	62	ARG
23	X	63	LYS
23	X	91	GLU
23	X	94	ASN
23	X	111	GLN
23	X	127	LEU
23	X	129	ARG
23	X	145	ASP
23	X	152	LYS
24	Y	2	LYS
24	Y	7	VAL
24	Y	8	THR

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Mol	Chain	Res	Type
24	Y	12	SER
24	Y	28	LYS
24	Y	32	SER
24	Y	34	LEU
24	Y	52	ASP
24	Y	55	VAL
24	Y	59	ARG
24	Y	65	GLN
24	Y	72	GLN
24	Y	87	ARG
24	Y	104	VAL
24	Y	105	VAL
24	Y	107	THR
24	Y	115	ARG
24	Y	127	GLN
25	Z	3	LYS
25	Z	11	VAL
25	Z	21	ARG
25	Z	26	VAL
25	Z	42	LEU
25	Z	57	MET
25	Z	59	LYS
25	Z	60	LYS
25	Z	67	LYS
25	Z	68	ILE
25	Z	76	ASN
25	Z	78	ASN
25	Z	83	THR
25	Z	88	ASP
25	Z	93	LYS
25	Z	96	VAL
25	Z	97	ASN
25	Z	100	VAL
25	Z	121	ARG
25	Z	123	LYS
26	a	14	HIS
26	a	16	SER
26	a	39	HIS
26	a	40	HIS
26	a	59	ARG
26	a	64	LYS
26	a	82	VAL

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Mol	Chain	Res	Type
26	a	84	GLU
26	a	122	VAL
26	a	127	LYS
26	a	132	ARG
27	b	9	THR
27	b	21	ILE
27	b	22	LYS
27	b	36	ASP
27	b	40	LEU
27	b	43	MET
27	b	44	ARG
27	b	51	LYS
27	b	72	ILE
28	c	18	LEU
28	c	28	VAL
28	c	37	MET
28	c	40	GLN
28	c	50	ASN
28	c	61	GLU
28	c	81	LEU
28	c	87	LYS
28	c	90	ARG
28	c	91	VAL
28	c	92	CYS
28	c	93	THR
28	c	94	LEU
28	c	101	ASP
29	d	19	GLU
29	d	20	VAL
29	d	23	ARG
29	d	26	THR
29	d	33	ILE
29	d	44	ARG
29	d	46	LEU
29	d	48	GLU
29	d	56	GLU
29	d	72	VAL
29	d	75	LYS
29	d	78	ARG
29	d	79	ASN
29	d	85	ARG
29	d	88	LEU

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Mol	Chain	Res	Type
29	d	89	SER
29	d	90	ARG
29	d	94	GLU
29	d	102	LEU
29	d	119	THR
30	e	8	VAL
30	e	9	LYS
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	30	LYS
30	e	41	ILE
30	e	46	ARG
30	e	47	ARG
30	e	48	ARG
30	e	49	PHE
30	e	53	ILE
30	e	64	LYS
30	e	78	LEU
30	e	79	VAL
30	e	80	HIS
30	e	98	GLU
30	e	106	LYS
30	e	107	ASN
30	e	109	LYS
30	e	113	GLU
30	e	123	THR
30	e	129	LEU
31	f	33	VAL
31	f	36	ARG
31	f	40	GLU
31	f	46	ARG
31	f	52	LYS
31	f	64	PRO
31	f	69	VAL
31	f	84	VAL
31	f	100	ARG
31	f	101	ILE
31	f	103	VAL
31	f	109	ARG
31	f	110	ILE
32	g	2	VAL

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Mol	Chain	Res	Type
32	g	5	LEU
32	g	8	ARG
32	g	11	LEU
32	g	14	ASN
32	g	23	SER
32	g	32	TYR
32	g	43	LYS
32	g	60	ARG
32	g	64	LEU
32	g	65	MET
32	g	66	ARG
32	g	73	HIS
32	g	74	VAL
32	g	88	ARG
32	g	100	GLN
32	g	115	LYS
33	h	28	LEU
33	h	51	ARG
33	h	58	LEU
33	h	59	THR
33	h	65	GLN
33	h	67	GLU
33	h	69	LEU
33	h	88	THR
33	h	96	ASN
33	h	97	LYS
33	h	104	THR
33	h	116	LEU
33	h	119	TYR
33	h	122	LYS
34	i	3	LEU
34	i	7	MET
34	i	9	VAL
34	i	18	THR
34	i	33	LEU
34	i	34	THR
34	i	44	ILE
34	i	85	ARG
34	i	86	LYS
34	i	87	ARG
34	i	103	LYS
35	j	3	LYS

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Mol	Chain	Res	Type
35	j	6	SER
35	j	10	LYS
35	j	12	ARG
35	j	20	ARG
35	j	25	LYS
35	j	45	ARG
35	j	46	LYS
35	j	48	ASN
35	j	63	ARG
35	j	64	MET
35	j	68	LYS
35	j	73	ARG
36	k	27	LYS
36	k	31	ASN
36	k	46	VAL
36	k	57	LYS
36	k	69	LEU
36	k	70	LYS
37	l	3	SER
37	l	8	ARG
37	l	11	ARG
37	l	16	LYS
37	l	23	ILE
37	l	36	ARG
37	l	46	ARG
38	m	79	GLU
38	m	84	GLN
38	m	85	LEU
38	m	97	ARG
38	m	98	LYS
38	m	106	ARG
38	m	111	ARG
38	m	118	THR
38	m	119	ASN
39	n	9	ARG
40	o	2	VAL
40	o	17	LYS
40	o	19	GLN
40	o	28	LYS
40	o	33	LEU
40	o	36	GLN
40	o	43	ARG

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Mol	Chain	Res	Type
40	o	55	ILE
40	o	61	LYS
40	o	67	VAL
40	o	69	ARG
40	o	77	CYS
40	o	82	MET
40	o	89	LYS
40	o	93	LEU
40	o	102	GLN
41	p	3	LYS
41	p	38	THR
41	p	52	VAL
41	p	54	ILE
41	p	59	SER
41	p	60	CYS
41	p	70	THR
41	p	74	THR
41	p	84	ARG
42	r	14	SER
42	r	18	ILE
42	r	21	ASN
42	r	26	SER
42	r	28	GLU
42	r	31	ASN
42	r	32	LEU
42	r	35	ARG
42	r	36	ASN
42	r	39	ARG
42	r	48	THR
42	r	60	VAL
42	r	67	ARG
42	r	78	VAL
42	r	83	ASN
42	r	105	ASP
42	r	106	LEU
42	r	108	MET
42	r	115	SER
42	r	118	LEU
43	s	38	LYS
43	s	44	ARG
43	s	50	LYS
43	s	62	ARG

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Mol	Chain	Res	Type
43	s	77	LYS
43	s	94	ASP
43	s	107	VAL
43	s	146	LYS
43	s	174	LEU
43	s	185	PHE
43	s	191	GLN
44	t	16	ARG
44	t	40	LYS
44	t	104	ILE
44	t	106	PHE
44	t	114	ARG
44	t	124	GLU
45	1	60	THR
45	1	63	SER
52	AA	2	SER
52	AA	8	LEU
52	AA	9	GLN
52	AA	23	THR
52	AA	44	ASP
52	AA	46	ILE
52	AA	50	ASN
52	AA	53	ARG
52	AA	56	GLU
52	AA	58	LEU
52	AA	60	LEU
52	AA	69	GLU
52	AA	75	SER
52	AA	84	GLN
52	AA	89	LYS
52	AA	109	THR
52	AA	111	GLN
52	AA	113	GLN
52	AA	124	VAL
52	AA	131	HIS
52	AA	134	LEU
52	AA	138	SER
52	AA	141	ASN
52	AA	142	LEU
52	AA	147	LEU
52	AA	148	CYS
52	AA	155	ARG

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Mol	Chain	Res	Type
52	AA	158	ASP
52	AA	159	ILE
52	AA	192	GLU
52	AA	200	ASP
53	BB	27	LYS
53	BB	38	MET
53	BB	43	ASN
53	BB	55	THR
53	BB	66	VAL
53	BB	69	VAL
53	BB	82	ARG
53	BB	99	ASN
53	BB	105	LEU
53	BB	107	ARG
53	BB	112	SER
53	BB	134	LEU
53	BB	136	ARG
53	BB	137	LEU
53	BB	149	GLN
53	BB	150	ILE
53	BB	151	ARG
53	BB	157	GLN
53	BB	169	MET
53	BB	172	MET
53	BB	173	THR
53	BB	175	GLU
53	BB	184	VAL
53	BB	187	LYS
53	BB	189	ILE
53	BB	202	GLN
53	BB	206	PRO
53	BB	208	HIS
53	BB	220	LYS
53	BB	225	LEU
53	BB	228	LEU
54	CC	78	LEU
54	CC	114	LYS
54	CC	120	GLN
54	CC	121	ARG
54	CC	137	VAL
54	CC	157	LEU
54	CC	162	ILE

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Mol	Chain	Res	Type
54	CC	167	ARG
54	CC	174	ILE
54	CC	176	LYS
54	CC	202	THR
54	CC	208	PRO
54	CC	227	TRP
54	CC	230	THR
54	CC	233	LEU
54	CC	249	SER
54	CC	251	LEU
54	CC	271	ASP
54	CC	275	LYS
55	DD	9	ARG
55	DD	14	ASP
55	DD	22	ASN
55	DD	25	LEU
55	DD	28	GLU
55	DD	31	GLU
55	DD	32	ASP
55	DD	42	THR
55	DD	55	THR
55	DD	58	VAL
55	DD	59	LEU
55	DD	64	ARG
55	DD	72	VAL
55	DD	110	LEU
55	DD	117	ARG
55	DD	119	CYS
55	DD	122	VAL
55	DD	127	MET
55	DD	134	CYS
55	DD	135	GLU
55	DD	142	LEU
55	DD	148	LYS
55	DD	149	SER
55	DD	154	ASP
55	DD	156	LEU
55	DD	167	TYR
55	DD	170	THR
55	DD	176	LEU
55	DD	182	LEU
55	DD	190	LEU

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Mol	Chain	Res	Type
55	DD	198	ILE
55	DD	204	LEU
55	DD	206	ASP
55	DD	212	GLU
55	DD	221	THR
55	DD	225	GLU
56	EE	3	ARG
56	EE	12	VAL
56	EE	17	HIS
56	EE	19	MET
56	EE	21	ASP
56	EE	24	THR
56	EE	32	SER
56	EE	38	LEU
56	EE	42	LEU
56	EE	48	LEU
56	EE	65	CYS
56	EE	66	MET
56	EE	67	GLN
56	EE	75	LYS
56	EE	95	THR
56	EE	98	ASN
56	EE	123	LEU
56	EE	130	PHE
56	EE	145	ARG
56	EE	148	ARG
56	EE	153	LEU
56	EE	155	LYS
56	EE	160	ILE
56	EE	171	ASP
56	EE	174	LYS
56	EE	180	LEU
56	EE	181	CYS
56	EE	205	PHE
56	EE	207	VAL
56	EE	220	THR
56	EE	227	VAL
56	EE	240	ARG
56	EE	245	ARG
56	EE	259	LYS
57	FF	29	GLN
57	FF	37	ASP

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Mol	Chain	Res	Type
57	FF	63	LYS
57	FF	68	ILE
57	FF	72	LEU
57	FF	81	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	106	GLU
57	FF	113	VAL
57	FF	116	ILE
57	FF	125	SER
57	FF	126	THR
57	FF	130	ARG
57	FF	136	ARG
57	FF	140	ASP
57	FF	141	VAL
57	FF	152	TRP
57	FF	156	THR
57	FF	164	ARG
57	FF	169	ILE
57	FF	173	LEU
57	FF	187	SER
57	FF	190	ILE
57	FF	192	LYS
57	FF	194	ASP
57	FF	197	GLU
57	FF	203	ASN
57	FF	204	ARG
58	GG	15	LEU
58	GG	26	THR
58	GG	30	LYS
58	GG	41	LEU
58	GG	56	ASN
58	GG	63	MET
58	GG	64	LYS
58	GG	68	LEU
58	GG	76	LEU
58	GG	88	ARG
58	GG	100	CYS
58	GG	120	ASP
58	GG	121	ILE
58	GG	136	LYS
58	GG	137	ARG

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Mol	Chain	Res	Type
58	GG	143	LYS
58	GG	151	ASP
58	GG	164	LYS
58	GG	178	ARG
58	GG	181	THR
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	196	LYS
58	GG	208	GLU
58	GG	213	LEU
58	GG	224	ARG
58	GG	227	GLN
58	GG	235	SER
59	HH	34	SER
59	HH	35	ASP
59	HH	36	LEU
59	HH	40	LEU
59	HH	69	LEU
59	HH	74	LYS
59	HH	82	GLU
59	HH	83	LEU
59	HH	93	VAL
59	HH	95	ILE
59	HH	106	ARG
59	HH	119	SER
59	HH	121	THR
59	HH	145	ARG
59	HH	160	LYS
59	HH	162	GLN
59	HH	188	GLU
60	II	6	ASP
60	II	7	ASN
60	II	10	LYS
60	II	23	LYS
60	II	26	LYS
60	II	29	LEU
60	II	56	ARG
60	II	60	LEU
60	II	70	GLU
60	II	74	ARG
60	II	75	LYS

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Mol	Chain	Res	Type
60	II	79	ILE
60	II	82	VAL
60	II	88	ASN
60	II	97	VAL
60	II	99	ASN
60	II	110	ARG
60	II	128	LYS
60	II	130	THR
60	II	133	GLU
60	II	140	LYS
60	II	165	GLN
60	II	168	GLN
60	II	172	LEU
60	II	175	ILE
60	II	177	SER
60	II	181	GLN
60	II	190	LEU
60	II	196	GLU
60	II	203	LYS
60	II	206	LYS
61	JJ	3	VAL
61	JJ	24	ARG
61	JJ	29	LEU
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	61	LEU
61	JJ	65	GLU
61	JJ	67	ASP
61	JJ	69	ARG
61	JJ	80	ARG
61	JJ	87	LEU
61	JJ	89	GLU
61	JJ	101	LYS
61	JJ	109	ARG
61	JJ	110	LEU
61	JJ	111	GLN
61	JJ	116	LYS
61	JJ	119	LEU
61	JJ	127	ARG
61	JJ	131	ARG
61	JJ	135	ILE
61	JJ	138	ARG

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Mol	Chain	Res	Type
61	JJ	139	LYS
61	JJ	152	ASP
61	JJ	169	ARG
61	JJ	174	LYS
62	KK	1	MET
62	KK	2	LEU
62	KK	3	MET
62	KK	13	GLU
62	KK	42	ASN
62	KK	43	LEU
62	KK	49	MET
62	KK	50	GLN
62	KK	60	GLU
62	KK	65	ARG
62	KK	66	HIS
62	KK	70	TYR
62	KK	72	THR
62	KK	81	ASP
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	42	LEU
63	LL	48	LYS
63	LL	56	ILE
63	LL	65	ASN
63	LL	66	VAL
63	LL	69	ARG
63	LL	72	ILE
63	LL	74	SER
63	LL	78	THR
63	LL	82	MET
63	LL	85	THR
63	LL	88	ILE
63	LL	91	ASP
63	LL	96	ILE
63	LL	103	GLU
63	LL	121	GLN
63	LL	122	ILE

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Mol	Chain	Res	Type
63	LL	127	THR
63	LL	134	LEU
64	MM	27	ILE
64	MM	31	LEU
64	MM	33	ARG
64	MM	35	ILE
64	MM	42	LEU
64	MM	45	ARG
64	MM	48	HIS
64	MM	74	ILE
64	MM	77	ILE
64	MM	78	LYS
64	MM	79	VAL
64	MM	88	TRP
64	MM	114	TYR
64	MM	127	TYR
65	NN	9	LYS
65	NN	12	SER
65	NN	13	GLN
65	NN	16	LEU
65	NN	25	TRP
65	NN	27	LYS
65	NN	52	VAL
65	NN	55	ARG
65	NN	57	SER
65	NN	60	VAL
65	NN	64	ARG
65	NN	70	LYS
65	NN	75	LEU
65	NN	78	LYS
65	NN	80	LEU
65	NN	84	LEU
65	NN	87	ASP
65	NN	91	LEU
65	NN	101	HIS
65	NN	102	LEU
65	NN	103	GLU
65	NN	107	LYS
65	NN	114	ARG
65	NN	120	SER
65	NN	134	VAL
65	NN	149	LEU

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Mol	Chain	Res	Type
66	OO	31	CYS
66	OO	46	ASP
66	OO	50	LYS
66	OO	51	GLU
66	OO	61	LYS
66	OO	65	ASP
66	OO	67	ASP
66	OO	69	SER
66	OO	70	SER
66	OO	80	ASP
66	OO	100	THR
66	OO	106	LYS
66	OO	116	LEU
66	OO	121	ARG
66	OO	122	SER
66	OO	128	ARG
66	OO	146	ARG
66	OO	151	LEU
67	PP	5	GLU
67	PP	6	GLN
67	PP	7	LYS
67	PP	10	ARG
67	PP	21	ASP
67	PP	28	MET
67	PP	29	SER
67	PP	37	TYR
67	PP	42	ARG
67	PP	43	ARG
67	PP	45	LEU
67	PP	47	ARG
67	PP	52	LYS
67	PP	64	LYS
67	PP	100	LYS
67	PP	101	THR
67	PP	104	GLN
67	PP	121	ILE
68	QQ	25	CYS
68	QQ	26	LYS
68	QQ	27	ARG
68	QQ	32	ILE
68	QQ	41	MET
68	QQ	47	LEU

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Mol	Chain	Res	Type
68	QQ	69	ARG
68	QQ	72	VAL
68	QQ	73	LYS
68	QQ	84	ILE
68	QQ	85	ARG
68	QQ	90	LYS
68	QQ	119	LEU
68	QQ	120	LEU
68	QQ	126	ARG
68	QQ	140	ARG
68	QQ	146	ARG
69	RR	5	ARG
69	RR	6	THR
69	RR	14	ARG
69	RR	31	ASN
69	RR	49	LYS
69	RR	55	THR
69	RR	58	MET
69	RR	77	GLU
69	RR	78	ARG
69	RR	82	ASP
69	RR	88	VAL
69	RR	91	LEU
69	RR	98	VAL
69	RR	99	ASP
69	RR	105	MET
69	RR	109	LEU
69	RR	121	GLN
69	RR	123	THR
69	RR	126	MET
69	RR	127	ASN
70	SS	7	GLU
70	SS	8	LYS
70	SS	10	GLN
70	SS	13	LEU
70	SS	17	ASN
70	SS	20	ILE
70	SS	21	ASP
70	SS	34	LYS
70	SS	52	LEU
70	SS	59	LEU
70	SS	63	GLU

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Mol	Chain	Res	Type
70	SS	64	VAL
70	SS	72	GLN
70	SS	78	LYS
70	SS	82	TRP
70	SS	86	ARG
70	SS	96	SER
70	SS	99	LEU
70	SS	118	ARG
70	SS	131	VAL
70	SS	134	GLN
70	SS	136	THR
71	TT	6	VAL
71	TT	8	ASP
71	TT	10	ASN
71	TT	16	ARG
71	TT	23	LYS
71	TT	28	LEU
71	TT	41	LYS
71	TT	50	GLU
71	TT	56	ARG
71	TT	62	ARG
71	TT	67	ARG
71	TT	74	SER
71	TT	84	ARG
71	TT	87	VAL
71	TT	93	SER
71	TT	103	VAL
71	TT	118	ASP
71	TT	123	LEU
71	TT	124	THR
71	TT	128	GLN
71	TT	131	LEU
72	UU	29	VAL
72	UU	31	SER
72	UU	39	LEU
72	UU	47	ASN
72	UU	48	LEU
72	UU	49	LYS
72	UU	56	MET
72	UU	68	THR
72	UU	76	THR
72	UU	82	MET

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Mol	Chain	Res	Type
72	UU	88	LEU
72	UU	93	SER
73	VV	9	VAL
73	VV	21	ASN
73	VV	40	ASP
73	VV	45	ARG
73	VV	51	LYS
73	VV	62	MET
73	VV	66	ASP
73	VV	69	ILE
73	VV	70	LEU
73	VV	74	LYS
74	WW	3	ARG
74	WW	14	ILE
74	WW	23	ARG
74	WW	31	SER
74	WW	40	VAL
74	WW	51	GLU
74	WW	52	ILE
74	WW	56	HIS
74	WW	78	ARG
74	WW	80	ASP
74	WW	84	LYS
74	WW	87	GLU
74	WW	98	GLN
74	WW	103	VAL
74	WW	104	LEU
75	XX	3	LYS
75	XX	5	ARG
75	XX	14	ARG
75	XX	19	ASP
75	XX	29	LYS
75	XX	37	LYS
75	XX	45	SER
75	XX	55	VAL
75	XX	61	GLN
75	XX	64	SER
75	XX	67	ARG
75	XX	68	LYS
75	XX	70	VAL
75	XX	90	CYS
75	XX	99	GLU

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Mol	Chain	Res	Type
75	XX	115	ILE
75	XX	119	ARG
75	XX	123	VAL
75	XX	128	VAL
75	XX	129	SER
76	YY	6	THR
76	YY	7	ILE
76	YY	8	ARG
76	YY	14	THR
76	YY	16	ARG
76	YY	20	ARG
76	YY	22	GLN
76	YY	32	LYS
76	YY	40	ILE
76	YY	46	LYS
76	YY	61	ARG
76	YY	69	THR
76	YY	72	PHE
76	YY	85	ASN
76	YY	93	ARG
76	YY	96	LEU
76	YY	98	GLU
76	YY	99	LYS
76	YY	100	LYS
76	YY	107	ARG
76	YY	111	LYS
76	YY	112	ASN
77	ZZ	44	LEU
77	ZZ	52	LYS
77	ZZ	67	LEU
77	ZZ	73	VAL
77	ZZ	76	ARG
77	ZZ	79	ILE
77	ZZ	83	LEU
77	ZZ	89	GLN
77	ZZ	92	LEU
77	ZZ	110	THR
77	ZZ	114	LYS
78	aa	2	THR
78	aa	10	ARG
78	aa	12	LYS
78	aa	19	GLN

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Mol	Chain	Res	Type
78	aa	21	ILE
78	aa	26	CYS
78	aa	38	LYS
78	aa	41	ILE
78	aa	44	ILE
78	aa	51	ARG
78	aa	95	ARG
79	bb	27	SER
79	bb	36	LYS
79	bb	37	CYS
79	bb	40	CYS
79	bb	44	THR
79	bb	72	ARG
79	bb	81	ARG
79	bb	83	GLN
79	bb	84	HIS
80	cc	20	LYS
80	cc	24	GLN
80	cc	26	GLN
80	cc	28	THR
80	cc	31	ARG
80	cc	34	PHE
80	cc	42	THR
80	cc	44	ARG
80	cc	56	LEU
80	cc	58	LEU
80	cc	60	GLU
80	cc	61	SER
80	cc	67	ARG
80	cc	68	LEU
81	dd	4	GLN
81	dd	5	GLN
81	dd	12	ARG
81	dd	14	PHE
81	dd	16	GLN
81	dd	26	ASN
81	dd	27	ARG
81	dd	39	CYS
81	dd	48	LYS
81	dd	49	ASP
81	dd	54	LYS
81	dd	56	ASP

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Mol	Chain	Res	Type
82	ee	15	GLN
82	ee	24	LYS
82	ee	26	LYS
82	ee	40	ARG
82	ee	52	LYS
82	ee	58	ASN
83	ff	81	THR
83	ff	130	HIS
84	gg	7	LEU
84	gg	17	TRP
84	gg	36	ARG
84	gg	47	ARG
84	gg	49	GLU
84	gg	59	LEU
84	gg	64	HIS
84	gg	79	LEU
84	gg	93	THR
84	gg	100	ARG
84	gg	115	SER
84	gg	119	GLN
84	gg	121	VAL
84	gg	131	LEU
84	gg	143	GLN
84	gg	165	ILE
84	gg	172	LYS
84	gg	173	LEU
84	gg	186	THR
84	gg	230	LEU
84	gg	261	LEU
84	gg	289	LEU
84	gg	298	LEU
84	gg	306	LEU
84	gg	309	VAL
86	ii	36	SER
86	ii	37	LEU
86	ii	44	GLN
86	ii	45	ILE
86	ii	58	THR
86	ii	60	SER
86	ii	61	ASN
86	ii	63	LYS
86	ii	65	ARG

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Mol	Chain	Res	Type
86	ii	69	LEU
86	ii	86	ASN
86	ii	103	GLU
86	ii	111	ASN
86	ii	120	ILE
86	ii	124	LEU
86	ii	152	ASP
86	ii	160	THR
86	ii	162	GLN
86	ii	179	LYS
86	ii	180	HIS
86	ii	182	ARG
86	ii	186	SER
86	ii	188	LEU
86	ii	189	ARG
86	ii	198	ARG
86	ii	211	GLN
86	ii	212	LEU
86	ii	214	ILE
86	ii	232	PHE
86	ii	241	MET
86	ii	246	LEU
86	ii	252	LYS
86	ii	265	ASN
86	ii	275	LEU
86	ii	292	ASP
86	ii	297	ASP
86	ii	300	LYS
86	ii	327	ASP
86	ii	340	GLU
86	ii	352	LYS
86	ii	361	GLU
86	ii	368	LEU
86	ii	375	LEU
86	ii	401	GLN
87	jj	40	GLU
87	jj	51	SER
87	jj	75	LEU
87	jj	78	ASN
87	jj	111	THR
87	jj	131	LEU
87	jj	153	GLN

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Mol	Chain	Res	Type
87	jj	154	ASN
87	jj	159	ILE
87	jj	161	GLU
87	jj	221	GLU
87	jj	222	LEU
87	jj	239	MET
87	jj	248	ASP
87	jj	253	LEU
87	jj	271	VAL
87	jj	282	LEU
87	jj	284	ASP
87	jj	289	LEU
87	jj	301	MET
87	jj	314	ASP
87	jj	320	GLU
87	jj	380	GLU
87	jj	409	VAL
87	jj	410	SER
87	jj	411	TYR
87	jj	416	ILE
87	jj	427	LEU
87	jj	455	ILE
87	jj	472	LEU
87	jj	534	VAL
87	jj	549	GLN
87	jj	552	LEU
87	jj	567	ARG
87	jj	574	ARG
87	jj	577	ILE
87	jj	578	ASN
87	jj	584	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	205	ASN
2	B	25	HIS
2	B	276	HIS
2	B	328	ASN
3	C	41	HIS
3	C	89	GLN

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Mol	Chain	Res	Type
3	C	112	HIS
3	C	329	ASN
4	D	157	ASN
4	D	175	HIS
5	E	39	HIS
5	E	153	HIS
5	E	178	ASN
5	E	217	GLN
5	E	246	GLN
5	E	252	GLN
5	E	264	GLN
5	E	280	HIS
6	F	41	GLN
6	F	118	GLN
6	F	121	ASN
7	G	43	GLN
7	G	66	GLN
7	G	153	GLN
7	G	240	ASN
8	H	102	ASN
8	H	106	GLN
9	I	123	GLN
9	I	144	ASN
10	J	112	HIS
11	L	175	ASN
13	N	15	GLN
13	N	57	GLN
14	O	46	ASN
15	P	56	GLN
15	P	75	GLN
15	P	137	ASN
17	R	141	HIS
18	S	50	GLN
18	S	66	GLN
19	T	79	GLN
21	V	27	ASN
23	X	108	GLN
24	Y	56	GLN
24	Y	96	HIS
25	Z	127	ASN
26	a	60	HIS
27	b	17	HIS

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Mol	Chain	Res	Type
28	c	15	ASN
30	e	24	GLN
30	e	63	ASN
31	f	21	GLN
33	h	20	GLN
36	k	31	ASN
40	o	25	GLN
41	p	56	HIS
42	r	21	ASN
42	r	83	ASN
43	s	105	ASN
43	s	126	GLN
43	s	200	ASN
44	t	65	GLN
44	t	70	GLN
44	t	156	ASN
52	AA	33	GLN
53	BB	124	HIS
53	BB	163	GLN
54	CC	172	ASN
54	CC	267	GLN
55	DD	145	GLN
55	DD	165	ASN
56	EE	17	HIS
56	EE	67	GLN
56	EE	157	ASN
56	EE	161	GLN
57	FF	95	HIS
58	GG	65	GLN
58	GG	70	HIS
59	HH	76	GLN
59	HH	97	GLN
59	HH	114	GLN
59	HH	193	GLN
60	II	88	ASN
61	JJ	27	GLN
62	KK	32	HIS
62	KK	50	GLN
63	LL	19	ASN
63	LL	39	ASN
63	LL	65	ASN
63	LL	121	GLN

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Mol	Chain	Res	Type
64	MM	28	HIS
64	MM	55	ASN
64	MM	82	ASN
65	NN	13	GLN
65	NN	69	ASN
66	OO	94	HIS
68	QQ	114	GLN
69	RR	118	GLN
70	SS	19	ASN
70	SS	134	GLN
71	TT	63	HIS
72	UU	81	GLN
73	VV	49	GLN
73	VV	81	GLN
74	WW	56	HIS
74	WW	82	GLN
74	WW	90	GLN
74	WW	98	GLN
75	XX	46	HIS
75	XX	73	GLN
78	aa	8	ASN
78	aa	19	GLN
78	aa	72	HIS
79	bb	26	GLN
79	bb	29	ASN
82	ee	44	ASN
84	gg	64	HIS
84	gg	117	ASN
84	gg	178	ASN
84	gg	237	ASN
84	gg	285	GLN
86	ii	11	ASN
86	ii	350	GLN
86	ii	380	ASN
86	ii	420	GLN
87	jj	153	GLN
87	jj	233	GLN
87	jj	468	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	24 (32%)	0
47	3	72/75 (96%)	29 (40%)	6 (8%)
48	5	3650/3662 (99%)	1260 (34%)	291 (7%)
49	7	120/120 (100%)	25 (20%)	2 (1%)
50	8	155/156 (99%)	49 (31%)	6 (3%)
51	9	1712/1719 (99%)	623 (36%)	115 (6%)
85	hh	11/12 (91%)	6 (54%)	0
All	All	5794/5820 (99%)	2016 (34%)	420 (7%)

All (2016) 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	14	A
46	2	16	C
46	2	19	G
46	2	20	U
46	2	20(A)	U
46	2	21	A
46	2	31	C
46	2	35	A
46	2	42	A
46	2	46	G
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	73	A
46	2	75	C
46	2	76	A
47	3	9	A
47	3	13	C
47	3	21	A
47	3	26	A
47	3	29	A
47	3	30	G
47	3	31	A

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Mol	Chain	Res	Type
47	3	34	U
47	3	35	U
47	3	39	U
47	3	40	C
47	3	41	U
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	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	12	A
48	5	13	U
48	5	17	A
48	5	20	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
48	5	59	A
48	5	64	A
48	5	65	A

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Mol	Chain	Res	Type
48	5	71	C
48	5	72	C
48	5	73	A
48	5	74	G
48	5	75	G
48	5	91	G
48	5	93	G
48	5	94	A
48	5	96	U
48	5	104	G
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	122	U
48	5	125	C
48	5	126	C
48	5	128	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	137	G
48	5	143	C
48	5	144	G
48	5	145	G
48	5	146	G
48	5	152	U
48	5	157	U
48	5	158	A
48	5	159	C
48	5	160	G
48	5	161	G
48	5	164	G
48	5	166	C
48	5	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	200	U
48	5	201	C
48	5	202	C
48	5	203	U
48	5	205	C
48	5	209	U
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	225	G
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	235	A
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	275	C
48	5	276	C
48	5	277	G
48	5	278	G
48	5	280	G
48	5	292	G
48	5	294	G
48	5	295	A

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Mol	Chain	Res	Type
48	5	296	A
48	5	297	U
48	5	300	A
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	322	C
48	5	325	U
48	5	328	A
48	5	330	G
48	5	331	G
48	5	334	A
48	5	336	A
48	5	340	C
48	5	345	C
48	5	349	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	363	A
48	5	365	U
48	5	379	G
48	5	385	A
48	5	386	A
48	5	387	G
48	5	388	A
48	5	399	G
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	422	C
48	5	423	G
48	5	429	A
48	5	431	G
48	5	432	U
48	5	440	U
48	5	446	C

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Mol	Chain	Res	Type
48	5	449	C
48	5	451	C
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	458	C
48	5	465	G
48	5	467	U
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	491	G
48	5	498	C
48	5	499	G
48	5	500	G
48	5	502	C
48	5	503	C
48	5	504	G
48	5	506	C
48	5	509	A
48	5	510	U
48	5	513	U
48	5	514	U
48	5	515	C
48	5	519	C
48	5	643	C
48	5	647	G
48	5	649	A
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

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Mol	Chain	Res	Type
48	5	685	C
48	5	686	A
48	5	689	U
48	5	690	C
48	5	694	C
48	5	695	G
48	5	696	C
48	5	697	G
48	5	701	G
48	5	703	G
48	5	707	C
48	5	716	C
48	5	718	C
48	5	722	G
48	5	728	U
48	5	729	G
48	5	730	G
48	5	737	C
48	5	742	G
48	5	744	G
48	5	745	G
48	5	746	A
48	5	747	A
48	5	748	G
48	5	749	G
48	5	911	U
48	5	914	U
48	5	915	A
48	5	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

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Mol	Chain	Res	Type
48	5	936	C
48	5	937	U
48	5	938	C
48	5	939	G
48	5	940	C
48	5	942	G
48	5	943	A
48	5	944	A
48	5	945	U
48	5	946	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	995	C
48	5	1051	G
48	5	1070	G
48	5	1072	C
48	5	1075	G
48	5	1076	C

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Mol	Chain	Res	Type
48	5	1083	U
48	5	1097	C
48	5	1173	G
48	5	1175	A
48	5	1176	C
48	5	1177	U
48	5	1181	C
48	5	1182	C
48	5	1183	C
48	5	1193	C
48	5	1204	C
48	5	1208	G
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	1267	C
48	5	1268	G
48	5	1269	G
48	5	1270	A
48	5	1272	C
48	5	1273	G

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Mol	Chain	Res	Type
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1278	C
48	5	1279	A
48	5	1280	C
48	5	1285	U
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	1314	C
48	5	1316	G
48	5	1320	U
48	5	1324	A
48	5	1325	C
48	5	1326	A
48	5	1329	G
48	5	1330	A
48	5	1337	A
48	5	1354	A
48	5	1355	G
48	5	1358	G
48	5	1359	G
48	5	1364	U
48	5	1365	C
48	5	1366	G
48	5	1367	C
48	5	1369	C
48	5	1370	G
48	5	1371	A
48	5	1372	A
48	5	1376	C
48	5	1377	G

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Mol	Chain	Res	Type
48	5	1378	C
48	5	1379	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1388	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1399	G
48	5	1407	C
48	5	1408	G
48	5	1409	C
48	5	1410	U
48	5	1411	C
48	5	1413	C
48	5	1414	C
48	5	1416	G
48	5	1418	C
48	5	1420	A
48	5	1421	G
48	5	1426	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	1465	G
48	5	1467	C
48	5	1469	C
48	5	1475	G
48	5	1477	C
48	5	1478	C
48	5	1482	G

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Mol	Chain	Res	Type
48	5	1483	C
48	5	1484	G
48	5	1486	C
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1503	A
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1523	A
48	5	1524	A
48	5	1531	U
48	5	1533	A
48	5	1534	A
48	5	1538	U
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1575	A
48	5	1578	U
48	5	1583	A
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1598	C
48	5	1601	A
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1616	U
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1632	A
48	5	1633	G
48	5	1634	A
48	5	1638	A
48	5	1640	C
48	5	1641	G

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Mol	Chain	Res	Type
48	5	1654	G
48	5	1656	U
48	5	1658	G
48	5	1661	C
48	5	1670	G
48	5	1671	U
48	5	1676	C
48	5	1677	U
48	5	1678	C
48	5	1679	A
48	5	1680	G
48	5	1692	C
48	5	1696	C
48	5	1697	G
48	5	1698	C
48	5	1699	A
48	5	1719	A
48	5	1720	C
48	5	1721	G
48	5	1723	A
48	5	1724	G
48	5	1725	U
48	5	1733	G
48	5	1734	G
48	5	1741	G
48	5	1742	A
48	5	1745	G
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

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Mol	Chain	Res	Type
48	5	1781	U
48	5	1785	C
48	5	1787	A
48	5	1800	U
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1812	C
48	5	1818	G
48	5	1819	G
48	5	1820	C
48	5	1821	G
48	5	1822	U
48	5	1827	C
48	5	1828	C
48	5	1830	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1840	G
48	5	1842	G
48	5	1848	C
48	5	1854	G
48	5	1855	G
48	5	1867	A
48	5	1869	G
48	5	1873	A
48	5	1882	U
48	5	1885	G
48	5	1889	U
48	5	1891	A
48	5	1892	A
48	5	1894	C
48	5	1897	A
48	5	1898	C
48	5	1899	G
48	5	1900	C
48	5	1910	G
48	5	1917	A
48	5	1918	U
48	5	1919	G

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Mol	Chain	Res	Type
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1929	A
48	5	1931	C
48	5	1939	A
48	5	1947	U
48	5	1948	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	1962	A
48	5	1963	C
48	5	1964	A
48	5	1968	G
48	5	1969	G
48	5	1972	G
48	5	1975	G
48	5	1976	G
48	5	1980	U
48	5	1981	G
48	5	1983	A
48	5	1984	A
48	5	1985	G
48	5	1986	U
48	5	1987	C
48	5	1988	G
48	5	1990	A
48	5	1991	A
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

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Mol	Chain	Res	Type
48	5	2008	U
48	5	2011	C
48	5	2018	C
48	5	2019	C
48	5	2020	U
48	5	2023	C
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2028	C
48	5	2040	A
48	5	2041	A
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2058	G
48	5	2062	C
48	5	2063	G
48	5	2064	G
48	5	2068	C
48	5	2069	A
48	5	2070	U
48	5	2071	A
48	5	2072	C
48	5	2079	G
48	5	2084	C
48	5	2087	C
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	2105	A
48	5	2107	C

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Mol	Chain	Res	Type
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	2244	C
48	5	2247	C
48	5	2248	C
48	5	2250	C
48	5	2251	G
48	5	2252	G
48	5	2253	A
48	5	2254	G
48	5	2255	C
48	5	2256	C
48	5	2257	C
48	5	2258	C
48	5	2259	G
48	5	2260	C
48	5	2261	G
48	5	2262	G
48	5	2263	A
48	5	2264	C
48	5	2265	G
48	5	2266	C

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Mol	Chain	Res	Type
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2275	G
48	5	2277	C
48	5	2279	A
48	5	2288	G
48	5	2289	C
48	5	2295	C
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2332	A
48	5	2333	G
48	5	2335	C
48	5	2344	U
48	5	2348	G
48	5	2351	C
48	5	2360	A
48	5	2364	G
48	5	2370	A
48	5	2371	U
48	5	2374	A
48	5	2391	G
48	5	2395	A
48	5	2396	A
48	5	2397	G
48	5	2399	G
48	5	2401	A
48	5	2416	G
48	5	2417	A
48	5	2421	G
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	2437	C
48	5	2440	U

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Mol	Chain	Res	Type
48	5	2441	C
48	5	2443	G
48	5	2447	U
48	5	2450	G
48	5	2467	U
48	5	2468	U
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	2502	G
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2507	A
48	5	2511	A
48	5	2512	A
48	5	2513	A
48	5	2514	G
48	5	2530	U
48	5	2537	A
48	5	2544	G
48	5	2546	G
48	5	2547	G
48	5	2549	G
48	5	2553	A
48	5	2554	U
48	5	2555	G
48	5	2557	G
48	5	2558	C
48	5	2564	G
48	5	2566	G
48	5	2572	C

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Mol	Chain	Res	Type
48	5	2575	U
48	5	2576	G
48	5	2583	C
48	5	2586	G
48	5	2587	A
48	5	2588	C
48	5	2589	C
48	5	2601	A
48	5	2602	G
48	5	2611	A
48	5	2612	G
48	5	2620	G
48	5	2622	G
48	5	2623	A
48	5	2624	G
48	5	2627	C
48	5	2638	G
48	5	2639	U
48	5	2640	G
48	5	2649	G
48	5	2658	G
48	5	2661	U
48	5	2662	G
48	5	2669	C
48	5	2670	C
48	5	2676	A
48	5	2686	G
48	5	2687	U
48	5	2688	G
48	5	2689	C
48	5	2694	G
48	5	2695	A
48	5	2696	A
48	5	2697	A
48	5	2708	U
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2721	G
48	5	2723	U

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Mol	Chain	Res	Type
48	5	2725	A
48	5	2726	G
48	5	2733	C
48	5	2735	G
48	5	2740	U
48	5	2742	G
48	5	2743	A
48	5	2744	A
48	5	2754	G
48	5	2755	A
48	5	2756	G
48	5	2757	A
48	5	2760	G
48	5	2761	U
48	5	2762	G
48	5	2763	U
48	5	2767	U
48	5	2768	C
48	5	2769	U
48	5	2770	C
48	5	2772	C
48	5	2778	G
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	2802	C
48	5	2806	A
48	5	2807	A
48	5	2808	G
48	5	2815	A
48	5	2820	C
48	5	2825	A
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2838	G

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Mol	Chain	Res	Type
48	5	2839	U
48	5	2842	G
48	5	2844	A
48	5	2846	G
48	5	2850	A
48	5	2855	G
48	5	2858	A
48	5	2859	G
48	5	2862	G
48	5	2874	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	3609	G
48	5	3615	G
48	5	3616	U
48	5	3617	G
48	5	3620	G
48	5	3625	G
48	5	3626	G
48	5	3628	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3659	G
48	5	3660	C
48	5	3662	A
48	5	3664	G
48	5	3668	C
48	5	3670	C
48	5	3671	G
48	5	3673	C

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Mol	Chain	Res	Type
48	5	3674	G
48	5	3680	U
48	5	3681	G
48	5	3682	A
48	5	3692	A
48	5	3696	C
48	5	3698	G
48	5	3709	U
48	5	3710	G
48	5	3711	A
48	5	3712	A
48	5	3713	U
48	5	3717	A
48	5	3718	A
48	5	3719	A
48	5	3729	U
48	5	3736	A
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	3761	C
48	5	3762	U
48	5	3764	U
48	5	3765	G
48	5	3766	A
48	5	3770	U
48	5	3773	U
48	5	3774	A
48	5	3775	A
48	5	3776	G
48	5	3777	G
48	5	3784	A
48	5	3786	U
48	5	3798	U
48	5	3799	A
48	5	3802	U
48	5	3810	C

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Mol	Chain	Res	Type
48	5	3811	G
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3828	A
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3842	C
48	5	3843	C
48	5	3859	G
48	5	3867	A
48	5	3871	A
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3881	G
48	5	3882	C
48	5	3889	G
48	5	3890	A
48	5	3892	U
48	5	3897	G
48	5	3898	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	3914	U
48	5	3915	U
48	5	3916	G
48	5	3917	A
48	5	3918	G
48	5	3925	U
48	5	3926	C
48	5	3927	U
48	5	3938	G
48	5	3939	G

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Mol	Chain	Res	Type
48	5	3943	A
48	5	3946	G
48	5	4069	U
48	5	4070	U
48	5	4073	A
48	5	4076	G
48	5	4077	A
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4091	G
48	5	4092	G
48	5	4093	G
48	5	4094	G
48	5	4097	G
48	5	4104	G
48	5	4105	A
48	5	4107	G
48	5	4110	C
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	4161	G
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4166	G
48	5	4170	A

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Mol	Chain	Res	Type
48	5	4171	C
48	5	4173	G
48	5	4182	G
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4197	G
48	5	4203	A
48	5	4205	A
48	5	4212	A
48	5	4213	A
48	5	4214	A
48	5	4218	U
48	5	4219	A
48	5	4225	G
48	5	4226	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4235	G
48	5	4237	C
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	4276	G
48	5	4279	A
48	5	4286	C
48	5	4291	G
48	5	4292	A
48	5	4296	U
48	5	4297	G
48	5	4302	U
48	5	4303	C
48	5	4304	A
48	5	4305	G

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Mol	Chain	Res	Type
48	5	4306	U
48	5	4312	U
48	5	4314	C
48	5	4317	A
48	5	4329	G
48	5	4330	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	4368	G
48	5	4371	G
48	5	4372	U
48	5	4373	G
48	5	4376	A
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4381	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	4404	U
48	5	4405	G
48	5	4419	U
48	5	4420	U
48	5	4421	C
48	5	4422	A
48	5	4424	A
48	5	4426	C
48	5	4433	G
48	5	4437	U
48	5	4438	U
48	5	4439	U
48	5	4441	A

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Mol	Chain	Res	Type
48	5	4444	C
48	5	4447	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4463	U
48	5	4464	A
48	5	4472	G
48	5	4473	A
48	5	4475	G
48	5	4476	C
48	5	4478	G
48	5	4482	U
48	5	4489	G
48	5	4491	G
48	5	4500	U
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4518	A
48	5	4519	C
48	5	4520	G
48	5	4522	G
48	5	4524	G
48	5	4527	G
48	5	4528	G
48	5	4529	G
48	5	4530	U
48	5	4531	U
48	5	4548	A
48	5	4549	G
48	5	4555	U
48	5	4556	U
48	5	4557	U
48	5	4560	C
48	5	4561	C
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G

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Mol	Chain	Res	Type
48	5	4583	C
48	5	4584	A
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4599	A
48	5	4606	G
48	5	4607	A
48	5	4608	G
48	5	4617	G
48	5	4618	G
48	5	4627	U
48	5	4636	U
48	5	4637	G
48	5	4641	U
48	5	4644	G
48	5	4647	G
48	5	4656	A
48	5	4657	U
48	5	4660	G
48	5	4661	G
48	5	4663	G
48	5	4667	C
48	5	4670	C
48	5	4671	C
48	5	4672	A
48	5	4677	U
48	5	4684	A
48	5	4687	A
48	5	4693	C
48	5	4694	G
48	5	4695	C
48	5	4697	U
48	5	4700	A
48	5	4702	G
48	5	4709	U
48	5	4712	C
48	5	4718	G
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4728	U

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Mol	Chain	Res	Type
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	4742	G
48	5	4744	A
48	5	4745	G
48	5	4746	C
48	5	4749	C
48	5	4750	G
48	5	4751	G
48	5	4753	U
48	5	4754	G
48	5	4756	C
48	5	4758	U
48	5	4759	C
48	5	4760	G
48	5	4764	A
48	5	4770	U
48	5	4771	C
48	5	4774	C
48	5	4869	U
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	U
48	5	4877	G
48	5	4878	C
48	5	4883	C
48	5	4884	G
48	5	4885	U
48	5	4886	C
48	5	4889	G
48	5	4890	G
48	5	4891	G
48	5	4895	C
48	5	4896	G

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Mol	Chain	Res	Type
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	4932	U
48	5	4934	A
48	5	4936	G
48	5	4937	C
48	5	4939	C
48	5	4942	C
48	5	4944	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	4963	G
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
48	5	4990	C
48	5	4991	U
48	5	5013	C
48	5	5014	A
48	5	5017	G

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Mol	Chain	Res	Type
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	5032	C
48	5	5034	A
48	5	5041	G
48	5	5047	C
48	5	5049	G
48	5	5050	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	3	C
49	7	7	G
49	7	8	G
49	7	11	A
49	7	21	G
49	7	25	G
49	7	33	U
49	7	34	C
49	7	40	U
49	7	41	G
49	7	42	A
49	7	53	U
49	7	54	A
49	7	64	G
49	7	78	C
49	7	79	U
49	7	94	C
49	7	97	G
49	7	99	G
49	7	100	A

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Mol	Chain	Res	Type
49	7	102	U
49	7	109	U
49	7	110	G
49	7	111	C
49	7	120	U
50	8	2	G
50	8	3	A
50	8	8	U
50	8	12	G
50	8	13	G
50	8	23	C
50	8	32	C
50	8	34	U
50	8	35	C
50	8	38	U
50	8	49	G
50	8	51	U
50	8	52	A
50	8	55	U
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	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	97	A
50	8	103	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	114	G

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Mol	Chain	Res	Type
50	8	115	G
50	8	116	C
50	8	117	C
50	8	119	C
50	8	122	G
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	150	C
50	8	153	C
51	9	2	A
51	9	3	C
51	9	4	C
51	9	5	U
51	9	8	U
51	9	9	U
51	9	11	A
51	9	16	G
51	9	17	C
51	9	25	A
51	9	26	U
51	9	31	U
51	9	33	G
51	9	41	G
51	9	42	A
51	9	44	U
51	9	45	A
51	9	46	A
51	9	48	C
51	9	49	C
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	62	G
51	9	65	C
51	9	66	G
51	9	67	C
51	9	68	A
51	9	70	G

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Mol	Chain	Res	Type
51	9	71	G
51	9	72	C
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	78	C
51	9	79	A
51	9	80	G
51	9	85	A
51	9	93	U
51	9	103	A
51	9	104	A
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	143	U
51	9	147	A
51	9	149	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C
51	9	175	A
51	9	179	C
51	9	181	A
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U

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Mol	Chain	Res	Type
51	9	190	G
51	9	191	A
51	9	192	C
51	9	202	G
51	9	206	G
51	9	215	G
51	9	216	C
51	9	217	A
51	9	289	G
51	9	291	G
51	9	292	A
51	9	293	C
51	9	302	A
51	9	304	C
51	9	305	U
51	9	306	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	310	C
51	9	312	G
51	9	313	A
51	9	314	U
51	9	316	G
51	9	319	C
51	9	320	G
51	9	321	C
51	9	322	C
51	9	324	C
51	9	325	C
51	9	326	C
51	9	327	G
51	9	328	U
51	9	338	G
51	9	343	A
51	9	347	G
51	9	350	C
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U

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Mol	Chain	Res	Type
51	9	369	C
51	9	370	G
51	9	372	U
51	9	377	G
51	9	384	U
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	421	G
51	9	426	A
51	9	434	G
51	9	435	A
51	9	438	G
51	9	448	A
51	9	449	A
51	9	450	C
51	9	459	C
51	9	460	A
51	9	461	U
51	9	464	A
51	9	465	A
51	9	466	G
51	9	469	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	475	C
51	9	482	G
51	9	487	U
51	9	489	A
51	9	492	C
51	9	493	A
51	9	496	C
51	9	508	A
51	9	509	G
51	9	512	A

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Mol	Chain	Res	Type
51	9	516	A
51	9	523	A
51	9	530	U
51	9	532	C
51	9	533	A
51	9	535	G
51	9	539	C
51	9	542	U
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	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	570	C
51	9	576	A
51	9	583	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	593	C
51	9	595	U
51	9	597	G
51	9	598	G
51	9	601	G
51	9	605	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	610	G
51	9	614	C

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Mol	Chain	Res	Type
51	9	617	G
51	9	620	G
51	9	621	C
51	9	627	U
51	9	628	A
51	9	629	A
51	9	631	U
51	9	632	C
51	9	634	A
51	9	637	U
51	9	643	A
51	9	644	G
51	9	654	A
51	9	655	A
51	9	656	G
51	9	659	G
51	9	660	C
51	9	663	C
51	9	664	A
51	9	666	U
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	674	C
51	9	679	A
51	9	683	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	698	G
51	9	733	C
51	9	735	C
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

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Mol	Chain	Res	Type
51	9	789	G
51	9	791	C
51	9	794	A
51	9	796	G
51	9	797	C
51	9	798	G
51	9	799	U
51	9	800	U
51	9	810	A
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	827	A
51	9	830	A
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	845	G
51	9	847	A
51	9	848	U
51	9	853	C
51	9	858	A
51	9	859	G
51	9	861	A
51	9	862	A
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	877	C
51	9	878	G
51	9	879	C
51	9	880	G
51	9	887	U
51	9	888	U

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Mol	Chain	Res	Type
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	908	A
51	9	909	G
51	9	910	G
51	9	912	C
51	9	913	A
51	9	914	U
51	9	916	A
51	9	917	U
51	9	919	A
51	9	920	A
51	9	921	G
51	9	933	G
51	9	934	G
51	9	938	A
51	9	943	U
51	9	955	A
51	9	960	U
51	9	961	G
51	9	963	A
51	9	968	U
51	9	971	G
51	9	985	G
51	9	990	A
51	9	991	G
51	9	992	A
51	9	999	G
51	9	1002	U
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1030	A
51	9	1033	G
51	9	1040	G
51	9	1041	G
51	9	1044	G
51	9	1049	A

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Mol	Chain	Res	Type
51	9	1052	A
51	9	1053	C
51	9	1060	A
51	9	1082	A
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1093	A
51	9	1096	G
51	9	1100	A
51	9	1101	U
51	9	1102	G
51	9	1109	C
51	9	1110	G
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	1123	C
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	1148	A
51	9	1149	A
51	9	1150	A
51	9	1153	C
51	9	1154	U
51	9	1157	G
51	9	1163	C
51	9	1164	G
51	9	1165	G
51	9	1166	G
51	9	1168	G

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Mol	Chain	Res	Type
51	9	1181	A
51	9	1194	A
51	9	1195	A
51	9	1197	G
51	9	1207	G
51	9	1208	A
51	9	1209	A
51	9	1210	G
51	9	1211	G
51	9	1212	G
51	9	1213	C
51	9	1214	A
51	9	1215	C
51	9	1216	C
51	9	1217	A
51	9	1224	G
51	9	1227	G
51	9	1230	C
51	9	1235	G
51	9	1240	A
51	9	1242	U
51	9	1250	A
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1258	A
51	9	1259	A
51	9	1260	A
51	9	1266	C
51	9	1267	C
51	9	1268	C
51	9	1270	G
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1276	A
51	9	1280	G
51	9	1282	A
51	9	1283	C
51	9	1284	A

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Mol	Chain	Res	Type
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
51	9	1294	G
51	9	1298	G
51	9	1299	A
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1304	U
51	9	1308	U
51	9	1309	C
51	9	1310	U
51	9	1312	G
51	9	1313	A
51	9	1314	U
51	9	1315	U
51	9	1316	C
51	9	1318	G
51	9	1322	G
51	9	1330	G
51	9	1331	C
51	9	1332	A
51	9	1333	U
51	9	1334	G
51	9	1342	U
51	9	1343	U
51	9	1344	A
51	9	1345	G
51	9	1348	G
51	9	1351	G
51	9	1371	U
51	9	1372	U
51	9	1376	A
51	9	1378	A
51	9	1386	A
51	9	1387	G

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Mol	Chain	Res	Type
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	1404	U
51	9	1405	A
51	9	1407	U
51	9	1408	U
51	9	1410	C
51	9	1412	C
51	9	1413	G
51	9	1414	A
51	9	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	1435	C
51	9	1437	C
51	9	1438	A
51	9	1439	A
51	9	1440	C
51	9	1442	U
51	9	1444	U
51	9	1447	G
51	9	1448	A
51	9	1449	G
51	9	1452	A
51	9	1454	A
51	9	1455	A
51	9	1456	G
51	9	1462	U
51	9	1463	U
51	9	1464	C

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Mol	Chain	Res	Type
51	9	1465	A
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	1487	A
51	9	1488	C
51	9	1490	G
51	9	1494	U
51	9	1495	G
51	9	1497	G
51	9	1498	A
51	9	1507	G
51	9	1509	U
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1523	C
51	9	1525	C
51	9	1527	C
51	9	1531	A
51	9	1533	A
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	1560	U
51	9	1567	G
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1585	U
51	9	1586	U

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Mol	Chain	Res	Type
51	9	1587	G
51	9	1588	A
51	9	1594	A
51	9	1595	U
51	9	1596	U
51	9	1599	U
51	9	1601	A
51	9	1602	U
51	9	1603	G
51	9	1604	G
51	9	1606	G
51	9	1612	G
51	9	1618	C
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1624	U
51	9	1625	U
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	1661	A
51	9	1663	A
51	9	1664	A
51	9	1665	G
51	9	1666	C
51	9	1667	U
51	9	1671	G
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	1699	A
51	9	1703	C

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Mol	Chain	Res	Type
51	9	1713	C
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1725	U
51	9	1729	U
51	9	1732	G
51	9	1745	A
51	9	1746	U
51	9	1748	G
51	9	1753	C
51	9	1756	C
51	9	1758	G
51	9	1760	G
51	9	1783	C
51	9	1786	U
51	9	1800	A
51	9	1801	A
51	9	1805	G
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	1840	U
51	9	1845	A
51	9	1846	G
51	9	1849	G
51	9	1850	A
51	9	1851	A
51	9	1852	C
51	9	1861	G
51	9	1862	G
51	9	1863	A

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Mol	Chain	Res	Type
51	9	1864	U
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1868	U
85	hh	42	C
85	hh	43	A
85	hh	46	G
85	hh	49	U
85	hh	51	A
85	hh	52	G

All (420) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	29	A
47	3	30	G
47	3	39	U
47	3	60	U
47	3	69	G
47	3	74	C
48	5	1	C
48	5	12	A
48	5	20	U
48	5	47	A
48	5	48	G
48	5	58	G
48	5	64	A
48	5	90	G
48	5	93	G
48	5	119	G
48	5	125	C
48	5	134	G
48	5	143	C
48	5	148	C
48	5	157	U
48	5	159	C
48	5	170	C
48	5	187	U
48	5	215	C
48	5	216	C
48	5	218	A

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Mol	Chain	Res	Type
48	5	219	G
48	5	224	U
48	5	226	G
48	5	234	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	277	G
48	5	286	U
48	5	294	G
48	5	296	A
48	5	333	U
48	5	352	G
48	5	385	A
48	5	387	G
48	5	406	C
48	5	417	G
48	5	451	C
48	5	454	U
48	5	486	C
48	5	497	G
48	5	505	G
48	5	509	A
48	5	664	G
48	5	684	G
48	5	686	A
48	5	693	C
48	5	727	C
48	5	728	U
48	5	733	A
48	5	746	A
48	5	747	A
48	5	917	A
48	5	928	C
48	5	930	G
48	5	931	C
48	5	932	A
48	5	935	A
48	5	943	A
48	5	944	A
48	5	956	A
48	5	957	G

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Mol	Chain	Res	Type
48	5	962	C
48	5	965	G
48	5	977	C
48	5	978	G
48	5	989	U
48	5	1071	C
48	5	1175	A
48	5	1176	C
48	5	1209	U
48	5	1211	G
48	5	1214	C
48	5	1232	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1241	C
48	5	1266	G
48	5	1268	G
48	5	1272	C
48	5	1279	A
48	5	1284	G
48	5	1292	C
48	5	1293	G
48	5	1296	G
48	5	1324	A
48	5	1329	G
48	5	1354	A
48	5	1365	C
48	5	1368	A
48	5	1370	G
48	5	1371	A
48	5	1376	C
48	5	1377	G
48	5	1379	C
48	5	1380	G
48	5	1387	A
48	5	1398	A
48	5	1407	C
48	5	1410	U
48	5	1419	G
48	5	1420	A

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Mol	Chain	Res	Type
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1474	C
48	5	1477	C
48	5	1485	C
48	5	1502	G
48	5	1523	A
48	5	1530	G
48	5	1533	A
48	5	1563	A
48	5	1611	C
48	5	1633	G
48	5	1672	U
48	5	1678	C
48	5	1679	A
48	5	1697	G
48	5	1724	G
48	5	1733	G
48	5	1746	A
48	5	1755	C
48	5	1804	A
48	5	1818	G
48	5	1819	G
48	5	1834	U
48	5	1835	G
48	5	1839	U
48	5	1854	G
48	5	1891	A
48	5	1892	A
48	5	1910	G
48	5	1918	U
48	5	1921	C
48	5	1947	U
48	5	1957	U
48	5	1959	U
48	5	1968	G
48	5	1974	U
48	5	1975	G
48	5	1980	U
48	5	1986	U
48	5	1987	C

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Mol	Chain	Res	Type
48	5	2003	G
48	5	2040	A
48	5	2046	G
48	5	2055	G
48	5	2056	G
48	5	2068	C
48	5	2083	C
48	5	2084	C
48	5	2088	A
48	5	2089	G
48	5	2093	A
48	5	2107	C
48	5	2116	C
48	5	2119	C
48	5	2123	C
48	5	2125	C
48	5	2246	C
48	5	2251	G
48	5	2253	A
48	5	2256	C
48	5	2257	C
48	5	2260	C
48	5	2262	G
48	5	2265	G
48	5	2266	C
48	5	2278	G
48	5	2313	A
48	5	2370	A
48	5	2396	A
48	5	2398	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2473	A
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	G
48	5	2505	C
48	5	2506	G
48	5	2513	A
48	5	2529	A

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Mol	Chain	Res	Type
48	5	2530	U
48	5	2546	G
48	5	2553	A
48	5	2554	U
48	5	2605	G
48	5	2623	A
48	5	2639	U
48	5	2661	U
48	5	2695	A
48	5	2696	A
48	5	2703	G
48	5	2724	G
48	5	2760	G
48	5	2768	C
48	5	2769	U
48	5	2794	C
48	5	2806	A
48	5	2827	G
48	5	2858	A
48	5	3593	C
48	5	3625	G
48	5	3663	A
48	5	3670	C
48	5	3673	C
48	5	3697	U
48	5	3709	U
48	5	3710	G
48	5	3712	A
48	5	3717	A
48	5	3752	C
48	5	3765	G
48	5	3784	A
48	5	3827	G
48	5	3876	A
48	5	3878	C
48	5	3888	G
48	5	3904	G
48	5	3913	G
48	5	4069	U
48	5	4075	U
48	5	4076	G
48	5	4084	G

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Mol	Chain	Res	Type
48	5	4115	G
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4127	A
48	5	4144	C
48	5	4162	C
48	5	4170	A
48	5	4204	C
48	5	4221	C
48	5	4232	U
48	5	4291	G
48	5	4331	G
48	5	4378	A
48	5	4379	A
48	5	4394	A
48	5	4395	U
48	5	4404	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4464	A
48	5	4475	G
48	5	4510	A
48	5	4524	G
48	5	4527	G
48	5	4528	G
48	5	4548	A
48	5	4555	U
48	5	4559	A
48	5	4560	C
48	5	4583	C
48	5	4626	A
48	5	4656	A
48	5	4670	C
48	5	4694	G
48	5	4699	U
48	5	4718	G
48	5	4719	G
48	5	4730	C
48	5	4872	G
48	5	4885	U

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Mol	Chain	Res	Type
48	5	4888	U
48	5	4889	G
48	5	4895	C
48	5	4900	C
48	5	4909	A
48	5	4935	C
48	5	4948	C
48	5	4951	G
48	5	4975	G
48	5	4990	C
48	5	5000	G
48	5	5022	U
48	5	5026	U
48	5	5027	C
48	5	5049	G
48	5	5059	C
48	5	5060	A
48	5	5061	A
49	7	1	G
49	7	109	U
50	8	2	G
50	8	37	A
50	8	51	U
50	8	94	G
50	8	110	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	8	U
51	9	58	C
51	9	72	C
51	9	76	U
51	9	92	A
51	9	98	C
51	9	110	U
51	9	113	G
51	9	139	C
51	9	140	C
51	9	149	A
51	9	160	U
51	9	183	G
51	9	215	G

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Mol	Chain	Res	Type
51	9	291	G
51	9	292	A
51	9	305	U
51	9	311	C
51	9	312	G
51	9	321	C
51	9	327	G
51	9	369	C
51	9	385	G
51	9	434	G
51	9	448	A
51	9	449	A
51	9	465	A
51	9	474	G
51	9	488	U
51	9	500	A
51	9	532	C
51	9	550	C
51	9	559	G
51	9	589	G
51	9	590	A
51	9	594	A
51	9	620	G
51	9	642	U
51	9	655	A
51	9	656	G
51	9	670	A
51	9	672	A
51	9	688	U
51	9	746	C
51	9	747	U
51	9	752	G
51	9	797	C
51	9	810	A
51	9	833	C
51	9	861	A
51	9	869	A
51	9	870	A
51	9	887	U
51	9	909	G
51	9	912	C
51	9	913	A

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Mol	Chain	Res	Type
51	9	916	A
51	9	925	G
51	9	1016	U
51	9	1109	C
51	9	1115	U
51	9	1137	U
51	9	1165	G
51	9	1215	C
51	9	1253	A
51	9	1259	A
51	9	1265	A
51	9	1267	C
51	9	1275	G
51	9	1283	C
51	9	1302	G
51	9	1309	C
51	9	1312	G
51	9	1313	A
51	9	1330	G
51	9	1342	U
51	9	1344	A
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1407	U
51	9	1418	C
51	9	1419	C
51	9	1432	U
51	9	1448	A
51	9	1454	A
51	9	1455	A
51	9	1463	U
51	9	1475	G
51	9	1477	U
51	9	1486	A
51	9	1487	A
51	9	1489	A
51	9	1555	U
51	9	1601	A
51	9	1621	U
51	9	1623	A
51	9	1636	G

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Mol	Chain	Res	Type
51	9	1637	A
51	9	1647	A
51	9	1663	A
51	9	1664	A
51	9	1665	G
51	9	1679	A
51	9	1680	G
51	9	1681	U
51	9	1683	C
51	9	1700	C
51	9	1721	U
51	9	1824	A
51	9	1826	G
51	9	1835	A
51	9	1837	G

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	-	-	-		
90	SF4	jj	601	87	0,12,12	-	-	-		
91	ADP	jj	603	-	28,29,29	1.52	5 (17%)	43,45,45	1.91	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
91	ADP	jj	602	-	28,29,29	1.51	5 (17%)	43,45,45	1.90	11 (25%)

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	-	-	0/6/5/5
91	ADP	jj	602	-	-	0/16/32/32	0/3/3/3
91	ADP	jj	603	-	-	2/16/32/32	0/3/3/3
90	SF4	jj	601	87	-	-	0/6/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	602	ADP	C5-C4	4.98	1.48	1.39
91	jj	603	ADP	C5-C4	4.96	1.47	1.39
91	jj	603	ADP	C5-C6	3.01	1.49	1.41
91	jj	602	ADP	C5-C6	2.96	1.49	1.41
91	jj	602	ADP	C8-N7	2.50	1.36	1.31
91	jj	603	ADP	C8-N7	2.48	1.36	1.31
91	jj	603	ADP	PA-O3A	2.29	1.62	1.59
91	jj	602	ADP	C5-N7	-2.26	1.35	1.39
91	jj	603	ADP	C5-N7	-2.23	1.35	1.39
91	jj	602	ADP	PA-O3A	2.21	1.61	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	jj	603	ADP	C5-C4-N3	-5.90	118.60	126.72
91	jj	602	ADP	C5-C4-N3	-5.87	118.64	126.72
91	jj	603	ADP	N3-C4-N9	4.63	135.04	127.17
91	jj	602	ADP	N3-C4-N9	4.61	135.00	127.17
91	jj	602	ADP	C2-N3-C4	3.95	121.48	111.83
91	jj	603	ADP	C2-N3-C4	3.95	121.47	111.83
91	jj	602	ADP	N3-C2-N1	-3.83	122.78	128.58
91	jj	603	ADP	N3-C2-N1	-3.78	122.86	128.58
91	jj	602	ADP	C4-C5-N7	-3.71	106.34	110.58
91	jj	603	ADP	C4-C5-N7	-3.69	106.37	110.58
91	jj	602	ADP	C5-N7-C8	2.82	107.88	103.45
91	jj	603	ADP	C5-N7-C8	2.78	107.82	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
91	jj	602	ADP	C4-N9-C8	2.75	108.62	105.74
91	jj	603	ADP	C4-N9-C8	2.70	108.58	105.74
91	jj	603	ADP	C3'-C2'-C1'	2.42	106.04	101.46
91	jj	602	ADP	C6-C5-N7	2.33	136.59	132.09
91	jj	603	ADP	C6-C5-N7	2.29	136.51	132.09
91	jj	602	ADP	N9-C8-N7	-2.21	110.80	113.94
91	jj	603	ADP	N9-C8-N7	-2.16	110.88	113.94
91	jj	602	ADP	C2-N1-C6	2.10	122.18	118.73
91	jj	602	ADP	C3'-C2'-C1'	2.09	105.42	101.46
91	jj	603	ADP	C2-N1-C6	2.07	122.14	118.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	jj	603	ADP	PB-O3A-PA-O1A
91	jj	603	ADP	PB-O3A-PA-O2A

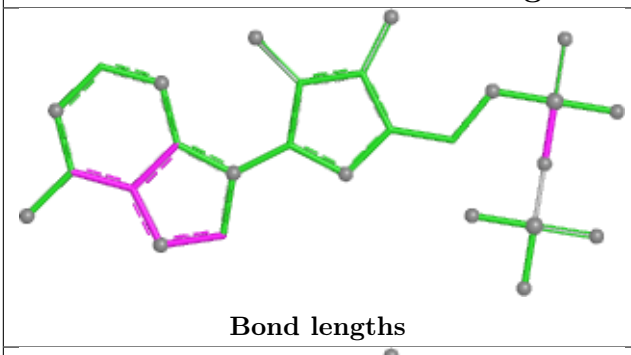
There are no ring outliers.

2 monomers are involved in 7 short contacts:

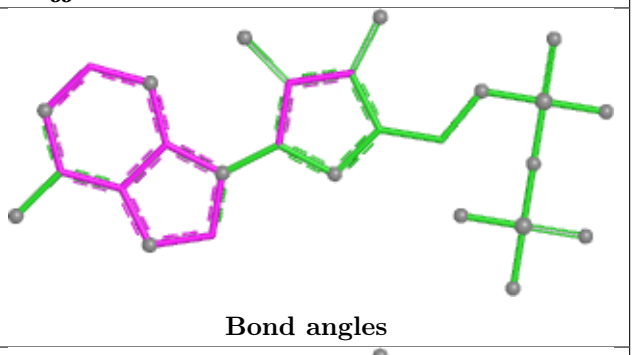
Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	jj	600	SF4	3	0
90	jj	601	SF4	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

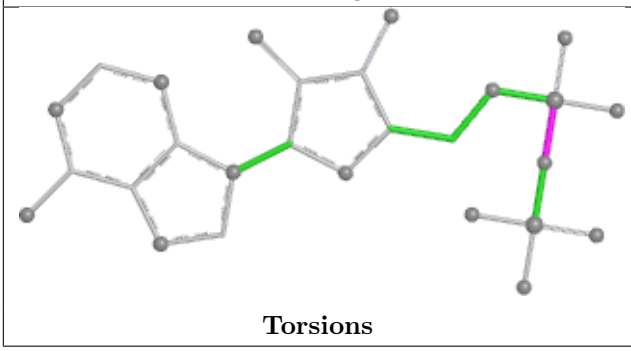
Ligand ADP jj 603



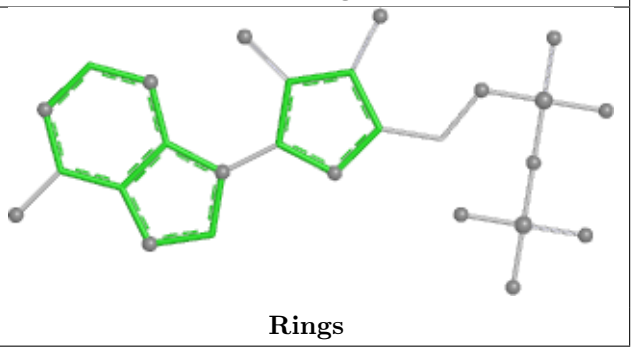
Bond lengths



Bond angles

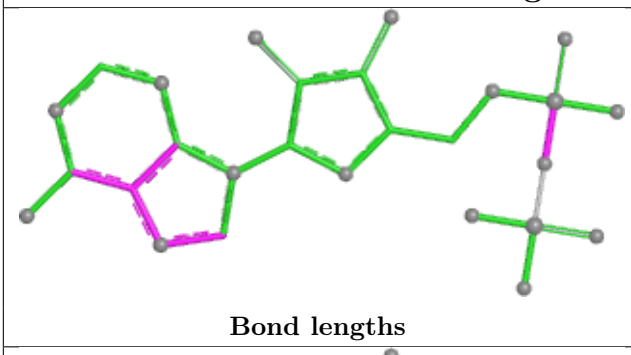


Torsions

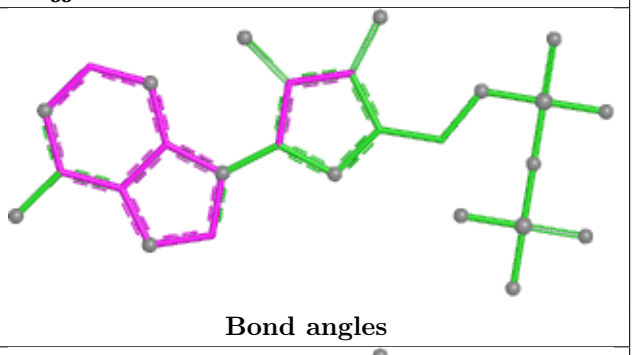


Rings

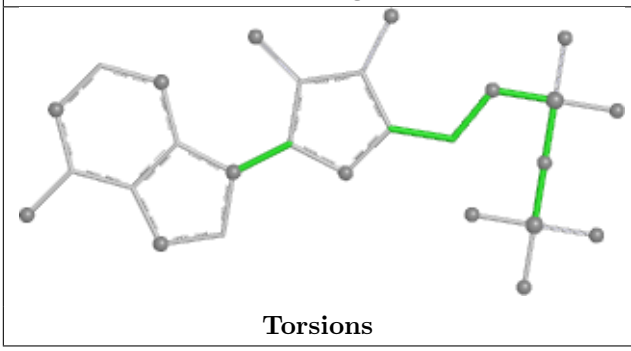
Ligand ADP jj 602



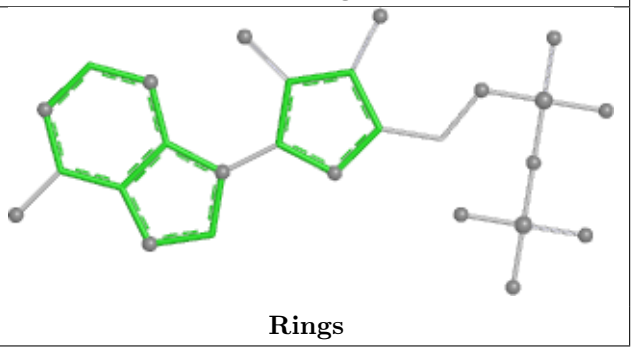
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	16
51	9	8
47	3	2
46	2	1
87	jj	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	753:C	O3'	785:C	P	23.51
1	9	126:G	O3'	139:C	P	21.53
1	9	698:G	O3'	730:C	P	20.02
1	5	4776:G	O3'	4859:C	P	17.98
1	9	1761:U	O3'	1771:G	P	17.66
1	5	757:G	O3'	906:C	P	17.38
1	5	2910:G	O3'	3583:U	P	16.73
1	5	519:C	O3'	642:G	P	16.70
1	5	2131:C	O3'	2243:C	P	14.45
1	5	3950:U	O3'	4065:G	P	14.15
1	5	997:C	O3'	1047:C	P	13.82
1	5	1051:G	O3'	1064:G	P	8.99
1	9	225:G	O3'	287:U	P	7.26
1	9	739:C	O3'	744:G	P	6.64
1	3	19:G	O3'	20:U	P	5.70
1	3	16:C	O3'	18:U	P	4.70
1	5	1222:A	O3'	1232:G	P	4.66
1	5	1100:U	O3'	1167:C	P	4.51
1	2	16:C	O3'	18:G	P	4.47
1	5	1699:A	O3'	1718:C	P	3.96
1	jj	416:ILE	C	417:SER	N	3.11
1	5	2016:C	O3'	2017:A	P	3.10
1	9	340:C	O3'	342:C	P	3.09
1	9	873:G	O3'	874:G	P	2.83
1	5	1840:G	O3'	1842:G	P	2.68
1	5	4939:C	O3'	4941:G	P	2.55
1	5	4942:C	O3'	4944:C	P	2.53
1	5	1823:G	O3'	1825:A	P	2.42

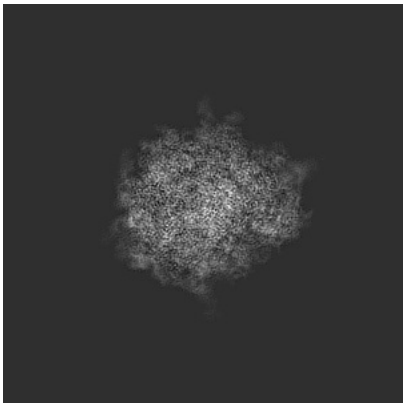
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3040. These allow visual inspection of the internal detail of the map and identification of artifacts.

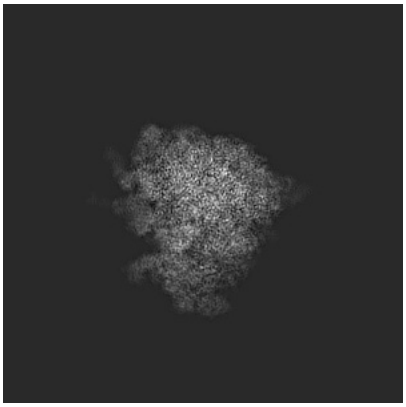
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

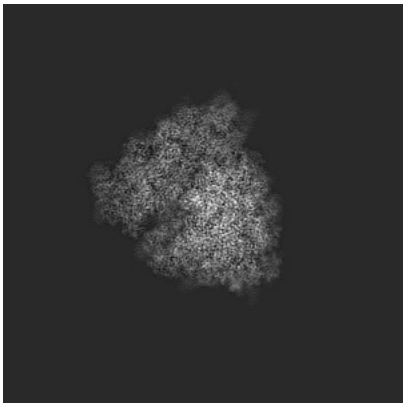
6.1.1 Primary map



X



Y



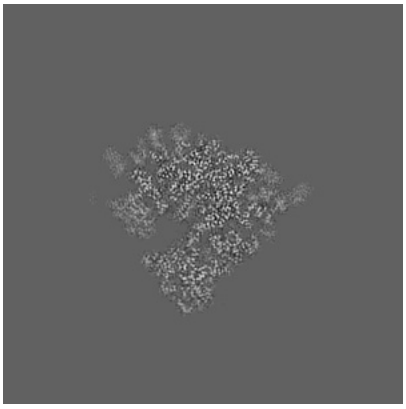
Z

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

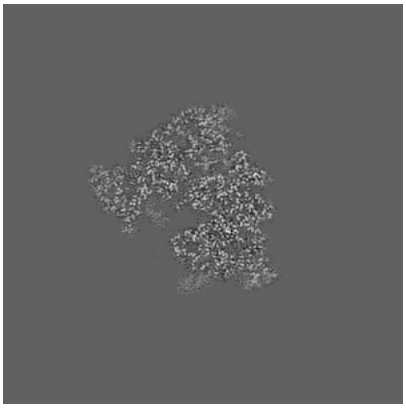
6.2 Central slices

6.2.1 Primary map

X Index: 210



Y Index: 210

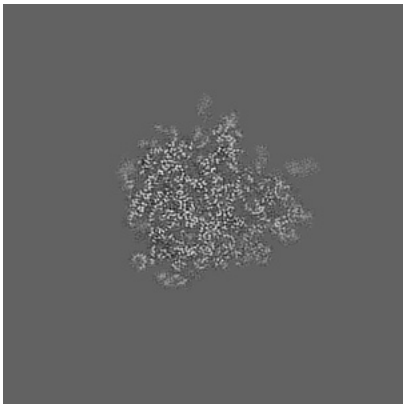


Z Index: 210

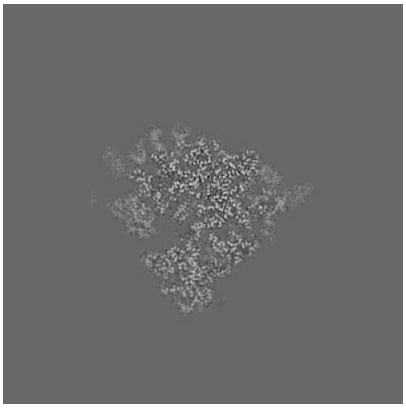
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

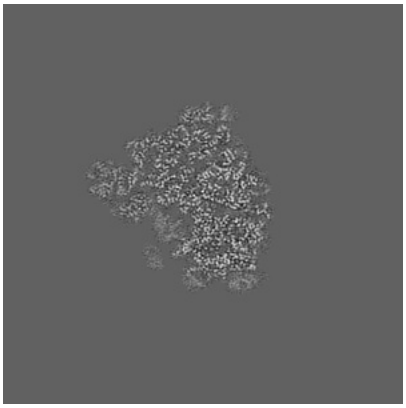
6.3.1 Primary map



X Index: 225



Y Index: 211

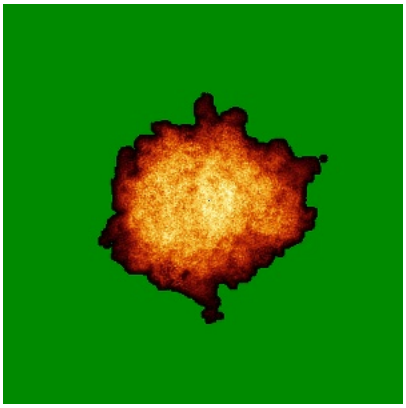


Z Index: 220

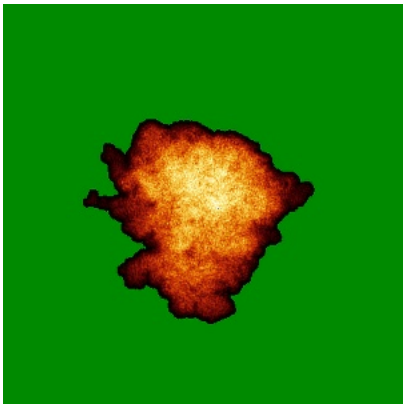
The images above show the largest variance slices of the map in three orthogonal directions.

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

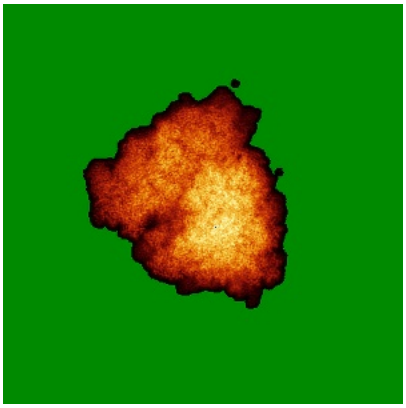
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

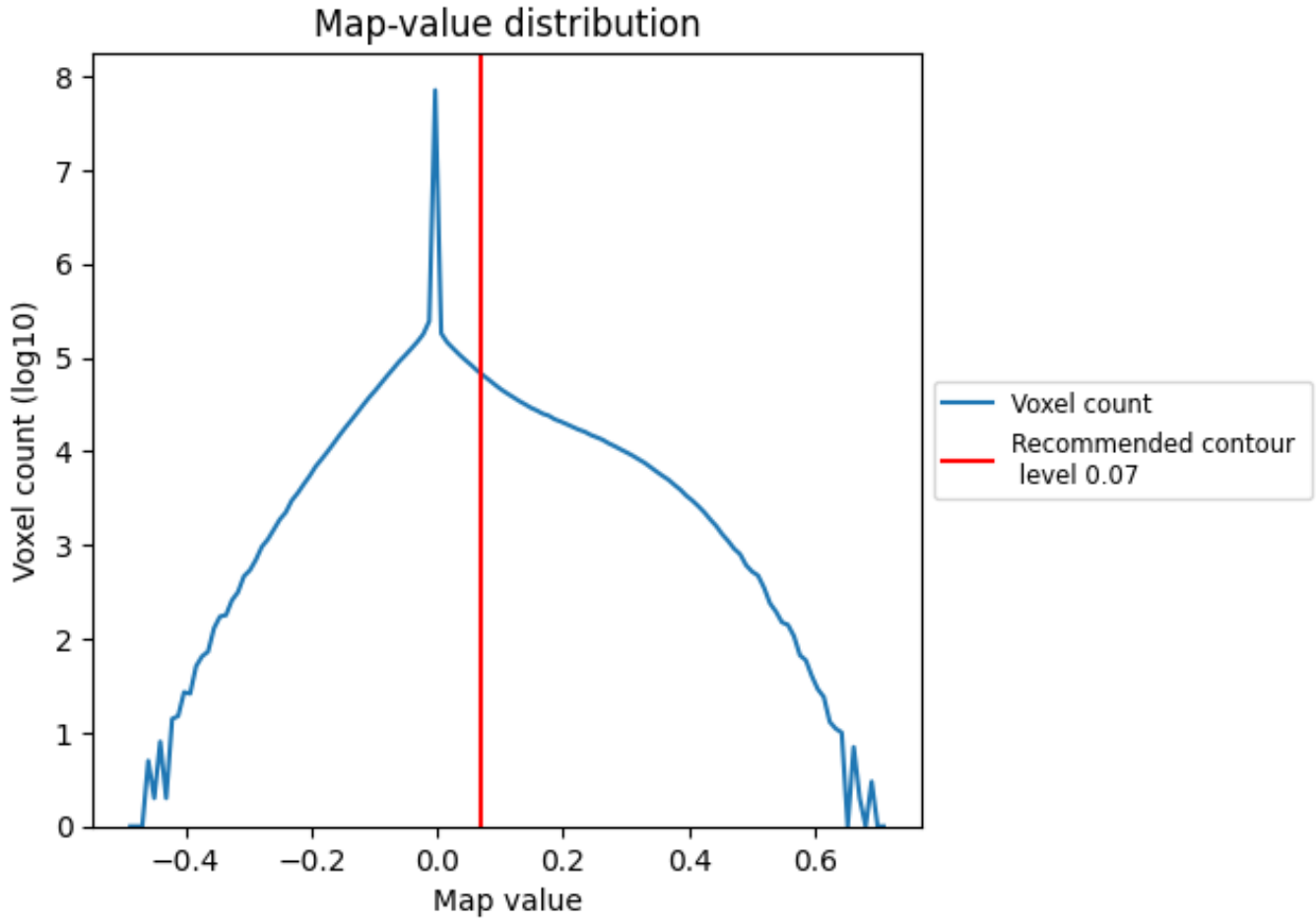
6.6 Mask visualisation (i)

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

7 Map analysis

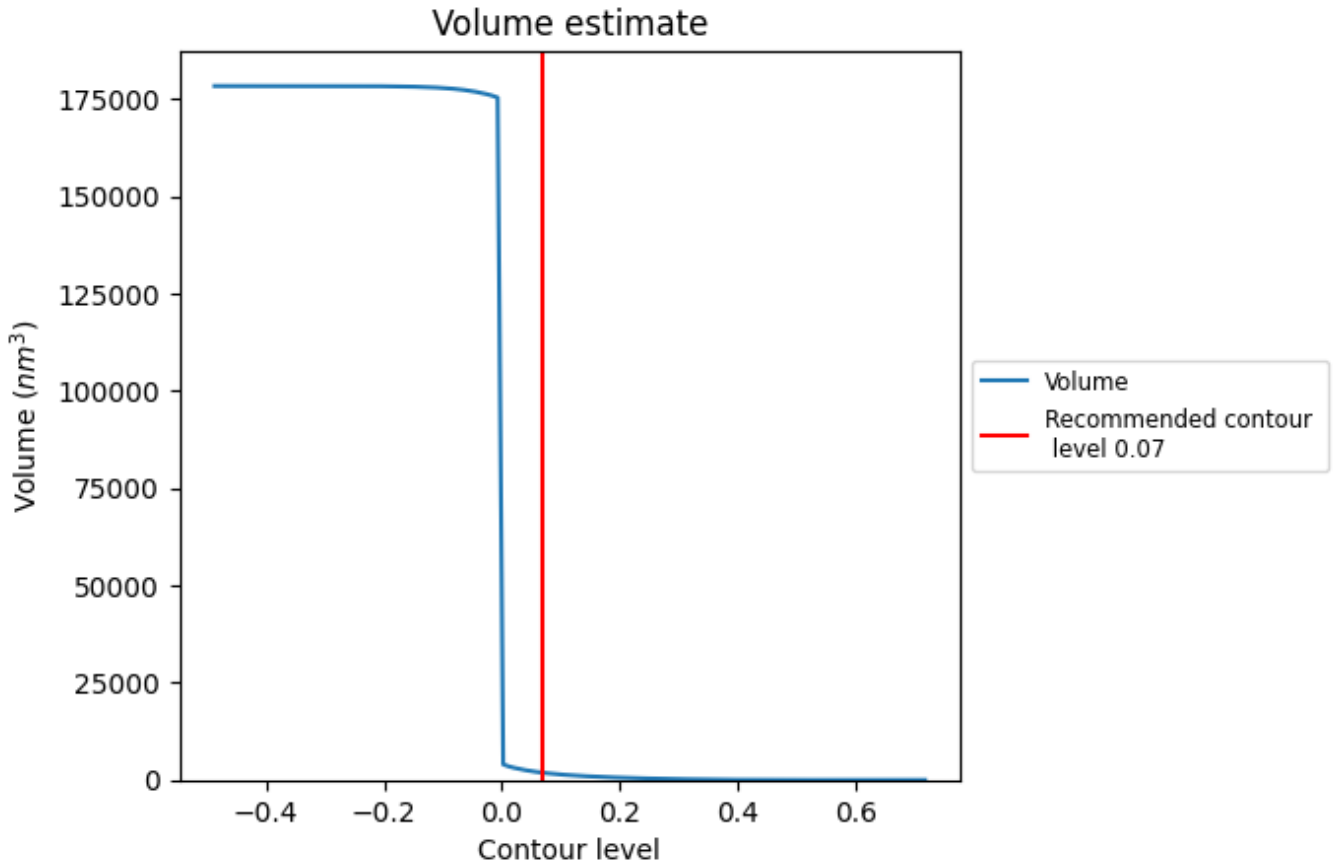
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

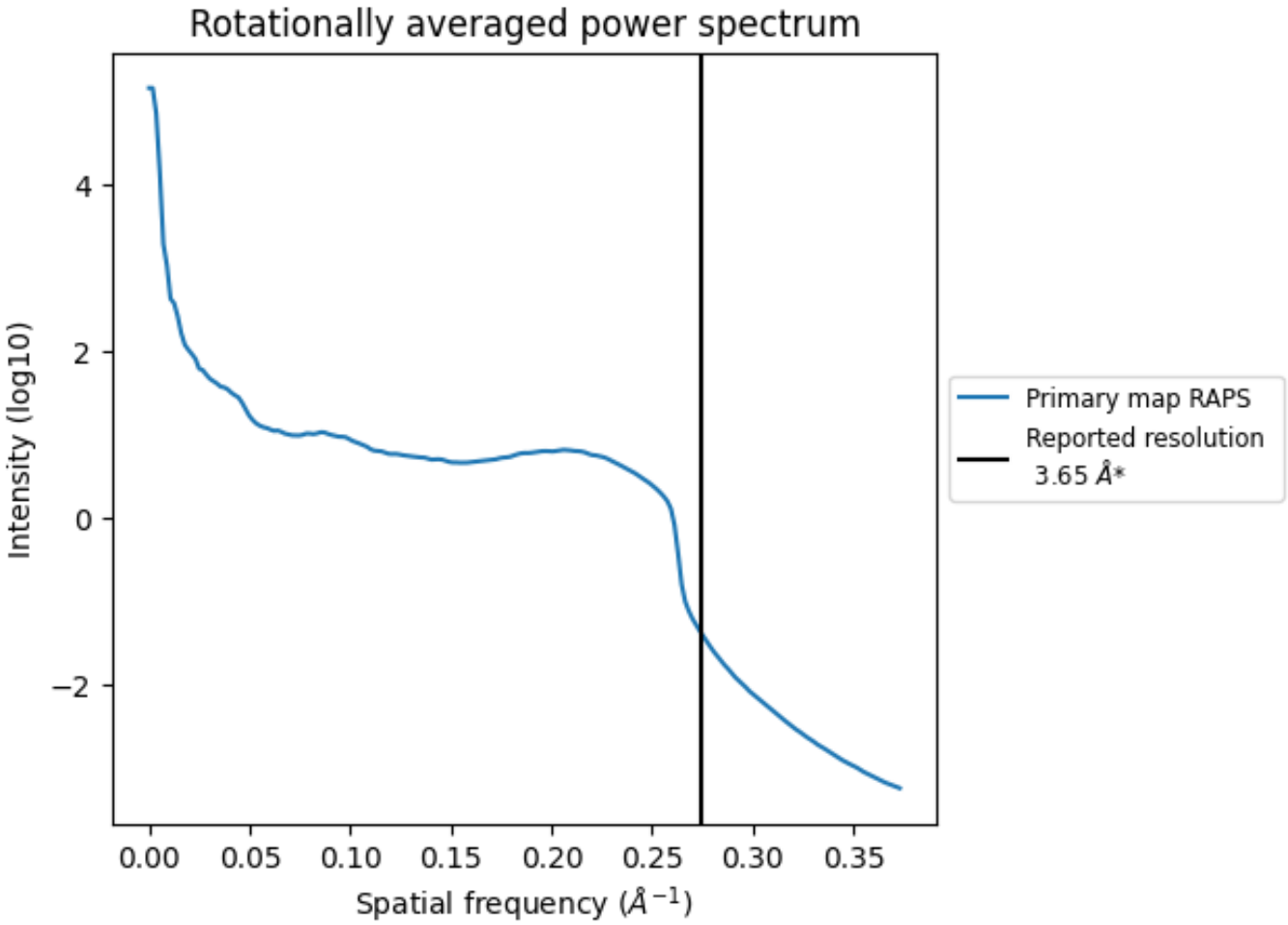
7.2 Volume estimate



The volume at the recommended contour level is 1855 nm^3; this corresponds to an approximate mass of 1676 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

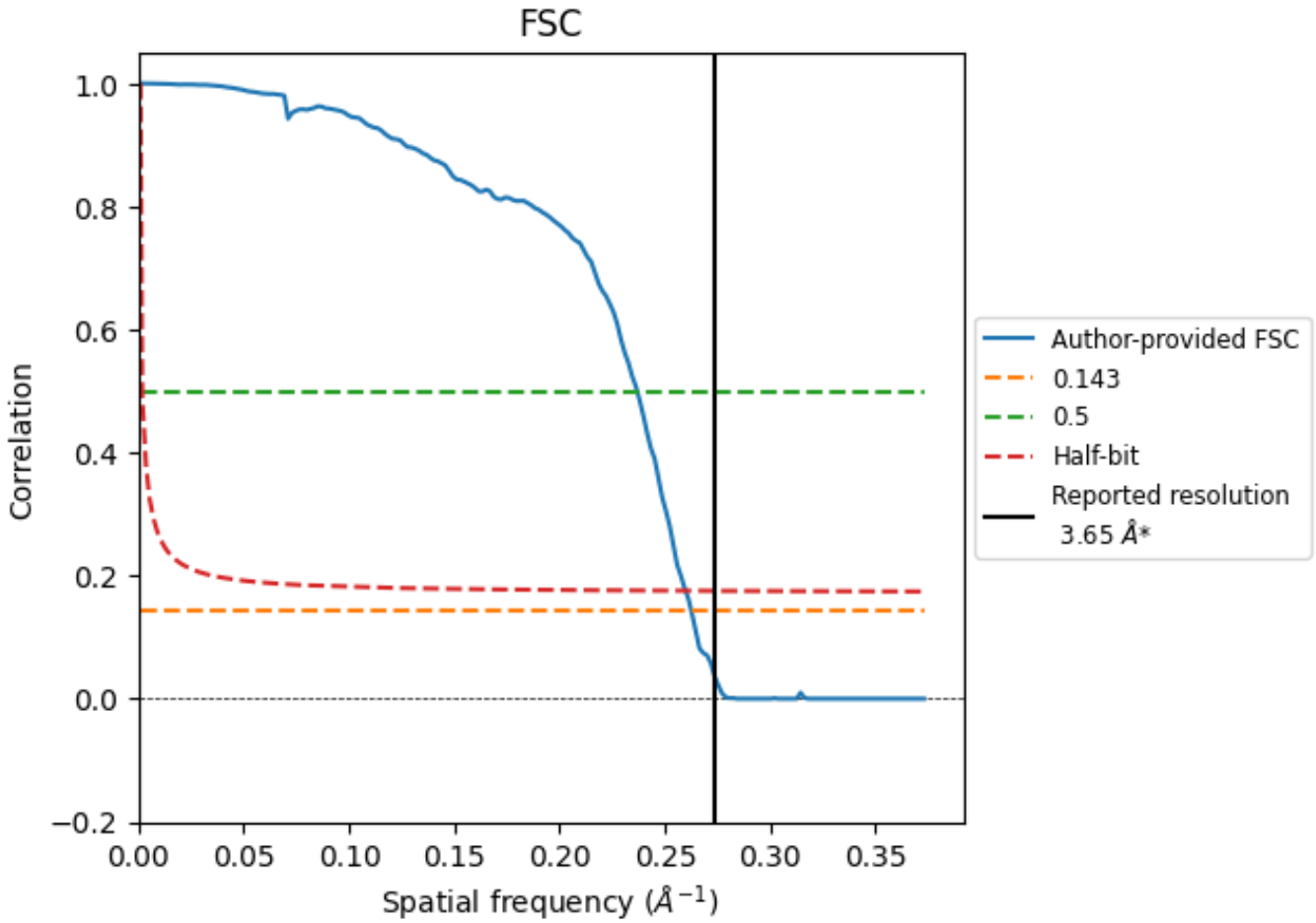


*Reported resolution corresponds to spatial frequency of 0.274 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.274 Å^{-1}

8.2 Resolution estimates (i)

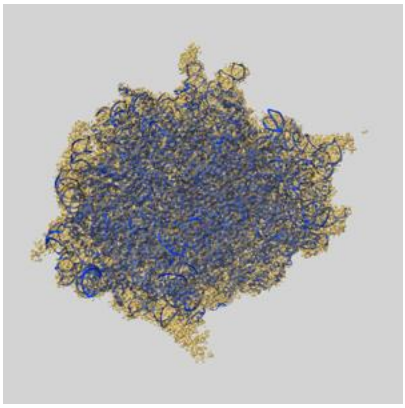
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.81	4.22	3.85
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

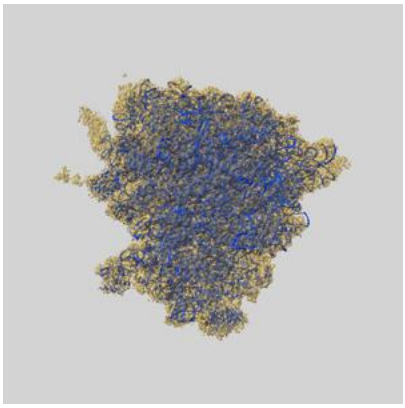
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3040 and PDB model 3JAI. Per-residue inclusion information can be found in section 3 on page 23.

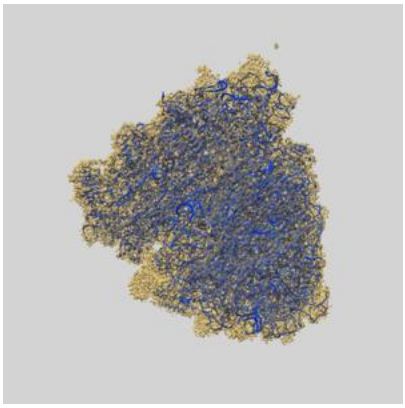
9.1 Map-model overlay



X



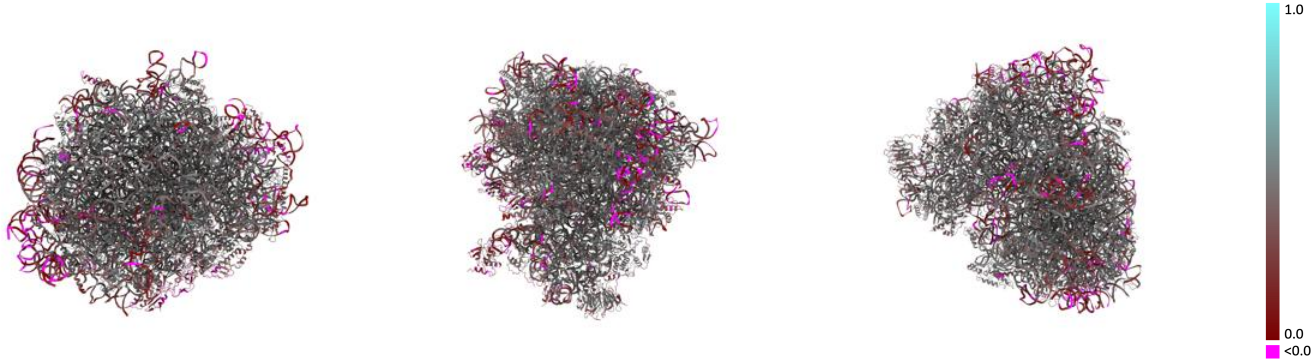
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

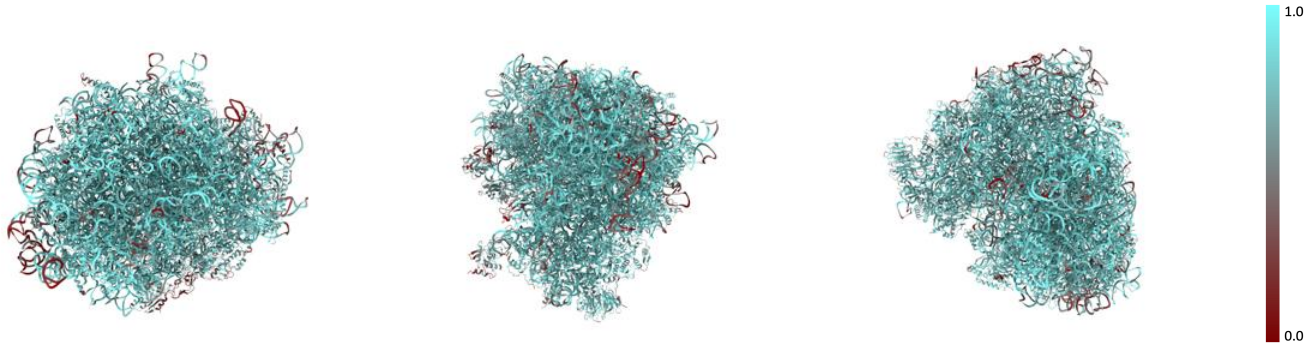
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

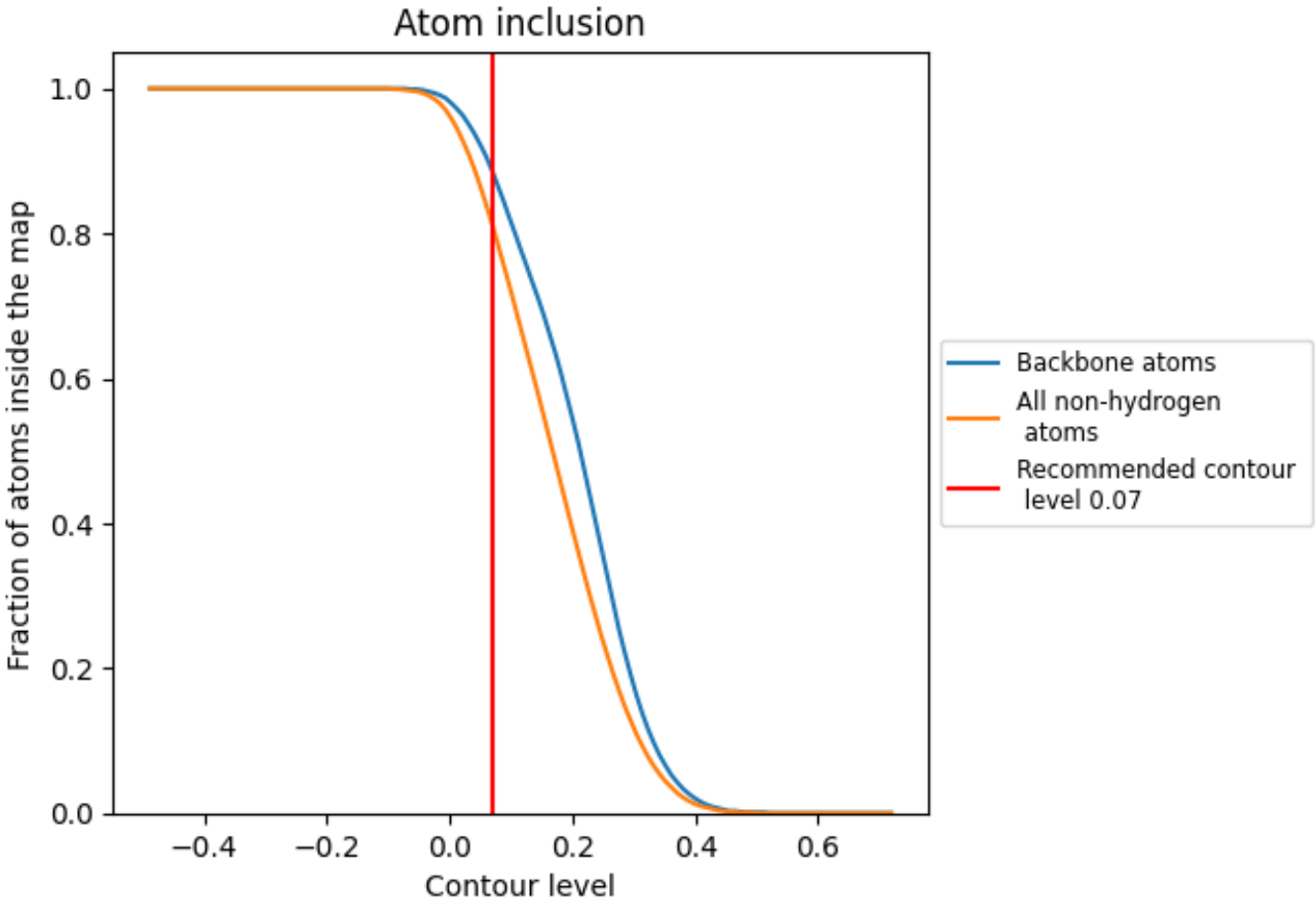
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8110	0.4030
1	0.7600	0.4260
2	0.8210	0.3620
3	0.6600	0.2310
5	0.8310	0.3780
7	0.9160	0.4410
8	0.8640	0.4060
9	0.8390	0.3840
A	0.8530	0.4850
AA	0.8050	0.4430
B	0.8470	0.4800
BB	0.7990	0.4590
C	0.8490	0.4760
CC	0.8050	0.4540
D	0.8340	0.4420
DD	0.7230	0.4000
E	0.7650	0.4120
EE	0.8080	0.4570
F	0.8180	0.4670
FF	0.7540	0.4220
G	0.7670	0.4160
GG	0.7370	0.3870
H	0.8130	0.4640
HH	0.7020	0.3610
I	0.8300	0.4730
II	0.7740	0.4220
J	0.8020	0.4350
JJ	0.7840	0.4300
KK	0.7280	0.3640
L	0.8120	0.4400
LL	0.7710	0.4380
M	0.8360	0.4580
MM	0.4580	0.1910
N	0.8690	0.4870
NN	0.8100	0.4550

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Chain	Atom inclusion	Q-score
O	0.8390	0.4720
OO	0.8200	0.4590
P	0.8370	0.4820
PP	0.7130	0.3720
Q	0.8480	0.4810
QQ	0.7840	0.4440
R	0.8180	0.4420
RR	0.7230	0.3950
S	0.8510	0.4770
SS	0.7870	0.4140
T	0.8350	0.4690
TT	0.7950	0.4250
U	0.7960	0.4300
UU	0.7080	0.3840
V	0.8110	0.4800
VV	0.7800	0.4310
W	0.8330	0.4770
WW	0.8360	0.4740
X	0.8250	0.4660
XX	0.8210	0.4710
Y	0.8240	0.4630
YY	0.7840	0.4190
Z	0.8430	0.4630
ZZ	0.7440	0.3880
a	0.8680	0.4870
aa	0.8340	0.4750
b	0.7400	0.4120
bb	0.7570	0.4290
c	0.8450	0.4690
cc	0.7270	0.4050
d	0.8330	0.4680
dd	0.8220	0.4600
e	0.8410	0.4750
ee	0.6840	0.3850
f	0.8590	0.4860
ff	0.5830	0.2490
g	0.8220	0.4560
gg	0.7070	0.3880
h	0.8130	0.4540
hh	0.8330	0.4170
i	0.8130	0.4520
ii	0.6690	0.3930

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Chain	Atom inclusion	Q-score
j	0.8860	0.4830
jj	0.7110	0.3920
k	0.7790	0.4280
l	0.8580	0.4850
m	0.8410	0.4610
n	0.8410	0.4620
o	0.8320	0.4780
p	0.8330	0.4680
r	0.8550	0.4750
s	0.4230	0.1690
t	0.5070	0.1640