



Full wwPDB EM Validation Report ⓘ

Aug 3, 2026 – 03:34 PM EDT

PDB ID : 3JAG / pdb_00003jag
EMDB ID : EMD-3038
Title : Structure of a mammalian ribosomal termination complex with ABCE1, eRF1(AAQ), and the UAA stop codon
Authors : Brown, A.; Shao, S.; Murray, J.; Hegde, R.S.; Ramakrishnan, V.
Deposited on : 2015-06-10
Resolution : 3.65 Å(reported)
Based on initial models : 3J92, 3BK7, 1DT9, 3J7P, 4V51

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
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) : 2.50

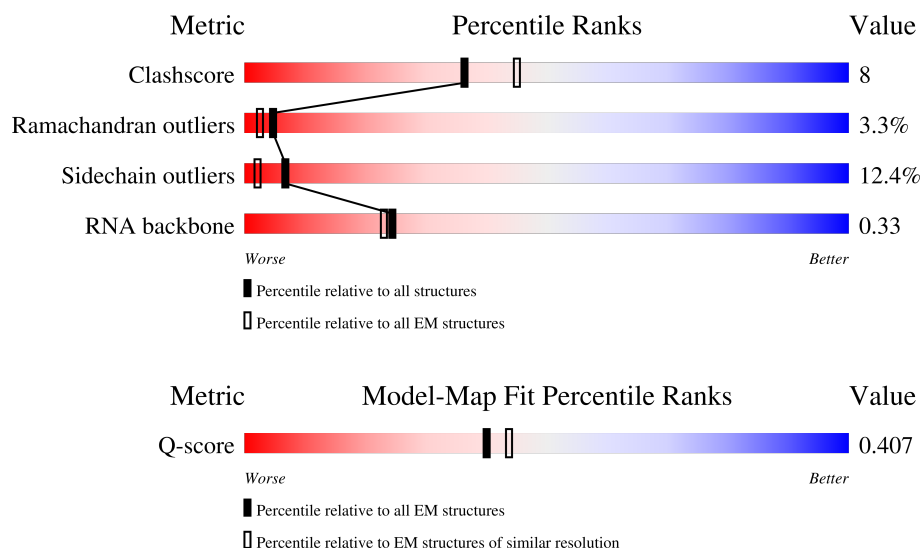
1 Overall quality at a glance

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.



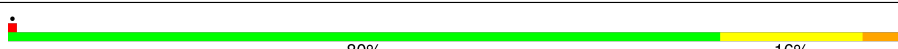
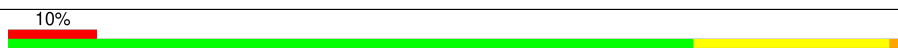
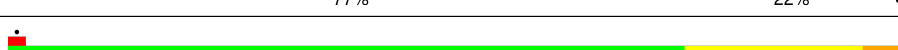
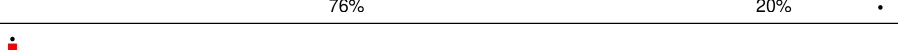
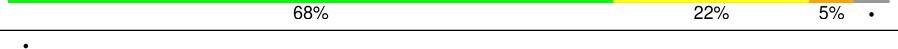
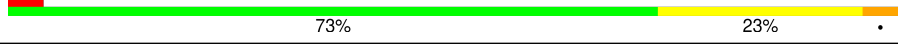
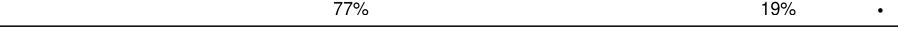
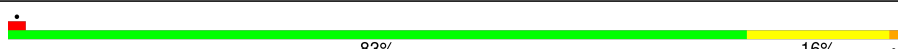
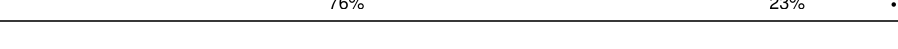
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11564 (3.15 - 4.15)

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

Mol	Chain	Length	Quality of chain
1	A	244	
2	B	394	
3	C	362	

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

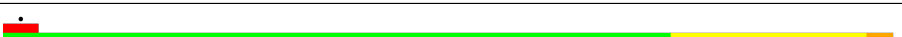
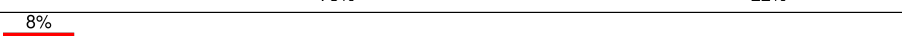
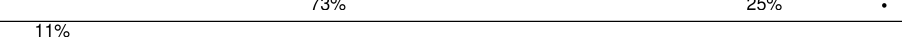
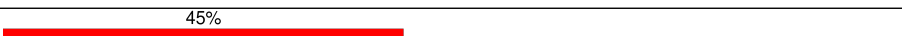
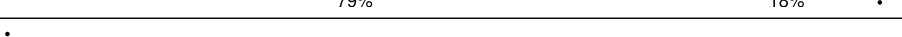
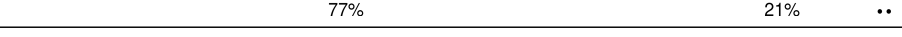
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Mol	Chain	Length	Quality of chain
29	d	107	
30	e	128	
31	f	109	
32	g	114	
33	h	122	
34	i	102	
35	j	86	
36	k	69	
37	l	50	
38	m	52	
39	n	23	
40	o	104	
41	p	91	
42	r	125	
43	s	198	
44	t	163	
45	1	15	
46	2	76	
47	3	75	
48	5	3662	
49	7	120	
50	8	156	
51	9	1719	
52	AA	208	
53	BB	213	

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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	69	
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	-

2 Entry composition [i](#)

There are 91 unique types of molecules in this entry. The entry contains 226469 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

- Molecule 3 is a protein called uL4.

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

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called uL18.

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

- Molecule 5 is a protein called eL6.

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

- Molecule 6 is a protein called uL30.

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

- Molecule 7 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called uL16.

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

- Molecule 10 is a protein called uL5.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called peptide.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA.

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

- Molecule 86 is a protein called eRF1.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	183	ALA	GLY	engineered mutation	UNP P62495
ii	184	ALA	GLY	engineered mutation	UNP P62495

- Molecule 87 is a protein called ABCE1.

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

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

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

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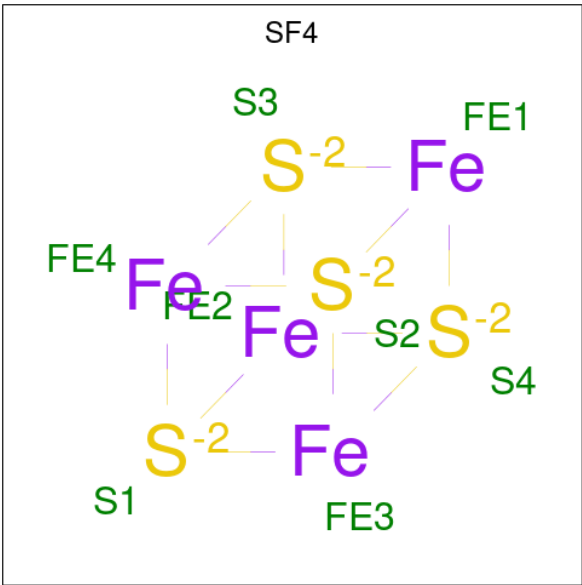
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Mol	Chain	Residues	Atoms		AltConf
88	5	146	Total 146	Mg 146	0
88	7	5	Total 5	Mg 5	0
88	8	2	Total 2	Mg 2	0
88	9	35	Total 35	Mg 35	0
88	hh	1	Total 1	Mg 1	0

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

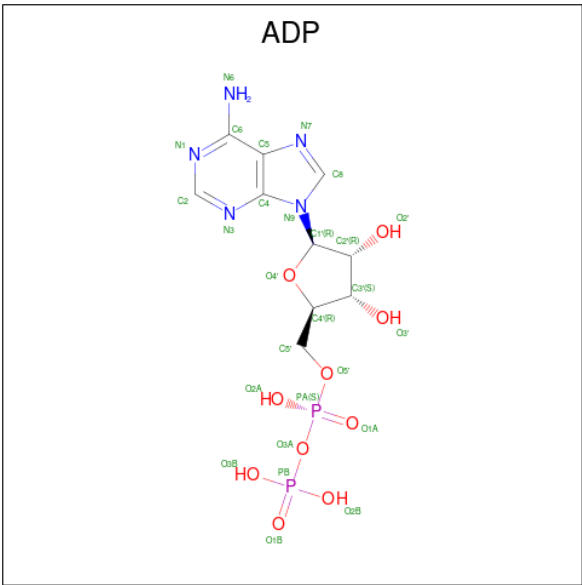
Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	p	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0

- Molecule 90 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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	

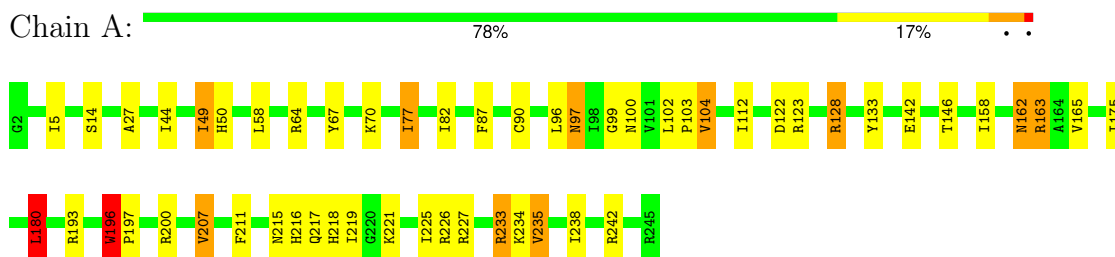
- Molecule 91 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



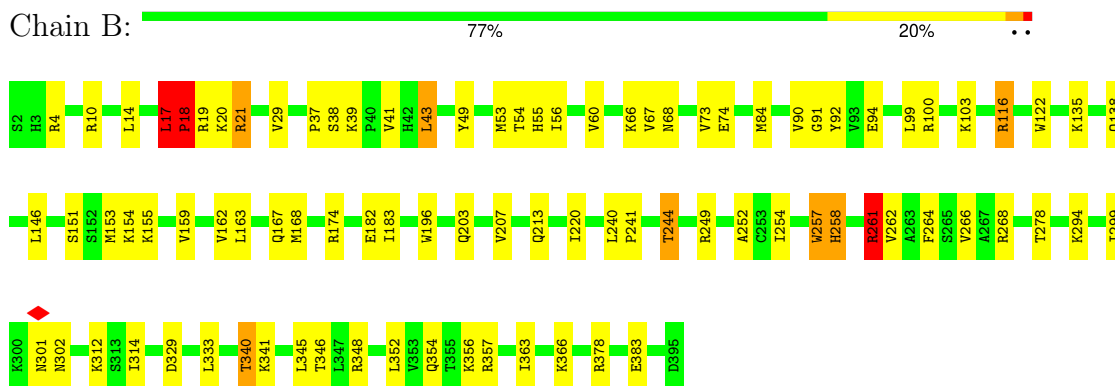
3 Residue-property plots

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.

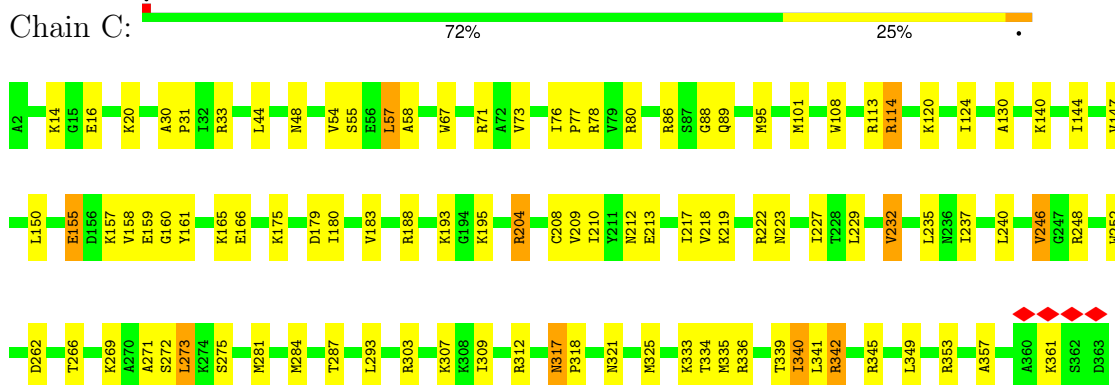
• Molecule 1: uL2



• Molecule 2: uL3

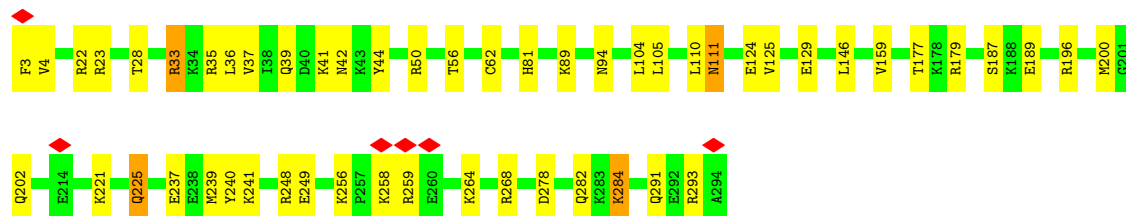


• Molecule 3: uL4



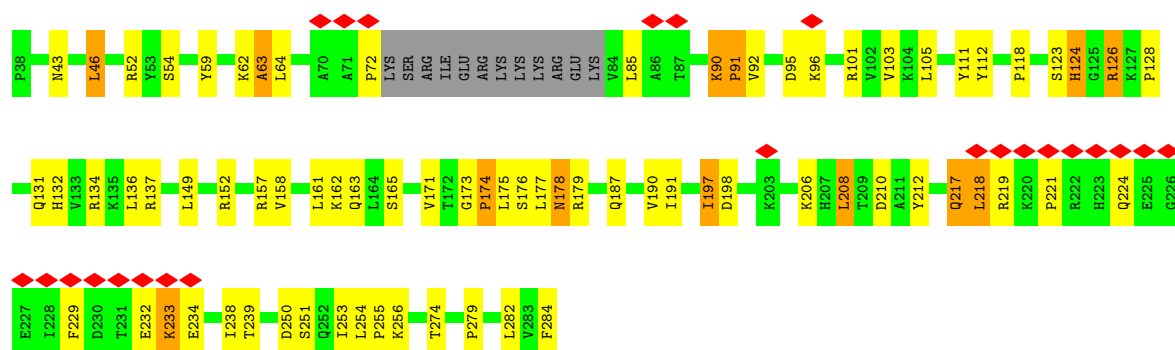
- Molecule 4: uL18

Chain D: 



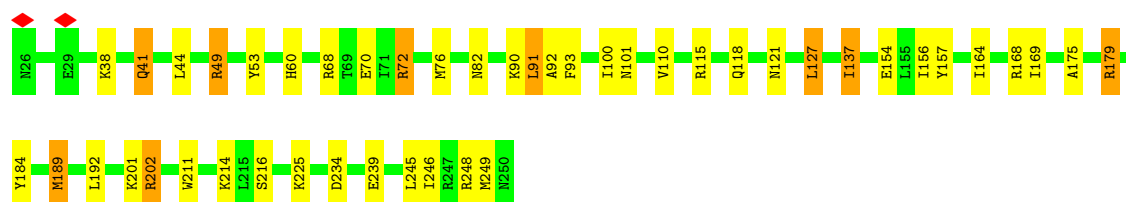
- Molecule 5: eL6

Chain E: 



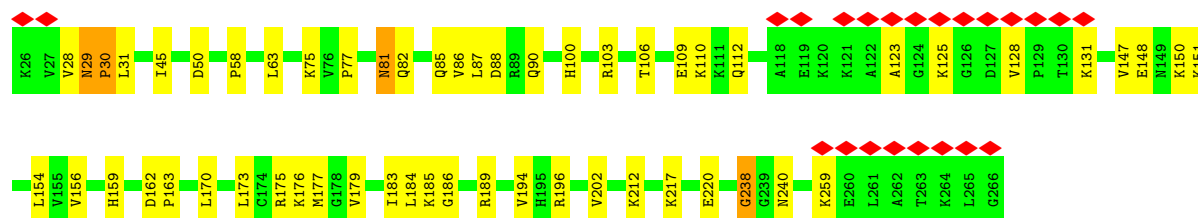
- Molecule 6: uL30

Chain F: 



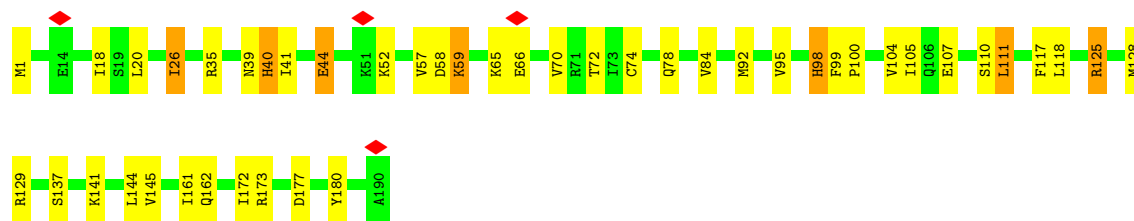
- Molecule 7: eL8

Chain G: 

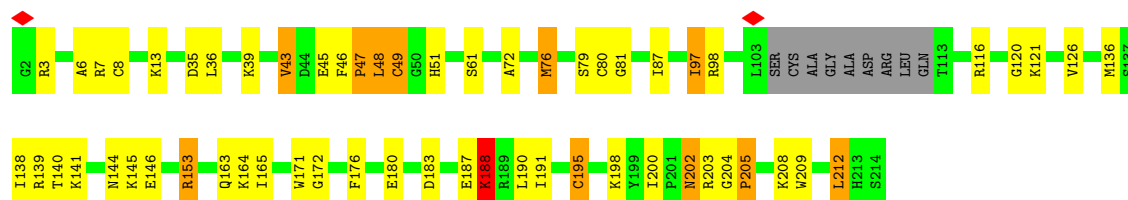


- Molecule 8: uL6

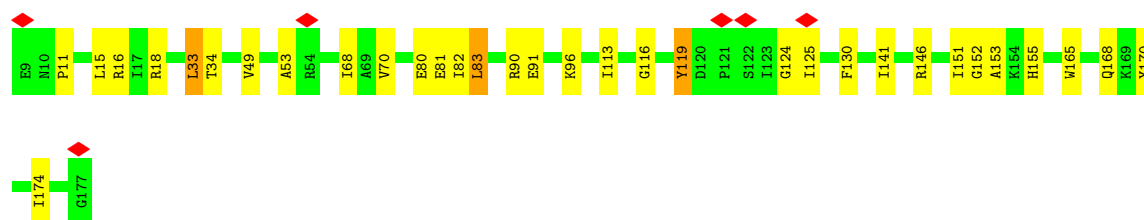
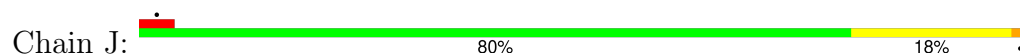
Chain H: 



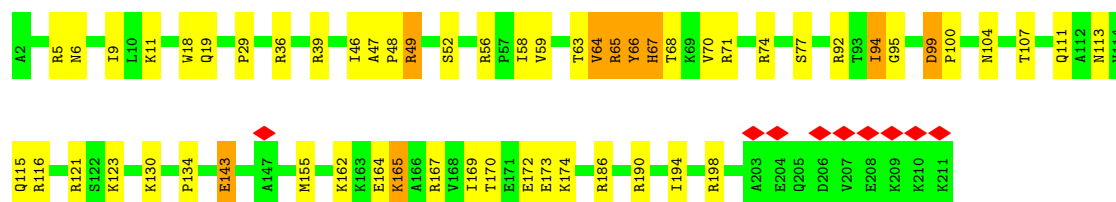
• Molecule 9: uL16



• Molecule 10: uL5



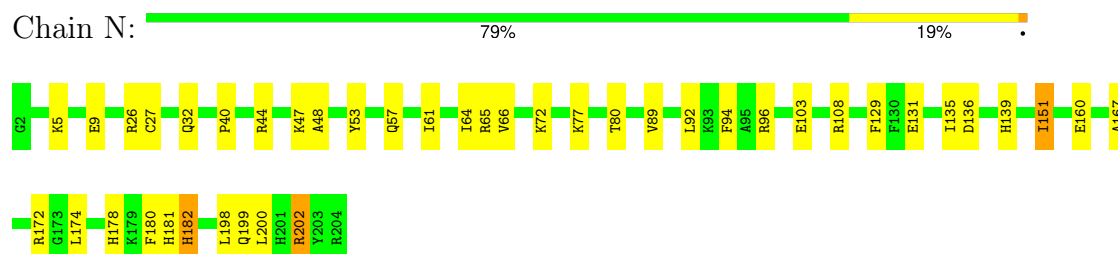
• Molecule 11: eL13



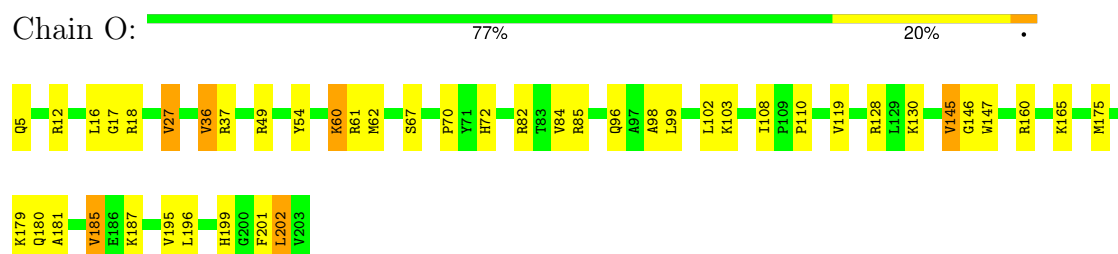
• Molecule 12: eL14



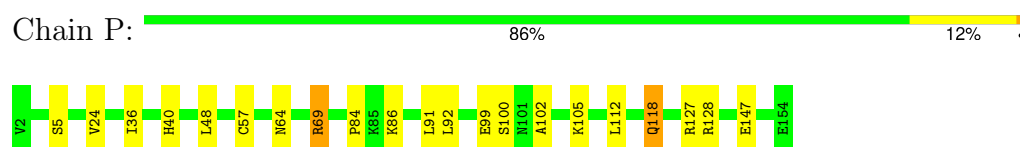
- Molecule 13: eL15



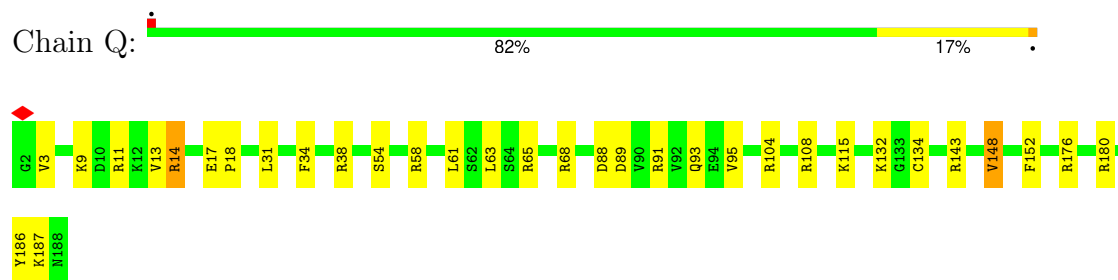
- Molecule 14: uL13



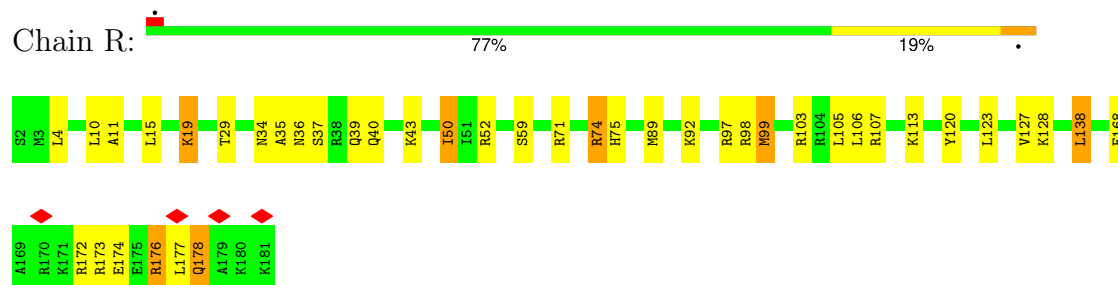
- Molecule 15: uL22



- Molecule 16: eL18

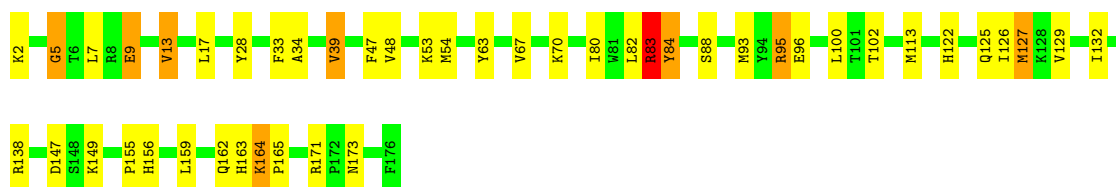


- Molecule 17: eL19



- Molecule 18: eL20

Chain S:  74% 21% 5% .



• Molecule 19: eL21

Chain T:  78% 20% .



• Molecule 20: eL22

Chain U:  84% 14% .



• Molecule 21: uL14

Chain V:  79% 20% .



• Molecule 22: eL24

Chain W:  89% 10% .



• Molecule 23: uL23

Chain X:  83% 16% .



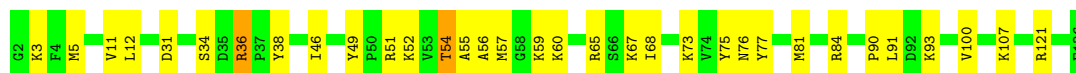
• Molecule 24: uL24

Chain Y:  81% 16% ..



• Molecule 25: eL27

Chain Z:  76% 23% .



• Molecule 26: uL15

Chain a:  79% 16% 5% .



• Molecule 27: eL29

Chain b:  11% 88% 9% .



• Molecule 28: eL30

Chain c:  80% 16% .



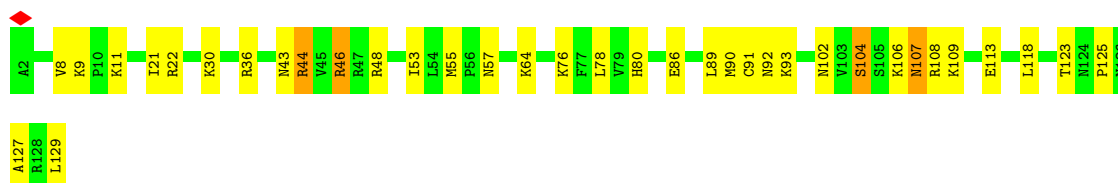
• Molecule 29: eL31

Chain d:  5% 75% 21% 5%

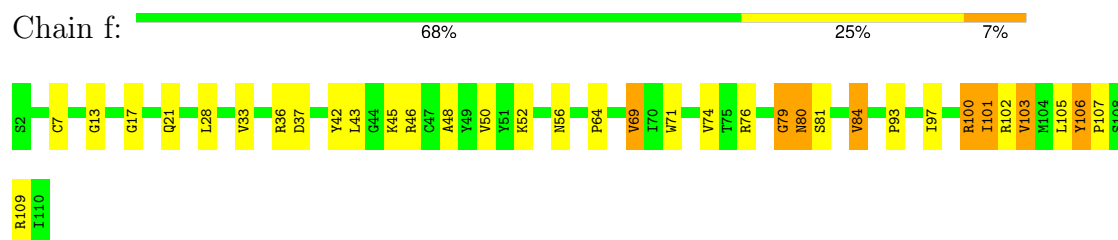


• Molecule 30: eL32

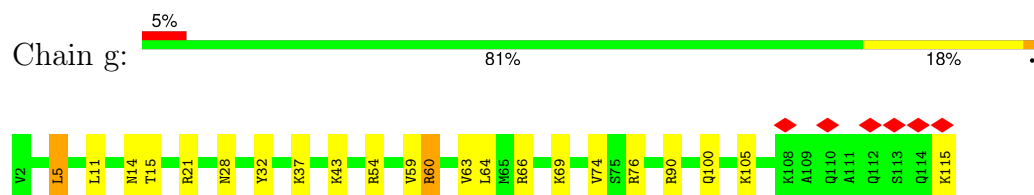
Chain e:  72% 25% .



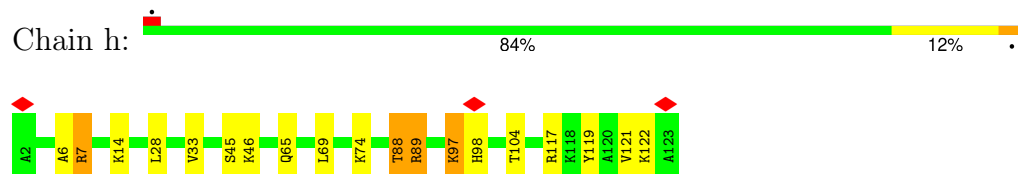
- Molecule 31: eL33



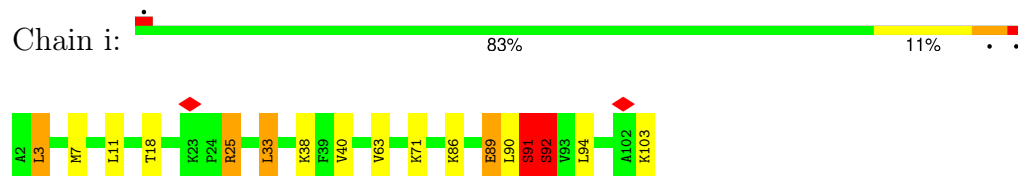
- Molecule 32: eL34



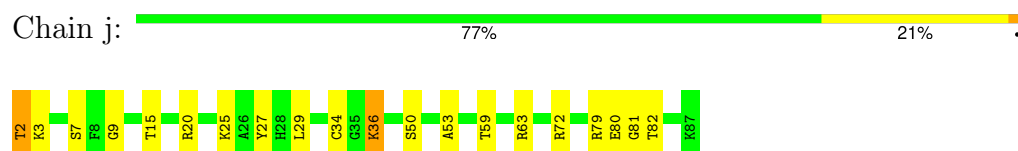
- Molecule 33: uL29



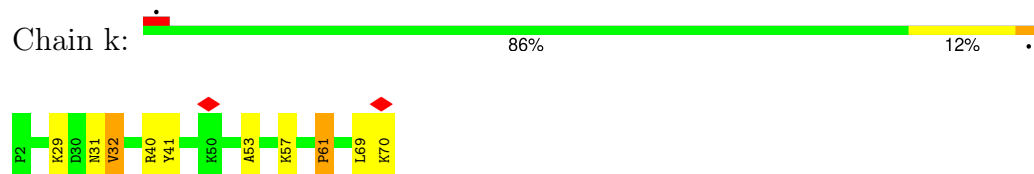
- Molecule 34: eL36



- Molecule 35: eL37

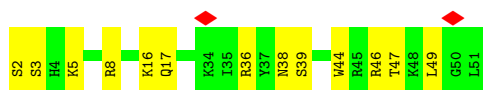


- Molecule 36: eL38

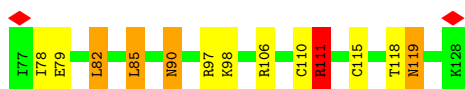
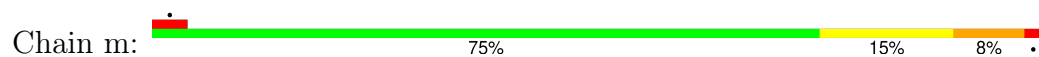


- Molecule 37: eL39

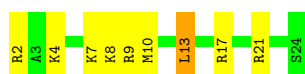




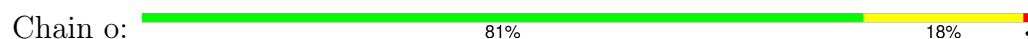
• Molecule 38: eL40



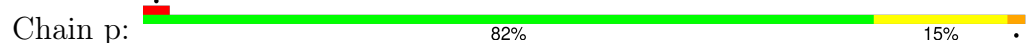
• Molecule 39: eL41



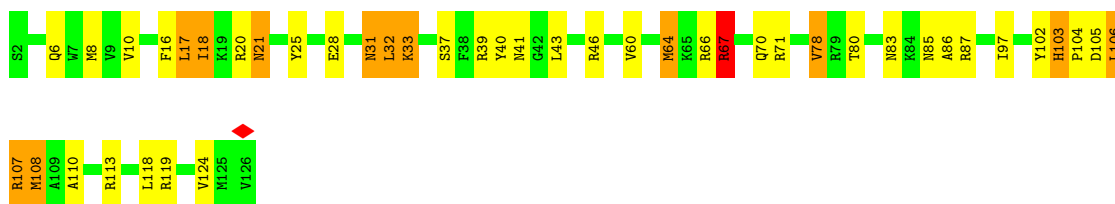
• Molecule 40: eL42



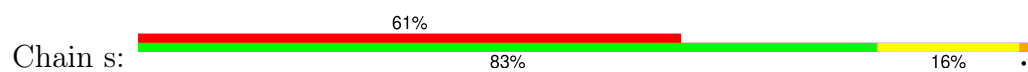
• Molecule 41: eL43

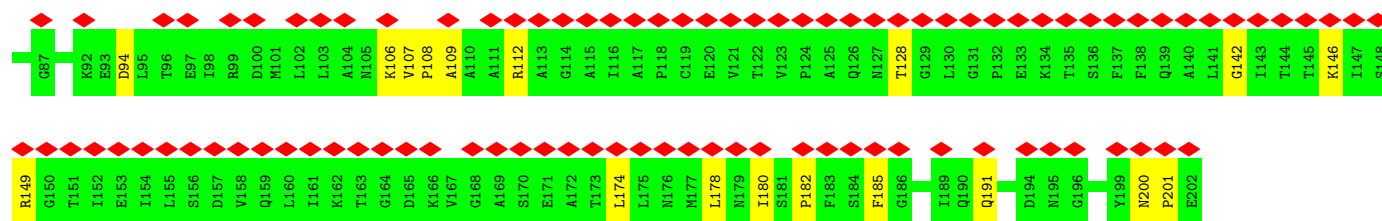


• Molecule 42: eL28

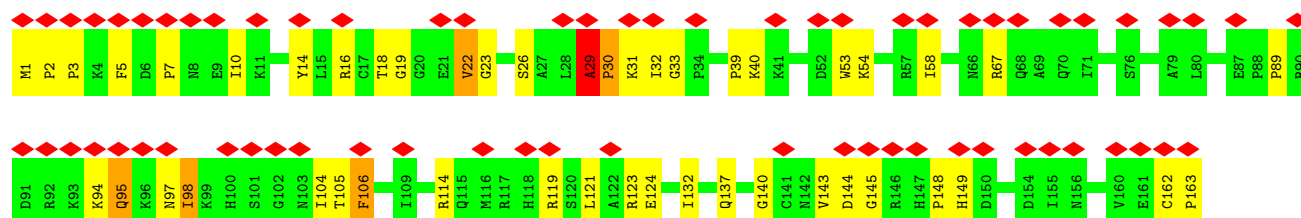
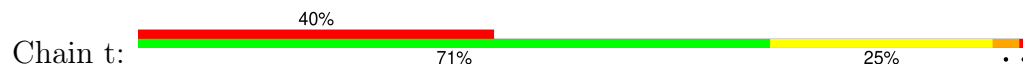


• Molecule 43: uL10

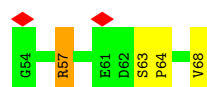




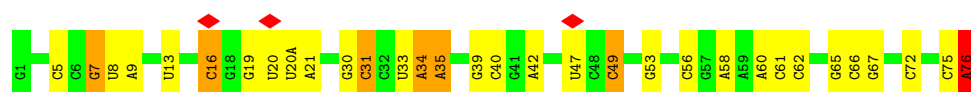
• Molecule 44: uL11



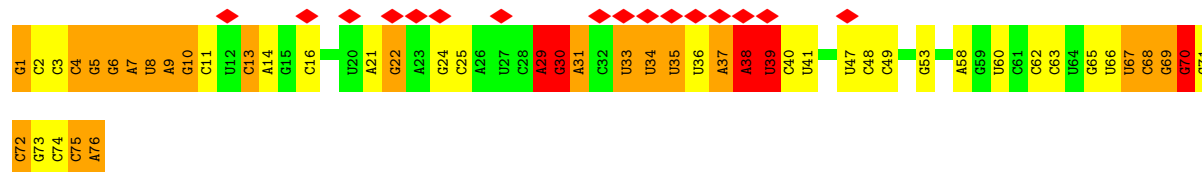
• Molecule 45: peptide



• Molecule 46: tRNA(Val)

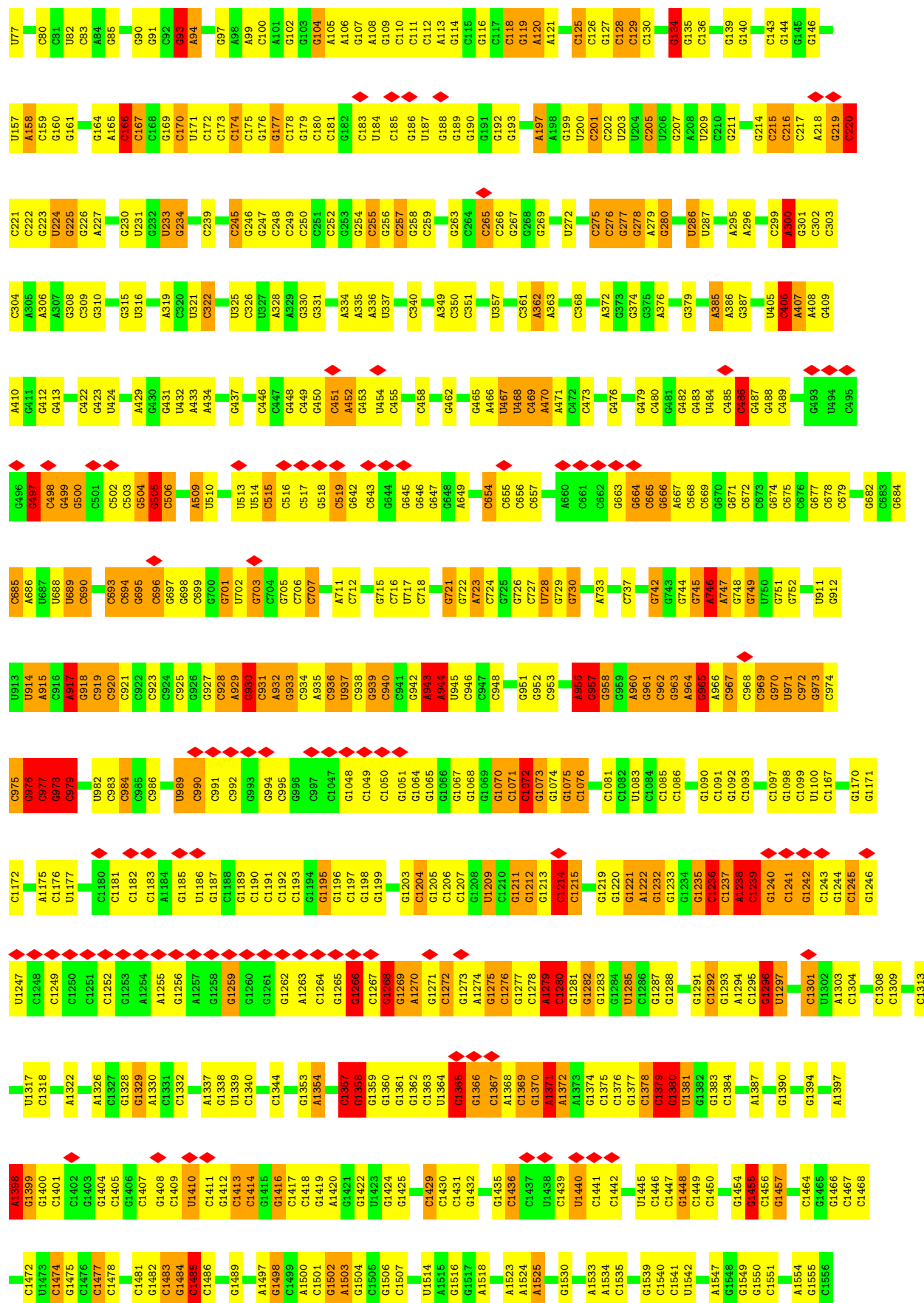


• Molecule 47: tRNA(Lys)

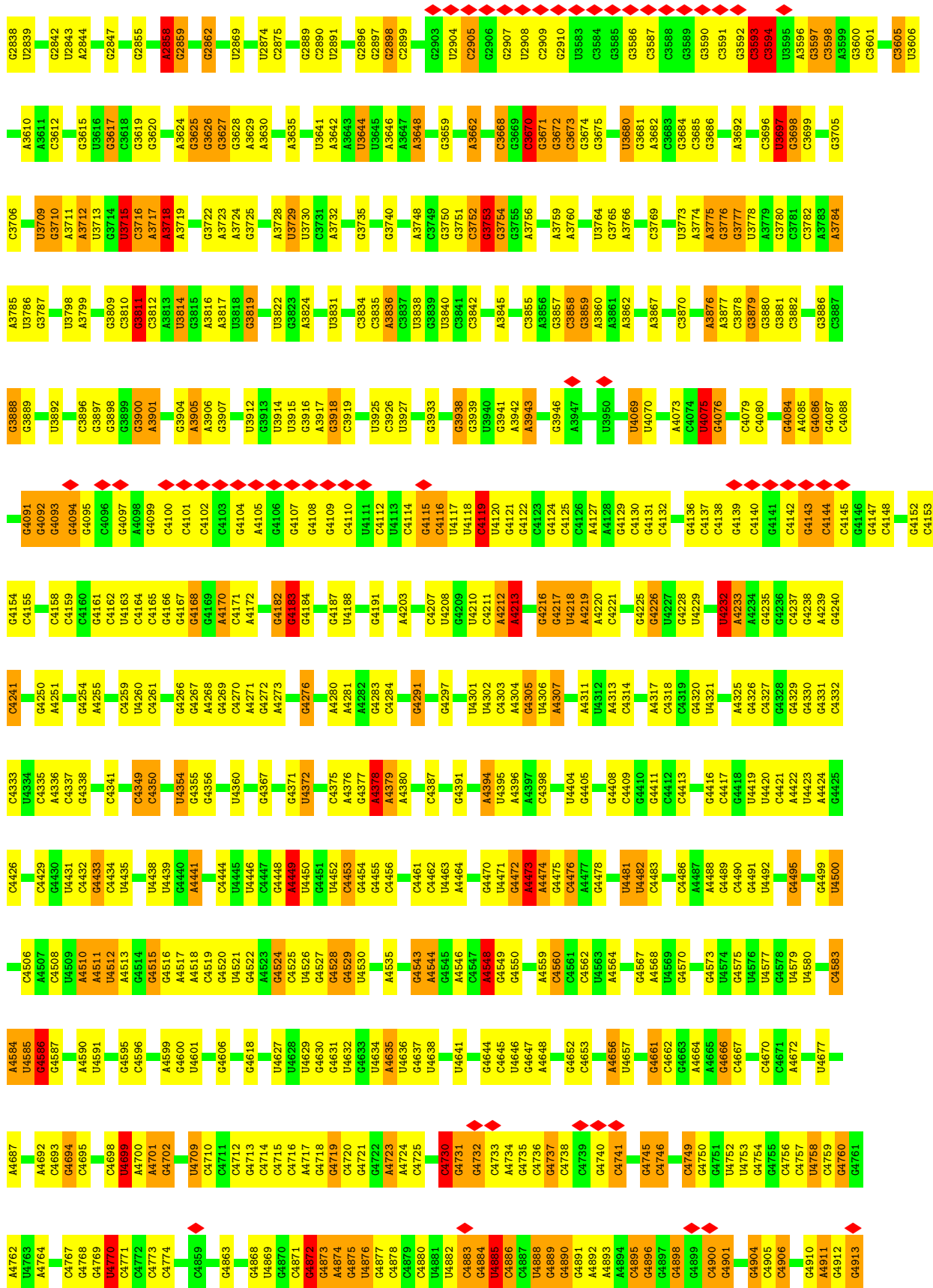


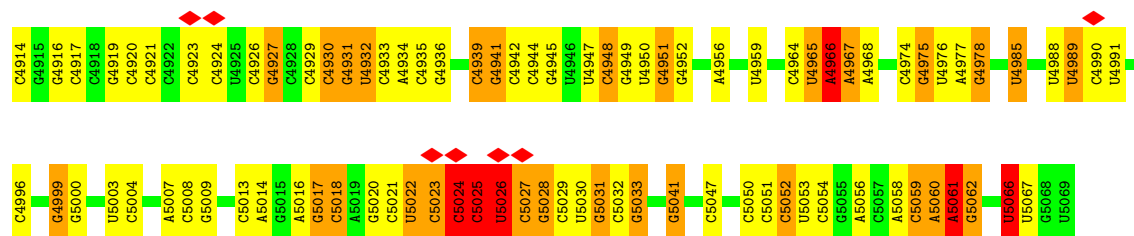
• Molecule 48: 28S ribosomal RNA





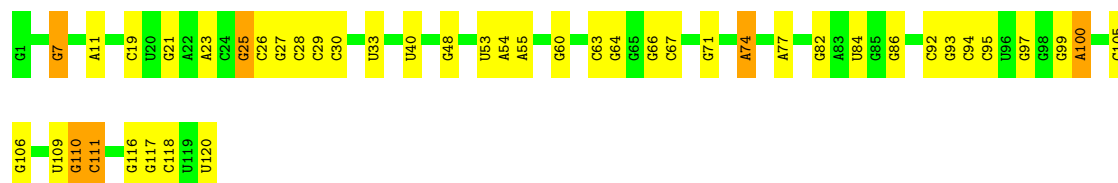
G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	A2764	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2703	G2704	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2720	G2721	G2722	G2723	G2724	A2725	G2726	G2727	G2728	G2729	U2730	G2731	G2732	G2733	U2734	U2740	A2743	A2744	G2752		
G2673	A2674	G2675	A2676	G2681	G2682	G2683	A2601	G2602	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2617	G2618	G2619	G2620	A2621	G2622	A2623	G2624	G2627	U2632	G2633	G2638	U2639	G2640	A2641	A2642	G2643	G2644	G2645	G2646	A2647	G2654	G2658	U2661	G2662	G2663	G2664	G2669	G2670	G2671	G2672									
G2586	A2587	G2588	G2589	G2594	A2601	G2602	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2617	G2618	G2619	G2620	A2621	G2622	A2623	G2624	G2627	U2632	G2633	G2638	U2639	G2640	A2641	A2642	G2643	G2644	G2645	G2646	A2647	G2654	G2658	U2661	G2662	G2663	G2664	G2669	G2670	G2671	G2672											
A2511	A2512	A2513	G2514	G2515	G2516	A2517	G2518	U2519	G2520	G2521	U2524	U2525	G2526	A2527	U2530	G2531	A2537	U2538	G2539	G2540	G2541	G2542	A2543	G2544	U2545	G2546	G2547	G2548	A2553	U2554	G2555	G2556	G2557	G2558	G2559	G2560	G2564	A2565	G2566	G2567	G2568	G2569	U2570	G2571	G2572	U2575	G2576	G2577	A2581	A2582	G2583							
G2427	A2428	A2429	G2433	G2434	G2435	G2439	U2440	G2441	G2446	G2450	G2457	G2458	G2459	G2465	G2466	U2467	U2468	G2469	G2470	G2471	A2472	G2473	G2474	G2475	G2476	A2477	G2478	G2479	G2481	G2482	U2485	G2488	G2489	U2490	G2491	G2492	G2493	U2494	U2495	G2496	G2497	G2498	G2499	G2502	G2503	G2504	G2505	G2506	A2507									
A2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	A2341	G2345	G2346	A2347	G2348	A2349	U2350	G2351	G2355	U2356	G2357	A2360	A2363	G2364	A2367	G2368	U2369	A2370	A2374	A2382	G2390	G2391	G2392	A2395	A2396	G2397	U2398	G2399	G2406	G2407	U2408	U2409	G2410	A2417	G2422	A2423	G2424	U2425	U2426											
A2253	G2254	G2255	G2256	G2257	G2258	G2259	G2260	G2261	G2262	A2263	G2264	G2265	G2266	U2267	G2268	G2269	G2270	G2271	G2272	G2274	G2275	A2276	G2277	G2278	A2282	G2288	G2289	G2290	G2294	G2295	G2296	G2297	G2298	G2299	A2300	G2301	G2302	G2303	G2311	U2312	A2313	G2314	G2315	G2319	G2322	G2323	G2324	G2325	G2328	G2331								
G2003	U2004	G2005	U2006	G2007	U2008	A2009	A2010	G2011	G2016	A2017	G2018	G2019	U2020	G2021	G2022	G2023	G2024	A2025	A2026	G2027	G2028	A2029	G2034	G2035	A2043	U2044	G2045	G2046	A2047	U2048	G2049	G2050	G2051	G2052	G2053	U2054	G2055	G2056	A2057	G2058	G2059	G2062	G2063	G2064	G2065	G2066	G2067	G2068	A2069	U2070	A2071	G2072	G2073	G2076				
C1926	G1835	G1836	G1837	G1838	G1839	G1840	G1842	G1846	G1847	G1848	G1854	G1855	G1856	A1857	G1858	G1859	G1861	G1862	C1863	A1864	G1865	G1866	G1867	G1868	G1869	G1872	A1873	A1874	G1878	G1879	U1882	G1885	G1886	G1889	A1891	G1892	A1893	A1894	G1895	U1896	G1897	G1898	G1899	A1900	G1904	A1907	G1910	A1911	G1912	G1913	U1918	G1919	G1920	U1921	G1922	A1923	C1924	A2002
U1754	G1755	U1756	U1757	G1758	G1759	U1760	G1761	G1762	G1763	G1764	A1765	G1766	A1767	G1768	U1771	G1772	U1773	G1774	A1775	A1776	C1777	A1780	U1781	U1782	C1783	A1787	G1798	G1799	U1800	A1804	A1805	C1808	G1811	G1812	G1815	G1818	G1819	C1820	G1821	U1822	G1823	A1825	G1826	C1827	G1828	G1829	G1830	G1831	C1832	G1833								
A1668	A1669	G1670	U1671	A1672	U1673	G1676	U1677	G1678	A1679	A1682	U1683	A1684	G1685	G1686	U1687	G1688	G1689	G1690	G1691	G1692	U1693	G1694	U1695	G1696	G1697	G1698	A1699	G1718	A1719	G1720	G1721	G1722	A1723	G1724	U1725	U1726	A1729	G1732	G1733	G1734	U1735	G1739	G1740	G1741	A1742	A1746	U1747	U1748	A1749	G1750	A1751	G1752	G1753					





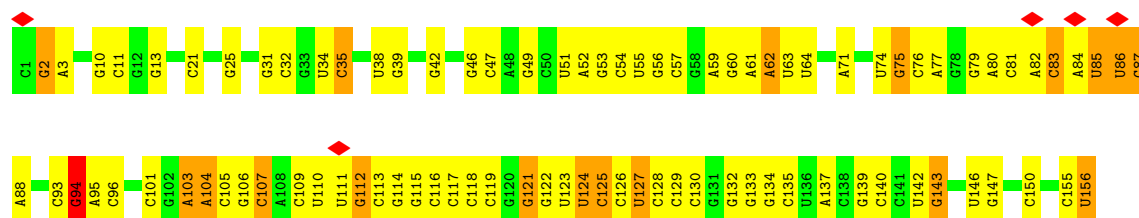
• Molecule 49: 5S ribosomal RNA

Chain 7: 63% 32% 5%



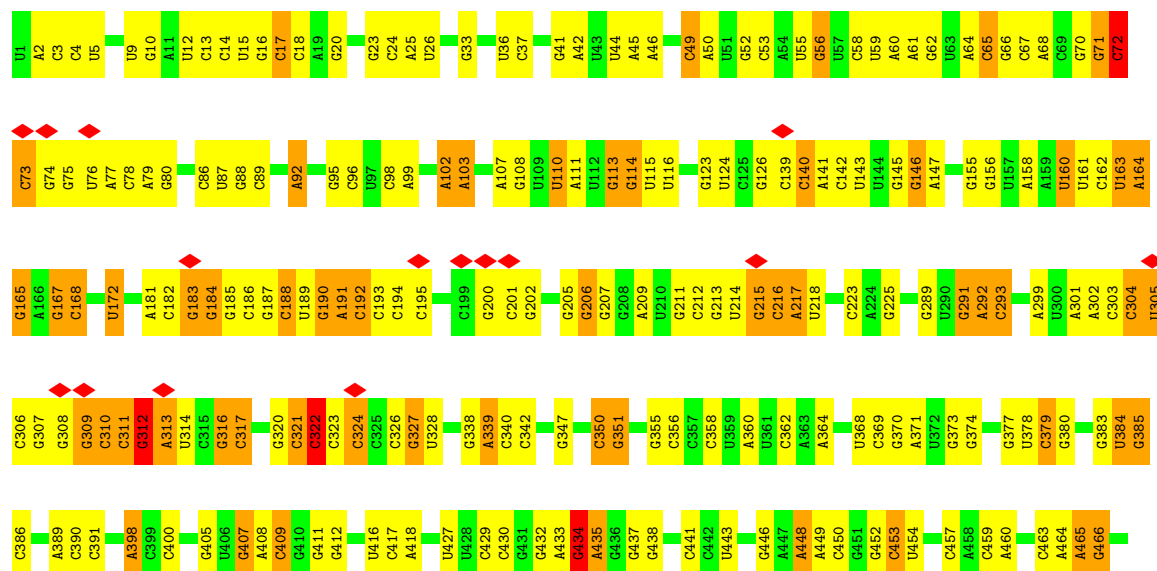
• Molecule 50: 5.8S ribosomal RNA

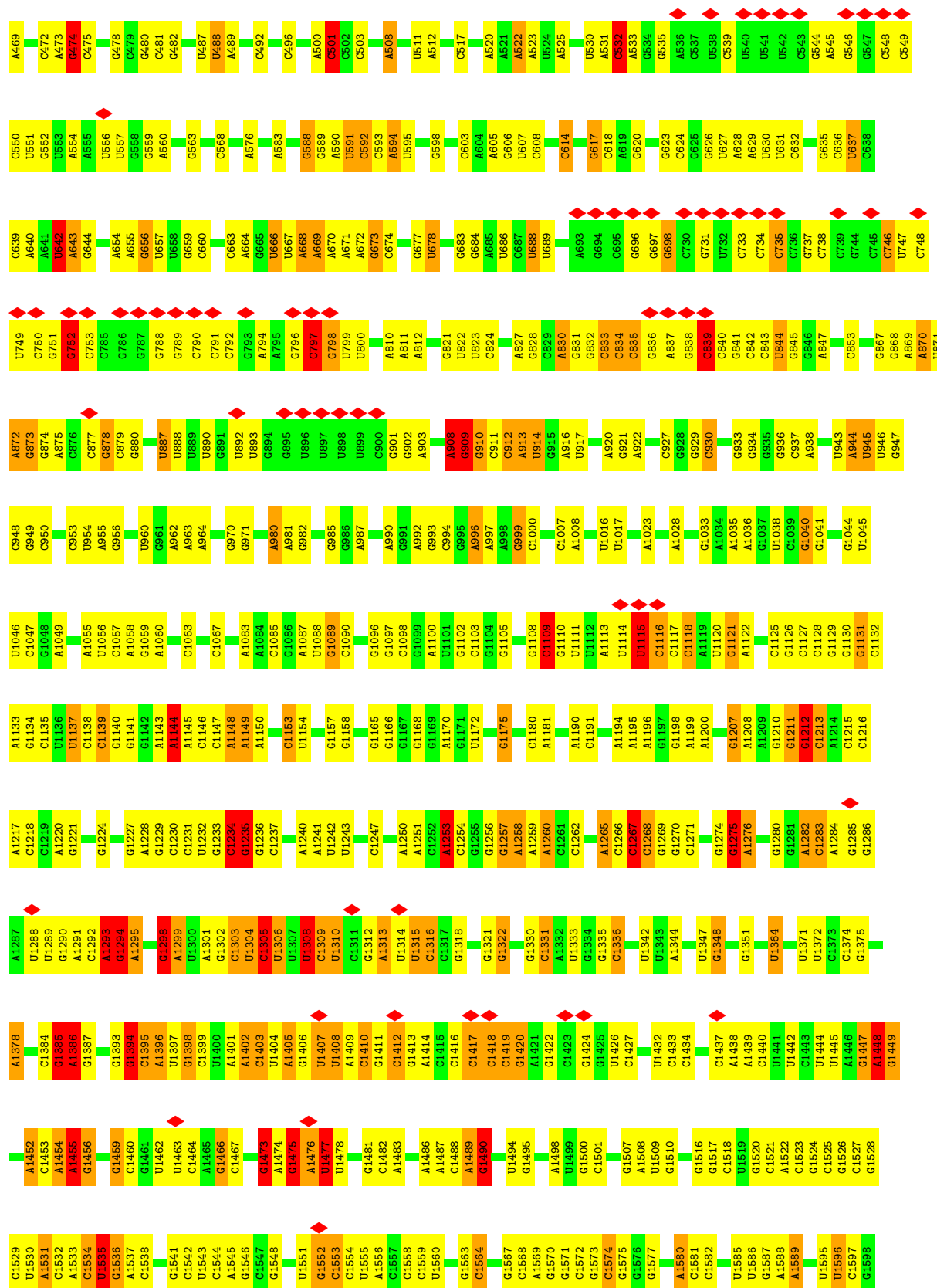
Chain 8: 42% 46% 12%

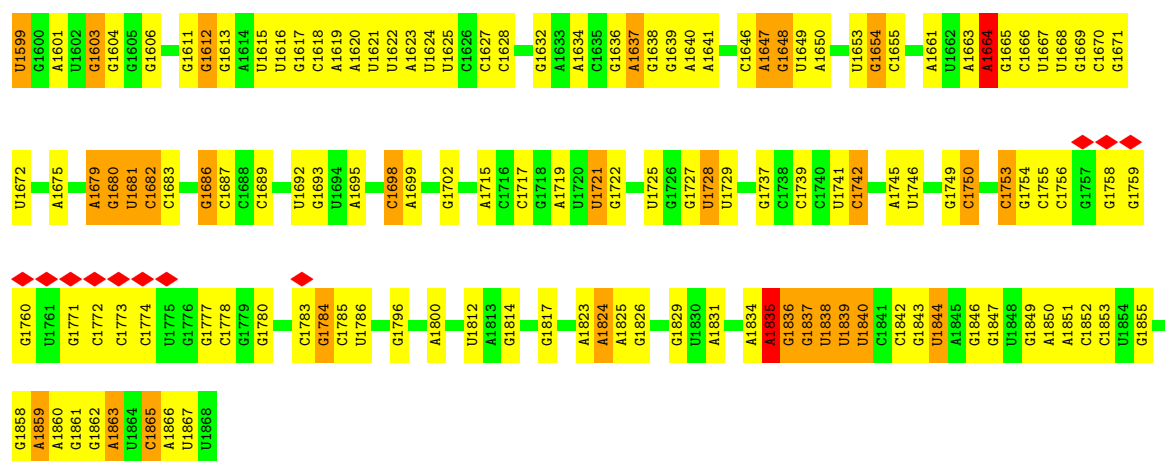


• Molecule 51: 18S ribosomal RNA

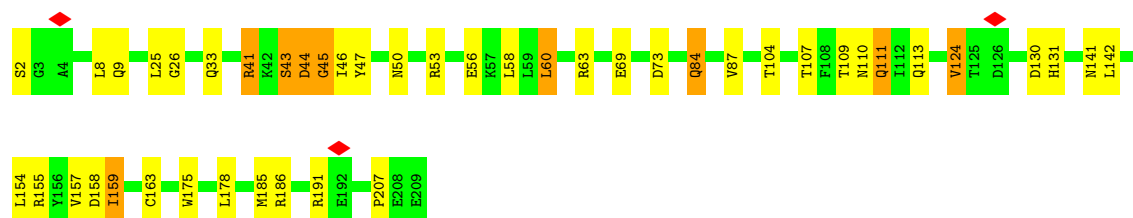
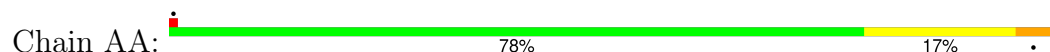
Chain 9: 5% 46% 40% 12%



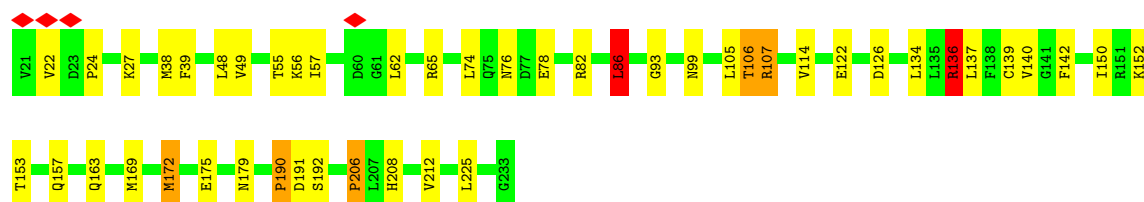
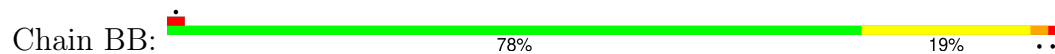




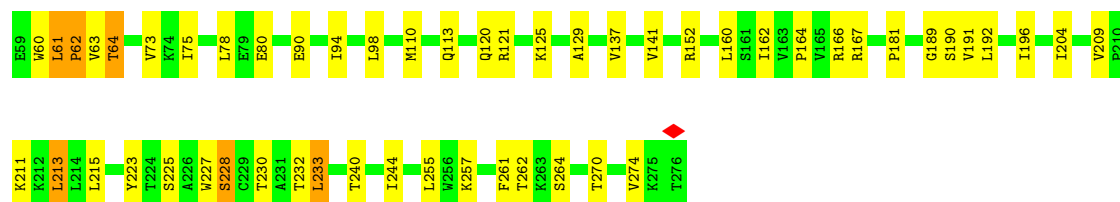
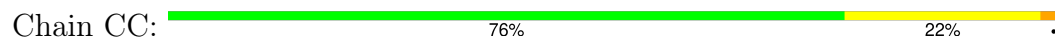
• Molecule 52: uS2



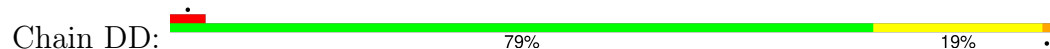
• Molecule 53: eS1

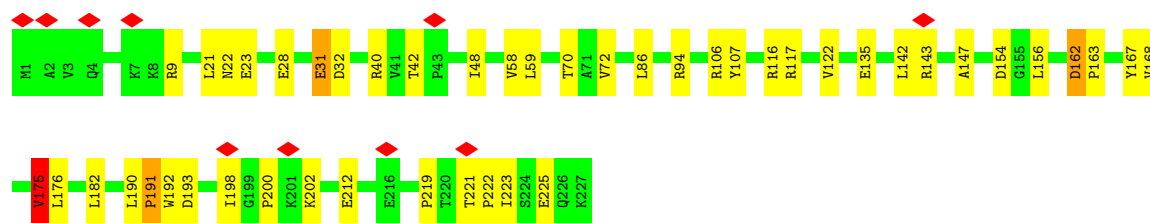


• Molecule 54: uS5

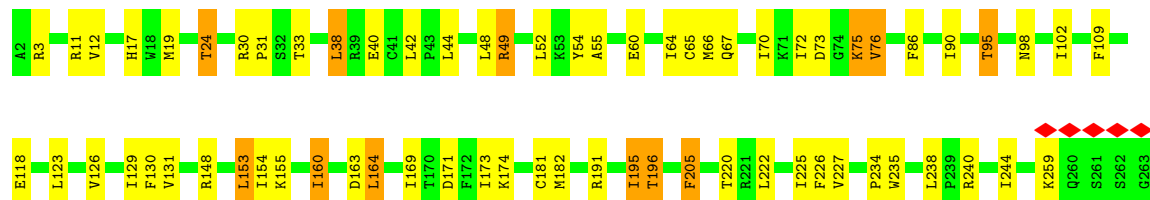
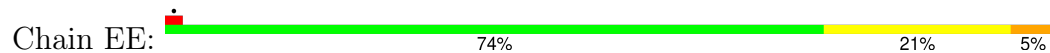


• Molecule 55: uS3

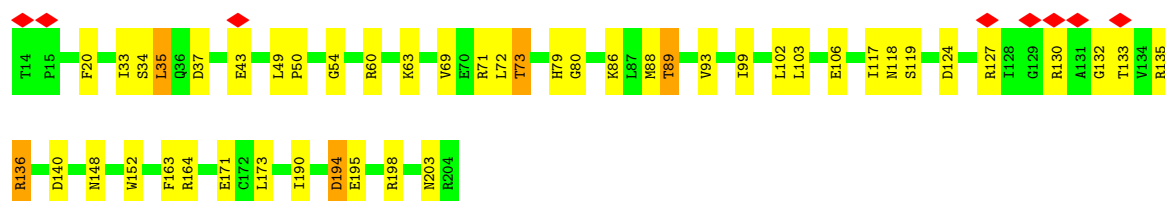
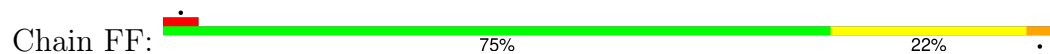




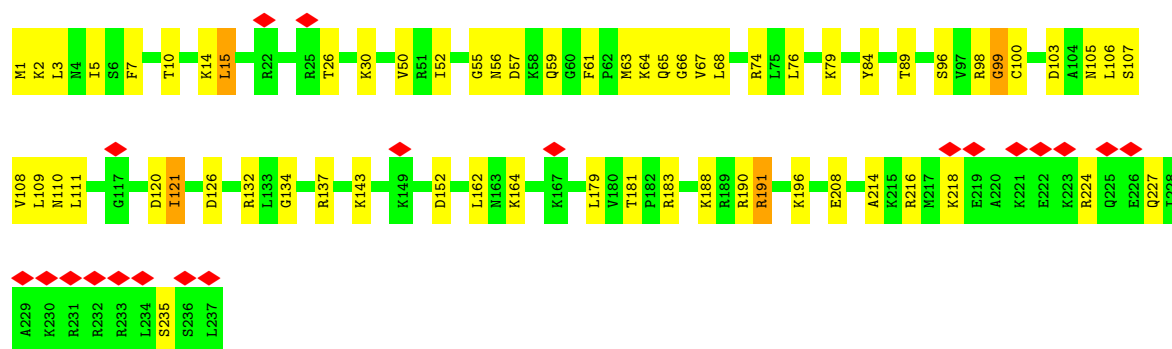
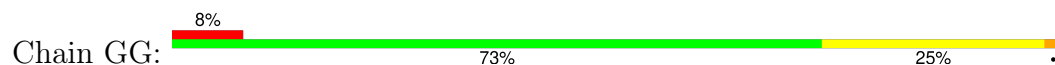
• Molecule 56: eS4



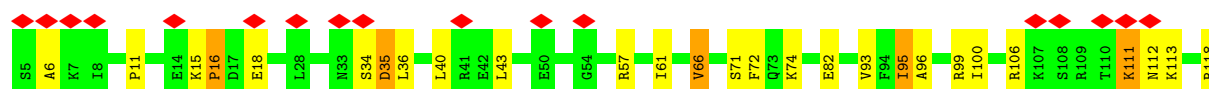
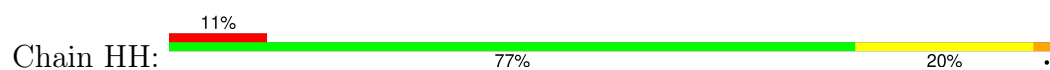
• Molecule 57: uS7

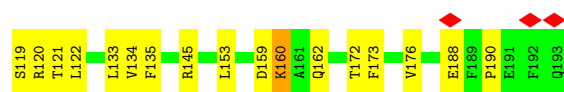


• Molecule 58: eS6

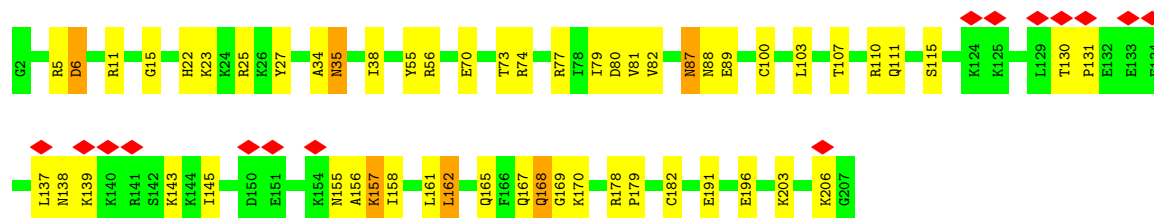
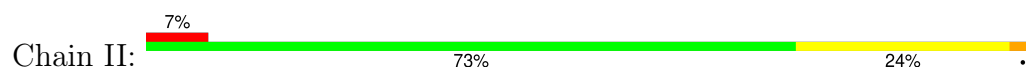


• Molecule 59: eS7

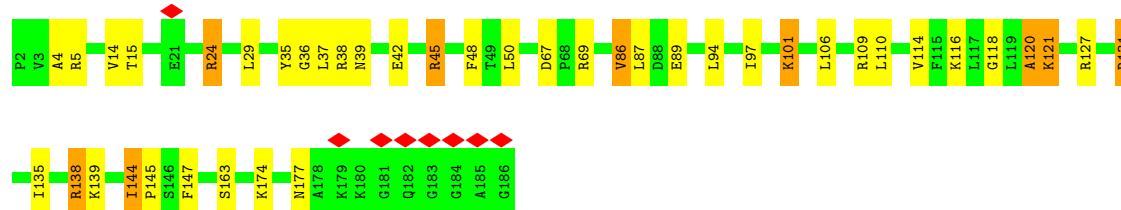
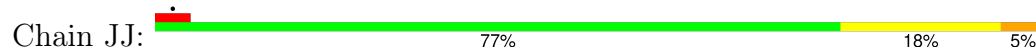




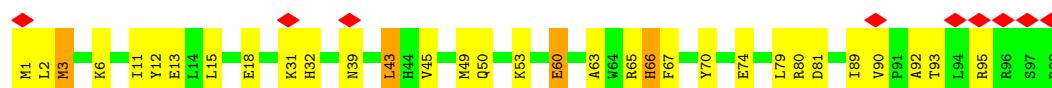
• Molecule 60: eS8



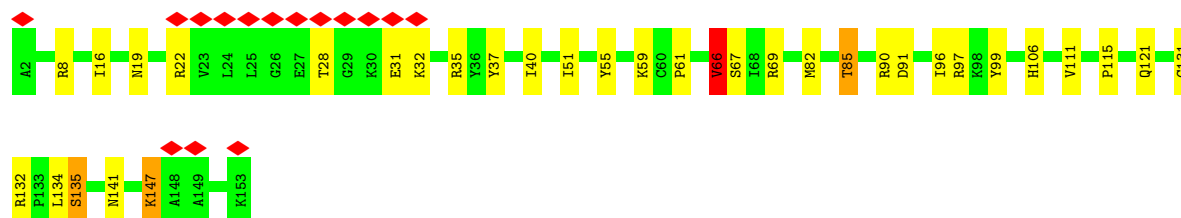
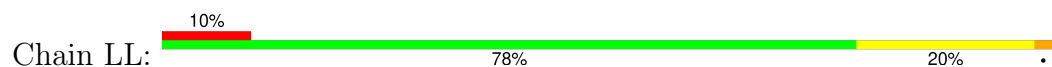
• Molecule 61: uS4



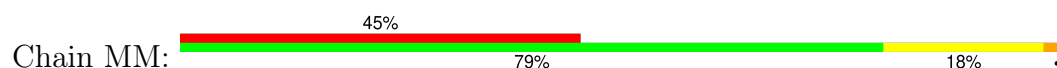
• Molecule 62: eS10

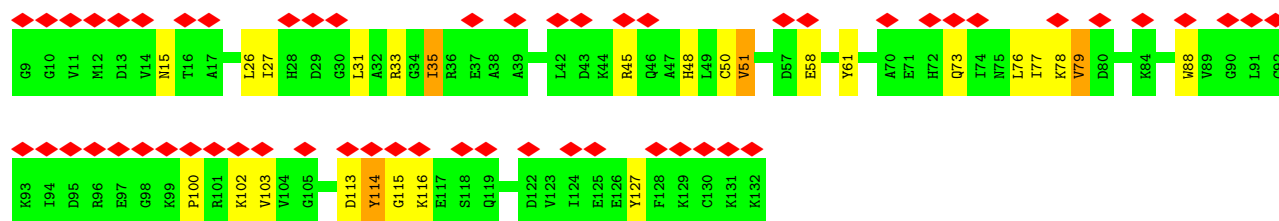


• Molecule 63: uS17

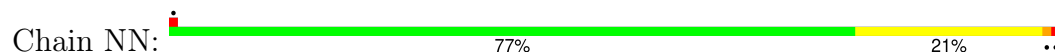


• Molecule 64: eS12

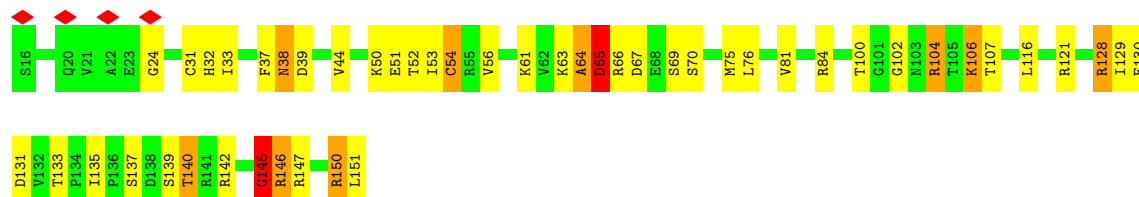




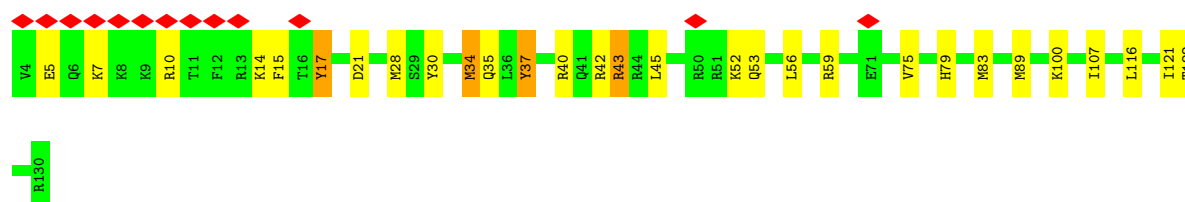
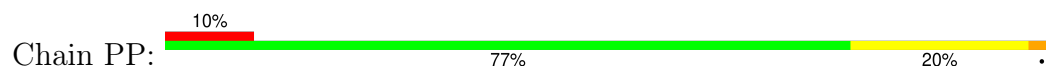
• Molecule 65: uS15



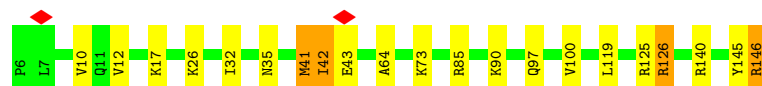
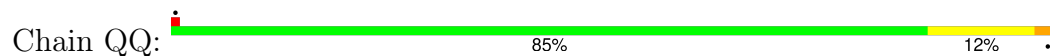
• Molecule 66: uS11



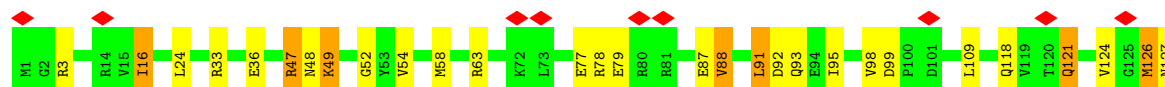
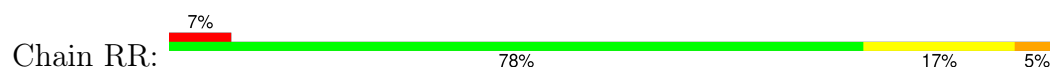
• Molecule 67: uS19



• Molecule 68: uS9



• Molecule 69: eS17



R128
K129

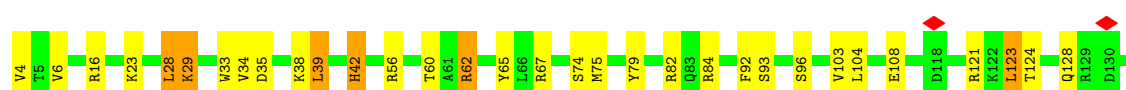
- Molecule 70: uS13

Chain SS:  77% 18%



- Molecule 71: eS19

Chain TT:  77% 18%



R143
K144

- Molecule 72: uS10

Chain UU:  9% 83% 14%



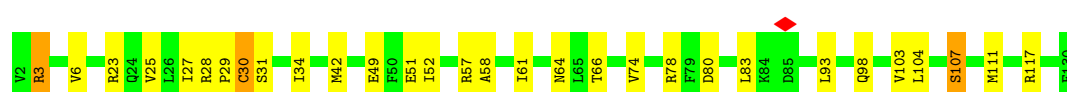
- Molecule 73: eS21

Chain VV:  77% 22%



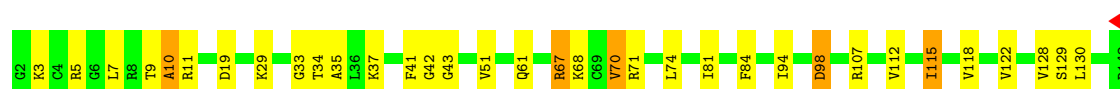
- Molecule 74: uS8

Chain WW:  77% 21%



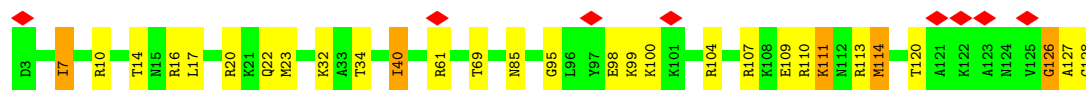
- Molecule 75: uS12

Chain XX:  76% 21%



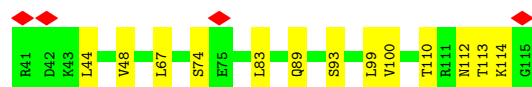
- Molecule 76: eS24

Chain YY: 



- Molecule 77: eS25

Chain ZZ: 



- Molecule 78: eS26

Chain aa: 



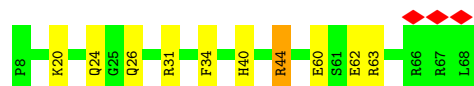
- Molecule 79: eS27

Chain bb: 



- Molecule 80: eS28

Chain cc: 



- Molecule 81: uS14

Chain dd: 

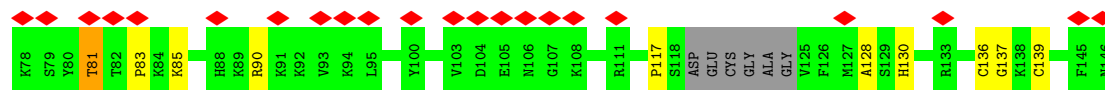
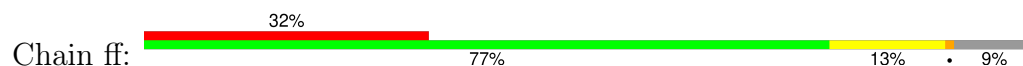


- Molecule 82: eS30

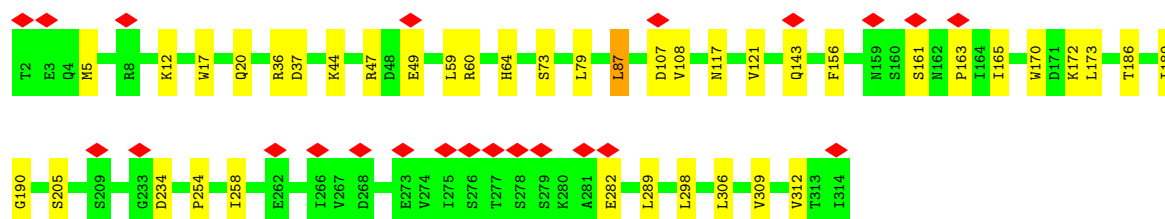
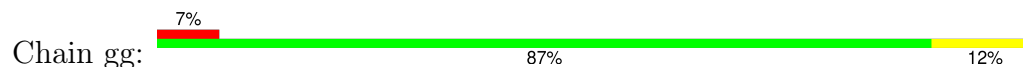
Chain ee: 



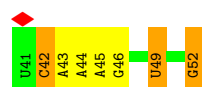
- Molecule 83: eS31



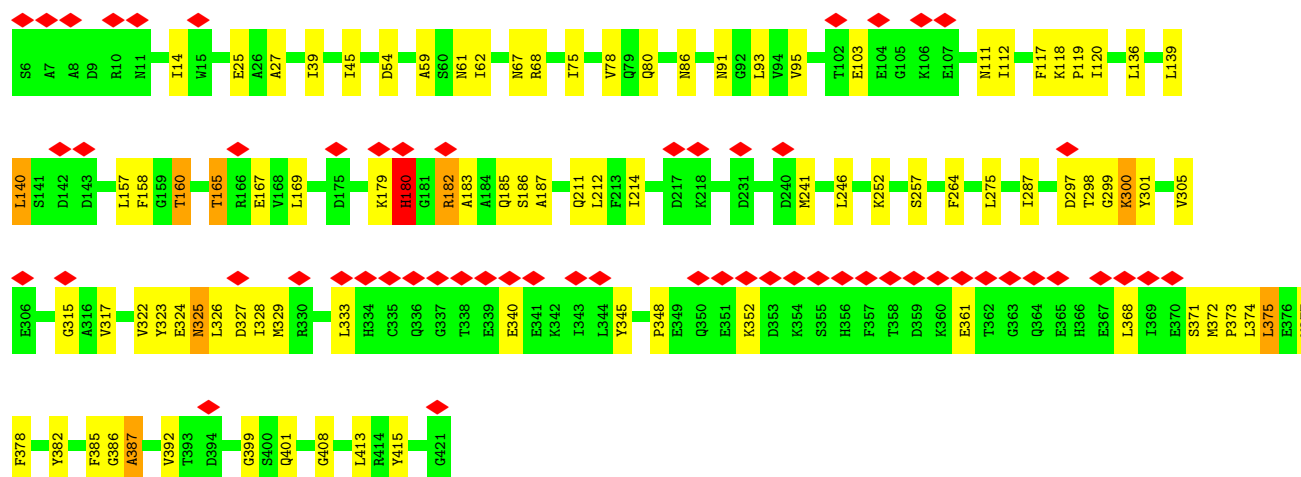
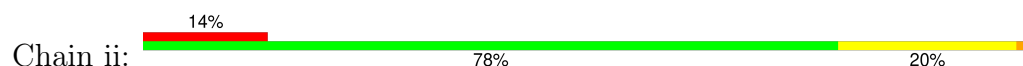
- Molecule 84: RACK1



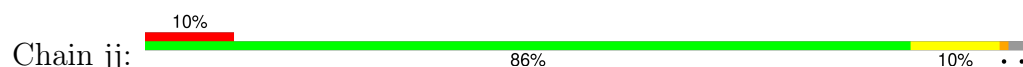
- Molecule 85: mRNA

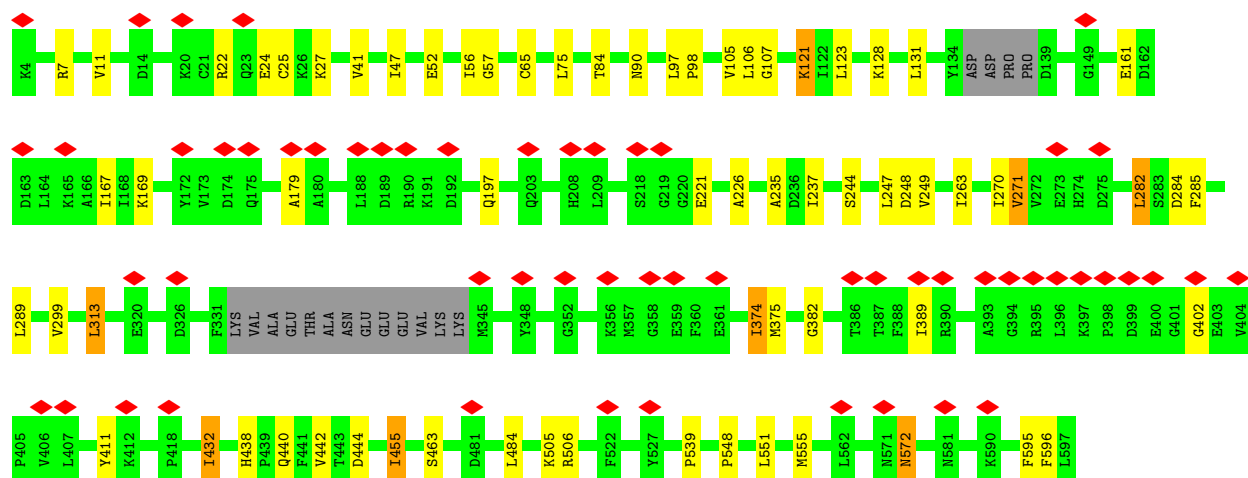


- Molecule 86: eRF1



- Molecule 87: ABCE1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	49979	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	2000, 2000	Depositor
Maximum defocus (nm)	3600, 3600	Depositor
Magnification	104478, 104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.759	Depositor
Minimum map value	-0.468	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ADP, ZN, MG, SF4

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	0.66	3/1906 (0.2%)	0.91	6/2556 (0.2%)
2	B	0.62	2/3216 (0.1%)	0.89	7/4311 (0.2%)
3	C	0.62	1/2937 (0.0%)	0.94	4/3946 (0.1%)
4	D	0.52	1/2432 (0.0%)	0.86	0/3257
5	E	0.63	0/1936	0.96	5/2600 (0.2%)
6	F	0.59	0/1905	0.85	0/2539
7	G	0.57	1/1967 (0.1%)	0.93	3/2647 (0.1%)
8	H	0.55	0/1535	0.84	0/2063
9	I	0.54	0/1693	0.85	2/2260 (0.1%)
10	J	0.51	0/1376	0.84	1/1841 (0.1%)
11	L	0.57	0/1734	0.91	1/2317 (0.0%)
12	M	0.57	1/1158 (0.1%)	0.92	1/1547 (0.1%)
13	N	0.60	0/1746	0.92	0/2338
14	O	0.64	1/1671 (0.1%)	0.94	1/2234 (0.0%)
15	P	0.67	1/1268 (0.1%)	0.91	2/1700 (0.1%)
16	Q	0.59	0/1530	0.89	1/2041 (0.0%)
17	R	0.57	1/1524 (0.1%)	0.90	0/2013
18	S	0.65	2/1493 (0.1%)	0.96	4/2002 (0.2%)
19	T	0.54	0/1326	0.82	2/1770 (0.1%)
20	U	0.47	0/822	0.74	0/1103
21	V	0.60	0/993	0.89	1/1332 (0.1%)
22	W	0.55	0/541	0.89	2/720 (0.3%)
23	X	0.58	1/993 (0.1%)	0.85	0/1334
24	Y	0.55	1/1132 (0.1%)	0.88	1/1504 (0.1%)
25	Z	0.54	0/1130	0.90	3/1507 (0.2%)
26	a	0.59	0/1191	0.91	2/1590 (0.1%)
27	b	0.57	1/619 (0.2%)	0.92	0/818
28	c	0.52	0/742	0.87	0/996
29	d	0.57	0/903	0.86	1/1216 (0.1%)
30	e	0.66	1/1071 (0.1%)	0.94	0/1429
31	f	0.63	0/895	0.98	3/1198 (0.3%)
32	g	0.60	1/916 (0.1%)	0.88	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.51	0/1021	0.92	0/1348
34	i	0.75	1/841 (0.1%)	2.32	6/1112 (0.5%)
35	j	0.66	0/720	0.98	0/952
36	k	0.53	0/575	0.85	1/761 (0.1%)
37	l	0.62	0/454	0.92	0/599
38	m	0.58	0/435	0.92	0/575
39	n	0.59	0/223	0.88	0/284
40	o	0.56	0/864	0.82	0/1140
41	p	0.59	1/718 (0.1%)	0.91	1/953 (0.1%)
42	r	0.66	2/1017 (0.2%)	0.95	1/1364 (0.1%)
43	s	0.57	0/1547	0.82	3/2088 (0.1%)
44	t	0.64	0/1257	0.97	3/1697 (0.2%)
45	1	0.60	0/129	0.89	2/173 (1.2%)
46	2	0.37	0/1805	0.77	1/2809 (0.0%)
47	3	0.46	0/1777	1.02	14/2763 (0.5%)
48	5	0.43	1/87790 (0.0%)	0.88	288/136937 (0.2%)
49	7	0.40	0/2858	0.75	1/4455 (0.0%)
50	8	0.42	0/3701	0.82	3/5766 (0.1%)
51	9	0.41	1/41013 (0.0%)	0.85	102/63919 (0.2%)
52	AA	0.56	2/1679 (0.1%)	0.87	0/2283
53	BB	0.53	0/1756	0.92	2/2350 (0.1%)
54	CC	0.53	0/1732	0.93	2/2347 (0.1%)
55	DD	0.54	0/1792	0.88	0/2412
56	EE	0.51	0/2115	0.90	1/2843 (0.0%)
57	FF	0.52	0/1531	0.91	0/2059
58	GG	0.58	2/1946 (0.1%)	0.84	1/2590 (0.0%)
59	HH	0.54	0/1544	0.91	1/2068 (0.0%)
60	II	0.57	1/1715 (0.1%)	0.87	0/2287
61	JJ	0.55	1/1550 (0.1%)	0.96	6/2069 (0.3%)
62	KK	0.59	0/851	0.93	1/1147 (0.1%)
63	LL	0.57	0/1259	0.83	1/1684 (0.1%)
64	MM	0.63	0/968	0.91	0/1296
65	NN	0.56	1/1232 (0.1%)	0.98	0/1656
66	OO	0.55	0/1029	0.97	1/1380 (0.1%)
67	PP	0.59	1/1079 (0.1%)	0.92	0/1437
68	QQ	0.50	0/1142	0.85	0/1528
69	RR	0.55	0/1060	0.90	0/1421
70	SS	0.55	1/1157 (0.1%)	0.94	1/1548 (0.1%)
71	TT	0.52	0/1120	0.98	1/1499 (0.1%)
72	UU	0.52	0/831	0.87	1/1115 (0.1%)
73	VV	0.52	0/645	0.90	0/865
74	WW	0.58	1/1051 (0.1%)	0.90	0/1406
75	XX	0.50	0/1116	0.90	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.53	0/1040	0.86	0/1382
77	ZZ	0.54	0/604	0.91	0/810
78	aa	0.53	0/794	0.93	0/1065
79	bb	0.51	0/665	0.76	0/891
80	cc	0.48	0/478	0.85	1/640 (0.2%)
81	dd	0.50	0/455	0.85	0/603
82	ee	0.52	0/462	0.80	0/607
83	ff	0.54	0/538	0.70	0/713
84	gg	0.48	0/2493	0.74	0/3394
85	hh	0.41	0/286	0.81	1/443 (0.2%)
86	ii	0.53	2/3333 (0.1%)	0.88	5/4483 (0.1%)
87	jj	0.53	2/4633 (0.0%)	0.85	1/6249 (0.0%)
All	All	0.49	39/242727 (0.0%)	0.89	506/355704 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
3	C	0	2
5	E	0	1
9	I	0	2
11	L	0	1
17	R	0	1
18	S	0	3
24	Y	0	1
26	a	0	2
31	f	0	2
34	i	0	3
38	m	0	1
42	r	0	1
51	9	0	3
52	AA	0	2
56	EE	0	2
57	FF	0	1
59	HH	0	1
66	OO	0	1
68	QQ	0	1
70	SS	0	1

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

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	i	91	SER	C-N	-15.41	1.12	1.33
87	jj	121	LYS	CE-NZ	11.46	1.83	1.49
14	O	96	GLN	CD-OE1	6.17	1.35	1.23
51	9	1306	U	O3'-P	-6.07	1.52	1.61
32	g	28	ASN	CG-OD1	5.89	1.34	1.23
58	GG	59	GLN	CD-OE1	5.69	1.34	1.23
24	Y	86	GLN	CD-OE1	5.59	1.34	1.23
48	5	957	G	O3'-P	5.54	1.69	1.61
23	X	93	ASN	CG-OD1	5.49	1.33	1.23
17	R	34	ASN	CG-OD1	5.47	1.33	1.23
27	b	27	GLN	CD-OE1	5.46	1.33	1.23
67	PP	35	GLN	CD-OE1	5.46	1.33	1.23
4	D	225	GLN	CD-OE1	5.39	1.33	1.23
3	C	212	ASN	CG-OD1	5.37	1.33	1.23
18	S	122	HIS	ND1-CE1	5.36	1.38	1.32
18	S	162	GLN	CD-OE1	5.33	1.33	1.23
74	WW	64	ASN	CG-OD1	5.33	1.33	1.23
86	ii	180	HIS	ND1-CE1	5.33	1.37	1.32
42	r	6	GLN	CD-OE1	5.32	1.33	1.23
1	A	216	HIS	ND1-CE1	5.32	1.37	1.32
30	e	102	ASN	CG-OD1	5.32	1.33	1.23
86	ii	180	HIS	CD2-NE2	-5.32	1.32	1.37
61	JJ	177	ASN	CG-OD1	5.31	1.33	1.23
15	P	40	HIS	ND1-CE1	5.30	1.37	1.32
70	SS	10	GLN	CD-OE1	5.30	1.33	1.23
58	GG	65	GLN	CD-OE1	5.28	1.33	1.23
42	r	41	ASN	CG-OD1	5.25	1.33	1.23
1	A	50	HIS	ND1-CE1	5.24	1.37	1.32
2	B	138	GLN	CD-OE1	5.24	1.33	1.23
41	p	33	GLN	CD-OE1	5.22	1.33	1.23
52	AA	141	ASN	CG-OD1	5.17	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	AA	84	GLN	CD-OE1	5.15	1.33	1.23
87	jj	197	GLN	CD-OE1	5.10	1.33	1.23
60	II	35	ASN	CG-OD1	5.08	1.33	1.23
12	M	56	GLN	CD-OE1	5.07	1.33	1.23
7	G	29	ASN	CG-OD1	5.06	1.33	1.23
65	NN	105	ASN	CG-OD1	5.06	1.33	1.23
2	B	68	ASN	CG-OD1	5.05	1.33	1.23
1	A	216	HIS	CD2-NE2	-5.02	1.32	1.37

All (506) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	i	92	SER	CA-C-N	-41.95	46.45	121.97
34	i	92	SER	C-N-CA	-41.95	46.45	121.97
34	i	91	SER	O-C-N	-36.48	74.06	122.59
48	5	1357	C	C4'-C3'-O3'	13.50	133.25	113.00
48	5	1358	G	C4'-C3'-O3'	13.49	133.24	113.00
48	5	4975	G	C2'-C3'-O3'	12.33	127.99	109.50
51	9	1305	C	C1'-C2'-O2'	-11.57	91.05	108.40
48	5	2046	G	C2'-C3'-O3'	10.82	125.73	109.50
48	5	5061	A	C2'-C3'-O3'	10.51	125.27	109.50
48	5	4872	G	C2'-C3'-O3'	10.34	125.02	109.50
48	5	2695	A	C2'-C3'-O3'	10.20	124.80	109.50
14	O	110	PRO	N-CA-C	10.15	123.08	110.70
51	9	1394	G	C2'-C3'-O3'	10.15	128.93	113.70
48	5	4951	G	C2'-C3'-O3'	10.11	124.67	109.50
51	9	1305	C	C4'-C3'-O3'	9.98	127.98	113.00
48	5	47	A	C4'-C3'-O3'	9.97	124.35	109.40
48	5	3718	A	C4'-C3'-O3'	9.91	127.86	113.00
34	i	91	SER	CA-C-N	9.79	140.23	121.54
34	i	91	SER	C-N-CA	9.79	140.23	121.54
48	5	4975	G	C4'-C3'-O3'	-9.77	94.75	109.40
48	5	1365	C	C4'-C3'-O3'	9.73	124.00	109.40
48	5	1847	C	C4'-C3'-O3'	-9.73	98.41	113.00
48	5	1398	A	C2'-C3'-O3'	9.61	123.91	109.50
51	9	312	G	C2'-C3'-O3'	9.58	123.87	109.50
48	5	385	A	C4'-C3'-O3'	9.43	123.54	109.40
48	5	1279	A	C2'-C3'-O3'	9.38	123.57	109.50
48	5	2068	C	C4'-C3'-O3'	9.36	123.44	109.40
7	G	30	PRO	CA-N-CD	-9.34	98.92	112.00
48	5	1696	C	C2'-C3'-O3'	9.33	123.49	109.50
48	5	2123	C	C2'-C3'-O3'	9.25	123.37	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1308	U	C2'-C3'-O3'	-9.21	99.89	113.70
51	9	72	C	C4'-C3'-O3'	9.03	122.94	109.40
51	9	594	A	C4'-C3'-O3'	8.99	122.88	109.40
51	9	1235	G	C4'-C3'-O3'	8.96	126.43	113.00
48	5	3888	G	C2'-C3'-O3'	8.95	127.13	113.70
2	B	37	PRO	CA-N-CD	-8.94	99.48	112.00
48	5	125	C	C2'-C3'-O3'	8.94	127.11	113.70
51	9	1448	A	C2'-C3'-O3'	-8.92	100.31	113.70
48	5	2028	C	C2'-C3'-O3'	-8.91	100.34	113.70
47	3	70	G	N9-C1'-C2'	-8.79	98.81	112.00
51	9	321	C	C4'-C3'-O3'	8.72	126.08	113.00
48	5	4378	A	C2'-C3'-O3'	8.70	122.54	109.50
34	i	92	SER	O-C-N	-8.69	111.04	122.59
51	9	1308	U	C4'-C3'-O3'	8.64	125.96	113.00
48	5	2083	C	C4'-C3'-O3'	8.63	125.95	113.00
51	9	678	U	C4'-C3'-O3'	-8.60	100.10	113.00
48	5	4266	G	C2'-C3'-O3'	-8.53	100.91	113.70
48	5	3753	G	N9-C1'-C2'	-8.52	99.22	112.00
48	5	1969	G	C4'-C3'-O3'	8.40	125.61	113.00
51	9	1305	C	N1-C1'-C2'	-8.39	99.41	112.00
48	5	48	G	C2'-C3'-O3'	8.38	122.08	109.50
48	5	1964	A	C4'-C3'-O3'	8.35	125.53	113.00
48	5	276	C	C4'-C3'-O3'	-8.35	100.48	113.00
47	3	70	G	C4'-C3'-O3'	8.34	125.52	113.00
51	9	291	G	C4'-C3'-O3'	8.34	121.91	109.40
48	5	1292	C	C2'-C3'-O3'	8.31	126.16	113.70
48	5	4528	G	C2'-C3'-O3'	8.30	126.15	113.70
48	5	1755	C	C2'-C3'-O3'	8.28	121.92	109.50
48	5	2858	A	C4'-C3'-O3'	8.27	125.40	113.00
48	5	1455	G	C2'-C3'-O3'	8.22	126.03	113.70
51	9	909	G	N9-C1'-C2'	-8.14	99.78	112.00
48	5	2769	U	C4'-C3'-O3'	8.13	121.59	109.40
51	9	870	A	C4'-C3'-O3'	8.12	121.58	109.40
3	C	340	ILE	N-CA-C	-8.10	104.60	111.56
48	5	3718	A	C2'-C3'-O3'	-8.09	101.57	113.70
3	C	232	VAL	CB-CA-C	-8.00	101.18	112.22
48	5	1410	U	C2'-C3'-O3'	7.95	121.42	109.50
3	C	67	TRP	N-CA-C	-7.92	98.08	109.96
48	5	1211	G	C2'-C3'-O3'	7.87	125.51	113.70
51	9	327	G	C2'-C3'-O3'	7.87	121.31	109.50
51	9	1835	A	C2'-C3'-O3'	7.85	121.27	109.50
48	5	1961	G	C4'-C3'-O3'	7.82	124.74	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	3	30	G	C4'-C3'-O3'	7.80	124.69	113.00
48	5	936	C	C2'-C3'-O3'	7.79	121.18	109.50
51	9	110	U	C2'-C3'-O3'	7.78	125.38	113.70
51	9	1647	A	C2'-C3'-O3'	7.78	121.18	109.50
48	5	2116	C	C2'-C3'-O3'	7.78	121.16	109.50
48	5	4170	A	C2'-C3'-O3'	7.77	121.15	109.50
51	9	1235	G	C2'-C3'-O3'	-7.76	102.05	113.70
48	5	5027	C	C2'-C3'-O3'	7.76	121.14	109.50
51	9	1664	A	C4'-C3'-O3'	7.75	121.03	109.40
51	9	797	C	C4'-C3'-O3'	7.75	121.03	109.40
51	9	1306	U	N1-C1'-C2'	-7.73	100.41	112.00
51	9	102	A	C2'-C3'-O3'	7.69	121.04	109.50
48	5	5060	A	C2'-C3'-O3'	7.64	125.16	113.70
48	5	3718	A	N9-C1'-C2'	-7.62	100.56	112.00
48	5	930	G	C4'-C3'-O3'	7.61	120.82	109.40
51	9	321	C	N1-C1'-C2'	-7.61	100.59	112.00
51	9	588	G	C2'-C3'-O3'	7.61	120.91	109.50
48	5	1500	A	C2'-C3'-O3'	7.60	125.10	113.70
48	5	1474	C	C2'-C3'-O3'	7.59	125.08	113.70
47	3	39	U	C2'-C3'-O3'	-7.58	102.34	113.70
51	9	1386	A	N9-C1'-C2'	-7.57	100.65	112.00
51	9	1386	A	C4'-C3'-O3'	7.53	124.30	113.00
50	8	94	G	C2'-C3'-O3'	7.51	120.77	109.50
51	9	688	U	C2'-C3'-O3'	7.49	120.74	109.50
48	5	956	A	C4'-C3'-O3'	7.49	120.63	109.40
48	5	957	G	C2'-C3'-O3'	7.47	120.71	109.50
48	5	1357	C	C2'-C3'-O3'	-7.45	102.52	113.70
51	9	1385	G	C4'-C3'-O3'	7.43	124.15	113.00
48	5	215	C	C4'-C3'-O3'	-7.42	101.86	113.00
48	5	4517	A	C4'-C3'-O3'	-7.42	101.87	113.00
86	ii	180	HIS	CB-CG-CD2	-7.41	121.57	131.20
48	5	1724	G	C4'-C3'-O3'	7.40	120.51	109.40
51	9	183	G	C4'-C3'-O3'	7.39	120.49	109.40
48	5	928	C	C2'-C3'-O3'	-7.36	102.66	113.70
48	5	4885	U	C2'-C3'-O3'	7.34	124.71	113.70
48	5	1292	C	C4'-C3'-O3'	-7.34	101.99	113.00
48	5	3811	G	C2'-C3'-O3'	-7.34	98.50	109.50
51	9	1235	G	N9-C1'-C2'	-7.33	101.00	112.00
48	5	1282	G	C1'-C2'-O2'	7.30	119.35	108.40
51	9	1109	C	C2'-C3'-O3'	7.27	120.41	109.50
48	5	275	C	C2'-C3'-O3'	7.27	124.60	113.70
48	5	406	C	C2'-C3'-O3'	7.26	124.60	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1212	G	C2'-C3'-O3'	-7.26	102.81	113.70
48	5	4948	C	C2'-C3'-O3'	7.21	124.52	113.70
48	5	215	C	C2'-C3'-O3'	7.18	124.47	113.70
48	5	2588	C	C2'-C3'-O3'	-7.18	102.94	113.70
51	9	1455	A	N9-C1'-C2'	-7.17	101.25	112.00
48	5	1477	C	C2'-C3'-O3'	7.16	124.45	113.70
48	5	1968	G	C2'-C3'-O3'	-7.16	102.97	113.70
48	5	5059	C	C2'-C3'-O3'	7.12	124.38	113.70
72	UU	93	SER	N-CA-C	7.10	114.39	108.07
48	5	1268	G	C4'-C3'-O3'	7.09	120.04	109.40
48	5	1964	A	C2'-C3'-O3'	-7.08	103.08	113.70
48	5	4730	C	C4'-C3'-O3'	7.05	119.98	109.40
48	5	1485	C	C2'-C3'-O3'	7.03	120.04	109.50
48	5	3670	C	C4'-C3'-O3'	7.02	123.53	113.00
61	JJ	144	ILE	N-CA-C	7.00	115.52	107.89
48	5	1964	A	N9-C1'-C2'	-6.99	101.52	112.00
15	P	40	HIS	CB-CG-CD2	-6.97	122.13	131.20
51	9	1294	G	N9-C1'-C2'	-6.97	101.54	112.00
51	9	1859	A	C4'-C3'-O3'	-6.96	102.56	113.00
48	5	3697	U	C2'-C3'-O3'	6.96	124.14	113.70
48	5	1818	G	C2'-C3'-O3'	6.94	124.11	113.70
48	5	2107	C	C2'-C3'-O3'	6.94	119.91	109.50
48	5	2093	A	C2'-C3'-O3'	6.92	119.88	109.50
47	3	30	G	N9-C1'-C2'	-6.91	101.64	112.00
48	5	944	A	C4'-C3'-O3'	-6.84	102.73	113.00
36	k	61	PRO	N-CA-C	6.83	119.03	110.70
48	5	1500	A	C4'-C3'-O3'	-6.82	102.76	113.00
47	3	38	A	C4'-C3'-O3'	6.80	123.20	113.00
48	5	4084	G	C2'-C3'-O3'	6.77	119.66	109.50
51	9	1115	U	C4'-C3'-O3'	6.77	119.56	109.40
2	B	258	HIS	N-CA-C	6.77	124.77	109.81
48	5	2256	C	C2'-C3'-O3'	6.76	119.63	109.50
24	Y	87	ARG	NE-CZ-NH2	6.75	125.27	119.20
18	S	164	LYS	N-CA-C	-6.73	101.58	109.93
48	5	2027	U	C1'-C2'-O2'	-6.73	98.30	108.40
1	A	50	HIS	CB-CG-CD2	-6.72	122.46	131.20
51	9	1234	C	C4'-C3'-O3'	6.72	123.08	113.00
50	8	124	U	C4'-C3'-O3'	6.71	119.46	109.40
48	5	4375	C	C2'-C3'-O3'	-6.69	103.66	113.70
48	5	1697	G	C4'-C3'-O3'	6.69	119.44	109.40
48	5	3753	G	C4'-C3'-O3'	6.69	123.04	113.00
48	5	1	C	C4'-C3'-O3'	6.67	119.41	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	93	G	C4'-C3'-O3'	6.67	123.01	113.00
1	A	216	HIS	CB-CG-CD2	-6.67	122.53	131.20
48	5	118	C	C4'-C3'-O3'	-6.67	103.00	113.00
51	9	1419	C	C2'-C3'-O3'	6.66	123.69	113.70
48	5	1974	U	C4'-C3'-O3'	6.64	119.36	109.40
44	t	140	GLY	N-CA-C	6.63	120.92	112.83
48	5	917	A	C4'-C3'-O3'	6.63	119.34	109.40
48	5	4888	U	C2'-C3'-O3'	6.60	119.40	109.50
48	5	2266	C	C2'-C3'-O3'	6.58	119.37	109.50
48	5	4656	A	C2'-C3'-O3'	6.56	119.34	109.50
48	5	1965	G	N9-C1'-C2'	-6.56	102.17	112.00
48	5	965	G	C2'-C3'-O3'	6.55	119.32	109.50
5	E	72	PRO	N-CA-CB	6.54	110.19	103.00
51	9	1294	G	C4'-C3'-O3'	6.53	122.80	113.00
51	9	1294	G	C2'-C3'-O3'	-6.51	103.93	113.70
48	5	4115	G	C4'-C3'-O3'	6.49	119.14	109.40
51	9	160	U	C2'-C3'-O3'	6.49	119.24	109.50
18	S	122	HIS	CB-CG-CD2	-6.48	122.78	131.20
51	9	666	U	N1-C1'-C2'	6.47	121.71	112.00
51	9	1253	A	C4'-C3'-O3'	6.47	119.10	109.40
47	3	38	A	N9-C1'-C2'	-6.43	102.35	112.00
48	5	1380	G	C4'-C3'-O3'	6.43	122.64	113.00
50	8	93	C	C4'-C3'-O3'	-6.42	103.37	113.00
51	9	322	C	N1-C1'-C2'	-6.41	102.39	112.00
48	5	1969	G	N9-C1'-C2'	-6.40	102.39	112.00
51	9	1386	A	C2'-C3'-O3'	-6.40	104.10	113.70
48	5	1967	A	C2'-C3'-O3'	-6.39	104.11	113.70
48	5	2827	G	C2'-C3'-O3'	-6.38	99.92	109.50
48	5	407	A	C4'-C3'-O3'	-6.38	103.43	113.00
9	I	49	CYS	N-CA-C	6.37	119.88	111.28
48	5	2313	A	C2'-C3'-O3'	6.35	119.03	109.50
48	5	2661	U	C2'-C3'-O3'	6.34	119.02	109.50
2	B	18	PRO	N-CA-C	-6.34	99.41	112.47
51	9	1419	C	C4'-C3'-O3'	-6.33	103.50	113.00
47	3	38	A	C2'-C3'-O3'	-6.33	104.20	113.70
48	5	1835	G	C4'-C3'-O3'	6.32	118.89	109.40
51	9	1475	G	C4'-C3'-O3'	6.31	118.86	109.40
86	ii	180	HIS	CB-CG-ND1	6.30	132.15	122.70
48	5	2027	U	C4'-C3'-O3'	6.29	122.44	113.00
48	5	300	A	N9-C1'-C2'	6.29	121.43	112.00
87	jj	121	LYS	CD-CE-NZ	-6.28	91.82	111.90
51	9	1109	C	C1'-C2'-O2'	6.26	121.19	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	2474	G	C2'-C3'-O3'	6.25	123.08	113.70
2	B	258	HIS	CA-C-N	-6.25	112.03	119.84
2	B	258	HIS	C-N-CA	-6.25	112.03	119.84
48	5	4075	U	C4'-C3'-O3'	6.25	118.77	109.40
48	5	1672	U	N1-C1'-C2'	6.24	121.36	112.00
48	5	90	G	C2'-C3'-O3'	6.22	123.04	113.70
51	9	1293	A	C2'-C3'-O3'	-6.20	104.39	113.70
51	9	908	A	N9-C1'-C2'	-6.19	102.72	112.00
48	5	4232	U	C4'-C3'-O3'	6.19	118.68	109.40
51	9	1212	G	N9-C1'-C2'	-6.19	102.72	112.00
48	5	1967	A	C4'-C3'-O3'	6.18	122.27	113.00
48	5	4144	C	C4'-C3'-O3'	6.14	118.61	109.40
44	t	29	ALA	CA-C-N	6.12	127.50	119.84
44	t	29	ALA	C-N-CA	6.12	127.50	119.84
48	5	2632	U	N1-C1'-C2'	6.12	121.18	112.00
48	5	2506	G	C4'-C3'-O3'	6.12	118.58	109.40
48	5	5024	C	C2'-C3'-O3'	6.10	118.65	109.50
25	Z	54	THR	N-CA-C	6.10	120.30	112.86
51	9	642	U	C4'-C3'-O3'	6.09	122.14	113.00
48	5	4473	A	C4'-C3'-O3'	-6.09	103.87	113.00
48	5	1636	U	C4'-C3'-O3'	-6.08	103.88	113.00
48	5	1236	C	C2'-C3'-O3'	6.07	122.81	113.70
48	5	3753	G	C2'-C3'-O3'	-6.07	104.60	113.70
51	9	872	A	C2'-C3'-O3'	6.07	118.60	109.50
48	5	3619	G	C4'-C3'-O3'	-6.06	103.91	113.00
51	9	1275	G	C2'-C3'-O3'	6.05	122.77	113.70
48	5	4882	U	C2'-C3'-O3'	6.04	118.55	109.50
48	5	1961	G	N9-C1'-C2'	-6.03	102.96	112.00
48	5	1975	G	C4'-C3'-O3'	6.01	118.42	109.40
48	5	3876	A	C2'-C3'-O3'	6.01	118.52	109.50
48	5	4435	U	C4'-C3'-O3'	-6.00	104.00	113.00
48	5	4966	A	N9-C1'-C2'	6.00	121.00	112.00
18	S	83	ARG	NE-CZ-NH2	5.99	124.59	119.20
43	s	200	ASN	CA-C-N	5.98	127.31	119.84
43	s	200	ASN	C-N-CA	5.98	127.31	119.84
48	5	1329	G	C4'-C3'-O3'	5.97	121.96	113.00
48	5	4429	C	C4'-C3'-O3'	-5.97	104.05	113.00
48	5	4900	C	C2'-C3'-O3'	5.96	118.45	109.50
48	5	372	A	C4'-C3'-O3'	-5.96	104.06	113.00
51	9	1824	A	C2'-C3'-O3'	5.94	122.62	113.70
53	BB	136	ARG	NE-CZ-NH2	5.94	124.55	119.20
48	5	497	G	C2'-C3'-O3'	-5.93	104.80	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1702	G	C1'-C2'-O2'	5.93	117.29	108.40
61	JJ	163	SER	N-CA-C	5.92	113.55	108.22
22	W	14	TYR	CA-C-N	5.92	127.24	119.84
22	W	14	TYR	C-N-CA	5.92	127.24	119.84
15	P	40	HIS	CB-CG-ND1	5.90	131.55	122.70
48	5	408	A	C2'-C3'-O3'	-5.90	104.85	113.70
48	5	1848	C	C2'-C3'-O3'	5.89	122.53	113.70
48	5	4307	A	C4'-C3'-O3'	-5.89	104.17	113.00
48	5	4237	C	C4'-C3'-O3'	-5.88	104.18	113.00
48	5	4449	A	C4'-C3'-O3'	5.88	118.22	109.40
48	5	1214	C	C4'-C3'-O3'	5.88	118.22	109.40
48	5	2027	U	N1-C1'-C2'	-5.88	103.19	112.00
48	5	3593	C	C4'-C3'-O3'	5.88	118.21	109.40
48	5	3715	U	C4'-C3'-O3'	5.87	121.81	113.00
48	5	2786	C	C2'-C3'-O3'	-5.87	104.89	113.70
63	LL	99	TYR	N-CA-C	-5.87	99.16	108.73
51	9	677	G	C4'-C3'-O3'	-5.87	104.20	113.00
51	9	1418	C	C4'-C3'-O3'	5.87	118.20	109.40
19	T	93	ILE	CB-CA-C	-5.87	104.35	112.04
48	5	2395	A	C2'-C3'-O3'	5.86	118.30	109.50
51	9	1473	G	C4'-C3'-O3'	5.86	121.79	113.00
48	5	1725	U	C1'-C2'-O2'	5.85	117.18	108.40
48	5	1232	G	C2'-C3'-O3'	5.85	118.27	109.50
51	9	1637	A	C2'-C3'-O3'	5.85	118.27	109.50
71	TT	42	HIS	CB-CA-C	-5.84	101.47	110.81
48	5	1477	C	C4'-C3'-O3'	-5.83	104.25	113.00
51	9	501	C	N1-C1'-C2'	5.82	120.73	112.00
48	5	1958	A	C2'-C3'-O3'	-5.82	104.97	113.70
51	9	532	C	C2'-C3'-O3'	5.80	122.40	113.70
48	5	664	G	C4'-C3'-O3'	5.79	118.08	109.40
48	5	2858	A	C1'-C2'-O2'	-5.78	99.73	108.40
48	5	3858	C	C4'-C3'-O3'	-5.78	104.34	113.00
51	9	908	A	C4'-C3'-O3'	5.77	121.66	113.00
48	5	1612	G	C2'-C3'-O3'	5.77	118.15	109.50
48	5	3859	G	C4'-C3'-O3'	-5.77	104.35	113.00
48	5	4543	G	C4'-C3'-O3'	-5.76	104.36	113.00
48	5	231	U	C4'-C3'-O3'	-5.75	104.38	113.00
48	5	977	C	C2'-C3'-O3'	5.74	122.31	113.70
86	ii	372	MET	CA-C-N	-5.74	114.02	119.76
86	ii	372	MET	C-N-CA	-5.74	114.02	119.76
48	5	1214	C	C2'-C3'-O3'	5.73	118.10	109.50
43	s	72	ASN	N-CA-C	5.73	116.87	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	261	ARG	N-CA-C	-5.73	99.81	108.46
48	5	4965	U	C4'-C3'-O3'	-5.72	104.41	113.00
48	5	497	G	C4'-C3'-O3'	5.72	121.58	113.00
1	A	50	HIS	CB-CG-ND1	5.71	131.27	122.70
48	5	976	G	C3'-C2'-O2'	5.71	119.27	110.70
48	5	4548	A	C4'-C3'-O3'	5.71	117.96	109.40
48	5	1329	G	C2'-C3'-O3'	5.69	122.23	113.70
31	f	93	PRO	N-CA-C	5.68	122.04	113.81
62	KK	66	HIS	N-CA-C	5.68	122.89	110.80
48	5	1279	A	C4'-C3'-O3'	-5.67	100.89	109.40
5	E	197	ILE	N-CA-C	-5.67	101.72	109.55
48	5	2554	U	C4'-C3'-O3'	5.67	121.51	113.00
48	5	265	C	C4'-C3'-O3'	5.67	117.90	109.40
48	5	964	A	O4'-C1'-C2'	-5.67	101.93	107.60
51	9	1385	G	C2'-C3'-O3'	-5.66	105.21	113.70
58	GG	121	ILE	CB-CA-C	5.66	114.88	109.33
47	3	30	G	C2'-C3'-O3'	-5.66	105.22	113.70
48	5	2468	U	C4'-C3'-O3'	5.65	117.88	109.40
80	cc	44	ARG	N-CA-C	5.65	117.44	108.79
48	5	1965	G	C2'-C3'-O3'	-5.64	105.24	113.70
1	A	216	HIS	CB-CG-ND1	5.64	131.16	122.70
48	5	3672	G	C2'-C3'-O3'	-5.64	105.24	113.70
51	9	1308	U	N1-C1'-C2'	-5.62	103.57	112.00
48	5	1624	G	C4'-C3'-O3'	5.62	117.83	109.40
51	9	1267	C	C1'-C2'-O2'	-5.62	99.98	108.40
46	2	76	A	C3'-C2'-O2'	5.61	119.11	110.70
48	5	220	C	C4'-C3'-O3'	-5.61	104.58	113.00
48	5	4473	A	N9-C1'-C2'	5.60	120.40	112.00
21	V	13	LYS	N-CA-C	5.60	118.57	111.69
51	9	215	G	C2'-C3'-O3'	5.59	117.89	109.50
48	5	5066	U	N1-C1'-C2'	5.59	120.39	112.00
48	5	4548	A	C2'-C3'-O3'	5.59	117.88	109.50
61	JJ	101	LYS	N-CA-C	5.59	117.56	109.07
51	9	146	G	C2'-C3'-O3'	5.58	117.88	109.50
48	5	4213	A	C4'-C3'-O3'	-5.58	104.62	113.00
48	5	1358	G	O4'-C1'-C2'	-5.58	102.02	107.60
47	3	39	U	N1-C1'-C2'	-5.57	103.64	112.00
51	9	1212	G	C4'-C3'-O3'	5.57	121.36	113.00
48	5	509	A	C2'-C3'-O3'	-5.57	105.35	113.70
51	9	1477	U	C2'-C3'-O3'	5.56	122.04	113.70
48	5	486	C	C2'-C3'-O3'	5.56	122.04	113.70
48	5	2246	C	C2'-C3'-O3'	5.55	122.02	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	752	G	C4'-C3'-O3'	5.55	117.72	109.40
10	J	119	TYR	CA-CB-CG	5.54	123.87	113.90
48	5	1280	C	C4'-C3'-O3'	-5.54	104.69	113.00
16	Q	176	ARG	N-CA-C	5.54	119.07	111.54
51	9	508	A	C1'-C2'-O2'	5.53	116.70	108.40
48	5	4335	C	C4'-C3'-O3'	-5.53	104.71	113.00
48	5	1429	C	C4'-C3'-O3'	-5.53	104.71	113.00
51	9	61	A	C4'-C3'-O3'	-5.52	104.72	113.00
48	5	451	C	C2'-C3'-O3'	5.51	117.77	109.50
48	5	2278	G	C2'-C3'-O3'	5.51	117.77	109.50
48	5	2119	C	C2'-C3'-O3'	5.51	117.77	109.50
48	5	2546	G	C3'-C2'-O2'	5.51	118.96	110.70
48	5	1633	G	C4'-C3'-O3'	5.50	121.25	113.00
48	5	2357	G	C4'-C3'-O3'	-5.50	104.75	113.00
48	5	134	G	C4'-C3'-O3'	5.50	117.64	109.40
51	9	317	C	C4'-C3'-O3'	-5.49	104.76	113.00
51	9	373	G	C4'-C3'-O3'	-5.49	104.76	113.00
48	5	746	A	C4'-C3'-O3'	5.49	117.63	109.40
48	5	4974	C	C4'-C3'-O3'	-5.48	104.78	113.00
48	5	1961	G	C2'-C3'-O3'	-5.48	105.48	113.70
61	JJ	163	SER	CA-C-N	5.46	124.65	118.97
61	JJ	163	SER	C-N-CA	5.46	124.65	118.97
48	5	505	G	C2'-C3'-O3'	5.46	121.89	113.70
51	9	1313	A	C4'-C3'-O3'	5.46	117.59	109.40
70	SS	26	ILE	N-CA-C	5.46	115.66	110.42
48	5	4211	C	C4'-C3'-O3'	-5.45	104.82	113.00
51	9	1298	G	C1'-C2'-O2'	-5.45	103.62	111.80
48	5	376	A	C1'-C2'-O2'	5.45	116.57	108.40
51	9	1844	U	C4'-C3'-O3'	-5.45	104.83	113.00
51	9	1234	C	N1-C1'-C2'	-5.45	103.83	112.00
48	5	932	A	C2'-C3'-O3'	5.44	117.67	109.50
48	5	2338	C	C4'-C3'-O3'	-5.44	104.84	113.00
48	5	4719	G	C4'-C3'-O3'	5.44	121.16	113.00
1	A	225	ILE	N-CA-C	5.44	115.38	107.88
18	S	122	HIS	CB-CG-ND1	5.44	130.85	122.70
9	I	121	LYS	N-CA-C	-5.43	103.08	110.36
48	5	2083	C	C2'-C3'-O3'	-5.43	105.56	113.70
51	9	1385	G	N9-C1'-C2'	-5.42	103.86	112.00
29	d	116	ASN	N-CA-C	5.42	119.05	111.90
41	p	52	VAL	CB-CA-C	-5.42	102.76	111.59
48	5	4666	G	C4'-C3'-O3'	-5.41	104.88	113.00
11	L	99	ASP	N-CA-C	-5.41	103.32	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1266	G	C2'-C3'-O3'	5.40	121.81	113.70
47	3	29	A	C2'-C3'-O3'	-5.40	105.59	113.70
5	E	217	GLN	N-CA-C	5.39	117.79	110.35
12	M	66	HIS	N-CA-C	5.39	119.35	112.34
48	5	1239	C	C3'-C2'-O2'	5.39	122.68	114.60
48	5	1542	U	C4'-C3'-O3'	-5.39	104.92	113.00
48	5	1848	C	C4'-C3'-O3'	-5.38	104.92	113.00
48	5	2260	C	C3'-C2'-O2'	5.38	118.77	110.70
19	T	27	LEU	N-CA-C	5.37	118.05	111.82
48	5	1457	G	C4'-C3'-O3'	-5.37	104.95	113.00
48	5	1921	C	C2'-C3'-O3'	5.36	117.55	109.50
25	Z	36	ARG	CA-C-N	5.36	124.87	119.19
25	Z	36	ARG	C-N-CA	5.36	124.87	119.19
48	5	286	U	N1-C1'-C2'	5.36	120.04	112.00
48	5	4116	C	C2'-C3'-O3'	5.36	117.54	109.50
48	5	1238	A	C3'-C2'-O2'	5.36	118.73	110.70
5	E	90	LYS	CA-C-N	5.35	126.53	119.84
5	E	90	LYS	C-N-CA	5.35	126.53	119.84
48	5	2427	G	C4'-C3'-O3'	-5.35	104.98	113.00
48	5	979	C	C2'-C3'-O3'	5.34	121.70	113.70
48	5	1966	C	N1-C1'-C2'	-5.33	104.00	112.00
48	5	38	A	C4'-C3'-O3'	-5.33	105.01	113.00
51	9	1535	U	C4'-C3'-O3'	-5.33	101.41	109.40
48	5	2257	C	C4'-C3'-O3'	5.32	117.38	109.40
48	5	2714	G	C4'-C3'-O3'	-5.31	105.03	113.00
48	5	2068	C	C2'-C3'-O3'	5.31	117.46	109.50
48	5	2797	C	N1-C1'-C2'	-5.30	106.05	114.00
48	5	1236	C	C3'-C2'-O2'	5.30	118.65	110.70
48	5	2807	A	C4'-C3'-O3'	-5.29	105.06	113.00
48	5	4228	G	C4'-C3'-O3'	-5.29	101.46	109.40
48	5	2732	G	C4'-C3'-O3'	-5.29	105.07	113.00
3	C	340	ILE	N-CA-CB	5.29	117.23	111.41
51	9	669	A	C4'-C3'-O3'	-5.28	105.07	113.00
61	JJ	86	VAL	N-CA-C	-5.28	106.52	111.48
48	5	2088	A	C2'-C3'-O3'	5.28	117.42	109.50
86	ii	301	TYR	N-CA-C	5.27	117.10	110.24
48	5	2724	G	C2'-C3'-O3'	-5.27	105.79	113.70
51	9	945	U	N1-C1'-C2'	5.27	119.91	112.00
2	B	17	LEU	N-CA-C	5.27	121.46	109.81
48	5	5041	G	C2'-C3'-O3'	-5.27	105.80	113.70
48	5	1296	G	C2'-C3'-O3'	5.26	117.40	109.50
48	5	2676	A	C1'-C2'-O2'	5.26	116.30	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3594	C	N1-C1'-C2'	5.26	119.90	112.00
1	A	90	CYS	N-CA-C	5.26	117.08	108.55
51	9	474	G	C4'-C3'-O3'	-5.26	105.11	113.00
51	9	980	A	C4'-C3'-O3'	-5.26	105.11	113.00
48	5	2262	G	C3'-C2'-O2'	5.25	118.57	110.70
51	9	1088	U	C2'-C3'-O3'	-5.24	101.64	109.50
48	5	1280	C	N1-C1'-C2'	5.24	119.86	112.00
48	5	943	A	C2'-C3'-O3'	5.23	117.35	109.50
48	5	509	A	C4'-C3'-O3'	-5.23	105.15	113.00
48	5	4770	U	C2'-C3'-O3'	-5.23	105.86	113.70
31	f	80	ASN	N-CA-C	5.22	121.92	110.80
26	a	120	GLN	CA-C-N	5.22	125.22	119.90
26	a	120	GLN	C-N-CA	5.22	125.22	119.90
48	5	93	G	C2'-C3'-O3'	-5.22	105.88	113.70
48	5	3673	C	C2'-C3'-O3'	5.22	117.32	109.50
47	3	1	G	C5'-C4'-O4'	5.21	117.62	109.80
48	5	4699	U	C4'-C3'-O3'	5.21	117.22	109.40
48	5	1990	A	C2'-C3'-O3'	5.21	121.51	113.70
48	5	3880	G	C4'-C3'-O3'	-5.21	105.19	113.00
48	5	4521	U	C4'-C3'-O3'	-5.21	105.19	113.00
51	9	434	G	C4'-C3'-O3'	5.21	120.81	113.00
48	5	5025	C	C2'-C3'-O3'	-5.20	105.90	113.70
48	5	4119	C	C2'-C3'-O3'	5.20	121.50	113.70
48	5	989	U	C3'-C2'-O2'	5.19	118.48	110.70
51	9	454	U	C4'-C3'-O3'	-5.19	105.22	113.00
31	f	17	GLY	N-CA-C	-5.18	104.07	112.31
48	5	2067	C	C4'-C3'-O3'	-5.17	105.25	113.00
48	5	1357	C	C3'-C2'-O2'	5.16	118.44	110.70
48	5	1729	A	C4'-C3'-O3'	-5.15	105.27	113.00
48	5	3625	G	C2'-C3'-O3'	5.15	121.42	113.70
48	5	4219	A	C4'-C3'-O3'	-5.15	105.27	113.00
48	5	4474	A	C3'-C2'-O2'	5.15	118.43	110.70
51	9	746	C	C3'-C2'-O2'	5.15	118.43	110.70
51	9	1275	G	C3'-C2'-O2'	5.15	118.42	110.70
56	EE	11	ARG	N-CA-C	-5.15	103.24	110.50
51	9	1859	A	N9-C1'-C2'	5.14	119.72	112.00
47	3	41	U	C3'-C2'-O2'	5.14	118.41	110.70
48	5	1804	A	C4'-C3'-O3'	5.14	117.11	109.40
48	5	5022	U	C3'-C2'-O2'	5.14	118.41	110.70
48	5	1239	C	C2'-C3'-O3'	5.14	117.20	109.50
48	5	2526	C	C4'-C3'-O3'	-5.13	105.31	113.00
48	5	2858	A	N9-C1'-C2'	-5.12	104.31	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	7	29	C	C4'-C3'-O3'	-5.12	105.31	113.00
48	5	931	C	C2'-C3'-O3'	5.12	121.39	113.70
48	5	1072	C	N1-C1'-C2'	5.12	121.68	114.00
54	CC	61	LEU	CA-C-N	-5.12	113.44	119.84
54	CC	61	LEU	C-N-CA	-5.12	113.44	119.84
51	9	1336	C	C4'-C3'-O3'	-5.12	105.32	113.00
53	BB	136	ARG	CG-CD-NE	5.12	123.26	112.00
48	5	2836	A	C4'-C3'-O3'	-5.12	105.32	113.00
48	5	4723	A	N9-C1'-C2'	5.12	119.68	112.00
51	9	522	A	C3'-C2'-O2'	5.11	118.36	110.70
85	hh	42	C	C4'-C3'-O3'	5.10	117.06	109.40
48	5	978	G	C2'-C3'-O3'	5.10	121.35	113.70
51	9	434	G	C2'-C3'-O3'	5.10	121.35	113.70
48	5	1530	G	C3'-C2'-O2'	5.10	118.35	110.70
48	5	4183	G	C2'-C3'-O3'	5.09	117.14	109.50
51	9	140	C	C3'-C2'-O2'	5.09	118.34	110.70
48	5	1912	G	C4'-C3'-O3'	-5.09	105.36	113.00
48	5	216	C	C3'-C2'-O2'	5.08	118.32	110.70
48	5	486	C	C3'-C2'-O2'	5.08	118.32	110.70
48	5	716	C	C4'-C3'-O3'	-5.08	105.38	113.00
7	G	77	PRO	CA-C-N	5.08	124.69	119.56
7	G	77	PRO	C-N-CA	5.08	124.69	119.56
48	5	1371	A	O4'-C1'-C2'	-5.08	102.53	107.60
48	5	93	G	C1'-C2'-O2'	-5.07	100.79	108.40
48	5	4544	A	C4'-C3'-O3'	-5.07	105.39	113.00
48	5	4889	G	C2'-C3'-O3'	5.07	117.11	109.50
48	5	20	U	C2'-C3'-O3'	5.07	117.11	109.50
48	5	1904	G	C3'-C2'-O2'	5.07	118.30	110.70
48	5	4069	U	C3'-C2'-O2'	5.07	118.30	110.70
48	5	4492	U	C3'-C2'-O2'	5.07	118.30	110.70
48	5	4978	G	C4'-C3'-O3'	-5.07	105.40	113.00
48	5	4586	G	C1'-C2'-O2'	5.07	116.00	108.40
48	5	2422	C	C3'-C2'-O2'	5.06	118.29	110.70
66	OO	37	PHE	N-CA-C	-5.06	102.21	110.20
48	5	4638	U	C1'-C2'-O2'	5.05	115.98	108.40
48	5	2356	U	C4'-C3'-O3'	-5.05	105.42	113.00
48	5	693	C	C2'-C3'-O3'	5.05	121.27	113.70
48	5	5026	U	N1-C1'-C2'	5.05	119.57	112.00
48	5	166	C	O4'-C1'-C2'	-5.04	102.56	107.60
48	5	2827	G	O4'-C4'-C3'	-5.04	101.06	106.10
48	5	977	C	C4'-C3'-O3'	-5.04	105.44	113.00
48	5	2505	C	C4'-C3'-O3'	5.04	116.97	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	3697	U	C3'-C2'-O2'	5.04	118.27	110.70
47	3	1	G	C5'-C4'-C3'	5.04	123.56	116.00
51	9	1490	G	C4'-C3'-O3'	-5.04	105.45	113.00
59	HH	112	ASN	N-CA-C	-5.03	105.99	112.68
51	9	686	U	C4'-C3'-O3'	-5.03	105.45	113.00
45	1	63	SER	CA-C-N	5.03	126.12	119.84
45	1	63	SER	C-N-CA	5.03	126.12	119.84
48	5	728	U	C4'-C3'-O3'	5.02	116.93	109.40
48	5	3784	A	C2'-C3'-O3'	5.02	117.03	109.50
42	r	124	VAL	N-CA-C	5.02	115.14	110.42
51	9	1144	A	N9-C1'-C2'	5.02	119.52	112.00
48	5	1440	U	C2'-C3'-O3'	5.01	121.22	113.70
48	5	1379	C	O4'-C1'-C2'	-5.01	100.79	105.80
51	9	839	C	N1-C1'-C2'	5.00	119.50	112.00

There are no chirality outliers.

All (42) planarity outliers are listed below:

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

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

5.2 Too-close contacts [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	20	0
2	B	3148	0	3267	35	0
3	C	2883	0	3053	43	0
4	D	2386	0	2419	23	0
5	E	1898	0	2035	45	0
6	F	1870	0	1994	20	0
7	G	1934	0	2087	36	0
8	H	1516	0	1597	19	0
9	I	1655	0	1704	38	0
10	J	1353	0	1386	17	0
11	L	1703	0	1820	33	0
12	M	1137	0	1211	25	0
13	N	1701	0	1749	17	0
14	O	1638	0	1777	25	0
15	P	1242	0	1274	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	Q	1506	0	1623	9	0
17	R	1508	0	1664	36	0
18	S	1454	0	1496	15	0
19	T	1298	0	1366	12	0
20	U	808	0	831	3	0
21	V	979	0	1039	3	0
22	W	528	0	541	3	0
23	X	976	0	1053	7	0
24	Y	1115	0	1205	6	0
25	Z	1107	0	1182	11	0
26	a	1162	0	1209	18	0
27	b	609	0	650	2	0
28	c	732	0	769	13	0
29	d	888	0	930	12	0
30	e	1053	0	1147	15	0
31	f	876	0	912	17	0
32	g	906	0	1000	6	0
33	h	1013	0	1147	13	0
34	i	830	0	914	13	0
35	j	705	0	737	10	0
36	k	569	0	637	3	0
37	l	444	0	483	3	0
38	m	429	0	467	8	0
39	n	222	0	264	10	0
40	o	851	0	921	5	0
41	p	708	0	757	8	0
42	r	1001	0	1060	34	0
43	s	1523	0	1577	21	0
44	t	1238	0	1295	8	0
45	1	125	0	117	4	0
46	2	1616	0	824	17	0
47	3	1593	0	811	112	0
48	5	78486	0	39661	1323	0
49	7	2558	0	1296	27	0
50	8	3314	0	1683	52	0
51	9	36680	0	18530	629	0
52	AA	1642	0	1646	16	0
53	BB	1729	0	1803	11	0
54	CC	1694	0	1782	38	0
55	DD	1764	0	1863	8	0
56	EE	2073	0	2175	23	0
57	FF	1509	0	1563	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	GG	1923	0	2089	21	0
59	HH	1521	0	1616	18	0
60	II	1686	0	1772	33	0
61	JJ	1525	0	1640	14	0
62	KK	827	0	854	6	0
63	LL	1238	0	1315	11	0
64	MM	958	0	993	3	0
65	NN	1208	0	1294	14	0
66	OO	1016	0	1039	15	0
67	PP	1060	0	1120	14	0
68	QQ	1124	0	1193	6	0
69	RR	1047	0	1103	20	0
70	SS	1139	0	1191	12	0
71	TT	1102	0	1142	13	0
72	UU	821	0	883	1	0
73	VV	636	0	634	4	0
74	WW	1034	0	1080	6	0
75	XX	1098	0	1167	11	0
76	YY	1023	0	1090	8	0
77	ZZ	598	0	656	3	0
78	aa	781	0	828	15	0
79	bb	651	0	672	3	0
80	cc	475	0	497	6	0
81	dd	445	0	439	6	0
82	ee	457	0	502	3	0
83	ff	527	0	545	10	0
84	gg	2436	0	2393	5	0
85	hh	256	0	129	4	0
86	ii	3280	0	3326	64	0
87	jj	4551	0	4687	40	0
88	5	146	0	0	0	0
88	7	5	0	0	0	0
88	8	2	0	0	0	0
88	9	35	0	0	0	0
88	C	1	0	0	0	0
88	I	1	0	0	0	0
88	P	1	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
89	aa	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	dd	1	0	0	0	0
89	ff	1	0	0	2	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	16	0	0	1	0
91	jj	54	0	24	0	0
All	All	226469	0	169875	3000	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (3000) 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)
78:aa:51:ARG:NH2	80:cc:40:HIS:CE1	1.70	1.58
87:jj:121:LYS:NZ	87:jj:121:LYS:CE	1.83	1.39
57:FF:194:ASP:O	57:FF:198:ARG:HG3	1.28	1.33
48:5:976:G:H2'	48:5:977:C:O4'	1.26	1.30
86:ii:374:LEU:CD2	86:ii:378:PHE:CE2	2.14	1.30
86:ii:374:LEU:HD21	86:ii:378:PHE:CE2	1.67	1.29
7:G:29:ASN:OD1	7:G:30:PRO:HD3	1.30	1.28
48:5:4213:A:N1	48:5:4218:U:O4	1.66	1.26
42:r:103:HIS:ND1	42:r:106:LEU:CD2	2.00	1.25
78:aa:26:CYS:SG	89:aa:201:ZN:ZN	1.27	1.23
51:9:1454:A:OP1	69:RR:3:ARG:NE	1.71	1.22
5:E:279:PRO:HG2	31:f:7:CYS:SG	1.79	1.21
48:5:2367:A:N1	48:5:2788:U:O4	1.72	1.21
9:I:191:ILE:CD1	9:I:200:ILE:HD12	1.71	1.21
48:5:2468:U:O4	48:5:2473:A:N1	1.72	1.20
42:r:103:HIS:ND1	42:r:106:LEU:HD23	1.57	1.20
48:5:1929:A:N1	48:5:2054:U:O4	1.73	1.20
54:CC:191:VAL:HA	54:CC:228:SER:OG	1.03	1.19
57:FF:194:ASP:OD1	57:FF:198:ARG:NE	1.77	1.18
48:5:1963:C:N3	48:5:4694:G:O6	1.74	1.17
51:9:1308:U:O2'	83:ff:128:ALA:HB2	1.45	1.14
9:I:191:ILE:HD12	9:I:200:ILE:CD1	1.78	1.14
57:FF:194:ASP:OD1	57:FF:198:ARG:CZ	1.95	1.14
5:E:59:TYR:CD2	5:E:64:LEU:HD12	1.84	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:52:LEU:HD13	56:EE:54:TYR:CD2	1.85	1.11
43:s:59:THR:HG23	48:5:1961:G:OP2	1.49	1.09
7:G:30:PRO:HD2	7:G:31:LEU:H	1.13	1.08
54:CC:191:VAL:CA	54:CC:228:SER:OG	1.99	1.08
51:9:1308:U:O2'	83:ff:128:ALA:CB	2.02	1.07
7:G:86:VAL:HG21	7:G:185:LYS:HE3	1.37	1.07
7:G:86:VAL:HG11	7:G:185:LYS:HG2	1.34	1.06
86:ii:323:TYR:CE2	86:ii:325:ASN:HB2	1.89	1.06
51:9:872:A:N1	51:9:914:U:O4	1.89	1.05
9:I:191:ILE:CD1	9:I:200:ILE:CD1	2.35	1.04
17:R:174:GLU:O	17:R:178:GLN:OE1	1.75	1.04
47:3:6:G:N2	47:3:67:U:O2	1.89	1.04
51:9:1454:A:P	69:RR:3:ARG:HE	1.80	1.03
28:c:83:THR:O	65:NN:151:ALA:O	1.77	1.02
48:5:1962:A:C2'	48:5:1963:C:H5'	1.88	1.02
48:5:2409:U:C4	48:5:2783:A:N1	2.28	1.02
48:5:1929:A:H61	48:5:2054:U:H3	1.04	1.02
51:9:1308:U:C4	51:9:1309:C:C6	2.49	1.01
17:R:178:GLN:OE1	17:R:178:GLN:N	1.94	1.01
48:5:1983:A:N1	48:5:2008:U:C4	2.30	1.00
9:I:191:ILE:HD11	9:I:200:ILE:HD12	1.38	1.00
48:5:1983:A:N1	48:5:2008:U:O4	1.95	0.99
51:9:830:A:N6	51:9:844:U:N3	2.08	0.99
78:aa:51:ARG:NH2	80:cc:40:HIS:ND1	2.10	0.99
7:G:156:VAL:HG11	7:G:184:LEU:HD12	1.40	0.99
43:s:57:LYS:NZ	48:5:1961:G:OP1	1.94	0.99
48:5:4694:G:N2	48:5:4694:G:OP1	1.94	0.99
54:CC:227:TRP:O	54:CC:228:SER:OG	1.80	0.99
47:3:39:U:O4'	57:FF:135:ARG:NH2	1.97	0.98
47:3:5:G:H2'	47:3:6:G:C8	1.98	0.98
86:ii:374:LEU:HD21	86:ii:378:PHE:CZ	1.98	0.98
3:C:161:TYR:CD1	3:C:166:GLU:HB3	1.99	0.98
51:9:1448:A:O2'	51:9:1449:G:C5'	2.12	0.97
48:5:77:U:O4	48:5:335:A:N1	1.96	0.97
51:9:1144:A:H2'	51:9:1145:A:C8	1.99	0.97
10:J:80:GLU:OE2	10:J:170:TYR:OH	1.81	0.97
11:L:170:THR:HG22	11:L:173:GLU:HG3	1.46	0.97
43:s:14:PHE:CE2	48:5:1960:A:C2	2.53	0.96
86:ii:323:TYR:CE1	86:ii:324:GLU:HG2	2.00	0.96
47:3:35:U:C1'	51:9:1641:A:OP1	2.14	0.96
4:D:200:MET:HE2	4:D:241:LYS:HG3	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:LEU:CD2	2:B:182:GLU:HG2	1.95	0.95
48:5:2409:U:O4	48:5:2783:A:N1	1.98	0.95
86:ii:345:TYR:CD1	86:ii:374:LEU:HD12	2.00	0.95
48:5:1563:A:N6	51:9:1028:A:N1	2.16	0.94
17:R:176:ARG:NH2	17:R:176:ARG:HB2	1.81	0.94
7:G:29:ASN:OD1	7:G:30:PRO:CD	2.16	0.94
51:9:872:A:N1	51:9:914:U:C4	2.36	0.93
51:9:830:A:N1	51:9:844:U:O4	2.02	0.93
54:CC:191:VAL:HA	54:CC:228:SER:CB	1.98	0.93
86:ii:345:TYR:HD1	86:ii:374:LEU:HD12	1.32	0.93
48:5:1278:C:H3'	48:5:1279:A:H4'	1.50	0.92
54:CC:60:TRP:O	54:CC:61:LEU:HD12	1.68	0.92
48:5:1968:G:H1	48:5:2018:C:H42	0.93	0.92
47:3:39:U:HO2'	47:3:40:C:H6	0.92	0.91
51:9:1681:U:O2'	51:9:1682:C:O4'	1.88	0.91
43:s:14:PHE:CZ	48:5:1960:A:N3	2.37	0.91
51:9:1407:U:H2'	51:9:1408:U:C5	2.05	0.91
47:3:6:G:H1	47:3:67:U:H3	1.18	0.91
48:5:976:G:C2'	48:5:977:C:O4'	2.18	0.91
78:aa:51:ARG:NH2	80:cc:40:HIS:HE1	1.46	0.91
47:3:68:C:O2'	47:3:69:G:O4'	1.88	0.91
56:EE:52:LEU:HD13	56:EE:54:TYR:HD2	1.28	0.91
5:E:279:PRO:CG	31:f:7:CYS:SG	2.58	0.91
8:H:100:PRO:HD3	87:jj:440:GLN:HE22	1.33	0.90
86:ii:374:LEU:HD23	86:ii:378:PHE:CE2	2.06	0.90
47:3:5:G:N1	47:3:68:C:O2	2.05	0.90
51:9:1305:C:O2'	51:9:1306:U:H5'	1.72	0.90
48:5:1968:G:H1	48:5:2018:C:N4	1.69	0.90
51:9:1233:G:C2'	51:9:1234:C:H5'	2.02	0.90
83:ff:139:CYS:HG	89:ff:200:ZN:ZN	0.64	0.89
87:jj:65:CYS:HG	90:jj:601:SF4:FE3	0.65	0.89
9:I:191:ILE:HD12	9:I:200:ILE:HD11	1.55	0.89
62:KK:15:LEU:HD22	62:KK:49:MET:HE1	1.54	0.89
57:FF:194:ASP:OD1	57:FF:198:ARG:NH1	2.05	0.89
54:CC:73:VAL:O	54:CC:73:VAL:HG12	1.71	0.88
11:L:164:GLU:N	11:L:164:GLU:OE2	2.06	0.88
4:D:33:ARG:NH2	49:7:7:G:O3'	2.06	0.88
48:5:2395:A:O2'	48:5:2806:A:H1'	1.72	0.88
48:5:2026:A:C2'	48:5:2027:U:H5'	2.04	0.88
47:3:66:U:C4	47:3:67:U:C5	2.61	0.88
47:3:5:G:C2	47:3:6:G:C5	2.61	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1267:C:O2'	51:9:1268:C:H5'	1.72	0.87
2:B:163:LEU:HD23	2:B:182:GLU:HG2	1.57	0.87
48:5:957:G:H1'	48:5:958:G:OP2	1.75	0.87
47:3:67:U:O2'	47:3:68:C:H5'	1.74	0.87
51:9:1454:A:OP1	69:RR:3:ARG:CZ	2.23	0.86
5:E:238:ILE:O	5:E:239:THR:OG1	1.92	0.86
86:ii:323:TYR:OH	86:ii:325:ASN:ND2	2.08	0.86
43:s:14:PHE:CE2	48:5:1960:A:H2	1.90	0.86
48:5:102:G:O2'	48:5:1381:U:O2'	1.93	0.86
48:5:2027:U:O2'	48:5:2028:C:H5'	1.74	0.86
48:5:3753:G:OP2	48:5:3776:G:O2'	1.92	0.86
48:5:1929:A:N6	48:5:2054:U:H3	1.72	0.86
11:L:94:ILE:C	33:h:119:TYR:CE1	2.54	0.85
48:5:2468:U:N3	48:5:2473:A:N6	2.24	0.85
51:9:1448:A:O2'	51:9:1449:G:H5''	1.76	0.85
51:9:1235:G:H2'	51:9:1236:G:H8	1.42	0.85
51:9:830:A:N6	51:9:844:U:H3	1.73	0.85
9:I:191:ILE:HD12	9:I:200:ILE:HD12	1.42	0.84
7:G:30:PRO:HD2	7:G:31:LEU:N	1.90	0.84
51:9:1305:C:C2'	51:9:1306:U:H5'	2.06	0.84
57:FF:194:ASP:O	57:FF:198:ARG:CG	2.20	0.84
43:s:57:LYS:NZ	48:5:1961:G:P	2.51	0.84
17:R:172:ARG:CB	51:9:909:G:OP2	2.26	0.83
48:5:1279:A:C3'	48:5:1280:C:H5''	2.08	0.83
48:5:4694:G:H21	48:5:4694:G:P	2.00	0.83
86:ii:374:LEU:CD2	86:ii:378:PHE:HE2	1.87	0.83
48:5:1963:C:C4	48:5:4694:G:O6	2.31	0.83
78:aa:51:ARG:HH21	80:cc:40:HIS:CE1	1.96	0.83
11:L:95:GLY:HA3	33:h:119:TYR:OH	1.79	0.83
48:5:5026:U:H5'	60:II:79:ILE:HD11	1.62	0.82
51:9:1233:G:O2'	51:9:1234:C:H5'	1.79	0.82
12:M:116:LYS:CG	14:O:196:LEU:HD21	2.10	0.82
17:R:174:GLU:O	17:R:178:GLN:CD	2.22	0.82
48:5:3914:U:H3	48:5:4378:A:N6	1.76	0.81
87:jj:121:LYS:NZ	87:jj:121:LYS:CD	2.42	0.81
48:5:723:A:H2	48:5:943:A:N1	1.79	0.81
48:5:4075:U:O2'	48:5:4076:G:H2'	1.80	0.81
56:EE:52:LEU:HD13	56:EE:54:TYR:CE2	2.15	0.81
7:G:156:VAL:HG11	7:G:184:LEU:CD1	2.10	0.81
48:5:3751:G:C2'	48:5:3752:C:H5'	2.11	0.81
17:R:176:ARG:HB2	17:R:176:ARG:HH21	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1367:C:C2	48:5:1370:G:H2'	2.16	0.80
47:3:5:G:H2'	47:3:6:G:H8	1.41	0.80
2:B:163:LEU:HD21	2:B:182:GLU:HG2	1.63	0.80
51:9:321:C:O2'	51:9:322:C:H5'	1.82	0.80
85:hh:49:U:O2	86:ii:61:ASN:O	1.98	0.80
47:3:38:A:C2	57:FF:135:ARG:NH1	2.50	0.79
47:3:4:C:C2	47:3:5:G:N7	2.50	0.79
47:3:6:G:O2'	47:3:7:A:O4'	1.99	0.79
86:ii:374:LEU:O	86:ii:377:TRP:HB3	1.81	0.79
7:G:156:VAL:CG1	7:G:184:LEU:HD12	2.13	0.79
59:HH:66:VAL:HG22	59:HH:96:ALA:HB1	1.64	0.79
51:9:1293:A:N6	51:9:1306:U:O2	2.16	0.79
28:c:86:GLY:N	65:NN:151:ALA:OXT	2.16	0.79
51:9:1235:G:H2'	51:9:1236:G:C8	2.18	0.79
51:9:1268:C:O2'	51:9:1269:G:O5'	2.00	0.79
48:5:2026:A:O2'	48:5:2027:U:H5'	1.82	0.78
86:ii:374:LEU:HD23	86:ii:378:PHE:CD2	2.18	0.78
48:5:504:G:N1	48:5:654:C:C2	2.52	0.78
48:5:723:A:C2	48:5:943:A:N1	2.51	0.78
51:9:656:G:O2'	54:CC:227:TRP:NE1	2.15	0.78
48:5:919:C:N4	48:5:920:C:C4	2.52	0.78
51:9:1102:G:N2	51:9:1103:C:C2	2.50	0.78
51:9:1293:A:N6	51:9:1306:U:C2	2.52	0.78
9:I:48:LEU:HD21	9:I:145:LYS:HG2	1.63	0.78
48:5:1213:G:C6	48:5:1215:C:C2	2.71	0.78
48:5:1279:A:H3'	48:5:1280:C:H5''	1.64	0.78
54:CC:60:TRP:C	54:CC:61:LEU:HD12	2.08	0.78
86:ii:327:ASP:HB3	86:ii:348:PRO:HG3	1.66	0.78
17:R:176:ARG:NH1	51:9:909:G:OP1	2.17	0.77
48:5:1379:C:H4'	48:5:1380:G:O4'	1.84	0.77
51:9:1385:G:O2'	51:9:1386:A:H5'	1.85	0.77
7:G:86:VAL:HG21	7:G:185:LYS:CE	2.15	0.77
48:5:1962:A:H2'	48:5:1963:C:H5'	1.66	0.77
54:CC:211:LYS:O	54:CC:215:LEU:HG	1.84	0.77
48:5:4371:G:O2'	48:5:4372:U:OP2	2.03	0.77
12:M:116:LYS:HG3	14:O:196:LEU:HD21	1.67	0.77
2:B:14:LEU:HD23	2:B:17:LEU:HD21	1.66	0.77
17:R:168:GLU:O	17:R:172:ARG:HG2	1.83	0.77
48:5:3914:U:H3	48:5:4378:A:H61	1.29	0.77
51:9:322:C:O2'	51:9:323:C:O5'	2.02	0.77
48:5:745:G:H2'	48:5:746:A:O4'	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:35:U:O4'	51:9:1641:A:OP1	2.03	0.76
47:3:39:U:O2'	47:3:40:C:H6	1.67	0.76
51:9:872:A:C6	51:9:914:U:O4	2.37	0.76
48:5:1563:A:C8	51:9:678:U:H4'	2.20	0.76
48:5:2468:U:C4	48:5:2473:A:N1	2.54	0.76
86:ii:78:VAL:HG23	86:ii:95:VAL:HG11	1.66	0.76
51:9:643:A:OP2	61:JJ:38:ARG:NH2	2.18	0.76
5:E:217:GLN:NE2	5:E:233:LYS:HD2	2.01	0.76
70:SS:11:HIS:O	70:SS:12:ILE:HD12	1.85	0.76
7:G:86:VAL:HG12	7:G:87:LEU:N	2.00	0.76
78:aa:51:ARG:HH21	80:cc:40:HIS:HE1	1.29	0.76
48:5:4723:A:H2'	48:5:4724:A:C8	2.21	0.75
51:9:913:A:OP1	59:HH:99:ARG:NH2	2.19	0.75
51:9:1293:A:C6	51:9:1306:U:C2	2.74	0.75
48:5:166:C:O2	48:5:167:C:H5	1.69	0.75
48:5:3629:A:H4'	51:9:1721:U:O2	1.85	0.75
2:B:174:ARG:NH1	48:5:4985:U:O2	2.19	0.75
47:3:35:U:H1'	51:9:1641:A:OP1	1.84	0.75
48:5:504:G:C2	48:5:654:C:O2	2.39	0.75
48:5:2793:G:C6	48:5:2797:C:C4	2.75	0.75
54:CC:204:ILE:HD13	54:CC:215:LEU:CD2	2.16	0.75
7:G:30:PRO:CD	7:G:31:LEU:H	1.96	0.74
13:N:202:ARG:NH2	48:5:1372:A:OP1	2.21	0.74
87:jj:7:ARG:NH1	87:jj:57:GLY:HA3	2.02	0.74
78:aa:28:ARG:NH1	78:aa:29:CYS:O	2.19	0.74
51:9:872:A:C6	51:9:914:U:C4	2.76	0.74
51:9:1406:G:H3'	51:9:1407:U:H4'	1.69	0.74
48:5:2769:U:C2	48:5:2770:C:C5	2.76	0.74
51:9:1454:A:P	69:RR:3:ARG:NE	2.51	0.74
9:I:49:CYS:SG	9:I:51:HIS:NE2	2.60	0.74
9:I:202:ASN:O	49:7:63:C:C5	2.40	0.74
48:5:3610:A:O2'	60:II:89:GLU:OE1	2.04	0.74
51:9:980:A:H2'	51:9:981:A:C8	2.23	0.74
86:ii:326:LEU:HD11	86:ii:408:GLY:O	1.88	0.73
47:3:33:U:P	57:FF:127:ARG:HH12	2.11	0.73
58:GG:3:LEU:HD13	58:GG:111:LEU:HD11	1.69	0.73
42:r:103:HIS:CE1	42:r:106:LEU:CD2	2.71	0.73
51:9:1211:G:C2'	51:9:1212:G:H5'	2.18	0.73
47:3:35:U:H1'	51:9:1641:A:P	2.28	0.73
2:B:163:LEU:CD2	2:B:182:GLU:CG	2.65	0.73
48:5:2367:A:N6	48:5:2798:A:O4'	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1308:U:H3	51:9:1309:C:H1'	1.53	0.73
47:3:13:C:N3	47:3:22:G:O6	2.22	0.73
48:5:3629:A:C4'	51:9:1721:U:O2	2.36	0.73
47:3:66:U:C5	47:3:67:U:C5	2.77	0.72
51:9:911:C:H2'	51:9:912:C:H5'	1.71	0.72
47:3:35:U:C1'	51:9:1641:A:P	2.77	0.72
51:9:309:G:N2	51:9:310:C:C2	2.58	0.72
48:5:166:C:O2	48:5:167:C:C5	2.42	0.72
11:L:170:THR:CG2	11:L:173:GLU:HG3	2.19	0.72
48:5:516:C:C2	48:5:646:G:N2	2.58	0.72
51:9:1308:U:O2'	51:9:1309:C:O5'	2.08	0.72
85:hh:49:U:C2	86:ii:61:ASN:O	2.42	0.72
30:e:91:CYS:O	30:e:93:LYS:N	2.23	0.71
47:3:4:C:HO2'	47:3:5:G:H8	1.36	0.71
51:9:103:A:OP2	51:9:356:C:N4	2.22	0.71
87:jj:98:PRO:HG2	87:jj:123:LEU:HD11	1.71	0.71
51:9:1235:G:H5'	51:9:1247:C:H42	1.53	0.71
51:9:1680:G:O2'	51:9:1681:U:H5'	1.89	0.71
4:D:200:MET:CE	4:D:241:LYS:HG3	2.19	0.71
26:a:4:ARG:NH2	48:5:2341:A:OP2	2.23	0.71
47:3:33:U:C5'	57:FF:127:ARG:HH12	2.02	0.71
59:HH:93:VAL:HG21	59:HH:133:LEU:HD23	1.72	0.71
47:3:35:U:O4'	51:9:1641:A:P	2.49	0.71
48:5:286:U:H2'	48:5:287:U:C6	2.26	0.71
3:C:161:TYR:CE1	3:C:166:GLU:HB3	2.25	0.71
48:5:4579:U:H2'	48:5:4580:U:C6	2.25	0.71
51:9:751:G:C2	51:9:792:C:N3	2.58	0.71
2:B:163:LEU:HD21	2:B:182:GLU:CG	2.20	0.71
10:J:119:TYR:HB3	70:SS:12:ILE:HD13	1.72	0.71
51:9:911:C:C2'	51:9:912:C:H5'	2.20	0.71
51:9:1386:A:H2'	51:9:1387:G:C8	2.26	0.71
48:5:1278:C:C3'	48:5:1279:A:H4'	2.19	0.71
48:5:1962:A:O2'	48:5:1963:C:H5'	1.89	0.71
48:5:4901:G:N2	48:5:4921:C:C2	2.59	0.71
48:5:973:G:N2	48:5:1282:G:O2'	2.23	0.71
47:3:76:A:N7	48:5:4371:G:C6	2.59	0.70
51:9:1308:U:O3'	83:ff:128:ALA:HB1	1.91	0.70
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.72	0.70
10:J:165:TRP:CH2	10:J:170:TYR:HE2	2.10	0.70
11:L:56:ARG:O	11:L:116:ARG:NH2	2.23	0.70
47:3:4:C:C2	47:3:5:G:C8	2.80	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:77:U:N3	48:5:335:A:N6	2.39	0.70
48:5:22:G:N2	50:8:35:C:C2	2.59	0.70
48:5:978:G:H2'	48:5:979:C:O4'	1.91	0.70
48:5:3723:A:H2'	48:5:3724:A:C8	2.26	0.70
54:CC:204:ILE:HD13	54:CC:215:LEU:HD21	1.72	0.70
48:5:4213:A:N1	48:5:4218:U:C4	2.57	0.70
47:3:1:G:N2	47:3:2:C:C2	2.59	0.70
49:7:30:C:C2	49:7:48:G:N2	2.59	0.70
47:3:68:C:C2	47:3:69:G:C8	2.79	0.70
48:5:181:C:N3	48:5:256:G:C2	2.60	0.70
48:5:4453:C:C2	48:5:4529:G:C2	2.80	0.70
48:5:499:G:N2	48:5:656:C:C2	2.60	0.70
48:5:977:C:C2	48:5:978:G:C8	2.80	0.69
51:9:1386:A:O2'	51:9:1387:G:H5'	1.90	0.69
48:5:504:G:C6	48:5:654:C:N3	2.60	0.69
48:5:956:A:H4'	48:5:957:G:OP2	1.93	0.69
47:3:68:C:C2	47:3:69:G:N7	2.60	0.69
51:9:1102:G:N1	51:9:1103:C:C4	2.60	0.69
48:5:1958:A:C2	48:5:2026:A:C2	2.80	0.69
51:9:872:A:C2	51:9:914:U:O4	2.45	0.69
52:AA:63:ARG:HG2	52:AA:185:MET:HE1	1.74	0.69
63:LL:131:CYS:SG	63:LL:132:ARG:N	2.64	0.69
4:D:200:MET:HE1	4:D:241:LYS:N	2.07	0.69
3:C:161:TYR:CD1	3:C:166:GLU:CB	2.74	0.69
42:r:103:HIS:ND1	42:r:106:LEU:HD21	2.07	0.69
47:3:76:A:C6	48:5:4371:G:C5	2.81	0.69
48:5:499:G:C2	48:5:656:C:C2	2.80	0.69
48:5:1929:A:N1	48:5:2054:U:C4	2.59	0.69
51:9:1407:U:H2'	51:9:1408:U:C6	2.28	0.69
48:5:166:C:O2	48:5:166:C:H2'	1.92	0.69
48:5:1964:A:C2'	48:5:1965:G:H5'	2.23	0.69
48:5:1380:G:O2'	48:5:1381:U:O2	2.09	0.69
48:5:3753:G:N2	48:5:3754:G:C4	2.61	0.69
48:5:5024:C:H2'	60:II:168:GLN:HG3	1.75	0.69
5:E:251:SER:O	5:E:255:PRO:CD	2.41	0.68
48:5:497:G:N2	48:5:657:C:C2	2.61	0.68
9:I:203:ARG:NH2	49:7:105:C:OP2	2.25	0.68
43:s:14:PHE:CE2	48:5:1960:A:N3	2.60	0.68
48:5:2409:U:C4	48:5:2783:A:C2	2.80	0.68
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.26	0.68
7:G:87:LEU:HD23	7:G:184:LEU:CD2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2084:C:H3'	48:5:2085:G:H5'	1.76	0.68
86:ii:322:VAL:HG13	86:ii:326:LEU:HD12	1.75	0.68
48:5:642:G:N2	48:5:643:C:C2	2.61	0.68
47:3:5:G:N1	47:3:6:G:C6	2.61	0.68
5:E:279:PRO:HG2	31:f:7:CYS:HG	1.59	0.68
48:5:2773:G:N2	48:5:2774:C:C2	2.62	0.68
48:5:3751:G:O2'	48:5:3752:C:H5'	1.92	0.68
30:e:30:LYS:NZ	48:5:2347:A:N3	2.42	0.68
48:5:1964:A:H2'	48:5:1965:G:H5'	1.75	0.68
4:D:200:MET:CE	4:D:237:GLU:O	2.43	0.67
17:R:176:ARG:NH1	51:9:909:G:H5'	2.09	0.67
10:J:83:LEU:HD12	10:J:170:TYR:OH	1.93	0.67
48:5:1280:C:C4	48:5:1282:G:C6	2.82	0.67
51:9:50:A:N1	51:9:488:U:O4	2.26	0.67
51:9:522:A:OP2	61:JJ:45:ARG:NH2	2.27	0.67
47:3:33:U:C5'	57:FF:127:ARG:NH1	2.57	0.67
48:5:1264:C:H2'	48:5:1265:G:O4'	1.94	0.67
48:5:1956:A:H2'	48:5:1957:U:C6	2.30	0.67
48:5:2367:A:N1	48:5:2788:U:C4	2.61	0.67
51:9:1448:A:O2'	51:9:1449:G:O5'	2.12	0.67
48:5:2632:U:H2'	48:5:2633:U:C6	2.29	0.67
67:PP:34:MET:HE2	67:PP:34:MET:HA	1.75	0.67
83:ff:139:CYS:SG	89:ff:200:ZN:ZN	1.80	0.67
47:3:34:U:O2	51:9:1641:A:H5'	1.94	0.67
48:5:1983:A:C2	48:5:2008:U:C4	2.82	0.67
51:9:1253:A:OP2	51:9:1526:G:N2	2.27	0.67
48:5:1635:C:C2'	48:5:1636:U:H5'	2.24	0.67
48:5:1968:G:O2'	48:5:1969:G:O5'	2.13	0.67
48:5:1358:G:C6	48:5:1379:C:N3	2.63	0.66
17:R:172:ARG:HB2	51:9:909:G:OP2	1.95	0.66
48:5:1724:G:H4'	48:5:1725:U:OP2	1.95	0.66
47:3:13:C:O2	47:3:22:G:N1	2.27	0.66
74:WW:52:ILE:HG22	74:WW:61:ILE:HG12	1.76	0.66
48:5:2654:C:C2	48:5:2681:G:N2	2.64	0.66
51:9:656:G:HO2'	54:CC:227:TRP:CD1	2.14	0.66
51:9:1649:U:C4	51:9:1675:A:N1	2.63	0.66
86:ii:375:LEU:HD12	86:ii:375:LEU:O	1.95	0.66
9:I:187:GLU:O	9:I:188:LYS:HE3	1.95	0.66
12:M:116:LYS:HG2	14:O:196:LEU:HD21	1.76	0.66
47:3:66:U:C4	47:3:67:U:C4	2.83	0.66
48:5:1983:A:C6	48:5:2008:U:O4	2.49	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:52:LEU:CD1	56:EE:54:TYR:HD2	2.04	0.66
48:5:2127:C:H2'	48:5:2128:G:C8	2.30	0.66
51:9:1293:A:C6	51:9:1306:U:O2	2.48	0.66
12:M:126:GLU:HG3	14:O:181:ALA:CB	2.26	0.66
43:s:14:PHE:HZ	48:5:1960:A:N3	1.91	0.66
48:5:2367:A:N6	48:5:2788:U:N3	2.44	0.66
48:5:5026:U:OP2	60:II:79:ILE:HD13	1.94	0.66
51:9:1420:G:HO2'	71:TT:4:VAL:N	1.93	0.66
17:R:176:ARG:HH11	51:9:909:G:H4'	1.59	0.66
48:5:977:C:C2'	48:5:978:G:H5'	2.25	0.66
48:5:986:C:C2	48:5:1068:G:N2	2.63	0.66
48:5:2288:G:N2	48:5:2290:C:C2	2.64	0.66
48:5:3712:A:C2	51:9:970:G:C6	2.84	0.66
87:jj:375:MET:HE1	87:jj:548:PRO:HB3	1.78	0.66
48:5:1268:G:H4'	48:5:1269:G:OP1	1.96	0.66
48:5:4481:U:H2'	48:5:4482:U:C6	2.30	0.66
7:G:87:LEU:HD23	7:G:184:LEU:HD21	1.77	0.66
35:j:59:THR:O	50:8:42:G:OP1	2.14	0.66
51:9:913:A:H62	59:HH:120:ARG:HG3	1.61	0.66
81:dd:21:CYS:SG	81:dd:23:VAL:N	2.69	0.66
86:ii:345:TYR:CD1	86:ii:374:LEU:CD1	2.79	0.66
2:B:261:ARG:HE	48:5:3870:C:H4'	1.61	0.65
45:1:68:VAL:C	46:2:76:A:O3'	2.39	0.65
47:3:37:A:C2'	47:3:38:A:H5'	2.25	0.65
86:ii:322:VAL:HG12	86:ii:323:TYR:O	1.96	0.65
10:J:83:LEU:HD12	10:J:170:TYR:CZ	2.30	0.65
16:Q:11:ARG:NH2	48:5:1690:C:OP2	2.29	0.65
45:1:57:ARG:NH2	48:5:3862:A:O2'	2.29	0.65
48:5:1279:A:C2'	48:5:1280:C:H5''	2.26	0.65
47:3:29:A:O2'	47:3:30:G:O5'	2.10	0.65
51:9:316:G:N2	51:9:317:C:C2	2.64	0.65
12:M:126:GLU:HG3	14:O:181:ALA:HB1	1.79	0.65
48:5:3668:C:C2	48:5:3675:G:C2	2.85	0.65
47:3:35:U:H1'	51:9:1640:A:O3'	1.97	0.65
51:9:1444:U:H2'	51:9:1445:U:C6	2.31	0.65
51:9:50:A:N1	51:9:488:U:C4	2.65	0.65
51:9:1454:A:C2	51:9:1476:A:H4'	2.31	0.65
51:9:1454:A:O2'	51:9:1455:A:OP2	2.12	0.65
42:r:46:ARG:NH1	48:5:666:G:C5	2.65	0.65
48:5:1958:A:N1	48:5:2026:A:N1	2.45	0.65
48:5:2367:A:N6	48:5:2788:U:H3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:412:G:N2	51:9:429:C:C2	2.65	0.65
51:9:1109:C:O2	51:9:1109:C:H2'	1.94	0.65
34:i:90:LEU:O	34:i:92:SER:N	2.30	0.65
47:3:66:U:H2'	47:3:67:U:O4'	1.97	0.65
48:5:1359:G:H2'	48:5:1360:G:C8	2.32	0.65
86:ii:385:PHE:O	86:ii:387:ALA:N	2.29	0.65
5:E:126:ARG:NH2	48:5:712:C:O2'	2.31	0.64
48:5:1563:A:C8	48:5:1563:A:O5'	2.49	0.64
48:5:2409:U:O4	48:5:2783:A:C6	2.50	0.64
51:9:913:A:N6	59:HH:120:ARG:HG3	2.12	0.64
48:5:1550:G:C2	48:5:1579:C:C2	2.85	0.64
48:5:2258:C:O2	48:5:2258:C:H2'	1.96	0.64
48:5:4600:G:P	87:jj:506:ARG:HH22	2.20	0.64
51:9:200:G:N2	51:9:201:C:C2	2.65	0.64
85:hh:49:U:N3	86:ii:61:ASN:O	2.29	0.64
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.78	0.64
48:5:482:G:H2'	48:5:483:G:C8	2.33	0.64
11:L:95:GLY:CA	33:h:119:TYR:OH	2.45	0.64
48:5:3662:A:H61	48:5:3680:U:H3	1.44	0.64
51:9:751:G:N2	51:9:792:C:C2	2.66	0.64
51:9:1406:G:C3'	51:9:1407:U:H4'	2.27	0.64
5:E:254:LEU:O	5:E:254:LEU:HD23	1.96	0.64
39:n:4:LYS:HE2	51:9:1844:U:O4	1.98	0.64
48:5:22:G:C2	50:8:35:C:N3	2.66	0.64
48:5:504:G:C6	48:5:654:C:C2	2.85	0.64
48:5:976:G:H4'	48:5:976:G:OP1	1.96	0.64
71:TT:33:TRP:O	71:TT:35:ASP:N	2.30	0.64
42:r:103:HIS:CE1	42:r:106:LEU:HD21	2.32	0.64
47:3:76:A:N6	48:5:4371:G:N7	2.45	0.64
48:5:1358:G:H8	48:5:1358:G:H3'	1.61	0.64
48:5:1962:A:C3'	48:5:1963:C:H5'	2.27	0.64
51:9:872:A:N6	51:9:914:U:C5	2.66	0.64
48:5:2090:U:P	48:5:2090:U:O4'	2.56	0.64
56:EE:102:ILE:HG23	56:EE:182:MET:HE1	1.79	0.64
81:dd:21:CYS:SG	81:dd:39:CYS:SG	2.95	0.64
3:C:114:ARG:HB2	3:C:114:ARG:CZ	2.28	0.63
47:3:38:A:C2	57:FF:135:ARG:CZ	2.81	0.63
48:5:111:C:C2	48:5:331:G:C2	2.86	0.63
48:5:1404:G:C2	48:5:1414:C:C2	2.85	0.63
51:9:1144:A:C2	51:9:1145:A:C2	2.85	0.63
86:ii:300:LYS:O	86:ii:413:LEU:HG	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1213:G:N1	48:5:1215:C:C2	2.67	0.63
48:5:1268:G:C2	48:5:1270:A:C8	2.86	0.63
48:5:1358:G:H2'	48:5:1359:G:O4'	1.97	0.63
48:5:5066:U:H2'	48:5:5067:U:C6	2.33	0.63
7:G:30:PRO:CD	7:G:31:LEU:N	2.59	0.63
48:5:1378:C:H3'	48:5:1379:C:C5'	2.29	0.63
51:9:200:G:N1	51:9:201:C:C4	2.66	0.63
86:ii:287:ILE:HD11	86:ii:392:VAL:HG21	1.81	0.63
76:YY:110:ARG:O	76:YY:113:ARG:O	2.16	0.63
7:G:86:VAL:CG1	7:G:87:LEU:N	2.61	0.63
7:G:87:LEU:CD2	7:G:184:LEU:HD21	2.29	0.63
47:3:68:C:N3	47:3:69:G:N7	2.47	0.63
48:5:1279:A:H3'	48:5:1280:C:C5'	2.29	0.63
9:I:191:ILE:HD11	9:I:200:ILE:CD1	2.18	0.63
11:L:116:ARG:NH1	11:L:155:MET:O	2.29	0.63
48:5:1635:C:H2'	48:5:1636:U:H5'	1.79	0.63
48:5:2108:G:C6	48:5:2125:C:N4	2.66	0.63
51:9:1453:C:H2'	51:9:1454:A:H4'	1.81	0.63
54:CC:73:VAL:O	54:CC:73:VAL:CG1	2.45	0.63
78:aa:8:ASN:O	78:aa:10:ARG:N	2.32	0.63
9:I:80:CYS:SG	9:I:81:GLY:N	2.71	0.63
48:5:1957:U:O2'	48:5:1958:A:H8	1.82	0.63
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.81	0.63
51:9:1308:U:HO2'	83:ff:128:ALA:HB2	1.62	0.63
47:3:67:U:C2'	47:3:68:C:H5'	2.29	0.62
49:7:30:C:N3	49:7:48:G:C2	2.67	0.62
5:E:279:PRO:CD	31:f:7:CYS:SG	2.87	0.62
10:J:83:LEU:CD1	10:J:170:TYR:CZ	2.82	0.62
3:C:271:ALA:O	3:C:272:SER:OG	2.12	0.62
7:G:86:VAL:HG12	7:G:87:LEU:H	1.65	0.62
12:M:126:GLU:CG	14:O:181:ALA:HB1	2.29	0.62
12:M:126:GLU:CD	12:M:130:LEU:HD13	2.25	0.62
14:O:72:HIS:N	48:5:4586:G:OP1	2.30	0.62
48:5:933:G:C2	48:5:940:C:C6	2.88	0.62
48:5:1241:C:N4	48:5:1270:A:O2'	2.33	0.62
48:5:5000:G:C2	48:5:5051:C:C2	2.87	0.62
51:9:474:G:N2	51:9:475:C:C2	2.67	0.62
51:9:1842:C:C2	51:9:1858:G:C2	2.88	0.62
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.82	0.62
48:5:969:C:O2'	48:5:970:G:N3	2.28	0.62
48:5:4461:C:O2	48:5:4516:G:C2	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1771:G:N2	51:9:1772:C:C2	2.67	0.62
51:9:1466:G:N2	51:9:1467:C:C2	2.68	0.62
51:9:1537:A:H2'	51:9:1538:C:O4'	2.00	0.62
51:9:1727:G:H2'	51:9:1728:U:O4'	1.99	0.62
48:5:106:A:H1'	48:5:336:A:C8	2.34	0.62
48:5:1358:G:O2'	48:5:1359:G:O4'	2.16	0.62
48:5:1367:C:N3	48:5:1369:C:OP2	2.32	0.62
48:5:1957:U:O2'	48:5:1958:A:OP2	2.18	0.62
48:5:1965:G:HO2'	48:5:1966:C:P	2.22	0.62
87:jj:98:PRO:HB2	87:jj:106:LEU:HD11	1.81	0.62
48:5:2547:G:N2	48:5:2548:C:C2	2.68	0.62
48:5:1964:A:O2'	48:5:1965:G:H5'	1.99	0.61
86:ii:117:PHE:CZ	86:ii:140:LEU:HD22	2.35	0.61
43:s:59:THR:CG2	48:5:1961:G:OP2	2.39	0.61
7:G:156:VAL:CG1	7:G:184:LEU:CD1	2.75	0.61
51:9:1386:A:H2'	51:9:1387:G:H8	1.62	0.61
48:5:222:C:H2'	48:5:223:G:O4'	2.00	0.61
48:5:1358:G:H3'	48:5:1358:G:C8	2.35	0.61
48:5:1378:C:H3'	48:5:1379:C:H5'	1.81	0.61
7:G:86:VAL:CG1	7:G:87:LEU:H	2.13	0.61
47:3:4:C:O2'	47:3:5:G:H8	1.83	0.61
43:s:14:PHE:CZ	48:5:1960:A:C2	2.87	0.61
48:5:2468:U:H3	48:5:2473:A:N6	1.97	0.61
48:5:2905:C:C2	48:5:3590:G:N2	2.69	0.61
51:9:309:G:N1	51:9:310:C:C4	2.68	0.61
48:5:181:C:C2	48:5:256:G:N2	2.69	0.61
48:5:1213:G:C2	48:5:1215:C:O2	2.53	0.61
48:5:4901:G:C2	48:5:4921:C:N3	2.69	0.61
1:A:27:ALA:O	1:A:128:ARG:NH2	2.34	0.61
25:Z:5:MET:HG2	25:Z:77:TYR:CE1	2.36	0.61
18:S:80:ILE:HD11	18:S:126:ILE:HD12	1.83	0.61
48:5:167:C:C2	48:5:269:G:N2	2.69	0.61
48:5:3723:A:C2	48:5:3724:A:C6	2.89	0.61
48:5:3751:G:H2'	48:5:3752:C:H5'	1.83	0.61
51:9:1453:C:C2'	51:9:1454:A:H4'	2.30	0.61
48:5:199:G:C6	48:5:201:C:N4	2.68	0.61
48:5:1854:G:N2	48:5:4394:A:O4'	2.33	0.61
51:9:1130:G:C2	51:9:1131:G:C8	2.89	0.61
42:r:103:HIS:ND1	42:r:106:LEU:HD22	2.11	0.60
48:5:1081:C:C2	48:5:1220:G:C2	2.88	0.60
48:5:1186:U:H2'	48:5:1187:G:O4'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1454:A:C2	51:9:1476:A:C4'	2.84	0.60
48:5:4600:G:OP1	87:jj:506:ARG:NH2	2.27	0.60
55:DD:31:GLU:OE1	55:DD:106:ARG:NH2	2.34	0.60
5:E:126:ARG:HH12	48:5:1285:U:P	2.23	0.60
48:5:4213:A:C2	48:5:4218:U:O4	2.50	0.60
1:A:180:LEU:HD21	41:p:26:VAL:HG21	1.83	0.60
47:3:10:G:N2	47:3:11:C:C2	2.69	0.60
48:5:515:C:C2	48:5:647:G:C2	2.90	0.60
48:5:1964:A:C5	48:5:1965:G:C8	2.90	0.60
48:5:1987:C:O2	48:5:1987:C:H2'	2.00	0.60
51:9:1129:G:H3'	51:9:1130:G:H8	1.66	0.60
51:9:1454:A:C2	51:9:1476:A:H5''	2.37	0.60
66:OO:75:MET:SD	80:cc:63:ARG:NH2	2.74	0.60
48:5:22:G:C2	50:8:35:C:C2	2.89	0.60
48:5:3612:C:H1'	48:5:5016:A:C8	2.36	0.60
63:LL:66:VAL:HG23	63:LL:131:CYS:SG	2.41	0.60
48:5:2616:C:C2	48:5:2722:G:C2	2.89	0.60
48:5:5061:A:O2'	48:5:5062:G:OP2	2.10	0.60
5:E:238:ILE:C	5:E:239:THR:HG1	1.99	0.60
4:D:200:MET:CE	4:D:240:TYR:HB2	2.31	0.60
48:5:77:U:H3	48:5:335:A:N6	2.00	0.60
51:9:1454:A:OP1	69:RR:49:LYS:HD2	2.01	0.60
47:3:37:A:H2'	47:3:38:A:H5'	1.83	0.60
47:3:39:U:O4'	57:FF:135:ARG:CZ	2.49	0.60
48:5:1957:U:O2'	48:5:1958:A:H5'	2.01	0.60
48:5:2758:G:O2'	48:5:2764:A:N3	2.27	0.60
49:7:30:C:C2	49:7:48:G:C2	2.90	0.60
54:CC:227:TRP:O	54:CC:228:SER:CB	2.50	0.60
42:r:46:ARG:NH1	48:5:666:G:C6	2.70	0.60
51:9:1416:C:H2'	51:9:1417:C:C2	2.37	0.60
48:5:1296:G:H1'	48:5:1297:U:P	2.42	0.59
48:5:1963:C:O2'	48:5:1964:A:OP1	2.20	0.59
48:5:4441:A:H5''	48:5:4441:A:H8	1.67	0.59
51:9:945:U:H2'	51:9:946:U:C6	2.38	0.59
48:5:1991:A:N6	48:5:2003:G:OP1	2.35	0.59
48:5:2446:C:C2	48:5:2515:G:C2	2.90	0.59
51:9:1401:A:C2	51:9:1402:A:C6	2.89	0.59
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.84	0.59
46:2:53:G:C2	46:2:62:C:C2	2.91	0.59
48:5:917:A:C2	48:5:919:C:C5	2.89	0.59
48:5:2084:C:H3'	48:5:2085:G:C5'	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:111:LEU:HD11	8:H:125:ARG:HB2	1.84	0.59
9:I:49:CYS:HB2	9:I:172:GLY:O	2.03	0.59
11:L:172:GLU:OE1	34:i:3:LEU:HG	2.01	0.59
48:5:3594:C:O2	48:5:3594:C:H2'	2.02	0.59
9:I:204:GLY:O	9:I:205:PRO:C	2.46	0.59
47:3:53:G:C2	47:3:62:C:C2	2.91	0.59
47:3:76:A:N7	48:5:4371:G:N1	2.51	0.59
48:5:4411:G:C2	48:5:4432:C:C2	2.90	0.59
51:9:1212:G:O2'	51:9:1213:C:O5'	2.20	0.59
3:C:157:LYS:O	3:C:160:GLY:N	2.35	0.59
11:L:165:LYS:HB2	11:L:165:LYS:NZ	2.17	0.59
48:5:300:A:C2	48:5:301:G:C5	2.91	0.59
48:5:1074:G:C2	48:5:1238:A:C2	2.90	0.59
48:5:3712:A:C6	51:9:970:G:C2	2.91	0.59
51:9:195:C:C2	51:9:205:G:N2	2.71	0.59
87:jj:382:GLY:C	87:jj:539:PRO:HB3	2.27	0.59
48:5:919:C:C4	48:5:920:C:C5	2.91	0.59
48:5:1266:G:H5''	48:5:2112:G:C2	2.38	0.59
48:5:1278:C:C6	48:5:1279:A:H1'	2.38	0.59
29:d:23:ARG:HD3	29:d:57:MET:HE1	1.85	0.59
48:5:4182:G:H5''	48:5:4183:G:OP2	2.03	0.59
48:5:4213:A:N6	48:5:4218:U:H3	2.01	0.59
51:9:1405:A:H2'	51:9:1406:G:O4'	2.03	0.59
9:I:183:ASP:O	9:I:187:GLU:HG3	2.03	0.59
48:5:1279:A:C2	48:5:1280:C:C2	2.90	0.59
48:5:1823:G:O3'	48:5:1825:A:P	2.60	0.59
51:9:1308:U:N3	51:9:1309:C:C1'	2.66	0.59
11:L:94:ILE:O	33:h:119:TYR:CE1	2.56	0.59
48:5:665:C:O2	48:5:665:C:H2'	2.02	0.59
48:5:642:G:N1	48:5:643:C:C4	2.71	0.58
48:5:2827:G:N3	48:5:2827:G:H2'	2.18	0.58
51:9:65:C:N4	58:GG:134:GLY:O	2.35	0.58
51:9:164:A:O2'	51:9:165:G:O4'	2.21	0.58
51:9:322:C:O2'	51:9:323:C:P	2.61	0.58
51:9:1144:A:C2'	51:9:1145:A:C8	2.83	0.58
48:5:5024:C:O3'	60:II:170:LYS:HE2	2.02	0.58
51:9:1408:U:O4	51:9:1409:A:N6	2.35	0.58
48:5:1213:G:O6	48:5:1215:C:C4	2.56	0.58
48:5:2256:C:O2	48:5:2256:C:H2'	2.03	0.58
48:5:245:C:O4'	48:5:245:C:O2	2.21	0.58
48:5:1268:G:C4	48:5:2111:G:C2	2.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:312:G:O2'	51:9:313:A:OP1	2.14	0.58
48:5:1074:G:N2	48:5:1075:G:C2	2.72	0.58
48:5:4723:A:C2	48:5:4724:A:C6	2.91	0.58
51:9:1305:C:C2'	51:9:1306:U:C5'	2.80	0.58
56:EE:163:ASP:O	56:EE:164:LEU:HB2	2.02	0.58
87:jj:374:ILE:HD11	87:jj:505:LYS:HA	1.86	0.58
5:E:198:ASP:O	5:E:256:LYS:HD3	2.02	0.58
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.37	0.58
28:c:84:ALA:HA	65:NN:151:ALA:C	2.28	0.58
48:5:166:C:O2	48:5:166:C:C2'	2.51	0.58
48:5:2026:A:H2'	48:5:2027:U:H5'	1.85	0.58
48:5:5026:U:C6	60:II:79:ILE:HG13	2.39	0.58
51:9:960:U:O2'	51:9:962:A:N7	2.29	0.58
51:9:1531:A:H2'	51:9:1532:C:C6	2.38	0.58
9:I:202:ASN:O	49:7:63:C:C4	2.57	0.58
30:e:108:ARG:HH22	30:e:127:ALA:HB3	1.69	0.58
48:5:685:C:H2'	48:5:685:C:O2	2.04	0.58
48:5:1358:G:C2'	48:5:1359:G:O4'	2.52	0.58
48:5:1430:C:C2	48:5:1455:G:C2	2.91	0.58
48:5:1840:G:H3'	48:5:1842:G:P	2.44	0.58
48:5:4892:A:N1	48:5:4927:G:O6	2.37	0.58
48:5:5026:U:OP2	60:II:79:ILE:CD1	2.52	0.58
48:5:5026:U:C5	60:II:79:ILE:HG13	2.39	0.58
51:9:750:C:O2	51:9:750:C:H2'	2.04	0.58
51:9:1351:G:O2'	51:9:1378:A:N1	2.35	0.58
51:9:1374:C:H2'	51:9:1375:G:O4'	2.03	0.58
53:BB:107:ARG:NH2	66:OO:133:THR:O	2.35	0.58
54:CC:64:THR:OG1	54:CC:90:GLU:HG3	2.04	0.58
51:9:1102:G:N2	51:9:1130:G:N2	2.51	0.58
51:9:1859:A:C2	51:9:1860:A:C6	2.92	0.58
54:CC:75:ILE:HG23	54:CC:80:GLU:OE1	2.04	0.58
48:5:973:G:N2	48:5:1282:G:HO2'	2.00	0.58
48:5:4207:C:C2	48:5:4226:G:C2	2.92	0.58
48:5:2654:C:C2	48:5:2681:G:C2	2.92	0.58
51:9:358:C:C2	51:9:405:G:C2	2.91	0.58
51:9:1233:G:H2'	51:9:1234:C:H5'	1.82	0.58
51:9:1444:U:O2'	51:9:1580:A:N1	2.37	0.58
51:9:1447:G:C6	51:9:1448:A:N6	2.71	0.58
48:5:516:C:N3	48:5:646:G:C2	2.72	0.57
48:5:3593:C:H4'	48:5:3594:C:OP2	2.03	0.57
48:5:4757:C:O2	48:5:4757:C:O4'	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:316:G:N1	51:9:317:C:C4	2.72	0.57
51:9:841:G:N2	51:9:842:C:C2	2.72	0.57
51:9:1211:G:O2'	51:9:1212:G:H5'	2.03	0.57
76:YY:113:ARG:O	76:YY:114:MET:HB2	2.04	0.57
5:E:128:PRO:HD2	5:E:131:GLN:OE1	2.03	0.57
9:I:187:GLU:O	9:I:188:LYS:HB2	2.04	0.57
12:M:130:LEU:HD21	14:O:180:GLN:OE1	2.04	0.57
44:t:30:PRO:O	44:t:32:ILE:N	2.37	0.57
48:5:1541:C:C2	48:5:1619:G:C2	2.91	0.57
48:5:2623:A:C2	48:5:2624:G:C5	2.92	0.57
51:9:623:G:N2	51:9:624:C:C2	2.72	0.57
54:CC:60:TRP:C	54:CC:61:LEU:CD1	2.77	0.57
48:5:685:C:O2	48:5:685:C:C2'	2.52	0.57
48:5:1682:A:C2	48:5:1683:U:C2	2.92	0.57
48:5:2554:U:H4'	48:5:2555:G:OP1	2.03	0.57
51:9:1760:G:C2	51:9:1773:C:C2	2.92	0.57
42:r:17:LEU:HD23	42:r:17:LEU:C	2.29	0.57
51:9:1137:U:N3	51:9:1148:A:N6	2.51	0.57
51:9:1613:G:C2	51:9:1627:C:C2	2.92	0.57
69:RR:124:VAL:HB	69:RR:126:MET:HE1	1.87	0.57
7:G:87:LEU:CD2	7:G:184:LEU:CD2	2.83	0.57
47:3:5:G:N2	47:3:6:G:C4	2.72	0.57
48:5:1269:G:C6	48:5:2111:G:N2	2.72	0.57
86:ii:91:ASN:HA	86:ii:119:PRO:HA	1.87	0.57
17:R:172:ARG:HG3	51:9:909:G:OP2	2.05	0.57
43:s:57:LYS:HZ1	48:5:1961:G:P	2.26	0.57
48:5:4213:A:H61	48:5:4218:U:H3	1.50	0.57
51:9:17:C:O2'	51:9:1194:A:N1	2.33	0.57
3:C:158:VAL:HA	3:C:161:TYR:CD2	2.40	0.57
48:5:127:G:N2	48:5:128:C:C2	2.73	0.57
48:5:1280:C:C2	48:5:1282:G:C5	2.93	0.57
48:5:1365:C:H4'	48:5:1366:G:OP1	2.05	0.57
48:5:1639:U:H3	48:5:1643:A:HO2'	1.51	0.57
51:9:1102:G:C2	51:9:1103:C:C4	2.92	0.57
51:9:1308:U:H3	51:9:1309:C:C1'	2.18	0.57
51:9:1488:C:O2'	51:9:1490:G:OP2	2.20	0.57
10:J:119:TYR:CB	70:SS:12:ILE:HD13	2.35	0.57
12:M:69:ARG:O	12:M:71:LYS:N	2.38	0.57
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.87	0.57
48:5:1279:A:H2'	48:5:1280:C:H5''	1.86	0.57
50:8:83:C:H4'	50:8:85:U:O2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:292:A:O2'	51:9:293:C:OP2	2.22	0.57
51:9:1454:A:N1	51:9:1476:A:C5'	2.68	0.57
40:o:39:ARG:NH1	48:5:295:A:OP2	2.31	0.56
47:3:68:C:HO2'	47:3:69:G:C1'	2.13	0.56
48:5:1965:G:O2'	48:5:1966:C:O5'	2.21	0.56
48:5:1999:A:H1'	48:5:2017:A:N1	2.20	0.56
48:5:2089:G:H2'	48:5:2089:G:N3	2.20	0.56
48:5:2301:G:N2	48:5:2302:C:C2	2.72	0.56
51:9:1526:G:N2	51:9:1527:C:C2	2.73	0.56
1:A:196:TRP:O	1:A:197:PRO:C	2.47	0.56
5:E:59:TYR:CE2	5:E:64:LEU:HD12	2.38	0.56
48:5:1279:A:C3'	48:5:1280:C:C5'	2.80	0.56
48:5:1279:A:O2'	48:5:1280:C:OP1	2.23	0.56
48:5:1757:U:H2'	48:5:1758:G:O4'	2.04	0.56
48:5:2297:G:N2	48:5:2338:C:C2	2.73	0.56
48:5:4769:G:H2'	48:5:4770:U:O4'	2.04	0.56
51:9:752:G:C6	51:9:790:C:N4	2.73	0.56
87:jj:7:ARG:CZ	87:jj:56:ILE:O	2.53	0.56
3:C:183:VAL:HG22	3:C:204:ARG:HB2	1.88	0.56
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.39	0.56
48:5:677:G:N2	48:5:678:C:C2	2.74	0.56
48:5:2256:C:O2	48:5:2256:C:C2'	2.53	0.56
48:5:3900:G:H5''	48:5:3901:A:H4'	1.87	0.56
48:5:4101:C:C2	48:5:4109:G:C2	2.94	0.56
51:9:1839:U:O4	78:aa:28:ARG:NH2	2.38	0.56
84:gg:5:MET:HE1	84:gg:312:VAL:HG13	1.87	0.56
86:ii:119:PRO:HB2	86:ii:165:THR:HG21	1.86	0.56
3:C:336:ARG:O	3:C:340:ILE:HG12	2.06	0.56
48:5:2258:C:O2	48:5:2258:C:C2'	2.54	0.56
14:O:160:ARG:NH2	48:5:4759:C:OP1	2.38	0.56
48:5:199:G:C2	48:5:220:C:O2	2.58	0.56
48:5:976:G:C2	48:5:977:C:C2	2.94	0.56
48:5:1358:G:C8	48:5:1358:G:C3'	2.87	0.56
48:5:2288:G:N1	48:5:2290:C:C4	2.73	0.56
48:5:2481:G:C2	48:5:2498:C:C2	2.94	0.56
51:9:434:G:H2'	51:9:435:A:C8	2.40	0.56
51:9:1455:A:O2'	51:9:1456:G:O5'	2.21	0.56
17:R:173:ARG:O	17:R:176:ARG:HB3	2.05	0.56
48:5:1404:G:N2	48:5:1414:C:C2	2.74	0.56
48:5:2773:G:N1	48:5:2774:C:C4	2.73	0.56
48:5:4583:C:C4	48:5:4718:G:C6	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:217:A:C2	51:9:309:G:N1	2.74	0.56
51:9:407:G:N3	51:9:407:G:H2'	2.21	0.56
52:AA:104:THR:O	52:AA:107:THR:HG23	2.06	0.56
48:5:1249:C:C2	48:5:1262:G:C2	2.94	0.56
48:5:1360:G:C6	48:5:1361:G:C5	2.94	0.56
48:5:2028:C:O2'	48:5:2029:A:C5'	2.53	0.56
50:8:155:C:H2'	50:8:156:U:O4'	2.05	0.56
51:9:913:A:N3	59:HH:66:VAL:HG11	2.21	0.56
51:9:1117:C:O2	51:9:1117:C:O4'	2.24	0.56
51:9:1760:G:N2	51:9:1773:C:C2	2.74	0.56
48:5:746:A:O2'	48:5:747:A:O5'	2.20	0.56
48:5:4092:G:N2	48:5:4158:C:C2	2.74	0.56
4:D:129:GLU:HG3	4:D:177:THR:HG21	1.86	0.56
48:5:976:G:C6	48:5:977:C:C4	2.93	0.56
48:5:1067:G:H2'	48:5:1068:G:O4'	2.05	0.56
48:5:1672:U:H2'	48:5:1673:U:C6	2.41	0.56
48:5:2089:G:O2'	48:5:2090:U:OP2	2.24	0.56
51:9:598:G:N2	51:9:639:C:C2	2.74	0.56
51:9:834:C:H3'	51:9:835:C:C4'	2.36	0.56
51:9:1308:U:C5	51:9:1309:C:C6	2.94	0.56
56:EE:31:PRO:CD	56:EE:38:LEU:HD13	2.36	0.56
87:jj:271:VAL:HG21	87:jj:282:LEU:HD13	1.87	0.56
17:R:172:ARG:CG	51:9:909:G:OP2	2.54	0.56
48:5:516:C:C2	48:5:646:G:C2	2.94	0.56
48:5:4723:A:C2	48:5:4724:A:C5	2.94	0.56
51:9:1403:C:O2	51:9:1403:C:C2'	2.53	0.56
54:CC:204:ILE:CD1	54:CC:215:LEU:HD23	2.36	0.56
48:5:497:G:C2	48:5:657:C:C2	2.94	0.55
48:5:977:C:C4	48:5:978:G:N7	2.74	0.55
48:5:1468:C:C2	48:5:1498:G:C2	2.94	0.55
67:PP:34:MET:HE3	67:PP:45:LEU:HD12	1.88	0.55
5:E:208:LEU:HD12	5:E:208:LEU:O	2.06	0.55
47:3:39:U:O2'	47:3:40:C:O5'	2.23	0.55
48:5:2524:U:H5''	48:5:2711:G:C2	2.42	0.55
48:5:2688:G:N2	48:5:2689:C:C2	2.74	0.55
48:5:4583:C:N4	48:5:4718:G:C6	2.75	0.55
48:5:4730:C:O5'	48:5:4731:G:N2	2.39	0.55
3:C:334:THR:HG21	6:F:53:TYR:OH	2.06	0.55
47:3:34:U:O2	51:9:1641:A:OP1	2.24	0.55
47:3:39:U:O2'	47:3:40:C:C6	2.49	0.55
48:5:466:A:C2	48:5:467:U:C4	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1205:G:N2	48:5:1206:C:C2	2.75	0.55
51:9:322:C:HO2'	51:9:323:C:P	2.30	0.55
71:TT:62:ARG:HD2	71:TT:62:ARG:C	2.31	0.55
47:3:76:A:N6	48:5:4371:G:C5	2.75	0.55
48:5:1483:C:O4'	48:5:1483:C:O2	2.22	0.55
48:5:2793:G:C5	48:5:2797:C:N4	2.74	0.55
48:5:5028:G:C6	48:5:5029:C:N4	2.75	0.55
51:9:167:G:C6	51:9:168:C:C5	2.94	0.55
51:9:350:C:O2'	51:9:383:G:N1	2.39	0.55
56:EE:55:ALA:HB1	56:EE:60:GLU:HB2	1.89	0.55
58:GG:188:LYS:HA	58:GG:191:ARG:HD3	1.87	0.55
75:XX:41:PHE:O	75:XX:43:GLY:N	2.39	0.55
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.39	0.55
17:R:176:ARG:HB2	17:R:176:ARG:CZ	2.37	0.55
18:S:53:LYS:NZ	49:7:74:A:O2'	2.40	0.55
48:5:1771:U:H2'	48:5:1772:C:O4'	2.06	0.55
48:5:3718:A:H2'	48:5:3719:A:C8	2.42	0.55
48:5:4281:A:C2	48:5:4283:G:C5	2.95	0.55
48:5:4416:G:N2	48:5:4417:C:C2	2.75	0.55
51:9:1262:C:O2'	81:dd:12:ARG:NH1	2.40	0.55
56:EE:234:PRO:HG3	56:EE:238:LEU:HD11	1.88	0.55
26:a:21:ARG:NH1	48:5:1317:U:OP1	2.40	0.55
48:5:1956:A:O2'	48:5:1957:U:H5'	2.07	0.55
48:5:1983:A:C2	48:5:2008:U:O4	2.58	0.55
51:9:853:C:O4'	51:9:853:C:O2	2.25	0.55
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.54	0.55
30:e:108:ARG:NH2	30:e:127:ALA:HB3	2.22	0.55
10:J:119:TYR:CD1	70:SS:12:ILE:HG12	2.41	0.55
48:5:1266:G:H5''	48:5:2112:G:N3	2.22	0.55
48:5:1975:G:O4'	48:5:1984:A:H1'	2.06	0.55
51:9:1406:G:H2'	51:9:1407:U:O3'	2.07	0.55
51:9:1454:A:OP1	69:RR:3:ARG:NH1	2.38	0.55
51:9:1784:G:N2	51:9:1785:C:C2	2.75	0.55
2:B:18:PRO:O	2:B:20:LYS:N	2.40	0.55
2:B:49:TYR:CE2	2:B:168:MET:HE1	2.41	0.55
39:n:13:LEU:HD11	39:n:17:ARG:CZ	2.37	0.55
48:5:181:C:N4	48:5:256:G:C6	2.75	0.55
48:5:2905:C:C2	48:5:3590:G:C2	2.95	0.55
51:9:598:G:C2	51:9:639:C:C2	2.94	0.55
51:9:953:C:H2'	51:9:954:U:O4'	2.07	0.55
59:HH:43:LEU:HD22	59:HH:72:PHE:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:165:LYS:HB2	11:L:165:LYS:HZ2	1.72	0.55
15:P:118:GLN:NE2	48:5:423:G:N3	2.55	0.55
17:R:59:SER:N	48:5:4646:U:OP1	2.39	0.55
29:d:78:ARG:HG2	29:d:78:ARG:HH11	1.72	0.55
32:g:21:ARG:NH2	48:5:2641:A:OP1	2.39	0.55
47:3:76:A:C5	48:5:4371:G:C5	2.95	0.55
48:5:1929:A:C2	48:5:2054:U:O4	2.57	0.55
54:CC:204:ILE:CD1	54:CC:215:LEU:CD2	2.84	0.55
57:FF:35:LEU:HD13	57:FF:117:ILE:HG12	1.89	0.55
83:ff:136:CYS:SG	83:ff:137:GLY:N	2.79	0.55
11:L:9:ILE:HG21	26:a:52:TYR:CE2	2.42	0.54
86:ii:327:ASP:HB3	86:ii:348:PRO:CG	2.36	0.54
48:5:2027:U:C2'	48:5:2028:C:H5'	2.38	0.54
48:5:4281:A:C2	48:5:4283:G:C6	2.94	0.54
48:5:5000:G:N2	48:5:5051:C:C2	2.75	0.54
51:9:698:G:N1	51:9:733:C:C2	2.76	0.54
51:9:834:C:N3	51:9:841:G:C2	2.75	0.54
61:JJ:35:TYR:O	61:JJ:37:LEU:N	2.41	0.54
23:X:127:LEU:HD12	23:X:127:LEU:C	2.32	0.54
48:5:1268:G:C2	48:5:2111:G:N2	2.76	0.54
48:5:1297:U:OP2	48:5:1297:U:O4'	2.26	0.54
48:5:3617:G:O2'	48:5:3620:G:N7	2.36	0.54
51:9:216:C:O2	51:9:216:C:O4'	2.24	0.54
48:5:93:G:O2'	48:5:94:A:O4'	2.24	0.54
48:5:975:C:C3'	48:5:976:G:O4'	2.55	0.54
4:D:258:LYS:O	4:D:259:ARG:HG3	2.07	0.54
5:E:62:LYS:O	5:E:63:ALA:HB3	2.06	0.54
6:F:93:PHE:CD2	6:F:246:ILE:HD11	2.42	0.54
25:Z:52:LYS:O	25:Z:65:ARG:NH2	2.40	0.54
48:5:1265:G:C2'	48:5:1266:G:H5'	2.37	0.54
48:5:2547:G:N1	48:5:2548:C:C4	2.76	0.54
48:5:5023:C:O2	48:5:5023:C:O4'	2.23	0.54
51:9:1447:G:N1	51:9:1448:A:C6	2.75	0.54
3:C:357:ALA:O	3:C:361:LYS:HG3	2.08	0.54
5:E:174:PRO:O	5:E:176:SER:N	2.40	0.54
9:I:98:ARG:HB3	9:I:120:GLY:HA3	1.90	0.54
48:5:3753:G:OP1	48:5:3777:G:H8	1.91	0.54
48:5:5025:C:OP2	60:II:170:LYS:HG3	2.06	0.54
51:9:887:U:O2	51:9:887:U:O4'	2.26	0.54
51:9:1139:C:O2	51:9:1139:C:O4'	2.26	0.54
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:II:38:ILE:HD11	60:II:81:VAL:HG23	1.90	0.54
7:G:86:VAL:HG13	7:G:183:ILE:O	2.07	0.54
47:3:16:C:O2	47:3:16:C:O4'	2.26	0.54
48:5:986:C:C2	48:5:1068:G:C2	2.96	0.54
48:5:2409:U:C5	48:5:2783:A:C2	2.95	0.54
48:5:4913:G:O2'	48:5:4914:C:O4'	2.24	0.54
51:9:643:A:OP1	51:9:643:A:H4'	2.08	0.54
51:9:830:A:N6	51:9:844:U:C2	2.74	0.54
47:3:66:U:C2	47:3:67:U:C6	2.96	0.54
48:5:2108:G:C2	48:5:2125:C:N3	2.76	0.54
48:5:4730:C:O2	48:5:4730:C:O4'	2.25	0.54
51:9:172:U:O2	51:9:172:U:C2'	2.56	0.54
51:9:751:G:O2'	51:9:752:G:O4'	2.25	0.54
51:9:1137:U:H3	51:9:1148:A:N6	2.06	0.54
86:ii:323:TYR:CE1	86:ii:324:GLU:CG	2.86	0.54
48:5:112:C:C2	48:5:330:G:C2	2.96	0.54
48:5:1381:U:O2	48:5:1381:U:O4'	2.26	0.54
48:5:2108:G:N1	48:5:2125:C:C4	2.76	0.54
51:9:1408:U:H2'	51:9:1409:A:C8	2.43	0.54
51:9:1649:U:O4	51:9:1675:A:C2	2.60	0.54
17:R:172:ARG:HB3	51:9:909:G:OP2	2.08	0.54
33:h:119:TYR:C	33:h:119:TYR:CD2	2.86	0.54
47:3:38:A:O2'	47:3:39:U:H5'	2.08	0.54
47:3:39:U:O2'	47:3:40:C:C5'	2.56	0.54
47:3:76:A:C6	48:5:4371:G:N7	2.76	0.54
48:5:2009:A:C8	86:ii:415:TYR:CD2	2.96	0.54
48:5:4885:U:H2'	48:5:4886:C:O4'	2.07	0.54
48:5:422:C:C2	50:8:13:G:C2	2.96	0.53
26:a:61:TYR:N	48:5:4354:U:O4	2.40	0.53
48:5:52:G:N2	48:5:53:C:C2	2.76	0.53
48:5:976:G:H2'	48:5:977:C:C1'	2.34	0.53
51:9:1126:G:N2	51:9:1127:C:C2	2.76	0.53
51:9:1654:G:N2	51:9:1655:C:C2	2.77	0.53
14:O:84:VAL:HG11	14:O:102:LEU:HD22	1.91	0.53
27:b:45:PHE:CE1	48:5:1815:G:N7	2.77	0.53
48:5:3641:U:H5	48:5:3646:A:N7	2.06	0.53
48:5:3782:C:N3	48:5:3811:G:C2	2.76	0.53
48:5:4138:C:C2	48:5:4147:G:C2	2.95	0.53
48:5:4543:G:H2'	48:5:4544:A:C8	2.43	0.53
48:5:5026:U:O4	60:II:103:LEU:HD13	2.08	0.53
51:9:1303:C:O2	51:9:1303:C:O4'	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1454:A:C2	51:9:1476:A:C5'	2.91	0.53
43:s:10:LYS:HE2	48:5:1961:G:OP1	2.07	0.53
48:5:4283:G:N2	48:5:4284:C:C2	2.77	0.53
49:7:66:G:C2	49:7:67:C:C2	2.96	0.53
51:9:71:G:O2'	51:9:72:C:OP1	2.24	0.53
51:9:1537:A:N1	51:9:1596:U:O4	2.41	0.53
47:3:33:U:P	57:FF:127:ARG:NH1	2.81	0.53
48:5:181:C:C2	48:5:256:G:C2	2.97	0.53
48:5:1811:G:N2	48:5:1812:C:C2	2.77	0.53
48:5:1965:G:C2	48:5:1966:C:C2	2.96	0.53
48:5:2301:G:N1	48:5:2302:C:C4	2.77	0.53
48:5:4093:G:C3'	48:5:4094:G:H5'	2.39	0.53
48:5:4305:G:C2'	48:5:4305:G:N3	2.71	0.53
51:9:384:U:O2'	63:LL:135:SER:C	2.52	0.53
51:9:944:A:C5	51:9:945:U:C5	2.96	0.53
59:HH:95:ILE:HD11	59:HH:133:LEU:HG	1.91	0.53
12:M:133:ALA:O	12:M:136:LEU:HB3	2.07	0.53
48:5:2045:G:O6	48:5:3870:C:O2'	2.25	0.53
48:5:3870:C:C2	48:5:3886:G:C2	2.95	0.53
51:9:384:U:O4	60:II:5:ARG:NH2	2.42	0.53
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.90	0.53
1:A:207:VAL:HG11	48:5:1633:G:C6	2.44	0.53
9:I:204:GLY:O	9:I:205:PRO:O	2.26	0.53
12:M:122:ILE:HG22	14:O:185:VAL:HG11	1.91	0.53
31:f:28:LEU:HG	31:f:101:ILE:HD11	1.90	0.53
48:5:1983:A:C2	48:5:2010:A:H5''	2.44	0.53
48:5:3751:G:O2'	48:5:3775:A:N6	2.41	0.53
48:5:3753:G:O2'	48:5:3754:G:C5'	2.56	0.53
48:5:4213:A:N6	48:5:4218:U:N3	2.53	0.53
48:5:4579:U:H2'	48:5:4580:U:O4'	2.08	0.53
51:9:163:U:OP1	58:GG:84:TYR:HA	2.08	0.53
28:c:34:THR:OG1	28:c:95:ALA:HB2	2.07	0.53
48:5:707:C:C2	48:5:1291:G:C2	2.97	0.53
48:5:1213:G:C6	48:5:1215:C:N3	2.76	0.53
48:5:3662:A:N6	48:5:3680:U:H3	2.07	0.53
3:C:325:MET:HE1	6:F:157:TYR:CZ	2.44	0.53
21:V:28:CYS:SG	21:V:30:ASP:OD1	2.67	0.53
48:5:2268:A:H4'	48:5:2269:C:H5'	1.90	0.53
48:5:2557:G:C2	48:5:2571:C:C2	2.96	0.53
51:9:1308:U:C4	51:9:1309:C:N1	2.75	0.53
51:9:1401:A:H2'	51:9:1402:A:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1454:A:H5'	69:RR:49:LYS:NZ	2.23	0.53
51:9:1835:A:C4	51:9:1863:A:N7	2.77	0.53
5:E:251:SER:O	5:E:255:PRO:HD2	2.08	0.53
29:d:79:ASN:OD1	29:d:79:ASN:N	2.41	0.53
47:3:31:A:H2'	57:FF:136:ARG:HH22	1.74	0.53
48:5:119:G:C8	48:5:119:G:H5''	2.44	0.53
48:5:1968:G:HO2'	48:5:1969:G:P	2.31	0.53
48:5:2110:C:C6	48:5:2110:C:OP1	2.62	0.53
48:5:2297:G:C2	48:5:2338:C:N3	2.77	0.53
48:5:4260:U:H2'	48:5:4261:C:C6	2.44	0.53
51:9:55:U:O2	51:9:55:U:C2'	2.56	0.53
51:9:522:A:O2'	61:JJ:131:ARG:NH2	2.41	0.53
51:9:1102:G:C2	51:9:1130:G:N2	2.77	0.53
58:GG:5:ILE:HG12	58:GG:111:LEU:HD12	1.91	0.53
2:B:163:LEU:HD23	2:B:182:GLU:CG	2.32	0.52
30:e:36:ARG:NH2	48:5:1661:C:OP1	2.40	0.52
41:p:17:ARG:NH2	48:5:1577:G:OP1	2.42	0.52
48:5:1485:C:O2	48:5:1485:C:O4'	2.26	0.52
48:5:1879:C:O2'	48:5:1891:A:N3	2.39	0.52
48:5:3900:G:N2	48:5:4562:C:C2	2.77	0.52
51:9:635:G:C6	51:9:636:C:C4	2.97	0.52
51:9:1528:G:N2	51:9:1529:C:C2	2.78	0.52
51:9:1599:U:O2	51:9:1599:U:O4'	2.27	0.52
51:9:1839:U:H2'	51:9:1840:U:C6	2.43	0.52
69:RR:126:MET:O	69:RR:127:ASN:ND2	2.43	0.52
24:Y:49:ILE:HD13	24:Y:80:ILE:HD13	1.92	0.52
28:c:84:ALA:C	65:NN:151:ALA:OXT	2.52	0.52
34:i:89:GLU:O	34:i:92:SER:HB2	2.09	0.52
48:5:1269:G:C5	48:5:2111:G:C2	2.98	0.52
48:5:2638:G:C2	48:5:2639:U:C4	2.98	0.52
48:5:2726:G:C6	48:5:2727:C:N4	2.77	0.52
48:5:3811:G:O2'	48:5:3814:U:OP2	2.28	0.52
48:5:4508:C:N3	48:5:4512:U:H5	2.07	0.52
48:5:4895:C:H1'	48:5:4896:G:C8	2.45	0.52
51:9:1401:A:C2	51:9:1402:A:N1	2.77	0.52
51:9:1408:U:C4	51:9:1409:A:N6	2.77	0.52
55:DD:21:LEU:HD22	55:DD:48:ILE:HD11	1.90	0.52
86:ii:14:ILE:HG12	86:ii:117:PHE:CE2	2.45	0.52
5:E:59:TYR:CZ	5:E:64:LEU:HB2	2.44	0.52
5:E:157:ARG:O	5:E:178:ASN:OD1	2.28	0.52
8:H:95:VAL:HG22	38:m:82:LEU:HD22	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:1:G:N1	47:3:2:C:C4	2.78	0.52
48:5:85:G:O2'	48:5:97:G:O6	2.27	0.52
48:5:919:C:N4	48:5:920:C:C5	2.77	0.52
48:5:1958:A:C2	48:5:2026:A:N1	2.78	0.52
48:5:4371:G:C5	48:5:4372:U:C4	2.98	0.52
51:9:427:U:O4'	51:9:427:U:O2	2.28	0.52
51:9:832:G:C2	51:9:843:C:C2	2.97	0.52
8:H:180:TYR:HB2	38:m:85:LEU:HD11	1.91	0.52
19:T:2:THR:N	48:5:4220:A:OP2	2.43	0.52
47:3:33:U:H5'	57:FF:127:ARG:NH1	2.24	0.52
51:9:1448:A:O2'	51:9:1449:G:P	2.67	0.52
75:XX:9:THR:O	75:XX:10:ALA:C	2.52	0.52
10:J:119:TYR:HE2	10:J:125:ILE:HD11	1.74	0.52
47:3:76:A:C5	48:5:4371:G:C6	2.98	0.52
48:5:1964:A:H2'	48:5:1965:G:C5'	2.40	0.52
48:5:4378:A:O2'	48:5:4379:A:H2'	2.09	0.52
51:9:1409:A:C6	51:9:1410:C:C5	2.98	0.52
58:GG:214:ALA:O	58:GG:218:LYS:N	2.39	0.52
2:B:21:ARG:NH2	48:5:4568:A:O3'	2.43	0.52
18:S:95:ARG:NH2	48:5:1951:G:O2'	2.42	0.52
48:5:256:G:N2	48:5:257:C:C2	2.78	0.52
48:5:3782:C:C2	48:5:3811:G:N2	2.77	0.52
51:9:1500:G:C6	51:9:1501:C:C4	2.97	0.52
51:9:1859:A:H2'	51:9:1860:A:C8	2.44	0.52
86:ii:322:VAL:CG1	86:ii:326:LEU:HD12	2.39	0.52
48:5:1277:G:N2	48:5:1278:C:C2	2.78	0.52
48:5:2627:C:O4'	48:5:2627:C:O2	2.27	0.52
48:5:5025:C:OP1	60:II:169:GLY:HA3	2.10	0.52
51:9:73:C:O2	51:9:73:C:O4'	2.27	0.52
51:9:1149:A:H2'	51:9:1149:A:N3	2.23	0.52
51:9:1236:G:C6	51:9:1237:C:C4	2.97	0.52
51:9:1384:C:C2'	51:9:1385:G:H5'	2.40	0.52
69:RR:126:MET:HA	69:RR:126:MET:HE3	1.91	0.52
86:ii:317:VAL:HG12	86:ii:413:LEU:CD2	2.40	0.52
1:A:162:ASN:HD22	1:A:162:ASN:C	2.18	0.52
6:F:49:ARG:NH1	48:5:974:C:O3'	2.43	0.52
8:H:98:HIS:ND1	87:jj:440:GLN:HG2	2.24	0.52
48:5:470:A:C5	48:5:471:A:C8	2.98	0.52
48:5:3594:C:O2	48:5:3594:C:C2'	2.57	0.52
48:5:4735:G:C2	48:5:4736:C:C2	2.98	0.52
48:5:4939:C:O3'	48:5:4941:G:P	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:8:106:G:N2	50:8:107:C:C2	2.78	0.52
51:9:1294:G:O2'	51:9:1295:A:O5'	2.22	0.52
2:B:29:VAL:HG13	2:B:348:ARG:HD3	1.92	0.52
10:J:53:ALA:HB2	10:J:68:ILE:HD12	1.92	0.52
41:p:4:ARG:NH1	48:5:1554:A:OP2	2.43	0.52
48:5:166:C:C2	48:5:167:C:H5	2.28	0.52
48:5:301:G:C6	48:5:302:C:C4	2.97	0.52
48:5:707:C:O2	48:5:1291:G:C2	2.63	0.52
51:9:195:C:C2	51:9:205:G:C2	2.98	0.52
51:9:1520:G:N3	51:9:1520:G:H2'	2.25	0.52
51:9:1553:C:O2	51:9:1553:C:O4'	2.25	0.52
58:GG:74:ARG:HA	58:GG:96:SER:HA	1.92	0.52
87:jj:389:ILE:HG23	87:jj:484:LEU:HD13	1.92	0.52
7:G:86:VAL:CG1	7:G:185:LYS:HG2	2.24	0.52
16:Q:186:TYR:CD2	48:5:4307:A:H4'	2.45	0.52
30:e:89:LEU:HD13	30:e:118:LEU:HD22	1.93	0.52
48:5:44:A:N3	48:5:94:A:H2	2.08	0.52
48:5:2693:G:C6	48:5:2694:G:N1	2.78	0.52
50:8:55:U:O4	50:8:62:A:N1	2.43	0.52
51:9:380:G:O6	60:II:178:ARG:NH2	2.43	0.52
51:9:1118:C:O2	51:9:1118:C:O4'	2.25	0.52
51:9:1597:C:H4'	51:9:1603:G:C6	2.45	0.52
47:3:3:C:C2'	47:3:4:C:H5'	2.40	0.51
48:5:4094:G:H2'	48:5:4095:G:O4'	2.10	0.51
48:5:4906:C:C2	48:5:4916:G:C2	2.98	0.51
51:9:488:U:O2	51:9:488:U:H2'	2.08	0.51
51:9:751:G:C6	51:9:792:C:N4	2.78	0.51
51:9:872:A:N6	51:9:914:U:C4	2.79	0.51
51:9:1275:G:O2'	51:9:1276:A:OP2	2.28	0.51
51:9:1398:G:N2	51:9:1399:C:C2	2.78	0.51
66:OO:106:LYS:HE3	66:OO:135:ILE:HG12	1.91	0.51
43:s:14:PHE:HE2	48:5:1960:A:C2	2.21	0.51
48:5:106:A:H2'	48:5:107:G:O4'	2.10	0.51
48:5:2826:U:H4'	48:5:2827:G:H5'	1.90	0.51
51:9:474:G:N1	51:9:475:C:C4	2.79	0.51
51:9:1617:G:N7	67:PP:43:ARG:NH1	2.58	0.51
54:CC:61:LEU:CD1	54:CC:61:LEU:N	2.73	0.51
55:DD:191:PRO:O	55:DD:193:ASP:N	2.44	0.51
87:jj:313:LEU:HD12	87:jj:572:ASN:HD22	1.75	0.51
11:L:165:LYS:NZ	11:L:165:LYS:CB	2.73	0.51
18:S:9:GLU:HG2	18:S:33:PHE:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2:16:C:O4'	46:2:16:C:O2	2.25	0.51
48:5:726:G:C6	48:5:727:C:N4	2.79	0.51
48:5:1171:G:C2	48:5:1191:C:C2	2.98	0.51
51:9:211:G:N2	51:9:212:C:C2	2.78	0.51
51:9:501:C:O2	51:9:501:C:C2'	2.58	0.51
51:9:1448:A:C2'	51:9:1449:G:H5''	2.40	0.51
51:9:1698:C:O2	51:9:1698:C:O4'	2.24	0.51
25:Z:54:THR:O	25:Z:56:ALA:N	2.43	0.51
31:f:102:ARG:NH2	48:5:4947:U:O4	2.42	0.51
44:t:121:LEU:HD22	44:t:132:ILE:HD13	1.92	0.51
48:5:962:C:OP2	48:5:2264:C:N3	2.43	0.51
48:5:1398:A:H1'	48:5:1399:G:C8	2.45	0.51
48:5:1726:U:H3	48:5:1836:G:H1	1.59	0.51
48:5:1872:G:O2'	48:5:4219:A:N3	2.38	0.51
48:5:2275:G:H5''	48:5:2275:G:H8	1.75	0.51
48:5:2505:C:O2	48:5:2505:C:O4'	2.28	0.51
48:5:4754:G:C2	48:5:4880:C:C2	2.99	0.51
51:9:71:G:H3'	51:9:72:C:H5''	1.92	0.51
51:9:501:C:O2	51:9:501:C:H2'	2.11	0.51
51:9:1130:G:N2	51:9:1131:G:C8	2.79	0.51
57:FF:73:THR:HG22	57:FF:89:THR:HG23	1.93	0.51
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	1.92	0.51
3:C:108:TRP:HZ2	11:L:19:GLN:HE21	1.57	0.51
13:N:65:ARG:HG3	13:N:129:PHE:CE2	2.46	0.51
47:3:10:G:N1	47:3:11:C:C4	2.78	0.51
47:3:35:U:O2'	47:3:36:U:H5'	2.11	0.51
48:5:1400:G:C6	48:5:1401:C:C4	2.99	0.51
48:5:2733:C:H2'	48:5:2734:U:O4'	2.11	0.51
48:5:4714:C:C5	48:5:4715:C:C5	2.99	0.51
51:9:1616:U:OP2	67:PP:43:ARG:NH2	2.42	0.51
5:E:124:HIS:O	48:5:1282:G:O6	2.29	0.51
5:E:279:PRO:HD2	31:f:7:CYS:SG	2.50	0.51
6:F:92:ALA:CB	6:F:127:LEU:HD21	2.40	0.51
26:a:25:HIS:ND1	48:5:1338:G:N2	2.59	0.51
48:5:986:C:N3	48:5:1068:G:C2	2.79	0.51
48:5:1072:C:O2	48:5:1072:C:C2'	2.59	0.51
51:9:322:C:OP2	51:9:322:C:H6	1.94	0.51
51:9:623:G:N1	51:9:624:C:C4	2.79	0.51
51:9:823:U:O2	51:9:823:U:O4'	2.28	0.51
51:9:1448:A:O2'	51:9:1449:G:C4'	2.59	0.51
9:I:46:PHE:CD1	9:I:140:THR:HA	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:7:LYS:HZ1	51:9:1843:G:P	2.34	0.51
48:5:1086:C:C2	48:5:1212:G:C2	2.99	0.51
48:5:1245:C:C4	48:5:1269:G:O6	2.64	0.51
48:5:1398:A:O2'	48:5:1399:G:OP2	2.24	0.51
48:5:5026:U:C4	60:II:170:LYS:HE3	2.45	0.51
51:9:1454:A:N1	51:9:1476:A:H5''	2.26	0.51
51:9:1500:G:C2	51:9:1501:C:C2	2.98	0.51
58:GG:1:MET:HE3	58:GG:106:LEU:HB2	1.93	0.51
61:JJ:94:LEU:HD12	61:JJ:97:ILE:HD12	1.91	0.51
63:LL:37:TYR:CE1	63:LL:51:ILE:HG23	2.46	0.51
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.38	0.51
31:f:42:TYR:HA	31:f:45:LYS:HG3	1.93	0.51
35:j:27:TYR:HA	35:j:34:CYS:HA	1.93	0.51
48:5:671:G:C6	48:5:672:C:C4	2.98	0.51
48:5:1269:G:C8	48:5:2111:G:C6	2.98	0.51
48:5:1378:C:OP1	48:5:1379:C:H3'	2.11	0.51
48:5:2043:A:O2'	48:5:4461:C:O2	2.27	0.51
48:5:2108:G:N2	48:5:2125:C:C2	2.79	0.51
48:5:4219:A:H2'	48:5:4220:A:C8	2.46	0.51
48:5:4749:C:O2	48:5:4749:C:O4'	2.27	0.51
51:9:833:C:H4'	51:9:834:C:OP1	2.10	0.51
87:jj:389:ILE:HG12	87:jj:484:LEU:HD22	1.92	0.51
21:V:82:ILE:HD12	21:V:104:VAL:HG22	1.93	0.51
48:5:1170:G:C2	48:5:1192:C:C2	2.98	0.51
51:9:830:A:N1	51:9:844:U:C4	2.78	0.51
51:9:1282:A:H3'	51:9:1283:C:C5'	2.40	0.51
51:9:1650:A:C4	51:9:1675:A:C6	2.99	0.51
3:C:342:ARG:HG3	3:C:342:ARG:HH11	1.76	0.51
6:F:245:LEU:HD23	6:F:249:MET:HG3	1.92	0.51
9:I:49:CYS:SG	9:I:51:HIS:CE1	3.04	0.51
47:3:9:A:O2'	47:3:10:G:N7	2.44	0.51
48:5:77:U:C4	48:5:335:A:N1	2.75	0.51
48:5:3753:G:C2	48:5:3754:G:C8	2.99	0.51
86:ii:323:TYR:CD1	86:ii:324:GLU:N	2.79	0.51
47:3:5:G:N3	47:3:6:G:C8	2.79	0.50
47:3:38:A:N1	57:FF:135:ARG:NH1	2.58	0.50
48:5:990:C:C4	48:5:1064:G:C2	2.99	0.50
48:5:1447:C:H2'	48:5:1448:G:O4'	2.10	0.50
48:5:2555:G:O6	48:5:2572:C:N4	2.42	0.50
48:5:3729:U:H2'	48:5:3730:U:C6	2.46	0.50
48:5:4692:A:C2	48:5:4693:C:N4	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:5026:U:C6	60:II:80:ASP:HB2	2.46	0.50
51:9:193:C:C2	51:9:207:G:C2	2.99	0.50
86:ii:375:LEU:HD12	86:ii:375:LEU:C	2.36	0.50
3:C:213:GLU:OE1	3:C:213:GLU:N	2.45	0.50
5:E:251:SER:O	5:E:255:PRO:HD3	2.10	0.50
9:I:191:ILE:CD1	9:I:200:ILE:HD11	2.21	0.50
11:L:65:ARG:HG2	11:L:66:TYR:CE2	2.47	0.50
14:O:27:VAL:HG13	14:O:98:ALA:HB1	1.93	0.50
48:5:1167:C:C2	48:5:1195:G:C2	2.99	0.50
48:5:3698:G:N2	48:5:3699:C:C2	2.79	0.50
48:5:3724:A:N6	48:5:3725:G:C6	2.79	0.50
51:9:62:G:O4'	51:9:172:U:N3	2.44	0.50
51:9:981:A:H2'	51:9:982:G:C8	2.46	0.50
51:9:1615:U:O4	67:PP:40:ARG:NH1	2.44	0.50
51:9:1679:A:O2'	51:9:1680:G:OP2	2.19	0.50
67:PP:17:TYR:OH	67:PP:37:TYR:HB3	2.11	0.50
69:RR:126:MET:N	69:RR:126:MET:SD	2.85	0.50
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.92	0.50
14:O:54:TYR:CE1	14:O:145:VAL:HG11	2.47	0.50
48:5:484:U:C4	48:5:486:C:C5	3.00	0.50
48:5:960:A:N6	48:5:1283:G:O6	2.45	0.50
48:5:2311:C:C2	48:5:2328:G:C2	2.99	0.50
48:5:2494:U:H2'	48:5:2495:U:O4'	2.11	0.50
48:5:2654:C:N3	48:5:2681:G:C2	2.79	0.50
50:8:119:C:C2	50:8:132:G:C2	2.99	0.50
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	1.92	0.50
9:I:47:PRO:HB3	9:I:171:TRP:CE2	2.46	0.50
20:U:100:LEU:HD22	20:U:112:LEU:HB3	1.92	0.50
26:a:59:ARG:NH2	26:a:61:TYR:OH	2.44	0.50
30:e:90:MET:HE1	42:r:113:ARG:HA	1.93	0.50
42:r:20:ARG:HG3	42:r:21:ASN:HB2	1.93	0.50
47:3:38:A:N3	57:FF:135:ARG:NH2	2.59	0.50
48:5:2557:G:C6	48:5:2558:C:C4	3.00	0.50
51:9:1364:U:O2	51:9:1364:U:O4'	2.28	0.50
86:ii:39:ILE:HD12	86:ii:93:LEU:HD23	1.94	0.50
5:E:59:TYR:CD2	5:E:64:LEU:CD1	2.76	0.50
17:R:176:ARG:HH11	51:9:909:G:C4'	2.24	0.50
39:n:21:ARG:NH2	51:9:1175:G:OP2	2.39	0.50
48:5:43:U:H2'	48:5:44:A:O5'	2.11	0.50
48:5:1263:A:C6	48:5:1264:C:C4	3.00	0.50
48:5:1910:G:N2	48:5:1911:C:C2	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2712:G:N2	48:5:2713:C:C2	2.79	0.50
48:5:4338:G:C4	48:5:4372:U:C5	3.00	0.50
51:9:409:C:C2	51:9:432:G:N2	2.80	0.50
51:9:1109:C:O2	51:9:1109:C:C2'	2.59	0.50
51:9:1616:U:O4	67:PP:40:ARG:NH1	2.44	0.50
24:Y:10:ASP:O	24:Y:11:ARG:C	2.54	0.50
39:n:8:LYS:HE3	51:9:1846:G:O6	2.12	0.50
48:5:1354:A:C5	48:5:1503:A:C2	3.00	0.50
48:5:1886:G:N2	48:5:1894:C:C2	2.80	0.50
48:5:4966:A:H2'	48:5:4967:A:C8	2.47	0.50
48:5:5026:U:OP2	60:II:77:ARG:NH2	2.45	0.50
51:9:113:G:N2	51:9:293:C:C2	2.80	0.50
55:DD:175:VAL:HG13	55:DD:182:LEU:HB2	1.92	0.50
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.94	0.50
3:C:114:ARG:CZ	48:5:1358:G:H5''	2.41	0.50
3:C:266:THR:HG22	3:C:269:LYS:HB3	1.94	0.50
11:L:74:ARG:NH2	48:5:76:A:N7	2.59	0.50
33:h:88:THR:O	33:h:89:ARG:C	2.54	0.50
42:r:85:ASN:O	42:r:87:ARG:N	2.45	0.50
47:3:33:U:OP1	57:FF:127:ARG:NH1	2.45	0.50
48:5:1412:G:N2	48:5:1413:C:C2	2.78	0.50
48:5:2065:G:H2'	48:5:2066:C:O4'	2.12	0.50
48:5:4462:C:C2	48:5:4515:G:C2	2.99	0.50
48:5:4548:A:N1	86:ii:183:ALA:HB2	2.27	0.50
48:5:4758:U:H2'	48:5:4759:C:O4'	2.12	0.50
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.46	0.50
48:5:28:C:C2	48:5:55:G:C2	3.00	0.50
48:5:1252:C:C2	48:5:1259:G:C2	3.00	0.50
48:5:1400:G:C2	48:5:1401:C:C2	2.99	0.50
48:5:1886:G:C2	48:5:1894:C:C2	3.00	0.50
48:5:1912:G:N2	48:5:1913:C:C2	2.80	0.50
48:5:3860:A:H61	48:5:4560:C:H5	1.60	0.50
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.47	0.50
51:9:1116:C:O2	51:9:1116:C:O4'	2.29	0.50
52:AA:159:ILE:HG23	52:AA:159:ILE:O	2.12	0.50
1:A:215:ASN:ND2	48:5:4546:A:N7	2.60	0.50
5:E:161:LEU:HD21	5:E:253:ILE:HD11	1.93	0.50
47:3:4:C:C2'	47:3:5:G:H8	2.25	0.50
48:5:977:C:N3	48:5:978:G:N7	2.59	0.50
48:5:1072:C:H1'	48:5:1073:G:C8	2.46	0.50
48:5:2046:G:C2	48:5:2047:A:C2	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2368:A:N6	48:5:2788:U:O2	2.45	0.50
48:5:2586:G:C8	48:5:2770:C:H1'	2.46	0.50
48:5:4510:A:O2'	48:5:4511:A:O4'	2.30	0.50
48:5:4699:U:C4	48:5:4702:G:C6	3.00	0.50
51:9:1842:C:C2	51:9:1858:G:N2	2.79	0.50
86:ii:160:THR:HG23	86:ii:169:LEU:HD11	1.93	0.50
12:M:38:VAL:HG21	12:M:55:MET:HE1	1.94	0.49
38:m:119:ASN:C	38:m:119:ASN:ND2	2.70	0.49
47:3:24:G:C6	47:3:25:C:C4	3.00	0.49
48:5:224:U:O2	48:5:224:U:O4'	2.26	0.49
48:5:1301:C:O2	48:5:1301:C:O4'	2.30	0.49
48:5:3717:A:O2'	48:5:3718:A:O5'	2.30	0.49
48:5:3879:G:O2'	48:5:3881:G:OP2	2.23	0.49
48:5:4699:U:C4	48:5:4701:A:N6	2.80	0.49
48:5:4709:U:C4	48:5:4710:C:C4	3.00	0.49
49:7:82:G:C2	49:7:95:C:C2	3.00	0.49
51:9:411:G:N2	51:9:430:C:C2	2.80	0.49
51:9:1321:G:H2'	51:9:1322:G:O4'	2.12	0.49
61:JJ:24:ARG:HG2	61:JJ:24:ARG:HH11	1.77	0.49
65:NN:55:ARG:NH1	65:NN:56:ASP:OD1	2.45	0.49
68:QQ:41:MET:N	68:QQ:41:MET:SD	2.85	0.49
5:E:174:PRO:O	5:E:177:LEU:N	2.43	0.49
6:F:164:ILE:HB	6:F:169:ILE:HD12	1.94	0.49
30:e:46:ARG:HA	30:e:55:MET:SD	2.53	0.49
44:t:94:LYS:HA	44:t:95:GLN:C	2.37	0.49
46:2:39:G:N2	46:2:40:C:C2	2.80	0.49
48:5:4583:C:C4	48:5:4718:G:N1	2.79	0.49
64:MM:113:ASP:O	64:MM:115:GLY:N	2.45	0.49
48:5:93:G:O2'	48:5:94:A:O5'	2.31	0.49
48:5:965:G:H2'	48:5:965:G:N3	2.27	0.49
48:5:1776:A:C6	48:5:1777:C:C4	3.00	0.49
48:5:2367:A:C2	48:5:2788:U:O4	2.60	0.49
51:9:635:G:C2	51:9:636:C:C2	3.00	0.49
56:EE:31:PRO:HD2	56:EE:38:LEU:HD13	1.93	0.49
86:ii:117:PHE:HZ	86:ii:140:LEU:HD22	1.76	0.49
3:C:341:LEU:HD21	5:E:46:LEU:HD21	1.94	0.49
11:L:66:TYR:O	11:L:68:THR:N	2.44	0.49
48:5:2557:G:C2	48:5:2558:C:C2	3.00	0.49
50:8:125:C:O2	50:8:125:C:O4'	2.30	0.49
51:9:217:A:C2	51:9:218:U:C6	3.00	0.49
51:9:412:G:C2	51:9:429:C:C2	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:656:G:HO2'	54:CC:227:TRP:NE1	2.04	0.49
51:9:1551:U:O2	51:9:1551:U:O4'	2.29	0.49
54:CC:204:ILE:HD13	54:CC:215:LEU:HD23	1.92	0.49
63:LL:82:MET:HB3	63:LL:85:THR:HG23	1.94	0.49
64:MM:50:CYS:SG	64:MM:51:VAL:N	2.86	0.49
86:ii:323:TYR:HE2	86:ii:325:ASN:HB2	1.64	0.49
5:E:152:ARG:NH1	48:5:4939:C:OP1	2.46	0.49
17:R:35:ALA:O	17:R:37:SER:N	2.45	0.49
18:S:173:ASN:HA	48:5:4762:A:H2	1.78	0.49
47:3:5:G:C2	47:3:6:G:N7	2.81	0.49
47:3:69:G:C2	47:3:70:G:C5	3.00	0.49
48:5:698:G:N2	48:5:699:C:C2	2.81	0.49
48:5:937:U:H2'	48:5:937:U:O2	2.12	0.49
48:5:984:C:C2	48:5:1070:G:C2	3.00	0.49
48:5:2065:G:C6	48:5:2066:C:C4	3.01	0.49
48:5:4441:A:H5''	48:5:4441:A:C8	2.48	0.49
50:8:127:U:C4	50:8:128:C:C5	3.00	0.49
8:H:100:PRO:CD	87:jj:440:GLN:HE22	2.15	0.49
13:N:135:ILE:HD12	13:N:151:ILE:HD13	1.95	0.49
48:5:202:C:C2	48:5:214:G:C2	3.00	0.49
48:5:2586:G:N7	48:5:2587:A:C6	2.80	0.49
48:5:4583:C:N3	48:5:4718:G:C2	2.81	0.49
49:7:93:G:C6	49:7:94:C:C4	3.00	0.49
50:8:56:G:C4	50:8:62:A:C2	3.01	0.49
51:9:1108:G:C2	51:9:1125:C:C2	3.00	0.49
51:9:1315:U:O2	51:9:1315:U:O4'	2.29	0.49
86:ii:324:GLU:O	86:ii:375:LEU:CD2	2.60	0.49
7:G:81:ASN:OD1	7:G:238:GLY:N	2.46	0.49
48:5:300:A:C2	48:5:301:G:C6	3.01	0.49
48:5:497:G:C2	48:5:657:C:N3	2.81	0.49
48:5:1214:C:H1'	48:5:1215:C:OP2	2.12	0.49
48:5:1984:A:N6	48:5:2011:C:O2'	2.46	0.49
48:5:4099:G:C6	48:5:4100:C:C4	3.00	0.49
51:9:191:A:H3'	51:9:192:C:H5''	1.94	0.49
51:9:1231:C:O2'	51:9:1253:A:N6	2.45	0.49
51:9:1455:A:H5''	69:RR:52:GLY:HA2	1.95	0.49
65:NN:55:ARG:HD2	79:bb:47:PHE:CD2	2.48	0.49
7:G:156:VAL:HG13	7:G:184:LEU:HG	1.95	0.49
18:S:47:PHE:HE1	18:S:125:GLN:HG2	1.76	0.49
43:s:57:LYS:CE	48:5:1961:G:OP2	2.61	0.49
48:5:209:U:C4	48:5:233:U:O4	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1755:C:O2	48:5:1755:C:O2'	2.23	0.49
48:5:2020:U:O2	48:5:2020:U:H2'	2.12	0.49
48:5:3717:A:N1	48:5:3933:G:H1'	2.28	0.49
51:9:1145:A:C5	51:9:1146:C:H1'	2.48	0.49
51:9:1212:G:O2'	51:9:1213:C:O4'	2.30	0.49
2:B:252:ALA:HB1	48:5:4524:G:N3	2.28	0.49
17:R:172:ARG:O	17:R:176:ARG:NH2	2.45	0.49
31:f:48:ALA:HB2	31:f:71:TRP:CZ3	2.48	0.49
42:r:32:LEU:HD13	42:r:110:ALA:HA	1.95	0.49
47:3:35:U:C1'	51:9:1640:A:O3'	2.60	0.49
48:5:742:G:N2	48:5:923:C:C2	2.81	0.49
48:5:919:C:N4	48:5:920:C:N4	2.60	0.49
48:5:1995:G:C6	48:5:1996:C:C4	3.01	0.49
48:5:2517:A:N3	48:5:2539:C:O2'	2.46	0.49
48:5:4476:C:O2'	48:5:4478:G:OP2	2.26	0.49
48:5:4559:A:O3'	48:5:4560:C:O2	2.31	0.49
48:5:4735:G:C6	48:5:4736:C:C4	3.01	0.49
48:5:4872:G:O2'	48:5:4873:G:OP1	2.29	0.49
51:9:14:C:O2	51:9:1198:G:C2	2.66	0.49
51:9:309:G:C2	51:9:310:C:C4	3.01	0.49
51:9:1308:U:C4	51:9:1309:C:C5	2.99	0.49
58:GG:52:ILE:O	58:GG:52:ILE:HG23	2.13	0.49
6:F:168:ARG:HD2	6:F:211:TRP:CD1	2.48	0.49
29:d:32:ARG:NH2	48:5:4996:C:OP1	2.46	0.49
48:5:2090:U:O4'	48:5:2090:U:OP2	2.31	0.49
48:5:2909:C:C2	48:5:3586:G:C2	3.00	0.49
51:9:1305:C:H2'	51:9:1306:U:C5'	2.43	0.49
1:A:44:ILE:HG22	1:A:87:PHE:CD1	2.47	0.48
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.95	0.48
5:E:149:LEU:HD11	5:E:191:ILE:HG13	1.94	0.48
6:F:92:ALA:HB3	6:F:127:LEU:HD21	1.94	0.48
34:i:90:LEU:C	34:i:92:SER:N	2.70	0.48
41:p:39:CYS:SG	41:p:41:PHE:HB2	2.53	0.48
47:3:5:G:N3	47:3:6:G:N7	2.61	0.48
48:5:2336:G:C6	48:5:2337:C:C4	3.01	0.48
48:5:2609:G:C2	48:5:2731:C:O2	2.66	0.48
48:5:3753:G:OP1	48:5:3777:G:C8	2.66	0.48
48:5:4136:G:C6	48:5:4137:C:C4	3.00	0.48
48:5:4586:G:H5''	48:5:4586:G:H8	1.77	0.48
51:9:88:G:C6	51:9:89:C:C4	3.01	0.48
51:9:1771:G:N1	51:9:1772:C:C4	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:FF:194:ASP:CG	57:FF:198:ARG:NH1	2.70	0.48
81:dd:21:CYS:SG	81:dd:22:ARG:N	2.86	0.48
86:ii:323:TYR:CD1	86:ii:324:GLU:HG2	2.45	0.48
4:D:200:MET:HE3	4:D:237:GLU:O	2.13	0.48
10:J:119:TYR:CB	70:SS:12:ILE:HG21	2.43	0.48
16:Q:65:ARG:NH1	48:5:1502:G:OP1	2.46	0.48
29:d:65:ASP:OD1	29:d:66:THR:N	2.46	0.48
30:e:43:ASN:O	30:e:44:ARG:C	2.55	0.48
45:1:68:VAL:C	46:2:76:A:O2'	2.56	0.48
48:5:505:G:C2	48:5:506:C:C2	3.01	0.48
48:5:1549:G:C2	48:5:1580:C:C2	3.01	0.48
48:5:2297:G:C2	48:5:2338:C:C2	3.02	0.48
48:5:3715:U:H2'	48:5:3716:C:C6	2.48	0.48
49:7:66:G:C6	49:7:67:C:C4	3.00	0.48
51:9:1344:A:N6	51:9:1386:A:H5''	2.28	0.48
51:9:1466:G:N1	51:9:1467:C:C4	2.81	0.48
51:9:1489:A:H4'	51:9:1490:G:OP2	2.12	0.48
52:AA:63:ARG:CG	52:AA:185:MET:HE1	2.43	0.48
70:SS:30:ILE:HD11	70:SS:45:LEU:HD21	1.95	0.48
84:gg:87:LEU:CD2	84:gg:108:VAL:HG11	2.42	0.48
2:B:378:ARG:HE	22:W:32:LEU:HD21	1.78	0.48
9:I:87:ILE:HG12	9:I:138:ILE:HG12	1.95	0.48
10:J:82:ILE:HG22	10:J:130:PHE:HE2	1.79	0.48
18:S:34:ALA:HB1	18:S:39:VAL:CG2	2.43	0.48
23:X:50:LYS:HG3	48:5:2475:G:C6	2.48	0.48
48:5:1072:C:O2	48:5:1072:C:H2'	2.13	0.48
48:5:1995:G:C2	48:5:1996:C:C2	3.01	0.48
50:8:139:G:C6	50:8:140:C:C4	3.01	0.48
51:9:963:A:H2'	51:9:964:A:O4'	2.14	0.48
51:9:1447:G:H2'	51:9:1448:A:C8	2.47	0.48
66:OO:102:GLY:O	66:OO:106:LYS:NZ	2.45	0.48
87:jj:595:PHE:C	87:jj:596:PHE:CD2	2.91	0.48
3:C:57:LEU:O	3:C:58:ALA:C	2.56	0.48
48:5:504:G:C2	48:5:654:C:C2	3.00	0.48
48:5:505:G:C6	48:5:506:C:C4	3.01	0.48
48:5:978:G:C6	48:5:979:C:C4	3.02	0.48
48:5:1541:C:C2	48:5:1619:G:N2	2.81	0.48
48:5:3586:G:C6	48:5:3587:C:C4	3.02	0.48
51:9:185:G:N2	51:9:186:C:C2	2.82	0.48
15:P:69:ARG:NH2	48:5:4568:A:N3	2.62	0.48
33:h:7:ARG:HG3	50:8:86:U:C5	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:24:G:H2'	47:3:25:C:O4'	2.13	0.48
47:3:39:U:H4'	66:OO:66:ARG:HH22	1.78	0.48
48:5:1754:U:O2	48:5:1754:U:O4'	2.30	0.48
48:5:1839:U:H2'	48:5:1840:G:O4'	2.14	0.48
48:5:4183:G:H2'	48:5:4183:G:N3	2.28	0.48
48:5:4635:A:C2	48:5:4664:A:C5	3.02	0.48
48:5:4767:C:C2	48:5:4868:G:C2	3.01	0.48
51:9:88:G:C2	51:9:89:C:C2	3.01	0.48
51:9:1190:A:H2'	51:9:1191:C:O4'	2.13	0.48
51:9:1236:G:C2	51:9:1237:C:C2	3.01	0.48
61:JJ:38:ARG:HA	82:ee:31:ARG:HB2	1.95	0.48
86:ii:183:ALA:O	86:ii:187:ALA:HB2	2.13	0.48
86:ii:287:ILE:HD13	86:ii:399:GLY:HA2	1.96	0.48
47:3:6:G:O2'	47:3:7:A:H5'	2.14	0.48
48:5:1270:A:H2'	48:5:1271:G:O5'	2.14	0.48
48:5:2028:C:O2'	48:5:2029:A:O4'	2.32	0.48
48:5:4276:G:N2	48:5:4333:C:C2	2.81	0.48
3:C:183:VAL:HG22	3:C:204:ARG:CB	2.44	0.48
7:G:30:PRO:HD2	7:G:31:LEU:HD22	1.96	0.48
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.95	0.48
40:o:66:ILE:HD13	40:o:91:PHE:CE1	2.48	0.48
48:5:4079:C:C2	48:5:4168:G:C2	3.02	0.48
48:5:4093:G:H3'	48:5:4094:G:H5'	1.94	0.48
48:5:4499:G:O6	86:ii:180:HIS:NE2	2.46	0.48
51:9:1717:C:C2	51:9:1817:G:C2	3.00	0.48
66:OO:145:GLY:O	66:OO:147:ARG:N	2.46	0.48
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.44	0.48
2:B:49:TYR:CZ	2:B:168:MET:HE1	2.49	0.48
6:F:110:VAL:HG21	6:F:137:ILE:HD12	1.96	0.48
37:l:5:LYS:NZ	48:5:2407:G:N7	2.61	0.48
46:2:53:G:N2	46:2:62:C:C2	2.81	0.48
47:3:34:U:O2'	47:3:35:U:O4'	2.32	0.48
48:5:1075:G:C2	48:5:1076:C:C2	3.02	0.48
48:5:1448:G:N2	48:5:1449:C:C2	2.81	0.48
48:5:2128:G:C6	48:5:2129:C:C4	3.02	0.48
48:5:4152:G:N2	48:5:4153:C:C2	2.81	0.48
48:5:4989:U:O2	48:5:4989:U:O4'	2.30	0.48
50:8:103:A:C8	50:8:104:A:C8	3.02	0.48
51:9:305:U:O2'	51:9:309:G:O4'	2.29	0.48
53:BB:62:LEU:HA	53:BB:65:ARG:HE	1.77	0.48
56:EE:173:ILE:HD11	56:EE:235:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:FF:35:LEU:HD13	57:FF:117:ILE:HG23	1.95	0.48
48:5:77:U:H3	48:5:336:A:N6	2.12	0.48
48:5:230:G:C2	48:5:239:C:C2	3.02	0.48
48:5:499:G:H2'	48:5:499:G:N3	2.28	0.48
48:5:671:G:C2	48:5:672:C:C2	3.02	0.48
48:5:1751:A:C2	48:5:1780:A:C2	3.02	0.48
48:5:2315:G:C2	48:5:2325:C:C2	3.01	0.48
48:5:3629:A:C1'	51:9:1721:U:O2	2.61	0.48
50:8:46:G:N2	50:8:47:C:C2	2.82	0.48
51:9:433:A:H2'	51:9:434:G:C8	2.49	0.48
51:9:1235:G:H5'	51:9:1247:C:N4	2.23	0.48
51:9:1406:G:C5	51:9:1407:U:H1'	2.48	0.48
67:PP:34:MET:CE	67:PP:42:ARG:HA	2.43	0.48
75:XX:67:ARG:HG2	75:XX:115:ILE:HD12	1.96	0.48
6:F:118:GLN:HB2	6:F:121:ASN:HD21	1.78	0.48
48:5:199:G:C6	48:5:220:C:N3	2.81	0.48
48:5:1198:G:H2'	48:5:1199:G:C8	2.48	0.48
48:5:1400:G:H2'	48:5:1401:C:O4'	2.14	0.48
48:5:1822:U:O2	48:5:1822:U:O4'	2.29	0.48
48:5:1964:A:C2'	48:5:1965:G:C5'	2.91	0.48
48:5:4883:C:O2'	48:5:4884:G:P	2.72	0.48
48:5:5020:G:C2	48:5:5021:C:C2	3.02	0.48
49:7:23:A:N3	49:7:118:C:O2'	2.44	0.48
51:9:15:U:H2'	51:9:16:G:O4'	2.14	0.48
51:9:1046:U:H2'	51:9:1047:C:O4'	2.14	0.48
51:9:1481:G:C6	51:9:1482:C:N3	2.82	0.48
60:II:11:ARG:NH1	60:II:15:GLY:O	2.41	0.48
65:NN:60:VAL:HG23	65:NN:66:VAL:HG21	1.96	0.48
66:OO:54:CYS:SG	66:OO:84:ARG:HG3	2.54	0.48
30:e:107:ASN:OD1	30:e:107:ASN:N	2.47	0.47
46:2:34:A:O2'	46:2:35:A:O4'	2.31	0.47
46:2:40:C:H4'	47:3:36:U:H1'	1.96	0.47
48:5:967:C:N3	48:5:2254:G:C6	2.81	0.47
48:5:2496:G:C2	48:5:2497:C:C2	3.02	0.47
48:5:3717:A:O2'	48:5:3718:A:O4'	2.32	0.47
48:5:4666:G:C6	48:5:4667:C:C4	3.01	0.47
51:9:1265:A:N3	51:9:1265:A:H2'	2.28	0.47
51:9:1308:U:O4	51:9:1309:C:C6	2.65	0.47
7:G:162:ASP:HB3	7:G:163:PRO:HD3	1.96	0.47
34:i:63:VAL:HG12	34:i:63:VAL:O	2.14	0.47
47:3:5:G:C4	47:3:6:G:N7	2.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:499:G:C2	48:5:500:G:C8	3.02	0.47
48:5:929:A:H3'	48:5:930:G:C5'	2.43	0.47
48:5:1189:G:C6	48:5:1190:C:C4	3.02	0.47
48:5:1221:G:O2'	48:5:1222:A:O5'	2.21	0.47
48:5:1655:C:H2'	48:5:1656:U:H5''	1.96	0.47
48:5:1904:G:C2	48:5:2073:C:C2	3.02	0.47
48:5:1987:C:O2	48:5:1987:C:C2'	2.61	0.47
48:5:3918:G:C6	48:5:3919:C:C4	3.02	0.47
48:5:4099:G:C2	48:5:4100:C:C2	3.02	0.47
48:5:4305:G:N3	48:5:4305:G:H2'	2.29	0.47
51:9:1408:U:C4	51:9:1409:A:C6	3.01	0.47
51:9:1537:A:C2	51:9:1596:U:N3	2.82	0.47
43:s:57:LYS:HE2	48:5:1961:G:OP2	2.14	0.47
46:2:30:G:C6	46:2:31:C:C4	3.02	0.47
48:5:199:G:N1	48:5:220:C:C2	2.82	0.47
48:5:1240:G:C2	48:5:1241:C:C2	3.02	0.47
48:5:1246:G:H2'	48:5:1247:U:O4'	2.14	0.47
48:5:2097:U:O2	48:5:2097:U:O4'	2.32	0.47
48:5:2539:C:H2'	48:5:2540:C:C6	2.49	0.47
48:5:4119:C:O2	48:5:4119:C:O4'	2.30	0.47
51:9:666:U:H2'	51:9:667:U:C6	2.50	0.47
51:9:1299:A:OP2	67:PP:59:ARG:NH2	2.47	0.47
60:II:162:LEU:HD11	60:II:191:GLU:HG2	1.97	0.47
87:jj:382:GLY:HA3	87:jj:539:PRO:HB3	1.96	0.47
3:C:209:VAL:HB	3:C:229:LEU:HD13	1.97	0.47
3:C:303:ARG:O	16:Q:38:ARG:NH1	2.46	0.47
14:O:17:GLY:HA3	48:5:2052:G:O3'	2.14	0.47
48:5:100:C:O4'	48:5:100:C:O2	2.30	0.47
48:5:300:A:H2'	48:5:301:G:C8	2.50	0.47
48:5:705:G:N2	48:5:706:C:C2	2.82	0.47
48:5:1238:A:H2'	48:5:1239:C:C6	2.49	0.47
48:5:1358:G:O6	48:5:1379:C:N3	2.47	0.47
48:5:2267:U:O4'	48:5:2267:U:O2	2.33	0.47
48:5:2336:G:C2	48:5:2337:C:C2	3.03	0.47
48:5:4919:G:C2	48:5:4920:C:C2	3.02	0.47
49:7:71:G:C2	49:7:105:C:C2	3.03	0.47
51:9:1308:U:N3	51:9:1309:C:H1'	2.23	0.47
51:9:1847:G:N2	51:9:1853:C:C2	2.83	0.47
12:M:126:GLU:CD	12:M:130:LEU:CD1	2.86	0.47
32:g:5:LEU:HD13	32:g:32:TYR:CE2	2.49	0.47
32:g:76:ARG:NH1	48:5:2582:A:OP1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:42:CYS:HA	48:5:2674:A:N6	2.30	0.47
42:r:64:MET:HE1	42:r:102:TYR:CG	2.50	0.47
47:3:5:G:C2	47:3:6:G:C4	3.03	0.47
48:5:499:G:C2	48:5:656:C:N3	2.82	0.47
48:5:1240:G:C6	48:5:1241:C:C4	3.03	0.47
48:5:1584:G:C6	48:5:1585:C:C4	3.01	0.47
48:5:1723:A:N1	48:5:1838:A:C2	2.83	0.47
48:5:2089:G:C6	48:5:2262:G:H2'	2.49	0.47
48:5:2496:G:C6	48:5:2497:C:C4	3.03	0.47
48:5:4759:C:H2'	48:5:4760:G:O4'	2.14	0.47
51:9:832:G:N2	51:9:843:C:C2	2.82	0.47
51:9:1535:U:O2	51:9:1535:U:H2'	2.15	0.47
51:9:1650:A:C5	51:9:1675:A:N1	2.82	0.47
51:9:1866:A:C5	78:aa:87:ARG:NH2	2.82	0.47
56:EE:54:TYR:CD1	76:YY:17:LEU:HD11	2.49	0.47
87:jj:169:LYS:HZ2	87:jj:226:ALA:HB3	1.80	0.47
19:T:57:TYR:CD1	19:T:76:VAL:HG21	2.49	0.47
48:5:1189:G:C2	48:5:1190:C:C2	3.03	0.47
51:9:92:A:C6	51:9:446:G:C6	3.03	0.47
51:9:1211:G:C3'	51:9:1212:G:H5'	2.43	0.47
51:9:1344:A:N6	51:9:1386:A:C5'	2.77	0.47
57:FF:73:THR:HG22	57:FF:89:THR:CG2	2.45	0.47
69:RR:24:LEU:HD22	69:RR:54:VAL:HG11	1.95	0.47
2:B:220:ILE:HB	2:B:346:THR:HB	1.97	0.47
3:C:86:ARG:HA	3:C:89:GLN:HG3	1.95	0.47
3:C:335:MET:HE1	48:5:944:A:H1'	1.97	0.47
4:D:35:ARG:HB2	48:5:4325:A:C2	2.49	0.47
6:F:156:ILE:HG22	6:F:189:MET:HE3	1.97	0.47
47:3:34:U:O2	51:9:1641:A:C5'	2.60	0.47
48:5:742:G:C2	48:5:923:C:C2	3.03	0.47
48:5:978:G:C2	48:5:979:C:C2	3.02	0.47
48:5:1099:C:H2'	48:5:1100:U:O4'	2.15	0.47
48:5:1367:C:O2	48:5:1367:C:H2'	2.14	0.47
48:5:2065:G:C2	48:5:2066:C:C2	3.03	0.47
48:5:2477:A:H2'	48:5:2478:C:C6	2.50	0.47
48:5:2542:G:C2	48:5:2775:C:C2	3.03	0.47
48:5:2612:G:C6	48:5:2613:C:C4	3.02	0.47
48:5:3697:U:O2'	48:5:3698:G:OP2	2.28	0.47
48:5:4740:G:C2	48:5:4741:C:C2	3.03	0.47
48:5:4773:C:C2	48:5:4863:G:C2	3.03	0.47
50:8:56:G:C2	50:8:57:C:C2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:86:C:C4	51:9:87:U:C5	3.03	0.47
51:9:1115:U:O2	51:9:1115:U:O4'	2.32	0.47
51:9:1260:A:C4	51:9:1620:A:N7	2.82	0.47
51:9:1308:U:O4	51:9:1309:C:C4	2.67	0.47
51:9:1648:G:C8	68:QQ:125:ARG:HB3	2.50	0.47
51:9:1666:C:H2'	51:9:1667:U:O4'	2.15	0.47
51:9:1754:G:C6	51:9:1755:C:C4	3.03	0.47
52:AA:2:SER:OG	52:AA:56:GLU:O	2.29	0.47
52:AA:157:VAL:HG23	52:AA:157:VAL:O	2.14	0.47
86:ii:323:TYR:HB3	86:ii:326:LEU:HG	1.96	0.47
12:M:126:GLU:OE2	12:M:130:LEU:HD13	2.14	0.47
42:r:46:ARG:HD2	48:5:666:G:C8	2.50	0.47
47:3:69:G:N1	47:3:70:G:C6	2.83	0.47
48:5:751:G:C2	48:5:752:G:N7	2.82	0.47
48:5:2128:G:C2	48:5:2129:C:C2	3.03	0.47
48:5:2698:G:C6	48:5:2699:C:C4	3.03	0.47
48:5:3628:G:C2	48:5:3834:C:C2	3.03	0.47
48:5:3709:U:O2'	48:5:3710:G:O4'	2.32	0.47
48:5:3896:C:O2	48:5:4564:A:N1	2.48	0.47
48:5:4472:G:C6	48:5:4473:A:N7	2.83	0.47
48:5:4916:G:C2	48:5:4917:C:C2	3.02	0.47
49:7:93:G:C2	49:7:94:C:C2	3.03	0.47
50:8:75:G:N2	50:8:76:C:C2	2.83	0.47
51:9:1551:U:H2'	51:9:1552:G:C8	2.50	0.47
70:SS:82:TRP:O	70:SS:84:LEU:N	2.48	0.47
26:a:75:LEU:O	26:a:76:ASP:C	2.57	0.47
28:c:82:GLY:HA2	28:c:91:VAL:HG12	1.95	0.47
48:5:299:C:C4	48:5:300:A:N7	2.83	0.47
48:5:1550:G:N1	48:5:1551:C:C2	2.83	0.47
48:5:2245:G:C2	48:5:2246:C:C2	3.03	0.47
48:5:2907:G:H2'	48:5:2908:U:O4'	2.15	0.47
48:5:3597:G:C2	48:5:3598:C:C2	3.03	0.47
48:5:3717:A:OP2	48:5:3735:G:N2	2.48	0.47
48:5:4102:C:C2	48:5:4108:G:C2	3.03	0.47
51:9:12:U:H2'	51:9:13:C:C6	2.50	0.47
51:9:1454:A:HO2'	51:9:1455:A:P	2.37	0.47
58:GG:3:LEU:HD22	58:GG:109:LEU:HB2	1.96	0.47
59:HH:133:LEU:HD21	59:HH:176:VAL:HG11	1.97	0.47
2:B:91:GLY:HA3	2:B:153:MET:HE3	1.97	0.47
5:E:126:ARG:HH21	48:5:712:C:C2'	2.28	0.47
13:N:5:LYS:HG2	34:i:40:VAL:HG11	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:94:PHE:CE2	13:N:96:ARG:HB2	2.50	0.47
42:r:97:ILE:HG21	42:r:107:ARG:HA	1.97	0.47
48:5:177:G:C2	48:5:178:C:C2	3.02	0.47
48:5:479:G:N2	48:5:480:C:C2	2.83	0.47
48:5:1557:C:C2	48:5:1571:G:C2	3.03	0.47
48:5:1613:A:H3'	48:5:1614:C:C5'	2.45	0.47
48:5:1995:G:C5	48:5:1996:C:C4	3.02	0.47
48:5:3626:G:C6	48:5:3836:A:C2	3.03	0.47
48:5:3629:A:O4'	51:9:1721:U:O2	2.33	0.47
48:5:4758:U:O2	48:5:4758:U:O4'	2.31	0.47
17:R:105:LEU:HD12	17:R:138:LEU:HD13	1.97	0.46
48:5:1171:G:C6	48:5:1172:C:C4	3.03	0.46
48:5:2028:C:O2'	48:5:2029:A:O5'	2.33	0.46
48:5:2844:A:O2'	48:5:4631:G:H4'	2.14	0.46
48:5:4092:G:C2	48:5:4158:C:C2	3.03	0.46
48:5:4411:G:C2	48:5:4432:C:O2	2.68	0.46
51:9:463:C:O2'	51:9:466:G:O6	2.23	0.46
51:9:639:C:H2'	51:9:640:A:C8	2.50	0.46
68:QQ:42:ILE:HD12	68:QQ:42:ILE:N	2.31	0.46
76:YY:113:ARG:O	76:YY:114:MET:CB	2.62	0.46
48:5:99:A:H2'	48:5:100:C:O2	2.14	0.46
48:5:105:A:C2	48:5:336:A:C8	3.04	0.46
48:5:177:G:C6	48:5:178:C:C4	3.02	0.46
48:5:497:G:H3'	48:5:498:C:H5''	1.97	0.46
48:5:1468:C:C2	48:5:1498:G:N2	2.83	0.46
48:5:3627:G:N2	48:5:3835:C:C2	2.83	0.46
48:5:4904:G:N2	48:5:4905:C:C2	2.84	0.46
50:8:53:G:C6	50:8:54:C:C4	3.03	0.46
51:9:1265:A:N3	51:9:1265:A:C2'	2.77	0.46
12:M:125:ASN:O	12:M:129:LYS:HG3	2.15	0.46
17:R:71:ARG:NH1	48:5:3605:C:OP2	2.38	0.46
38:m:119:ASN:C	38:m:119:ASN:HD22	2.23	0.46
48:5:181:C:C4	48:5:256:G:N1	2.84	0.46
48:5:1357:C:H5''	48:5:1358:G:OP1	2.16	0.46
48:5:4489:G:C6	48:5:4490:C:C4	3.03	0.46
48:5:4652:G:N2	48:5:4653:C:C2	2.84	0.46
51:9:194:C:C2	51:9:206:G:C2	3.04	0.46
51:9:697:G:C2	51:9:734:C:C2	3.03	0.46
51:9:834:C:H3'	51:9:835:C:H4'	1.96	0.46
51:9:1141:G:N2	51:9:1147:C:C2	2.84	0.46
65:NN:40:LEU:HD21	65:NN:53:ILE:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:PP:83:MET:HE2	67:PP:116:LEU:HD11	1.97	0.46
26:a:25:HIS:CG	48:5:1338:G:H22	2.33	0.46
43:s:54:LEU:HD23	43:s:60:MET:HE1	1.97	0.46
47:3:37:A:N1	57:FF:133:THR:HG23	2.30	0.46
48:5:488:G:N2	48:5:489:C:C2	2.84	0.46
48:5:994:G:C2	48:5:1050:C:C2	3.03	0.46
48:5:1448:G:C6	48:5:1449:C:N4	2.83	0.46
48:5:1661:C:C2	48:5:2345:G:N1	2.84	0.46
51:9:14:C:C2	51:9:1198:G:C2	3.04	0.46
51:9:50:A:C2	51:9:488:U:O4	2.68	0.46
51:9:187:G:C6	51:9:188:C:C4	3.04	0.46
51:9:962:A:N1	51:9:1055:A:O2'	2.48	0.46
51:9:987:A:C2	53:BB:114:VAL:HG21	2.51	0.46
51:9:1459:G:C6	51:9:1460:C:C4	3.04	0.46
51:9:1534:C:H1'	51:9:1536:G:C4	2.51	0.46
54:CC:94:ILE:HD11	54:CC:98:LEU:HD12	1.97	0.46
61:JJ:118:GLY:O	61:JJ:120:ALA:N	2.48	0.46
13:N:172:ARG:NH1	48:5:62:A:OP1	2.49	0.46
17:R:176:ARG:HH12	51:9:909:G:H5'	1.81	0.46
47:3:24:G:C2	47:3:25:C:C2	3.02	0.46
48:5:209:U:N3	48:5:233:U:C4	2.83	0.46
48:5:977:C:O2'	48:5:978:G:H5'	2.16	0.46
48:5:984:C:C2	48:5:1070:G:N2	2.83	0.46
48:5:1235:G:H2'	48:5:1236:C:H5'	1.96	0.46
48:5:1998:A:O2'	48:5:1999:A:O4'	2.33	0.46
48:5:2088:A:O2'	48:5:2089:G:P	2.74	0.46
48:5:4919:G:C6	48:5:4920:C:C4	3.04	0.46
51:9:123:G:C2	51:9:342:C:C2	3.03	0.46
51:9:834:C:C2	51:9:841:G:N2	2.84	0.46
51:9:1308:U:O4	51:9:1309:C:C2	2.68	0.46
51:9:1524:G:N2	51:9:1525:C:C2	2.83	0.46
3:C:130:ALA:HB3	3:C:246:VAL:HG13	1.97	0.46
5:E:59:TYR:CE1	5:E:64:LEU:HB2	2.50	0.46
7:G:50:ASP:C	7:G:50:ASP:OD1	2.58	0.46
9:I:61:SER:HA	9:I:126:VAL:HG23	1.97	0.46
12:M:24:LEU:HB2	12:M:43:THR:HG21	1.98	0.46
12:M:104:MET:HE2	14:O:199:HIS:HB3	1.97	0.46
13:N:57:GLN:HB3	13:N:139:HIS:CE1	2.50	0.46
39:n:4:LYS:CE	51:9:1844:U:O4	2.64	0.46
48:5:504:G:O6	48:5:654:C:C4	2.69	0.46
48:5:2468:U:N3	48:5:2473:A:C6	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2771:G:C6	48:5:2772:C:C4	3.04	0.46
48:5:3586:G:C2	48:5:3587:C:C2	3.03	0.46
48:5:4136:G:C2	48:5:4137:C:C2	3.04	0.46
48:5:4916:G:C6	48:5:4917:C:C4	3.04	0.46
51:9:182:C:H2'	51:9:184:G:H1'	1.96	0.46
51:9:980:A:C2	51:9:981:A:C6	3.03	0.46
51:9:1129:G:H3'	51:9:1130:G:C8	2.48	0.46
51:9:1624:U:O2	51:9:1624:U:O4'	2.34	0.46
51:9:1865:C:OP1	78:aa:87:ARG:NH2	2.49	0.46
78:aa:50:VAL:HG23	78:aa:64:LEU:HD11	1.98	0.46
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.98	0.46
5:E:112:TYR:CZ	42:r:108:MET:HE1	2.51	0.46
7:G:100:HIS:HA	7:G:103:ARG:HD2	1.98	0.46
10:J:165:TRP:CH2	10:J:170:TYR:CE2	2.99	0.46
19:T:130:ARG:NH2	48:5:1836:G:OP1	2.48	0.46
35:j:2:THR:O	35:j:7:SER:OG	2.32	0.46
47:3:31:A:H2'	57:FF:136:ARG:NH2	2.31	0.46
48:5:721:G:C2	48:5:948:C:C2	3.03	0.46
48:5:977:C:H2'	48:5:978:G:O4'	2.15	0.46
48:5:1878:G:N2	48:5:1879:C:C2	2.83	0.46
48:5:4452:U:O2'	86:ii:185:GLN:HG3	2.16	0.46
48:5:4454:G:HO2'	48:5:4500:U:HO2'	1.59	0.46
51:9:873:G:N1	51:9:914:U:C5	2.84	0.46
51:9:1537:A:C2	51:9:1538:C:C2	3.03	0.46
56:EE:195:ILE:O	56:EE:196:THR:CB	2.64	0.46
66:OO:65:ASP:OD1	66:OO:65:ASP:N	2.48	0.46
87:jj:121:LYS:NZ	87:jj:121:LYS:HG2	2.31	0.46
3:C:218:VAL:O	3:C:218:VAL:HG12	2.14	0.46
4:D:44:TYR:CD1	48:5:1823:G:H4'	2.51	0.46
5:E:217:GLN:HE22	5:E:233:LYS:HD2	1.79	0.46
5:E:254:LEU:N	5:E:255:PRO:HD2	2.30	0.46
7:G:58:PRO:CD	23:X:46:PHE:HD2	2.28	0.46
31:f:43:LEU:HD22	31:f:76:ARG:HA	1.97	0.46
37:l:2:SER:N	48:5:2406:G:N7	2.64	0.46
48:5:1241:C:C2'	48:5:1242:G:OP1	2.64	0.46
48:5:1362:G:N2	48:5:1363:C:C2	2.83	0.46
48:5:1818:G:O2'	48:5:1819:G:OP1	2.23	0.46
48:5:1899:G:N2	48:5:1900:C:C2	2.83	0.46
48:5:4473:A:C2	48:5:4474:A:C5	3.03	0.46
48:5:4737:G:C2	48:5:4738:C:C2	3.03	0.46
51:9:321:C:H2'	51:9:322:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1231:C:H2'	51:9:1232:U:O4'	2.16	0.46
51:9:1304:U:OP2	83:ff:90:ARG:NH2	2.49	0.46
51:9:1865:C:O2'	78:aa:95:ARG:NH1	2.49	0.46
53:BB:86:LEU:HA	53:BB:99:ASN:O	2.15	0.46
6:F:91:LEU:HD22	6:F:92:ALA:N	2.31	0.46
43:s:180:ILE:HG22	43:s:182:PRO:HD3	1.98	0.46
48:5:1270:A:H2'	48:5:1271:G:O4'	2.16	0.46
48:5:1910:G:C6	48:5:1911:C:N4	2.84	0.46
48:5:4109:G:C6	48:5:4110:C:C4	3.04	0.46
48:5:4731:G:H4'	48:5:4732:G:H5'	1.98	0.46
51:9:437:G:C2	51:9:457:C:C2	3.03	0.46
51:9:1476:A:H3'	51:9:1477:U:C5'	2.46	0.46
51:9:1759:G:C2	51:9:1774:C:C2	3.04	0.46
70:SS:113:ARG:HG2	70:SS:113:ARG:HH11	1.80	0.46
14:O:18:ARG:NH1	48:5:2053:C:O3'	2.47	0.46
35:j:9:GLY:HA2	48:5:2792:C:O2	2.16	0.46
48:5:1098:G:C2	48:5:1099:C:C2	3.04	0.46
48:5:1279:A:C4	48:5:1280:C:C4	3.04	0.46
48:5:1539:G:C6	48:5:1540:C:C4	3.03	0.46
48:5:1958:A:O2'	48:5:1959:U:H5''	2.15	0.46
48:5:1995:G:C6	48:5:1996:C:N3	2.84	0.46
48:5:2752:G:H2'	48:5:2753:G:O4'	2.16	0.46
48:5:2843:U:O2'	48:5:4632:U:OP1	2.29	0.46
48:5:2898:G:C6	48:5:2899:C:C4	3.04	0.46
48:5:4524:G:N2	48:5:4525:C:C2	2.84	0.46
48:5:4913:G:HO2'	48:5:4914:C:C1'	2.28	0.46
51:9:156:G:H4'	58:GG:108:VAL:HG23	1.97	0.46
51:9:409:C:C2	51:9:432:G:C2	3.03	0.46
51:9:1347:U:H2'	51:9:1348:G:C8	2.50	0.46
86:ii:374:LEU:O	86:ii:377:TRP:CB	2.58	0.46
35:j:34:CYS:SG	35:j:36:LYS:HB3	2.56	0.45
46:2:7:G:C6	46:2:49:C:N4	2.84	0.45
48:5:2:G:C2	48:5:3:C:C2	3.04	0.45
48:5:715:G:H1	48:5:953:C:H42	1.63	0.45
48:5:971:U:H2'	48:5:972:C:H5'	1.98	0.45
48:5:1399:G:H2'	48:5:1400:G:O4'	2.16	0.45
48:5:2729:C:H2'	48:5:2730:U:O4'	2.15	0.45
49:7:27:G:C2	49:7:28:C:C2	3.05	0.45
49:7:117:G:C2	49:7:118:C:C2	3.04	0.45
50:8:115:G:N2	50:8:116:C:C2	2.84	0.45
51:9:642:U:H4'	51:9:643:A:OP1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1309:C:HO2'	51:9:1310:U:P	2.39	0.45
58:GG:66:GLY:N	58:GG:100:CYS:SG	2.89	0.45
61:JJ:120:ALA:O	61:JJ:121:LYS:CB	2.64	0.45
87:jj:123:LEU:HD13	87:jj:270:ILE:HD13	1.98	0.45
87:jj:244:SER:HA	87:jj:247:LEU:HD12	1.98	0.45
4:D:41:LYS:CG	19:T:93:ILE:HD11	2.46	0.45
48:5:302:C:N4	48:5:303:C:N4	2.64	0.45
48:5:747:A:C2	48:5:749:G:H1'	2.50	0.45
48:5:1613:A:H3'	48:5:1614:C:H5'	1.98	0.45
48:5:2567:G:C2	48:5:2568:C:C2	3.04	0.45
48:5:3600:G:C2	48:5:3601:C:C2	3.05	0.45
48:5:4080:C:C2	48:5:4167:G:C2	3.04	0.45
48:5:4303:C:O2	48:5:4303:C:O4'	2.34	0.45
51:9:52:G:C6	51:9:53:C:C4	3.05	0.45
51:9:830:A:H2'	51:9:831:G:O4'	2.17	0.45
51:9:1835:A:N9	51:9:1863:A:N7	2.63	0.45
60:II:34:ALA:HB2	60:II:56:ARG:HG3	1.98	0.45
86:ii:297:ASP:O	86:ii:299:GLY:N	2.49	0.45
25:Z:46:ILE:HD11	25:Z:49:TYR:CE2	2.52	0.45
39:n:7:LYS:NZ	51:9:1843:G:OP1	2.46	0.45
39:n:21:ARG:HH22	51:9:1175:G:P	2.38	0.45
47:3:76:A:C8	48:5:4341:C:N4	2.82	0.45
48:5:179:G:C2	48:5:180:C:C2	3.05	0.45
48:5:278:G:H4'	48:5:279:A:OP2	2.16	0.45
48:5:744:G:C2	48:5:921:C:C2	3.04	0.45
48:5:918:G:H2'	48:5:918:G:N3	2.32	0.45
48:5:1270:A:C5	48:5:1271:G:H1'	2.52	0.45
48:5:2270:G:C6	48:5:2271:C:C4	3.05	0.45
48:5:2465:C:H2'	48:5:2466:G:O4'	2.16	0.45
48:5:2640:G:N7	48:5:2694:G:O6	2.49	0.45
48:5:2768:C:O2	48:5:2768:C:O4'	2.31	0.45
48:5:3705:G:C6	48:5:3706:C:C4	3.05	0.45
48:5:4583:C:C2	48:5:4718:G:N2	2.84	0.45
48:5:4587:G:C2	48:5:4716:C:C2	3.05	0.45
48:5:5020:G:C6	48:5:5021:C:C4	3.04	0.45
51:9:1229:G:C2	51:9:1230:C:C2	3.04	0.45
51:9:1669:G:C6	51:9:1670:C:C4	3.04	0.45
57:FF:20:PHE:CZ	57:FF:69:VAL:HG11	2.52	0.45
62:KK:12:TYR:CD2	62:KK:79:LEU:HD22	2.52	0.45
66:OO:139:SER:OG	66:OO:140:THR:N	2.49	0.45
86:ii:182:ARG:HH11	86:ii:182:ARG:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:42:ASN:OD1	4:D:42:ASN:N	2.48	0.45
9:I:97:ILE:HD13	9:I:126:VAL:HG11	1.97	0.45
17:R:176:ARG:NH1	51:9:909:G:C5'	2.77	0.45
30:e:57:ASN:O	48:5:2319:C:H1'	2.16	0.45
42:r:64:MET:HE3	42:r:64:MET:HB3	1.72	0.45
47:3:66:U:O4	47:3:67:U:C4	2.70	0.45
48:5:325:U:H2'	48:5:326:C:C6	2.51	0.45
48:5:1584:G:C2	48:5:1585:C:C2	3.05	0.45
48:5:1823:G:C3'	48:5:1825:A:P	3.04	0.45
48:5:1874:A:H5'	48:5:4218:U:O2	2.17	0.45
48:5:2245:G:C6	48:5:2246:C:C4	3.04	0.45
48:5:4740:G:C6	48:5:4741:C:C4	3.04	0.45
48:5:5020:G:H2'	48:5:5021:C:O4'	2.16	0.45
51:9:56:G:OP1	76:YY:111:LYS:NZ	2.39	0.45
51:9:592:C:O2	51:9:592:C:O4'	2.33	0.45
51:9:916:A:C5	65:NN:73:ARG:HD3	2.52	0.45
51:9:1038:U:O2'	51:9:1180:C:N3	2.49	0.45
57:FF:49:LEU:HD13	57:FF:50:PRO:HD2	1.99	0.45
58:GG:67:VAL:HG23	58:GG:99:GLY:HA2	1.98	0.45
59:HH:15:LYS:N	59:HH:16:PRO:HD2	2.32	0.45
75:XX:94:ILE:HD11	75:XX:122:VAL:HG11	1.97	0.45
86:ii:374:LEU:HD22	86:ii:378:PHE:HE2	1.75	0.45
1:A:97:ASN:N	1:A:97:ASN:OD1	2.49	0.45
1:A:122:ASP:C	1:A:122:ASP:OD1	2.59	0.45
2:B:100:ARG:NH1	48:5:4911:A:OP2	2.50	0.45
3:C:78:ARG:HB3	3:C:88:GLY:HA2	1.98	0.45
25:Z:100:VAL:HG13	25:Z:107:LYS:HA	1.97	0.45
28:c:77:ASN:OD1	28:c:78:ASN:N	2.49	0.45
47:3:3:C:H2'	47:3:4:C:H5'	1.99	0.45
48:5:469:C:C2	48:5:470:A:C8	3.05	0.45
48:5:476:G:N2	48:5:679:C:C2	2.85	0.45
48:5:3600:G:C6	48:5:3601:C:C4	3.05	0.45
48:5:3782:C:C2	48:5:3811:G:C2	3.05	0.45
48:5:4489:G:C2	48:5:4490:C:C2	3.04	0.45
50:8:56:G:C6	50:8:57:C:C4	3.05	0.45
50:8:118:C:C2	50:8:133:G:C2	3.04	0.45
51:9:443:U:O2'	58:GG:89:THR:HG22	2.17	0.45
51:9:1131:G:N1	51:9:1132:C:C4	2.84	0.45
51:9:1229:G:C6	51:9:1230:C:C4	3.05	0.45
54:CC:233:LEU:C	54:CC:233:LEU:HD12	2.42	0.45
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:LL:96:ILE:N	63:LL:96:ILE:HD12	2.32	0.45
67:PP:34:MET:HE1	67:PP:42:ARG:HA	1.99	0.45
74:WW:6:VAL:HG13	74:WW:29:PRO:HG2	1.97	0.45
86:ii:300:LYS:O	86:ii:413:LEU:CG	2.65	0.45
29:d:38:PHE:HB3	29:d:78:ARG:HD2	1.99	0.45
39:n:7:LYS:NZ	51:9:1843:G:P	2.89	0.45
48:5:190:G:C2	48:5:252:C:C2	3.05	0.45
48:5:963:G:H2'	48:5:963:G:N3	2.32	0.45
48:5:994:G:C2	48:5:995:C:C2	3.05	0.45
48:5:1297:U:P	48:5:1297:U:O4'	2.75	0.45
48:5:1732:C:C2	48:5:1798:G:C2	3.04	0.45
48:5:1855:G:C6	48:5:1856:C:C4	3.05	0.45
51:9:673:G:C2	51:9:674:C:C2	3.05	0.45
51:9:1057:C:O2	51:9:1057:C:O4'	2.35	0.45
51:9:1386:A:OP1	51:9:1483:A:N3	2.50	0.45
56:EE:86:PHE:HE2	56:EE:226:PHE:CD2	2.34	0.45
9:I:3:ARG:NH2	48:5:4431:U:OP2	2.50	0.45
28:c:85:CYS:SG	28:c:94:LEU:HD22	2.56	0.45
29:d:38:PHE:CE1	48:5:4634:U:C2	3.05	0.45
31:f:13:GLY:HA2	31:f:97:ILE:HD12	1.98	0.45
42:r:17:LEU:HD23	42:r:18:ILE:N	2.32	0.45
43:s:128:THR:HG22	43:s:178:LEU:HD21	1.98	0.45
44:t:97:ASN:N	44:t:98:ILE:HA	2.32	0.45
48:5:994:G:C6	48:5:995:C:C4	3.04	0.45
48:5:2370:A:N1	48:5:2390:G:O2'	2.50	0.45
48:5:2618:G:C2	48:5:2720:C:C2	3.04	0.45
48:5:2909:C:O2	48:5:3586:G:C2	2.70	0.45
48:5:4482:U:N3	48:5:4483:C:C5	2.84	0.45
48:5:5031:G:N2	48:5:5032:C:C2	2.85	0.45
51:9:301:A:N3	60:II:73:THR:HG21	2.31	0.45
51:9:841:G:N1	51:9:842:C:C4	2.85	0.45
58:GG:61:PHE:CE2	58:GG:96:SER:HB3	2.52	0.45
66:OO:31:CYS:HA	66:OO:44:VAL:HA	1.99	0.45
87:jj:24:GLU:O	87:jj:27:LYS:N	2.48	0.45
3:C:262:ASP:O	3:C:271:ALA:O	2.34	0.45
7:G:63:LEU:HD12	13:N:32:GLN:HB3	1.99	0.45
9:I:139:ARG:NH1	9:I:195:CYS:SG	2.90	0.45
10:J:119:TYR:C	70:SS:12:ILE:HD13	2.41	0.45
31:f:50:VAL:HG22	31:f:69:VAL:CG1	2.47	0.45
42:r:66:ARG:O	42:r:67:ARG:HB3	2.16	0.45
48:5:1196:G:C6	48:5:1197:C:C4	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1213:G:C4	48:5:1215:C:H1'	2.52	0.45
48:5:1365:C:O2	48:5:1366:G:C8	2.70	0.45
48:5:1416:G:N2	48:5:1417:C:C2	2.85	0.45
48:5:2026:A:HO2'	48:5:2027:U:H5'	1.79	0.45
48:5:2559:G:C6	48:5:2560:C:C4	3.04	0.45
48:5:2898:G:C2	48:5:2899:C:C2	3.05	0.45
48:5:3648:A:H1'	48:5:3785:A:N6	2.31	0.45
48:5:4109:G:C2	48:5:4110:C:C2	3.05	0.45
50:8:53:G:C2	50:8:54:C:C2	3.05	0.45
51:9:1058:A:H2'	51:9:1059:G:C8	2.52	0.45
51:9:1407:U:C2'	51:9:1408:U:C6	2.97	0.45
63:LL:59:LYS:O	63:LL:141:ASN:ND2	2.46	0.45
87:jj:105:VAL:HG23	87:jj:263:ILE:HD11	1.98	0.45
87:jj:121:LYS:NZ	87:jj:121:LYS:CG	2.80	0.45
3:C:76:ILE:HG22	3:C:77:PRO:HD2	1.98	0.45
13:N:180:PHE:O	13:N:182:HIS:N	2.50	0.45
18:S:127:MET:HE1	19:T:155:PRO:HA	1.97	0.45
47:3:5:G:C6	47:3:6:G:O6	2.70	0.45
48:5:1196:G:C2	48:5:1197:C:C2	3.04	0.45
48:5:1404:G:C6	48:5:1405:C:C4	3.04	0.45
48:5:1448:G:C2	48:5:1449:C:C2	3.05	0.45
48:5:2408:U:C1'	48:5:2409:U:C5	3.00	0.45
48:5:2715:G:C2	48:5:2716:C:C2	3.05	0.45
48:5:3662:A:N6	48:5:3680:U:N3	2.60	0.45
48:5:4142:C:C4	48:5:4143:G:N1	2.85	0.45
48:5:4476:C:O2	48:5:4476:C:O4'	2.35	0.45
51:9:52:G:C2	51:9:53:C:C2	3.04	0.45
51:9:433:A:H5''	60:II:22:HIS:HB3	1.99	0.45
51:9:696:G:C2	51:9:735:C:C2	3.05	0.45
51:9:1228:A:H2'	51:9:1229:G:C8	2.51	0.45
51:9:1386:A:O2'	51:9:1387:G:C5'	2.63	0.45
51:9:1516:G:O3'	67:PP:122:THR:HG21	2.16	0.45
56:EE:55:ALA:HB2	56:EE:64:ILE:HD12	1.99	0.45
1:A:211:PHE:CD1	1:A:219:ILE:HG23	2.53	0.45
17:R:99:MET:HE3	17:R:127:VAL:HG12	1.98	0.45
42:r:18:ILE:HG23	42:r:25:TYR:HB2	1.98	0.45
45:1:68:VAL:C	46:2:76:A:HO2'	2.25	0.45
48:5:917:A:C6	48:5:919:C:N4	2.85	0.45
48:5:1963:C:HO2'	48:5:1964:A:P	2.40	0.45
48:5:5017:G:C2	48:5:5018:C:C2	3.05	0.45
49:7:117:G:C6	49:7:118:C:C4	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:832:G:C6	51:9:833:C:C4	3.05	0.45
51:9:1139:C:H2'	51:9:1140:G:O4'	2.17	0.45
51:9:1298:G:O2'	51:9:1299:A:O5'	2.35	0.45
51:9:1398:G:C6	51:9:1399:C:C4	3.05	0.45
56:EE:160:ILE:HG21	56:EE:169:ILE:HG22	1.99	0.45
71:TT:60:THR:HG23	71:TT:75:MET:HE2	1.99	0.45
85:hh:52:G:OP1	86:ii:62:ILE:HG23	2.17	0.45
11:L:18:TRP:CE3	13:N:198:LEU:HD12	2.53	0.44
14:O:61:ARG:HA	14:O:70:PRO:HD2	1.99	0.44
39:n:10:MET:CE	51:9:1172:U:H4'	2.47	0.44
47:3:5:G:O2'	47:3:6:G:H5'	2.17	0.44
48:5:2730:U:H2'	48:5:2731:C:C6	2.52	0.44
48:5:2858:A:O2'	48:5:2859:G:O4'	2.34	0.44
48:5:4461:C:N3	48:5:4516:G:C6	2.86	0.44
50:8:75:G:C6	50:8:76:C:N4	2.85	0.44
51:9:322:C:OP2	51:9:322:C:C6	2.70	0.44
51:9:1131:G:N2	51:9:1132:C:C2	2.85	0.44
51:9:1268:C:O2'	51:9:1269:G:P	2.75	0.44
82:ee:8:ARG:O	82:ee:9:VAL:C	2.60	0.44
3:C:210:ILE:N	3:C:210:ILE:HD12	2.33	0.44
8:H:137:SER:HB3	8:H:145:VAL:HG23	1.99	0.44
13:N:178:HIS:HA	13:N:181:HIS:CE1	2.53	0.44
23:X:76:ILE:HG21	23:X:112:ALA:HB2	1.99	0.44
48:5:158:A:C4	48:5:277:G:C6	3.05	0.44
48:5:1171:G:C2	48:5:1172:C:C2	3.05	0.44
48:5:1245:C:C5	48:5:1269:G:C6	3.06	0.44
48:5:1280:C:N3	48:5:1282:G:C6	2.84	0.44
48:5:2089:G:HO2'	48:5:2090:U:P	2.39	0.44
48:5:4075:U:H4'	48:5:4076:G:OP1	2.17	0.44
48:5:4147:G:C6	48:5:4148:C:C4	3.05	0.44
48:5:4495:G:C2	48:5:4506:C:C2	3.06	0.44
51:9:1045:U:H2'	51:9:1046:U:O4'	2.17	0.44
51:9:1145:A:C6	51:9:1146:C:H1'	2.52	0.44
51:9:1717:C:C2	51:9:1817:G:N2	2.86	0.44
54:CC:191:VAL:CA	54:CC:228:SER:CB	2.81	0.44
86:ii:157:LEU:HD22	86:ii:264:PHE:CD2	2.51	0.44
3:C:158:VAL:HG12	3:C:217:ILE:HD12	1.98	0.44
12:M:132:ARG:O	12:M:135:LEU:HB3	2.17	0.44
46:2:65:G:N2	46:2:66:C:C2	2.86	0.44
48:5:654:C:O2	48:5:654:C:H2'	2.17	0.44
48:5:1466:G:N2	48:5:1467:C:C2	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1835:G:O2'	48:5:1836:G:OP2	2.33	0.44
48:5:2315:G:C2	48:5:2325:C:O2	2.71	0.44
48:5:3723:A:C2	48:5:3724:A:C5	3.05	0.44
48:5:3941:G:H2'	48:5:3942:A:O4'	2.16	0.44
48:5:4584:A:H2'	48:5:4585:U:O4'	2.18	0.44
51:9:167:G:N1	51:9:168:C:C4	2.86	0.44
51:9:673:G:C6	51:9:674:C:C4	3.04	0.44
51:9:797:C:O2	51:9:798:G:O2'	2.34	0.44
51:9:1526:G:N1	51:9:1527:C:C4	2.85	0.44
51:9:1739:C:C2	51:9:1796:G:C2	3.05	0.44
51:9:1749:G:C2	51:9:1750:C:C2	3.05	0.44
8:H:39:ASN:O	8:H:40:HIS:HB3	2.17	0.44
11:L:58:ILE:HG23	11:L:70:VAL:CG1	2.47	0.44
30:e:36:ARG:NH1	48:5:2322:G:OP1	2.49	0.44
47:3:69:G:C2	47:3:70:G:C6	3.05	0.44
48:5:211:G:H4'	48:5:234:G:C8	2.52	0.44
48:5:1268:G:O4'	48:5:2111:G:C5	2.71	0.44
48:5:1383:G:C6	48:5:1384:C:C4	3.05	0.44
48:5:1835:G:H4'	48:5:1836:G:O5'	2.18	0.44
48:5:2664:G:N2	48:5:2671:C:C2	2.86	0.44
48:5:4212:A:C2	48:5:4218:U:C5	3.06	0.44
48:5:4303:C:O2	48:5:4303:C:O5'	2.34	0.44
51:9:123:G:N2	51:9:342:C:C2	2.86	0.44
51:9:303:C:H2'	51:9:304:C:O4'	2.17	0.44
51:9:1267:C:C2	51:9:1516:G:N2	2.86	0.44
51:9:1416:C:O3'	51:9:1417:C:O4'	2.36	0.44
51:9:1448:A:HO2'	51:9:1449:G:C4'	2.30	0.44
51:9:1649:U:C4	51:9:1675:A:C2	3.06	0.44
61:JJ:144:ILE:HA	61:JJ:145:PRO:HD3	1.89	0.44
63:LL:55:TYR:CE2	63:LL:115:PRO:HG2	2.52	0.44
66:OO:116:LEU:HD22	78:aa:53:ILE:HD11	1.99	0.44
5:E:111:TYR:CE2	42:r:119:ARG:HD3	2.53	0.44
7:G:147:VAL:HG13	7:G:179:VAL:HG21	2.00	0.44
11:L:9:ILE:O	11:L:9:ILE:HG23	2.18	0.44
11:L:29:PRO:CB	48:5:1371:A:H2'	2.47	0.44
17:R:99:MET:CE	17:R:128:LYS:HA	2.47	0.44
28:c:84:ALA:C	65:NN:151:ALA:C	2.85	0.44
42:r:64:MET:HE1	42:r:102:TYR:CD2	2.53	0.44
48:5:744:G:H2'	48:5:745:G:C8	2.52	0.44
48:5:939:G:H2'	48:5:939:G:N3	2.33	0.44
48:5:1268:G:C4	48:5:2111:G:N2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1308:C:H2'	48:5:1309:C:C6	2.53	0.44
48:5:2294:G:N2	48:5:2295:C:C2	2.85	0.44
48:5:2457:G:C2	48:5:2458:C:C2	3.06	0.44
48:5:2468:U:C4	48:5:2473:A:N6	2.80	0.44
48:5:2612:G:C2	48:5:2613:C:C2	3.05	0.44
48:5:2779:C:O2'	50:8:112:G:OP1	2.25	0.44
48:5:2889:G:C2	48:5:2890:C:C2	3.05	0.44
48:5:2889:G:C6	48:5:2890:C:C4	3.05	0.44
48:5:4583:C:C2	48:5:4718:G:C2	3.04	0.44
48:5:4717:A:H2'	48:5:4718:G:O4'	2.17	0.44
48:5:4876:U:O2	48:5:4876:U:O4'	2.35	0.44
48:5:4966:A:H2'	48:5:4967:A:O4'	2.17	0.44
51:9:1447:G:O6	51:9:1448:A:N6	2.51	0.44
53:BB:212:VAL:HG23	53:BB:212:VAL:O	2.15	0.44
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.99	0.44
82:ee:37:GLN:O	82:ee:41:ARG:HG2	2.17	0.44
86:ii:382:TYR:O	86:ii:385:PHE:O	2.35	0.44
3:C:161:TYR:HD1	3:C:166:GLU:CB	2.29	0.44
7:G:86:VAL:CG2	7:G:185:LYS:HE3	2.26	0.44
17:R:92:LYS:NZ	48:5:2606:G:O3'	2.50	0.44
29:d:33:ILE:HD11	29:d:41:ARG:HB3	1.99	0.44
48:5:1721:G:C6	48:5:1722:C:C4	3.06	0.44
48:5:1855:G:C2	48:5:1856:C:C2	3.05	0.44
48:5:2021:G:C6	48:5:2022:C:C4	3.06	0.44
48:5:2481:G:C6	48:5:2482:C:C4	3.05	0.44
48:5:3680:U:O2	48:5:3680:U:H2'	2.17	0.44
48:5:3724:A:C6	48:5:3725:G:C5	3.06	0.44
48:5:4232:U:H1'	48:5:4233:A:OP2	2.18	0.44
48:5:4240:G:C6	48:5:4241:C:C4	3.05	0.44
48:5:4416:G:N1	48:5:4417:C:C4	2.86	0.44
48:5:4462:C:C2	48:5:4515:G:N2	2.86	0.44
48:5:4890:G:C2	48:5:4930:C:C2	3.05	0.44
50:8:134:G:C6	50:8:135:C:C4	3.06	0.44
51:9:1229:G:H2'	51:9:1230:C:O4'	2.17	0.44
51:9:1466:G:C6	51:9:1467:C:N4	2.86	0.44
51:9:1476:A:H3'	51:9:1477:U:H5''	2.00	0.44
55:DD:175:VAL:HG13	55:DD:182:LEU:CB	2.47	0.44
61:JJ:35:TYR:CD1	61:JJ:106:LEU:HD23	2.53	0.44
63:LL:55:TYR:CD2	63:LL:115:PRO:HG2	2.52	0.44
9:I:176:PHE:CE2	9:I:190:LEU:HD21	2.53	0.44
18:S:83:ARG:HH21	18:S:83:ARG:CG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:99:ILE:HG21	24:Y:104:VAL:HG23	1.99	0.44
34:i:90:LEU:O	34:i:92:SER:C	2.61	0.44
37:l:38:ASN:O	48:5:362:A:N1	2.51	0.44
44:t:143:VAL:O	44:t:145:GLY:N	2.50	0.44
48:5:223:G:H4'	48:5:225:G:C8	2.52	0.44
48:5:254:G:C2	48:5:255:C:C2	3.06	0.44
48:5:642:G:C2	48:5:643:C:C4	3.05	0.44
48:5:1236:C:O2'	48:5:1237:C:O5'	2.24	0.44
48:5:1358:G:H2'	48:5:1359:G:C8	2.53	0.44
48:5:1404:G:C2	48:5:1405:C:C2	3.06	0.44
48:5:1431:C:C2	48:5:1454:G:C2	3.05	0.44
48:5:1667:G:H5'	48:5:1688:G:OP1	2.18	0.44
48:5:1826:G:C6	48:5:1827:C:C4	3.05	0.44
48:5:2021:G:C2	48:5:2022:C:C2	3.06	0.44
48:5:2594:C:O2	48:5:2752:G:C2	2.71	0.44
48:5:4250:G:C2	48:5:4259:C:C2	3.05	0.44
48:5:4433:G:N2	48:5:4434:C:C2	2.86	0.44
48:5:4898:G:N2	48:5:4923:C:C2	2.86	0.44
50:8:139:G:C2	50:8:140:C:C2	3.05	0.44
51:9:190:G:O2'	51:9:209:A:N6	2.50	0.44
51:9:841:G:C2	51:9:842:C:C2	3.05	0.44
51:9:1267:C:C2	51:9:1516:G:C2	3.05	0.44
51:9:1563:G:C2	51:9:1564:C:C2	3.06	0.44
51:9:1655:C:OP1	71:TT:92:PHE:N	2.46	0.44
51:9:1679:A:H3'	57:FF:60:ARG:HD2	2.00	0.44
51:9:1749:G:C6	51:9:1750:C:C4	3.06	0.44
51:9:1777:G:C6	51:9:1778:C:C4	3.05	0.44
52:AA:87:VAL:HG12	52:AA:175:TRP:CZ2	2.52	0.44
52:AA:155:ARG:NE	73:VV:61:ARG:O	2.48	0.44
62:KK:15:LEU:O	62:KK:18:GLU:O	2.36	0.44
81:dd:6:LEU:HA	81:dd:9:SER:HB2	1.99	0.44
4:D:282:GLN:OE1	48:5:1185:G:N2	2.51	0.44
6:F:225:LYS:HE3	48:5:1907:A:H4'	2.00	0.44
7:G:58:PRO:HD3	23:X:46:PHE:HD2	1.83	0.44
12:M:62:LEU:HD23	12:M:82:ILE:HG13	1.99	0.44
17:R:176:ARG:HH21	17:R:176:ARG:CB	2.23	0.44
36:k:40:ARG:HE	36:k:41:TYR:HE1	1.66	0.44
40:o:104:ILE:HG21	46:2:56:C:N4	2.33	0.44
42:r:106:LEU:O	42:r:107:ARG:C	2.60	0.44
48:5:80:C:C2	48:5:104:G:C2	3.05	0.44
48:5:174:C:C2	48:5:263:G:C2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:688:U:H2'	48:5:689:U:C6	2.53	0.44
48:5:751:G:N2	48:5:912:G:C4	2.85	0.44
48:5:1270:A:C2'	48:5:1271:G:O5'	2.66	0.44
48:5:1691:G:C6	48:5:1692:C:C4	3.06	0.44
48:5:2542:G:N2	48:5:2775:C:C2	2.86	0.44
48:5:2567:G:C6	48:5:2568:C:C4	3.06	0.44
48:5:3597:G:C6	48:5:3598:C:C4	3.06	0.44
48:5:4661:G:C6	48:5:4662:C:C4	3.04	0.44
48:5:4666:G:C2	48:5:4667:C:C2	3.05	0.44
50:8:10:G:C2	50:8:11:C:C2	3.06	0.44
51:9:200:G:C2	51:9:201:C:C4	3.06	0.44
51:9:752:G:N1	51:9:790:C:C4	2.85	0.44
51:9:1102:G:C2	51:9:1103:C:C5	3.06	0.44
51:9:1541:G:C6	51:9:1542:C:C4	3.06	0.44
51:9:1669:G:C2	51:9:1670:C:C2	3.05	0.44
51:9:1741:U:H2'	51:9:1742:C:O4'	2.17	0.44
51:9:1754:G:C2	51:9:1755:C:C2	3.05	0.44
57:FF:99:ILE:HG23	77:ZZ:67:LEU:HD21	2.00	0.44
86:ii:157:LEU:HD23	86:ii:158:PHE:N	2.32	0.44
87:jj:98:PRO:N	87:jj:299:VAL:HG11	2.32	0.44
5:E:132:HIS:CE1	48:5:711:A:H1'	2.52	0.44
5:E:134:ARG:NH1	5:E:165:SER:O	2.51	0.44
11:L:71:ARG:NH2	48:5:74:G:O3'	2.51	0.44
35:j:50:SER:HB2	35:j:53:ALA:HB3	2.00	0.44
43:s:57:LYS:CE	48:5:1961:G:P	3.06	0.44
47:3:4:C:O2'	47:3:5:G:O4'	2.35	0.44
48:5:205:C:C4	48:5:211:G:C6	3.06	0.44
48:5:956:A:H3'	48:5:957:G:C8	2.52	0.44
48:5:1048:G:C6	48:5:1049:C:C4	3.06	0.44
48:5:1213:G:C6	48:5:1215:C:C4	3.06	0.44
48:5:1947:U:O2	48:5:1947:U:H2'	2.18	0.44
48:5:2122:G:O2'	48:5:2123:C:P	2.76	0.44
48:5:3752:C:H2'	48:5:3777:G:C8	2.53	0.44
48:5:4094:G:H2'	48:5:4095:G:C1'	2.48	0.44
48:5:4139:G:C6	48:5:4140:C:C4	3.06	0.44
51:9:187:G:C2	51:9:188:C:C2	3.05	0.44
51:9:323:C:H3'	51:9:324:C:C5'	2.48	0.44
51:9:636:C:C4	51:9:637:U:C4	3.06	0.44
51:9:927:C:O2	79:bb:51:GLN:NE2	2.51	0.44
51:9:1121:G:C6	51:9:1122:A:C5	3.05	0.44
51:9:1228:A:O2'	51:9:1634:A:N3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1308:U:O3'	83:ff:128:ALA:CB	2.64	0.44
51:9:1616:U:H2'	51:9:1617:G:O4'	2.18	0.44
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.99	0.44
86:ii:75:ILE:HA	86:ii:78:VAL:HG12	2.00	0.44
5:E:126:ARG:NH1	48:5:1285:U:P	2.89	0.43
12:M:126:GLU:CG	14:O:181:ALA:CB	2.92	0.43
31:f:7:CYS:HB2	31:f:103:VAL:HG22	2.00	0.43
42:r:33:LYS:HD2	42:r:40:TYR:CE2	2.53	0.43
42:r:85:ASN:HD22	48:5:689:U:H4'	1.82	0.43
48:5:113:A:H2'	48:5:114:G:O4'	2.18	0.43
48:5:933:G:C2	48:5:939:G:C2	3.06	0.43
48:5:1048:G:C2	48:5:1049:C:C2	3.05	0.43
48:5:1064:G:C2	48:5:1065:G:C4	3.06	0.43
48:5:1205:G:C2	48:5:1206:C:C2	3.06	0.43
48:5:1424:G:H2'	48:5:1425:G:O4'	2.18	0.43
48:5:2270:G:C2	48:5:2271:C:C2	3.06	0.43
48:5:2439:G:H2'	48:5:2439:G:N3	2.32	0.43
48:5:4495:G:N2	48:5:4506:C:C2	2.86	0.43
48:5:4919:G:N2	48:5:4920:C:C2	2.86	0.43
48:5:4966:A:C2	48:5:4967:A:C2	3.06	0.43
51:9:145:G:N1	51:9:146:G:C6	2.86	0.43
51:9:1258:A:C2	51:9:1664:A:C8	3.06	0.43
51:9:1476:A:C8	69:RR:3:ARG:HB2	2.53	0.43
51:9:1777:G:C2	51:9:1778:C:C2	3.05	0.43
52:AA:43:SER:O	52:AA:45:GLY:N	2.51	0.43
53:BB:190:PRO:O	53:BB:192:SER:N	2.50	0.43
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.81	0.43
71:TT:56:ARG:HG2	71:TT:56:ARG:HH11	1.83	0.43
3:C:158:VAL:HA	3:C:161:TYR:HD2	1.82	0.43
4:D:111:ASN:ND2	4:D:111:ASN:C	2.76	0.43
4:D:200:MET:HE1	4:D:241:LYS:H	1.82	0.43
6:F:72:ARG:NH1	48:5:1209:U:O2'	2.51	0.43
8:H:44:GLU:HB3	8:H:58:ASP:HB2	2.00	0.43
9:I:200:ILE:HD13	9:I:212:LEU:HD21	2.00	0.43
11:L:172:GLU:OE1	34:i:3:LEU:CG	2.65	0.43
25:Z:36:ARG:HG2	25:Z:38:TYR:CE1	2.53	0.43
48:5:1721:G:C2	48:5:1722:C:C2	3.06	0.43
48:5:1957:U:H3'	48:5:1957:U:OP2	2.18	0.43
48:5:2614:C:O2	48:5:2726:G:C2	2.71	0.43
48:5:2847:G:N2	48:5:3842:C:C2	2.87	0.43
48:5:4423:U:O2	48:5:4423:U:O4'	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:5029:C:H2'	48:5:5030:U:O4'	2.18	0.43
51:9:996:A:H2'	51:9:997:A:C8	2.53	0.43
51:9:1675:A:N3	51:9:1675:A:O4'	2.51	0.43
52:AA:60:LEU:HD13	52:AA:159:ILE:HD11	2.00	0.43
56:EE:48:LEU:HD21	56:EE:70:ILE:HD11	2.00	0.43
57:FF:71:ARG:NH1	57:FF:148:ASN:OD1	2.50	0.43
16:Q:148:VAL:HG13	16:Q:152:PHE:CZ	2.53	0.43
42:r:46:ARG:NH1	48:5:666:G:N7	2.67	0.43
48:5:82:U:H2'	48:5:83:C:O4'	2.18	0.43
48:5:665:C:O2	48:5:665:C:C2'	2.66	0.43
48:5:917:A:C2	48:5:918:G:N2	2.86	0.43
48:5:1237:C:O2	48:5:1237:C:O4'	2.34	0.43
48:5:1277:G:N1	48:5:1278:C:C4	2.86	0.43
48:5:1279:A:H3'	48:5:1280:C:C6	2.54	0.43
48:5:1280:C:C2	48:5:1282:G:C4	3.07	0.43
48:5:1449:C:H2'	48:5:1450:C:O4'	2.18	0.43
48:5:1963:C:N3	48:5:4694:G:C6	2.74	0.43
48:5:2609:G:N1	48:5:2731:C:C2	2.87	0.43
48:5:2862:G:N3	48:5:3624:A:H2'	2.33	0.43
51:9:922:A:OP1	74:WW:28:ARG:NH2	2.52	0.43
51:9:1454:A:OP1	69:RR:49:LYS:CD	2.65	0.43
51:9:1537:A:N1	51:9:1596:U:C4	2.86	0.43
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.54	0.43
10:J:141:ILE:HD11	49:7:55:A:C2	2.53	0.43
29:d:57:MET:O	29:d:59:THR:N	2.52	0.43
48:5:258:G:C2	48:5:259:C:C2	3.06	0.43
48:5:1755:C:C3'	48:5:1756:U:H5''	2.49	0.43
48:5:2481:G:C2	48:5:2482:C:C2	3.07	0.43
48:5:2559:G:C2	48:5:2560:C:C2	3.06	0.43
48:5:3905:A:C2	48:5:4449:A:C6	3.06	0.43
48:5:4320:G:H2'	48:5:4321:U:O4'	2.18	0.43
48:5:4326:G:C6	48:5:4327:C:C4	3.06	0.43
48:5:4644:G:C6	48:5:4645:C:C4	3.07	0.43
48:5:5003:U:H2'	48:5:5004:C:O4'	2.17	0.43
48:5:5032:C:N4	48:5:5033:G:C6	2.87	0.43
51:9:496:C:OP2	56:EE:49:ARG:NH1	2.52	0.43
51:9:1333:U:H4'	55:DD:147:ALA:HB2	1.99	0.43
52:AA:69:GLU:HB3	54:CC:270:THR:HG21	2.00	0.43
53:BB:172:MET:HE3	53:BB:212:VAL:HG12	2.01	0.43
54:CC:64:THR:OG1	54:CC:90:GLU:CG	2.66	0.43
67:PP:53:GLN:HE22	67:PP:83:MET:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:11:VAL:HG23	87:jj:90:ASN:HB3	2.00	0.43
3:C:108:TRP:HB2	13:N:200:LEU:HD13	2.00	0.43
4:D:3:PHE:HB2	48:5:1755:C:C6	2.53	0.43
9:I:45:GLU:O	9:I:46:PHE:CG	2.72	0.43
26:a:79:TRP:CZ2	26:a:122:VAL:HG13	2.53	0.43
34:i:92:SER:N	34:i:94:LEU:H	2.12	0.43
48:5:322:C:O2	48:5:4356:G:C2	2.71	0.43
48:5:1357:C:O2'	48:5:1358:G:O4'	2.32	0.43
48:5:1383:G:C2	48:5:1384:C:C2	3.07	0.43
48:5:1422:G:C2	48:5:1464:C:C2	3.07	0.43
48:5:1557:C:C2	48:5:1571:G:N2	2.86	0.43
48:5:1563:A:N7	51:9:678:U:O4'	2.51	0.43
48:5:1563:A:N7	51:9:678:U:C4'	2.81	0.43
48:5:2458:C:H2'	48:5:2459:G:O4'	2.19	0.43
48:5:2698:G:C2	48:5:2699:C:C2	3.07	0.43
50:8:86:U:O2'	50:8:87:G:H2'	2.18	0.43
50:8:115:G:C2	50:8:116:C:C2	3.07	0.43
51:9:1035:A:H2'	51:9:1036:A:O4'	2.18	0.43
51:9:1612:G:C2	51:9:1628:C:C2	3.07	0.43
54:CC:129:ALA:HB2	54:CC:213:LEU:HD11	2.00	0.43
69:RR:33:ARG:NH1	84:gg:107:ASP:OD2	2.52	0.43
87:jj:595:PHE:C	87:jj:596:PHE:HD2	2.27	0.43
15:P:102:ALA:CB	15:P:112:LEU:HD11	2.49	0.43
28:c:84:ALA:O	65:NN:151:ALA:HB1	2.18	0.43
48:5:192:G:C2	48:5:250:C:C2	3.07	0.43
48:5:423:G:H2'	48:5:424:U:O4'	2.18	0.43
48:5:1265:G:OP1	48:5:2115:G:N1	2.52	0.43
48:5:1271:G:H3'	48:5:1272:C:H5'	2.00	0.43
48:5:1278:C:C2	48:5:1279:A:O2'	2.61	0.43
48:5:1431:C:C2	48:5:1454:G:N2	2.86	0.43
48:5:1757:U:C2	48:5:1758:G:C8	3.06	0.43
48:5:1874:A:C5'	48:5:4218:U:O2	2.66	0.43
48:5:2457:G:C6	48:5:2458:C:C4	3.07	0.43
48:5:2715:G:C6	48:5:2716:C:C4	3.07	0.43
48:5:3670:C:O2'	48:5:3671:G:O4'	2.36	0.43
48:5:4216:G:C2'	48:5:4217:G:H5'	2.48	0.43
48:5:4525:C:H2'	48:5:4526:U:O4'	2.19	0.43
51:9:5:U:C2	51:9:20:G:N2	2.86	0.43
51:9:194:C:C2	51:9:206:G:N2	2.87	0.43
51:9:378:U:H2'	51:9:379:C:O4'	2.19	0.43
51:9:908:A:C2'	51:9:909:G:O5'	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:GG:57:ASP:HB2	58:GG:98:ARG:HD2	2.01	0.43
60:II:178:ARG:O	60:II:179:PRO:C	2.61	0.43
86:ii:374:LEU:O	86:ii:377:TRP:N	2.52	0.43
87:jj:167:ILE:HD12	87:jj:235:ALA:CB	2.48	0.43
8:H:172:ILE:HD12	38:m:90:ASN:HB3	1.99	0.43
24:Y:50:ARG:NH2	50:8:83:C:O2	2.51	0.43
25:Z:73:LYS:HG2	25:Z:75:TYR:CZ	2.53	0.43
35:j:80:GLU:O	35:j:82:THR:HG23	2.19	0.43
47:3:72:C:C6	47:3:72:C:H5''	2.54	0.43
48:5:674:G:C6	48:5:675:C:C4	3.07	0.43
48:5:975:C:H2'	48:5:976:G:C1'	2.49	0.43
48:5:1379:C:O2	48:5:1379:C:O4'	2.37	0.43
48:5:1549:G:N2	48:5:1580:C:C2	2.87	0.43
48:5:2690:C:H2'	48:5:2691:U:O4'	2.19	0.43
48:5:3870:C:C2	48:5:3886:G:N2	2.87	0.43
48:5:4470:G:N2	48:5:4486:C:C2	2.87	0.43
50:8:2:G:H2'	50:8:2:G:N3	2.33	0.43
51:9:62:G:H1'	51:9:172:U:O2	2.18	0.43
51:9:113:G:C2	51:9:293:C:C2	3.06	0.43
51:9:909:G:H2'	51:9:910:G:C8	2.54	0.43
51:9:1233:G:C6	51:9:1234:C:C4	3.06	0.43
51:9:1308:U:N3	51:9:1309:C:N1	2.67	0.43
51:9:1834:A:C2	51:9:1836:G:C4	3.06	0.43
53:BB:139:CYS:N	53:BB:172:MET:HE1	2.34	0.43
54:CC:110:MET:HE2	54:CC:125:LYS:HD3	2.00	0.43
57:FF:102:LEU:HD11	77:ZZ:100:VAL:HG21	2.00	0.43
58:GG:7:PHE:CD2	58:GG:10:THR:HG23	2.53	0.43
7:G:194:VAL:HG21	7:G:196:ARG:NH1	2.33	0.43
8:H:95:VAL:CG1	38:m:78:ILE:HD11	2.49	0.43
14:O:12:ARG:O	18:S:171:ARG:NH2	2.52	0.43
26:a:98:ALA:HB2	26:a:121:PRO:HB2	2.00	0.43
43:s:34:ASN:OD1	48:5:1969:G:OP1	2.37	0.43
44:t:30:PRO:O	44:t:33:GLY:N	2.49	0.43
47:3:8:U:H5	47:3:14:A:N7	2.16	0.43
48:5:52:G:N1	48:5:53:C:C4	2.87	0.43
48:5:698:G:N1	48:5:699:C:C4	2.87	0.43
48:5:1075:G:C6	48:5:1076:C:C4	3.07	0.43
48:5:1436:C:O5'	48:5:2119:C:N4	2.52	0.43
48:5:1723:A:N1	48:5:1838:A:N1	2.66	0.43
48:5:2606:G:C6	48:5:2607:C:C4	3.07	0.43
48:5:5017:G:C6	48:5:5018:C:C4	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1056:U:O2	51:9:1063:C:N4	2.52	0.43
51:9:1134:G:N2	51:9:1135:C:C2	2.87	0.43
51:9:1241:A:C2	51:9:1517:G:O4'	2.72	0.43
51:9:1589:A:N3	51:9:1653:U:O2'	2.50	0.43
74:WW:30:CYS:SG	74:WW:31:SER:N	2.91	0.43
2:B:43:LEU:HG	2:B:183:ILE:HG21	2.01	0.43
8:H:59:LYS:HB2	8:H:70:VAL:HG22	2.01	0.43
10:J:119:TYR:HB3	70:SS:12:ILE:HG21	2.01	0.43
25:Z:51:ARG:HB2	25:Z:65:ARG:HD2	2.01	0.43
26:a:146:LEU:HD13	34:i:7:MET:HG2	2.00	0.43
27:b:8:THR:OG1	27:b:9:THR:N	2.52	0.43
29:d:28:ASN:C	29:d:28:ASN:OD1	2.60	0.43
35:j:81:GLY:HA3	48:5:134:G:C5	2.54	0.43
46:2:7:G:C2	46:2:49:C:C2	3.07	0.43
48:5:1239:C:O2'	48:5:1240:G:P	2.76	0.43
48:5:4075:U:HO2'	48:5:4076:G:P	2.42	0.43
48:5:4629:U:H2'	48:5:4630:G:O4'	2.18	0.43
48:5:4901:G:N1	48:5:4921:C:C4	2.87	0.43
50:8:142:U:H2'	50:8:143:G:O4'	2.19	0.43
51:9:910:G:C6	51:9:911:C:C4	3.07	0.43
51:9:1105:G:C2	51:9:1128:C:C2	3.07	0.43
51:9:1137:U:HO2'	52:AA:155:ARG:HH22	1.65	0.43
51:9:1650:A:C6	51:9:1675:A:C2	3.07	0.43
51:9:1753:C:C2	51:9:1780:G:C2	3.07	0.43
51:9:1843:G:H2'	51:9:1844:U:O4'	2.19	0.43
2:B:241:PRO:O	2:B:244:THR:OG1	2.36	0.43
5:E:59:TYR:CE2	5:E:64:LEU:CD1	3.01	0.43
16:Q:17:GLU:HB2	16:Q:18:PRO:HD2	2.00	0.43
29:d:46:LEU:HD12	29:d:72:VAL:HG11	2.01	0.43
32:g:69:LYS:N	48:5:2769:U:OP1	2.50	0.43
47:3:4:C:N3	47:3:5:G:N7	2.67	0.43
48:5:35:U:O2'	48:5:1525:A:N1	2.50	0.43
48:5:674:G:C2	48:5:675:C:C2	3.07	0.43
48:5:920:C:H2'	48:5:921:C:O4'	2.19	0.43
48:5:967:C:OP1	48:5:2254:G:N1	2.52	0.43
48:5:1085:C:C2	48:5:1213:G:N1	2.86	0.43
48:5:1322:A:N6	48:5:4446:U:OP1	2.52	0.43
48:5:1739:G:C6	48:5:1740:C:N4	2.87	0.43
48:5:3590:G:C6	48:5:3591:C:C4	3.07	0.43
48:5:3938:G:O6	48:5:4172:A:N1	2.52	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)
51:9:452:G:N2	51:9:453:C:C2	2.87	0.43
51:9:1315:U:C4	51:9:1316:C:C4	3.07	0.43
51:9:1481:G:C2	51:9:1482:C:C2	3.07	0.43
51:9:1771:G:C6	51:9:1772:C:N4	2.87	0.43
51:9:1784:G:N1	51:9:1785:C:C4	2.87	0.43
59:HH:122:LEU:C	59:HH:122:LEU:HD13	2.44	0.43
66:OO:64:ALA:O	66:OO:66:ARG:N	2.52	0.43
86:ii:329:MET:HG2	86:ii:373:PRO:HA	2.01	0.43
8:H:117:PHE:CZ	8:H:118:LEU:HD23	2.53	0.42
9:I:153:ARG:HA	9:I:165:ILE:HD11	2.00	0.42
11:L:65:ARG:HG2	11:L:66:TYR:CD2	2.54	0.42
14:O:196:LEU:HB3	14:O:202:LEU:HD22	2.01	0.42
17:R:178:GLN:N	17:R:178:GLN:CD	2.73	0.42
18:S:96:GLU:OE2	18:S:138:ARG:N	2.50	0.42
30:e:104:SER:HB3	48:5:2303:C:OP1	2.19	0.42
31:f:79:GLY:O	31:f:81:SER:N	2.52	0.42
35:j:72:ARG:NH2	50:8:94:G:OP2	2.51	0.42
42:r:31:ASN:C	42:r:31:ASN:ND2	2.76	0.42
47:3:4:C:O2	47:3:5:G:C8	2.70	0.42
48:5:914:U:H2'	48:5:915:A:O4'	2.19	0.42
48:5:1277:G:C2	48:5:1278:C:C2	3.07	0.42
48:5:1358:G:H2'	48:5:1359:G:H8	1.83	0.42
48:5:1379:C:H4'	48:5:1380:G:C8	2.53	0.42
48:5:1466:G:C6	48:5:1467:C:C4	3.07	0.42
48:5:1846:G:C2	48:5:1847:C:C2	3.07	0.42
48:5:1968:G:N1	48:5:2018:C:N4	2.50	0.42
48:5:2034:G:C6	48:5:2035:C:C4	3.07	0.42
48:5:2703:G:C2	48:5:2704:C:C2	3.07	0.42
48:5:4147:G:C2	48:5:4148:C:C2	3.07	0.42
48:5:4737:G:C6	48:5:4738:C:C4	3.06	0.42
51:9:1335:G:C6	51:9:1336:C:C4	3.06	0.42
51:9:1395:C:O2'	51:9:1396:A:OP1	2.34	0.42
51:9:1466:G:C2	51:9:1467:C:C4	3.07	0.42
51:9:1568:C:H2'	51:9:1569:A:C8	2.54	0.42
51:9:1771:G:C2	51:9:1772:C:C4	3.08	0.42
57:FF:127:ARG:HG3	57:FF:127:ARG:HH11	1.84	0.42
70:SS:81:ASP:N	70:SS:81:ASP:OD1	2.52	0.42
71:TT:56:ARG:HD2	71:TT:79:TYR:CE2	2.54	0.42
74:WW:42:MET:HE2	74:WW:49:GLU:HA	2.00	0.42
75:XX:67:ARG:CG	75:XX:115:ILE:HD12	2.49	0.42
75:XX:84:PHE:HB2	75:XX:118:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:112:TYR:CE1	42:r:108:MET:HE1	2.54	0.42
41:p:50:ARG:HD2	41:p:54:ILE:HD11	2.01	0.42
48:5:1070:G:C6	48:5:1071:C:N4	2.87	0.42
48:5:1808:C:C2	48:5:1831:G:C2	3.07	0.42
48:5:1826:G:C2	48:5:1827:C:C2	3.07	0.42
48:5:2468:U:O4	48:5:2473:A:C2	2.59	0.42
48:5:2569:G:H2'	48:5:2570:U:O4'	2.18	0.42
48:5:4932:U:H2'	48:5:4933:C:O4'	2.18	0.42
49:7:25:G:C6	49:7:26:C:C4	3.08	0.42
49:7:110:G:C2	49:7:111:C:C2	3.07	0.42
50:8:10:G:C6	50:8:11:C:C4	3.07	0.42
51:9:358:C:C2	51:9:405:G:N2	2.87	0.42
51:9:398:A:C8	51:9:398:A:H5'	2.54	0.42
51:9:1459:G:C2	51:9:1460:C:C2	3.06	0.42
51:9:1500:G:H2'	51:9:1501:C:O4'	2.19	0.42
53:BB:136:ARG:HH21	53:BB:136:ARG:HG3	1.84	0.42
57:FF:194:ASP:CG	57:FF:198:ARG:HH11	2.26	0.42
66:OO:67:ASP:HB2	66:OO:70:SER:HB3	2.01	0.42
75:XX:70:VAL:HG21	75:XX:94:ILE:HG21	2.01	0.42
8:H:98:HIS:ND1	87:jj:440:GLN:CG	2.82	0.42
31:f:50:VAL:HG21	31:f:102:ARG:HD2	2.00	0.42
42:r:16:PHE:CE2	42:r:43:LEU:HD11	2.54	0.42
47:3:67:U:H2'	47:3:68:C:C6	2.54	0.42
48:5:119:G:H3'	48:5:120:A:H5'	2.01	0.42
48:5:197:A:N3	48:5:222:C:O2'	2.50	0.42
48:5:1275:G:N2	48:5:1276:C:C2	2.88	0.42
48:5:2473:A:C6	48:5:2506:G:N7	2.87	0.42
48:5:3590:G:N1	48:5:3591:C:C2	2.87	0.42
48:5:3753:G:O2'	48:5:3754:G:H5'	2.19	0.42
48:5:4291:G:H5''	48:5:4291:G:N3	2.34	0.42
51:9:164:A:H2'	51:9:165:G:C2	2.54	0.42
51:9:448:A:H5''	60:II:25:ARG:HA	2.00	0.42
51:9:1134:G:C2	51:9:1135:C:C2	3.07	0.42
51:9:1298:G:O2'	51:9:1299:A:O4'	2.37	0.42
51:9:1452:A:C5'	69:RR:48:ASN:HD21	2.32	0.42
51:9:1571:G:C2	51:9:1572:C:C2	3.07	0.42
71:TT:28:LEU:O	71:TT:29:LYS:HB2	2.20	0.42
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.54	0.42
6:F:175:ALA:O	6:F:179:ARG:HB2	2.19	0.42
8:H:92:MET:SD	8:H:161:ILE:HD11	2.59	0.42
32:g:59:VAL:HG21	32:g:63:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:179:G:C6	48:5:180:C:C4	3.06	0.42
48:5:517:C:C2	48:5:645:G:N2	2.87	0.42
48:5:1332:C:C2	48:5:2355:G:N2	2.87	0.42
48:5:1925:G:C6	48:5:1926:C:C4	3.08	0.42
48:5:2086:G:C6	48:5:2087:C:C4	3.08	0.42
48:5:2606:G:C2	48:5:2607:C:C2	3.07	0.42
48:5:2793:G:C6	48:5:2797:C:N4	2.88	0.42
48:5:4461:C:C2	48:5:4516:G:C2	3.07	0.42
50:8:31:G:C6	50:8:32:C:C4	3.08	0.42
51:9:614:C:C2	51:9:626:G:C2	3.07	0.42
51:9:666:U:C5	51:9:1150:A:C5	3.08	0.42
51:9:827:A:C5	51:9:828:G:C8	3.08	0.42
51:9:999:G:C6	51:9:1000:C:C4	3.07	0.42
51:9:1126:G:C2	51:9:1127:C:C2	3.07	0.42
51:9:1530:U:H2'	51:9:1531:A:O4'	2.19	0.42
71:TT:104:LEU:HD22	71:TT:121:ARG:HG2	2.00	0.42
75:XX:74:LEU:HD21	75:XX:81:ILE:HD12	2.00	0.42
79:bb:46:VAL:HG11	79:bb:64:CYS:SG	2.60	0.42
6:F:184:TYR:HB3	6:F:202:ARG:HG2	2.01	0.42
23:X:80:PRO:CD	33:h:33:VAL:HG22	2.49	0.42
25:Z:38:TYR:CE1	25:Z:76:ASN:OD1	2.73	0.42
48:5:28:C:C2	48:5:55:G:N2	2.88	0.42
48:5:93:G:H2'	48:5:94:A:C8	2.55	0.42
48:5:165:A:H3'	48:5:166:C:H6	1.83	0.42
48:5:247:G:C2	48:5:248:C:C2	3.07	0.42
48:5:469:C:H2'	48:5:470:A:O4'	2.20	0.42
48:5:1466:G:C2	48:5:1467:C:C2	3.08	0.42
48:5:1748:U:C2	48:5:1783:C:C2	3.08	0.42
48:5:1787:A:N3	48:5:4210:U:O2'	2.52	0.42
48:5:2256:C:H1'	48:5:2257:C:OP2	2.20	0.42
48:5:2391:G:N2	48:5:2392:C:C2	2.87	0.42
48:5:2424:G:O5'	48:5:2424:G:H8	2.02	0.42
48:5:3942:A:H2'	48:5:3943:A:O4'	2.19	0.42
48:5:4326:G:C2	48:5:4327:C:C2	3.08	0.42
50:8:31:G:C2	50:8:32:C:C2	3.08	0.42
51:9:211:G:C2	51:9:212:C:C2	3.08	0.42
51:9:668:A:N1	51:9:1143:A:C5	2.87	0.42
51:9:839:C:O2	51:9:839:C:C2'	2.66	0.42
51:9:1233:G:C2	51:9:1234:C:C2	3.08	0.42
51:9:1541:G:C2	51:9:1542:C:C2	3.07	0.42
54:CC:60:TRP:CE2	54:CC:62:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:GG:63:MET:HG3	58:GG:98:ARG:HD3	2.02	0.42
61:JJ:14:VAL:HG23	61:JJ:48:PHE:CD1	2.54	0.42
65:NN:62:GLN:HB2	65:NN:65:PHE:CD2	2.55	0.42
73:VV:20:SER:HB3	73:VV:59:ILE:HD11	2.01	0.42
75:XX:33:GLY:O	75:XX:35:ALA:N	2.52	0.42
13:N:48:ALA:HB1	13:N:53:TYR:HB3	2.01	0.42
17:R:11:ALA:HB1	17:R:50:ILE:HD13	2.02	0.42
17:R:97:ARG:NH2	48:5:2725:A:OP1	2.53	0.42
44:t:162:CYS:N	44:t:163:PRO:CD	2.83	0.42
48:5:973:G:C6	48:5:974:C:C4	3.08	0.42
48:5:1506:G:C2	48:5:1507:C:C2	3.08	0.42
48:5:1904:G:N2	48:5:2073:C:C2	2.88	0.42
48:5:2645:G:C6	48:5:2646:C:C4	3.07	0.42
48:5:2712:G:N1	48:5:2713:C:C4	2.87	0.42
48:5:2793:G:H5''	48:5:2794:C:H5''	2.00	0.42
48:5:4131:G:C2	48:5:4132:C:C2	3.08	0.42
48:5:4891:G:C2	48:5:4929:C:C2	3.08	0.42
49:7:86:G:C2	49:7:92:C:C2	3.08	0.42
51:9:1398:G:C2	51:9:1399:C:C2	3.08	0.42
56:EE:126:VAL:CG1	56:EE:160:ILE:HD11	2.49	0.42
59:HH:118:ARG:O	59:HH:119:SER:C	2.61	0.42
75:XX:9:THR:O	75:XX:11:ARG:N	2.52	0.42
2:B:340:THR:OG1	2:B:341:LYS:N	2.52	0.42
3:C:235:LEU:HD22	3:C:240:LEU:HD11	2.02	0.42
20:U:84:LYS:HB2	20:U:110:TYR:CE2	2.54	0.42
26:a:97:ALA:O	26:a:98:ALA:HB3	2.20	0.42
32:g:37:LYS:HB2	32:g:60:ARG:CD	2.50	0.42
42:r:64:MET:O	42:r:78:VAL:HG12	2.19	0.42
48:5:22:G:N1	50:8:35:C:C4	2.88	0.42
48:5:106:A:O2'	48:5:335:A:N3	2.46	0.42
48:5:258:G:C6	48:5:259:C:C4	3.07	0.42
48:5:1755:C:H3'	48:5:1756:U:H5''	2.02	0.42
48:5:2322:G:C6	48:5:2323:C:C4	3.08	0.42
48:5:2396:A:N6	48:5:2814:C:O2	2.53	0.42
48:5:2712:G:C2	48:5:2713:C:C2	3.08	0.42
48:5:4433:G:C2	48:5:4434:C:C2	3.07	0.42
48:5:4920:C:H2'	48:5:4921:C:C6	2.55	0.42
48:5:5026:U:O4	60:II:103:LEU:CD1	2.68	0.42
50:8:60:G:O6	50:8:96:C:O2'	2.30	0.42
51:9:95:G:C6	51:9:96:C:C4	3.08	0.42
51:9:947:G:C2	51:9:948:C:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1134:G:C6	51:9:1135:C:C4	3.06	0.42
51:9:1207:G:C6	51:9:1837:G:C6	3.08	0.42
51:9:1447:G:C6	51:9:1448:A:C6	3.07	0.42
51:9:1486:A:H2'	51:9:1487:A:O4'	2.19	0.42
51:9:1692:U:H2'	51:9:1693:G:C8	2.54	0.42
51:9:1834:A:N3	51:9:1834:A:C2'	2.82	0.42
52:AA:111:GLN:O	54:CC:63:VAL:HG11	2.20	0.42
52:AA:124:VAL:HG13	52:AA:130:ASP:HB2	2.01	0.42
60:II:6:ASP:OD1	60:II:6:ASP:N	2.53	0.42
71:TT:56:ARG:HD2	71:TT:79:TYR:CD2	2.54	0.42
2:B:116:ARG:HD2	2:B:122:TRP:CD2	2.55	0.42
3:C:195:LYS:NZ	50:8:21:C:OP1	2.52	0.42
10:J:33:LEU:CD2	10:J:70:VAL:HB	2.50	0.42
14:O:85:ARG:HG3	14:O:99:LEU:HD11	2.02	0.42
31:f:100:ARG:HG2	48:5:4752:U:OP2	2.19	0.42
38:m:115:CYS:SG	38:m:118:THR:OG1	2.76	0.42
40:o:38:LYS:HA	47:3:75:C:N4	2.34	0.42
47:3:72:C:H5''	47:3:72:C:H6	1.84	0.42
48:5:193:G:C2	48:5:249:C:C2	3.07	0.42
48:5:518:G:C6	48:5:519:C:C4	3.08	0.42
48:5:973:G:N2	48:5:974:C:C2	2.88	0.42
48:5:1205:G:N1	48:5:1206:C:C4	2.88	0.42
48:5:1662:C:H2'	48:5:1663:C:C6	2.55	0.42
48:5:2339:G:C6	48:5:2340:C:C4	3.08	0.42
48:5:2576:G:C6	48:5:2577:C:C4	3.07	0.42
48:5:3642:A:OP1	48:5:3644:U:OP1	2.38	0.42
48:5:3765:G:O2'	48:5:3766:A:C8	2.63	0.42
48:5:4207:C:C2	48:5:4226:G:N2	2.88	0.42
48:5:4455:G:C6	48:5:4456:C:C4	3.08	0.42
48:5:4901:G:C2	48:5:4921:C:C2	3.07	0.42
50:8:60:G:N2	50:8:64:U:C2	2.87	0.42
51:9:23:G:C2	51:9:24:C:C2	3.08	0.42
51:9:211:G:C6	51:9:212:C:N4	2.88	0.42
51:9:666:U:C2	51:9:667:U:C5	3.07	0.42
51:9:751:G:N1	51:9:792:C:C4	2.88	0.42
51:9:912:C:H3'	51:9:913:A:H5''	2.01	0.42
51:9:993:G:C2	51:9:994:C:C2	3.08	0.42
51:9:1568:C:OP1	71:TT:96:SER:OG	2.28	0.42
53:BB:39:PHE:CE2	53:BB:74:LEU:HD23	2.55	0.42
53:BB:48:LEU:C	53:BB:48:LEU:HD12	2.45	0.42
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:GG:2:LYS:HB3	58:GG:15:LEU:HD21	2.02	0.42
68:QQ:125:ARG:O	68:QQ:126:ARG:NH2	2.53	0.42
87:jj:382:GLY:CA	87:jj:539:PRO:HB3	2.50	0.42
2:B:14:LEU:HD22	2:B:264:PHE:CE2	2.54	0.42
2:B:41:VAL:HG21	2:B:196:TRP:CG	2.55	0.42
8:H:26:ILE:HB	8:H:35:ARG:HG2	2.02	0.42
11:L:170:THR:HG23	11:L:173:GLU:H	1.85	0.42
13:N:103:GLU:OE1	13:N:167:ALA:HB3	2.19	0.42
13:N:160:GLU:OE1	13:N:160:GLU:N	2.50	0.42
34:i:25:ARG:CG	34:i:25:ARG:HH11	2.33	0.42
36:k:40:ARG:NE	36:k:41:TYR:HE1	2.17	0.42
40:o:31:ASP:O	40:o:33:LEU:N	2.53	0.42
48:5:2:G:C6	48:5:3:C:C4	3.07	0.42
48:5:301:G:C2	48:5:302:C:C2	3.08	0.42
48:5:303:C:H2'	48:5:304:C:O4'	2.20	0.42
48:5:479:G:C2	48:5:480:C:C2	3.08	0.42
48:5:674:G:N2	48:5:675:C:C2	2.88	0.42
48:5:744:G:H2'	48:5:745:G:H8	1.85	0.42
48:5:751:G:N2	48:5:752:G:C5	2.88	0.42
48:5:1275:G:C2	48:5:1276:C:C2	3.07	0.42
48:5:1539:G:C2	48:5:1540:C:C2	3.08	0.42
48:5:2645:G:C2	48:5:2646:C:C2	3.08	0.42
48:5:3752:C:O2'	48:5:3753:G:P	2.78	0.42
48:5:3816:A:O2'	48:5:3819:G:N3	2.42	0.42
48:5:4724:A:C6	48:5:4725:C:C4	3.08	0.42
50:8:76:C:H2'	50:8:77:A:O4'	2.20	0.42
50:8:115:G:C6	50:8:116:C:C4	3.08	0.42
51:9:591:U:O2	51:9:591:U:O4'	2.36	0.42
51:9:1153:C:O2	51:9:1153:C:O4'	2.37	0.42
51:9:1309:C:O2'	51:9:1310:U:C5'	2.68	0.42
51:9:1481:G:C6	51:9:1482:C:C4	3.07	0.42
51:9:1563:G:C6	51:9:1564:C:C4	3.07	0.42
51:9:1719:A:N6	51:9:1814:G:O2'	2.51	0.42
52:AA:41:ARG:HD3	52:AA:47:TYR:CZ	2.55	0.42
54:CC:274:VAL:HG13	54:CC:274:VAL:O	2.20	0.42
5:E:254:LEU:HD23	5:E:254:LEU:C	2.43	0.42
13:N:48:ALA:HB1	13:N:53:TYR:CB	2.50	0.42
14:O:146:GLY:O	14:O:147:TRP:C	2.62	0.42
14:O:201:PHE:HB2	14:O:202:LEU:HD13	2.02	0.42
19:T:80:VAL:O	19:T:82:GLY:N	2.53	0.42
48:5:127:G:C2	48:5:128:C:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:199:G:C2	48:5:201:C:N3	2.88	0.42
48:5:207:G:O4'	48:5:406:C:H5'	2.19	0.42
48:5:279:A:O2'	48:5:280:G:OP2	2.32	0.42
48:5:351:C:C2	50:8:25:G:N2	2.88	0.42
48:5:717:U:H3	48:5:951:G:H1	1.68	0.42
48:5:1416:G:C2	48:5:1417:C:C2	3.07	0.42
48:5:2052:G:C6	48:5:2053:C:C4	3.08	0.42
48:5:2268:A:C4'	48:5:2269:C:H5'	2.50	0.42
48:5:2468:U:C2	48:5:2469:C:C5	3.08	0.42
48:5:2771:G:C2	48:5:2772:C:C2	3.08	0.42
48:5:3918:G:C2	48:5:3919:C:C2	3.08	0.42
48:5:5008:C:H2'	48:5:5009:G:O4'	2.20	0.42
50:8:134:G:C2	50:8:135:C:C2	3.08	0.42
51:9:339:A:C6	51:9:340:C:C4	3.08	0.42
51:9:1838:U:O2	66:OO:150:ARG:HD2	2.20	0.42
59:HH:135:PHE:CD1	59:HH:135:PHE:C	2.97	0.42
60:II:156:ALA:O	60:II:158:ILE:N	2.53	0.42
2:B:151:SER:O	2:B:155:LYS:HG3	2.20	0.41
5:E:126:ARG:NH1	48:5:1285:U:OP2	2.53	0.41
5:E:173:GLY:O	5:E:174:PRO:C	2.61	0.41
6:F:60:HIS:HA	48:5:944:A:N7	2.35	0.41
26:a:84:GLU:O	26:a:88:VAL:HG23	2.20	0.41
28:c:84:ALA:HA	65:NN:151:ALA:O	2.19	0.41
46:2:65:G:C2	46:2:66:C:C2	3.08	0.41
48:5:169:G:C2	48:5:170:C:C2	3.08	0.41
48:5:1098:G:C6	48:5:1099:C:C4	3.07	0.41
48:5:1213:G:C5	48:5:1215:C:N1	2.88	0.41
48:5:1359:G:C5	48:5:1360:G:C5	3.07	0.41
48:5:1412:G:C6	48:5:1413:C:C4	3.08	0.41
48:5:1484:G:C2'	48:5:1484:G:N3	2.82	0.41
48:5:1612:G:H2'	48:5:1612:G:N3	2.35	0.41
48:5:1811:G:C2	48:5:1812:C:C2	3.08	0.41
48:5:1970:A:C2	48:5:2016:C:C5	3.08	0.41
48:5:1983:A:N1	48:5:2010:A:OP2	2.53	0.41
48:5:2066:C:O2'	48:5:2067:C:H5'	2.19	0.41
48:5:2618:G:N2	48:5:2720:C:C2	2.88	0.41
48:5:4269:G:C6	48:5:4270:C:C4	3.08	0.41
48:5:4453:C:C2	48:5:4529:G:N2	2.88	0.41
48:5:4713:G:C6	48:5:4714:C:C4	3.08	0.41
51:9:531:A:H3'	51:9:532:C:H5''	2.02	0.41
51:9:936:G:C6	51:9:937:C:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1863:A:C2	78:aa:76:SER:HA	2.55	0.41
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	2.02	0.41
61:JJ:114:VAL:HG12	61:JJ:120:ALA:HB2	2.00	0.41
86:ii:59:ALA:O	86:ii:62:ILE:HG13	2.19	0.41
86:ii:120:ILE:HG22	86:ii:139:LEU:HD13	2.02	0.41
2:B:91:GLY:CA	2:B:153:MET:HE3	2.51	0.41
6:F:41:GLN:HG3	48:5:2095:A:N1	2.34	0.41
9:I:76:MET:HG3	9:I:87:ILE:HD11	2.02	0.41
38:m:110:CYS:SG	38:m:111:ARG:N	2.93	0.41
48:5:219:G:H4'	48:5:219:G:OP1	2.19	0.41
48:5:254:G:C6	48:5:255:C:C4	3.08	0.41
48:5:695:G:H3'	48:5:696:C:H5'	2.01	0.41
48:5:1090:G:C2	48:5:1091:C:C2	3.08	0.41
48:5:1203:G:C2	48:5:1204: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	3.09	0.41
48:5:2076:G:C2	48:5:2077:C:C2	3.09	0.41
48:5:4131:G:C6	48:5:4132:C:C4	3.09	0.41
48:5:4139:G:C2	48:5:4140:C:C2	3.07	0.41
48:5:4152:G:C2	48:5:4153:C:C2	3.09	0.41
48:5:4473:A:C2	48:5:4474:A:C4	3.08	0.41
48:5:5028:G:C2	48:5:5029:C:C2	3.08	0.41
49:7:30:C:C4	49:7:48:G:N1	2.88	0.41
51:9:617:G:N2	51:9:618:C:C2	2.89	0.41
51:9:752:G:C2	51:9:790:C:N3	2.87	0.41
51:9:999:G:C2	51:9:1000:C:C2	3.08	0.41
6:F:41:GLN:CG	48:5:2095:A:N1	2.83	0.41
12:M:56:GLN:HE21	12:M:56:GLN:HB3	1.71	0.41
12:M:127:VAL:HG12	12:M:131:GLN:HE21	1.84	0.41
13:N:40:PRO:HG3	48:5:8:U:H5''	2.02	0.41
18:S:28:TYR:CD2	18:S:54:MET:HE1	2.55	0.41
26:a:21:ARG:HB2	48:5:1318:C:OP1	2.20	0.41
41:p:4:ARG:NH2	48:5:1555:G:O6	2.54	0.41
48:5:130:C:C2	48:5:139:G:N2	2.88	0.41
48:5:351:C:C2	50:8:25:G:C2	3.07	0.41
48:5:1957:U:O2'	48:5:1958:A:P	2.78	0.41
48:5:2076:G:C6	48:5:2077:C:C4	3.08	0.41
48:5:2468:U:C4	48:5:2473:A:C6	3.07	0.41
48:5:2874:U:H4'	48:5:2875:C:OP2	2.20	0.41
50:8:71:A:C2	50:8:88:A:H1'	2.56	0.41
51:9:107:A:H2'	51:9:108:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:630:U:O2	51:9:630:U:C2'	2.69	0.41
51:9:839:C:O2	51:9:839:C:H2'	2.19	0.41
51:9:993:G:C6	51:9:994:C:C4	3.08	0.41
51:9:1217:A:H2'	51:9:1218:C:C6	2.55	0.41
51:9:1613:G:N2	51:9:1627:C:C2	2.89	0.41
67:PP:83:MET:HE3	67:PP:89:MET:SD	2.60	0.41
72:UU:46:LYS:HD3	72:UU:97:ILE:HG23	2.03	0.41
3:C:30:ALA:HB1	3:C:31:PRO:HD2	2.03	0.41
3:C:114:ARG:NE	48:5:1358:G:O3'	2.50	0.41
9:I:72:ALA:HB2	9:I:136:MET:HE1	2.02	0.41
24:Y:87:ARG:HH21	24:Y:87:ARG:HG3	1.85	0.41
26:a:54:GLY:N	48:5:93:G:OP2	2.51	0.41
28:c:51:ASN:OD1	28:c:51:ASN:C	2.63	0.41
30:e:53:ILE:HG22	48:5:437:G:H5'	2.03	0.41
47:3:67:U:H2'	47:3:68:C:H6	1.86	0.41
48:5:199:G:C2	48:5:201:C:C4	3.08	0.41
48:5:479:G:C6	48:5:480:C:C4	3.08	0.41
48:5:689:U:N3	48:5:690:C:C5	2.89	0.41
48:5:1339:U:H2'	48:5:1340:C:C6	2.55	0.41
48:5:1981:G:O2'	48:5:1982:G:C8	2.73	0.41
48:5:2711:G:H3'	48:5:2712:G:H5''	2.03	0.41
48:5:2771:G:H2'	48:5:2772:C:O4'	2.21	0.41
48:5:3627:G:C2	48:5:3835:C:C2	3.09	0.41
48:5:4874:A:H3'	48:5:4875:G:C5'	2.50	0.41
48:5:4967:A:C2	48:5:4968:A:C4	3.08	0.41
50:8:46:G:O2'	50:8:61:A:N1	2.48	0.41
51:9:14:C:OP2	54:CC:232:THR:HG21	2.20	0.41
51:9:1518:C:O2	51:9:1518:C:O5'	2.38	0.41
52:AA:33:GLN:HB3	52:AA:154:LEU:HD12	2.02	0.41
57:FF:86:LYS:O	57:FF:89:THR:N	2.53	0.41
60:II:87:ASN:OD1	60:II:87:ASN:C	2.63	0.41
71:TT:65:TYR:HA	71:TT:123:LEU:HD22	2.01	0.41
86:ii:305:VAL:HG11	86:ii:328:ILE:HG21	2.01	0.41
87:jj:596:PHE:CD2	87:jj:596:PHE:N	2.88	0.41
2:B:29:VAL:HG23	2:B:346:THR:HG21	2.01	0.41
3:C:210:ILE:HG21	3:C:252:TRP:CZ3	2.56	0.41
4:D:146:LEU:HD11	4:D:159:VAL:CG1	2.50	0.41
4:D:284:LYS:HD2	9:I:209:TRP:CZ2	2.55	0.41
11:L:172:GLU:OE1	34:i:3:LEU:HD23	2.20	0.41
11:L:172:GLU:C	11:L:172:GLU:CD	2.89	0.41
25:Z:12:LEU:HB2	25:Z:81:MET:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3:39:U:C2	47:3:40:C:C5	3.07	0.41
48:5:190:G:C2	48:5:252:C:O2	2.74	0.41
48:5:450:G:O2'	48:5:452:A:H4'	2.21	0.41
48:5:1075:G:N2	48:5:1076:C:C2	2.89	0.41
48:5:1280:C:C2'	48:5:1282:G:C8	3.04	0.41
48:5:1358:G:N3	48:5:1359:G:N7	2.68	0.41
48:5:3591:C:C4	48:5:3592:G:C8	3.08	0.41
48:5:3712:A:N6	51:9:970:G:C2	2.88	0.41
48:5:4408:G:C6	48:5:4409:C:C4	3.08	0.41
48:5:4579:U:O2	48:5:4580:U:C2	2.74	0.41
48:5:4587:G:N2	48:5:4716:C:C2	2.88	0.41
51:9:17:C:H2'	51:9:18:C:C6	2.55	0.41
51:9:23:G:C6	51:9:24:C:C4	3.08	0.41
51:9:832:G:C2	51:9:833:C:C2	3.08	0.41
51:9:936:G:C2	51:9:937:C:C2	3.08	0.41
51:9:1260:A:C6	51:9:1619:A:C6	3.09	0.41
51:9:1308:U:C2'	51:9:1309:C:O5'	2.69	0.41
54:CC:164:PRO:HB2	73:VV:11:LEU:HD11	2.02	0.41
69:RR:36:GLU:HG2	69:RR:47:ARG:HD2	2.03	0.41
69:RR:91:LEU:HD12	69:RR:92:ASP:N	2.35	0.41
8:H:99:PHE:HA	87:jj:440:GLN:OE1	2.20	0.41
17:R:4:LEU:HD11	17:R:29:THR:HG23	2.01	0.41
19:T:64:VAL:HG13	19:T:72:VAL:HG13	2.03	0.41
23:X:99:ILE:HG23	23:X:133:GLU:HB3	2.03	0.41
24:Y:85:VAL:HG12	24:Y:97:VAL:HB	2.03	0.41
48:5:129:C:C2	48:5:140:G:N2	2.89	0.41
48:5:1075:G:H2'	48:5:1076:C:C6	2.55	0.41
48:5:1264:C:C4	48:5:1265:G:N7	2.89	0.41
48:5:1360:G:H2'	48:5:1361:G:O4'	2.21	0.41
48:5:1550:G:C2	48:5:1579:C:O2	2.73	0.41
48:5:1633:G:H5'	48:5:1634:A:OP1	2.20	0.41
48:5:1685:G:C6	48:5:1686:C:C4	3.09	0.41
48:5:1819:G:H5''	48:5:1819:G:C8	2.56	0.41
48:5:2050:G:C2	48:5:2051:C:C2	3.08	0.41
48:5:2052:G:C2	48:5:2053:C:C2	3.09	0.41
48:5:3684:G:C6	48:5:3685:C:N4	2.89	0.41
48:5:4413:C:O2	48:5:4413:C:O4'	2.39	0.41
48:5:4652:G:C2	48:5:4653:C:C2	3.08	0.41
48:5:4904:G:C6	48:5:4905:C:C4	3.08	0.41
49:7:27:G:C6	49:7:28:C:C4	3.09	0.41
51:9:1108:G:N2	51:9:1125:C:C2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1473:G:N2	51:9:1475:G:OP2	2.51	0.41
54:CC:190:SER:OG	54:CC:191:VAL:N	2.53	0.41
59:HH:43:LEU:HD21	59:HH:71:SER:HB3	2.01	0.41
62:KK:49:MET:HA	62:KK:49:MET:HE2	2.02	0.41
87:jj:106:LEU:HD23	87:jj:107:GLY:N	2.35	0.41
2:B:54:THR:OG1	2:B:55:HIS:N	2.54	0.41
7:G:159:HIS:CE1	7:G:185:LYS:HE2	2.56	0.41
11:L:74:ARG:NH2	48:5:76:A:C8	2.89	0.41
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.56	0.41
18:S:13:VAL:HG22	18:S:63:TYR:HB3	2.03	0.41
19:T:41:ASP:HA	19:T:61:THR:HA	2.03	0.41
26:a:90:ALA:O	26:a:91:ALA:HB3	2.21	0.41
36:k:32:VAL:HG11	36:k:53:ALA:HB1	2.02	0.41
48:5:93:G:O2'	48:5:94:A:C5'	2.69	0.41
48:5:730:G:N2	48:5:939:G:N2	2.68	0.41
48:5:1245:C:C5	48:5:1269:G:O6	2.72	0.41
48:5:1374:G:C2	48:5:1375:C:C2	3.09	0.41
48:5:1412:G:C2	48:5:1413:C:C2	3.09	0.41
48:5:1668:A:C4	48:5:2282:A:C2	3.09	0.41
48:5:2006:U:H2'	48:5:2007:G:O4'	2.21	0.41
48:5:2058:G:C6	48:5:2059:C:C4	3.09	0.41
48:5:2703:G:C6	48:5:2704:C:C4	3.08	0.41
48:5:4093:G:C6	48:5:4094:G:N7	2.89	0.41
48:5:4931:G:H2'	48:5:4931:G:N3	2.36	0.41
48:5:5031:G:C6	48:5:5032:C:C4	3.09	0.41
51:9:172:U:O2	51:9:172:U:O2'	2.30	0.41
51:9:949:G:C2	51:9:950:C:C2	3.08	0.41
51:9:1089:G:C6	51:9:1090:C:C4	3.09	0.41
51:9:1097:G:C6	51:9:1098:C:C4	3.09	0.41
51:9:1518:C:O2	51:9:1518:C:O4'	2.37	0.41
51:9:1654:G:C6	51:9:1655:C:C4	3.09	0.41
62:KK:53:LYS:HD3	62:KK:60:GLU:HG3	2.03	0.41
64:MM:35:ILE:HD13	64:MM:61:TYR:CE1	2.56	0.41
1:A:233:ARG:O	1:A:235:VAL:N	2.53	0.41
2:B:92:TYR:HB2	2:B:159:VAL:HB	2.03	0.41
8:H:144:LEU:HD22	8:H:161:ILE:CD1	2.51	0.41
30:e:90:MET:CE	42:r:113:ARG:HA	2.50	0.41
46:2:30:G:C2	46:2:31:C:C2	3.08	0.41
46:2:33:U:C5	68:QQ:146:ARG:NH1	2.88	0.41
48:5:990:C:C4	48:5:991:C:C5	3.09	0.41
48:5:1075:G:C6	48:5:1076:C:N4	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1383:G:C5	48:5:1384:C:C4	3.09	0.41
48:5:1925:G:C2	48:5:1926:C:C2	3.08	0.41
48:5:2478:C:N4	48:5:2479:G:O6	2.54	0.41
48:5:2688:G:N1	48:5:2689:C:C4	2.88	0.41
48:5:3612:C:H1'	48:5:5016:A:H8	1.85	0.41
48:5:4745:G:N2	48:5:4746:C:N4	2.69	0.41
49:7:19:C:C2	49:7:60:G:C2	3.09	0.41
51:9:385:G:N3	51:9:385:G:H2'	2.36	0.41
51:9:1227:G:C2	51:9:1228:A:C8	3.09	0.41
51:9:1308:U:O2'	51:9:1309:C:P	2.79	0.41
51:9:1331:C:OP2	51:9:1490:G:OP1	2.38	0.41
51:9:1573:G:C2	51:9:1574:C:C2	3.08	0.41
56:EE:64:ILE:HG23	76:YY:17:LEU:HD13	2.03	0.41
57:FF:103:LEU:HD22	77:ZZ:67:LEU:HD22	2.02	0.41
63:LL:35:ARG:NH2	63:LL:55:TYR:O	2.50	0.41
76:YY:7:ILE:HD11	76:YY:40:ILE:CD1	2.50	0.41
1:A:49:ILE:HG22	1:A:58:LEU:HB2	2.02	0.41
1:A:207:VAL:HG12	48:5:3919:C:H4'	2.02	0.41
2:B:220:ILE:HG12	2:B:278:THR:HG23	2.02	0.41
2:B:257:TRP:CE2	48:5:4518:A:N7	2.88	0.41
3:C:349:LEU:O	3:C:353:ARG:HG3	2.21	0.41
14:O:60:LYS:HG2	48:5:2046:G:C5	2.56	0.41
15:P:64:ASN:HD21	48:5:3892:U:H4'	1.86	0.41
26:a:92:LYS:O	26:a:94:LYS:N	2.52	0.41
33:h:45:SER:O	33:h:46:LYS:C	2.64	0.41
44:t:29:ALA:HB3	44:t:30:PRO:CD	2.50	0.41
48:5:127:G:C6	48:5:128:C:C4	3.09	0.41
48:5:258:G:N2	48:5:259:C:C2	2.89	0.41
48:5:467:U:C4	48:5:468:U:C5	3.09	0.41
48:5:476:G:C2	48:5:679:C:C2	3.09	0.41
48:5:517:C:C2	48:5:645:G:C2	3.09	0.41
48:5:1092:G:C6	48:5:1093:C:C4	3.09	0.41
48:5:1328:G:O2'	48:5:2349:A:OP1	2.36	0.41
48:5:1550:G:C2	48:5:1551:C:C2	3.08	0.41
48:5:1550:G:C6	48:5:1551:C:C4	3.08	0.41
48:5:1699:A:N6	48:5:2094:G:O2'	2.54	0.41
48:5:1957:U:O2'	48:5:1958:A:C8	2.69	0.41
48:5:2027:U:HO2'	48:5:2028:C:H5'	1.80	0.41
48:5:2465:C:H1'	48:5:3672:G:N2	2.36	0.41
48:5:2481:G:N2	48:5:2498:C:C2	2.89	0.41
48:5:2743:A:H2'	48:5:2744:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2767:U:C4	48:5:2769:U:O4	2.74	0.41
48:5:2811:G:N1	48:5:2814:C:OP2	2.46	0.41
48:5:3685:C:H2'	48:5:3686:G:O4'	2.20	0.41
48:5:4129:G:C2	48:5:4130:C:C2	3.08	0.41
48:5:4129:G:C6	48:5:4130:C:C4	3.08	0.41
48:5:4473:A:H2'	48:5:4474:A:C8	2.56	0.41
48:5:4595:G:C6	48:5:4596:C:C4	3.09	0.41
48:5:4977:A:H2'	48:5:4978:G:O4'	2.20	0.41
48:5:4999:G:C2	48:5:5052:C:C2	3.09	0.41
48:5:5026:U:H3'	60:II:79:ILE:CD1	2.50	0.41
50:8:121:G:C2	50:8:130:C:C2	3.09	0.41
50:8:128:C:C5	50:8:129:C:C5	3.09	0.41
51:9:36:U:C2	51:9:520:A:C2	3.09	0.41
51:9:114:G:O6	51:9:351:G:H1'	2.21	0.41
51:9:389:A:C6	51:9:390:C:C4	3.09	0.41
51:9:463:C:H2'	51:9:465:A:C8	2.56	0.41
51:9:913:A:H61	59:HH:119:SER:C	2.29	0.41
51:9:929:G:C6	51:9:930:C:C4	3.08	0.41
51:9:1097:G:C2	51:9:1098:C:C2	3.09	0.41
51:9:1199:A:H2'	51:9:1200:A:C8	2.56	0.41
51:9:1393:G:C6	51:9:1394:G:C6	3.09	0.41
51:9:1411:G:H3'	51:9:1412:C:H4'	2.03	0.41
51:9:1455:A:OP2	51:9:1455:A:H3'	2.21	0.41
51:9:1571:G:C6	51:9:1572:C:C4	3.09	0.41
51:9:1654:G:C2	51:9:1655:C:C2	3.08	0.41
51:9:1654:G:N1	51:9:1655:C:C4	2.89	0.41
51:9:1686:G:C2	51:9:1687:C:C2	3.08	0.41
51:9:1686:G:N2	51:9:1687:C:C2	2.89	0.41
59:HH:118:ARG:O	59:HH:121:THR:HG22	2.20	0.41
60:II:55:TYR:HB2	60:II:182:CYS:O	2.21	0.41
60:II:79:ILE:HG23	60:II:103:LEU:HB2	2.01	0.41
83:ff:81:THR:HG22	83:ff:83:PRO:HD2	2.03	0.41
84:gg:73:SER:HB3	84:gg:117:ASN:HD21	1.86	0.41
87:jj:438:HIS:O	87:jj:442:VAL:HG23	2.21	0.41
2:B:84:MET:HE1	2:B:183:ILE:HD11	2.02	0.41
8:H:117:PHE:CE1	8:H:118:LEU:HD23	2.56	0.41
11:L:94:ILE:C	33:h:119:TYR:HE1	2.18	0.41
19:T:48:VAL:HG21	19:T:94:GLU:HG2	2.02	0.41
26:a:132:ARG:NH1	48:5:1468:C:OP1	2.47	0.41
28:c:82:GLY:HA2	28:c:91:VAL:CG1	2.51	0.41
31:f:74:VAL:HG13	31:f:84:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:33:A:C6	48:5:34:A:C6	3.09	0.41
48:5:80:C:C2	48:5:104:G:N2	2.89	0.41
48:5:167:C:C2	48:5:269:G:C2	3.09	0.41
48:5:176:G:H2'	48:5:177:G:O4'	2.20	0.41
48:5:961:G:N3	48:5:961:G:C2'	2.84	0.41
48:5:975:C:N4	48:5:1279:A:C2	2.89	0.41
48:5:1484:G:N3	48:5:1484:G:H2'	2.36	0.41
48:5:1691:G:C2	48:5:1692:C:C2	3.08	0.41
48:5:2682:G:C2	48:5:2683:C:C2	3.09	0.41
48:5:3705:G:C2	48:5:3706:C:C2	3.09	0.41
48:5:3857:G:C6	48:5:3858:C:C4	3.08	0.41
48:5:4371:G:C8	48:5:4372:U:C5	3.09	0.41
48:5:4455:G:C2	48:5:4456:C:C2	3.09	0.41
51:9:49:C:O2	51:9:478:G:C2	2.73	0.41
51:9:223:C:C2	51:9:299:A:C2	3.09	0.41
51:9:480:G:C2	51:9:481:C:C2	3.09	0.41
51:9:832:G:C2	51:9:843:C:N3	2.89	0.41
51:9:841:G:C6	51:9:842:C:C4	3.09	0.41
51:9:936:G:C2	51:9:1007:C:C2	3.09	0.41
51:9:1040:G:H8	51:9:1040:G:H5''	1.85	0.41
51:9:1528:G:N1	51:9:1529:C:C4	2.89	0.41
87:jj:555:MET:HB2	87:jj:595:PHE:CE1	2.55	0.41
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.56	0.40
2:B:249:ARG:NH2	48:5:3845:A:OP2	2.54	0.40
16:Q:14:ARG:NH2	48:5:2083:C:OP2	2.54	0.40
18:S:84:TYR:CE2	18:S:93:MET:HE3	2.56	0.40
29:d:33:ILE:HD11	29:d:41:ARG:CB	2.51	0.40
42:r:46:ARG:CD	48:5:666:G:C8	3.04	0.40
42:r:103:HIS:N	42:r:104:PRO:HD3	2.36	0.40
48:5:368:C:C2	48:5:374:G:C2	3.09	0.40
48:5:701:G:N3	48:5:701:G:H2'	2.37	0.40
48:5:952:G:C2	48:5:953:C:C2	3.09	0.40
48:5:1563:A:N7	51:9:678:U:H4'	2.35	0.40
48:5:1963:C:O2'	48:5:1964:A:P	2.79	0.40
48:5:2050:G:C6	48:5:2051:C:C4	3.09	0.40
48:5:2322:G:C2	48:5:2323:C:C2	3.09	0.40
48:5:2363:A:C2	48:5:3860:A:C4	3.09	0.40
48:5:2519:U:C2	48:5:2520:C:C5	3.09	0.40
48:5:2581:A:H2'	48:5:2582:A:C8	2.55	0.40
48:5:4091:G:N2	48:5:4159:C:C2	2.89	0.40
48:5:4462:C:N3	48:5:4515:G:C2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1143:A:H2'	51:9:1144:A:C8	2.56	0.40
51:9:1220:A:N6	51:9:1221:G:C6	2.89	0.40
56:EE:49:ARG:HB3	56:EE:55:ALA:HB3	2.03	0.40
60:II:139:LYS:HD2	60:II:145:ILE:HD12	2.02	0.40
68:QQ:12:VAL:HG11	68:QQ:90:LYS:HB3	2.02	0.40
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	2.03	0.40
73:VV:9:VAL:HG13	73:VV:10:ASP:N	2.36	0.40
86:ii:59:ALA:HA	86:ii:62:ILE:HG13	2.03	0.40
1:A:67:TYR:HB3	48:5:4086:G:C6	2.57	0.40
4:D:258:LYS:O	4:D:259:ARG:CG	2.70	0.40
17:R:177:LEU:HB2	17:R:178:GLN:OE1	2.21	0.40
33:h:119:TYR:C	33:h:119:TYR:HD2	2.27	0.40
35:j:2:THR:OG1	48:5:3642:A:O3'	2.39	0.40
47:3:4:C:O2'	47:3:5:G:P	2.79	0.40
48:5:977:C:H2'	48:5:978:G:H5'	2.02	0.40
48:5:1070:G:C2	48:5:1071:C:C2	3.09	0.40
48:5:1092:G:C2	48:5:1093:C:C2	3.09	0.40
48:5:1275:G:C6	48:5:1276:C:C4	3.09	0.40
48:5:1358:G:N1	48:5:1379:C:O2	2.54	0.40
48:5:1448:G:C2	48:5:2097:U:C4	3.09	0.40
48:5:2410:C:C2	48:5:2435:G:N2	2.89	0.40
48:5:2576:G:C2	48:5:2577:C:C2	3.09	0.40
48:5:4644:G:C2	48:5:4645:C:C2	3.09	0.40
51:9:310:C:H2'	51:9:311:C:C6	2.56	0.40
51:9:452:G:C2	51:9:453:C:C2	3.10	0.40
51:9:1126:G:C6	51:9:1127:C:C4	3.09	0.40
51:9:1686:G:C6	51:9:1687:C:C4	3.08	0.40
54:CC:204:ILE:HD11	54:CC:215:LEU:HD23	2.03	0.40
3:C:180:ILE:HD11	3:C:227:ILE:HD11	2.03	0.40
9:I:6:ALA:O	9:I:7:ARG:C	2.65	0.40
17:R:120:TYR:CD1	17:R:120:TYR:C	2.99	0.40
19:T:42:ILE:HD13	19:T:89:ILE:HD11	2.03	0.40
22:W:44:ARG:CG	22:W:44:ARG:HH11	2.33	0.40
22:W:44:ARG:HH11	22:W:44:ARG:HG2	1.87	0.40
25:Z:51:ARG:NH1	48:5:2755:A:OP2	2.54	0.40
33:h:6:ALA:O	33:h:7:ARG:C	2.63	0.40
41:p:42:CYS:SG	41:p:43:GLY:N	2.94	0.40
48:5:29:G:C6	48:5:30:C:C4	3.09	0.40
48:5:199:G:C2	48:5:201:C:C2	3.09	0.40
48:5:462:G:C2	48:5:694:C:C2	3.10	0.40
48:5:1213:G:C2	48:5:1215:C:C2	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1761:G:C2	48:5:1762:C:C2	3.09	0.40
48:5:2123:C:O2'	48:5:2124:G:OP2	2.19	0.40
48:5:4154:G:C2	48:5:4155:C:C2	3.09	0.40
48:5:4187:G:H2'	48:5:4188:U:O4'	2.21	0.40
48:5:4699:U:O4	48:5:4702:G:C6	2.75	0.40
48:5:4709:U:C4	48:5:4710:C:N4	2.89	0.40
48:5:4713:G:C2	48:5:4714:C:C2	3.09	0.40
48:5:5028:G:C2	48:5:5029:C:N3	2.89	0.40
49:7:77:A:C2	49:7:100:A:C4	3.09	0.40
51:9:452:G:C6	51:9:453:C:C4	3.10	0.40
51:9:878:G:C6	51:9:909:G:C6	3.09	0.40
51:9:1126:G:N1	51:9:1127:C:C4	2.90	0.40
51:9:1293:A:C2'	51:9:1294:G:O5'	2.70	0.40
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.44	0.40
51:9:1855:G:OP2	66:OO:147:ARG:NH1	2.49	0.40
87:jj:84:THR:HG21	87:jj:97:LEU:HG	2.04	0.40
1:A:103:PRO:HA	1:A:163:ARG:HA	2.03	0.40
5:E:90:LYS:N	5:E:91:PRO:HD3	2.36	0.40
9:I:140:THR:OG1	9:I:141:LYS:N	2.51	0.40
11:L:39:ARG:NH2	48:5:1362:G:OP1	2.55	0.40
15:P:36:ILE:HD12	15:P:48:LEU:HD11	2.04	0.40
18:S:93:MET:SD	18:S:113:MET:HE1	2.61	0.40
34:i:33:LEU:HD11	34:i:38:LYS:HB2	2.03	0.40
43:s:112:ARG:NH1	48:5:1968:G:OP1	2.54	0.40
48:5:158:A:C5	48:5:277:G:C6	3.09	0.40
48:5:247:G:C6	48:5:248:C:C4	3.09	0.40
48:5:488:G:C6	48:5:489:C:C4	3.09	0.40
48:5:702:U:H2'	48:5:703:G:H4'	2.03	0.40
48:5:975:C:H3'	48:5:976:G:O4'	2.21	0.40
48:5:1090:G:C2	48:5:1207:C:C2	3.10	0.40
48:5:1203:G:C6	48:5:1204:C:C4	3.09	0.40
48:5:1506:G:C6	48:5:1507:C:C4	3.10	0.40
48:5:1739:G:C2	48:5:1740:C:N3	2.90	0.40
48:5:1936:C:C5	49:7:84:U:C4	3.10	0.40
48:5:2086:G:C2	48:5:2087:C:C2	3.09	0.40
48:5:2468:U:O2	48:5:2469:C:C5	2.75	0.40
48:5:2622:G:C6	48:5:2623:A:N7	2.89	0.40
48:5:2831:G:C2	48:5:3855:C:C2	3.09	0.40
48:5:4240:G:C2	48:5:4241:C:C2	3.09	0.40
48:5:4276:G:C2	48:5:4333:C:C2	3.09	0.40
48:5:4349:C:H3'	48:5:4350:C:C5'	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:374:G:C2	51:9:391:C:C2	3.10	0.40
51:9:1559:C:C2	51:9:1577:G:C2	3.10	0.40
58:GG:55:GLY:N	58:GG:63:MET:HE2	2.36	0.40
76:YY:126:GLY:O	76:YY:128:GLY:N	2.55	0.40
84:gg:173:LEU:HD22	84:gg:189:ILE:HG12	2.04	0.40
3:C:317:ASN:HA	3:C:318:PRO:HD3	1.96	0.40
11:L:49:ARG:NH1	33:h:117:ARG:O	2.55	0.40
14:O:36:VAL:HG11	14:O:108:ILE:HD12	2.02	0.40
17:R:176:ARG:HH11	51:9:909:G:C5'	2.35	0.40
20:U:87:THR:HG23	20:U:102:VAL:HG21	2.02	0.40
47:3:5:G:N1	47:3:6:G:C5	2.83	0.40
48:5:102:G:C2'	48:5:1381:U:O2'	2.68	0.40
48:5:747:A:C2	48:5:918:G:N1	2.89	0.40
48:5:963:G:N3	48:5:963:G:C2'	2.84	0.40
48:5:1693:U:H2'	48:5:1694:C:O4'	2.21	0.40
48:5:4714:C:C6	48:5:4715:C:C5	3.10	0.40
50:8:146:U:H2'	50:8:147:G:O4'	2.21	0.40
51:9:830:A:C6	51:9:844:U:N3	2.82	0.40
51:9:1257:G:H4'	51:9:1258:A:C5'	2.52	0.40
51:9:1403:C:O2	51:9:1403:C:H2'	2.22	0.40
51:9:1661:A:C8	81:dd:14:PHE:HD2	2.39	0.40
51:9:1667:U:H2'	51:9:1668:U:C6	2.56	0.40
56:EE:75:LYS:O	56:EE:76:VAL:HB	2.22	0.40
60:II:156:ALA:O	60:II:157:LYS:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	242/244 (99%)	215 (89%)	23 (10%)	4 (2%)	7 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	392/394 (100%)	354 (90%)	33 (8%)	5 (1%)	9	36
3	C	360/362 (99%)	322 (89%)	30 (8%)	8 (2%)	5	27
4	D	290/292 (99%)	263 (91%)	25 (9%)	2 (1%)	18	48
5	E	232/248 (94%)	179 (77%)	34 (15%)	19 (8%)	0	6
6	F	223/225 (99%)	206 (92%)	16 (7%)	1 (0%)	30	58
7	G	239/241 (99%)	206 (86%)	25 (10%)	8 (3%)	3	21
8	H	188/190 (99%)	170 (90%)	16 (8%)	2 (1%)	11	39
9	I	200/213 (94%)	181 (90%)	14 (7%)	5 (2%)	4	25
10	J	167/169 (99%)	144 (86%)	15 (9%)	8 (5%)	2	14
11	L	208/210 (99%)	182 (88%)	15 (7%)	11 (5%)	1	13
12	M	136/138 (99%)	124 (91%)	12 (9%)	0	100	100
13	N	201/203 (99%)	186 (92%)	15 (8%)	0	100	100
14	O	197/199 (99%)	190 (96%)	7 (4%)	0	100	100
15	P	151/153 (99%)	141 (93%)	9 (6%)	1 (1%)	18	48
16	Q	185/187 (99%)	172 (93%)	11 (6%)	2 (1%)	11	39
17	R	178/180 (99%)	166 (93%)	10 (6%)	2 (1%)	11	39
18	S	173/175 (99%)	158 (91%)	11 (6%)	4 (2%)	5	26
19	T	157/159 (99%)	139 (88%)	15 (10%)	3 (2%)	6	30
20	U	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	1	14
21	V	129/131 (98%)	116 (90%)	12 (9%)	1 (1%)	16	45
22	W	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
23	X	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	14	43
24	Y	132/134 (98%)	115 (87%)	15 (11%)	2 (2%)	8	33
25	Z	133/135 (98%)	114 (86%)	13 (10%)	6 (4%)	2	15
26	a	145/147 (99%)	124 (86%)	16 (11%)	5 (3%)	3	21
27	b	73/75 (97%)	66 (90%)	6 (8%)	1 (1%)	9	34
28	c	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
29	d	105/107 (98%)	90 (86%)	13 (12%)	2 (2%)	6	30
30	e	126/128 (98%)	117 (93%)	6 (5%)	3 (2%)	4	25
31	f	107/109 (98%)	93 (87%)	9 (8%)	5 (5%)	2	15
32	g	112/114 (98%)	107 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	3	21
34	i	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	2	17
35	j	84/86 (98%)	73 (87%)	10 (12%)	1 (1%)	10	38
36	k	67/69 (97%)	57 (85%)	7 (10%)	3 (4%)	2	15
37	l	48/50 (96%)	40 (83%)	4 (8%)	4 (8%)	0	6
38	m	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
39	n	21/23 (91%)	21 (100%)	0	0	100	100
40	o	102/104 (98%)	89 (87%)	10 (10%)	3 (3%)	3	22
41	p	89/91 (98%)	79 (89%)	10 (11%)	0	100	100
42	r	123/125 (98%)	100 (81%)	18 (15%)	5 (4%)	2	17
43	s	196/198 (99%)	162 (83%)	24 (12%)	10 (5%)	1	14
44	t	161/163 (99%)	100 (62%)	34 (21%)	27 (17%)	0	2
45	1	13/15 (87%)	10 (77%)	1 (8%)	2 (15%)	0	2
52	AA	206/208 (99%)	174 (84%)	23 (11%)	9 (4%)	2	16
53	BB	211/213 (99%)	172 (82%)	25 (12%)	14 (7%)	1	10
54	CC	216/218 (99%)	187 (87%)	22 (10%)	7 (3%)	3	21
55	DD	225/227 (99%)	187 (83%)	29 (13%)	9 (4%)	2	17
56	EE	260/262 (99%)	215 (83%)	29 (11%)	16 (6%)	1	11
57	FF	189/191 (99%)	163 (86%)	18 (10%)	8 (4%)	2	16
58	GG	235/237 (99%)	205 (87%)	27 (12%)	3 (1%)	9	36
59	HH	187/189 (99%)	153 (82%)	22 (12%)	12 (6%)	1	11
60	II	204/206 (99%)	171 (84%)	26 (13%)	7 (3%)	3	21
61	JJ	183/185 (99%)	156 (85%)	20 (11%)	7 (4%)	2	18
62	KK	96/98 (98%)	64 (67%)	21 (22%)	11 (12%)	0	3
63	LL	150/152 (99%)	131 (87%)	14 (9%)	5 (3%)	3	21
64	MM	122/124 (98%)	85 (70%)	29 (24%)	8 (7%)	1	10
65	NN	148/150 (99%)	126 (85%)	16 (11%)	6 (4%)	2	17
66	OO	134/136 (98%)	104 (78%)	15 (11%)	15 (11%)	0	3
67	PP	125/127 (98%)	111 (89%)	11 (9%)	3 (2%)	4	25
68	QQ	139/141 (99%)	116 (84%)	17 (12%)	6 (4%)	2	16
69	RR	127/129 (98%)	108 (85%)	14 (11%)	5 (4%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	SS	135/137 (98%)	116 (86%)	11 (8%)	8 (6%)	1	12
71	TT	139/141 (99%)	128 (92%)	8 (6%)	3 (2%)	5	27
72	UU	102/104 (98%)	88 (86%)	8 (8%)	6 (6%)	1	12
73	VV	81/83 (98%)	70 (86%)	7 (9%)	4 (5%)	1	14
74	WW	127/129 (98%)	110 (87%)	10 (8%)	7 (6%)	1	13
75	XX	139/141 (99%)	125 (90%)	10 (7%)	4 (3%)	3	22
76	YY	124/126 (98%)	102 (82%)	15 (12%)	7 (6%)	1	13
77	ZZ	73/75 (97%)	59 (81%)	12 (16%)	2 (3%)	4	24
78	aa	96/98 (98%)	78 (81%)	9 (9%)	9 (9%)	0	5
79	bb	81/83 (98%)	66 (82%)	9 (11%)	6 (7%)	1	8
80	cc	59/61 (97%)	48 (81%)	10 (17%)	1 (2%)	7	31
81	dd	51/53 (96%)	44 (86%)	6 (12%)	1 (2%)	6	29
82	ee	55/57 (96%)	40 (73%)	13 (24%)	2 (4%)	2	19
83	ff	59/69 (86%)	51 (86%)	6 (10%)	2 (3%)	3	21
84	gg	311/313 (99%)	269 (86%)	33 (11%)	9 (3%)	3	22
86	ii	414/416 (100%)	383 (92%)	25 (6%)	6 (1%)	9	34
87	jj	569/594 (96%)	518 (91%)	40 (7%)	11 (2%)	6	30
All	All	12494/12710 (98%)	10874 (87%)	1202 (10%)	418 (3%)	5	21

All (418) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	TRP
5	E	91	PRO
5	E	95	ASP
5	E	118	PRO
5	E	175	LEU
5	E	221	PRO
7	G	45	ILE
7	G	128	VAL
8	H	40	HIS
8	H	110	SER
9	I	188	LYS
11	L	64	VAL
11	L	67	HIS
16	Q	148	VAL

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Mol	Chain	Res	Type
17	R	36	ASN
18	S	165	PRO
25	Z	84	ARG
26	a	90	ALA
29	d	94	GLU
30	e	92	ASN
31	f	80	ASN
34	i	91	SER
34	i	92	SER
35	j	36	LYS
36	k	61	PRO
40	o	32	SER
42	r	86	ALA
43	s	201	PRO
44	t	29	ALA
44	t	30	PRO
44	t	31	LYS
44	t	53	TRP
44	t	89	PRO
44	t	144	ASP
44	t	148	PRO
44	t	149	HIS
52	AA	44	ASP
52	AA	186	ARG
53	BB	57	ILE
55	DD	192	TRP
55	DD	202	LYS
55	DD	223	ILE
56	EE	118	GLU
56	EE	164	LEU
57	FF	80	GLY
59	HH	18	GLU
59	HH	66	VAL
59	HH	159	ASP
59	HH	190	PRO
60	II	157	LYS
61	JJ	4	ALA
61	JJ	36	GLY
61	JJ	121	LYS
62	KK	95	ARG
64	MM	79	VAL
64	MM	102	LYS

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Mol	Chain	Res	Type
64	MM	114	TYR
65	NN	24	THR
66	OO	56	VAL
66	OO	65	ASP
66	OO	140	THR
68	QQ	43	GLU
68	QQ	64	ALA
69	RR	88	VAL
69	RR	93	GLN
71	TT	29	LYS
71	TT	34	VAL
72	UU	107	GLU
73	VV	33	PRO
75	XX	34	THR
76	YY	104	ARG
77	ZZ	113	THR
82	ee	9	VAL
84	gg	161	SER
84	gg	282	GLU
86	ii	298	THR
86	ii	386	GLY
86	ii	387	ALA
87	jj	455	ILE
1	A	217	GLN
2	B	18	PRO
2	B	302	ASN
3	C	16	GLU
3	C	73	VAL
3	C	273	LEU
3	C	275	SER
4	D	187	SER
5	E	85	LEU
5	E	92	VAL
5	E	96	LYS
5	E	210	ASP
5	E	234	GLU
9	I	47	PRO
10	J	116	GLY
10	J	155	HIS
11	L	143	GLU
16	Q	14	ARG
17	R	19	LYS

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Mol	Chain	Res	Type
18	S	88	SER
18	S	155	PRO
19	T	44	GLY
19	T	81	LYS
20	U	98	ASP
23	X	131	ASP
25	Z	34	SER
25	Z	55	ALA
30	e	44	ARG
31	f	79	GLY
31	f	107	PRO
33	h	7	ARG
33	h	74	LYS
37	l	49	LEU
42	r	67	ARG
42	r	71	ARG
42	r	107	ARG
43	s	62	ARG
43	s	69	LEU
43	s	70	GLU
43	s	106	LYS
43	s	109	ALA
44	t	5	PHE
44	t	22	VAL
44	t	26	SER
44	t	39	PRO
44	t	54	LYS
44	t	58	ILE
44	t	106	PHE
52	AA	45	GLY
52	AA	191	ARG
53	BB	86	LEU
53	BB	140	VAL
53	BB	152	LYS
53	BB	153	THR
53	BB	179	ASN
53	BB	191	ASP
54	CC	228	SER
55	DD	175	VAL
55	DD	219	PRO
56	EE	95	THR
56	EE	171	ASP

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Mol	Chain	Res	Type
56	EE	196	THR
57	FF	34	SER
57	FF	54	GLY
58	GG	105	ASN
58	GG	152	ASP
59	HH	160	LYS
60	II	155	ASN
62	KK	3	MET
62	KK	39	ASN
62	KK	63	ALA
62	KK	67	PHE
63	LL	66	VAL
64	MM	15	ASN
65	NN	138	ASN
66	OO	24	GLY
66	OO	104	ARG
66	OO	129	ILE
66	OO	146	ARG
67	PP	14	LYS
67	PP	75	VAL
68	QQ	35	ASN
68	QQ	100	VAL
70	SS	12	ILE
70	SS	133	GLY
71	TT	39	LEU
72	UU	50	VAL
72	UU	52	GLY
73	VV	41	LYS
74	WW	107	SER
75	XX	42	GLY
76	YY	34	THR
76	YY	95	GLY
76	YY	114	MET
76	YY	120	THR
76	YY	127	ALA
78	aa	9	GLY
78	aa	10	ARG
78	aa	25	ASN
78	aa	62	TYR
79	bb	4	ALA
79	bb	6	ASP
79	bb	82	LYS

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Mol	Chain	Res	Type
84	gg	254	PRO
86	ii	315	GLY
87	jj	25	CYS
87	jj	47	ILE
1	A	14	SER
1	A	180	LEU
5	E	174	PRO
5	E	232	GLU
7	G	85	GLN
10	J	11	PRO
11	L	63	THR
20	U	47	ILE
21	V	14	PHE
26	a	76	ASP
30	e	125	PRO
31	f	37	ASP
33	h	89	ARG
34	i	3	LEU
34	i	11	LEU
36	k	32	VAL
40	o	33	LEU
40	o	77	CYS
43	s	108	PRO
43	s	142	GLY
44	t	67	ARG
44	t	105	THR
44	t	137	GLN
53	BB	106	THR
53	BB	206	PRO
55	DD	200	PRO
56	EE	24	THR
56	EE	76	VAL
56	EE	98	ASN
56	EE	109	PHE
56	EE	153	LEU
56	EE	154	ILE
57	FF	37	ASP
57	FF	119	SER
57	FF	163	PHE
59	HH	16	PRO
59	HH	111	LYS
60	II	27	TYR

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Mol	Chain	Res	Type
60	II	137	LEU
60	II	138	ASN
61	JJ	120	ALA
61	JJ	138	ARG
62	KK	31	LYS
62	KK	92	ALA
63	LL	28	THR
63	LL	147	LYS
64	MM	100	PRO
65	NN	3	ARG
65	NN	108	ASP
66	OO	32	HIS
68	QQ	17	LYS
69	RR	63	ARG
70	SS	11	HIS
70	SS	83	PHE
73	VV	45	ARG
73	VV	48	GLY
74	WW	3	ARG
74	WW	30	CYS
74	WW	58	ALA
74	WW	78	ARG
75	XX	10	ALA
77	ZZ	112	ASN
78	aa	8	ASN
78	aa	15	ARG
78	aa	61	ALA
79	bb	75	GLU
80	cc	26	GLN
84	gg	12	LYS
84	gg	60	ARG
86	ii	27	ALA
87	jj	22	ARG
87	jj	179	ALA
3	C	155	GLU
3	C	222	ARG
3	C	248	ARG
5	E	224	GLN
9	I	79	SER
9	I	205	PRO
10	J	153	ALA
11	L	100	PRO

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Mol	Chain	Res	Type
19	T	144	ASN
20	U	27	HIS
20	U	97	ARG
25	Z	31	ASP
25	Z	91	LEU
26	a	92	LYS
26	a	98	ALA
29	d	58	GLY
37	l	39	SER
37	l	47	THR
42	r	33	LYS
44	t	2	PRO
44	t	18	THR
44	t	119	ARG
52	AA	207	PRO
54	CC	264	SER
55	DD	143	ARG
56	EE	30	ARG
60	II	143	LYS
61	JJ	5	ARG
61	JJ	147	PHE
62	KK	93	THR
66	OO	39	ASP
66	OO	64	ALA
66	OO	128	ARG
69	RR	121	GLN
70	SS	7	GLU
72	UU	48	LEU
72	UU	118	ASP
74	WW	66	THR
75	XX	129	SER
83	ff	85	LYS
87	jj	285	PHE
2	B	19	ARG
2	B	38	SER
2	B	301	ASN
3	C	309	ILE
5	E	54	SER
5	E	63	ALA
5	E	179	ARG
5	E	218	LEU
7	G	123	ALA

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Mol	Chain	Res	Type
7	G	125	LYS
10	J	124	GLY
11	L	6	ASN
11	L	52	SER
11	L	134	PRO
20	U	67	LYS
24	Y	11	ARG
24	Y	63	LYS
31	f	106	TYR
33	h	97	LYS
36	k	29	LYS
37	l	44	TRP
43	s	34	ASN
44	t	7	PRO
44	t	19	GLY
45	1	57	ARG
52	AA	43	SER
52	AA	110	ASN
53	BB	22	VAL
53	BB	76	ASN
54	CC	62	PRO
54	CC	255	LEU
54	CC	261	PHE
56	EE	40	GLU
56	EE	131	VAL
57	FF	132	GLY
58	GG	99	GLY
59	HH	6	ALA
59	HH	57	ARG
59	HH	100	ILE
60	II	131	PRO
62	KK	32	HIS
62	KK	43	LEU
63	LL	19	ASN
63	LL	32	LYS
64	MM	116	LYS
65	NN	27	LYS
66	OO	38	ASN
66	OO	54	CYS
67	PP	15	PHE
69	RR	95	ILE
70	SS	59	LEU

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Mol	Chain	Res	Type
70	SS	92	ASP
72	UU	105	SER
74	WW	93	LEU
78	aa	65	PRO
79	bb	51	GLN
81	dd	11	PRO
82	ee	22	GLN
84	gg	37	ASP
84	gg	205	SER
5	E	103	VAL
5	E	229	PHE
6	F	239	GLU
7	G	82	GLN
10	J	146	ARG
11	L	5	ARG
11	L	167	ARG
11	L	169	ILE
44	t	10	ILE
55	DD	191	PRO
59	HH	35	ASP
62	KK	90	VAL
64	MM	103	VAL
65	NN	60	VAL
68	QQ	32	ILE
70	SS	10	GLN
83	ff	117	PRO
87	jj	402	GLY
7	G	238	GLY
10	J	152	GLY
26	a	22	ILE
27	b	21	ILE
56	EE	90	ILE
57	FF	33	ILE
66	OO	33	ILE
66	OO	145	GLY
76	YY	126	GLY
79	bb	38	PRO
84	gg	163	PRO
84	gg	190	GLY
87	jj	237	ILE
7	G	186	GLY
25	Z	90	PRO

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Mol	Chain	Res	Type
44	t	23	GLY
53	BB	24	PRO
64	MM	58	GLU
87	jj	41	VAL
87	jj	432	ILE
4	D	125	VAL
9	I	43	VAL
18	S	5	GLY
43	s	73	PRO
44	t	3	PRO
45	1	64	PRO
53	BB	93	GLY
53	BB	190	PRO
86	ii	118	LYS
10	J	174	ILE
44	t	98	ILE
52	AA	159	ILE
54	CC	181	PRO
54	CC	189	GLY
55	DD	222	PRO
59	HH	11	PRO
78	aa	64	LEU
15	P	84	PRO
52	AA	26	GLY
56	EE	195	ILE
87	jj	249	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/187 (100%)	158 (84%)	29 (16%)	2	14
2	B	336/342 (98%)	290 (86%)	46 (14%)	3	18
3	C	302/302 (100%)	258 (85%)	44 (15%)	3	16
4	D	247/247 (100%)	217 (88%)	30 (12%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	208/221 (94%)	181 (87%)	27 (13%)	4	19
6	F	194/195 (100%)	168 (87%)	26 (13%)	4	19
7	G	206/206 (100%)	180 (87%)	26 (13%)	4	20
8	H	169/169 (100%)	142 (84%)	27 (16%)	2	14
9	I	174/180 (97%)	154 (88%)	20 (12%)	5	23
10	J	142/142 (100%)	128 (90%)	14 (10%)	7	29
11	L	176/176 (100%)	148 (84%)	28 (16%)	2	14
12	M	117/117 (100%)	101 (86%)	16 (14%)	3	18
13	N	171/171 (100%)	150 (88%)	21 (12%)	4	21
14	O	171/171 (100%)	149 (87%)	22 (13%)	4	19
15	P	134/134 (100%)	120 (90%)	14 (10%)	7	27
16	Q	163/163 (100%)	142 (87%)	21 (13%)	4	19
17	R	159/159 (100%)	139 (87%)	20 (13%)	4	20
18	S	156/156 (100%)	134 (86%)	22 (14%)	3	17
19	T	139/139 (100%)	124 (89%)	15 (11%)	6	25
20	U	89/89 (100%)	82 (92%)	7 (8%)	11	35
21	V	101/101 (100%)	81 (80%)	20 (20%)	1	8
22	W	55/55 (100%)	50 (91%)	5 (9%)	9	31
23	X	107/107 (100%)	96 (90%)	11 (10%)	7	27
24	Y	124/124 (100%)	109 (88%)	15 (12%)	5	21
25	Z	117/117 (100%)	108 (92%)	9 (8%)	12	36
26	a	119/119 (100%)	109 (92%)	10 (8%)	10	33
27	b	62/62 (100%)	56 (90%)	6 (10%)	8	29
28	c	79/79 (100%)	68 (86%)	11 (14%)	3	17
29	d	98/98 (100%)	83 (85%)	15 (15%)	3	14
30	e	114/114 (100%)	95 (83%)	19 (17%)	2	13
31	f	88/88 (100%)	75 (85%)	13 (15%)	3	16
32	g	98/98 (100%)	84 (86%)	14 (14%)	3	17
33	h	109/109 (100%)	99 (91%)	10 (9%)	8	30
34	i	86/86 (100%)	79 (92%)	7 (8%)	11	34
35	j	73/73 (100%)	65 (89%)	8 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	64/64 (100%)	60 (94%)	4 (6%)	16	41
37	l	47/47 (100%)	41 (87%)	6 (13%)	4	20
38	m	48/48 (100%)	39 (81%)	9 (19%)	1	9
39	n	22/22 (100%)	19 (86%)	3 (14%)	3	18
40	o	92/92 (100%)	80 (87%)	12 (13%)	4	19
41	p	74/74 (100%)	67 (90%)	7 (10%)	8	30
42	r	109/109 (100%)	88 (81%)	21 (19%)	1	8
43	s	166/166 (100%)	154 (93%)	12 (7%)	13	38
44	t	136/136 (100%)	125 (92%)	11 (8%)	11	34
45	1	13/13 (100%)	13 (100%)	0	100	100
52	AA	174/174 (100%)	155 (89%)	19 (11%)	6	25
53	BB	194/194 (100%)	168 (87%)	26 (13%)	4	19
54	CC	184/184 (100%)	163 (89%)	21 (11%)	5	23
55	DD	190/190 (100%)	160 (84%)	30 (16%)	2	14
56	EE	223/223 (100%)	191 (86%)	32 (14%)	3	17
57	FF	161/161 (100%)	139 (86%)	22 (14%)	3	18
58	GG	207/207 (100%)	175 (84%)	32 (16%)	2	14
59	HH	169/169 (100%)	154 (91%)	15 (9%)	9	31
60	II	178/178 (100%)	156 (88%)	22 (12%)	4	20
61	JJ	161/161 (100%)	139 (86%)	22 (14%)	3	18
62	KK	89/89 (100%)	74 (83%)	15 (17%)	2	12
63	LL	136/136 (100%)	118 (87%)	18 (13%)	4	19
64	MM	104/104 (100%)	88 (85%)	16 (15%)	2	14
65	NN	130/130 (100%)	110 (85%)	20 (15%)	2	14
66	OO	106/106 (100%)	82 (77%)	24 (23%)	1	6
67	PP	116/116 (100%)	100 (86%)	16 (14%)	3	18
68	QQ	117/117 (100%)	106 (91%)	11 (9%)	8	30
69	RR	117/117 (100%)	101 (86%)	16 (14%)	3	18
70	SS	119/119 (100%)	100 (84%)	19 (16%)	2	14
71	TT	112/112 (100%)	95 (85%)	17 (15%)	3	15
72	UU	94/94 (100%)	83 (88%)	11 (12%)	5	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	VV	67/67 (100%)	58 (87%)	9 (13%)	4	19
74	WW	112/112 (100%)	98 (88%)	14 (12%)	4	20
75	XX	113/113 (100%)	96 (85%)	17 (15%)	3	15
76	YY	108/108 (100%)	90 (83%)	18 (17%)	2	13
77	ZZ	66/66 (100%)	57 (86%)	9 (14%)	3	18
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%)	47 (87%)	7 (13%)	4	19
81	dd	47/47 (100%)	38 (81%)	9 (19%)	1	9
82	ee	47/47 (100%)	40 (85%)	7 (15%)	3	15
83	ff	59/62 (95%)	57 (97%)	2 (3%)	32	53
84	gg	272/272 (100%)	249 (92%)	23 (8%)	10	32
86	ii	358/358 (100%)	323 (90%)	35 (10%)	7	29
87	jj	507/522 (97%)	487 (96%)	20 (4%)	28	51
All	All	10892/10936 (100%)	9545 (88%)	1347 (12%)	7	20

All (1347) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	49	ILE
1	A	64	ARG
1	A	70	LYS
1	A	77	ILE
1	A	96	LEU
1	A	97	ASN
1	A	100	ASN
1	A	102	LEU
1	A	104	VAL
1	A	123	ARG
1	A	128	ARG
1	A	142	GLU
1	A	158	ILE
1	A	162	ASN
1	A	163	ARG
1	A	165	VAL
1	A	175	ILE

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Mol	Chain	Res	Type
1	A	180	LEU
1	A	193	ARG
1	A	200	ARG
1	A	207	VAL
1	A	218	HIS
1	A	221	LYS
1	A	226	ARG
1	A	227	ARG
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
2	B	4	ARG
2	B	10	ARG
2	B	21	ARG
2	B	39	LYS
2	B	43	LEU
2	B	53	MET
2	B	56	ILE
2	B	60	VAL
2	B	66	LYS
2	B	67	VAL
2	B	73	VAL
2	B	74	GLU
2	B	90	VAL
2	B	94	GLU
2	B	99	LEU
2	B	103	LYS
2	B	116	ARG
2	B	135	LYS
2	B	146	LEU
2	B	154	LYS
2	B	162	VAL
2	B	167	GLN
2	B	203	GLN
2	B	207	VAL
2	B	213	GLN
2	B	240	LEU
2	B	244	THR
2	B	258	HIS
2	B	261	ARG
2	B	262	VAL
2	B	268	ARG

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Mol	Chain	Res	Type
2	B	294	LYS
2	B	299	ILE
2	B	312	LYS
2	B	314	ILE
2	B	329	ASP
2	B	333	LEU
2	B	340	THR
2	B	345	LEU
2	B	352	LEU
2	B	354	GLN
2	B	356	LYS
2	B	357	ARG
2	B	363	ILE
2	B	366	LYS
2	B	383	GLU
3	C	14	LYS
3	C	20	LYS
3	C	33	ARG
3	C	44	LEU
3	C	54	VAL
3	C	55	SER
3	C	57	LEU
3	C	71	ARG
3	C	80	ARG
3	C	95	MET
3	C	101	MET
3	C	113	ARG
3	C	114	ARG
3	C	120	LYS
3	C	124	ILE
3	C	140	LYS
3	C	144	ILE
3	C	147	VAL
3	C	150	LEU
3	C	155	GLU
3	C	159	GLU
3	C	165	LYS
3	C	175	LYS
3	C	179	ASP
3	C	188	ARG
3	C	193	LYS
3	C	204	ARG

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Mol	Chain	Res	Type
3	C	208	CYS
3	C	219	LYS
3	C	223	ASN
3	C	232	VAL
3	C	237	ILE
3	C	246	VAL
3	C	273	LEU
3	C	281	MET
3	C	284	MET
3	C	287	THR
3	C	307	LYS
3	C	312	ARG
3	C	317	ASN
3	C	321	ASN
3	C	333	LYS
3	C	342	ARG
3	C	345	ARG
4	D	4	VAL
4	D	33	ARG
4	D	36	LEU
4	D	37	VAL
4	D	39	GLN
4	D	50	ARG
4	D	56	THR
4	D	81	HIS
4	D	89	LYS
4	D	94	ASN
4	D	104	LEU
4	D	110	LEU
4	D	111	ASN
4	D	124	GLU
4	D	179	ARG
4	D	189	GLU
4	D	196	ARG
4	D	202	GLN
4	D	221	LYS
4	D	225	GLN
4	D	239	MET
4	D	248	ARG
4	D	249	GLU
4	D	256	LYS
4	D	264	LYS

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Mol	Chain	Res	Type
4	D	268	ARG
4	D	278	ASP
4	D	284	LYS
4	D	291	GLN
4	D	293	ARG
5	E	43	ASN
5	E	46	LEU
5	E	52	ARG
5	E	101	ARG
5	E	105	LEU
5	E	124	HIS
5	E	126	ARG
5	E	136	LEU
5	E	137	ARG
5	E	158	VAL
5	E	162	LYS
5	E	163	GLN
5	E	171	VAL
5	E	178	ASN
5	E	187	GLN
5	E	190	VAL
5	E	197	ILE
5	E	206	LYS
5	E	208	LEU
5	E	212	TYR
5	E	218	LEU
5	E	219	ARG
5	E	233	LYS
5	E	250	ASP
5	E	274	THR
5	E	282	LEU
5	E	284	PHE
6	F	38	LYS
6	F	41	GLN
6	F	44	LEU
6	F	49	ARG
6	F	68	ARG
6	F	70	GLU
6	F	72	ARG
6	F	76	MET
6	F	82	ASN
6	F	90	LYS

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Mol	Chain	Res	Type
6	F	91	LEU
6	F	100	ILE
6	F	101	ASN
6	F	115	ARG
6	F	127	LEU
6	F	137	ILE
6	F	154	GLU
6	F	179	ARG
6	F	189	MET
6	F	192	LEU
6	F	201	LYS
6	F	202	ARG
6	F	214	LYS
6	F	216	SER
6	F	234	ASP
6	F	248	ARG
7	G	28	VAL
7	G	75	LYS
7	G	81	ASN
7	G	88	ASP
7	G	90	GLN
7	G	106	THR
7	G	109	GLU
7	G	110	LYS
7	G	112	GLN
7	G	131	LYS
7	G	148	GLU
7	G	150	LYS
7	G	151	LYS
7	G	154	LEU
7	G	170	LEU
7	G	173	LEU
7	G	175	ARG
7	G	176	LYS
7	G	177	MET
7	G	189	ARG
7	G	202	VAL
7	G	212	LYS
7	G	217	LYS
7	G	220	GLU
7	G	240	ASN
7	G	259	LYS

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Mol	Chain	Res	Type
8	H	1	MET
8	H	18	ILE
8	H	20	LEU
8	H	26	ILE
8	H	41	ILE
8	H	44	GLU
8	H	52	LYS
8	H	57	VAL
8	H	59	LYS
8	H	65	LYS
8	H	66	GLU
8	H	72	THR
8	H	74	CYS
8	H	78	GLN
8	H	84	VAL
8	H	98	HIS
8	H	104	VAL
8	H	105	ILE
8	H	107	GLU
8	H	111	LEU
8	H	125	ARG
8	H	128	MET
8	H	129	ARG
8	H	141	LYS
8	H	162	GLN
8	H	173	ARG
8	H	177	ASP
9	I	8	CYS
9	I	13	LYS
9	I	35	ASP
9	I	36	LEU
9	I	39	LYS
9	I	43	VAL
9	I	48	LEU
9	I	76	MET
9	I	97	ILE
9	I	116	ARG
9	I	144	ASN
9	I	146	GLU
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS

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Mol	Chain	Res	Type
9	I	180	GLU
9	I	195	CYS
9	I	198	LYS
9	I	208	LYS
9	I	212	LEU
10	J	15	LEU
10	J	16	ARG
10	J	18	ARG
10	J	33	LEU
10	J	34	THR
10	J	49	VAL
10	J	81	GLU
10	J	83	LEU
10	J	90	ARG
10	J	91	GLU
10	J	96	LYS
10	J	113	ILE
10	J	151	ILE
10	J	168	GLN
11	L	11	LYS
11	L	36	ARG
11	L	46	ILE
11	L	49	ARG
11	L	59	VAL
11	L	64	VAL
11	L	65	ARG
11	L	67	HIS
11	L	77	SER
11	L	92	ARG
11	L	94	ILE
11	L	99	ASP
11	L	104	ASN
11	L	107	THR
11	L	111	GLN
11	L	113	ASN
11	L	115	GLN
11	L	121	ARG
11	L	123	LYS
11	L	130	LYS
11	L	143	GLU
11	L	162	LYS
11	L	165	LYS

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Mol	Chain	Res	Type
11	L	174	LYS
11	L	186	ARG
11	L	190	ARG
11	L	194	ILE
11	L	198	ARG
12	M	4	ARG
12	M	8	GLU
12	M	25	VAL
12	M	32	ASP
12	M	33	GLN
12	M	37	LEU
12	M	38	VAL
12	M	43	THR
12	M	48	GLN
12	M	56	GLN
12	M	57	LEU
12	M	61	ILE
12	M	89	THR
12	M	96	GLU
12	M	105	THR
12	M	119	ARG
13	N	9	GLU
13	N	26	ARG
13	N	27	CYS
13	N	44	ARG
13	N	47	LYS
13	N	61	ILE
13	N	64	ILE
13	N	66	VAL
13	N	72	LYS
13	N	77	LYS
13	N	80	THR
13	N	89	VAL
13	N	92	LEU
13	N	108	ARG
13	N	131	GLU
13	N	136	ASP
13	N	151	ILE
13	N	174	LEU
13	N	182	HIS
13	N	199	GLN
13	N	202	ARG

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Mol	Chain	Res	Type
14	O	5	GLN
14	O	16	LEU
14	O	27	VAL
14	O	36	VAL
14	O	37	ARG
14	O	49	ARG
14	O	60	LYS
14	O	62	MET
14	O	67	SER
14	O	82	ARG
14	O	103	LYS
14	O	119	VAL
14	O	128	ARG
14	O	130	LYS
14	O	145	VAL
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	185	VAL
14	O	187	LYS
14	O	195	VAL
14	O	202	LEU
15	P	5	SER
15	P	24	VAL
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	92	LEU
15	P	99	GLU
15	P	100	SER
15	P	105	LYS
15	P	118	GLN
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	9	LYS
16	Q	13	VAL
16	Q	31	LEU
16	Q	54	SER
16	Q	58	ARG

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Mol	Chain	Res	Type
16	Q	61	LEU
16	Q	63	LEU
16	Q	68	ARG
16	Q	88	ASP
16	Q	89	ASP
16	Q	91	ARG
16	Q	93	GLN
16	Q	95	VAL
16	Q	108	ARG
16	Q	115	LYS
16	Q	132	LYS
16	Q	134	CYS
16	Q	143	ARG
16	Q	180	ARG
16	Q	187	LYS
17	R	10	LEU
17	R	15	LEU
17	R	39	GLN
17	R	40	GLN
17	R	43	LYS
17	R	50	ILE
17	R	52	ARG
17	R	74	ARG
17	R	75	HIS
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	123	LEU
17	R	138	LEU
17	R	176	ARG
17	R	178	GLN
18	S	2	LYS
18	S	7	LEU
18	S	9	GLU
18	S	13	VAL
18	S	17	LEU
18	S	39	VAL
18	S	48	VAL

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Mol	Chain	Res	Type
18	S	67	VAL
18	S	70	LYS
18	S	82	LEU
18	S	83	ARG
18	S	84	TYR
18	S	95	ARG
18	S	100	LEU
18	S	102	THR
18	S	127	MET
18	S	129	VAL
18	S	132	ILE
18	S	147	ASP
18	S	149	LYS
18	S	156	HIS
18	S	159	LEU
19	T	5	LYS
19	T	9	ARG
19	T	14	MET
19	T	33	ILE
19	T	52	MET
19	T	60	LYS
19	T	81	LYS
19	T	96	ILE
19	T	118	GLU
19	T	131	GLN
19	T	142	ARG
19	T	144	ASN
19	T	146	LYS
19	T	154	ILE
19	T	159	MET
20	U	33	ILE
20	U	45	GLU
20	U	65	ARG
20	U	67	LYS
20	U	69	LYS
20	U	97	ARG
20	U	99	TRP
21	V	15	ARG
21	V	16	ILE
21	V	18	LEU
21	V	31	ASN
21	V	35	LYS

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Mol	Chain	Res	Type
21	V	45	ILE
21	V	46	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	91	LYS
21	V	99	GLU
21	V	106	VAL
21	V	109	LYS
21	V	111	GLU
21	V	113	LYS
21	V	123	LYS
22	W	4	GLU
22	W	27	LYS
22	W	41	LEU
22	W	43	LYS
22	W	44	ARG
23	X	39	LYS
23	X	50	LYS
23	X	52	LEU
23	X	59	LYS
23	X	63	LYS
23	X	94	ASN
23	X	111	GLN
23	X	129	ARG
23	X	145	ASP
23	X	147	LEU
23	X	152	LYS
24	Y	2	LYS
24	Y	7	VAL
24	Y	8	THR
24	Y	28	LYS
24	Y	34	LEU
24	Y	52	ASP
24	Y	55	VAL
24	Y	59	ARG
24	Y	65	GLN
24	Y	72	GLN
24	Y	79	VAL

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Mol	Chain	Res	Type
24	Y	87	ARG
24	Y	104	VAL
24	Y	115	ARG
24	Y	126	ARG
25	Z	3	LYS
25	Z	11	VAL
25	Z	57	MET
25	Z	59	LYS
25	Z	60	LYS
25	Z	67	LYS
25	Z	68	ILE
25	Z	93	LYS
25	Z	121	ARG
26	a	16	SER
26	a	40	HIS
26	a	59	ARG
26	a	77	LYS
26	a	82	VAL
26	a	84	GLU
26	a	116	LYS
26	a	121	PRO
26	a	122	VAL
26	a	140	VAL
27	b	21	ILE
27	b	22	LYS
27	b	27	GLN
27	b	28	ARG
27	b	43	MET
27	b	51	LYS
28	c	28	VAL
28	c	37	MET
28	c	40	GLN
28	c	50	ASN
28	c	61	GLU
28	c	77	ASN
28	c	78	ASN
28	c	81	LEU
28	c	87	LYS
28	c	91	VAL
28	c	94	LEU
29	d	19	GLU
29	d	23	ARG

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Mol	Chain	Res	Type
29	d	26	THR
29	d	36	VAL
29	d	48	GLU
29	d	56	GLU
29	d	75	LYS
29	d	78	ARG
29	d	79	ASN
29	d	86	VAL
29	d	90	ARG
29	d	94	GLU
29	d	102	LEU
29	d	107	THR
29	d	116	ASN
30	e	8	VAL
30	e	9	LYS
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	46	ARG
30	e	48	ARG
30	e	64	LYS
30	e	76	LYS
30	e	78	LEU
30	e	80	HIS
30	e	86	GLU
30	e	104	SER
30	e	106	LYS
30	e	107	ASN
30	e	109	LYS
30	e	113	GLU
30	e	123	THR
30	e	129	LEU
31	f	21	GLN
31	f	33	VAL
31	f	36	ARG
31	f	46	ARG
31	f	52	LYS
31	f	56	ASN
31	f	64	PRO
31	f	69	VAL
31	f	84	VAL
31	f	100	ARG

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Mol	Chain	Res	Type
31	f	101	ILE
31	f	103	VAL
31	f	109	ARG
32	g	5	LEU
32	g	11	LEU
32	g	14	ASN
32	g	15	THR
32	g	43	LYS
32	g	54	ARG
32	g	60	ARG
32	g	64	LEU
32	g	66	ARG
32	g	74	VAL
32	g	90	ARG
32	g	100	GLN
32	g	105	LYS
32	g	115	LYS
33	h	14	LYS
33	h	28	LEU
33	h	65	GLN
33	h	69	LEU
33	h	88	THR
33	h	97	LYS
33	h	98	HIS
33	h	104	THR
33	h	121	VAL
33	h	122	LYS
34	i	18	THR
34	i	25	ARG
34	i	33	LEU
34	i	71	LYS
34	i	86	LYS
34	i	89	GLU
34	i	103	LYS
35	j	2	THR
35	j	3	LYS
35	j	15	THR
35	j	20	ARG
35	j	25	LYS
35	j	29	LEU
35	j	63	ARG
35	j	79	ARG

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Mol	Chain	Res	Type
36	k	31	ASN
36	k	57	LYS
36	k	69	LEU
36	k	70	LYS
37	l	3	SER
37	l	8	ARG
37	l	16	LYS
37	l	17	GLN
37	l	36	ARG
37	l	46	ARG
38	m	79	GLU
38	m	82	LEU
38	m	85	LEU
38	m	90	ASN
38	m	97	ARG
38	m	98	LYS
38	m	106	ARG
38	m	111	ARG
38	m	119	ASN
39	n	2	ARG
39	n	9	ARG
39	n	13	LEU
40	o	17	LYS
40	o	19	GLN
40	o	24	THR
40	o	28	LYS
40	o	33	LEU
40	o	36	GLN
40	o	55	ILE
40	o	61	LYS
40	o	69	ARG
40	o	82	MET
40	o	89	LYS
40	o	102	GLN
41	p	3	LYS
41	p	16	THR
41	p	24	LYS
41	p	52	VAL
41	p	54	ILE
41	p	60	CYS
41	p	84	ARG
42	r	8	MET

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Mol	Chain	Res	Type
42	r	10	VAL
42	r	17	LEU
42	r	18	ILE
42	r	21	ASN
42	r	28	GLU
42	r	31	ASN
42	r	32	LEU
42	r	37	SER
42	r	39	ARG
42	r	60	VAL
42	r	64	MET
42	r	67	ARG
42	r	78	VAL
42	r	80	THR
42	r	83	ASN
42	r	103	HIS
42	r	105	ASP
42	r	106	LEU
42	r	108	MET
42	r	118	LEU
43	s	38	LYS
43	s	44	ARG
43	s	50	LYS
43	s	62	ARG
43	s	77	LYS
43	s	94	ASP
43	s	107	VAL
43	s	146	LYS
43	s	149	ARG
43	s	174	LEU
43	s	185	PHE
43	s	191	GLN
44	t	1	MET
44	t	14	TYR
44	t	16	ARG
44	t	22	VAL
44	t	40	LYS
44	t	95	GLN
44	t	104	ILE
44	t	106	PHE
44	t	114	ARG
44	t	123	ARG

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Mol	Chain	Res	Type
44	t	124	GLU
52	AA	8	LEU
52	AA	9	GLN
52	AA	25	LEU
52	AA	41	ARG
52	AA	44	ASP
52	AA	46	ILE
52	AA	50	ASN
52	AA	53	ARG
52	AA	58	LEU
52	AA	60	LEU
52	AA	84	GLN
52	AA	109	THR
52	AA	111	GLN
52	AA	113	GLN
52	AA	124	VAL
52	AA	131	HIS
52	AA	142	LEU
52	AA	158	ASP
52	AA	178	LEU
53	BB	27	LYS
53	BB	38	MET
53	BB	49	VAL
53	BB	55	THR
53	BB	56	LYS
53	BB	78	GLU
53	BB	82	ARG
53	BB	86	LEU
53	BB	105	LEU
53	BB	106	THR
53	BB	107	ARG
53	BB	122	GLU
53	BB	126	ASP
53	BB	134	LEU
53	BB	136	ARG
53	BB	137	LEU
53	BB	142	PHE
53	BB	150	ILE
53	BB	157	GLN
53	BB	163	GLN
53	BB	169	MET
53	BB	172	MET

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Mol	Chain	Res	Type
53	BB	175	GLU
53	BB	206	PRO
53	BB	208	HIS
53	BB	225	LEU
54	CC	64	THR
54	CC	78	LEU
54	CC	113	GLN
54	CC	120	GLN
54	CC	121	ARG
54	CC	137	VAL
54	CC	141	VAL
54	CC	152	ARG
54	CC	160	LEU
54	CC	162	ILE
54	CC	166	ARG
54	CC	167	ARG
54	CC	192	LEU
54	CC	213	LEU
54	CC	225	SER
54	CC	230	THR
54	CC	233	LEU
54	CC	240	THR
54	CC	244	ILE
54	CC	257	LYS
54	CC	262	THR
55	DD	9	ARG
55	DD	22	ASN
55	DD	23	GLU
55	DD	28	GLU
55	DD	31	GLU
55	DD	32	ASP
55	DD	40	ARG
55	DD	42	THR
55	DD	58	VAL
55	DD	59	LEU
55	DD	72	VAL
55	DD	94	ARG
55	DD	107	TYR
55	DD	116	ARG
55	DD	117	ARG
55	DD	122	VAL
55	DD	135	GLU

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Mol	Chain	Res	Type
55	DD	142	LEU
55	DD	154	ASP
55	DD	156	LEU
55	DD	162	ASP
55	DD	167	TYR
55	DD	168	VAL
55	DD	175	VAL
55	DD	176	LEU
55	DD	190	LEU
55	DD	198	ILE
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	24	THR
56	EE	33	THR
56	EE	38	LEU
56	EE	42	LEU
56	EE	49	ARG
56	EE	65	CYS
56	EE	66	MET
56	EE	67	GLN
56	EE	73	ASP
56	EE	75	LYS
56	EE	95	THR
56	EE	123	LEU
56	EE	130	PHE
56	EE	148	ARG
56	EE	153	LEU
56	EE	155	LYS
56	EE	160	ILE
56	EE	174	LYS
56	EE	181	CYS
56	EE	191	ARG
56	EE	205	PHE
56	EE	220	THR
56	EE	222	LEU
56	EE	225	ILE
56	EE	227	VAL

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Mol	Chain	Res	Type
56	EE	240	ARG
56	EE	244	ILE
56	EE	259	LYS
57	FF	35	LEU
57	FF	63	LYS
57	FF	72	LEU
57	FF	73	THR
57	FF	79	HIS
57	FF	88	MET
57	FF	89	THR
57	FF	93	VAL
57	FF	106	GLU
57	FF	118	ASN
57	FF	124	ASP
57	FF	130	ARG
57	FF	136	ARG
57	FF	140	ASP
57	FF	152	TRP
57	FF	164	ARG
57	FF	171	GLU
57	FF	173	LEU
57	FF	190	ILE
57	FF	194	ASP
57	FF	195	GLU
57	FF	203	ASN
58	GG	14	LYS
58	GG	15	LEU
58	GG	26	THR
58	GG	30	LYS
58	GG	50	VAL
58	GG	56	ASN
58	GG	64	LYS
58	GG	68	LEU
58	GG	76	LEU
58	GG	79	LYS
58	GG	103	ASP
58	GG	107	SER
58	GG	110	ASN
58	GG	120	ASP
58	GG	121	ILE
58	GG	126	ASP
58	GG	132	ARG

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Mol	Chain	Res	Type
58	GG	137	ARG
58	GG	143	LYS
58	GG	162	LEU
58	GG	164	LYS
58	GG	179	LEU
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	216	ARG
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	74	LYS
59	HH	82	GLU
59	HH	95	ILE
59	HH	106	ARG
59	HH	113	LYS
59	HH	145	ARG
59	HH	153	LEU
59	HH	160	LYS
59	HH	162	GLN
59	HH	172	THR
59	HH	188	GLU
60	II	6	ASP
60	II	23	LYS
60	II	35	ASN
60	II	70	GLU
60	II	74	ARG
60	II	82	VAL
60	II	87	ASN
60	II	88	ASN
60	II	100	CYS
60	II	107	THR
60	II	110	ARG
60	II	111	GLN

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Mol	Chain	Res	Type
60	II	115	SER
60	II	130	THR
60	II	161	LEU
60	II	162	LEU
60	II	165	GLN
60	II	167	GLN
60	II	168	GLN
60	II	196	GLU
60	II	203	LYS
60	II	206	LYS
61	JJ	15	THR
61	JJ	24	ARG
61	JJ	29	LEU
61	JJ	39	ASN
61	JJ	42	GLU
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	67	ASP
61	JJ	69	ARG
61	JJ	86	VAL
61	JJ	87	LEU
61	JJ	89	GLU
61	JJ	101	LYS
61	JJ	109	ARG
61	JJ	110	LEU
61	JJ	116	LYS
61	JJ	127	ARG
61	JJ	131	ARG
61	JJ	135	ILE
61	JJ	138	ARG
61	JJ	139	LYS
61	JJ	174	LYS
62	KK	1	MET
62	KK	2	LEU
62	KK	3	MET
62	KK	6	LYS
62	KK	13	GLU
62	KK	43	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	65	ARG
62	KK	66	HIS

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Mol	Chain	Res	Type
62	KK	70	TYR
62	KK	74	GLU
62	KK	80	ARG
62	KK	81	ASP
62	KK	89	ILE
63	LL	8	ARG
63	LL	16	ILE
63	LL	22	ARG
63	LL	31	GLU
63	LL	40	ILE
63	LL	66	VAL
63	LL	67	SER
63	LL	69	ARG
63	LL	85	THR
63	LL	90	ARG
63	LL	91	ASP
63	LL	97	ARG
63	LL	106	HIS
63	LL	111	VAL
63	LL	121	GLN
63	LL	134	LEU
63	LL	135	SER
63	LL	147	LYS
64	MM	26	LEU
64	MM	27	ILE
64	MM	31	LEU
64	MM	33	ARG
64	MM	35	ILE
64	MM	45	ARG
64	MM	48	HIS
64	MM	51	VAL
64	MM	73	GLN
64	MM	76	LEU
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	12	SER
65	NN	13	GLN
65	NN	27	LYS

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Mol	Chain	Res	Type
65	NN	52	VAL
65	NN	60	VAL
65	NN	62	GLN
65	NN	64	ARG
65	NN	75	LEU
65	NN	77	SER
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	101	HIS
65	NN	102	LEU
65	NN	103	GLU
65	NN	110	ASP
65	NN	121	ARG
65	NN	130	LYS
65	NN	132	LYS
65	NN	133	ARG
66	OO	38	ASN
66	OO	50	LYS
66	OO	51	GLU
66	OO	52	THR
66	OO	53	ILE
66	OO	61	LYS
66	OO	63	LYS
66	OO	65	ASP
66	OO	69	SER
66	OO	76	LEU
66	OO	81	VAL
66	OO	100	THR
66	OO	104	ARG
66	OO	106	LYS
66	OO	107	THR
66	OO	121	ARG
66	OO	128	ARG
66	OO	130	GLU
66	OO	131	ASP
66	OO	137	SER
66	OO	142	ARG
66	OO	146	ARG
66	OO	150	ARG
66	OO	151	LEU
67	PP	5	GLU

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Mol	Chain	Res	Type
67	PP	7	LYS
67	PP	10	ARG
67	PP	17	TYR
67	PP	21	ASP
67	PP	28	MET
67	PP	30	TYR
67	PP	34	MET
67	PP	37	TYR
67	PP	43	ARG
67	PP	52	LYS
67	PP	56	LEU
67	PP	79	HIS
67	PP	100	LYS
67	PP	107	ILE
67	PP	121	ILE
68	QQ	10	VAL
68	QQ	26	LYS
68	QQ	41	MET
68	QQ	73	LYS
68	QQ	85	ARG
68	QQ	97	GLN
68	QQ	119	LEU
68	QQ	126	ARG
68	QQ	140	ARG
68	QQ	145	TYR
68	QQ	146	ARG
69	RR	16	ILE
69	RR	47	ARG
69	RR	49	LYS
69	RR	58	MET
69	RR	77	GLU
69	RR	78	ARG
69	RR	79	GLU
69	RR	87	GLU
69	RR	88	VAL
69	RR	91	LEU
69	RR	98	VAL
69	RR	99	ASP
69	RR	109	LEU
69	RR	118	GLN
69	RR	121	GLN
69	RR	126	MET

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Mol	Chain	Res	Type
70	SS	8	LYS
70	SS	13	LEU
70	SS	34	LYS
70	SS	36	VAL
70	SS	52	LEU
70	SS	59	LEU
70	SS	63	GLU
70	SS	64	VAL
70	SS	78	LYS
70	SS	81	ASP
70	SS	82	TRP
70	SS	95	TYR
70	SS	113	ARG
70	SS	115	LYS
70	SS	118	ARG
70	SS	125	HIS
70	SS	131	VAL
70	SS	134	GLN
70	SS	136	THR
71	TT	6	VAL
71	TT	16	ARG
71	TT	23	LYS
71	TT	28	LEU
71	TT	38	LYS
71	TT	39	LEU
71	TT	62	ARG
71	TT	67	ARG
71	TT	74	SER
71	TT	82	ARG
71	TT	84	ARG
71	TT	93	SER
71	TT	103	VAL
71	TT	108	GLU
71	TT	123	LEU
71	TT	124	THR
71	TT	128	GLN
72	UU	33	GLU
72	UU	36	CYS
72	UU	48	LEU
72	UU	49	LYS
72	UU	55	ARG
72	UU	56	MET

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Mol	Chain	Res	Type
72	UU	68	THR
72	UU	79	ARG
72	UU	84	ILE
72	UU	93	SER
72	UU	111	GLU
73	VV	9	VAL
73	VV	34	MET
73	VV	38	GLU
73	VV	40	ASP
73	VV	47	ASN
73	VV	51	LYS
73	VV	62	MET
73	VV	69	ILE
73	VV	74	LYS
74	WW	3	ARG
74	WW	23	ARG
74	WW	25	VAL
74	WW	51	GLU
74	WW	57	ARG
74	WW	74	VAL
74	WW	80	ASP
74	WW	83	LEU
74	WW	98	GLN
74	WW	103	VAL
74	WW	104	LEU
74	WW	107	SER
74	WW	111	MET
74	WW	117	ARG
75	XX	3	LYS
75	XX	5	ARG
75	XX	7	LEU
75	XX	19	ASP
75	XX	29	LYS
75	XX	37	LYS
75	XX	61	GLN
75	XX	67	ARG
75	XX	68	LYS
75	XX	70	VAL
75	XX	71	ARG
75	XX	98	ASP
75	XX	107	ARG
75	XX	112	VAL

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Mol	Chain	Res	Type
75	XX	115	ILE
75	XX	128	VAL
75	XX	130	LEU
76	YY	7	ILE
76	YY	10	ARG
76	YY	14	THR
76	YY	16	ARG
76	YY	20	ARG
76	YY	22	GLN
76	YY	23	MET
76	YY	32	LYS
76	YY	40	ILE
76	YY	61	ARG
76	YY	69	THR
76	YY	85	ASN
76	YY	98	GLU
76	YY	99	LYS
76	YY	100	LYS
76	YY	107	ARG
76	YY	109	GLU
76	YY	111	LYS
77	ZZ	44	LEU
77	ZZ	48	VAL
77	ZZ	74	SER
77	ZZ	83	LEU
77	ZZ	89	GLN
77	ZZ	93	SER
77	ZZ	99	LEU
77	ZZ	110	THR
77	ZZ	114	LYS
78	aa	12	LYS
78	aa	18	VAL
78	aa	19	GLN
78	aa	23	CYS
78	aa	26	CYS
78	aa	30	VAL
78	aa	41	ILE
78	aa	51	ARG
78	aa	52	ASP
78	aa	74	CYS
78	aa	87	ARG
79	bb	3	LEU

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Mol	Chain	Res	Type
79	bb	27	SER
79	bb	36	LYS
79	bb	37	CYS
79	bb	40	CYS
79	bb	60	SER
79	bb	63	LEU
79	bb	72	ARG
79	bb	84	HIS
80	cc	20	LYS
80	cc	24	GLN
80	cc	31	ARG
80	cc	34	PHE
80	cc	44	ARG
80	cc	60	GLU
80	cc	62	GLU
81	dd	5	GLN
81	dd	6	LEU
81	dd	21	CYS
81	dd	26	ASN
81	dd	27	ARG
81	dd	36	LEU
81	dd	39	CYS
81	dd	54	LYS
81	dd	56	ASP
82	ee	12	VAL
82	ee	15	GLN
82	ee	16	THR
82	ee	18	LYS
82	ee	24	LYS
82	ee	37	GLN
82	ee	52	LYS
83	ff	81	THR
83	ff	130	HIS
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	44	LYS
84	gg	47	ARG
84	gg	49	GLU
84	gg	59	LEU
84	gg	64	HIS
84	gg	79	LEU

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Mol	Chain	Res	Type
84	gg	87	LEU
84	gg	121	VAL
84	gg	143	GLN
84	gg	156	PHE
84	gg	165	ILE
84	gg	170	TRP
84	gg	172	LYS
84	gg	186	THR
84	gg	234	ASP
84	gg	258	ILE
84	gg	289	LEU
84	gg	298	LEU
84	gg	306	LEU
84	gg	309	VAL
86	ii	25	GLU
86	ii	45	ILE
86	ii	54	ASP
86	ii	67	ASN
86	ii	68	ARG
86	ii	80	GLN
86	ii	86	ASN
86	ii	103	GLU
86	ii	111	ASN
86	ii	112	ILE
86	ii	136	LEU
86	ii	140	LEU
86	ii	160	THR
86	ii	165	THR
86	ii	167	GLU
86	ii	179	LYS
86	ii	180	HIS
86	ii	182	ARG
86	ii	186	SER
86	ii	211	GLN
86	ii	212	LEU
86	ii	214	ILE
86	ii	241	MET
86	ii	246	LEU
86	ii	252	LYS
86	ii	257	SER
86	ii	275	LEU
86	ii	300	LYS

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Mol	Chain	Res	Type
86	ii	333	LEU
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	52	GLU
87	jj	75	LEU
87	jj	128	LYS
87	jj	131	LEU
87	jj	161	GLU
87	jj	221	GLU
87	jj	248	ASP
87	jj	271	VAL
87	jj	282	LEU
87	jj	284	ASP
87	jj	289	LEU
87	jj	313	LEU
87	jj	374	ILE
87	jj	411	TYR
87	jj	432	ILE
87	jj	444	ASP
87	jj	455	ILE
87	jj	463	SER
87	jj	551	LEU
87	jj	572	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (126) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
3	C	41	HIS
3	C	89	GLN
3	C	223	ASN
3	C	329	ASN
4	D	9	ASN
4	D	131	ASN
4	D	191	ASN
5	E	163	GLN
5	E	217	GLN
5	E	252	GLN

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Mol	Chain	Res	Type
5	E	262	GLN
5	E	264	GLN
5	E	275	ASN
6	F	58	HIS
6	F	165	ASN
7	G	43	GLN
7	G	85	GLN
7	G	208	ASN
9	I	73	ASN
11	L	27	ASN
11	L	87	HIS
11	L	175	ASN
11	L	205	GLN
12	M	56	GLN
12	M	131	GLN
13	N	109	HIS
15	P	34	GLN
15	P	56	GLN
16	Q	44	ASN
16	Q	93	GLN
17	R	39	GLN
17	R	40	GLN
17	R	141	HIS
18	S	50	GLN
18	S	77	ASN
18	S	108	GLN
19	T	58	HIS
19	T	79	GLN
20	U	95	ASN
21	V	77	HIS
22	W	30	GLN
23	X	73	HIS
23	X	107	HIS
24	Y	56	GLN
24	Y	127	GLN
25	Z	97	ASN
26	a	39	HIS
26	a	62	HIS
26	a	74	ASN
27	b	12	GLN
27	b	60	ASN
28	c	50	ASN

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Mol	Chain	Res	Type
29	d	34	HIS
29	d	93	ASN
30	e	63	ASN
31	f	21	GLN
33	h	30	GLN
34	i	80	HIS
35	j	76	HIS
38	m	119	ASN
38	m	120	ASN
40	o	25	GLN
41	p	72	ASN
42	r	12	ASN
43	s	126	GLN
43	s	176	ASN
43	s	200	ASN
44	t	156	ASN
53	BB	40	ASN
53	BB	75	GLN
53	BB	202	GLN
54	CC	134	ASN
55	DD	145	GLN
55	DD	159	HIS
55	DD	165	ASN
55	DD	226	GLN
56	EE	17	HIS
57	FF	82	ASN
58	GG	65	GLN
60	II	168	GLN
61	JJ	132	GLN
62	KK	7	ASN
63	LL	121	GLN
64	MM	73	GLN
65	NN	69	ASN
66	OO	26	ASN
67	PP	6	GLN
67	PP	104	GLN
69	RR	74	GLN
69	RR	83	ASN
69	RR	127	ASN
70	SS	19	ASN
71	TT	126	GLN
73	VV	21	ASN

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Mol	Chain	Res	Type
74	WW	5	ASN
74	WW	70	ASN
74	WW	90	GLN
74	WW	98	GLN
75	XX	16	HIS
75	XX	97	ASN
75	XX	127	ASN
76	YY	19	GLN
76	YY	112	ASN
78	aa	8	ASN
79	bb	65	GLN
80	cc	40	HIS
82	ee	44	ASN
83	ff	88	HIS
84	gg	15	ASN
84	gg	117	ASN
84	gg	215	GLN
86	ii	30	ASN
86	ii	79	GLN
86	ii	80	GLN
86	ii	132	HIS
86	ii	170	HIS
86	ii	247	GLN
86	ii	266	GLN
86	ii	325	ASN
86	ii	380	ASN
87	jj	233	GLN
87	jj	460	GLN
87	jj	468	GLN
87	jj	549	GLN
87	jj	571	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	22 (29%)	1 (1%)
47	3	72/75 (96%)	36 (50%)	13 (18%)
48	5	3649/3662 (99%)	1192 (32%)	270 (7%)
49	7	119/120 (99%)	19 (15%)	1 (0%)
50	8	155/156 (99%)	48 (30%)	6 (3%)
51	9	1712/1719 (99%)	569 (33%)	113 (6%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
85	hh	11/12 (91%)	7 (63%)	0
All	All	5792/5820 (99%)	1893 (32%)	404 (6%)

All (1893) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	5	C
46	2	7	G
46	2	8	U
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G
46	2	20	U
46	2	20(A)	U
46	2	21	A
46	2	31	C
46	2	35	A
46	2	42	A
46	2	47	U
46	2	49	C
46	2	58	A
46	2	60	A
46	2	61	C
46	2	67	G
46	2	72	C
46	2	75	C
46	2	76	A
47	3	4	C
47	3	5	G
47	3	6	G
47	3	7	A
47	3	8	U
47	3	9	A
47	3	10	G
47	3	13	C
47	3	21	A
47	3	22	G
47	3	29	A
47	3	30	G
47	3	31	A
47	3	33	U

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Mol	Chain	Res	Type
47	3	34	U
47	3	35	U
47	3	37	A
47	3	38	A
47	3	39	U
47	3	47	U
47	3	48	C
47	3	49	C
47	3	58	A
47	3	60	U
47	3	63	C
47	3	65	G
47	3	67	U
47	3	68	C
47	3	69	G
47	3	70	G
47	3	71	G
47	3	72	C
47	3	73	G
47	3	74	C
47	3	75	C
47	3	76	A
48	5	2	G
48	5	8	U
48	5	9	C
48	5	10	A
48	5	12	A
48	5	13	U
48	5	20	U
48	5	21	G
48	5	25	A
48	5	30	C
48	5	39	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A

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Mol	Chain	Res	Type
48	5	67	C
48	5	68	U
48	5	69	A
48	5	71	C
48	5	72	C
48	5	73	A
48	5	74	G
48	5	91	G
48	5	93	G
48	5	94	A
48	5	104	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	116	G
48	5	118	C
48	5	119	G
48	5	120	A
48	5	121	A
48	5	125	C
48	5	126	C
48	5	128	C
48	5	129	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	146	G
48	5	157	U
48	5	158	A
48	5	159	C
48	5	160	G
48	5	161	G
48	5	164	G
48	5	166	C
48	5	167	C
48	5	170	C
48	5	171	U
48	5	172	C
48	5	173	C
48	5	174	C

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Mol	Chain	Res	Type
48	5	175	C
48	5	177	G
48	5	183	C
48	5	184	U
48	5	185	C
48	5	186	G
48	5	187	U
48	5	188	G
48	5	189	G
48	5	197	A
48	5	200	U
48	5	201	C
48	5	203	U
48	5	205	C
48	5	216	C
48	5	217	C
48	5	218	A
48	5	219	G
48	5	220	C
48	5	221	C
48	5	224	U
48	5	225	G
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	246	G
48	5	255	C
48	5	257	C
48	5	265	C
48	5	266	C
48	5	267	G
48	5	272	U
48	5	275	C
48	5	276	C
48	5	277	G
48	5	278	G
48	5	280	G
48	5	296	A
48	5	300	A
48	5	306	A
48	5	309	C

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Mol	Chain	Res	Type
48	5	310	G
48	5	315	G
48	5	316	U
48	5	319	A
48	5	321	U
48	5	322	C
48	5	328	A
48	5	334	A
48	5	337	U
48	5	340	C
48	5	349	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	362	A
48	5	363	A
48	5	379	G
48	5	385	A
48	5	386	A
48	5	387	G
48	5	405	U
48	5	406	C
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	429	A
48	5	431	G
48	5	432	U
48	5	433	A
48	5	434	A
48	5	446	C
48	5	448	G
48	5	449	C
48	5	451	C
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	458	C
48	5	465	G

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Mol	Chain	Res	Type
48	5	467	U
48	5	468	U
48	5	469	C
48	5	470	A
48	5	473	C
48	5	485	C
48	5	486	C
48	5	487	G
48	5	498	C
48	5	499	G
48	5	500	G
48	5	502	C
48	5	503	C
48	5	504	G
48	5	506	C
48	5	509	A
48	5	510	U
48	5	513	U
48	5	514	U
48	5	515	C
48	5	519	C
48	5	649	A
48	5	654	C
48	5	655	C
48	5	663	G
48	5	664	G
48	5	665	C
48	5	666	G
48	5	667	A
48	5	668	C
48	5	669	C
48	5	682	G
48	5	684	G
48	5	685	C
48	5	686	A
48	5	689	U
48	5	690	C
48	5	694	C
48	5	695	G
48	5	696	C
48	5	697	G
48	5	701	G

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Mol	Chain	Res	Type
48	5	703	G
48	5	707	C
48	5	718	C
48	5	721	G
48	5	722	G
48	5	723	A
48	5	724	C
48	5	728	U
48	5	729	G
48	5	730	G
48	5	737	C
48	5	742	G
48	5	745	G
48	5	746	A
48	5	747	A
48	5	748	G
48	5	749	G
48	5	911	U
48	5	914	U
48	5	915	A
48	5	918	G
48	5	919	C
48	5	920	C
48	5	925	C
48	5	927	G
48	5	928	C
48	5	929	A
48	5	930	G
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	935	A
48	5	936	C
48	5	937	U
48	5	938	C
48	5	939	G
48	5	940	C
48	5	942	G
48	5	943	A
48	5	944	A
48	5	945	U

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Mol	Chain	Res	Type
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	975	C
48	5	976	G
48	5	977	C
48	5	978	G
48	5	979	C
48	5	982	U
48	5	983	C
48	5	984	C
48	5	989	U
48	5	990	C
48	5	992	C
48	5	1051	G
48	5	1070	G
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1083	U
48	5	1097	C
48	5	1175	A
48	5	1176	C
48	5	1177	U
48	5	1181	C
48	5	1182	C
48	5	1183	C

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Mol	Chain	Res	Type
48	5	1193	C
48	5	1195	G
48	5	1204	C
48	5	1209	U
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1219	G
48	5	1221	G
48	5	1222	A
48	5	1233	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1240	G
48	5	1241	C
48	5	1242	G
48	5	1243	C
48	5	1244	G
48	5	1245	C
48	5	1255	A
48	5	1256	G
48	5	1259	G
48	5	1266	G
48	5	1267	C
48	5	1268	G
48	5	1269	G
48	5	1270	A
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1279	A
48	5	1280	C
48	5	1281	G
48	5	1285	U
48	5	1287	G
48	5	1288	G

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Mol	Chain	Res	Type
48	5	1293	G
48	5	1294	A
48	5	1295	C
48	5	1296	G
48	5	1297	U
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1329	G
48	5	1330	A
48	5	1337	A
48	5	1344	C
48	5	1354	A
48	5	1358	G
48	5	1364	U
48	5	1365	C
48	5	1366	G
48	5	1367	C
48	5	1368	A
48	5	1369	C
48	5	1370	G
48	5	1371	A
48	5	1372	A
48	5	1376	C
48	5	1377	G
48	5	1378	C
48	5	1379	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1390	G
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1399	G
48	5	1407	C
48	5	1408	G
48	5	1409	C
48	5	1410	U
48	5	1411	C

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Mol	Chain	Res	Type
48	5	1413	C
48	5	1414	C
48	5	1416	G
48	5	1418	C
48	5	1420	A
48	5	1429	C
48	5	1432	G
48	5	1435	G
48	5	1436	C
48	5	1439	C
48	5	1440	U
48	5	1441	C
48	5	1442	C
48	5	1445	U
48	5	1446	C
48	5	1448	G
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1472	C
48	5	1475	G
48	5	1477	C
48	5	1478	C
48	5	1481	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1501	C
48	5	1502	G
48	5	1503	A
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1524	A
48	5	1525	A

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Mol	Chain	Res	Type
48	5	1533	A
48	5	1534	A
48	5	1535	C
48	5	1547	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1578	U
48	5	1582	U
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1601	A
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G
48	5	1626	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1636	U
48	5	1638	A
48	5	1641	G
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1670	G
48	5	1676	C
48	5	1677	U
48	5	1678	C
48	5	1679	A
48	5	1691	G
48	5	1692	C
48	5	1696	C
48	5	1697	G
48	5	1698	C
48	5	1699	A
48	5	1719	A
48	5	1720	C
48	5	1721	G

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Mol	Chain	Res	Type
48	5	1722	C
48	5	1724	G
48	5	1725	U
48	5	1733	G
48	5	1734	G
48	5	1735	U
48	5	1741	G
48	5	1742	A
48	5	1746	A
48	5	1750	G
48	5	1753	G
48	5	1754	U
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1758	G
48	5	1760	G
48	5	1761	G
48	5	1764	G
48	5	1767	A
48	5	1768	C
48	5	1772	C
48	5	1776	A
48	5	1777	C
48	5	1781	U
48	5	1787	A
48	5	1799	G
48	5	1800	U
48	5	1804	A
48	5	1805	A
48	5	1812	C
48	5	1815	G
48	5	1818	G
48	5	1819	G
48	5	1820	C
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1830	G
48	5	1832	C
48	5	1833	G
48	5	1834	U

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Mol	Chain	Res	Type
48	5	1835	G
48	5	1836	G
48	5	1840	G
48	5	1842	G
48	5	1847	C
48	5	1848	C
48	5	1855	G
48	5	1867	A
48	5	1869	G
48	5	1882	U
48	5	1885	G
48	5	1891	A
48	5	1892	A
48	5	1897	A
48	5	1898	C
48	5	1899	G
48	5	1900	C
48	5	1910	G
48	5	1918	U
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1932	A
48	5	1947	U
48	5	1952	G
48	5	1955	G
48	5	1956	A
48	5	1957	U
48	5	1958	A
48	5	1959	U
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1964	A
48	5	1965	G
48	5	1966	C
48	5	1967	A
48	5	1968	G
48	5	1969	G
48	5	1975	G

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Mol	Chain	Res	Type
48	5	1976	G
48	5	1977	C
48	5	1979	A
48	5	1980	U
48	5	1981	G
48	5	1983	A
48	5	1984	A
48	5	1985	G
48	5	1986	U
48	5	1987	C
48	5	1988	G
48	5	1990	A
48	5	1991	A
48	5	1992	U
48	5	1993	C
48	5	1997	U
48	5	1998	A
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2010	A
48	5	2011	C
48	5	2019	C
48	5	2020	U
48	5	2021	G
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2027	U
48	5	2028	C
48	5	2044	U
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2068	C

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Mol	Chain	Res	Type
48	5	2069	A
48	5	2070	U
48	5	2071	A
48	5	2079	G
48	5	2084	C
48	5	2085	G
48	5	2089	G
48	5	2090	U
48	5	2091	C
48	5	2092	G
48	5	2093	A
48	5	2094	G
48	5	2095	A
48	5	2097	U
48	5	2100	A
48	5	2101	C
48	5	2107	C
48	5	2108	G
48	5	2109	G
48	5	2110	C
48	5	2111	G
48	5	2112	G
48	5	2113	G
48	5	2114	G
48	5	2115	G
48	5	2116	C
48	5	2117	G
48	5	2118	G
48	5	2119	C
48	5	2120	G
48	5	2121	C
48	5	2122	G
48	5	2123	C
48	5	2124	G
48	5	2125	C
48	5	2126	G
48	5	2127	C
48	5	2129	C
48	5	2130	G
48	5	2131	C
48	5	2247	C
48	5	2248	C

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Mol	Chain	Res	Type
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
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2274	C
48	5	2275	G
48	5	2277	C
48	5	2279	A
48	5	2288	G
48	5	2289	C
48	5	2299	G
48	5	2300	A
48	5	2301	G
48	5	2312	U
48	5	2313	A
48	5	2314	G
48	5	2331	G
48	5	2332	A
48	5	2333	G
48	5	2335	C
48	5	2337	C
48	5	2348	G
48	5	2351	C
48	5	2360	A
48	5	2364	G

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Mol	Chain	Res	Type
48	5	2370	A
48	5	2374	A
48	5	2382	A
48	5	2395	A
48	5	2396	A
48	5	2397	G
48	5	2399	G
48	5	2417	A
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2428	A
48	5	2429	A
48	5	2433	G
48	5	2434	G
48	5	2440	U
48	5	2441	C
48	5	2450	G
48	5	2458	C
48	5	2469	C
48	5	2471	G
48	5	2473	A
48	5	2474	G
48	5	2475	G
48	5	2485	U
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2499	C
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2507	A
48	5	2511	A
48	5	2512	A
48	5	2513	A
48	5	2514	G
48	5	2521	G

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Mol	Chain	Res	Type
48	5	2527	A
48	5	2530	U
48	5	2531	C
48	5	2537	A
48	5	2544	G
48	5	2546	G
48	5	2547	G
48	5	2553	A
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2568	C
48	5	2571	C
48	5	2575	U
48	5	2577	C
48	5	2583	C
48	5	2586	G
48	5	2587	A
48	5	2588	C
48	5	2589	C
48	5	2601	A
48	5	2602	G
48	5	2611	A
48	5	2620	G
48	5	2623	A
48	5	2627	C
48	5	2638	G
48	5	2640	G
48	5	2643	G
48	5	2647	A
48	5	2658	G
48	5	2661	U
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2673	G
48	5	2676	A
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2688	G

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Mol	Chain	Res	Type
48	5	2694	G
48	5	2695	A
48	5	2696	A
48	5	2697	A
48	5	2704	C
48	5	2708	U
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2733	C
48	5	2740	U
48	5	2743	A
48	5	2752	G
48	5	2754	G
48	5	2755	A
48	5	2756	G
48	5	2760	G
48	5	2761	U
48	5	2762	G
48	5	2767	U
48	5	2768	C
48	5	2769	U
48	5	2770	C
48	5	2772	C
48	5	2787	A
48	5	2788	U
48	5	2789	A
48	5	2790	U
48	5	2794	C
48	5	2795	A
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2824	C
48	5	2825	A

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Mol	Chain	Res	Type
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2838	G
48	5	2839	U
48	5	2842	G
48	5	2855	G
48	5	2858	A
48	5	2859	G
48	5	2862	G
48	5	2869	U
48	5	2896	G
48	5	2897	G
48	5	2898	G
48	5	2904	U
48	5	2905	C
48	5	2910	G
48	5	3594	C
48	5	3596	A
48	5	3597	G
48	5	3598	C
48	5	3605	C
48	5	3606	U
48	5	3615	G
48	5	3617	G
48	5	3625	G
48	5	3626	G
48	5	3627	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3659	G
48	5	3662	A
48	5	3668	C
48	5	3670	C
48	5	3671	G
48	5	3673	C
48	5	3674	G
48	5	3680	U
48	5	3681	G
48	5	3682	A

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Mol	Chain	Res	Type
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	3715	U
48	5	3716	C
48	5	3717	A
48	5	3718	A
48	5	3722	G
48	5	3728	A
48	5	3729	U
48	5	3732	A
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3752	C
48	5	3753	G
48	5	3754	G
48	5	3756	A
48	5	3759	A
48	5	3760	A
48	5	3764	U
48	5	3769	C
48	5	3773	U
48	5	3774	A
48	5	3775	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3784	A
48	5	3786	U
48	5	3787	G
48	5	3798	U
48	5	3799	A
48	5	3809	G
48	5	3810	C
48	5	3811	G
48	5	3812	C

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Mol	Chain	Res	Type
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3824	A
48	5	3831	U
48	5	3836	A
48	5	3838	U
48	5	3840	U
48	5	3859	G
48	5	3867	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3882	C
48	5	3889	G
48	5	3897	G
48	5	3898	G
48	5	3900	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3912	U
48	5	3915	U
48	5	3916	G
48	5	3917	A
48	5	3918	G
48	5	3925	U
48	5	3926	C
48	5	3927	U
48	5	3938	G
48	5	3939	G
48	5	3943	A
48	5	3946	G
48	5	4069	U
48	5	4070	U
48	5	4073	A
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G

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Mol	Chain	Res	Type
48	5	4087	G
48	5	4088	C
48	5	4091	G
48	5	4092	G
48	5	4093	G
48	5	4094	G
48	5	4097	G
48	5	4104	G
48	5	4105	A
48	5	4107	G
48	5	4112	C
48	5	4114	C
48	5	4115	G
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4143	G
48	5	4144	C
48	5	4145	C
48	5	4161	G
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4165	C
48	5	4166	G
48	5	4168	G
48	5	4170	A
48	5	4171	C
48	5	4182	G
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4203	A
48	5	4208	U
48	5	4212	A
48	5	4213	A

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Mol	Chain	Res	Type
48	5	4216	G
48	5	4217	G
48	5	4218	U
48	5	4225	G
48	5	4226	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4235	G
48	5	4238	G
48	5	4239	A
48	5	4241	C
48	5	4251	A
48	5	4254	G
48	5	4255	A
48	5	4267	G
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4276	G
48	5	4291	G
48	5	4297	G
48	5	4302	U
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4311	A
48	5	4313	A
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4329	G
48	5	4330	G
48	5	4331	G
48	5	4332	C
48	5	4336	A
48	5	4337	C
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4360	U

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Mol	Chain	Res	Type
48	5	4367	G
48	5	4372	U
48	5	4376	A
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4394	A
48	5	4395	U
48	5	4396	A
48	5	4398	C
48	5	4405	G
48	5	4419	U
48	5	4420	U
48	5	4421	C
48	5	4422	A
48	5	4424	A
48	5	4426	C
48	5	4433	G
48	5	4438	U
48	5	4439	U
48	5	4441	A
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4463	U
48	5	4464	A
48	5	4471	U
48	5	4472	G
48	5	4473	A
48	5	4475	G
48	5	4476	C
48	5	4481	U
48	5	4482	U
48	5	4488	A
48	5	4491	G
48	5	4495	G
48	5	4500	U

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Mol	Chain	Res	Type
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4522	G
48	5	4524	G
48	5	4527	G
48	5	4528	G
48	5	4529	G
48	5	4530	U
48	5	4535	A
48	5	4548	A
48	5	4549	G
48	5	4550	G
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4577	U
48	5	4583	C
48	5	4584	A
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4591	U
48	5	4599	A
48	5	4601	U
48	5	4606	G
48	5	4618	G
48	5	4627	U
48	5	4635	A
48	5	4636	U
48	5	4637	G
48	5	4641	U
48	5	4647	G
48	5	4648	A
48	5	4656	A
48	5	4657	U
48	5	4661	G

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Mol	Chain	Res	Type
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4687	A
48	5	4694	G
48	5	4695	C
48	5	4698	C
48	5	4699	U
48	5	4700	A
48	5	4701	A
48	5	4702	G
48	5	4709	U
48	5	4712	C
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4730	C
48	5	4731	G
48	5	4732	G
48	5	4733	C
48	5	4734	A
48	5	4737	G
48	5	4741	C
48	5	4745	G
48	5	4746	C
48	5	4749	C
48	5	4750	G
48	5	4753	U
48	5	4756	C
48	5	4758	U
48	5	4760	G
48	5	4764	A
48	5	4768	G
48	5	4770	U
48	5	4771	C
48	5	4774	C
48	5	4869	U
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G

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Mol	Chain	Res	Type
48	5	4876	U
48	5	4877	G
48	5	4878	C
48	5	4883	C
48	5	4884	G
48	5	4885	U
48	5	4886	C
48	5	4889	G
48	5	4890	G
48	5	4893	A
48	5	4895	C
48	5	4896	G
48	5	4898	G
48	5	4900	C
48	5	4901	G
48	5	4904	G
48	5	4906	C
48	5	4910	G
48	5	4911	A
48	5	4912	G
48	5	4913	G
48	5	4924	C
48	5	4926	C
48	5	4927	G
48	5	4930	C
48	5	4931	G
48	5	4932	U
48	5	4934	A
48	5	4936	G
48	5	4939	C
48	5	4941	G
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	4956	A
48	5	4959	U
48	5	4964	C

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Mol	Chain	Res	Type
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	4999	G
48	5	5007	A
48	5	5013	C
48	5	5014	A
48	5	5017	G
48	5	5018	C
48	5	5022	U
48	5	5023	C
48	5	5024	C
48	5	5025	C
48	5	5026	U
48	5	5027	C
48	5	5028	G
48	5	5031	G
48	5	5033	G
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5052	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5058	A
48	5	5059	C
48	5	5060	A
48	5	5061	A
48	5	5062	G
48	5	5066	U
49	7	7	G
49	7	11	A
49	7	21	G
49	7	25	G

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Mol	Chain	Res	Type
49	7	33	U
49	7	40	U
49	7	53	U
49	7	54	A
49	7	64	G
49	7	74	A
49	7	97	G
49	7	99	G
49	7	100	A
49	7	106	G
49	7	109	U
49	7	110	G
49	7	111	C
49	7	116	G
49	7	120	U
50	8	2	G
50	8	3	A
50	8	34	U
50	8	35	C
50	8	38	U
50	8	39	G
50	8	49	G
50	8	51	U
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	74	U
50	8	75	G
50	8	79	G
50	8	80	A
50	8	81	C
50	8	82	A
50	8	83	C
50	8	84	A
50	8	85	U
50	8	86	U
50	8	87	G
50	8	94	G
50	8	95	A
50	8	101	C
50	8	103	A

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Mol	Chain	Res	Type
50	8	104	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	113	C
50	8	114	G
50	8	117	C
50	8	121	G
50	8	122	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	150	C
50	8	156	U
51	9	3	C
51	9	4	C
51	9	9	U
51	9	10	G
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
51	9	41	G
51	9	42	A
51	9	44	U
51	9	45	A
51	9	46	A
51	9	49	C
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	64	A
51	9	65	C

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Mol	Chain	Res	Type
51	9	66	G
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	72	C
51	9	73	C
51	9	74	G
51	9	75	G
51	9	76	U
51	9	77	A
51	9	78	C
51	9	79	A
51	9	80	G
51	9	99	A
51	9	103	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	114	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	140	C
51	9	141	A
51	9	142	C
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	164	A
51	9	165	G
51	9	167	G
51	9	168	C
51	9	172	U
51	9	183	G
51	9	184	G
51	9	188	C

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Mol	Chain	Res	Type
51	9	189	U
51	9	190	G
51	9	191	A
51	9	192	C
51	9	202	G
51	9	206	G
51	9	213	G
51	9	214	U
51	9	216	C
51	9	217	A
51	9	225	G
51	9	289	G
51	9	291	G
51	9	292	A
51	9	293	C
51	9	302	A
51	9	304	C
51	9	305	U
51	9	306	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	310	C
51	9	312	G
51	9	313	A
51	9	314	U
51	9	316	G
51	9	320	G
51	9	322	C
51	9	324	C
51	9	326	C
51	9	327	G
51	9	328	U
51	9	338	G
51	9	339	A
51	9	347	G
51	9	350	C
51	9	351	G
51	9	355	G
51	9	360	A
51	9	362	C
51	9	364	A

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Mol	Chain	Res	Type
51	9	368	U
51	9	369	C
51	9	370	G
51	9	371	A
51	9	377	G
51	9	379	C
51	9	384	U
51	9	385	G
51	9	386	C
51	9	398	A
51	9	400	C
51	9	407	G
51	9	408	A
51	9	409	C
51	9	416	U
51	9	417	C
51	9	418	A
51	9	434	G
51	9	435	A
51	9	438	G
51	9	441	C
51	9	448	A
51	9	449	A
51	9	450	C
51	9	453	C
51	9	459	C
51	9	460	A
51	9	464	A
51	9	465	A
51	9	466	G
51	9	469	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	482	G
51	9	487	U
51	9	488	U
51	9	489	A
51	9	492	C
51	9	500	A
51	9	501	C
51	9	503	C

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Mol	Chain	Res	Type
51	9	508	A
51	9	511	U
51	9	512	A
51	9	517	C
51	9	523	A
51	9	525	A
51	9	530	U
51	9	532	C
51	9	533	A
51	9	535	G
51	9	539	C
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	552	G
51	9	554	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	563	G
51	9	568	C
51	9	576	A
51	9	583	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	593	C
51	9	594	A
51	9	595	U
51	9	603	C
51	9	605	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	614	C

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Mol	Chain	Res	Type
51	9	617	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	631	U
51	9	632	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	654	A
51	9	655	A
51	9	656	G
51	9	657	U
51	9	659	G
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	683	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	698	G
51	9	731	G
51	9	735	C
51	9	737	G
51	9	738	C
51	9	747	U
51	9	748	C
51	9	749	U
51	9	752	G
51	9	753	C
51	9	788	G
51	9	789	G
51	9	791	C
51	9	794	A
51	9	796	G

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Mol	Chain	Res	Type
51	9	797	C
51	9	798	G
51	9	799	U
51	9	800	U
51	9	810	A
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	833	C
51	9	834	C
51	9	835	C
51	9	836	G
51	9	837	A
51	9	838	G
51	9	839	C
51	9	840	C
51	9	844	U
51	9	845	G
51	9	847	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	873	G
51	9	874	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	879	C
51	9	880	G
51	9	887	U
51	9	888	U
51	9	890	U
51	9	892	U
51	9	893	U
51	9	901	G
51	9	902	G
51	9	903	A
51	9	908	A
51	9	910	G

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Mol	Chain	Res	Type
51	9	912	C
51	9	913	A
51	9	914	U
51	9	917	U
51	9	920	A
51	9	921	G
51	9	930	C
51	9	933	G
51	9	934	G
51	9	938	A
51	9	943	U
51	9	944	A
51	9	955	A
51	9	956	G
51	9	971	G
51	9	985	G
51	9	990	A
51	9	992	A
51	9	996	A
51	9	999	G
51	9	1008	A
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1033	G
51	9	1040	G
51	9	1041	G
51	9	1044	G
51	9	1049	A
51	9	1060	A
51	9	1067	C
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1096	G
51	9	1100	A
51	9	1109	C
51	9	1110	G
51	9	1111	U
51	9	1113	A
51	9	1114	U
51	9	1115	U

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Mol	Chain	Res	Type
51	9	1116	C
51	9	1118	C
51	9	1120	U
51	9	1121	G
51	9	1131	G
51	9	1133	A
51	9	1137	U
51	9	1138	C
51	9	1139	C
51	9	1144	A
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1157	G
51	9	1158	G
51	9	1165	G
51	9	1166	G
51	9	1168	G
51	9	1170	A
51	9	1175	G
51	9	1181	A
51	9	1195	A
51	9	1196	A
51	9	1207	G
51	9	1208	A
51	9	1210	G
51	9	1211	G
51	9	1212	G
51	9	1213	C
51	9	1215	C
51	9	1216	C
51	9	1224	G
51	9	1234	C
51	9	1235	G
51	9	1240	A
51	9	1242	U
51	9	1243	U
51	9	1250	A
51	9	1251	A
51	9	1253	A
51	9	1254	C

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Mol	Chain	Res	Type
51	9	1256	G
51	9	1257	G
51	9	1258	A
51	9	1259	A
51	9	1260	A
51	9	1265	A
51	9	1266	C
51	9	1267	C
51	9	1268	C
51	9	1270	G
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1276	A
51	9	1280	G
51	9	1282	A
51	9	1283	C
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1288	U
51	9	1289	U
51	9	1290	G
51	9	1291	A
51	9	1292	C
51	9	1293	A
51	9	1294	G
51	9	1295	A
51	9	1299	A
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1304	U
51	9	1305	C
51	9	1308	U
51	9	1309	C
51	9	1310	U
51	9	1312	G
51	9	1313	A
51	9	1314	U
51	9	1315	U
51	9	1316	C

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Mol	Chain	Res	Type
51	9	1318	G
51	9	1322	G
51	9	1330	G
51	9	1331	C
51	9	1342	U
51	9	1348	G
51	9	1364	U
51	9	1371	U
51	9	1372	U
51	9	1378	A
51	9	1385	G
51	9	1386	A
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1398	G
51	9	1402	A
51	9	1403	C
51	9	1404	U
51	9	1405	A
51	9	1407	U
51	9	1408	U
51	9	1410	C
51	9	1412	C
51	9	1413	G
51	9	1414	A
51	9	1417	C
51	9	1418	C
51	9	1419	C
51	9	1420	G
51	9	1422	G
51	9	1424	G
51	9	1426	U
51	9	1427	C
51	9	1432	U
51	9	1433	C
51	9	1434	C
51	9	1437	C
51	9	1438	A
51	9	1439	A
51	9	1440	C

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Mol	Chain	Res	Type
51	9	1442	U
51	9	1447	G
51	9	1448	A
51	9	1449	G
51	9	1452	A
51	9	1454	A
51	9	1455	A
51	9	1456	G
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1464	C
51	9	1466	G
51	9	1473	G
51	9	1474	A
51	9	1475	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1490	G
51	9	1494	U
51	9	1495	G
51	9	1498	A
51	9	1507	G
51	9	1508	A
51	9	1509	U
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1523	C
51	9	1531	A
51	9	1533	A
51	9	1535	U
51	9	1536	G
51	9	1544	C
51	9	1545	A
51	9	1546	G
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1554	C
51	9	1555	U

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Mol	Chain	Res	Type
51	9	1556	A
51	9	1558	C
51	9	1560	U
51	9	1564	C
51	9	1567	G
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1582	C
51	9	1585	U
51	9	1586	U
51	9	1587	G
51	9	1588	A
51	9	1589	A
51	9	1595	U
51	9	1596	U
51	9	1599	U
51	9	1601	A
51	9	1603	G
51	9	1604	G
51	9	1606	G
51	9	1612	G
51	9	1618	C
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1639	G
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1672	U
51	9	1680	G
51	9	1681	U
51	9	1682	C

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Mol	Chain	Res	Type
51	9	1683	C
51	9	1686	G
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1725	U
51	9	1728	U
51	9	1729	U
51	9	1737	G
51	9	1742	C
51	9	1745	A
51	9	1746	U
51	9	1750	C
51	9	1753	C
51	9	1756	C
51	9	1758	G
51	9	1783	C
51	9	1784	G
51	9	1786	U
51	9	1800	A
51	9	1812	U
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1839	U
51	9	1840	U
51	9	1849	G
51	9	1850	A
51	9	1851	A
51	9	1852	C
51	9	1861	G
51	9	1862	G

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

All (404) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	2	34	A
47	3	4	C
47	3	5	G
47	3	6	G
47	3	7	A
47	3	9	A
47	3	29	A
47	3	30	G
47	3	38	A
47	3	60	U
47	3	67	U
47	3	68	C
47	3	69	G
47	3	74	C
48	5	1	C
48	5	12	A
48	5	20	U
48	5	42	A
48	5	47	A
48	5	48	G
48	5	58	G
48	5	64	A
48	5	72	C
48	5	93	G
48	5	119	G
48	5	120	A
48	5	125	C
48	5	126	C
48	5	134	G

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Mol	Chain	Res	Type
48	5	143	C
48	5	157	U
48	5	159	C
48	5	170	C
48	5	187	U
48	5	200	U
48	5	215	C
48	5	216	C
48	5	218	A
48	5	219	G
48	5	224	U
48	5	226	G
48	5	245	C
48	5	265	C
48	5	266	C
48	5	275	C
48	5	296	A
48	5	308	G
48	5	315	G
48	5	361	C
48	5	385	A
48	5	387	G
48	5	406	C
48	5	409	G
48	5	451	C
48	5	454	U
48	5	486	C
48	5	497	G
48	5	502	C
48	5	505	G
48	5	664	G
48	5	684	G
48	5	693	C
48	5	728	U
48	5	733	A
48	5	746	A
48	5	747	A
48	5	917	A
48	5	930	G
48	5	931	C
48	5	932	A
48	5	935	A

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Mol	Chain	Res	Type
48	5	943	A
48	5	956	A
48	5	957	G
48	5	965	G
48	5	977	C
48	5	978	G
48	5	989	U
48	5	1071	C
48	5	1211	G
48	5	1214	C
48	5	1232	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1241	C
48	5	1266	G
48	5	1268	G
48	5	1272	C
48	5	1279	A
48	5	1280	C
48	5	1292	C
48	5	1296	G
48	5	1329	G
48	5	1357	C
48	5	1365	C
48	5	1368	A
48	5	1370	G
48	5	1371	A
48	5	1376	C
48	5	1379	C
48	5	1380	G
48	5	1390	G
48	5	1398	A
48	5	1407	C
48	5	1410	U
48	5	1419	G
48	5	1420	A
48	5	1435	G
48	5	1440	U
48	5	1445	U
48	5	1455	G

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Mol	Chain	Res	Type
48	5	1474	C
48	5	1477	C
48	5	1481	C
48	5	1485	C
48	5	1502	G
48	5	1523	A
48	5	1533	A
48	5	1563	A
48	5	1601	A
48	5	1625	G
48	5	1633	G
48	5	1654	G
48	5	1678	C
48	5	1696	C
48	5	1697	G
48	5	1724	G
48	5	1733	G
48	5	1746	A
48	5	1755	C
48	5	1756	U
48	5	1804	A
48	5	1818	G
48	5	1819	G
48	5	1835	G
48	5	1891	A
48	5	1921	C
48	5	1956	A
48	5	1957	U
48	5	1958	A
48	5	1961	G
48	5	1964	A
48	5	1965	G
48	5	1966	C
48	5	1967	A
48	5	1968	G
48	5	1974	U
48	5	1975	G
48	5	1986	U
48	5	2009	A
48	5	2019	C
48	5	2028	C
48	5	2046	G

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Mol	Chain	Res	Type
48	5	2068	C
48	5	2083	C
48	5	2084	C
48	5	2088	A
48	5	2089	G
48	5	2093	A
48	5	2107	C
48	5	2110	C
48	5	2116	C
48	5	2119	C
48	5	2123	C
48	5	2125	C
48	5	2246	C
48	5	2251	G
48	5	2253	A
48	5	2256	C
48	5	2257	C
48	5	2260	C
48	5	2262	G
48	5	2263	A
48	5	2265	G
48	5	2266	C
48	5	2269	C
48	5	2278	G
48	5	2313	A
48	5	2370	A
48	5	2396	A
48	5	2398	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2473	A
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	G
48	5	2505	C
48	5	2506	G
48	5	2513	A
48	5	2530	U
48	5	2546	G
48	5	2553	A

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Mol	Chain	Res	Type
48	5	2554	U
48	5	2586	G
48	5	2588	C
48	5	2661	U
48	5	2687	U
48	5	2695	A
48	5	2696	A
48	5	2754	G
48	5	2760	G
48	5	2769	U
48	5	2782	U
48	5	2794	C
48	5	2806	A
48	5	2827	G
48	5	2858	A
48	5	3593	C
48	5	3625	G
48	5	3648	A
48	5	3670	C
48	5	3673	C
48	5	3697	U
48	5	3709	U
48	5	3710	G
48	5	3713	U
48	5	3715	U
48	5	3717	A
48	5	3752	C
48	5	3753	G
48	5	3809	G
48	5	3810	C
48	5	3811	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	4069	U
48	5	4075	U
48	5	4084	G
48	5	4086	G
48	5	4115	G
48	5	4119	C
48	5	4120	U
48	5	4121	G

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Mol	Chain	Res	Type
48	5	4124	G
48	5	4144	C
48	5	4170	A
48	5	4221	C
48	5	4232	U
48	5	4254	G
48	5	4272	G
48	5	4331	G
48	5	4378	A
48	5	4395	U
48	5	4404	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4475	G
48	5	4510	A
48	5	4527	G
48	5	4528	G
48	5	4548	A
48	5	4560	C
48	5	4583	C
48	5	4656	A
48	5	4694	G
48	5	4699	U
48	5	4719	G
48	5	4730	C
48	5	4872	G
48	5	4885	U
48	5	4888	U
48	5	4889	G
48	5	4895	C
48	5	4900	C
48	5	4926	C
48	5	4935	C
48	5	4948	C
48	5	4951	G
48	5	4965	U
48	5	4975	G
48	5	4990	C
48	5	5022	U
48	5	5026	U
48	5	5027	C

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Mol	Chain	Res	Type
48	5	5059	C
48	5	5060	A
48	5	5061	A
49	7	109	U
50	8	2	G
50	8	51	U
50	8	94	G
50	8	110	U
50	8	111	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	72	C
51	9	92	A
51	9	98	C
51	9	102	A
51	9	110	U
51	9	113	G
51	9	139	C
51	9	140	C
51	9	160	U
51	9	164	A
51	9	181	A
51	9	183	G
51	9	215	G
51	9	291	G
51	9	292	A
51	9	304	C
51	9	305	U
51	9	311	C
51	9	312	G
51	9	322	C
51	9	327	G
51	9	369	C
51	9	385	G
51	9	400	C
51	9	407	G
51	9	434	G
51	9	448	A
51	9	464	A
51	9	465	A
51	9	473	A

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Mol	Chain	Res	Type
51	9	488	U
51	9	500	A
51	9	532	C
51	9	550	C
51	9	559	G
51	9	589	G
51	9	594	A
51	9	620	G
51	9	627	U
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U
51	9	746	C
51	9	747	U
51	9	752	G
51	9	797	C
51	9	798	G
51	9	810	A
51	9	833	C
51	9	867	G
51	9	868	G
51	9	869	A
51	9	870	A
51	9	887	U
51	9	912	C
51	9	913	A
51	9	1016	U
51	9	1087	A
51	9	1109	C
51	9	1113	A
51	9	1115	U
51	9	1137	U
51	9	1165	G
51	9	1212	G
51	9	1253	A
51	9	1265	A
51	9	1275	G
51	9	1283	C
51	9	1294	G
51	9	1298	G
51	9	1302	G

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

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

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

5.5 Carbohydrates [i](#)

There are no 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	601	87	0,12,12	-	-	-		
91	ADP	jj	603	-	28,29,29	1.51	5 (17%)	43,45,45	1.90	11 (25%)
90	SF4	jj	600	87	0,12,12	-	-	-		
91	ADP	jj	602	-	28,29,29	1.51	5 (17%)	43,45,45	1.91	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
91	ADP	jj	602	-	-	1/16/32/32	0/3/3/3
91	ADP	jj	603	-	-	1/16/32/32	0/3/3/3
90	SF4	jj	600	87	-	-	0/6/5/5
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	4.94	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	jj	603	ADP	C5-C6	2.97	1.49	1.41
91	jj	602	ADP	C5-C6	2.94	1.49	1.41
91	jj	602	ADP	C8-N7	2.43	1.36	1.31
91	jj	603	ADP	C8-N7	2.41	1.36	1.31
91	jj	602	ADP	PA-O3A	2.33	1.62	1.59
91	jj	603	ADP	C5-N7	-2.31	1.34	1.39
91	jj	603	ADP	PA-O3A	2.24	1.61	1.59
91	jj	602	ADP	C5-N7	-2.24	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	jj	603	ADP	C5-C4-N3	-5.90	118.60	126.72
91	jj	602	ADP	C5-C4-N3	-5.84	118.67	126.72
91	jj	603	ADP	N3-C4-N9	4.72	135.20	127.17
91	jj	602	ADP	N3-C4-N9	4.65	135.07	127.17
91	jj	602	ADP	C2-N3-C4	3.94	121.46	111.83
91	jj	603	ADP	C2-N3-C4	3.93	121.42	111.83
91	jj	602	ADP	N3-C2-N1	-3.84	122.77	128.58
91	jj	603	ADP	N3-C2-N1	-3.77	122.87	128.58
91	jj	602	ADP	C4-C5-N7	-3.66	106.39	110.58
91	jj	603	ADP	C4-C5-N7	-3.54	106.53	110.58
91	jj	602	ADP	C4-N9-C8	2.83	108.71	105.74
91	jj	602	ADP	C5-N7-C8	2.78	107.82	103.45
91	jj	603	ADP	C5-N7-C8	2.74	107.76	103.45
91	jj	603	ADP	C4-N9-C8	2.74	108.62	105.74
91	jj	603	ADP	C3'-C2'-C1'	2.38	105.97	101.46
91	jj	602	ADP	C6-C5-N7	2.30	136.53	132.09
91	jj	602	ADP	C3'-C2'-C1'	2.24	105.71	101.46
91	jj	602	ADP	N9-C8-N7	-2.20	110.82	113.94
91	jj	603	ADP	C6-C5-N7	2.19	136.31	132.09
91	jj	603	ADP	N9-C8-N7	-2.15	110.88	113.94
91	jj	602	ADP	C2-N1-C6	2.09	122.17	118.73
91	jj	603	ADP	C2-N1-C6	2.06	122.12	118.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

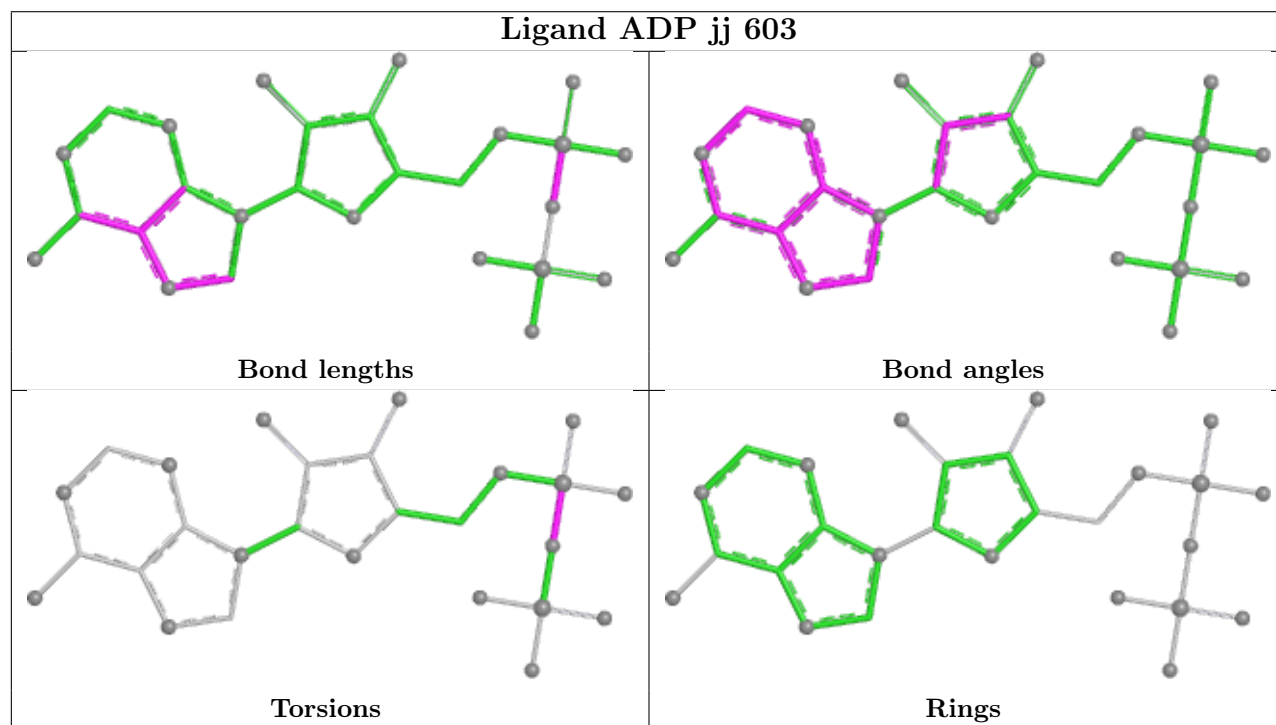
Mol	Chain	Res	Type	Atoms
91	jj	602	ADP	PB-O3A-PA-O1A
91	jj	603	ADP	PB-O3A-PA-O1A

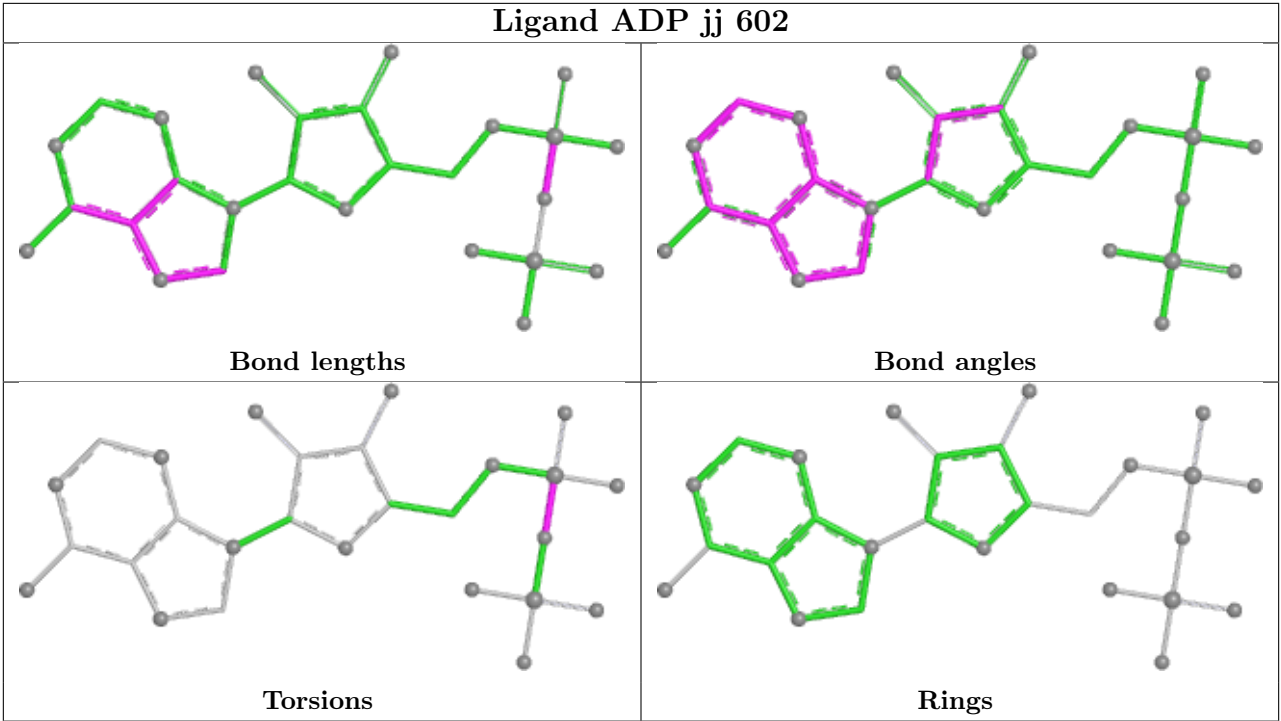
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	jj	601	SF4	1	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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
34	i	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	23.46
1	9	126:G	O3'	139:C	P	21.86
1	9	698:G	O3'	730:C	P	19.70
1	5	4776:G	O3'	4859:C	P	18.03
1	9	1761:U	O3'	1771:G	P	17.54

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	757:G	O3'	906:C	P	17.52
1	5	519:C	O3'	642:G	P	16.75
1	5	2910:G	O3'	3583:U	P	16.46
1	5	3950:U	O3'	4065:G	P	14.50
1	5	2131:C	O3'	2243:C	P	14.48
1	5	997:C	O3'	1047:C	P	13.94
1	5	1051:G	O3'	1064:G	P	8.92
1	9	225:G	O3'	287:U	P	6.78
1	9	739:C	O3'	744:G	P	6.41
1	3	19:G	O3'	20:U	P	6.17
1	5	1222:A	O3'	1232:G	P	5.11
1	5	2016:C	O3'	2017:A	P	4.58
1	3	16:C	O3'	18:U	P	4.19
1	5	1100:U	O3'	1167:C	P	4.11
1	5	1699:A	O3'	1718:C	P	4.05
1	2	16:C	O3'	18:G	P	3.96
1	jj	416:ILE	C	417:SER	N	3.66
1	5	1840:G	O3'	1842:G	P	3.22
1	9	873:G	O3'	874:G	P	3.09
1	9	340:C	O3'	342:C	P	3.05
1	5	4942:C	O3'	4944:C	P	2.85
1	5	4939:C	O3'	4941:G	P	2.68
1	5	1823:G	O3'	1825:A	P	2.60
1	i	91:SER	C	92:SER	N	1.12

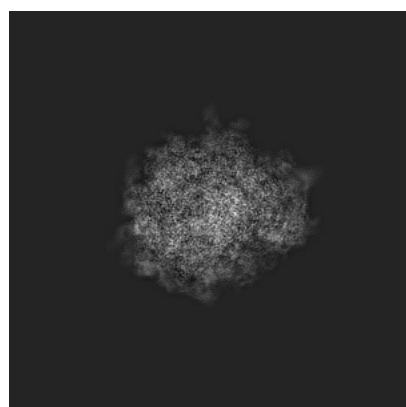
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3038. These allow visual inspection of the internal detail of the map and identification of artifacts.

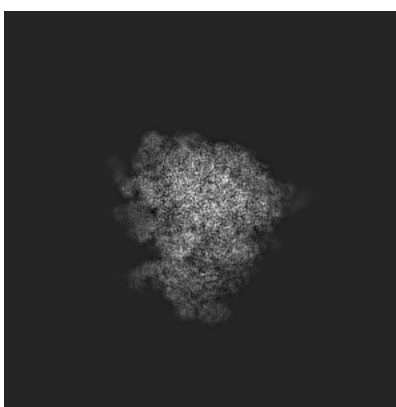
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

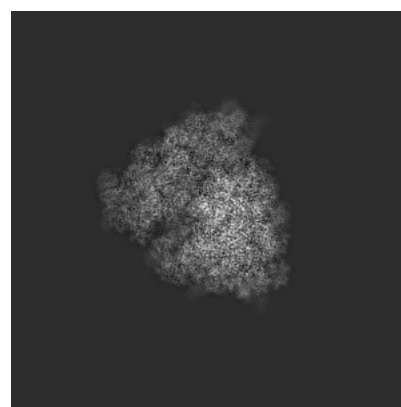
6.1.1 Primary map



X



Y

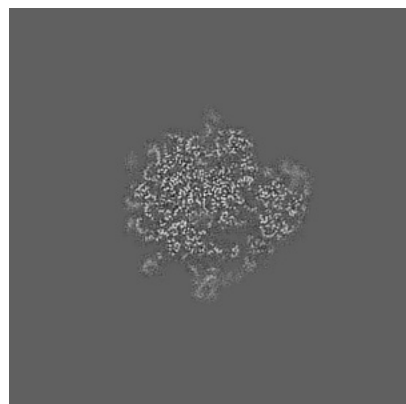


Z

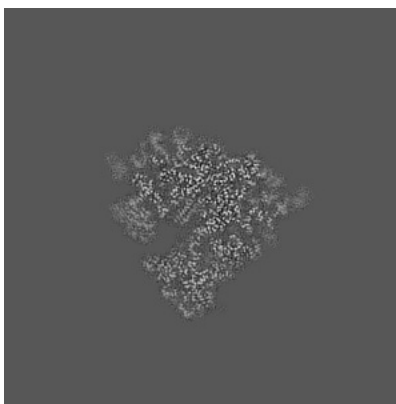
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 210



Y Index: 210



Z Index: 210

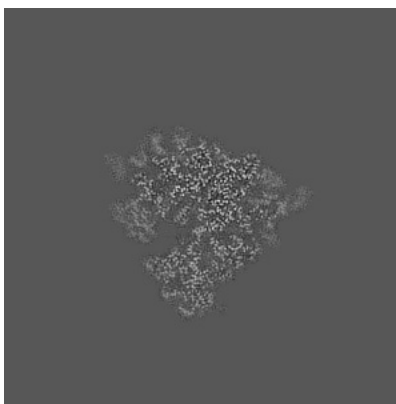
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

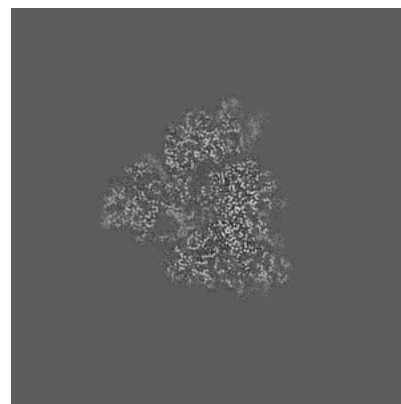
6.3.1 Primary map



X Index: 228



Y Index: 211

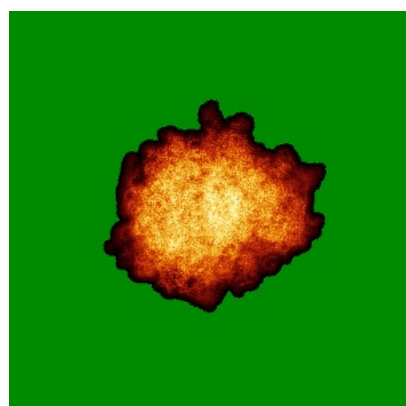


Z Index: 195

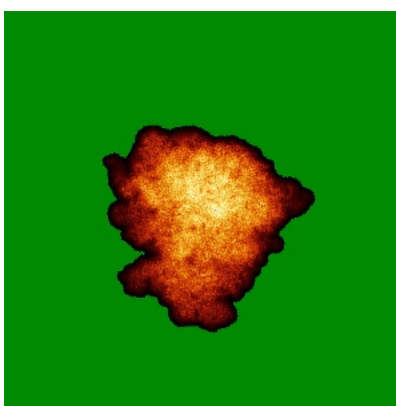
The images above show the largest variance slices of the map in three orthogonal directions.

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

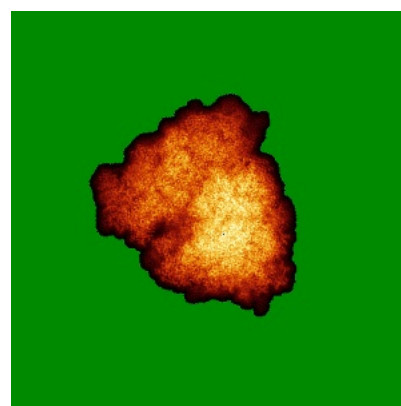
6.4.1 Primary map



X



Y

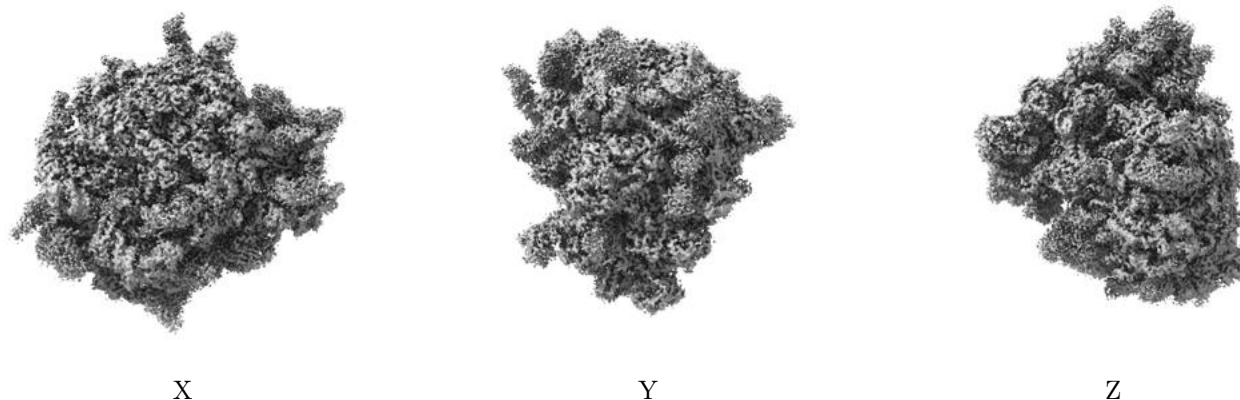


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

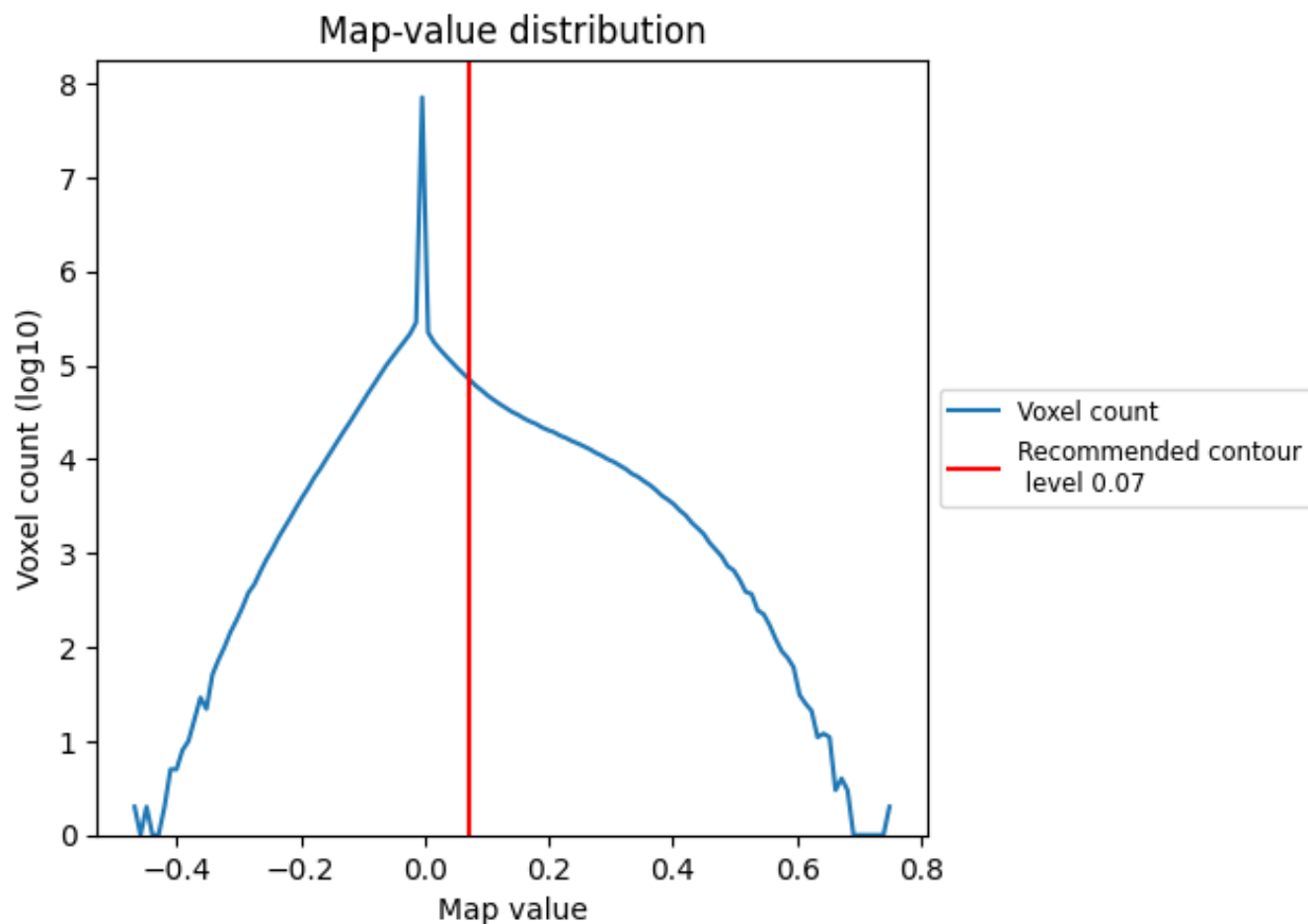
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

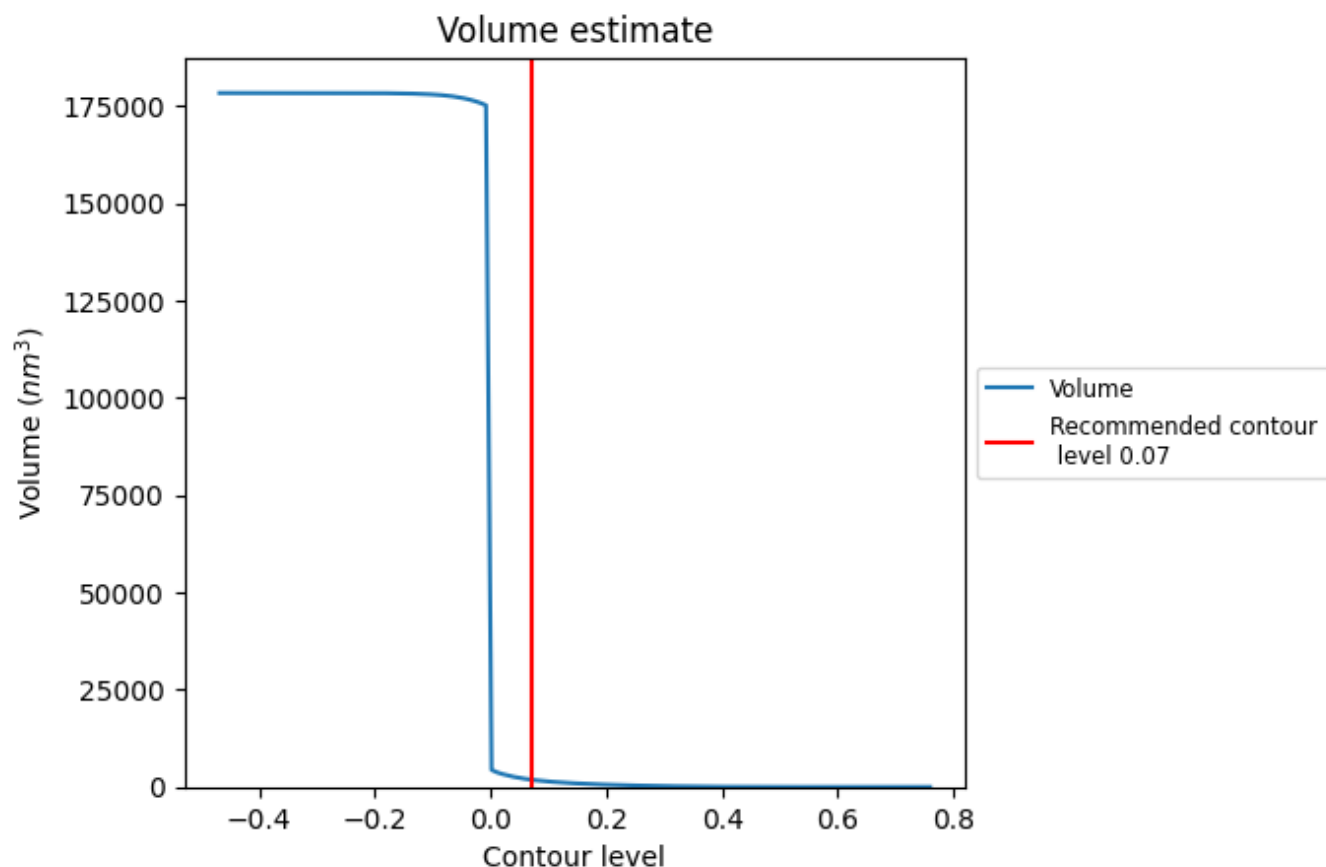
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

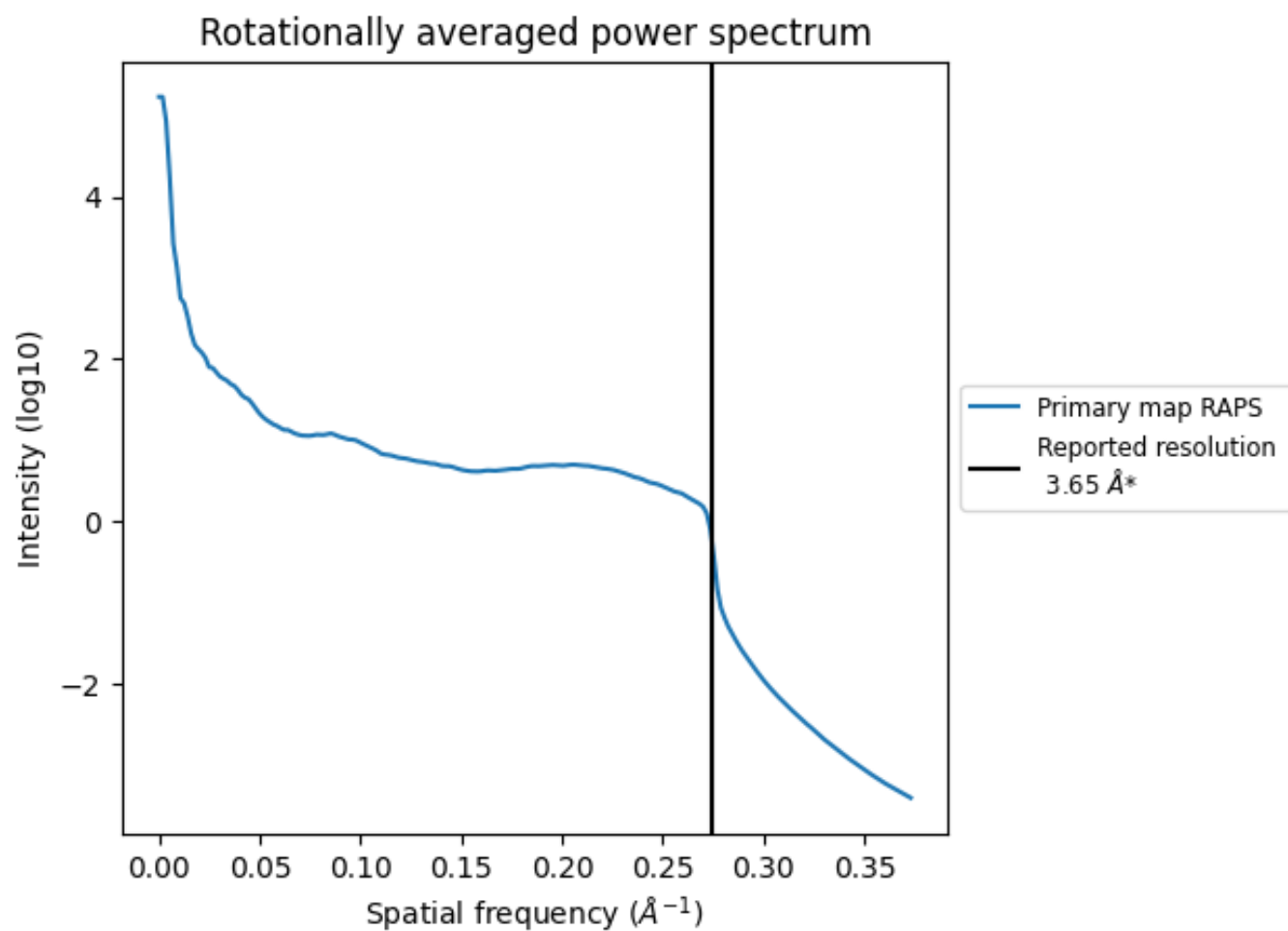
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1869 nm³; this corresponds to an approximate mass of 1688 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

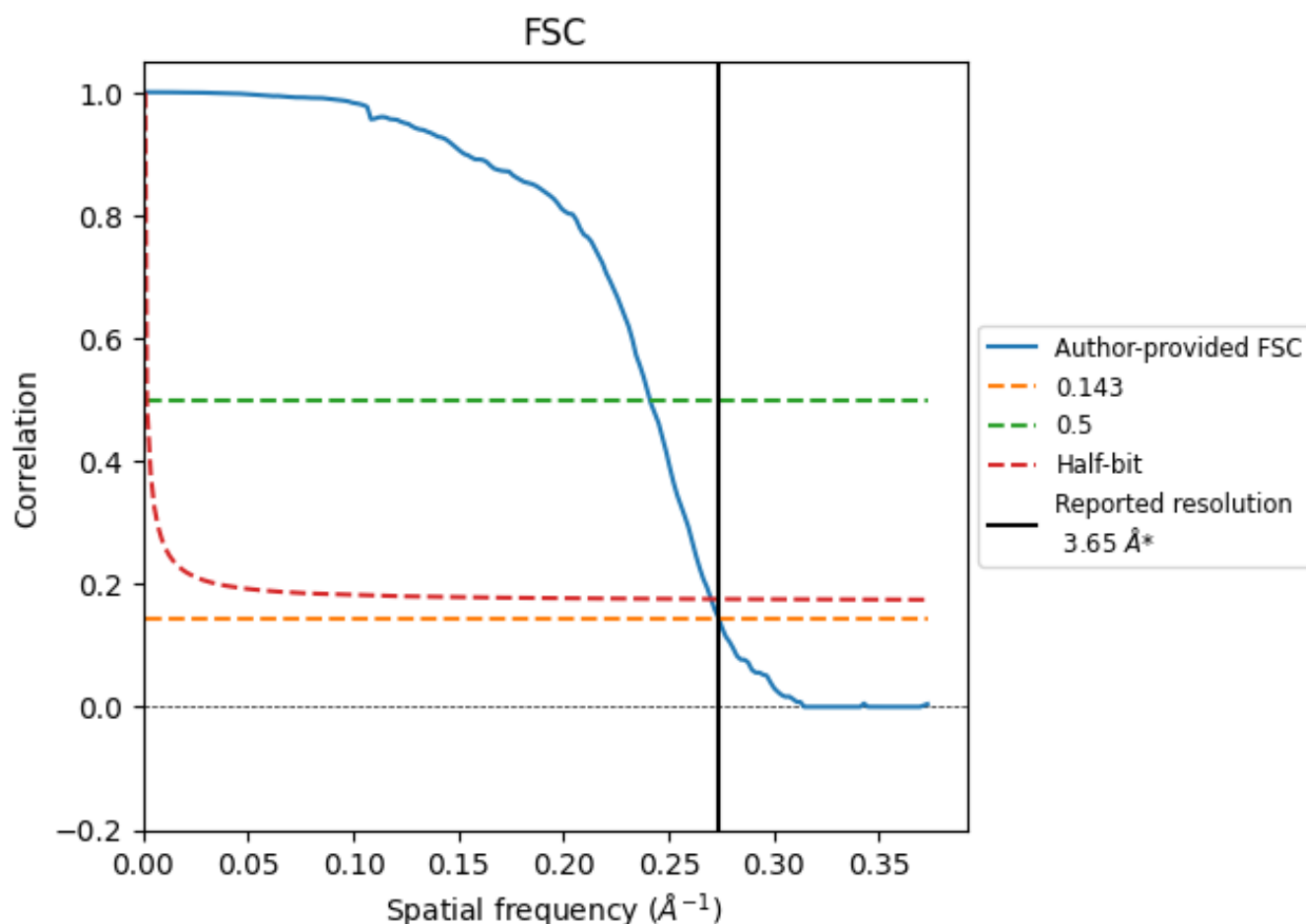


*Reported resolution corresponds to spatial frequency of 0.274 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.274 Å⁻¹

8.2 Resolution estimates [i](#)

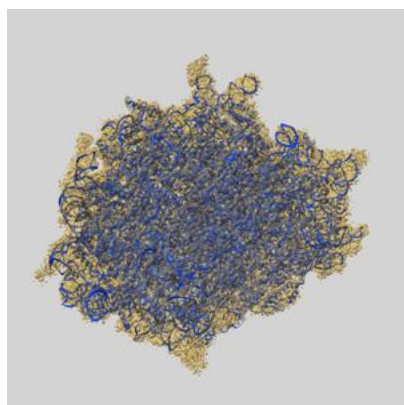
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.65	4.15	3.70
Unmasked-calculated*	-	-	-

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

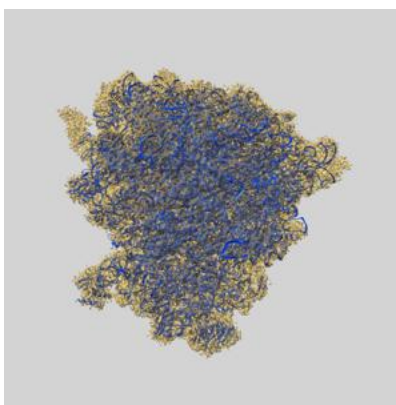
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3038 and PDB model 3JAG. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

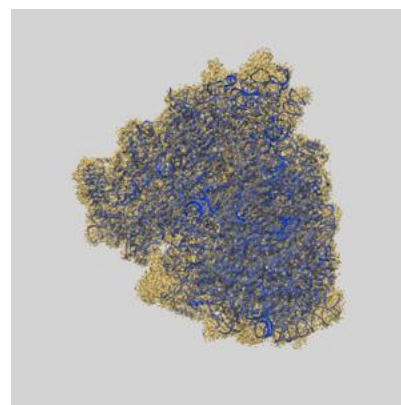
9.1 Map-model overlay [i](#)



X



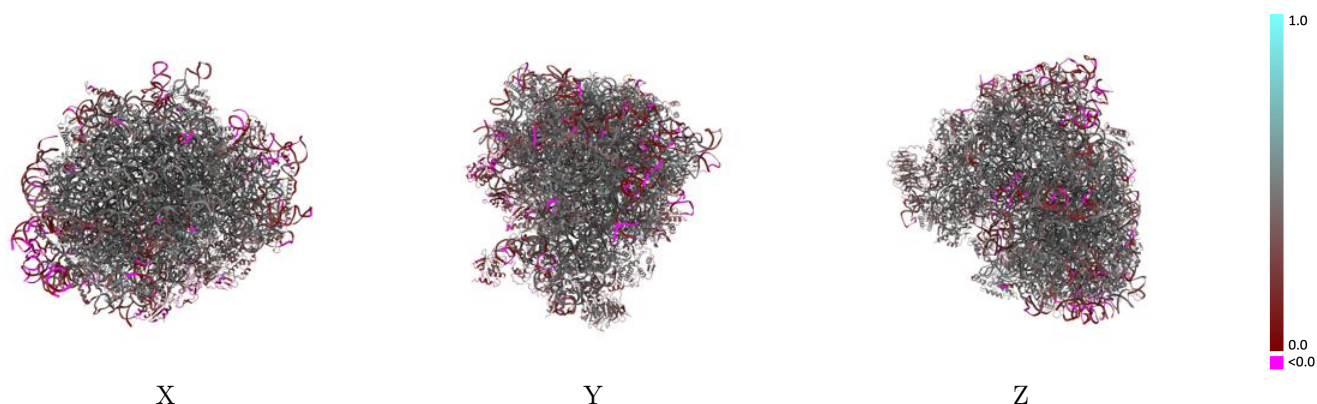
Y



Z

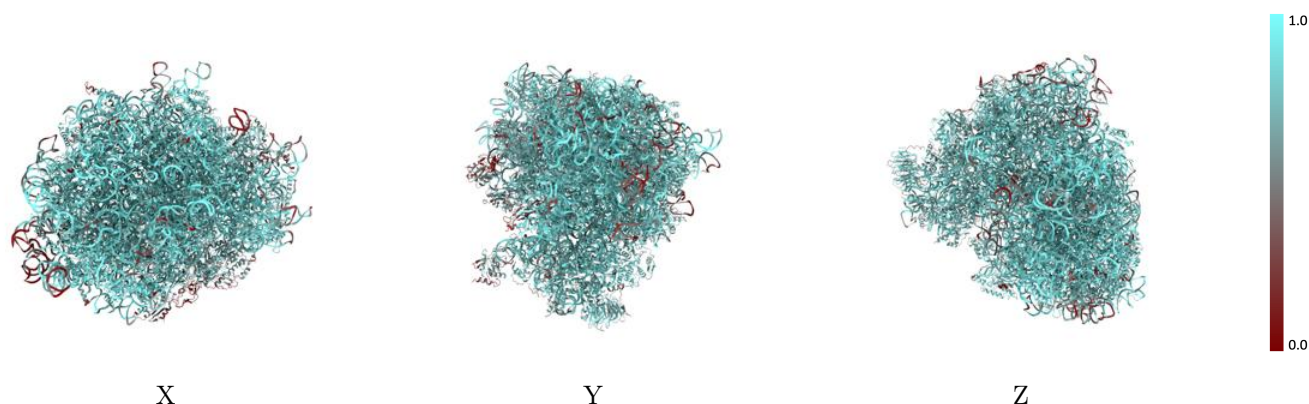
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



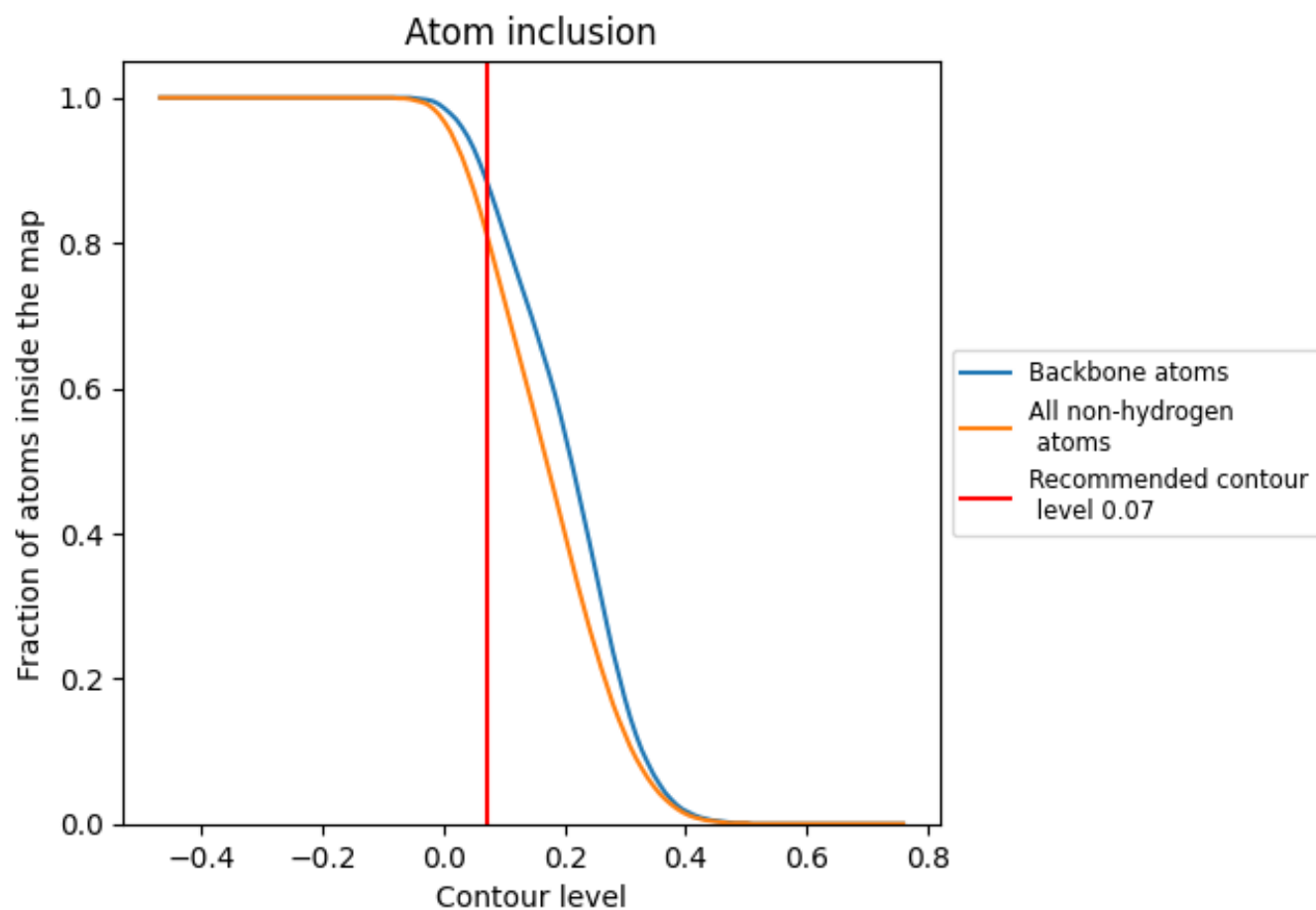
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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	 0.8150	 0.4070
1	 0.6450	 0.3920
2	 0.8280	 0.3460
3	 0.5520	 0.2200
5	 0.8480	 0.3910
7	 0.9380	 0.4610
8	 0.8870	 0.4200
9	 0.8600	 0.3980
A	 0.8420	 0.4900
AA	 0.7840	 0.4370
B	 0.8460	 0.4860
BB	 0.7820	 0.4540
C	 0.8440	 0.4820
CC	 0.7930	 0.4590
D	 0.8290	 0.4450
DD	 0.7190	 0.3880
E	 0.7710	 0.4070
EE	 0.8160	 0.4600
F	 0.8400	 0.4760
FF	 0.7330	 0.4060
G	 0.7540	 0.4060
GG	 0.7310	 0.3680
H	 0.8150	 0.4630
HH	 0.6820	 0.3600
I	 0.8160	 0.4650
II	 0.7770	 0.4170
J	 0.7870	 0.4180
JJ	 0.7860	 0.4310
KK	 0.7140	 0.3420
L	 0.8090	 0.4410
LL	 0.7600	 0.4370
M	 0.8540	 0.4690
MM	 0.4280	 0.1740
N	 0.8590	 0.4940
NN	 0.8050	 0.4650



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Chain	Atom inclusion	Q-score
O	 0.8330	 0.4750
OO	 0.7930	 0.4520
P	 0.8580	 0.4900
PP	 0.7050	 0.3530
Q	 0.8500	 0.4930
QQ	 0.7910	 0.4260
R	 0.8080	 0.4500
RR	 0.7110	 0.3590
S	 0.8530	 0.4820
SS	 0.7760	 0.3960
T	 0.8290	 0.4660
TT	 0.7830	 0.4150
U	 0.7940	 0.4020
UU	 0.7000	 0.3770
V	 0.8140	 0.4800
VV	 0.7670	 0.4250
W	 0.8370	 0.4770
WW	 0.8290	 0.4810
X	 0.8160	 0.4610
XX	 0.8090	 0.4770
Y	 0.8200	 0.4590
YY	 0.7730	 0.4000
Z	 0.8400	 0.4620
ZZ	 0.7360	 0.3890
a	 0.8760	 0.4960
aa	 0.8190	 0.4660
b	 0.7520	 0.4230
bb	 0.7500	 0.4230
c	 0.8310	 0.4650
cc	 0.7200	 0.4130
d	 0.8180	 0.4620
dd	 0.8320	 0.4540
e	 0.8560	 0.4900
ee	 0.6820	 0.3810
f	 0.8800	 0.4970
ff	 0.5010	 0.2120
g	 0.8180	 0.4590
gg	 0.7130	 0.3710
h	 0.8000	 0.4410
hh	 0.8250	 0.4200
i	 0.8150	 0.4370
ii	 0.6320	 0.3670

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Chain	Atom inclusion	Q-score
j	 0.8780	 0.4900
jj	 0.6430	 0.3640
k	 0.7650	 0.4000
l	 0.8440	 0.4800
m	 0.8290	 0.4620
n	 0.8210	 0.4510
o	 0.8210	 0.4670
p	 0.8040	 0.4750
r	 0.8630	 0.4900
s	 0.3310	 0.1170
t	 0.4520	 0.1540