



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 17, 2019 – 08:08 AM EST

PDB ID : 6HCF
EMDB ID: : EMD-0192
Title : Structure of the rabbit 80S ribosome stalled on globin mRNA at the stop codon
Authors : Juszkievicz, S.; Chandrasekaran, V.; Lin, Z.; Kraatz, S.; Ramakrishnan, V.;
Hegde, R.S.
Deposited on : 2018-08-14
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

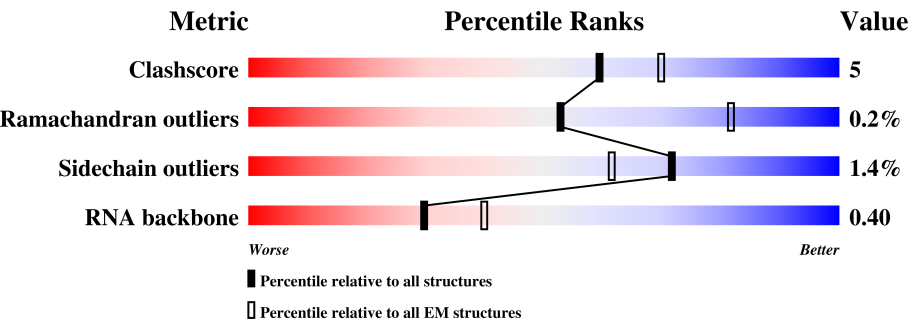
MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 Å.

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
















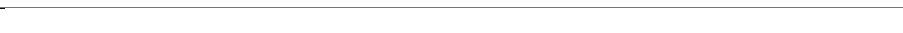

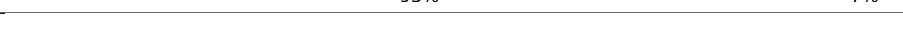
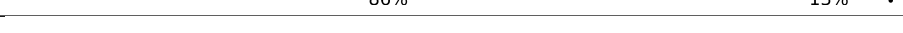
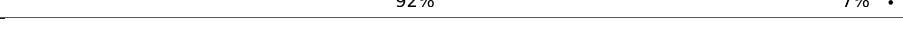



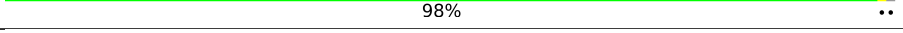

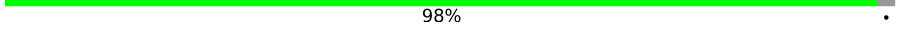

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A1	1869	56% 31% 5% • 7%
2	B1	295	65% 8% 26%
3	C1	264	67% 13% 19%
4	D1	293	68% 8% 25%
5	E1	243	78% 16% 6%
6	F1	263	90% 10%
7	G1	204	83% 7% 9%
8	H1	249	78% 18% 5%

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Mol	Chain	Length	Quality of chain
9	I1	194	 90%6%5%
10	J1	208	 86%13%.
11	K1	194	 85%9%.5%
12	L1	165	 53%5%42%
13	M1	158	 78%12%9%
14	N1	132	 67%20%.11%
15	O1	151	 92%7%.
16	P1	168	 70%10%.19%
17	Q1	145	 73%9%.17%
18	R1	146	 87%9%..
19	S1	135	 85%13%.
20	T1	152	 88%7%5%
21	U1	145	 87%10%..
22	V1	119	 76%8%16%
23	W1	83	 93%7%
24	X1	130	 86%13%.
25	Y1	143	 92%7%.
26	Z1	130	 83%12%5%
27	a1	125	 60%40%
28	b1	115	 88%12%
29	c1	84	 98%..
30	d1	69	 90%10%
31	e1	56	 98%.
32	f1	133	 40%.59%
33	g1	156	 43%.56%



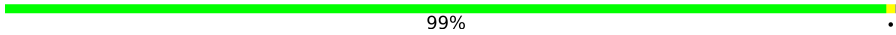



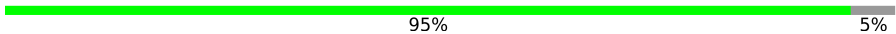
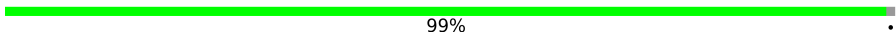

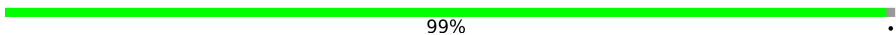
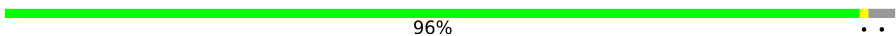


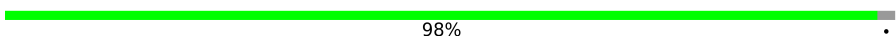

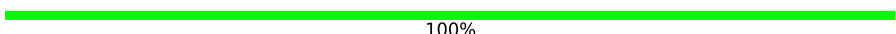
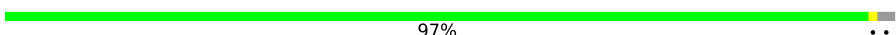
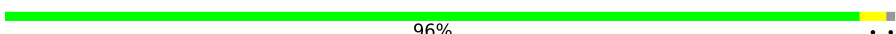


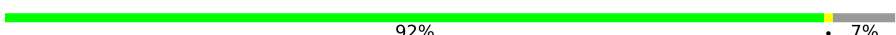




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Mol	Chain	Length	Quality of chain
34	h1	317	98% ..
35	j1	439	94% • 5%
36	k1	599	95% • •
37	52	3634	56% 34% 8% •
38	72	120	56% 38% • •
39	82	156	58% 34% • •
40	A3	257	69% 23% • • •
41	B3	403	83% 15% •
42	C3	425	79% 6% 15%
43	E3	291	64% 9% • 26%
44	F3	247	81% 11% 9%
45	H3	192	90% 9% •
46	L3	211	91% 8%
47	M3	218	56% 7% 37%
48	N3	204	81% 18%
49	O3	203	91% 6% •
50	P3	184	78% 5% 17%
51	Q3	188	91% 8% • •
52	R3	196	72% 17% • 8%
53	S3	176	89% 10% •
54	T3	160	89% 11% •
55	U3	128	63% 13% • 23%
56	V3	140	80% 13% • 6%
57	W3	157	55% 11% • 32%
58	X3	156	69% 6% 24%




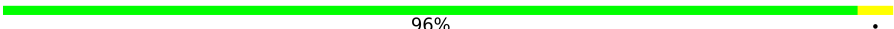
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Mol	Chain	Length	Quality of chain
59	Y3	145	 78%14%8%
60	Z3	136	 72%25%...
61	a3	148	 99%..
62	b3	226	 45%54%
63	c3	115	 83%15%
64	d3	125	 84%14%
65	e3	135	 95%5%
66	f3	110	 99%.
67	g3	117	 89%5%..
68	h3	123	 99%.
69	i3	105	 96%..
70	j3	97	 88%11%
71	k3	70	 94%..
72	l3	51	 98%.
73	m3	102	 50%49%
74	n3	25	 100%
75	o3	106	 97%..
76	p3	92	 96%..
77	r3	137	 89%9%
78	s3	318	 58%38%
79	t3	165	 92%7%
80	23	76	 66%26%8%
81	w3	23	 52%43%.
82	J3	178	 86%10%.
83	G3	319	 61%10%27%

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Mol	Chain	Length	Quality of chain
84	D3	297	 84%14%..
85	I3	214	 83%11%..
86	1	22	 68%9%23%
87	u3	217	 96%.

2 Entry composition

There are 91 unique types of molecules in this entry. The entry contains 226754 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	1732	Total	C	N	O	P	0	0
			36969	16502	6637	12099	1731		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 5 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 10 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 12 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 15 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 18 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R1	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 22 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V1	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W1	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X1	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y1	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z1	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a1	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b1	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 30 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d1	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 31 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f1	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 33 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g1	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 34 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h1	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a protein called eRF1(AAQ).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j1	419	Total	C	N	O	S	0	0
			3309	2106	562	629	12		

- Molecule 36 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k1	577	Total	C	N	O	S	0	0
			4555	2914	780	830	31		

- Molecule 37 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	52	3634	Total	C	N	O	P	0	0
			77819	34651	14241	25293	3634		

- Molecule 38 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	72	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 39 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	82	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 40 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A3	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 41 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B3	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 42 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	C3	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 43 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	E3	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 44 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	F3	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	61	ARG	GLY	conflict	UNP G1TUB1
F3	93	ARG	GLY	conflict	UNP G1TUB1
F3	131	MET	VAL	conflict	UNP G1TUB1
F3	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 45 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	H3	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 46 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L3	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 47 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M3	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 48 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N3	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 49 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O3	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 50 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	P3	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 51 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Q3	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 52 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	R3	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 53 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S3	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 54 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T3	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 55 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U3	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 56 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	V3	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 57 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	W3	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 58 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	X3	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 59 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Y3	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Z3	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 61 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	a3	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 62 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	b3	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 63 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c3	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 64 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	d3	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 65 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	e3	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 66 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	f3	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 67 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	g3	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 68 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	h3	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 69 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	i3	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j3	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 71 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k3	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 72 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	l3	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 73 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	m3	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 74 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	n3	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 75 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o3	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 76 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	p3	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 77 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	r3	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 78 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	s3	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 79 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	t3	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 80 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	23	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 81 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	w3	23	Total	C	N	O	P	0	0
			493	222	94	154	23		

- Molecule 82 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	J3	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 83 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	G3	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

- Molecule 84 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	D3	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 85 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	I3	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 86 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
86	1	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 87 is a protein called uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	u3	217	Total	C	N	O	S	0	0
			1741	1113	312	307	9		

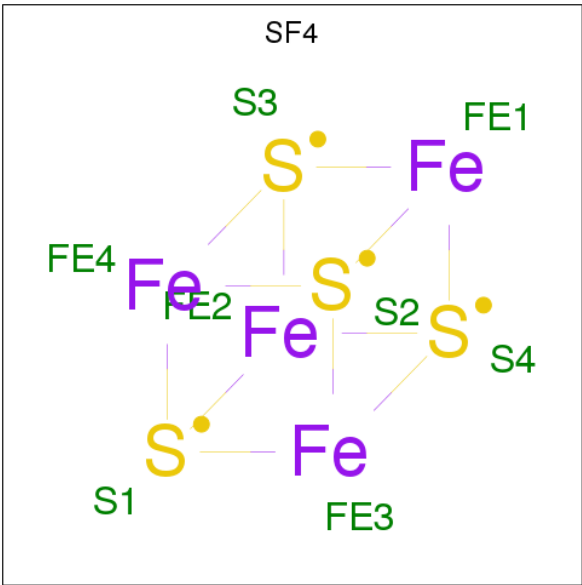
- Molecule 88 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	G1	1	Total 1	Mg 1	0
88	A1	77	Total 77	Mg 77	0
88	g3	1	Total 1	Mg 1	0
88	w3	1	Total 1	Mg 1	0
88	P3	1	Total 1	Mg 1	0
88	72	7	Total 7	Mg 7	0
88	52	204	Total 204	Mg 204	0
88	M1	1	Total 1	Mg 1	0
88	V3	1	Total 1	Mg 1	0
88	82	5	Total 5	Mg 5	0
88	a3	1	Total 1	Mg 1	0

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

Mol	Chain	Residues	Atoms		AltConf
89	g1	1	Total 1	Zn 1	0
89	g3	1	Total 1	Zn 1	0
89	e1	1	Total 1	Zn 1	0
89	p3	1	Total 1	Zn 1	0
89	m3	1	Total 1	Zn 1	0
89	b1	1	Total 1	Zn 1	0
89	j3	1	Total 1	Zn 1	0
89	o3	1	Total 1	Zn 1	0

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



Mol	Chain	Residues	Atoms			AltConf
90	k1	1	Total	Fe	S	0
			16	8	8	
90	k1	1	Total	Fe	S	0
			16	8	8	

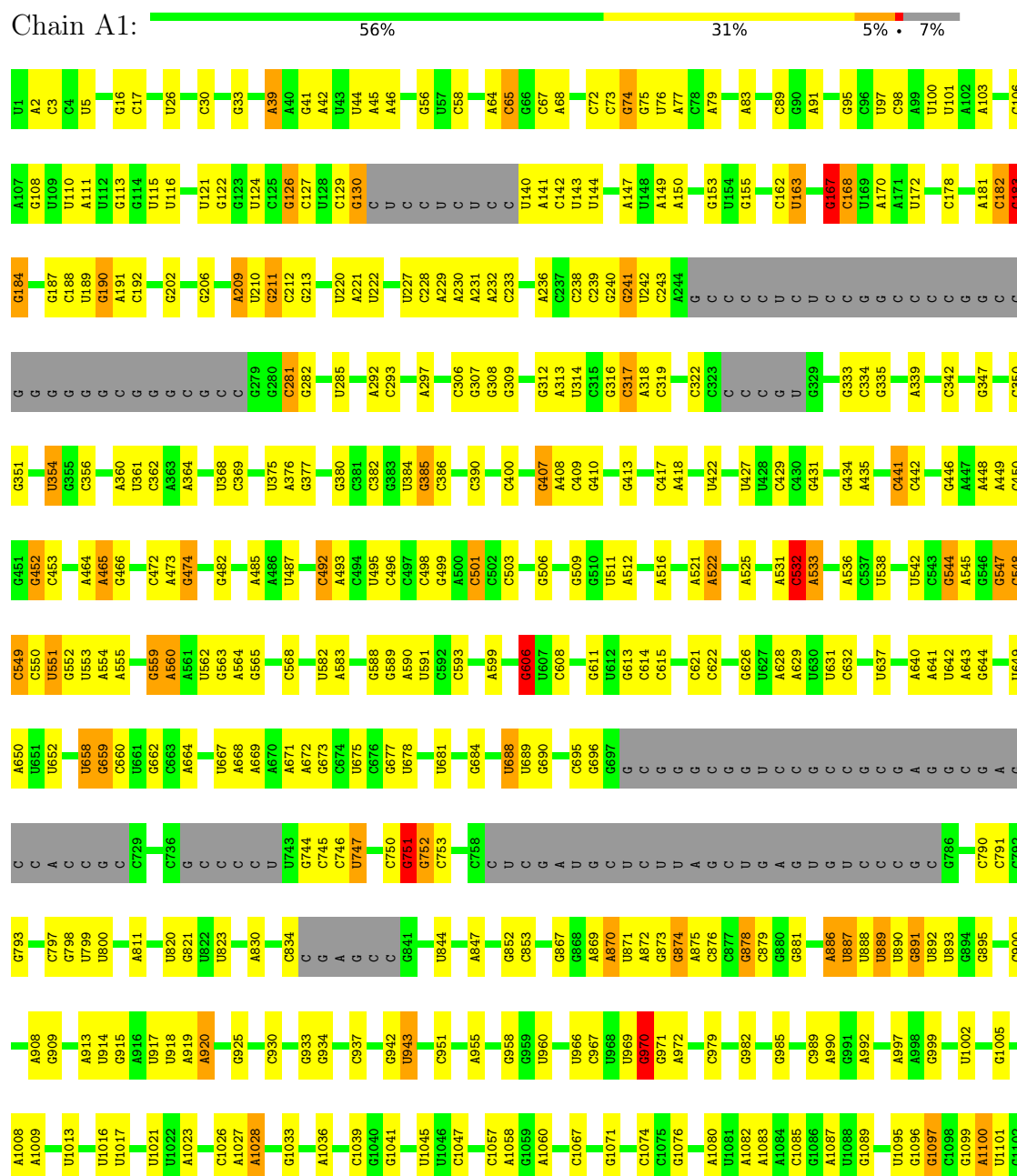
- Molecule 91 is water.

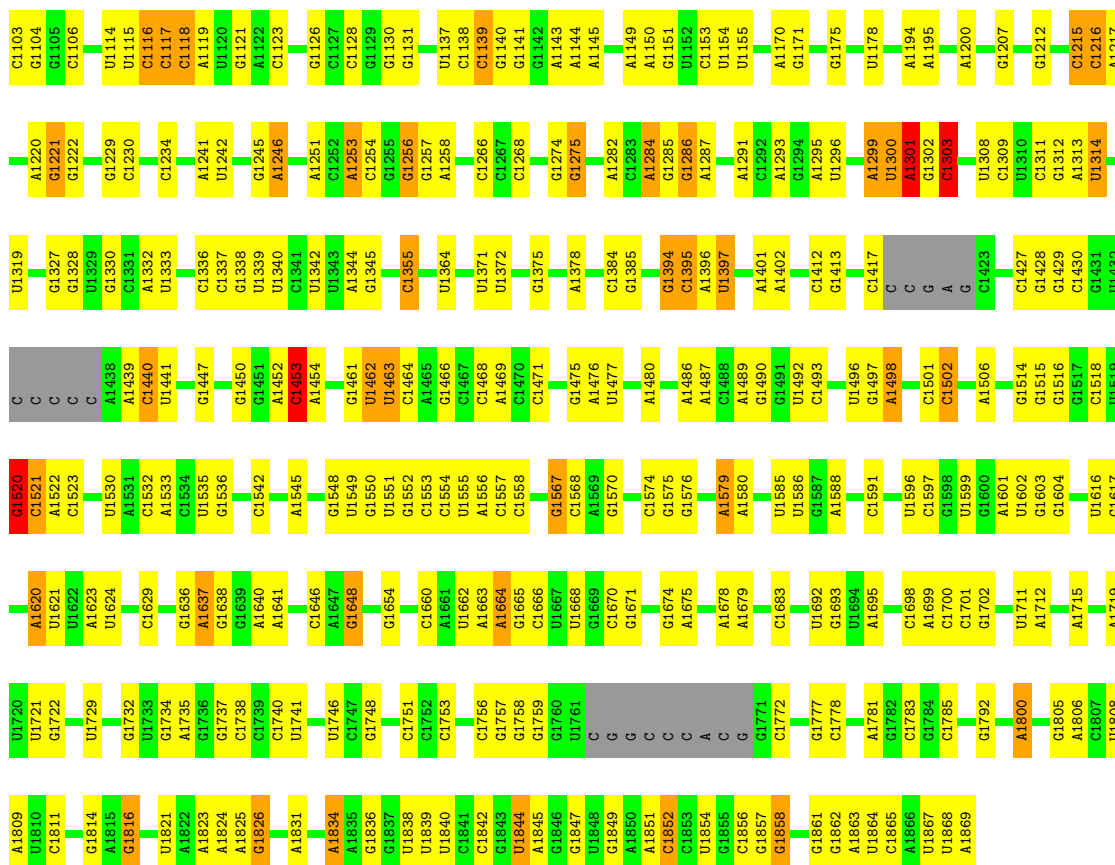
Mol	Chain	Residues	Atoms		AltConf
91	52	3	Total	O	0
			3	3	
91	1	1	Total	O	0
			1	1	

3 Residue-property plots

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

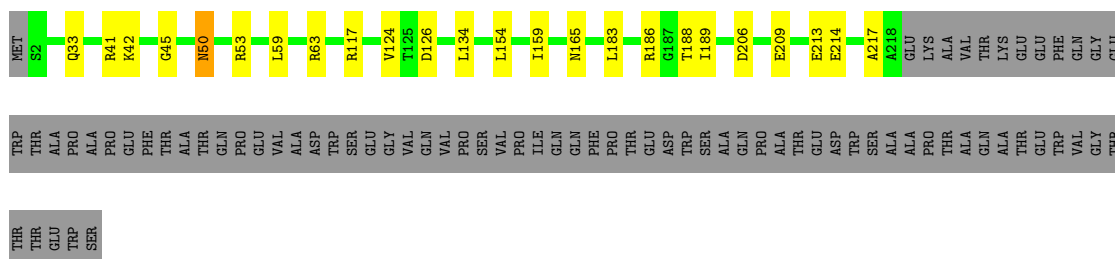
• Molecule 1: 18S ribosomal RNA





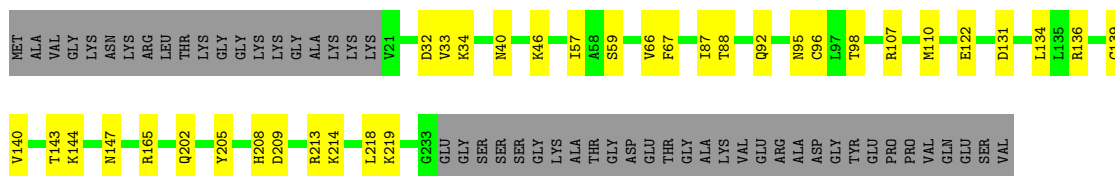
- Molecule 2: uS2

Chain B1:



- Molecule 3: 40S ribosomal protein S3a

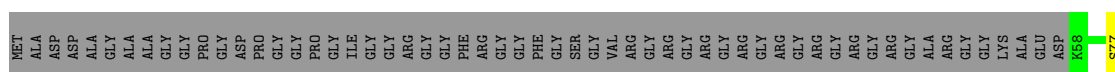
Chain C1:



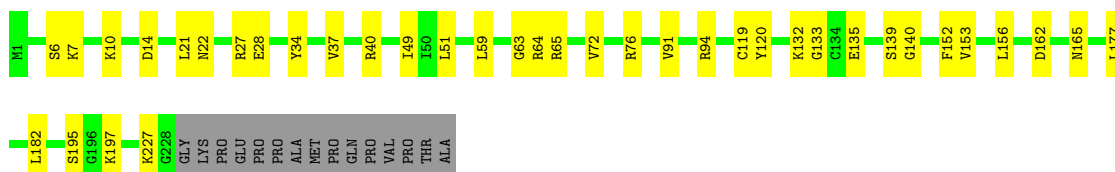
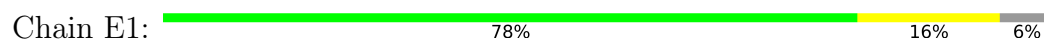
- Molecule 4: uS5

Chain D1:

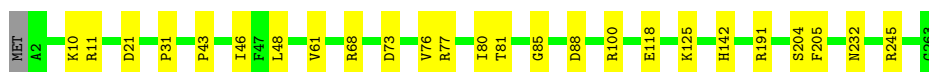




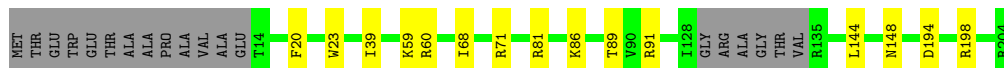
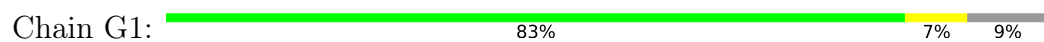
- Molecule 5: uS3



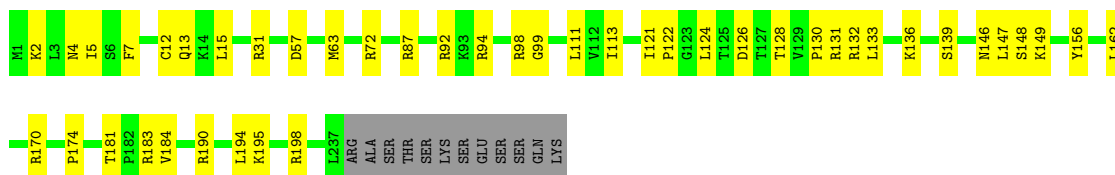
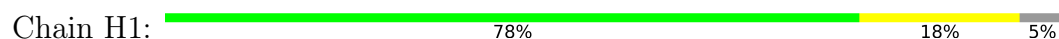
- Molecule 6: eS4



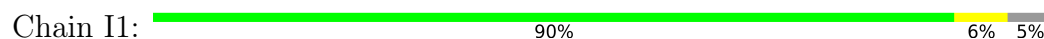
- Molecule 7: Ribosomal protein S5



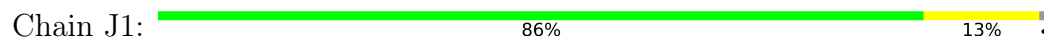
- Molecule 8: 40S ribosomal protein S6



- Molecule 9: 40S ribosomal protein S7



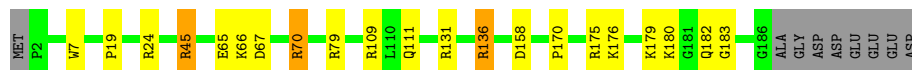
- Molecule 10: eS8





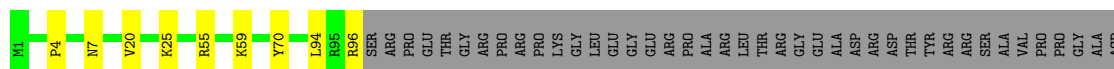
- Molecule 11: Ribosomal protein S9 (Predicted)

Chain K1: 85% 9% 5%



- Molecule 12: eS10

Chain L1: 53% 5% 42%



- Molecule 13: Ribosomal protein S11

Chain M1: 78% 12% 9%



- Molecule 14: 40S ribosomal protein S12

Chain N1: 67% 20% 11%



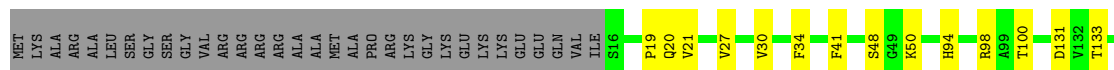
- Molecule 15: uS15

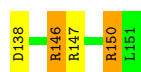
Chain O1: 92% 7% 1%



- Molecule 16: uS11

Chain P1: 70% 10% 19%





- Molecule 17: uS19

Chain Q1: 73% 9% 17%



- Molecule 18: Ribosomal protein S16

Chain R1: 87% 9% ..



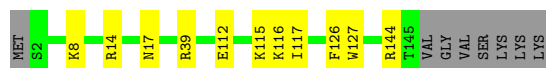
- Molecule 19: eS17

Chain S1: 85% 13% .



- Molecule 20: uS13

Chain T1: 88% 7% 5%



- Molecule 21: eS19

Chain U1: 87% 10% ..



- Molecule 22: uS10

Chain V1: 76% 8% 16%

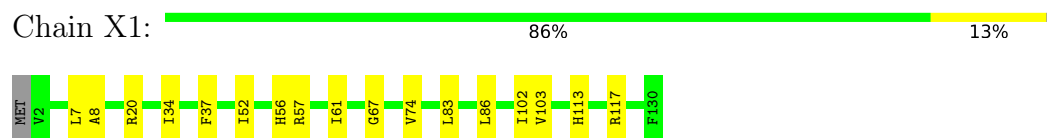


- Molecule 23: eS21

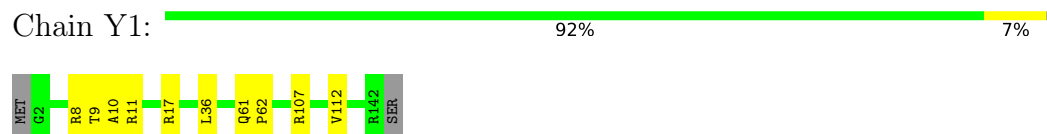
Chain W1: 93% 7%



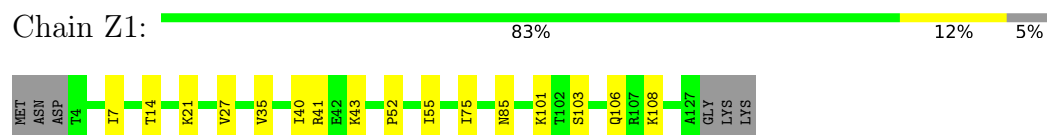
- Molecule 24: Ribosomal protein S15a



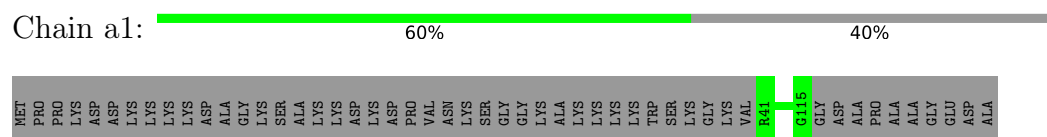
- Molecule 25: uS12



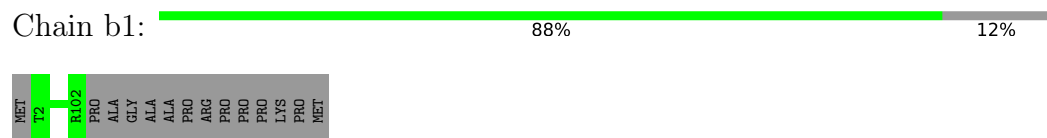
- Molecule 26: eS24



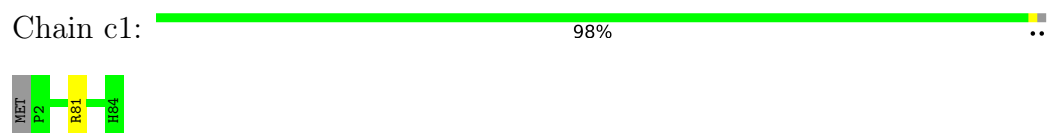
- Molecule 27: eS25



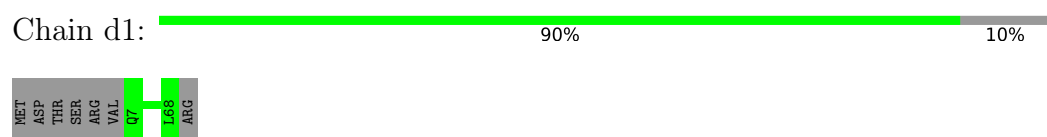
- Molecule 28: eS26



- Molecule 29: 40S ribosomal protein S27



- Molecule 30: Ribosomal protein S28



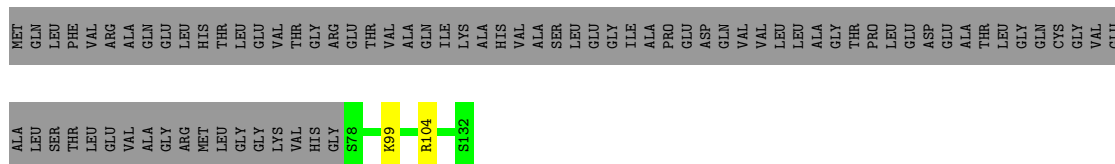
- Molecule 31: uS14





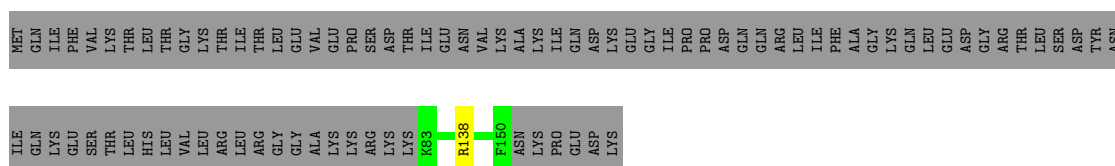
- Molecule 32: 40S ribosomal protein S30

Chain f1: 40% 59%



- Molecule 33: Ribosomal protein S27a

Chain g1: 43% 56%



- Molecule 34: RACK1

Chain h1: 98% ..



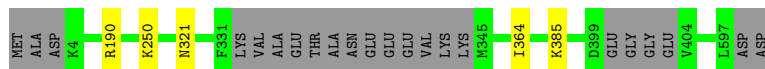
- Molecule 35: eRF1(AAQ)

Chain j1: 94% 5%



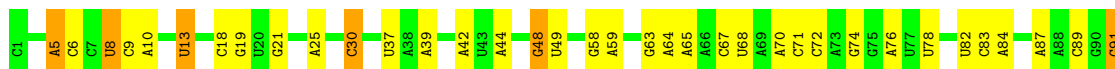
- Molecule 36: ATP binding cassette subfamily E member 1

Chain k1: 95% ..



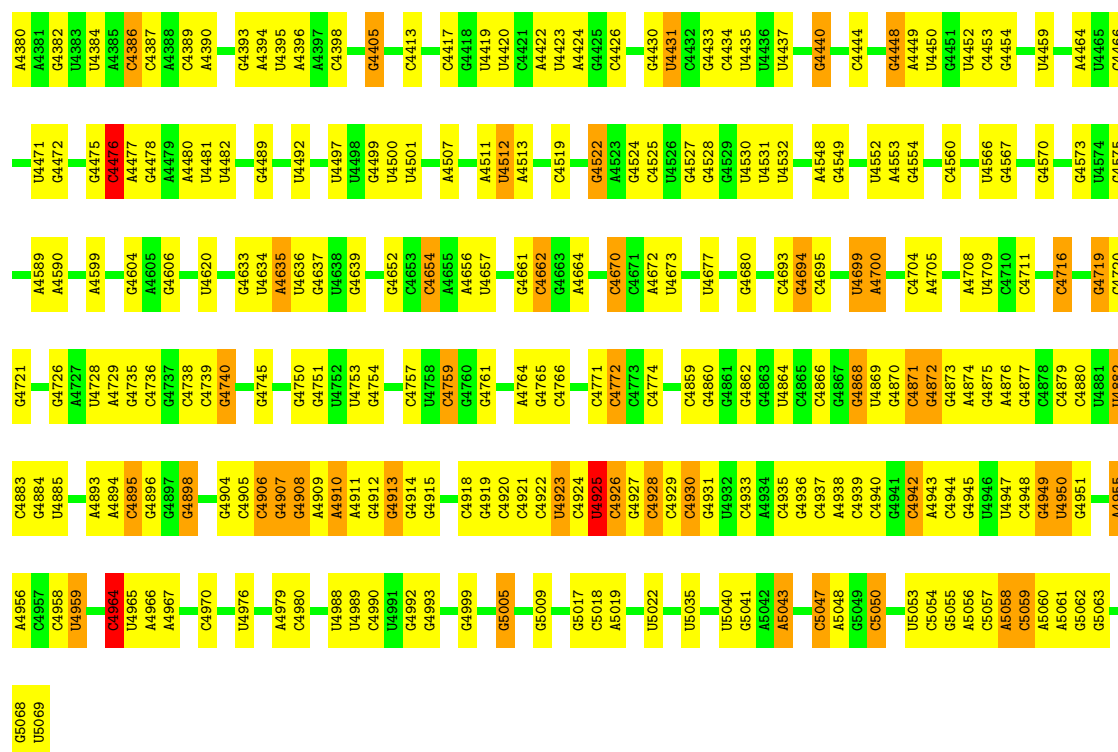
- Molecule 37: 28S ribosomal RNA

Chain 52: 56% 34% 8%

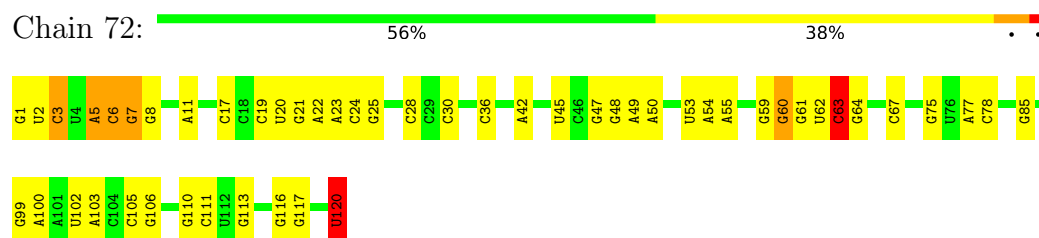


C1920	G1818	C1731	G1614	G1517	G1426	G1338	G1234	G1094	C941	C719	G497	C390	C276	C172	C92
C1921	G1819	G1734	G1624	A1518	C1429	U1341	G1235	A1095	G942	G720	C498	C390	G277	C173	G93
G1922	A1820	G1735	G1625	A1518	C1429	U1341	G1236	A1095	A943	G721	G499	A395	G280	C174	G94
C1924	G1821	G1736	G1626	C1521	G1434	C1346	G1237	U1100	A945	G722	G500	A396	G280	C175	G95
C1928	U1822	C1740	G1627	G1522	G1435	C1347	A1238	U1101	U946	G729	G504	A407	G292	G176	U96
A1929	G1823	G1741	A1631	A1523	C1436	C1347	G1239	U1102	C947	G730	G505	A407	G293	G179	C100
U1930	G1824	A1742	A1632	A1524	C1437	C1352	G1244	C1103	G948	G731	G506	A410	G294	C180	A101
C1931	C1828	A1746	G1633	U1531	U1440	G1353	G1245	C1104	G949	G732	U510	G411	U297	C181	G102
A1932	G1829	G1750	G1634	U1531	A1441	G1354	G1246	C1105	G950	A733	C515	G412	G301	G182	G104
G1933	U1834	G1751	C1635	A1534	U1356	U1356	G1272	C1106	G951	G737	C516	G413	A300	G191	A105
A1934	G1835	G1752	G1636	C1535	U1357	U1357	G1273	C1107	A855	C737	C517	G417	G301	G107	A106
C1935	A1837	G1753	A1637	C1536	C1446	G1358	C1276	C1108	A856	C738	C518	G417	G302	A197	G109
A1939	U1838	U1754	U1638	U1538	G1453	G1359	G1277	C1109	G959	C739	G641	G423	C303	U200	U108
G1940	G1842	C1755	U1639	G1539	G1454	G1360	G1278	C1110	A960	G740	G642	G423	A306	C201	G109
A1941	U1843	U1756	A1643	C1540	G1455	G1361	A1278	G1161	G961	G741	G648	G441	A307	G204	G114
U1942	G1844	G1758	G1456	G1543	C1456	G1362	G1280	G1162	G962	G743	A649	U440	G308	U204	C115
A1943	G1847	G1759	U1457	G1547	G1457	G1370	G1281	C1165	G969	G747	G661	U446	G309	G214	G119
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G1948	G1853	C1763	A1652	G1548	A1459	A1372	G1283	G1168	A966	G749	G664	C448	G311	G217	U122
G1951	G1854	G1764	G1654	G1549	G1460	A1373	U1285	G1169	C968	U750	G665	C449	G312	C218	U122
G1952	C1855	G1765	G1655	G1550	G1461	G1377	G1286	U1177	C969	G751	G666	C450	G315	C219	G126
A1956	C1856	A1767	G1658	G1551	C1462	G1378	G1287	G1178	G970	G755	A667	C451	U316	C220	C126
U1957	C1857	C1768	U1659	G1552	C1463	C1379	G1291	C1181	U971	C756	G668	A452	U321	C133	C134
A1958	U1858	G1769	U1660	A1553	C1464	G1380	C1292	G1182	G971A	G757	G669	U454	C322	G224	G135
U1959	G1859	C1772	C1661	G1556	G1472	U1381	G1293	C1183	C972	G758	G670	C455	C323	G225	C136
A1960	U1866	U1773	G1662	C1557	U1473	A1387	A1294	G1184	G978	G759	G671	A463	A324	C228	G137
G1961	A1867	G1774	C1663	A1558	G1474	A1388	U1295	G1185	U982	G760	G672	A463	U325	G229	G142
A1962	U1868	U1775	G1664	C1566	G1475	A1389	G1296	G1186	C904	G761	G673	U464	U326	G230	C143
C1963	G1869	A1776	C1665	C1476	C1477	G1390	U1297	G1187	C983	C905	G674	U465	U327	G231	C144
U1964	C1870	C1777	G1666	C1478	C1479	A1391	G1298	G1193	C984	C906	G675	U466	A334	G232	G145
G1968	G1878	A1767	A1668	G1570	G1479	A1392	G1299	G1194	C985	C907	G676	U467	C339	G233	G146
G1969	U1882	U1790	U1673	U1571	C1480	G1393	G1300	G1195	U989	U913	G679	U468	C340	G234	A147
A1970	C1882	C1791	C1674	G1573	C1481	G1394	C1301	G1196	C990	U914	G680	C474	G341	G236	C148
U1971	U1889	U1792	C1675	G1574	G1482	U1395	U1302	G1199	G1064	A915	G684	G475	C345	G237	U149
G1976	G1890	U1793	C1676	G1577	G1483	G1396	C1303	G1200	C916	C916	G685	C480	C346	G246	U150
C1977	A1891	U1796	U1677	U1578	G1484	A1397	C1304	U1201	A917	G918	G687	C481	A347	C250	G151
G1978	C1893	U1796	A1679	C1585	C1485	G1399	C1305	G1202	G918	G918	U688	C481A	G348	G257	U152
A1979	U1800	U1800	A1684	U1590	G1486	G1400	C1309	G1203	C922B	C922B	U688	C482	C349	C257	G153
U1980	A1801	A1801	U1684	U1591	G1487	G1403	C1310	G1205	C923	C923	G691	G483	C350	G260	G156
G1981	U1802	U1802	U1687	U1592	G1488	C1404	C1318	U1209	C924	C924	G696	G484	C351	G261	U157
U1982	G1803	G1803	U1688	G1592	G1489	C1405	G1321	G1210	G925	G925	G697	U485	C358	G262	A158
A1983	A1804	A1804	G1689	U1596	G1490	G1406	G1321	C1210	G926	G926	G697	C486	C358	G263	C159
U1984	U1806	U1806	G1690	G1597	G1493	G1406C	A1324	G1211	G929	G929	G700	G487	C367	G264	G160
A1990	G1807	C1807	G1691	U1602	A1497	C1411	G1325	G1212	A929	A929	G700	G488	C367	C265	G161
A1991	C1808	C1808	C1720	G1605	G1498	G1411A	A1326	G1213	G930	G930	C704	G489	C379	C266	U162
U1992	G1809	G1809	C1720	G1605	C1501	C1414	G1329	G1215	A932	A932	G705	C490	G379	G267	G164
C1993	G1810	G1810	G1724	U1609	G1502	C1419	A1330	C1216	G934	G934	C709	C493	A383	G268	C168
C1994	U1811	U1811	U1725	U1609	G1505	G1419	G1331	G1219	C935	C935	C713	C494	A384	U272	C169
G1995	C1812	C1812	A1729	G1612	C1505	A1420	A1332	G1220	C935A	C935A	C714	C495	A386	C275	C170
U1997	U1918	U1918	A1730	A1613	U1514	G1425	A1333	G1221	G1090	G1090	G714	G496	C387		U171

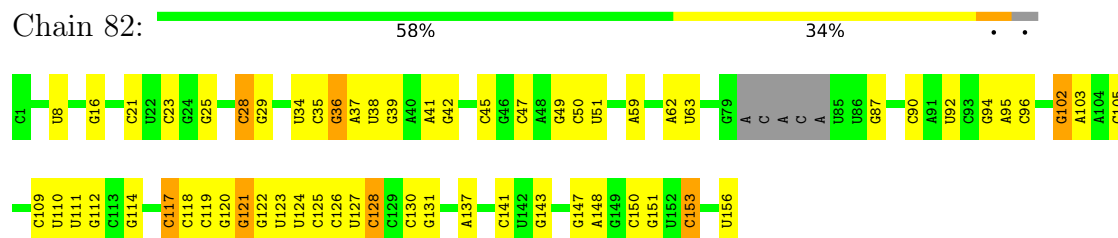
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C2076	C2081	U2084	G2085	A2088	G2089	G2091	G2092	G2093	G2094	A2097	G2014	G2015	C2016	C2019	U2020	C2021	C2022	G2023	G2024	A2025	A2026	G2112	G2113	C2158	G2159	G2160	G2261	G2262	A2263	U2267	A2268	G2269	G2270	G2274	G2275	C2276	G2277	G2278	G2279	G2280	U2281	G2284	A2285	G2286	C2289	G2294	G2295	A2300	G2301	C2392	C2393	G2396	A2397	G2398	G2399	G2400	G2407	G2408	C2461	U2469	U2495	G2496	U2499	U2500	C2501	A2502	G2503	G2504	C2505	G2506	A2507	U2508	A2511	A2512	A2513	G2516	G2521	G2528	A2529	C2532	C2533	G2534	G2535	A2536	G2537	U2538	C2539	G2542	A2543	G2544	U2545	G2549	G2550	A2551	G2552	G2555	G2556	C2561	G2562	U2563	G2566	U2570	C2571	A2572	G2573	G2574	U2575	G2576	C2577	G2578	U2580	A2581	A2582	C2583	A2587	C2588	C2589	G2590	U2591	U2592	C2593	C2594	C2595	C2596	C2597	C2600	A2601	C2604	C2607	G2608	G2609	G2610	A2611	G2620	A2621	G2622	A2623	G2624	C2627	U2631	U2633	G2639	G2647	C2653	C2654	C2655	G2656	C2657	G2658	A2659	G2662	G2663	G2664	U2665	G2667	G2668	C2669	C2670	A2674	G2675	A2676	G2677	C2683	C2684	C2685	G2686	G2687	G2688	C2689	G2693	A2694	A2695	A2696	A2697	U2701	G2702	G2703	G2706	U2707	G2708	C2709	G2710	G2711	G2712	G2713	G2714	G2715	C2716	C2719	G2722	U2723	A2724	A2725	G2726	G2732	G2735	C2738	C2739	U2740	G2742	A2743	A2744	U2747	G2748	C2749	G2750	G2751	G2752	G2753	G2754	A2755	G2756	A2757	G2758	G2759	G2760	U2761	G2762	A2763	A2764	A2765	G2766	U2767	C2768	U2769	G2778	C2779	G2780	A2781	U2782	G2783	A2784	G2785	G2786	G2787	G2788	C2789	G2790	A2791	G2792	G2793	G2794	A2795	G2796	G2797	G2798	G2799	U2800	U2801	C2804	C2805	A2806	A2807	G2808	U2809	U2810	G2811	A2812	A2813	G2817	U2821	G2822	G2823	U2826	G2827	U2837	G2838	G2842	A2843	A2844	A2845	A2846	A2847	A2848	A2849	A2850	G2851	G2854	G2855	G2856	A2857	A2858	G2862	G2863	A2864	C2872	U2873	U2874	G2875	G2876	G2877	G2878	C2879	G2880	G2881	A2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	U2891	A2895	G2896	G2897	G2898	C2899	A2900	G2901	A2902	A2903	G2904	A2905	A2906	G2907	A2908	C2909	U2910	C2911	C2912	C2913	U2914	C2915	C2916	C2917	C2918	C2919	C2920	U2921	C2922	C2923	C2924	C2925	C2926	A3635	G3636	G3637	G3638	A3642	A3643	G3644	A3645	A3646	A3649	C3650	A3651	G3654	C3660	G3661	A3662	G3663	G3664	C3667	C3668	G3673	A3674	G3675	A3676	A3677	A3678	U3679	A3680	A3682	C3683	G3684	C3685	U3688	G3689	U3690	G3691	A3692	C3696	G3705	C3706	U3707	C3708	U3709	G3710	G3711	A3712	U3713	A3714	G3715	U3822	G3823	G3824	G3825	C3716	A3717	U3729	U3730	C3731	A3732	C3733	U3734	G3735	A3736	G3743	G3744	U3822	A3825	C3834	C3837	U3838	G3839	U3840	C3841	C3842	C3843	U3844	A3845	U3846	A3847	C3848	A3849	A3850	A3851	G3852	A3853	G3857	C3858	A3865	C3866	A3867	G3868	C3869	C3870	A3871	A3872	A3873	A3874	A3875	A3876	A3877	C3878	C3879	G3880	G3881	C3882	G3883	G3884	U3885	C3886	A3887	A3888	A3889	G3890	C3891	A3892	A3893	G3894	C3895	G3896	C3897	A3901	A3902	A3903	A3904	C3905	A3906	G3907	A3908	C3909	U3910	C3911	C3912	C3913	U3914	C3915	C3916	C3917	C3918	C3919	U3920	U3921	U3922	U3923	U3924	U3925	U3926	U3927	U3928	U3929	U3930	U3931	U3932	U3933	U3934	U3935	U3936	U3937	U3938	U3939	U3940	U3941	U3942	U3943	U3944	U3945	U3946	U3947	U3948	U3949	U3950	U3951	U3952	U3953	U3954	U3955	U3956	U3957	U3958	U3959	U3960	U3961	U3962	U3963	U3964	U3965	U3966	U3967	U3968	U3969	U3970	U3971	U3972	U3973	U3974	U3975	U3976	U3977	U3978	U3979	U3980	U3981	U3982	U3983	U3984	U3985	U3986	U3987	U3988	U3989	U3990	U3991	U3992	U3993	U3994	U3995	U3996	U3997	U3998	U3999	U4000	U4001	U4002	U4003	U4004	U4005	U4006	U4007	U4008	U4009	U4010	U4011	U4012	U4013	U4014	U4015	U4016	U4017	U4018	U4019	U4020	U4021	U4022	U4023	U4024	U4025	U4026	U4027	U4028	U4029	U4030	U4031	U4032	U4033	U4034	U4035	U4036	U4037	U4038	U4039	U4040	U4041	U4042	U4043	U4044	U4045	U4046	U4047	U4048	U4049	U4050	U4051	U4052	U4053	U4054	U4055	U4056	U4057	U4058	U4059	U4060	U4061	U4062	U4063	U4064	U4065	U4066	U4067	U4068	U4069	U4070	U4071	U4072	U4073	U4074	U4075	U4076	U4077	U4078	U4079	U4080	U4081	U4082	U4083	U4084	U4085	U4086	U4087	U4088	U4089	U4090	U4091	U4092	U4093	U4094	U4095	U4096	U4097	U4098	U4099	U4100	U4101	U4102	U4103	U4104	U4105	U4106	U4107	U4108	U4109	U4110	U4111	U4112	U4113	U4114	U4115	U4116	U4117	U4118	U4119	U4120	U4121	U4122	U4123	U4124	U4125	U4126	U4127	U4128	U4129	U4130	U4131	U4132	U4133	U4134	U4135	U4136	U4137	U4138	U4139	U4140	U4141	U4142	U4143	U4144	U4145	U4146	U4147	U4148	U4149	U4150	U4151	U4152	U4153	U4154	U4155	U4156	U4157	U4158	U4159	U4160	U4161	U4162	U4163	U4164	U4165	U4166	U4167	U4168	U4169	U4170	U4171	U4172	U4173	U4174	U4175	U4176	U4177	U4178	U4179	U4180	U4181	U4182	U4183	U4184	U4185	U4186	U4187	U4188	U4189	U4190	U4191	U4192	U4193	U4194	U4195	U4196	U4197	U4198	U4199	U4200	U4201	U4202	U4203	U4204	U4205	U4206	U4207	U4208	U4209	U4210	U4211	U4212	U4213	U4214	U4215	U4216	U4217	U4218	U4219	U4220	U4221	U4222	U4223	U4224	U4225	U4226	U4227	U4228	U4229	U4230	U4231	U4232	U4233	U4234	U4235	U4236	U4237	U4238	U4239	U4240	U4241	U4242	U4243	U4244	U4245	U4246	U4247	U4248	U4249	U4250	U4251	U4252	U4253	U4254	U4255	U4256	U4257	U4258	U4259	U4260	U4261	U4262	U4263	U4264	U4265	U4266	U4267	U4268	U4269	U4270	U4271	U4272	U4273	U4274	U4275	U4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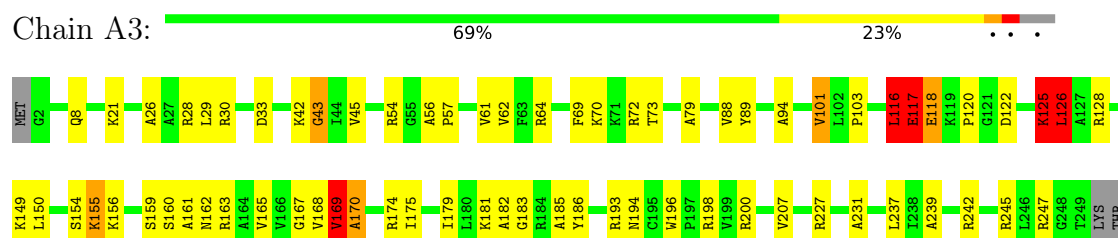
• Molecule 38: 5S ribosomal RNA



• Molecule 39: 5.8S ribosomal RNA



• Molecule 40: Ribosomal protein L8



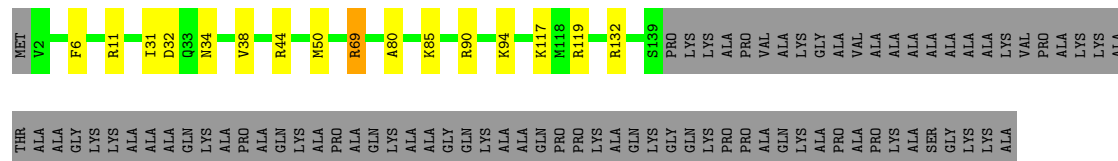
- Molecule 46: eL13

Chain L3:  91% 8%



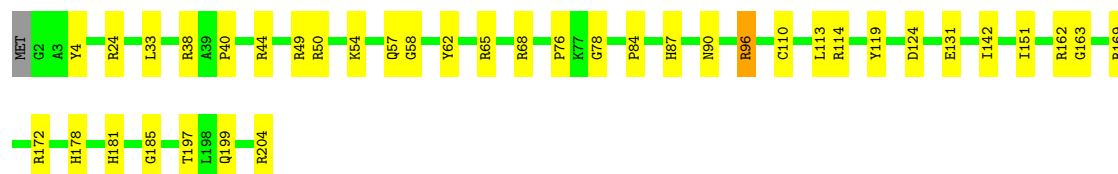
- Molecule 47: Ribosomal protein L14

Chain M3: 



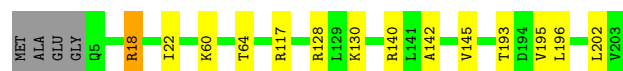
- Molecule 48: Ribosomal protein L15

Chain N3: 81% 18%




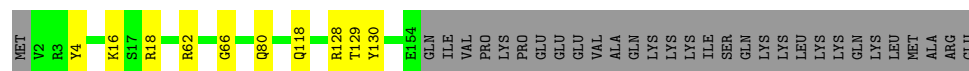
- Molecule 49: uL13

Chain O3: 91% 6%



- Molecule 50: uL22

Chain P3: 



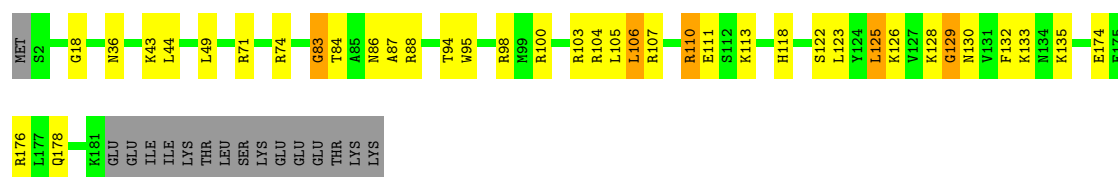
- Molecule 51: eL18

Chain Q3:  91% 8% ..



- Molecule 52: eL19

Chain R3: 72% 17% 8%



- Molecule 53: eL20

Chain S3: 89% 10% .



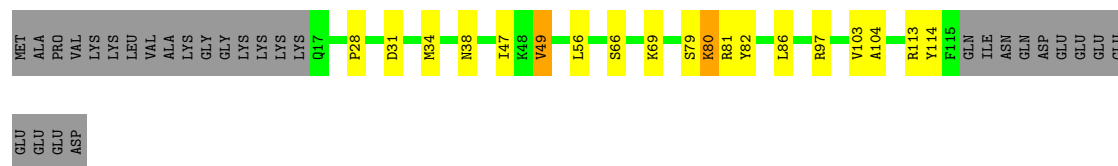
- Molecule 54: eL21

Chain T3: 89% 11% .



- Molecule 55: eL22

Chain U3: 63% 13% 23%



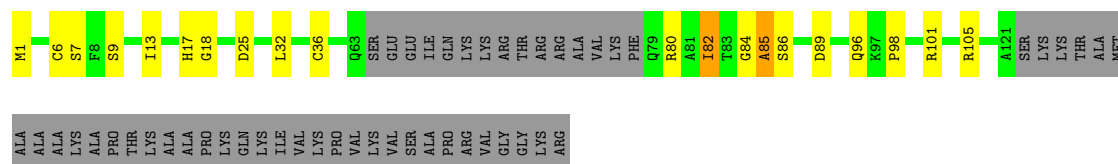
- Molecule 56: Ribosomal protein L23

Chain V3: 80% 13% 6%



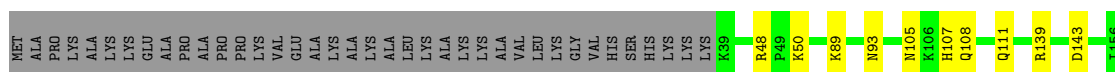
- Molecule 57: eL24

Chain W3: 55% 11% 32%

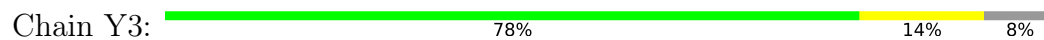


- Molecule 58: uL23

Chain X3: 69% 6% 24%



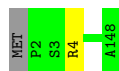
- Molecule 59: Ribosomal protein L26



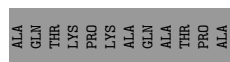
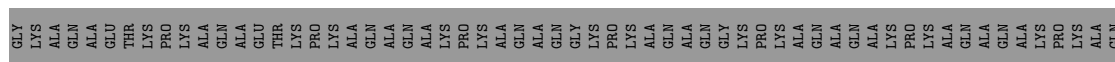
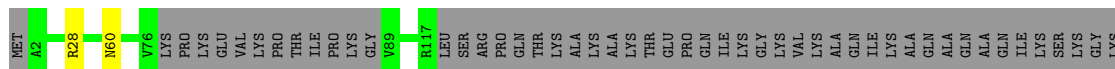
- Molecule 60: 60S ribosomal protein L27



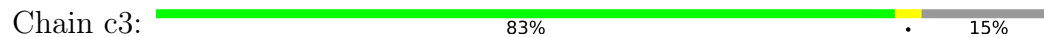
- Molecule 61: uL15



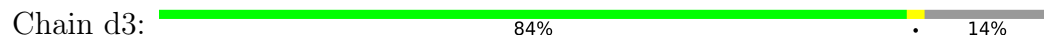
- Molecule 62: eL29

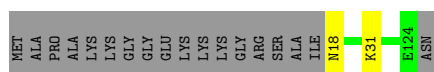


- Molecule 63: eL30



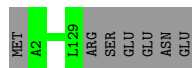
- Molecule 64: eL31





- Molecule 65: eL32

Chain e3: 95% 5%



- Molecule 66: eL33

Chain f3: 99% .



- Molecule 67: eL34

Chain g3: 89% 5% . .



- Molecule 68: uL29

Chain h3: 99% .



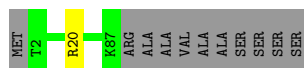
- Molecule 69: 60S ribosomal protein L36

Chain i3: 96% . .



- Molecule 70: Ribosomal protein L37

Chain j3: 88% . 11%



- Molecule 71: eL38

Chain k3: 94% . .



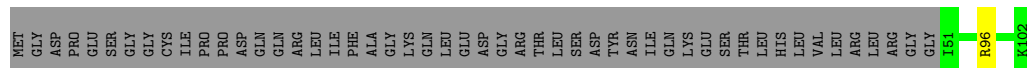
- Molecule 72: eL39

Chain l3:  98%



- Molecule 73: eL40

Chain m3:  50% 49%



- Molecule 74: eL41

Chain n3:  100%

There are no outlier residues recorded for this chain.

- Molecule 75: eL42

Chain o3:  97%



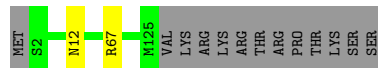
- Molecule 76: eL43

Chain p3:  96%



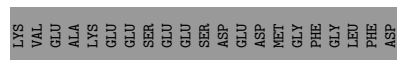
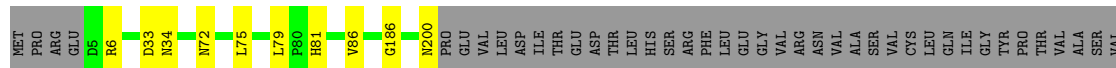
- Molecule 77: eL28

Chain r3:  89% 9%



- Molecule 78: uL10

Chain s3:  58% 38%



- Molecule 79: Ribosomal protein L12

Chain t3: 92% . 7%



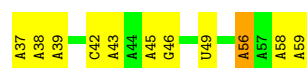
- Molecule 80: P-site tRNA

Chain 23:  66% 26% 8%



- Molecule 81: mRNA

Chain w3:  52% 43% .



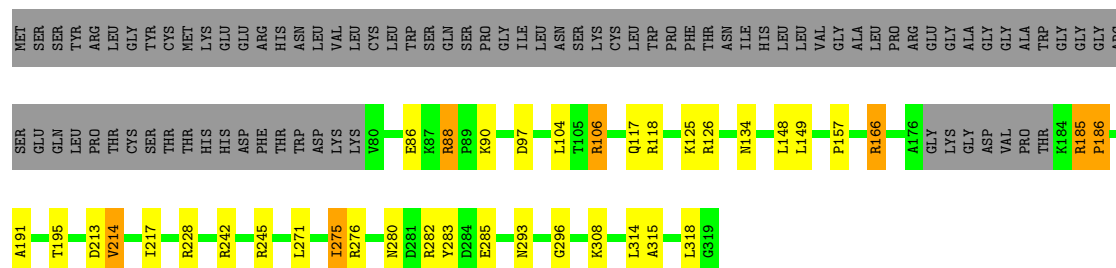
- Molecule 82: Ribosomal protein L11

Chain J3: 86% 10% .

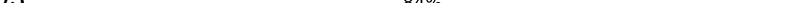


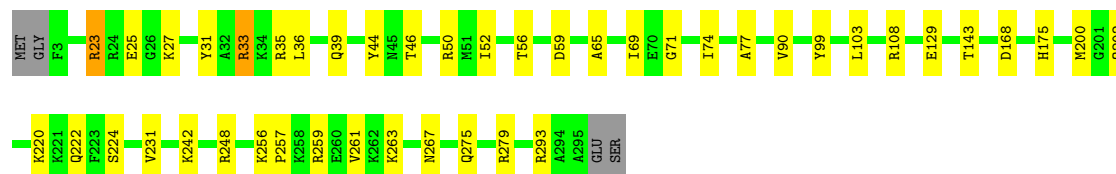
- Molecule 83: eL8

Chain G3:  61% 10% 27%

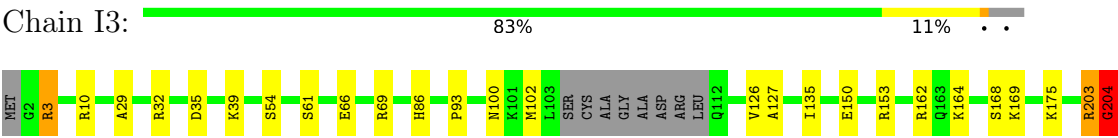


- Molecule 84: 60S ribosomal protein L5

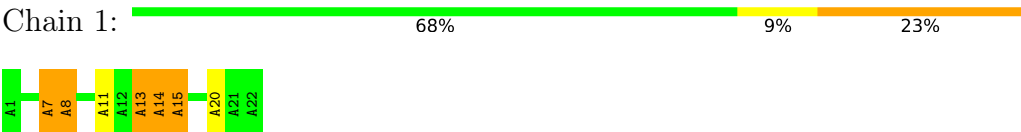
Chain D3:  84% 14%



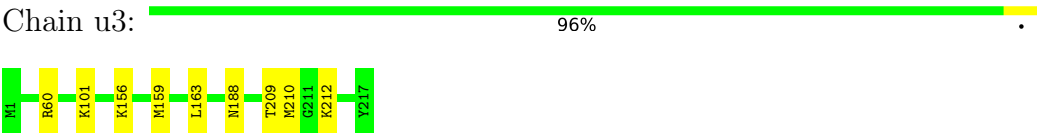
- Molecule 85: 60S ribosomal protein L10



● Molecule 86: nascent chain



● Molecule 87: uL1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	71954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.79	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A1	1.76	9/41324 (0.0%)	1.12	170/64370 (0.3%)
10	J1	0.42	0/1715	0.57	0/2287
11	K1	0.38	0/1550	0.60	0/2069
12	L1	0.37	0/834	0.59	0/1125
13	M1	0.45	0/1195	0.57	0/1597
14	N1	0.32	0/918	0.65	1/1233 (0.1%)
15	O1	0.39	0/1226	0.55	0/1649
16	P1	0.39	0/1029	0.57	0/1380
17	Q1	0.42	0/1017	0.60	0/1358
18	R1	0.41	0/1146	0.59	0/1534
19	S1	0.35	0/1082	0.55	0/1452
2	B1	0.39	0/1747	0.57	0/2374
20	T1	0.39	0/1208	0.59	0/1618
21	U1	0.39	0/1115	0.57	0/1493
22	V1	0.33	0/805	0.54	0/1081
23	W1	0.40	0/643	0.59	0/860
24	X1	0.42	0/1051	0.58	0/1406
25	Y1	0.43	0/1116	0.59	0/1490
26	Z1	0.36	0/1028	0.53	0/1366
27	a1	0.37	0/604	0.67	0/810
28	b1	0.42	0/828	0.54	0/1109
29	c1	0.36	0/665	0.57	0/891
3	C1	0.38	0/1756	0.58	1/2350 (0.0%)
30	d1	0.38	0/490	0.55	0/656
31	e1	0.44	0/470	0.57	0/623
32	f1	0.35	0/447	0.51	0/587
33	g1	0.28	0/567	0.57	0/753
34	h1	0.34	0/2493	0.58	0/3394
35	j1	0.35	0/3363	0.57	1/4523 (0.0%)
36	k1	0.36	0/4640	0.57	0/6264
37	52	2.86	72/87026 (0.1%)	1.46	556/135683 (0.4%)
38	72	5.70	7/2858 (0.2%)	1.28	21/4455 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	82	1.02	0/3581	1.12	14/5577 (0.3%)
4	D1	0.44	0/1753	0.58	0/2369
40	A3	0.56	2/1936 (0.1%)	0.85	7/2596 (0.3%)
41	B3	0.51	0/3240	0.63	3/4339 (0.1%)
42	C3	0.53	0/2937	0.63	1/3946 (0.0%)
43	E3	2.24	3/1762 (0.2%)	0.69	3/2362 (0.1%)
44	F3	0.57	0/1911	0.61	0/2549
45	H3	0.47	0/1535	0.60	0/2063
46	L3	0.50	0/1733	0.62	0/2316
47	M3	0.52	0/1158	0.59	0/1547
48	N3	0.58	0/1746	0.64	0/2338
49	O3	0.53	0/1662	0.65	1/2222 (0.0%)
5	E1	0.38	0/1796	0.59	0/2417
50	P3	0.55	0/1268	0.59	0/1700
51	Q3	1.98	2/1539 (0.1%)	0.95	4/2054 (0.2%)
52	R3	0.46	0/1524	0.71	1/2013 (0.0%)
53	S3	1.00	1/1501 (0.1%)	0.82	5/2012 (0.2%)
54	T3	0.53	0/1326	0.56	0/1770
55	U3	1.95	3/823 (0.4%)	1.37	7/1104 (0.6%)
56	V3	0.49	0/993	0.60	0/1332
57	W3	0.43	0/873	0.60	0/1158
58	X3	0.45	0/984	0.55	0/1323
59	Y3	0.51	0/1132	0.60	0/1504
6	F1	0.39	0/2118	0.57	1/2849 (0.0%)
60	Z3	0.61	0/1130	0.99	4/1507 (0.3%)
61	a3	0.52	0/1191	0.59	0/1590
62	b3	1.83	2/861 (0.2%)	0.84	4/1138 (0.4%)
63	c3	0.46	0/771	0.84	3/1034 (0.3%)
64	d3	0.51	0/903	0.62	0/1216
65	e3	0.52	0/1071	0.60	0/1429
66	f3	0.59	0/895	0.63	0/1198
67	g3	5.33	4/916 (0.4%)	1.34	7/1220 (0.6%)
68	h3	0.47	0/1021	0.59	0/1348
69	i3	0.43	0/841	0.59	0/1112
7	G1	0.38	0/1492	0.56	0/2005
70	j3	0.54	0/720	0.61	0/952
71	k3	0.42	0/575	0.80	1/761 (0.1%)
72	l3	0.47	0/459	0.58	0/608
73	m3	0.46	0/435	0.55	0/575
74	n3	0.40	0/240	0.66	0/305
75	o3	0.45	0/864	0.58	0/1140
76	p3	0.55	0/718	0.74	0/953
77	r3	0.53	0/1010	0.63	0/1354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	s3	0.50	1/1530 (0.1%)	0.89	5/2064 (0.2%)
79	t3	0.31	0/1174	0.64	0/1582
8	H1	0.36	0/1946	0.62	0/2590
80	23	0.61	0/1805	1.13	10/2809 (0.4%)
81	w3	0.62	0/553	1.24	3/859 (0.3%)
82	J3	0.41	0/1385	0.58	0/1852
83	G3	1.53	2/1910 (0.1%)	0.98	6/2569 (0.2%)
84	D3	0.48	0/2437	0.61	0/3264
85	I3	1.09	2/1702 (0.1%)	0.76	4/2272 (0.2%)
86	1	0.45	0/109	0.65	0/151
87	u3	0.29	0/1769	0.64	1/2371 (0.0%)
9	I1	0.34	0/1510	0.60	1/2022 (0.0%)
All	All	2.04	110/242730 (0.0%)	1.12	846/355150 (0.2%)

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
14	N1	0	1
16	P1	0	1
17	Q1	0	2
2	B1	0	1
25	Y1	0	1
35	j1	0	1
36	k1	0	1
40	A3	0	5
42	C3	0	1
47	M3	0	1
48	N3	0	2
52	R3	0	5
53	S3	0	1
55	U3	0	1
57	W3	0	1
60	Z3	0	3
63	c3	0	1
67	g3	0	8
71	k3	0	1
76	p3	0	2
78	s3	0	4
79	t3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
83	G3	0	3
85	I3	0	1
87	u3	0	2
All	All	0	51

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	52	732	A	N3-C4	183.88	2.45	1.34
37	52	1805	A	N3-C4	177.26	2.41	1.34
37	52	732	A	C6-N1	163.87	2.50	1.35
1	A1	970	G	C6-N1	162.13	2.53	1.39
37	52	2631	U	C2-N3	160.48	2.50	1.37
37	52	1805	A	C6-N1	156.94	2.45	1.35
38	72	63	C	N3-C4	154.05	2.41	1.33
1	A1	970	G	N1-C2	147.61	2.55	1.37
67	g3	2	VAL	CA-CB	146.99	4.63	1.54
38	72	63	C	C2-N3	141.19	2.48	1.35
37	52	2399	G	N3-C4	141.09	2.34	1.35
37	52	119	G	N3-C4	140.75	2.33	1.35
38	72	63	C	N1-C6	137.18	2.19	1.37
37	52	1805	A	C5-C4	131.27	2.30	1.38
1	A1	970	G	N3-C4	130.54	2.26	1.35
37	52	2631	U	N1-C2	129.16	2.54	1.38
37	52	2084	U	C2-N3	128.31	2.27	1.37
37	52	732	A	C5-C4	128.19	2.28	1.38
37	52	2631	U	N3-C4	126.02	2.51	1.38
37	52	119	G	C2-N3	125.48	2.33	1.32
37	52	2399	G	C2-N3	124.99	2.32	1.32
37	52	732	A	N1-C2	123.46	2.45	1.34
37	52	1805	A	N1-C2	119.68	2.42	1.34
37	52	732	A	C2-N3	119.42	2.41	1.33
37	52	1805	A	C5-C6	119.25	2.48	1.41
37	52	1239	C	N3-C4	118.39	2.16	1.33
37	52	2631	U	N1-C6	118.04	2.44	1.38
1	A1	970	G	C5-C4	117.47	2.20	1.38
37	52	2631	U	C4-C5	115.89	2.47	1.43
1	A1	970	G	C2-N3	115.81	2.25	1.32
37	52	1805	A	C2-N3	114.82	2.36	1.33
37	52	119	G	C6-N1	114.36	2.19	1.39
37	52	2399	G	C6-N1	111.66	2.17	1.39
37	52	732	A	C5-C6	109.08	2.39	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	52	2631	U	C5-C6	108.90	2.32	1.34
37	52	1239	C	C2-N3	104.51	2.19	1.35
38	72	63	C	C4-C5	101.90	2.24	1.43
37	52	2084	U	N3-C4	100.66	2.29	1.38
37	52	2084	U	N1-C2	99.49	2.28	1.38
37	52	119	G	N1-C2	98.55	2.16	1.37
37	52	2399	G	N1-C2	97.15	2.15	1.37
37	52	2084	U	N1-C6	95.12	2.23	1.38
38	72	63	C	C5-C6	94.73	2.10	1.34
37	52	2399	G	C5-C4	94.70	2.04	1.38
37	52	119	G	C5-C4	94.11	2.04	1.38
37	52	1239	C	N1-C6	93.42	1.93	1.37
1	A1	970	G	C5-C6	91.55	2.33	1.42
43	E3	65	TYR	CZ-OH	90.99	2.92	1.37
37	52	2084	U	C4-C5	90.19	2.24	1.43
38	72	63	C	N1-C2	89.67	2.29	1.40
37	52	2084	U	C5-C6	85.62	2.11	1.34
37	52	3712	A	N1-C2	82.20	2.08	1.34
37	52	3712	A	C2-N3	81.69	2.07	1.33
51	Q3	14	ARG	CD-NE	74.39	2.73	1.46
37	52	3712	A	N3-C4	72.93	1.78	1.34
37	52	2399	G	C5-C6	72.47	2.14	1.42
37	52	119	G	C5-C6	72.33	2.14	1.42
37	52	2395	A	N3-C4	67.97	1.75	1.34
37	52	1239	C	C4-C5	65.61	1.95	1.43
37	52	3712	A	C6-N1	65.61	1.81	1.35
37	52	2395	A	C6-N1	63.03	1.79	1.35
83	G3	185	ARG	CD-NE	62.84	2.53	1.46
67	g3	4	ARG	CD-NE	62.73	2.53	1.46
37	52	1239	C	C5-C6	61.86	1.83	1.34
37	52	1239	C	N1-C2	60.57	2.00	1.40
62	b3	28	ARG	CA-CB	51.95	2.68	1.53
37	52	2395	A	C5-C4	51.00	1.74	1.38
55	U3	49	VAL	CA-CB	49.08	2.57	1.54
37	52	2395	A	N1-C2	47.55	1.77	1.34
37	52	2395	A	C2-N3	44.38	1.73	1.33
37	52	2395	A	C5-C6	43.04	1.79	1.41
85	I3	203	ARG	C-N	35.14	1.96	1.33
53	S3	68	PHE	CA-C	31.88	2.35	1.52
85	I3	204	GLY	N-CA	20.28	1.76	1.46
55	U3	49	VAL	CB-CG1	16.45	1.87	1.52
55	U3	49	VAL	CB-CG2	14.16	1.82	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
78	s3	186	GLY	C-N	14.10	1.66	1.34
83	G3	185	ARG	NE-CZ	11.39	1.47	1.33
67	g3	4	ARG	NE-CZ	10.90	1.47	1.33
37	52	1805	A	C8-N7	9.35	1.38	1.31
1	A1	970	G	C8-N7	9.17	1.36	1.30
43	E3	65	TYR	CE1-CZ	9.04	1.50	1.38
37	52	3712	A	C5-C4	-8.66	1.32	1.38
43	E3	65	TYR	CE2-CZ	8.06	1.49	1.38
37	52	3712	A	C5-C6	-7.77	1.34	1.41
37	52	1969	G	C8-N7	-7.48	1.26	1.30
37	52	3712	A	N9-C4	7.39	1.42	1.37
67	g3	4	ARG	CG-CD	7.32	1.70	1.51
37	52	2598	A	N7-C5	-7.04	1.35	1.39
51	Q3	14	ARG	NE-CZ	7.03	1.42	1.33
37	52	732	A	C8-N7	6.87	1.36	1.31
37	52	119	G	C8-N7	6.84	1.35	1.30
37	52	1805	A	N9-C8	6.75	1.43	1.37
37	52	2675	G	N7-C5	-6.72	1.35	1.39
62	b3	28	ARG	CB-CG	6.66	1.70	1.52
38	72	5	A	N9-C4	-6.66	1.33	1.37
37	52	2597	G	N9-C8	-6.53	1.33	1.37
40	A3	117	GLU	CB-CG	-6.35	1.40	1.52
37	52	2598	A	N9-C4	6.24	1.41	1.37
37	52	1969	G	N7-C5	-6.08	1.35	1.39
1	A1	970	G	N9-C8	6.02	1.42	1.37
37	52	347	A	N9-C4	-5.63	1.34	1.37
37	52	1805	A	N9-C4	-5.34	1.34	1.37
37	52	3681	G	N3-C4	-5.29	1.31	1.35
1	A1	970	G	N9-C4	-5.26	1.33	1.38
40	A3	169	VAL	CB-CG2	-5.18	1.42	1.52
37	52	1324	A	N7-C5	-5.17	1.36	1.39
37	52	2399	G	N7-C5	-5.17	1.36	1.39
37	52	2675	G	N9-C8	-5.17	1.34	1.37
37	52	1577	G	C8-N7	-5.14	1.27	1.30

All (846) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	3712	A	N1-C2-N3	-240.10	9.25	129.30
37	52	3712	A	C2-N3-C4	88.07	154.63	110.60
37	52	3712	A	C6-N1-C2	69.39	160.23	118.60
37	52	3712	A	C4-C5-C6	-48.11	92.95	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	970	G	C4-C5-N7	-38.17	95.53	110.80
37	52	732	A	N7-C8-N9	36.92	132.26	113.80
37	52	2395	A	N1-C2-N3	-36.03	111.29	129.30
37	52	2399	G	N3-C4-N9	35.69	147.41	126.00
37	52	2399	G	C4-C5-N7	-35.19	96.72	110.80
37	52	732	A	N1-C2-N3	-34.77	111.92	129.30
37	52	1805	A	C4-C5-N7	-34.65	93.38	110.70
37	52	119	G	N3-C4-N9	34.04	146.43	126.00
37	52	2399	G	C2-N3-C4	34.00	128.90	111.90
37	52	119	G	C4-C5-N7	-33.42	97.43	110.80
37	52	1805	A	N7-C8-N9	33.38	130.49	113.80
37	52	119	G	C2-N3-C4	33.31	128.55	111.90
37	52	2399	G	N3-C4-C5	-32.89	112.15	128.60
37	52	1805	A	N1-C2-N3	-32.84	112.88	129.30
37	52	732	A	C4-C5-N7	-32.69	94.36	110.70
37	52	3712	A	N3-C4-N9	32.62	153.49	127.40
37	52	2395	A	C2-N3-C4	31.59	126.40	110.60
37	52	119	G	N3-C4-C5	-31.55	112.82	128.60
1	A1	970	G	C2-N3-C4	31.21	127.50	111.90
1	A1	970	G	N7-C8-N9	30.41	128.31	113.10
37	52	732	A	C2-N3-C4	29.93	125.56	110.60
37	52	1805	A	C2-N3-C4	29.81	125.50	110.60
37	52	2399	G	N1-C2-N3	-28.58	106.75	123.90
37	52	119	G	N1-C2-N3	-28.49	106.81	123.90
1	A1	168	C	OP1-P-OP2	-28.26	77.20	119.60
1	A1	168	C	O5'-P-OP1	-28.05	77.04	110.70
37	52	3712	A	N3-C4-C5	-27.25	107.72	126.80
37	52	119	G	N7-C8-N9	27.14	126.67	113.10
37	52	1239	C	N3-C4-C5	-26.87	111.15	121.90
1	A1	970	G	N1-C2-N3	-26.72	107.87	123.90
37	52	2399	G	N7-C8-N9	26.47	126.34	113.10
67	g3	4	ARG	CD-NE-CZ	24.95	158.52	123.60
83	G3	185	ARG	CD-NE-CZ	24.43	157.81	123.60
37	52	732	A	N9-C4-C5	-24.34	96.06	105.80
51	Q3	14	ARG	CD-NE-CZ	23.70	156.79	123.60
37	52	3712	A	C5-C6-N1	-22.89	106.25	117.70
37	52	1239	C	N1-C2-N3	-22.43	103.50	119.20
37	52	1805	A	N9-C4-C5	-22.28	96.89	105.80
37	52	732	A	N3-C4-N9	21.79	144.83	127.40
37	52	3712	A	C4-C5-N7	21.70	121.55	110.70
38	72	63	C	N3-C4-C5	-21.04	113.48	121.90
1	A1	970	G	N9-C4-C5	-21.03	96.99	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1805	A	C6-C5-N7	20.98	146.99	132.30
55	U3	49	VAL	CG1-CB-CG2	-20.82	77.59	110.90
1	A1	970	G	N3-C4-N9	20.77	138.46	126.00
38	72	63	C	C6-N1-C2	20.76	128.60	120.30
38	72	63	C	N1-C2-N3	-20.59	104.79	119.20
37	52	2395	A	N7-C8-N9	19.99	123.80	113.80
37	52	1239	C	C6-N1-C2	19.69	128.18	120.30
37	52	2399	G	C5-C6-N1	19.68	121.34	111.50
83	G3	185	ARG	NE-CZ-NH1	19.64	130.12	120.30
55	U3	49	VAL	CA-CB-CG1	19.63	140.35	110.90
1	A1	970	G	C6-C5-N7	19.14	141.88	130.40
37	52	1805	A	N3-C4-N9	19.04	142.63	127.40
37	52	119	G	C5-C6-N1	19.04	121.02	111.50
37	52	3712	A	C6-C5-N7	18.81	145.46	132.30
85	I3	203	ARG	C-N-CA	18.40	160.94	122.30
55	U3	49	VAL	CA-CB-CG2	18.36	138.43	110.90
37	52	3712	A	N9-C4-C5	-17.64	98.74	105.80
38	72	63	C	N1-C2-O2	16.69	128.91	118.90
67	g3	4	ARG	NE-CZ-NH1	16.51	128.55	120.30
37	52	1239	C	C2-N3-C4	16.50	128.15	119.90
37	52	3712	A	N1-C6-N6	16.16	128.30	118.60
62	b3	28	ARG	CA-CB-CG	15.94	148.47	113.40
78	s3	186	GLY	O-C-N	-15.85	97.34	122.70
51	Q3	14	ARG	NE-CZ-NH1	15.70	128.15	120.30
1	A1	167	G	OP1-P-O3'	15.25	138.76	105.20
37	52	2399	G	N9-C4-C5	-14.98	99.41	105.40
53	S3	68	PHE	O-C-N	-14.90	98.86	122.70
53	S3	68	PHE	CB-CA-C	14.88	140.15	110.40
37	52	2399	G	C6-C5-N7	14.66	139.19	130.40
37	52	1239	C	N1-C2-O2	14.38	127.53	118.90
37	52	732	A	C6-C5-N7	14.21	142.25	132.30
1	A1	281	C	N1-C2-O2	14.17	127.40	118.90
37	52	2395	A	C6-N1-C2	13.83	126.90	118.60
37	52	2399	G	N3-C2-N2	13.77	129.53	119.90
1	A1	168	C	O5'-P-OP2	13.74	127.19	110.70
38	72	63	C	C2-N3-C4	13.57	126.69	119.90
1	A1	167	G	OP2-P-O3'	-13.47	75.57	105.20
37	52	119	G	C6-C5-N7	13.46	138.48	130.40
1	A1	281	C	C2-N1-C1'	13.41	133.55	118.80
37	52	2397	G	N1-C6-O6	-13.29	111.93	119.90
37	52	1805	A	C5-N7-C8	13.23	110.52	103.90
83	G3	185	ARG	NE-CZ-NH2	-13.14	113.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	4123	C	C6-N1-C2	-12.56	115.28	120.30
37	52	3712	A	C5-N7-C8	-12.54	97.63	103.90
37	52	119	G	N9-C4-C5	-12.48	100.41	105.40
37	52	4123	C	C2-N1-C1'	12.41	132.45	118.80
67	g3	4	ARG	NE-CZ-NH2	-12.33	114.14	120.30
37	52	2395	A	C4-C5-N7	-12.20	104.60	110.70
51	Q3	14	ARG	CG-CD-NE	12.09	137.18	111.80
37	52	2399	G	C5-N7-C8	11.86	110.23	104.30
37	52	2395	A	N3-C4-N9	11.78	136.82	127.40
37	52	4123	C	N1-C2-O2	11.64	125.88	118.90
37	52	732	A	N3-C4-C5	-11.63	118.66	126.80
1	A1	281	C	N3-C2-O2	-11.56	113.81	121.90
37	52	2258	C	N1-C2-O2	11.54	125.82	118.90
37	52	732	A	C4-C5-C6	11.53	122.77	117.00
37	52	2021	G	C8-N9-C4	-11.48	101.81	106.40
37	52	4119	C	N1-C2-O2	11.35	125.71	118.90
37	52	2397	G	C5-C6-O6	11.31	135.39	128.60
37	52	1239	C	C4-C5-C6	11.14	122.97	117.40
37	52	4123	C	N3-C2-O2	-11.08	114.14	121.90
37	52	4120	U	C2-N1-C1'	11.06	130.98	117.70
37	52	732	A	C5-N7-C8	11.06	109.43	103.90
1	A1	887	U	C2-N1-C1'	11.01	130.91	117.70
1	A1	887	U	N1-C2-O2	10.99	130.49	122.80
55	U3	49	VAL	CB-CA-C	10.98	132.27	111.40
40	A3	126	LEU	CA-CB-CG	10.90	140.38	115.30
78	s3	186	GLY	CA-C-N	10.81	140.98	117.20
37	52	119	G	N1-C2-N2	10.78	125.91	116.20
78	s3	186	GLY	C-N-CA	10.78	148.65	121.70
62	b3	28	ARG	CB-CA-C	10.70	131.79	110.40
1	A1	356	C	N1-C2-O2	10.68	125.31	118.90
37	52	1805	A	C6-N1-C2	10.66	124.99	118.60
80	23	20	U	N1-C2-O2	10.59	130.21	122.80
37	52	327	U	C2-N1-C1'	10.57	130.38	117.70
37	52	3810	C	N1-C2-O2	10.54	125.22	118.90
37	52	2597	G	N3-C4-C5	-10.50	123.35	128.60
80	23	20	U	C2-N1-C1'	10.45	130.24	117.70
37	52	2021	G	O4'-C1'-N9	10.43	116.54	108.20
1	A1	970	G	C5-N7-C8	10.41	109.50	104.30
37	52	119	G	N3-C2-N2	10.37	127.16	119.90
37	52	2021	G	C4-N9-C1'	10.30	139.89	126.50
37	52	2021	G	N3-C4-C5	-10.22	123.49	128.60
67	g3	4	ARG	CG-CD-NE	10.17	133.16	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
80	23	20	U	N3-C2-O2	-10.13	115.11	122.20
37	52	1915	C	N1-C2-O2	10.05	124.93	118.90
37	52	2258	C	N3-C2-O2	-9.92	114.95	121.90
37	52	2021	G	C2-N3-C4	9.90	116.85	111.90
37	52	3810	C	C6-N1-C2	-9.84	116.37	120.30
38	72	63	C	C4-C5-C6	9.81	122.30	117.40
37	52	2399	G	N1-C6-O6	-9.80	114.02	119.90
37	52	2019	C	N1-C2-O2	9.79	124.78	118.90
37	52	2597	G	C4-N9-C1'	9.74	139.16	126.50
37	52	1915	C	N3-C2-O2	-9.67	115.13	121.90
37	52	4119	C	N3-C2-O2	-9.66	115.13	121.90
37	52	2397	G	C6-C5-N7	9.63	136.18	130.40
37	52	2598	A	C8-N9-C4	-9.56	101.98	105.80
37	52	2581	A	O5'-P-OP2	9.55	122.16	110.70
1	A1	970	G	N3-C2-N2	9.53	126.57	119.90
83	G3	185	ARG	CG-CD-NE	9.50	131.75	111.80
1	A1	887	U	N3-C2-O2	-9.45	115.58	122.20
55	U3	49	VAL	N-CA-C	-9.43	85.53	111.00
37	52	732	A	C6-N1-C2	9.35	124.21	118.60
1	A1	970	G	N1-C2-N2	9.31	124.58	116.20
43	E3	65	TYR	CE1-CZ-CE2	-9.31	104.91	119.80
37	52	2397	G	N9-C4-C5	9.31	109.12	105.40
37	52	2581	A	O5'-P-OP1	-9.31	97.33	105.70
37	52	1996	C	C5-C6-N1	9.30	125.65	121.00
37	52	1639	U	C2-N1-C1'	9.28	128.83	117.70
1	A1	356	C	C2-N1-C1'	9.27	129.00	118.80
1	A1	281	C	C6-N1-C1'	-9.24	109.71	120.80
37	52	3810	C	C5-C6-N1	9.21	125.61	121.00
37	52	119	G	C5-N7-C8	9.15	108.88	104.30
37	52	1805	A	N3-C4-C5	-9.13	120.41	126.80
37	52	4948	C	C2-N1-C1'	9.10	128.81	118.80
37	52	2397	G	N3-C4-N9	-9.08	120.55	126.00
37	52	119	G	C5-C6-O6	-9.07	123.16	128.60
37	52	3810	C	C2-N1-C1'	8.98	128.68	118.80
1	A1	281	C	C6-N1-C2	-8.95	116.72	120.30
37	52	2395	A	N3-C4-C5	-8.95	120.54	126.80
37	52	4123	C	C5-C6-N1	8.91	125.45	121.00
1	A1	1520	G	N3-C4-N9	8.89	131.34	126.00
37	52	1915	C	C6-N1-C2	-8.87	116.75	120.30
37	52	4948	C	N1-C2-O2	8.86	124.22	118.90
37	52	1239	C	N3-C2-O2	8.85	128.09	121.90
37	52	1239	C	C5-C6-N1	8.81	125.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	501	C	N1-C2-O2	8.79	124.18	118.90
37	52	119	G	C4-C5-C6	8.79	124.07	118.80
1	A1	356	C	N3-C2-O2	-8.75	115.78	121.90
37	52	2399	G	C4-C5-C6	8.72	124.03	118.80
37	52	1915	C	C2-N1-C1'	8.71	128.38	118.80
37	52	2397	G	C4-C5-N7	-8.65	107.34	110.80
37	52	2674	A	OP1-P-OP2	-8.64	106.64	119.60
37	52	4928	C	N1-C2-O2	8.62	124.07	118.90
1	A1	1520	G	N3-C4-C5	-8.55	124.32	128.60
37	52	275	C	C6-N1-C2	-8.54	116.89	120.30
1	A1	1518	C	C2-N1-C1'	8.47	128.12	118.80
1	A1	970	G	N3-C4-C5	-8.47	124.37	128.60
85	I3	203	ARG	CA-C-O	-8.46	102.32	120.10
37	52	2395	A	N9-C4-C5	-8.38	102.45	105.80
37	52	2399	G	N1-C2-N2	8.35	123.71	116.20
67	g3	2	VAL	CA-CB-CG1	8.35	123.42	110.90
37	52	358	C	N1-C2-O2	8.34	123.91	118.90
37	52	327	U	N3-C2-O2	-8.29	116.39	122.20
37	52	2258	C	C6-N1-C2	-8.28	116.99	120.30
37	52	4119	C	C2-N1-C1'	8.27	127.89	118.80
1	A1	1518	C	N1-C2-O2	8.27	123.86	118.90
1	A1	1520	G	C4-N9-C1'	8.25	137.23	126.50
53	S3	68	PHE	N-CA-CB	-8.24	95.76	110.60
1	A1	369	C	N1-C2-O2	8.24	123.84	118.90
37	52	4928	C	C2-N1-C1'	8.16	127.78	118.80
37	52	2597	G	C8-N9-C4	-8.15	103.14	106.40
37	52	2597	G	N7-C8-N9	8.15	117.17	113.10
37	52	3810	C	N3-C2-O2	-8.14	116.20	121.90
37	52	3941	G	N3-C4-C5	-8.14	124.53	128.60
37	52	4928	C	N3-C2-O2	-8.14	116.20	121.90
37	52	4120	U	C5-C6-N1	8.10	126.75	122.70
1	A1	1518	C	N3-C2-O2	-8.09	116.24	121.90
37	52	4120	U	N1-C2-O2	8.07	128.45	122.80
37	52	2019	C	C5-C6-N1	8.05	125.03	121.00
37	52	3941	G	C4-N9-C1'	8.02	136.92	126.50
37	52	257	C	N1-C2-O2	7.97	123.68	118.90
37	52	4948	C	N3-C2-O2	-7.91	116.36	121.90
1	A1	970	G	C8-N9-C4	7.86	109.55	106.40
51	Q3	14	ARG	NE-CZ-NH2	-7.82	116.39	120.30
37	52	3941	G	N3-C4-N9	7.80	130.68	126.00
37	52	358	C	N3-C2-O2	-7.80	116.44	121.90
37	52	3661	G	C4-C5-N7	7.78	113.91	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	s3	75	LEU	CA-CB-CG	7.78	133.18	115.30
1	A1	887	U	C6-N1-C1'	-7.77	110.32	121.20
37	52	737	C	N1-C2-O2	7.74	123.54	118.90
37	52	1239	C	C5-C4-N4	7.70	125.59	120.20
37	52	2019	C	C6-N1-C2	-7.69	117.22	120.30
37	52	1556	C	N1-C2-O2	7.68	123.51	118.90
43	E3	65	TYR	CD1-CE1-CZ	7.68	126.71	119.80
37	52	2583	C	C6-N1-C2	-7.67	117.23	120.30
37	52	1070	G	C4-N9-C1'	7.66	136.46	126.50
1	A1	1303	C	N1-C2-O2	7.65	123.49	118.90
55	U3	49	VAL	N-CA-CB	7.64	128.32	111.50
37	52	672	C	N1-C2-O2	7.64	123.48	118.90
38	72	1	G	N3-C4-C5	-7.59	124.80	128.60
1	A1	1624	U	N3-C2-O2	-7.59	116.89	122.20
85	I3	203	ARG	CA-C-N	7.58	131.36	116.20
37	52	327	U	N1-C2-O2	7.56	128.09	122.80
1	A1	1624	U	C2-N1-C1'	7.54	126.74	117.70
37	52	2552	G	N3-C4-N9	7.51	130.51	126.00
37	52	4120	U	C6-N1-C1'	-7.50	110.70	121.20
37	52	1639	U	N1-C2-O2	7.50	128.05	122.80
37	52	2598	A	N3-C4-C5	-7.50	121.55	126.80
67	g3	2	VAL	CA-CB-CG2	7.46	122.09	110.90
37	52	2021	G	N7-C8-N9	7.45	116.83	113.10
37	52	2597	G	N3-C4-N9	7.41	130.44	126.00
37	52	3843	C	N1-C2-O2	7.38	123.33	118.90
1	A1	501	C	C2-N1-C1'	7.38	126.92	118.80
38	72	63	C	C6-N1-C1'	-7.38	111.95	120.80
37	52	4123	C	C6-N1-C1'	-7.36	111.97	120.80
37	52	2019	C	C2-N3-C4	7.33	123.57	119.90
1	A1	501	C	N3-C2-O2	-7.33	116.77	121.90
37	52	2528	G	C4-N9-C1'	7.32	136.02	126.50
1	A1	369	C	C2-N1-C1'	7.30	126.83	118.80
37	52	737	C	N3-C2-O2	-7.30	116.79	121.90
1	A1	751	G	P-O3'-C3'	7.28	128.44	119.70
37	52	1305	C	C6-N1-C2	-7.28	117.39	120.30
38	72	1	G	N3-C4-N9	7.28	130.37	126.00
37	52	2084	U	C2-N3-C4	-7.27	122.64	127.00
37	52	1612	G	C4-N9-C1'	7.27	135.95	126.50
37	52	2046	G	P-O3'-C3'	7.26	128.41	119.70
37	52	48	G	P-O3'-C3'	7.25	128.40	119.70
37	52	1310	C	C6-N1-C2	-7.25	117.40	120.30
43	E3	65	TYR	CZ-CE2-CD2	7.25	126.32	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1805	A	C8-N9-C4	7.24	108.69	105.80
1	A1	751	G	OP1-P-O3'	7.21	121.05	105.20
37	52	2597	G	C8-N9-C1'	-7.19	117.65	127.00
37	52	1556	C	N3-C2-O2	-7.16	116.89	121.90
37	52	1239	C	N3-C4-N4	7.13	122.99	118.00
37	52	2598	A	C4-C5-C6	7.13	120.56	117.00
37	52	2022	C	O5'-P-OP2	-7.12	99.29	105.70
37	52	2395	A	C6-C5-N7	7.11	137.28	132.30
39	82	36	G	C4-N9-C1'	7.09	135.72	126.50
53	S3	68	PHE	CA-C-O	7.07	134.95	120.10
1	A1	1520	G	C8-N9-C1'	-7.06	117.83	127.00
37	52	3941	G	C8-N9-C1'	-7.05	117.84	127.00
37	52	2580	U	OP2-P-O3'	-7.04	89.70	105.20
52	R3	125	LEU	CB-CG-CD1	-7.04	99.03	111.00
1	A1	1664	A	P-O3'-C3'	7.02	128.12	119.70
37	52	4528	G	C4-N9-C1'	7.01	135.62	126.50
37	52	2078	C	C5-C6-N1	7.01	124.51	121.00
37	52	3661	G	N9-C4-C5	-7.00	102.60	105.40
1	A1	241	G	N3-C4-N9	7.00	130.20	126.00
37	52	2580	U	OP1-P-O3'	6.98	120.57	105.20
37	52	2084	U	C6-N1-C2	6.98	125.19	121.00
37	52	2597	G	C4-C5-C6	6.97	122.98	118.80
37	52	2875	C	P-O3'-C3'	6.95	128.04	119.70
1	A1	1303	C	N3-C2-O2	-6.93	117.05	121.90
37	52	1996	C	C6-N1-C2	-6.92	117.53	120.30
37	52	2581	A	C5'-C4'-C3'	6.92	127.08	116.00
1	A1	1303	C	C2-N1-C1'	6.92	126.41	118.80
37	52	3809	G	N3-C4-N9	6.91	130.15	126.00
37	52	3651	A	O5'-P-OP1	-6.89	99.49	105.70
37	52	4138	C	N1-C2-O2	6.89	123.04	118.90
1	A1	183	G	N3-C4-N9	6.89	130.13	126.00
71	k3	56	LEU	CA-CB-CG	6.89	131.14	115.30
37	52	4119	C	C6-N1-C2	-6.86	117.56	120.30
37	52	119	G	N1-C6-O6	-6.84	115.80	119.90
37	52	3661	G	C5-C6-O6	-6.84	124.50	128.60
37	52	2504	C	C6-N1-C2	-6.83	117.57	120.30
1	A1	356	C	C6-N1-C1'	-6.83	112.61	120.80
80	23	20	U	C6-N1-C1'	-6.80	111.68	121.20
37	52	3637	U	N3-C2-O2	-6.77	117.46	122.20
37	52	4117	U	N3-C2-O2	-6.76	117.47	122.20
37	52	2580	U	C4-C5-C6	6.74	123.74	119.70
1	A1	183	G	C4-N9-C1'	6.72	135.24	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	970	G	C4-N9-C1'	-6.71	117.78	126.50
37	52	1639	U	N3-C2-O2	-6.70	117.51	122.20
87	u3	163	LEU	CA-CB-CG	6.70	130.71	115.30
37	52	2021	G	C8-N9-C1'	-6.70	118.29	127.00
37	52	2258	C	C2-N1-C1'	6.69	126.16	118.80
37	52	2397	G	C8-N9-C1'	6.69	135.69	127.00
1	A1	75	G	N3-C4-N9	6.68	130.01	126.00
37	52	2089	G	P-O3'-C3'	6.67	127.70	119.70
37	52	1612	G	C8-N9-C1'	-6.66	118.34	127.00
49	O3	18	ARG	NE-CZ-NH2	-6.66	116.97	120.30
37	52	2875	C	OP2-P-O3'	6.66	119.85	105.20
1	A1	281	C	C5-C6-N1	6.65	124.33	121.00
1	A1	1858	G	C4-N9-C1'	6.65	135.15	126.50
37	52	48	G	OP2-P-O3'	6.65	119.83	105.20
37	52	1210	C	N1-C2-O2	6.64	122.88	118.90
1	A1	75	G	C4-N9-C1'	6.63	135.12	126.50
37	52	2631	U	C2-N3-C4	-6.63	123.02	127.00
37	52	2399	G	C5-C6-O6	-6.63	124.62	128.60
37	52	1210	C	C2-N1-C1'	6.62	126.09	118.80
37	52	327	U	C6-N1-C1'	-6.62	111.94	121.20
37	52	2768	C	O4'-C1'-N1	6.61	113.49	108.20
1	A1	688	U	P-O3'-C3'	6.61	127.63	119.70
37	52	358	C	C2-N1-C1'	6.60	126.06	118.80
1	A1	751	G	N3-C4-N9	6.58	129.95	126.00
1	A1	293	C	N1-C2-O2	6.58	122.85	118.90
1	A1	1057	C	C2-N1-C1'	6.58	126.04	118.80
37	52	2750	G	C6-C5-N7	-6.58	126.45	130.40
37	52	1517	G	C4-N9-C1'	6.57	135.04	126.50
37	52	2574	G	O5'-P-OP1	6.57	118.58	110.70
60	Z3	80	LEU	CA-CB-CG	6.55	130.37	115.30
37	52	1305	C	C2-N1-C1'	6.55	126.00	118.80
37	52	4243	C	N3-C2-O2	-6.54	117.32	121.90
1	A1	1518	C	C6-N1-C2	-6.54	117.69	120.30
37	52	672	C	N3-C2-O2	-6.53	117.33	121.90
37	52	2084	U	N3-C4-C5	6.52	118.51	114.60
1	A1	369	C	N3-C2-O2	-6.52	117.33	121.90
37	52	2528	G	C8-N9-C1'	-6.52	118.52	127.00
1	A1	1637	A	P-O3'-C3'	6.51	127.51	119.70
1	A1	212	C	C6-N1-C2	-6.51	117.70	120.30
39	82	36	G	N3-C4-C5	-6.50	125.35	128.60
37	52	2572	C	C5-C4-N4	-6.49	115.66	120.20
37	52	2489	C	N1-C2-O2	6.49	122.79	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
78	s3	79	LEU	CA-CB-CG	-6.48	100.40	115.30
40	A3	117	GLU	CB-CA-C	-6.47	97.45	110.40
37	52	2580	U	N3-C4-O4	6.47	123.93	119.40
37	52	1805	A	C4-N9-C1'	-6.47	114.66	126.30
37	52	1651	G	C4-N9-C1'	6.46	134.90	126.50
37	52	3959	U	P-O3'-C3'	6.46	127.45	119.70
37	52	4880	C	C2-N1-C1'	6.45	125.89	118.80
37	52	217	C	N1-C2-O2	6.43	122.76	118.90
37	52	4243	C	N1-C2-O2	6.43	122.76	118.90
1	A1	1118	C	C2-N1-C1'	6.43	125.87	118.80
39	82	36	G	N3-C4-N9	6.42	129.85	126.00
37	52	2014	C	N1-C2-O2	6.42	122.75	118.90
37	52	2580	U	P-O3'-C3'	6.41	127.39	119.70
37	52	4926	C	C2-N1-C1'	6.39	125.83	118.80
37	52	100	C	C2-N1-C1'	6.39	125.83	118.80
37	52	2078	C	C6-N1-C2	-6.39	117.74	120.30
1	A1	1314	U	C2-N1-C1'	6.38	125.36	117.70
37	52	1961	G	C8-N9-C4	-6.38	103.85	106.40
1	A1	532	C	C6-N1-C2	-6.37	117.75	120.30
37	52	4423	U	N3-C2-O2	-6.37	117.74	122.20
37	52	4948	C	C6-N1-C1'	-6.37	113.16	120.80
1	A1	474	G	C4-N9-C1'	6.36	134.76	126.50
37	52	4926	C	N1-C2-O2	6.35	122.71	118.90
63	c3	30	GLY	N-CA-C	6.35	128.97	113.10
37	52	1573	G	O5'-P-OP1	-6.35	99.99	105.70
37	52	1070	G	C8-N9-C1'	-6.34	118.76	127.00
80	23	30	G	N3-C4-N9	6.34	129.80	126.00
37	52	2084	U	C5-C6-N1	-6.33	119.53	122.70
37	52	4942	C	N1-C2-O2	6.32	122.69	118.90
37	52	2019	C	N3-C2-O2	-6.32	117.48	121.90
1	A1	241	G	N3-C4-C5	-6.31	125.44	128.60
37	52	4919	G	N3-C4-N9	6.30	129.78	126.00
1	A1	751	G	C4-N9-C1'	6.30	134.68	126.50
1	A1	970	G	C4-C5-C6	6.30	122.58	118.80
1	A1	1300	U	N3-C2-O2	-6.29	117.79	122.20
37	52	1632	A	C2-N3-C4	6.29	113.75	110.60
37	52	4919	G	N3-C4-C5	-6.29	125.45	128.60
1	A1	1130	G	N3-C4-C5	-6.27	125.46	128.60
37	52	2552	G	N3-C4-C5	-6.27	125.46	128.60
1	A1	1636	G	C4-N9-C1'	6.27	134.65	126.50
37	52	1185	G	C8-N9-C4	-6.26	103.89	106.40
37	52	4560	C	N3-C2-O2	-6.26	117.52	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	c3	94	LEU	CA-CB-CG	6.25	129.68	115.30
37	52	986	C	N1-C2-O2	6.24	122.64	118.90
37	52	4759	C	C2-N1-C1'	6.24	125.66	118.80
37	52	1979	A	P-O3'-C3'	6.24	127.19	119.70
37	52	1639	U	C6-N1-C1'	-6.23	112.47	121.20
37	52	1961	G	N3-C4-C5	-6.23	125.48	128.60
62	b3	28	ARG	N-CA-C	-6.23	94.17	111.00
38	72	63	C	N3-C2-O2	6.22	126.25	121.90
14	N1	64	LEU	CA-CB-CG	6.21	129.59	115.30
37	52	4869	U	C2-N1-C1'	6.21	125.16	117.70
1	A1	870	A	P-O3'-C3'	6.21	127.15	119.70
37	52	1612	G	N3-C4-N9	6.21	129.72	126.00
37	52	449	C	P-O3'-C3'	6.20	127.14	119.70
37	52	4303	C	C2-N1-C1'	6.19	125.61	118.80
37	52	2528	G	N3-C4-N9	6.18	129.71	126.00
37	52	1961	G	C4-N9-C1'	6.18	134.53	126.50
37	52	2597	G	C6-C5-N7	-6.17	126.70	130.40
37	52	3888	G	P-O3'-C3'	6.17	127.11	119.70
37	52	294	G	C4-N9-C1'	6.17	134.51	126.50
37	52	4413	C	N1-C2-O2	6.15	122.59	118.90
37	52	2811	G	C8-N9-C4	-6.15	103.94	106.40
37	52	4413	C	N3-C2-O2	-6.15	117.60	121.90
37	52	4528	G	C8-N9-C1'	-6.13	119.03	127.00
37	52	1968	G	C8-N9-C4	-6.13	103.95	106.40
1	A1	1130	G	N3-C4-N9	6.12	129.67	126.00
62	b3	28	ARG	N-CA-CB	6.12	121.61	110.60
37	52	2594	C	C6-N1-C2	-6.10	117.86	120.30
1	A1	1397	U	N3-C2-O2	-6.09	117.94	122.20
85	I3	204	GLY	N-CA-C	6.09	128.33	113.10
39	82	36	G	C8-N9-C1'	-6.08	119.09	127.00
37	52	1456	C	C6-N1-C2	-6.07	117.87	120.30
37	52	1612	G	C6-C5-N7	-6.06	126.76	130.40
1	A1	1364	U	C2-N1-C1'	6.06	124.97	117.70
37	52	2397	G	C4-N9-C1'	-6.06	118.62	126.50
38	72	63	C	N3-C4-N4	6.06	122.24	118.00
37	52	180	C	N1-C2-O2	6.06	122.53	118.90
37	52	4759	C	N3-C2-O2	-6.06	117.66	121.90
39	82	153	C	N1-C2-O2	6.05	122.53	118.90
37	52	4413	C	C2-N1-C1'	6.04	125.45	118.80
1	A1	183	G	C8-N9-C1'	-6.03	119.17	127.00
37	52	104	G	C4-N9-C1'	6.03	134.33	126.50
37	52	1805	A	O4'-C1'-N9	-6.02	103.38	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	72	1	G	C4-N9-C1'	6.02	134.33	126.50
1	A1	1394	G	P-O3'-C3'	6.02	126.92	119.70
37	52	1469	C	C6-N1-C2	-6.00	117.90	120.30
37	52	2550	G	N7-C8-N9	6.00	116.10	113.10
1	A1	1453	C	C2-N1-C1'	6.00	125.40	118.80
37	52	275	C	N3-C2-O2	-6.00	117.70	121.90
37	52	1556	C	C2-N1-C1'	5.99	125.39	118.80
37	52	2754	G	C5'-C4'-O4'	5.99	116.29	109.10
1	A1	1314	U	N3-C2-O2	-5.99	118.01	122.20
1	A1	465	A	P-O3'-C3'	5.99	126.88	119.70
1	A1	1333	U	N3-C2-O2	-5.97	118.02	122.20
37	52	4423	U	C2-N1-C1'	5.97	124.87	117.70
1	A1	75	G	C8-N9-C1'	-5.97	119.24	127.00
37	52	4454	G	C4-N9-C1'	5.97	134.26	126.50
37	52	4120	U	N3-C2-O2	-5.97	118.02	122.20
37	52	4919	G	C4-N9-C1'	5.96	134.25	126.50
37	52	1185	G	N3-C4-C5	-5.96	125.62	128.60
37	52	704	C	C2-N1-C1'	5.96	125.35	118.80
37	52	966	A	N7-C8-N9	5.95	116.78	113.80
37	52	1485	C	N1-C2-O2	5.95	122.47	118.90
37	52	3809	G	N3-C4-C5	-5.94	125.63	128.60
1	A1	823	U	C2-N1-C1'	5.93	124.82	117.70
37	52	1215	C	N1-C2-O2	5.93	122.46	118.90
37	52	3712	A	C8-N9-C1'	-5.93	117.02	127.70
37	52	2598	A	C2-N3-C4	5.93	113.56	110.60
37	52	3941	G	C2-N3-C4	5.92	114.86	111.90
80	23	29	C	O4'-C1'-N1	5.92	112.94	108.20
1	A1	501	C	C6-N1-C2	-5.92	117.93	120.30
37	52	4266	G	C4-N9-C1'	5.92	134.19	126.50
37	52	1070	G	N7-C8-N9	5.91	116.06	113.10
37	52	2750	G	C4-N9-C1'	5.91	134.18	126.50
37	52	2740	U	N3-C2-O2	-5.91	118.06	122.20
37	52	4173	G	C6-C5-N7	-5.90	126.86	130.40
37	52	3842	C	N1-C2-O2	5.90	122.44	118.90
37	52	959	G	P-O3'-C3'	5.89	126.76	119.70
37	52	972	C	N1-C2-O2	5.89	122.43	118.90
37	52	2597	G	P-O3'-C3'	5.88	126.76	119.70
37	52	2749	C	C6-N1-C2	-5.87	117.95	120.30
37	52	1961	G	N7-C8-N9	5.87	116.03	113.10
40	A3	43	GLY	N-CA-C	5.86	127.75	113.10
37	52	257	C	C2-N1-C1'	5.86	125.24	118.80
37	52	2577	C	C6-N1-C2	-5.86	117.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	2726	G	C4-N9-C1'	5.86	134.11	126.50
37	52	2594	C	N3-C2-O2	-5.85	117.80	121.90
37	52	327	U	C5-C6-N1	5.85	125.63	122.70
1	A1	1300	U	N1-C2-O2	5.85	126.89	122.80
37	52	257	C	N3-C2-O2	-5.85	117.81	121.90
37	52	2583	C	C5-C6-N1	5.85	123.92	121.00
38	72	63	C	C5-C6-N1	5.85	123.92	121.00
37	52	2258	C	C5-C6-N1	5.84	123.92	121.00
1	A1	183	G	N3-C4-C5	-5.84	125.68	128.60
37	52	1181	C	N1-C2-O2	5.84	122.40	118.90
37	52	1720	C	C6-N1-C2	-5.83	117.97	120.30
37	52	495	C	N1-C2-O2	5.83	122.40	118.90
37	52	115	C	N1-C2-O2	5.83	122.40	118.90
37	52	276	C	C6-N1-C2	-5.83	117.97	120.30
37	52	2407	G	C4-N9-C1'	5.83	134.08	126.50
37	52	914	U	C5-C6-N1	5.83	125.61	122.70
37	52	4759	C	N1-C2-O2	5.83	122.39	118.90
37	52	3712	A	C4-N9-C1'	5.82	136.78	126.30
37	52	4243	C	C2-N1-C1'	5.82	125.20	118.80
1	A1	1475	G	C4-N9-C1'	5.81	134.06	126.50
37	52	37	U	C2-N1-C1'	5.81	124.67	117.70
37	52	3948	C	N1-C2-O2	5.81	122.39	118.90
40	A3	126	LEU	CB-CA-C	-5.81	99.16	110.20
1	A1	853	C	C2-N1-C1'	5.80	125.19	118.80
1	A1	538	U	N1-C2-O2	5.79	126.85	122.80
37	52	30	C	C6-N1-C2	-5.79	117.98	120.30
37	52	2578	G	C4-C5-N7	5.79	113.12	110.80
37	52	4232	U	P-O3'-C3'	5.79	126.65	119.70
37	52	1467	C	C6-N1-C2	-5.79	117.99	120.30
37	52	1915	C	C5-C6-N1	5.78	123.89	121.00
80	23	72	C	N1-C2-O2	5.78	122.37	118.90
1	A1	1397	U	N1-C2-O2	5.78	126.84	122.80
37	52	1182	C	N1-C2-O2	5.78	122.37	118.90
37	52	2303	C	C6-N1-C2	-5.77	117.99	120.30
1	A1	874	G	P-O3'-C3'	5.77	126.62	119.70
37	52	2470	C	N1-C2-O2	5.77	122.36	118.90
37	52	4942	C	N3-C2-O2	-5.77	117.86	121.90
37	52	327	U	C6-N1-C2	-5.77	117.54	121.00
37	52	4964	C	C6-N1-C2	-5.77	117.99	120.30
37	52	1571	G	C2-N3-C4	5.76	114.78	111.90
37	52	3842	C	C2-N1-C1'	5.76	125.14	118.80
1	A1	751	G	N3-C4-C5	-5.76	125.72	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	823	U	N3-C2-O2	-5.76	118.17	122.20
1	A1	659	G	C4-N9-C1'	5.76	133.98	126.50
1	A1	182	C	P-O3'-C3'	5.75	126.61	119.70
1	A1	241	G	C2-N3-C4	5.75	114.78	111.90
37	52	4138	C	N3-C2-O2	-5.75	117.87	121.90
37	52	1912	G	C4-N9-C1'	5.75	133.98	126.50
1	A1	75	G	N3-C4-C5	-5.75	125.72	128.60
1	A1	752	G	O5'-P-OP1	-5.74	100.53	105.70
63	c3	30	GLY	C-N-CA	5.74	136.06	121.70
1	A1	1772	C	C6-N1-C2	-5.74	118.00	120.30
37	52	3649	A	C4-N9-C1'	5.74	136.63	126.30
1	A1	1624	U	N1-C2-O2	5.73	126.81	122.80
37	52	1762	C	C6-N1-C2	-5.73	118.01	120.30
37	52	4928	C	C6-N1-C2	-5.73	118.01	120.30
1	A1	1738	C	C6-N1-C2	-5.73	118.01	120.30
37	52	104	G	C8-N9-C1'	-5.73	119.56	127.00
37	52	1550	G	C4-N9-C1'	5.72	133.94	126.50
37	52	4662	C	C6-N1-C2	-5.72	118.01	120.30
37	52	275	C	P-O3'-C3'	5.71	126.55	119.70
1	A1	751	G	C8-N9-C1'	-5.71	119.58	127.00
37	52	1651	G	C6-C5-N7	-5.70	126.98	130.40
37	52	2014	C	C2-N1-C1'	5.70	125.07	118.80
1	A1	1551	U	C2-N1-C1'	5.69	124.53	117.70
39	82	47	C	C6-N1-C2	-5.69	118.02	120.30
37	52	4948	C	C6-N1-C2	-5.69	118.02	120.30
37	52	934	C	C6-N1-C2	-5.67	118.03	120.30
1	A1	1117	C	N1-C2-O2	5.67	122.30	118.90
37	52	4866	C	C6-N1-C2	-5.66	118.04	120.30
37	52	3843	C	C2-N1-C1'	5.66	125.02	118.80
38	72	113	G	C4-N9-C1'	5.66	133.85	126.50
80	23	30	G	C4-N9-C1'	5.65	133.85	126.50
1	A1	1811	C	C6-N1-C2	-5.65	118.04	120.30
1	A1	958	G	C4-N9-C1'	5.65	133.84	126.50
37	52	498	C	P-O3'-C3'	5.65	126.48	119.70
37	52	1969	G	C5-C6-O6	5.64	131.99	128.60
37	52	1632	A	N3-C4-N9	5.64	131.91	127.40
1	A1	1624	U	C6-N1-C2	-5.63	117.62	121.00
1	A1	1834	A	C4-N9-C1'	5.63	136.43	126.30
1	A1	1253	A	P-O3'-C3'	5.62	126.45	119.70
41	B3	309	LEU	CA-CB-CG	5.62	128.24	115.30
37	52	311	G	C4-N9-C1'	5.62	133.81	126.50
37	52	1517	G	N3-C4-C5	-5.62	125.79	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1969	G	N1-C2-N2	-5.62	111.14	116.20
37	52	672	C	C2-N1-C1'	5.62	124.98	118.80
37	52	2594	C	C2-N1-C1'	5.61	124.97	118.80
37	52	1663	C	C6-N1-C2	-5.61	118.06	120.30
1	A1	532	C	N1-C2-O2	5.61	122.26	118.90
37	52	37	U	N3-C2-O2	-5.61	118.28	122.20
37	52	1928	C	N3-C2-O2	-5.60	117.98	121.90
37	52	204	U	N3-C2-O2	-5.60	118.28	122.20
37	52	37	U	N1-C2-O2	5.60	126.72	122.80
37	52	729	G	N3-C4-C5	-5.60	125.80	128.60
37	52	4194	U	N3-C2-O2	-5.60	118.28	122.20
37	52	4560	C	N1-C2-O2	5.59	122.25	118.90
1	A1	427	U	C2-N1-C1'	5.58	124.40	117.70
37	52	4869	U	N3-C2-O2	-5.57	118.30	122.20
37	52	685	C	O5'-P-OP2	-5.57	100.69	105.70
37	52	4871	C	C2-N1-C1'	5.57	124.92	118.80
37	52	339	C	C6-N1-C2	-5.56	118.08	120.30
37	52	4925	U	P-O3'-C3'	5.56	126.37	119.70
37	52	115	C	C2-N1-C1'	5.56	124.91	118.80
37	52	704	C	N1-C2-O2	5.56	122.23	118.90
37	52	4476	C	C2-N1-C1'	5.56	124.91	118.80
37	52	3625	G	P-O3'-C3'	5.55	126.37	119.70
37	52	1286	C	N1-C2-O2	5.55	122.23	118.90
1	A1	1518	C	C6-N1-C1'	-5.55	114.14	120.80
37	52	930	G	P-O3'-C3'	5.55	126.36	119.70
37	52	4528	G	N3-C4-N9	5.55	129.33	126.00
37	52	1853	G	C4-N9-C1'	5.54	133.71	126.50
37	52	2014	C	C6-N1-C2	-5.54	118.08	120.30
37	52	3843	C	N3-C2-O2	-5.54	118.02	121.90
1	A1	1660	C	C2-N1-C1'	5.53	124.88	118.80
37	52	4047	A	OP1-P-O3'	5.53	117.37	105.20
37	52	2014	C	N3-C2-O2	-5.53	118.03	121.90
37	52	4939	C	N1-C2-O2	5.53	122.22	118.90
37	52	2675	G	C8-N9-C1'	-5.53	119.82	127.00
37	52	2753	G	P-O3'-C3'	5.52	126.33	119.70
1	A1	1826	G	C4-N9-C1'	5.52	133.68	126.50
37	52	2631	U	N3-C4-C5	5.52	117.91	114.60
37	52	3638	G	C6-C5-N7	-5.51	127.09	130.40
37	52	1639	U	C5-C6-N1	5.51	125.46	122.70
37	52	2489	C	C6-N1-C2	-5.51	118.09	120.30
37	52	4999	G	C4-N9-C1'	5.51	133.66	126.50
37	52	4117	U	C2-N1-C1'	5.51	124.31	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1301	A	C2-N3-C4	5.50	113.35	110.60
37	52	1968	G	N7-C8-N9	5.50	115.85	113.10
37	52	4405	G	C4-N9-C1'	5.50	133.65	126.50
37	52	1674	C	C6-N1-C2	-5.49	118.10	120.30
37	52	3937	C	C6-N1-C2	-5.49	118.10	120.30
1	A1	1440	C	N1-C2-O2	5.49	122.19	118.90
37	52	4448	G	P-O3'-C3'	5.49	126.29	119.70
37	52	4928	C	C6-N1-C1'	-5.49	114.21	120.80
39	82	141	C	C6-N1-C2	-5.48	118.11	120.30
1	A1	606	G	C4-N9-C1'	5.47	133.62	126.50
37	52	217	C	N3-C2-O2	-5.47	118.07	121.90
37	52	4716	C	C6-N1-C2	-5.47	118.11	120.30
38	72	63	C	C5-C4-N4	5.47	124.03	120.20
37	52	2594	C	N1-C2-O2	5.47	122.18	118.90
37	52	2020	U	C5-C6-N1	5.46	125.43	122.70
37	52	294	G	N3-C4-N9	5.46	129.28	126.00
37	52	3600	G	C4-N9-C1'	5.46	133.60	126.50
37	52	3876	A	P-O3'-C3'	5.46	126.25	119.70
37	52	4100	C	C6-N1-C2	-5.46	118.12	120.30
37	52	1310	C	C5-C6-N1	5.46	123.73	121.00
37	52	257	C	C6-N1-C2	-5.45	118.12	120.30
1	A1	30	C	C6-N1-C2	-5.45	118.12	120.30
1	A1	1785	C	N1-C2-O2	5.45	122.17	118.90
1	A1	1309	C	N1-C2-O2	5.45	122.17	118.90
37	52	311	G	C6-C5-N7	-5.45	127.13	130.40
37	52	1420	A	C2-N3-C4	5.45	113.32	110.60
37	52	934	C	N3-C2-O2	-5.44	118.09	121.90
37	52	732	A	O4'-C1'-N9	5.44	112.55	108.20
37	52	4528	G	N3-C4-C5	-5.43	125.88	128.60
37	52	4223	C	C6-N1-C2	-5.43	118.13	120.30
37	52	1420	A	N3-C4-N9	5.43	131.74	127.40
37	52	448	G	C4-N9-C1'	5.42	133.55	126.50
37	52	3709	U	C2-N1-C1'	5.42	124.21	117.70
39	82	153	C	N3-C2-O2	-5.42	118.11	121.90
37	52	2441	C	C6-N1-C2	-5.42	118.13	120.30
37	52	115	C	N3-C2-O2	-5.41	118.11	121.90
81	w3	56	A	C2-N3-C4	5.40	113.30	110.60
1	A1	853	C	N3-C2-O2	-5.39	118.12	121.90
1	A1	1664	A	OP1-P-O3'	5.39	117.07	105.20
37	52	1517	G	C8-N9-C1'	-5.39	119.99	127.00
37	52	1239	C	C6-N1-C1'	-5.39	114.33	120.80
37	52	2021	G	N9-C4-C5	5.39	107.56	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	2008	U	C2-N1-C1'	5.39	124.17	117.70
1	A1	1751	C	C5-C6-N1	5.38	123.69	121.00
37	52	1084	C	C5-C6-N1	5.38	123.69	121.00
37	52	4926	C	N3-C2-O2	-5.38	118.13	121.90
1	A1	652	U	N3-C2-O2	-5.38	118.43	122.20
37	52	2580	U	C5'-C4'-O4'	-5.38	102.64	109.10
37	52	2550	G	C6-C5-N7	-5.38	127.17	130.40
37	52	1305	C	N3-C2-O2	-5.38	118.13	121.90
60	Z3	73	LYS	CB-CA-C	5.38	121.15	110.40
1	A1	549	C	C6-N1-C2	-5.37	118.15	120.30
37	52	1651	G	C8-N9-C1'	-5.37	120.01	127.00
37	52	3943	A	C2-N3-C4	5.37	113.29	110.60
37	52	4654	C	C6-N1-C2	-5.37	118.15	120.30
1	A1	1364	U	N1-C2-O2	5.37	126.56	122.80
37	52	4527	G	C4-N9-C1'	5.37	133.48	126.50
1	A1	474	G	C8-N9-C1'	-5.37	120.02	127.00
37	52	1286	C	C2-N1-C1'	5.37	124.70	118.80
37	52	236	G	N3-C2-N2	-5.36	116.15	119.90
39	82	28	C	C6-N1-C2	-5.36	118.16	120.30
53	S3	68	PHE	CB-CG-CD1	5.34	124.54	120.80
37	52	3618	C	C6-N1-C2	-5.34	118.16	120.30
37	52	1370	G	P-O3'-C3'	5.34	126.11	119.70
35	j1	368	LEU	CA-CB-CG	5.33	127.56	115.30
37	52	1969	G	N3-C2-N2	5.33	123.63	119.90
37	52	3809	G	C4-N9-C1'	5.33	133.43	126.50
37	52	1666	C	C6-N1-C2	-5.33	118.17	120.30
37	52	2787	A	C4-N9-C1'	5.32	135.88	126.30
37	52	1070	G	C6-C5-N7	-5.32	127.21	130.40
83	G3	275	ILE	CG1-CB-CG2	-5.32	99.70	111.40
39	82	117	C	N1-C2-O2	5.32	122.09	118.90
37	52	125	C	P-O3'-C3'	5.31	126.08	119.70
1	A1	1314	U	N1-C2-O2	5.31	126.52	122.80
37	52	2581	A	C8-N9-C4	-5.31	103.68	105.80
37	52	4243	C	C6-N1-C2	-5.31	118.18	120.30
37	52	2489	C	N3-C2-O2	-5.30	118.19	121.90
80	23	20	U	C5-C6-N1	5.30	125.35	122.70
9	I1	36	LEU	CA-CB-CG	5.30	127.48	115.30
37	52	257	C	C5-C6-N1	5.29	123.65	121.00
1	A1	532	C	N3-C2-O2	-5.29	118.20	121.90
81	w3	56	A	C4-N9-C1'	5.29	135.82	126.30
1	A1	1395	C	O4'-C1'-N1	5.29	112.43	108.20
37	52	2851	G	C6-C5-N7	-5.29	127.23	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	1890	G	C4-C5-N7	5.29	112.92	110.80
1	A1	1453	C	N1-C2-O2	5.29	122.07	118.90
39	82	117	C	N3-C2-O2	-5.29	118.20	121.90
1	A1	1118	C	N1-C2-O2	5.28	122.07	118.90
1	A1	1256	G	C4-N9-C1'	5.28	133.36	126.50
60	Z3	14	LEU	CA-CB-CG	5.28	127.44	115.30
1	A1	1520	G	C6-C5-N7	-5.28	127.23	130.40
1	A1	142	C	N1-C2-O2	5.28	122.06	118.90
37	52	1084	C	C6-N1-C2	-5.27	118.19	120.30
39	82	42	G	C6-C5-N7	-5.27	127.24	130.40
37	52	4305	G	C4-N9-C1'	5.27	133.35	126.50
37	52	966	A	C5-N7-C8	-5.27	101.27	103.90
37	52	1636	U	C2-N1-C1'	5.27	124.02	117.70
37	52	1571	G	O4'-C1'-N9	5.27	112.41	108.20
37	52	1474	C	C6-N1-C2	-5.26	118.19	120.30
37	52	13	U	N3-C2-O2	-5.26	118.52	122.20
37	52	204	U	N1-C2-O2	5.26	126.48	122.80
1	A1	1858	G	C6-C5-N7	-5.26	127.25	130.40
39	82	121	G	C4-N9-C1'	5.26	133.34	126.50
37	52	2577	C	C5-C6-N1	5.26	123.63	121.00
37	52	986	C	N3-C2-O2	-5.25	118.23	121.90
37	52	1485	C	C2-N1-C1'	5.24	124.57	118.80
37	52	2598	A	N3-C4-N9	5.24	131.59	127.40
37	52	4165	C	C6-N1-C2	-5.24	118.20	120.30
37	52	149	A	C4-N9-C1'	5.24	135.72	126.30
37	52	168	C	N1-C2-O2	5.23	122.04	118.90
37	52	4119	C	C6-N1-C1'	-5.23	114.53	120.80
37	52	923	C	O5'-P-OP1	5.23	116.97	110.70
37	52	4871	C	N1-C2-O2	5.23	122.04	118.90
1	A1	1620	A	C4-N9-C1'	5.23	135.71	126.30
37	52	4440	G	C4-N9-C1'	5.22	133.29	126.50
1	A1	967	C	C6-N1-C2	-5.22	118.21	120.30
37	52	176	G	N3-C4-N9	-5.22	122.87	126.00
37	52	4527	G	N3-C4-N9	5.22	129.13	126.00
40	A3	29	LEU	CA-CB-CG	5.22	127.30	115.30
1	A1	1057	C	N3-C2-O2	-5.21	118.25	121.90
37	52	3600	G	N3-C4-N9	5.21	129.13	126.00
41	B3	214	ASP	CB-CG-OD1	5.21	122.99	118.30
37	52	2035	C	C6-N1-C2	-5.21	118.22	120.30
37	52	1481	C	C2-N1-C1'	5.21	124.53	118.80
37	52	1632	A	C4-N9-C1'	5.21	135.68	126.30
1	A1	1858	G	C8-N9-C1'	-5.21	120.23	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	853	C	N1-C2-O2	5.21	122.02	118.90
1	A1	1116	C	N1-C2-O2	5.21	122.02	118.90
37	52	1805	A	C4-C5-C6	5.21	119.60	117.00
37	52	1211	G	P-O3'-C3'	5.21	125.95	119.70
37	52	2019	C	C2-N1-C1'	5.21	124.53	118.80
1	A1	1074	C	C6-N1-C2	-5.20	118.22	120.30
37	52	2753	G	O3'-P-O5'	5.20	113.89	104.00
37	52	2750	G	C4-C5-N7	5.20	112.88	110.80
37	52	4948	C	O4'-C1'-N1	5.20	112.36	108.20
37	52	1556	C	C6-N1-C2	-5.20	118.22	120.30
37	52	4303	C	N3-C2-O2	-5.20	118.26	121.90
37	52	4173	G	C5-C6-O6	-5.19	125.48	128.60
1	A1	791	C	C6-N1-C2	-5.19	118.22	120.30
1	A1	1130	G	C2-N3-C4	5.19	114.49	111.90
37	52	2528	G	N3-C4-C5	-5.19	126.01	128.60
1	A1	915	G	O4'-C1'-N9	5.18	112.35	108.20
37	52	2021	G	N9-C1'-C2'	5.18	120.74	114.00
1	A1	369	C	C6-N1-C2	-5.18	118.23	120.30
80	23	30	G	C8-N9-C1'	-5.18	120.26	127.00
37	52	30	C	C5-C6-N1	5.18	123.59	121.00
1	A1	688	U	OP2-P-O3'	5.18	116.59	105.20
1	A1	1751	C	C6-N1-C2	-5.17	118.23	120.30
37	52	1912	G	C8-N9-C1'	-5.17	120.28	127.00
37	52	2627	C	C6-N1-C2	-5.17	118.23	120.30
37	52	2750	G	N7-C8-N9	5.17	115.69	113.10
1	A1	870	A	OP2-P-O3'	5.17	116.57	105.20
1	A1	937	C	C6-N1-C2	-5.17	118.23	120.30
37	52	1467	C	C5-C6-N1	5.17	123.58	121.00
37	52	453	G	N3-C4-N9	5.17	129.10	126.00
1	A1	958	G	O4'-C1'-N9	5.16	112.33	108.20
1	A1	1333	U	N1-C2-O2	5.16	126.42	122.80
37	52	294	G	N3-C4-C5	-5.16	126.02	128.60
37	52	4774	C	N1-C2-O2	5.16	122.00	118.90
3	C1	34	LYS	C-N-CA	5.16	134.59	121.70
37	52	2502	A	P-O3'-C3'	5.16	125.89	119.70
37	52	2097	A	C4-N9-C1'	5.15	135.58	126.30
37	52	2726	G	C8-N9-C1'	-5.15	120.30	127.00
1	A1	1364	U	N3-C2-O2	-5.15	118.59	122.20
37	52	2596	G	N1-C2-N2	-5.15	111.56	116.20
37	52	3809	G	C8-N9-C1'	-5.15	120.30	127.00
37	52	3938	G	C8-N9-C4	5.15	108.46	106.40
37	52	4201	G	C4-N9-C1'	5.15	133.20	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	2787	A	N3-C4-N9	5.15	131.52	127.40
37	52	4527	G	N3-C4-C5	-5.15	126.03	128.60
37	52	4880	C	N1-C2-O2	5.15	121.99	118.90
60	Z3	51	ARG	CD-NE-CZ	5.14	130.80	123.60
1	A1	1097	G	C4-N9-C1'	5.14	133.18	126.50
37	52	1774	C	C6-N1-C2	-5.14	118.24	120.30
37	52	13	U	N1-C2-O2	5.14	126.40	122.80
1	A1	1636	G	C6-C5-N7	-5.14	127.32	130.40
37	52	2838	G	C4-N9-C1'	5.14	133.18	126.50
37	52	1485	C	N3-C2-O2	-5.13	118.31	121.90
37	52	495	C	C6-N1-C2	-5.13	118.25	120.30
37	52	1899	G	C4-N9-C1'	5.13	133.17	126.50
1	A1	1139	C	N1-C2-O2	5.13	121.98	118.90
37	52	3842	C	N3-C2-O2	-5.13	118.31	121.90
38	72	5	A	N3-C4-C5	5.13	130.39	126.80
37	52	1286	C	C6-N1-C2	-5.13	118.25	120.30
37	52	3939	G	P-O3'-C3'	5.13	125.85	119.70
41	B3	17	LEU	CA-CB-CG	5.13	127.09	115.30
37	52	2441	C	C5-C6-N1	5.12	123.56	121.00
1	A1	1300	U	C2-N1-C1'	5.12	123.84	117.70
37	52	1202	C	C6-N1-C2	-5.12	118.25	120.30
37	52	2740	U	C2-N1-C1'	5.12	123.84	117.70
37	52	4232	U	OP2-P-O3'	5.12	116.45	105.20
83	G3	104	LEU	CA-CB-CG	5.12	127.07	115.30
37	52	2709	C	C6-N1-C2	-5.11	118.25	120.30
37	52	1106	A	P-O3'-C3'	5.11	125.83	119.70
37	52	1517	G	N3-C4-N9	5.11	129.06	126.00
40	A3	125	LYS	C-N-CA	5.10	134.46	121.70
37	52	1070	G	N3-C4-N9	5.10	129.06	126.00
37	52	1929	A	C2-N3-C4	5.10	113.15	110.60
37	52	4454	G	C8-N9-C1'	-5.10	120.37	127.00
37	52	4423	U	N1-C2-O2	5.10	126.37	122.80
1	A1	538	U	N3-C2-O2	-5.09	118.63	122.20
37	52	4173	G	N1-C6-O6	5.09	122.96	119.90
38	72	1	G	C2-N3-C4	5.09	114.45	111.90
37	52	266	C	O5'-P-OP2	-5.08	101.12	105.70
1	A1	887	U	C5-C6-N1	5.08	125.24	122.70
37	52	1853	G	C8-N9-C1'	-5.08	120.40	127.00
37	52	3810	C	C2-N3-C4	5.08	122.44	119.90
37	52	4158	C	O5'-P-OP1	-5.08	101.13	105.70
37	52	385	A	OP1-P-O3'	5.08	116.37	105.20
37	52	486	C	C5-C6-N1	5.08	123.54	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	52	3661	G	O4'-C1'-N9	-5.08	104.14	108.20
37	52	3673	C	N1-C2-O2	5.08	121.94	118.90
37	52	4078	C	C6-N1-C2	-5.07	118.27	120.30
37	52	3888	G	C8-N9-C4	-5.06	104.37	106.40
37	52	2295	C	C6-N1-C2	-5.06	118.28	120.30
38	72	67	C	C6-N1-C2	-5.06	118.28	120.30
1	A1	465	A	OP2-P-O3'	5.06	116.33	105.20
37	52	4929	C	C6-N1-C2	-5.06	118.28	120.30
37	52	4719	G	OP1-P-O3'	5.05	116.32	105.20
37	52	3685	C	C6-N1-C2	-5.05	118.28	120.30
37	52	498	C	OP2-P-O3'	5.05	116.30	105.20
38	72	120	U	C5-C6-N1	5.04	125.22	122.70
42	C3	289	LEU	CA-CB-CG	5.04	126.89	115.30
37	52	1577	G	C8-N9-C1'	-5.04	120.45	127.00
37	52	236	G	N1-C2-N3	5.04	126.92	123.90
37	52	934	C	N1-C2-O2	5.04	121.92	118.90
55	U3	80	LYS	CD-CE-NZ	5.04	123.28	111.70
67	g3	43	LYS	C-N-CA	5.03	134.28	121.70
1	A1	1016	U	N3-C2-O2	-5.03	118.68	122.20
37	52	729	G	N3-C4-N9	5.03	129.02	126.00
37	52	4774	C	N3-C2-O2	-5.03	118.38	121.90
38	72	36	C	C6-N1-C2	-5.03	118.29	120.30
39	82	38	U	N3-C2-O2	-5.03	118.68	122.20
37	52	515	C	C6-N1-C2	-5.03	118.29	120.30
37	52	449	C	OP2-P-O3'	5.02	116.25	105.20
37	52	3876	A	OP2-P-O3'	5.02	116.25	105.20
37	52	1286	C	N3-C2-O2	-5.02	118.39	121.90
37	52	1674	C	N3-C2-O2	-5.02	118.39	121.90
37	52	2504	C	C5-C6-N1	5.02	123.51	121.00
37	52	4879	C	C6-N1-C2	-5.02	118.29	120.30
81	w3	37	A	N7-C8-N9	5.02	116.31	113.80
37	52	4123	C	N3-C4-C5	-5.02	119.89	121.90
1	A1	659	G	C8-N9-C1'	-5.01	120.48	127.00
1	A1	1139	C	C6-N1-C2	-5.01	118.30	120.30
37	52	294	G	C8-N9-C1'	-5.01	120.48	127.00
37	52	1305	C	N1-C2-O2	5.01	121.91	118.90
40	A3	117	GLU	N-CA-C	5.01	124.53	111.00
6	F1	73	ASP	CB-CG-OD1	5.01	122.81	118.30
37	52	2008	U	N3-C2-O2	-5.01	118.69	122.20
37	52	4272	G	N3-C4-C5	-5.01	126.09	128.60
38	72	113	G	C8-N9-C1'	-5.01	120.49	127.00
37	52	1082	C	N1-C2-O2	5.01	121.91	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	293	C	C2-N1-C1'	5.00	124.30	118.80
37	52	1663	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	A3	116	LEU	Peptide
40	A3	117	GLU	Peptide
40	A3	168	VAL	Peptide
40	A3	170	ALA	Peptide
40	A3	94	ALA	Peptide
2	B1	42	LYS	Peptide
42	C3	339	THR	Peptide
83	G3	157	PRO	Peptide
83	G3	186	PRO	Peptide
83	G3	214	VAL	Peptide
85	I3	204	GLY	Peptide
47	M3	69	ARG	Peptide
14	N1	37	GLU	Peptide
48	N3	76	PRO	Peptide
48	N3	78	GLY	Peptide
16	P1	21	VAL	Peptide
17	Q1	17	TYR	Peptide
17	Q1	37	TYR	Peptide
52	R3	106	LEU	Peptide
52	R3	113	LYS	Peptide
52	R3	123	LEU	Peptide
52	R3	129	GLY	Peptide
52	R3	83	GLY	Peptide
53	S3	68	PHE	Peptide
55	U3	86	LEU	Peptide
57	W3	85	ALA	Peptide
25	Y1	61	GLN	Peptide
60	Z3	18	TYR	Peptide
60	Z3	79	HIS	Peptide
60	Z3	92	ASP	Peptide
63	c3	87	LYS	Peptide
67	g3	2	VAL	Peptide
67	g3	4	ARG	Sidechain
67	g3	43	LYS	Mainchain
67	g3	44	SER	Peptide

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Mol	Chain	Res	Type	Group
67	g3	73	HIS	Peptide
67	g3	93	ARG	Peptide
67	g3	94	ALA	Peptide
67	g3	99	GLU	Peptide
35	j1	315	GLY	Peptide
36	k1	364	ILE	Peptide
71	k3	43	TYR	Peptide
76	p3	50	ARG	Peptide
76	p3	52	VAL	Peptide
78	s3	33	ASP	Peptide
78	s3	72	ASN	Peptide
78	s3	81	HIS	Peptide
78	s3	86	VAL	Peptide
79	t3	53	TRP	Peptide
87	u3	209	THR	Peptide
87	u3	60	ARG	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	A1	36969	0	18687	184	0
2	B1	1710	0	1708	13	0
3	C1	1729	0	1803	19	0
4	D1	1716	0	1806	12	0
5	E1	1768	0	1866	21	0
6	F1	2076	0	2177	13	0
7	G1	1471	0	1522	8	0
8	H1	1923	0	2089	36	0
9	I1	1488	0	1582	6	0
10	J1	1686	0	1772	18	0
11	K1	1525	0	1640	13	0
12	L1	810	0	836	5	0
13	M1	1175	0	1249	12	0
14	N1	908	0	939	16	0
15	O1	1202	0	1289	7	0
16	P1	1016	0	1039	15	0
17	Q1	997	0	1044	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R1	1128	0	1195	9	0
19	S1	1068	0	1121	11	0
20	T1	1190	0	1249	6	0
21	U1	1097	0	1132	9	0
22	V1	795	0	862	4	0
23	W1	636	0	637	3	0
24	X1	1034	0	1080	12	0
25	Y1	1098	0	1167	7	0
26	Z1	1011	0	1083	9	0
27	a1	598	0	656	0	0
28	b1	814	0	865	0	0
29	c1	651	0	672	0	0
30	d1	488	0	514	0	0
31	e1	459	0	449	0	0
32	f1	443	0	492	0	0
33	g1	555	0	564	0	0
34	h1	2436	0	2393	0	0
35	j1	3309	0	3350	0	0
36	k1	4555	0	4696	0	0
37	52	77819	0	39310	602	0
38	72	2558	0	1296	36	0
39	82	3208	0	1629	12	0
40	A3	1898	0	1993	46	0
41	B3	3172	0	3310	37	0
42	C3	2883	0	3053	14	0
43	E3	1729	0	1887	30	0
44	F3	1875	0	1995	21	0
45	H3	1516	0	1597	8	0
46	L3	1702	0	1820	14	0
47	M3	1137	0	1211	12	0
48	N3	1701	0	1749	26	0
49	O3	1630	0	1778	12	0
50	P3	1242	0	1274	7	0
51	Q3	1515	0	1634	29	0
52	R3	1508	0	1664	30	0
53	S3	1462	0	1508	37	0
54	T3	1298	0	1366	12	0
55	U3	809	0	833	41	0
56	V3	979	0	1039	9	0
57	W3	860	0	903	20	0
58	X3	967	0	1040	8	0
59	Y3	1115	0	1205	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	Z3	1107	0	1182	41	0
61	a3	1162	0	1209	0	0
62	b3	848	0	920	0	0
63	c3	761	0	794	0	0
64	d3	888	0	930	0	0
65	e3	1053	0	1147	0	0
66	f3	876	0	912	0	0
67	g3	906	0	1001	0	0
68	h3	1013	0	1147	0	0
69	i3	830	0	916	0	0
70	j3	705	0	737	0	0
71	k3	569	0	637	0	0
72	l3	447	0	480	0	0
73	m3	429	0	465	0	0
74	n3	239	0	289	0	0
75	o3	851	0	922	0	0
76	p3	708	0	757	0	0
77	r3	994	0	1051	0	0
78	s3	1507	0	1564	0	0
79	t3	1160	0	1218	0	0
80	23	1616	0	824	7	0
81	w3	493	0	249	0	0
82	J3	1362	0	1399	9	0
83	G3	1879	0	2027	37	0
84	D3	2391	0	2424	27	0
85	I3	1664	0	1711	25	0
86	1	110	0	112	9	0
87	u3	1741	0	1854	0	0
88	52	204	0	0	0	0
88	72	7	0	0	0	0
88	82	5	0	0	0	0
88	A1	77	0	0	0	0
88	G1	1	0	0	0	0
88	M1	1	0	0	0	0
88	P3	1	0	0	0	0
88	V3	1	0	0	0	0
88	a3	1	0	0	0	0
88	g3	1	0	0	0	0
88	w3	1	0	0	0	0
89	b1	1	0	0	0	0
89	e1	1	0	0	0	0
89	g1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
89	g3	1	0	0	0	0
89	j3	1	0	0	0	0
89	m3	1	0	0	0	0
89	o3	1	0	0	0	0
89	p3	1	0	0	0	0
90	k1	16	0	0	0	0
91	1	1	0	0	0	0
91	52	3	0	0	0	0
All	All	226754	0	171197	1304	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 5.

All (1304) 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)
37:52:2395:A:C6	37:52:2395:A:C5	1.79	1.66
37:52:1239:C:C5	37:52:1239:C:C6	1.83	1.60
37:52:2395:A:N3	37:52:2395:A:C2	1.73	1.56
37:52:2395:A:C4	37:52:2395:A:N3	1.75	1.52
55:U3:49:VAL:CG2	55:U3:49:VAL:CB	1.82	1.51
37:52:2395:A:N1	37:52:2395:A:C2	1.77	1.50
55:U3:49:VAL:CG1	55:U3:49:VAL:CB	1.87	1.49
37:52:1239:C:C4	37:52:1239:C:C5	1.95	1.49
37:52:2395:A:N1	37:52:2395:A:C6	1.79	1.49
85:I3:204:GLY:CA	85:I3:204:GLY:N	1.76	1.49
37:52:3712:A:C4	37:52:3712:A:N3	1.78	1.49
37:52:3712:A:C6	37:52:3712:A:N1	1.81	1.45
37:52:119:G:C4	37:52:119:G:C5	2.04	1.42
38:72:63:C:C5	38:72:63:C:C6	2.10	1.39
37:52:2399:G:C5	37:52:2399:G:C4	2.04	1.39
37:52:2084:U:C6	37:52:2084:U:C5	2.11	1.36
37:52:1239:C:N1	37:52:1239:C:C6	1.93	1.36
37:52:2399:G:C5	37:52:2399:G:C6	2.14	1.34
37:52:119:G:C6	37:52:119:G:C5	2.14	1.34
38:72:63:C:N3	85:I3:204:GLY:N	1.73	1.33
37:52:3712:A:C6	37:52:3712:A:N3	1.97	1.33
37:52:3712:A:C4	37:52:3712:A:N1	1.96	1.32
37:52:119:G:N3	83:G3:185:ARG:NE	1.78	1.30
37:52:1239:C:C2	37:52:1239:C:N1	2.00	1.29
1:A1:970:G:C5	1:A1:970:G:C4	2.20	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:72:63:C:C5	38:72:63:C:C4	2.24	1.26
37:52:2084:U:C4	37:52:2084:U:C5	2.24	1.24
37:52:1239:C:N3	43:E3:65:TYR:OH	1.69	1.24
37:52:3712:A:C2	37:52:3712:A:N3	2.07	1.23
37:52:3712:A:C2	37:52:3712:A:N1	2.08	1.22
37:52:732:A:C4	37:52:732:A:C5	2.28	1.21
37:52:1805:A:C4	37:52:1805:A:C5	2.30	1.18
85:I3:203:ARG:C	85:I3:204:GLY:N	1.96	1.18
37:52:2631:U:C5	37:52:2631:U:C6	2.32	1.18
1:A1:970:G:N1	37:52:3712:A:N1	1.92	1.17
1:A1:970:G:C5	1:A1:970:G:C6	2.33	1.16
37:52:2399:G:C2	37:52:2399:G:N1	2.15	1.14
37:52:119:G:N1	37:52:119:G:C2	2.16	1.14
37:52:1239:C:C4	37:52:1239:C:N3	2.16	1.11
37:52:2399:G:N1	37:52:2399:G:C6	2.17	1.11
37:52:732:A:C6	37:52:732:A:C5	2.39	1.10
37:52:1239:C:C2	37:52:1239:C:N3	2.19	1.10
38:72:63:C:C6	38:72:63:C:N1	2.19	1.10
37:52:119:G:C6	37:52:119:G:N1	2.19	1.09
55:U3:49:VAL:CG2	55:U3:49:VAL:CG1	2.31	1.07
37:52:2084:U:N1	37:52:2084:U:C6	2.23	1.06
55:U3:49:VAL:CA	55:U3:49:VAL:HB	1.85	1.05
1:A1:970:G:C2	1:A1:970:G:N3	2.25	1.05
1:A1:970:G:C4	1:A1:970:G:N3	2.26	1.03
55:U3:49:VAL:HG11	55:U3:49:VAL:HG21	1.38	1.03
37:52:2084:U:N3	37:52:2084:U:C2	2.27	1.02
38:72:63:C:C2	85:I3:204:GLY:N	2.26	1.02
37:52:2084:U:N1	37:52:2084:U:C2	2.28	1.02
37:52:1805:A:C5	37:52:1805:A:C6	2.48	1.01
37:52:2631:U:C5	37:52:2631:U:C4	2.47	1.01
37:52:2084:U:C4	37:52:2084:U:N3	2.29	1.01
37:52:732:A:N1	53:S3:69:GLU:N	2.09	1.00
38:72:63:C:C2	38:72:63:C:N1	2.29	0.99
37:52:119:G:C2	83:G3:185:ARG:NE	2.31	0.98
37:52:119:G:C4	83:G3:185:ARG:NE	2.31	0.98
37:52:2399:G:C2	37:52:2399:G:N3	2.32	0.97
37:52:119:G:N3	37:52:119:G:C2	2.33	0.97
38:72:63:C:C4	85:I3:204:GLY:N	2.32	0.97
37:52:119:G:C4	37:52:119:G:N3	2.34	0.96
37:52:2399:G:N3	37:52:2399:G:C4	2.34	0.96
37:52:732:A:N1	53:S3:68:PHE:HA	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:2631:U:C5	55:U3:49:VAL:HA	2.02	0.94
53:S3:68:PHE:C	53:S3:68:PHE:CA	2.35	0.93
37:52:2631:U:N3	55:U3:49:VAL:HB	1.83	0.93
37:52:1805:A:N3	37:52:1805:A:C2	2.36	0.92
37:52:2631:U:C6	55:U3:49:VAL:HA	2.04	0.92
1:A1:970:G:N1	37:52:3712:A:N3	2.18	0.91
37:52:732:A:N3	37:52:732:A:C2	2.41	0.89
37:52:1805:A:N3	37:52:1805:A:C4	2.41	0.89
38:72:63:C:N3	38:72:63:C:C4	2.41	0.89
37:52:1239:C:C2	43:E3:65:TYR:OH	2.26	0.88
37:52:2084:U:C2	51:Q3:14:ARG:NE	2.40	0.88
37:52:732:A:N3	53:S3:68:PHE:N	2.22	0.88
37:52:1805:A:C2	37:52:1805:A:N1	2.42	0.88
1:A1:970:G:N1	37:52:3712:A:C2	2.42	0.87
55:U3:49:VAL:HG21	55:U3:49:VAL:CG1	2.02	0.87
1:A1:970:G:C2	37:52:3712:A:N1	2.43	0.87
37:52:2631:U:N1	37:52:2631:U:C6	2.44	0.86
37:52:732:A:N1	37:52:732:A:C2	2.45	0.85
37:52:1805:A:N1	37:52:1805:A:C6	2.45	0.85
37:52:732:A:C4	37:52:732:A:N3	2.45	0.85
37:52:1239:C:C4	43:E3:65:TYR:OH	2.30	0.84
1:A1:970:G:C2	37:52:3712:A:C2	2.68	0.82
55:U3:49:VAL:CA	55:U3:49:VAL:CB	2.57	0.82
38:72:63:C:N3	38:72:63:C:C2	2.48	0.81
37:52:2084:U:C4	51:Q3:14:ARG:NE	2.49	0.81
80:23:50:U:H3	80:23:64:G:H1	1.30	0.80
37:52:2631:U:N3	37:52:2631:U:C2	2.50	0.80
1:A1:970:G:C4	37:52:3712:A:C2	2.69	0.80
37:52:2631:U:C2	55:U3:49:VAL:HB	2.16	0.80
37:52:2794:C:N3	86:1:11:ALA:HB3	1.97	0.80
1:A1:970:G:C6	37:52:3712:A:C2	2.70	0.79
37:52:732:A:C6	37:52:732:A:N1	2.50	0.79
37:52:1239:C:N3	43:E3:65:TYR:CZ	2.51	0.79
37:52:2631:U:N3	37:52:2631:U:C4	2.51	0.78
37:52:2084:U:N1	51:Q3:14:ARG:NE	2.31	0.78
37:52:2753:G:H2'	60:Z3:51:ARG:HH21	1.47	0.77
37:52:1239:C:C2	43:E3:65:TYR:CZ	2.71	0.77
1:A1:970:G:C6	1:A1:970:G:N1	2.53	0.77
37:52:2084:U:C6	51:Q3:14:ARG:NE	2.51	0.77
1:A1:970:G:C6	37:52:3712:A:N3	2.52	0.77
37:52:119:G:C5	83:G3:185:ARG:NE	2.52	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:2581:A:H5''	60:Z3:73:LYS:HB3	1.67	0.77
1:A1:970:G:C5	37:52:3712:A:C2	2.73	0.76
37:52:2631:U:N1	37:52:2631:U:C2	2.54	0.75
8:H1:130:PRO:O	57:W3:84:GLY:N	2.19	0.75
37:52:2084:U:N3	51:Q3:14:ARG:NE	2.35	0.75
37:52:732:A:C6	53:S3:68:PHE:C	2.60	0.75
37:52:2084:U:C5	51:Q3:14:ARG:NE	2.55	0.74
37:52:2631:U:C2	55:U3:49:VAL:CB	2.71	0.74
37:52:732:A:C5	53:S3:68:PHE:C	2.61	0.73
1:A1:970:G:C2	1:A1:970:G:N1	2.55	0.73
40:A3:118:GLU:H	40:A3:162:ASN:HD22	1.35	0.73
16:P1:34:PHE:HB3	16:P1:41:PHE:HB2	1.70	0.72
1:A1:970:G:C4	37:52:3712:A:N3	2.58	0.72
37:52:732:A:C2	53:S3:68:PHE:C	2.63	0.72
37:52:4124:G:N7	40:A3:64:ARG:NH2	2.37	0.72
37:52:119:G:C6	83:G3:185:ARG:NE	2.58	0.71
38:72:63:C:N1	85:I3:204:GLY:N	2.38	0.71
40:A3:181:LYS:HG3	40:A3:183:GLY:H	1.55	0.71
38:72:6:C:H42	84:D3:71:GLY:HA2	1.55	0.71
83:G3:185:ARG:NE	83:G3:185:ARG:CD	2.53	0.71
1:A1:970:G:C5	37:52:3712:A:N3	2.59	0.71
37:52:732:A:N1	53:S3:68:PHE:C	2.45	0.70
84:D3:200:MET:HB3	84:D3:202:GLN:HE22	1.57	0.70
37:52:1239:C:C4	43:E3:65:TYR:CZ	2.80	0.70
37:52:2753:G:H5''	60:Z3:51:ARG:HG2	1.74	0.70
37:52:2753:G:H3'	60:Z3:51:ARG:HE	1.58	0.69
37:52:119:G:N1	83:G3:185:ARG:NE	2.40	0.69
1:A1:970:G:C6	37:52:3712:A:N1	2.59	0.69
48:N3:163:GLY:O	48:N3:172:ARG:NH2	2.26	0.68
1:A1:1033:G:H1	1:A1:1080:A:HO2'	1.41	0.68
37:52:2754:G:N3	60:Z3:51:ARG:NH1	2.41	0.68
1:A1:659:G:HO2'	1:A1:662:G:HO2'	1.37	0.68
1:A1:970:G:N3	37:52:3712:A:C2	2.62	0.68
60:Z3:128:LYS:HA	60:Z3:131:PHE:HD2	1.58	0.68
37:52:732:A:C4	53:S3:68:PHE:C	2.67	0.68
39:82:151:G:OP2	83:G3:118:ARG:NH1	2.27	0.67
40:A3:28:ARG:HD2	40:A3:30:ARG:HE	1.59	0.67
55:U3:79:SER:HB3	55:U3:82:TYR:HB2	1.76	0.67
37:52:989:U:H3	37:52:1065:G:H1	1.41	0.67
37:52:4212:A:N1	54:T3:3:ASN:ND2	2.42	0.67
37:52:4745:G:H1	37:52:4955:A:H61	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:122:G:H1	1:A1:342:C:H42	1.40	0.67
37:52:2399:G:N2	37:52:2400:G:N3	2.43	0.67
14:N1:58:GLU:HB3	14:N1:61:TYR:HB3	1.76	0.67
37:52:4431:U:OP2	85:I3:3:ARG:NH2	2.28	0.66
37:52:914:U:N3	37:52:918:G:N7	2.40	0.66
1:A1:658:U:O2	25:Y1:17:ARG:NH2	2.28	0.66
6:F1:191:ARG:HH21	6:F1:245:ARG:HD3	1.60	0.66
37:52:1758:G:H1	37:52:1774:C:H42	1.41	0.66
37:52:2575:U:O2	37:52:2589:C:N4	2.29	0.65
40:A3:118:GLU:HB3	40:A3:120:PRO:HD2	1.77	0.65
15:O1:136:PRO:HG2	15:O1:139:TRP:HB2	1.78	0.65
37:52:1952:G:N2	37:52:2032:U:O2	2.28	0.65
37:52:2837:U:OP1	41:B3:249:ARG:NH1	2.29	0.65
37:52:2393:C:N4	37:52:2822:G:O6	2.30	0.65
37:52:1963:C:H42	37:52:4694:G:H1	1.45	0.65
14:N1:33:ARG:HH12	14:N1:89:VAL:HG11	1.60	0.65
37:52:2631:U:C2	55:U3:49:VAL:CA	2.79	0.65
37:52:732:A:C4	53:S3:68:PHE:O	2.50	0.65
37:52:2631:U:C4	55:U3:49:VAL:CB	2.80	0.65
37:52:732:A:N3	53:S3:68:PHE:C	2.51	0.64
38:72:63:C:C5	85:I3:204:GLY:N	2.65	0.64
37:52:1280:C:O2'	42:C3:321:ASN:ND2	2.30	0.64
44:F3:93:ARG:HE	44:F3:108:LEU:HD13	1.61	0.64
37:52:4122:G:C5	60:Z3:135:ARG:HD2	2.32	0.64
45:H3:129:ARG:HG2	45:H3:153:LEU:HD22	1.80	0.64
60:Z3:16:GLY:O	60:Z3:19:SER:OG	2.15	0.64
37:52:2597:G:N2	37:52:2749:C:O2	2.30	0.64
55:U3:47:ILE:HD12	55:U3:56:LEU:HD13	1.79	0.64
42:C3:330:PRO:HB3	44:F3:46:ARG:HH21	1.63	0.64
37:52:230:G:OP1	59:Y3:15:ARG:NH1	2.31	0.64
37:52:95:G:OP2	46:L3:11:LYS:NZ	2.29	0.64
37:52:2084:U:C2	51:Q3:14:ARG:CD	2.80	0.64
37:52:1332:C:H2'	37:52:1333:A:H8	1.63	0.63
13:M1:93:LEU:HD21	25:Y1:8:ARG:HH11	1.63	0.63
38:72:63:C:C6	85:I3:204:GLY:N	2.66	0.63
1:A1:1104:G:H1	1:A1:1128:C:H42	1.46	0.63
80:23:14:A:N6	80:23:21:A:O2'	2.32	0.63
1:A1:1858:G:OP2	16:P1:146:ARG:NH2	2.31	0.63
37:52:3688:U:OP2	40:A3:198:ARG:NH2	2.31	0.63
40:A3:162:ASN:OD1	40:A3:162:ASN:N	2.32	0.63
37:52:2046:G:H5'	49:O3:60:LYS:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:2654:C:O3'	60:Z3:76:ASN:ND2	2.32	0.63
37:52:732:A:C6	53:S3:68:PHE:HA	2.34	0.63
37:52:2631:U:N3	55:U3:49:VAL:CB	2.60	0.62
13:M1:11:GLN:HB3	13:M1:56:ILE:HD11	1.79	0.62
37:52:1182:C:OP2	37:52:1183:C:N4	2.32	0.62
37:52:3894:A:H61	37:52:4566:U:H3	1.48	0.62
40:A3:122:ASP:OD1	40:A3:122:ASP:N	2.30	0.62
52:R3:126:LYS:O	52:R3:132:PHE:N	2.32	0.62
38:72:85:G:OP1	44:F3:221:LYS:NZ	2.32	0.62
1:A1:39:A:H5'	11:K1:7:TRP:HE1	1.65	0.62
37:52:2624:G:N2	37:52:2633:U:O2	2.33	0.62
1:A1:970:G:C2	37:52:3712:A:N3	2.68	0.62
42:C3:329:ASN:ND2	44:F3:187:GLU:OE2	2.32	0.61
10:J1:123:ARG:NH1	10:J1:134:GLU:OE1	2.33	0.61
20:T1:127:TRP:O	20:T1:144:ARG:NH2	2.33	0.61
8:H1:131:ARG:O	57:W3:85:ALA:N	2.34	0.61
37:52:732:A:C6	53:S3:69:GLU:N	2.69	0.61
43:E3:191:ARG:NH2	43:E3:217:ASP:OD1	2.33	0.61
1:A1:522:A:O3'	11:K1:131:ARG:NH2	2.33	0.61
53:S3:34:ALA:HB1	53:S3:39:VAL:HG23	1.82	0.61
37:52:2455:G:N2	37:52:2471:G:N7	2.46	0.61
37:52:3896:C:O2'	41:B3:268:ARG:NH1	2.34	0.61
44:F3:114:ARG:HD3	51:Q3:5:ILE:HD11	1.83	0.61
37:52:2262:G:OP2	52:R3:107:ARG:NH1	176.19	0.61
37:52:2812:A:OP1	52:R3:88:ARG:NH1	2.33	0.61
37:52:3892:U:O2'	50:P3:80:GLN:NE2	2.34	0.61
37:52:732:A:C4	53:S3:68:PHE:CA	2.83	0.60
41:B3:322:HIS:O	41:B3:342:LYS:NZ	2.32	0.60
56:V3:31:ASN:HD21	56:V3:115:SER:HB2	1.66	0.60
39:82:21:C:OP1	42:C3:195:LYS:NZ	2.34	0.60
1:A1:943:U:OP1	3:C1:214:LYS:NZ	2.34	0.60
1:A1:678:U:H5''	15:O1:127:ARG:HH12	1.67	0.60
37:52:1552:G:O2'	37:52:1574:G:N2	2.30	0.60
37:52:3940:U:OP2	48:N3:24:ARG:NH2	2.34	0.60
1:A1:377:G:OP1	10:J1:98:LYS:NZ	2.34	0.60
82:J3:46:GLN:NE2	82:J3:72:CYS:SG	2.74	0.60
37:52:2658:G:N2	37:52:2675:G:O2'	2.33	0.60
14:N1:33:ARG:HA	14:N1:110:VAL:HB	1.83	0.60
37:52:2663:G:OP2	52:R3:118:HIS:NE2	2.35	0.60
37:52:1906:U:OP1	44:F3:217:GLY:N	2.35	0.60
37:52:2631:U:C4	55:U3:49:VAL:CA	2.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:312:G:N2	37:52:326:C:O2	2.34	0.60
37:52:732:A:C6	53:S3:68:PHE:CA	2.84	0.60
60:Z3:38:TYR:OH	60:Z3:74:VAL:O	2.18	0.60
37:52:3707:U:O2	37:52:3744:G:N2	2.35	0.60
37:52:1857:C:N3	37:52:1878:G:N2	2.50	0.60
1:A1:942:G:N2	16:P1:138:ASP:OD2	2.35	0.60
6:F1:43:PRO:HD2	6:F1:46:ILE:HD12	1.84	0.60
37:52:3787:G:H21	37:52:3789:C:H42	1.47	0.59
1:A1:1284:A:N6	1:A1:1313:A:O2'	2.34	0.59
8:H1:146:ASN:O	57:W3:101:ARG:NH1	2.34	0.59
45:H3:94:SER:HB3	45:H3:142:ASP:HB3	1.83	0.59
1:A1:1096:G:OP1	24:X1:20:ARG:NH1	2.35	0.59
59:Y3:21:ALA:O	59:Y3:26:ARG:NH2	2.35	0.59
37:52:1764:G:O2'	37:52:1767:A:N7	2.35	0.59
37:52:2794:C:H42	86:1:11:ALA:HB3	1.67	0.59
6:F1:11:ARG:NH2	6:F1:21:ASP:OD1	2.36	0.59
24:X1:102:ILE:H	24:X1:113:HIS:HD2	1.50	0.59
4:D1:209:VAL:HG11	4:D1:233:LEU:HD11	1.84	0.59
47:M3:80:ALA:O	47:M3:85:LYS:NZ	2.35	0.59
26:Z1:7:ILE:HD12	26:Z1:43:LYS:HD2	1.84	0.59
37:52:4661:G:N2	37:52:5005:G:OP1	2.36	0.59
44:F3:151:GLU:O	44:F3:247:ASN:ND2	2.35	0.59
37:52:1187:G:H1'	84:D3:275:GLN:HE21	1.66	0.59
37:52:3973:G:H1	37:52:4038:C:H42	1.51	0.59
1:A1:521:A:OP1	11:K1:45:ARG:NH1	2.35	0.59
58:X3:48:ARG:HH12	58:X3:50:LYS:HG3	1.66	0.59
37:52:713:C:H2'	37:52:714:G:H8	1.67	0.59
43:E3:185:ASN:ND2	43:E3:274:LEU:O	2.34	0.59
37:52:3711:A:N6	37:52:3736:A:OP2	2.36	0.59
48:N3:114:ARG:NH1	48:N3:151:ILE:O	2.36	0.59
47:M3:119:ARG:NH2	49:O3:193:THR:OG1	2.35	0.59
59:Y3:50:ARG:HB2	59:Y3:115:ARG:HH22	1.66	0.59
1:A1:1854:U:OP1	16:P1:150:ARG:NH1	2.35	0.59
45:H3:26:ILE:HG22	45:H3:35:ARG:HG2	1.84	0.59
52:R3:84:THR:OG1	52:R3:87:ALA:N	2.36	0.59
41:B3:165:HIS:ND1	41:B3:166:THR:O	2.36	0.58
37:52:732:A:C2	53:S3:68:PHE:CA	2.86	0.58
37:52:1970:A:N6	37:52:2016:C:OP2	2.36	0.58
37:52:2420:A:N6	37:52:2424:G:N7	2.52	0.58
37:52:2709:C:OP2	52:R3:43:LYS:NZ	2.36	0.58
37:52:1239:C:N1	43:E3:65:TYR:OH	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X1:52:ILE:HG22	24:X1:61:ILE:HG12	1.85	0.58
80:23:21:A:N6	80:23:46:G:O2'	2.36	0.58
37:52:1763:C:H2'	37:52:1769:G:H22	1.69	0.58
1:A1:1082:A:HO2'	1:A1:1842:C:HO2'	1.51	0.58
40:A3:149:LYS:HD2	40:A3:156:LYS:HE2	1.85	0.58
46:L3:25:TRP:HE1	48:N3:199:GLN:HB3	1.67	0.58
37:52:2023:C:OP1	53:S3:83:ARG:NH1	54.34	0.58
1:A1:64:A:H2	1:A1:83:A:H62	1.51	0.58
11:K1:170:PRO:O	11:K1:175:ARG:NH1	2.37	0.58
59:Y3:46:SER:O	59:Y3:122:LYS:NZ	2.35	0.58
37:52:2084:U:C4	51:Q3:14:ARG:CD	2.87	0.58
37:52:3942:A:N6	37:52:4067:U:O4	2.35	0.58
57:W3:6:CYS:SG	57:W3:7:SER:N	2.77	0.58
37:52:2581:A:O5'	60:Z3:75:TYR:N	2.37	0.58
37:52:4772:C:N4	37:52:4864:U:O2	2.37	0.58
1:A1:442:C:N3	1:A1:452:G:N2	2.52	0.58
2:B1:188:THR:HG22	2:B1:189:ILE:HG13	1.85	0.58
42:C3:232:VAL:HG21	42:C3:256:ALA:HB1	1.85	0.58
53:S3:11:LYS:HD2	53:S3:29:ARG:HD2	1.86	0.58
26:Z1:14:THR:HG22	26:Z1:21:LYS:HG3	1.86	0.58
37:52:102:G:O2'	37:52:1381:U:O2'	2.20	0.58
37:52:3968:U:H3	37:52:4053:A:H61	1.49	0.58
37:52:982:U:OP2	37:52:983:C:N4	2.35	0.58
1:A1:1567:G:H1'	21:U1:37:VAL:HG21	1.85	0.58
37:52:191:G:O6	37:52:250:C:N4	2.36	0.58
37:52:1079:C:N4	37:52:1221:G:O6	2.37	0.58
37:52:2658:G:N3	37:52:2675:G:N2	2.51	0.58
37:52:2059:C:O2	53:S3:118:ARG:NH1	2.37	0.57
10:J1:174:CYS:SG	10:J1:175:ILE:N	2.77	0.57
82:J3:152:GLY:O	82:J3:156:ARG:NH1	2.36	0.57
37:52:3965:A:N6	37:52:4048:A:N3	2.52	0.57
37:52:960:A:H62	43:E3:129:LEU:H	1.52	0.57
37:52:2779:C:H5'	58:X3:105:ASN:HD22	1.69	0.57
37:52:1590:C:O2	37:52:1605:G:N2	2.37	0.57
37:52:2577:C:OP1	60:Z3:111:ARG:NE	2.36	0.57
37:52:4389:C:H2'	37:52:4390:A:H8	1.69	0.57
39:82:36:G:H3'	45:H3:89:ARG:HD2	167.64	0.57
3:C1:57:ILE:HG22	3:C1:59:SER:H	1.69	0.57
8:H1:162:LEU:HD22	8:H1:170:ARG:HB2	1.87	0.57
85:I3:61:SER:HA	85:I3:126:VAL:HG23	1.86	0.57
85:I3:93:PRO:HA	85:I3:127:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L1:59:LYS:HB3	12:L1:70:TYR:HB2	1.85	0.57
37:52:1239:C:C6	43:E3:65:TYR:CZ	2.92	0.57
37:52:1823:G:O2'	84:D3:44:TYR:O	2.23	0.57
7:G1:20:PHE:HB3	7:G1:23:TRP:HB2	1.86	0.57
37:52:3939:G:HO2'	37:52:4076:G:H1	1.50	0.57
1:A1:1629:C:OP1	20:T1:39:ARG:NH2	2.37	0.57
37:52:2631:U:N1	55:U3:49:VAL:CA	2.68	0.57
3:C1:66:VAL:HG22	3:C1:87:ILE:HG22	1.86	0.57
5:E1:133:GLY:HA3	5:E1:156:LEU:H	1.69	0.57
58:X3:107:HIS:O	58:X3:111:GLN:NE2	2.37	0.57
1:A1:1497:G:N7	12:L1:25:LYS:NZ	2.49	0.57
59:Y3:50:ARG:NH1	59:Y3:112:ASP:OD2	2.38	0.57
5:E1:28:GLU:OE2	5:E1:65:ARG:NH2	2.38	0.56
37:52:1239:C:C6	43:E3:65:TYR:OH	2.57	0.56
7:G1:71:ARG:NH1	7:G1:148:ASN:OD1	2.37	0.56
1:A1:1095:U:O2	1:A1:1151:G:N2	2.38	0.56
83:G3:148:LEU:HD23	83:G3:271:LEU:HD21	1.87	0.56
38:72:105:C:OP2	85:I3:203:ARG:NH2	2.39	0.56
21:U1:115:LYS:HA	21:U1:121:ARG:HA	1.87	0.56
60:Z3:47:ASP:HB3	60:Z3:69:LYS:HB3	1.86	0.56
37:52:119:G:C6	83:G3:185:ARG:CD	2.89	0.56
24:X1:37:PHE:HE1	24:X1:103:VAL:HG11	1.70	0.56
37:52:2400:G:H1	37:52:2804:C:H42	1.54	0.56
37:52:956:A:H62	37:52:1283:G:H1'	1.71	0.56
38:72:77:A:H62	38:72:99:G:H21	1.54	0.56
43:E3:164:ARG:NH1	43:E3:276:SER:OG	2.38	0.56
44:F3:104:VAL:HG13	44:F3:135:VAL:HG12	1.87	0.56
11:K1:179:LYS:O	11:K1:183:GLY:N	2.36	0.56
56:V3:83:ARG:NH1	56:V3:120:PRO:O	2.35	0.56
37:52:1755:C:O2'	37:52:1757:U:OP2	2.23	0.56
1:A1:1229:G:N2	1:A1:1530:U:O2	2.39	0.56
1:A1:611:G:H1	1:A1:632:C:H42	1.51	0.56
41:B3:57:VAL:HG22	41:B3:73:VAL:HG12	1.86	0.56
1:A1:121:U:O3'	6:F1:77:ARG:NH1	2.38	0.56
37:52:4162:C:N3	83:G3:125:LYS:NZ	2.48	0.56
37:52:417:G:O2'	39:82:16:G:N2	2.34	0.56
37:52:1239:C:C5	43:E3:65:TYR:OH	2.58	0.56
48:N3:68:ARG:NH1	48:N3:124:ASP:O	2.38	0.56
37:52:8:U:H5'	48:N3:40:PRO:HG3	1.86	0.56
37:52:2084:U:N3	51:Q3:14:ARG:CD	2.69	0.56
37:52:4633:G:O2'	37:52:4635:A:OP2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:41:ARG:HE	2:B1:45:GLY:HA2	1.69	0.56
37:52:2100:G:H1	42:C3:310:HIS:HA	1.71	0.56
21:U1:11:GLN:OE1	21:U1:62:ARG:NH1	2.37	0.56
1:A1:1514:G:H2'	1:A1:1515:G:H8	1.69	0.56
1:A1:506:G:OP1	26:Z1:108:LYS:NZ	2.35	0.56
2:B1:50:ASN:OD1	2:B1:53:ARG:NH1	2.39	0.56
37:52:2631:U:C6	55:U3:49:VAL:CB	2.89	0.56
37:52:2756:G:O6	60:Z3:65:ARG:NH2	2.38	0.56
37:52:4970:C:N4	37:52:5063:G:O6	2.38	0.56
39:82:147:G:H2'	39:82:148:A:H8	1.70	0.56
37:52:3928:A:OP1	48:N3:90:ASN:ND2	2.39	0.56
37:52:1177:U:H2'	37:52:1178:G:H8	1.70	0.55
37:52:1239:C:C1'	37:52:1239:C:C6	2.88	0.55
37:52:1928:C:N4	37:52:2054:U:O2	2.39	0.55
37:52:2739:C:O2	40:A3:174:ARG:NH1	2.39	0.55
37:52:4882:U:OP1	47:M3:117:LYS:NZ	2.39	0.55
6:F1:100:ARG:HH21	6:F1:118:GLU:HG2	1.71	0.55
21:U1:56:ARG:NH2	21:U1:99:VAL:O	2.39	0.55
37:52:2756:G:C2	37:52:2757:A:H1'	2.42	0.55
83:G3:282:ARG:NH1	83:G3:285:GLU:OE2	2.38	0.55
1:A1:140:U:O2'	8:H1:149:LYS:NZ	2.39	0.55
37:52:3965:A:H61	37:52:4045:G:H21	1.53	0.55
1:A1:599:A:H2'	1:A1:606:G:H21	1.71	0.55
6:F1:48:LEU:HD23	6:F1:61:VAL:HG13	1.88	0.55
37:52:181:C:N4	37:52:182:G:O6	2.39	0.55
37:52:4949:G:H4'	37:52:4950:U:H5'	1.88	0.55
8:H1:12:CYS:SG	8:H1:13:GLN:N	2.79	0.55
55:U3:103:VAL:HG21	55:U3:113:ARG:HE	1.71	0.55
26:Z1:41:ARG:NH2	26:Z1:52:PRO:O	2.40	0.55
37:52:386:A:O2'	59:Y3:87:ARG:NH2	2.36	0.55
38:72:63:C:N3	85:I3:203:ARG:C	2.59	0.55
19:S1:31:ASN:HD21	19:S1:55:THR:HG22	1.71	0.55
37:52:2631:U:N3	55:U3:49:VAL:CA	2.70	0.55
37:52:4735:G:H1	37:52:4964:C:H42	1.55	0.55
37:52:4872:G:OP2	47:M3:94:LYS:NZ	2.39	0.55
37:52:495:C:N4	37:52:496:G:O6	2.40	0.55
1:A1:1121:G:N2	3:C1:202:GLN:O	2.39	0.55
26:Z1:103:SER:OG	26:Z1:106:GLN:OE1	2.25	0.55
37:52:1239:C:C5	43:E3:65:TYR:CZ	2.95	0.55
37:52:1818:G:O2'	37:52:1820:U:OP2	2.24	0.55
37:52:2439:G:N2	37:52:2539:C:O2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A3:160:SER:OG	40:A3:161:ALA:N	2.40	0.55
38:72:62:U:OP1	84:D3:279:ARG:NH2	2.40	0.55
37:52:2754:G:C4	60:Z3:51:ARG:HD3	2.42	0.55
37:52:2794:C:N4	86:1:11:ALA:HB3	2.22	0.55
37:52:679:C:H2'	37:52:680:G:H8	1.71	0.55
18:R1:123:ASP:O	18:R1:126:ARG:NH2	2.40	0.55
37:52:2022:C:H4'	53:S3:83:ARG:HA	49.38	0.55
37:52:2794:C:C4	86:1:11:ALA:HB3	2.42	0.54
43:E3:96:THR:HG22	43:E3:109:VAL:HG22	1.89	0.54
1:A1:453:C:O2'	8:H1:92:ARG:O	2.24	0.54
40:A3:159:SER:OG	40:A3:160:SER:N	2.39	0.54
38:72:5:A:H4'	84:D3:52:ILE:HD13	1.88	0.54
48:N3:33:LEU:O	48:N3:65:ARG:NH1	2.41	0.54
37:52:2631:U:N1	55:U3:49:VAL:CB	2.70	0.54
1:A1:878:G:H22	1:A1:908:A:H2	1.55	0.54
14:N1:38:ALA:HA	14:N1:42:LEU:HD13	1.90	0.54
1:A1:678:U:OP1	15:O1:127:ARG:NH2	2.41	0.54
37:52:3717:A:OP2	37:52:3735:G:N2	2.41	0.54
37:52:738(A):C:O2'	37:52:740:G:OP2	2.26	0.54
40:A3:26:ALA:HB3	40:A3:28:ARG:HE	1.73	0.54
84:D3:261:VAL:HG12	84:D3:263:LYS:H	1.72	0.54
14:N1:99:LYS:H	14:N1:101:ARG:HH12	1.54	0.54
37:52:732:A:C5	53:S3:68:PHE:CA	2.91	0.54
37:52:119:G:O6	83:G3:166:ARG:NH1	2.41	0.54
37:52:1689:G:O6	37:52:1847:C:N4	2.40	0.54
37:52:2590:G:H21	60:Z3:65:ARG:HH21	1.54	0.54
1:A1:232:A:OP2	1:A1:889:U:O2'	2.25	0.54
6:F1:204:SER:OG	6:F1:205:PHE:N	2.40	0.54
8:H1:98:ARG:NH1	8:H1:99:GLY:O	2.40	0.54
10:J1:148:LYS:HA	10:J1:151:GLU:HB2	1.88	0.54
37:52:1759:G:H1	37:52:1773:U:H3	1.54	0.54
37:52:2490:U:O2'	37:52:2491:C:O4'	2.24	0.54
37:52:2647:A:H62	37:52:2686:G:H8	1.55	0.54
37:52:322:C:N4	37:52:4355:G:O6	2.40	0.54
40:A3:179:ILE:HG21	40:A3:185:ALA:HB2	1.90	0.54
41:B3:234:ARG:NH1	41:B3:271:GLN:O	2.40	0.54
8:H1:181:THR:HG22	8:H1:184:VAL:HG23	1.89	0.54
37:52:1720:C:OP1	37:52:1835:G:N2	2.40	0.54
39:82:130:C:H2'	39:82:131:G:H8	1.72	0.54
1:A1:970:G:N3	37:52:3712:A:N3	2.56	0.54
37:52:1103:C:N4	37:52:1195:G:O2'	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:3605:C:OP2	52:R3:71:ARG:NH1	2.41	0.54
37:52:4195:G:OP2	37:52:4195:G:N2	2.41	0.54
84:D3:39:GLN:NE2	84:D3:46:THR:O	2.40	0.54
52:R3:103:ARG:HH21	52:R3:128:LYS:HB2	1.72	0.54
37:52:119:G:C2	83:G3:185:ARG:CD	2.91	0.54
1:A1:167:G:O3'	57:W3:80:ARG:NH2	2.41	0.54
37:52:2045:G:N2	37:52:2046:G:N7	2.56	0.54
37:52:2581:A:H8	60:Z3:73:LYS:HG3	1.73	0.54
1:A1:970:G:H22	37:52:3709:U:H6	1.55	0.54
37:52:4459:U:O2'	41:B3:265:SER:OG	2.25	0.54
1:A1:1568:C:OP1	21:U1:96:SER:OG	2.26	0.54
41:B3:254:ILE:HG23	41:B3:266:VAL:HG11	1.88	0.54
14:N1:82:ASN:O	14:N1:86:GLY:N	2.41	0.54
18:R1:19:ALA:HB2	18:R1:75:GLY:HA3	1.89	0.54
37:52:1996:C:H42	37:52:2000:G:H1	1.56	0.53
37:52:2749:C:H2'	37:52:2750:G:H8	1.72	0.53
37:52:63:G:OP2	48:N3:169:ARG:NH1	2.39	0.53
17:Q1:85:ILE:HD13	17:Q1:111:MET:HB3	1.90	0.53
55:U3:49:VAL:CB	55:U3:49:VAL:HA	2.37	0.53
37:52:3961:G:H1	37:52:3964:U:H5''	1.72	0.53
37:52:2041:A:N7	37:52:4434:C:O2'	2.41	0.53
37:52:729:G:C6	37:52:732:A:H1'	2.43	0.53
1:A1:951:C:O2'	16:P1:50:LYS:NZ	2.41	0.53
20:T1:115:LYS:HE2	20:T1:126:PHE:HB2	1.90	0.53
37:52:346:G:OP1	59:Y3:8:THR:OG1	2.26	0.53
37:52:4254:G:H22	37:52:4257:A:H2	1.56	0.53
1:A1:316:G:H3'	8:H1:183:ARG:HH22	1.72	0.53
60:Z3:12:LEU:HB2	60:Z3:81:MET:HB3	1.91	0.53
60:Z3:28:ASN:N	60:Z3:28:ASN:OD1	2.41	0.53
37:52:4240:G:N2	37:52:4285:U:O2	2.41	0.53
37:52:4704:C:H2'	37:52:4705:A:H8	1.73	0.53
1:A1:1520:G:N2	1:A1:1521:C:N3	2.56	0.53
43:E3:105:GLY:HA2	43:E3:108:ARG:HH22	1.73	0.53
83:G3:90:LYS:NZ	83:G3:97:ASP:OD2	2.36	0.53
37:52:1398:A:N6	37:52:1399:G:N3	2.56	0.53
37:52:1570:G:N2	52:R3:129:GLY:O	2.42	0.53
13:M1:120:VAL:HG22	13:M1:145:VAL:HG11	1.89	0.53
37:52:2475:G:C5	58:X3:50:LYS:HD2	2.44	0.53
37:52:175:C:O2	37:52:262:G:N2	2.41	0.53
38:72:20:U:O2	38:72:59:G:N2	2.42	0.53
40:A3:182:ALA:O	40:A3:186:TYR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:1239:C:N1	43:E3:65:TYR:CZ	2.77	0.53
1:A1:380:G:OP1	10:J1:56:ARG:NH2	2.41	0.53
10:J1:6:ASP:N	10:J1:6:ASP:OD1	2.40	0.53
37:52:1485:C:H2'	46:L3:198:ARG:HH12	1.73	0.53
37:52:732:A:N3	53:S3:68:PHE:CA	2.72	0.53
37:52:2422:C:HO2'	37:52:3857:G:HO2'	1.55	0.53
1:A1:106:C:H4'	1:A1:410:G:H21	1.74	0.53
37:52:4735:G:N2	37:52:4736:C:N3	2.57	0.53
1:A1:1327:G:H1	1:A1:1502:C:H42	1.56	0.53
1:A1:492:C:N3	1:A1:509:G:N2	2.57	0.53
14:N1:95:ASP:HB3	14:N1:101:ARG:HH11	1.73	0.53
37:52:2794:C:N3	86:1:11:ALA:CB	2.69	0.53
1:A1:1617:G:N1	1:A1:1620:A:OP2	2.42	0.53
4:D1:196:ILE:HB	4:D1:223:TYR:HB2	1.89	0.53
37:52:2703:G:OP1	55:U3:113:ARG:NH1	2.42	0.53
37:52:3939:G:O2'	37:52:4076:G:N1	2.37	0.53
37:52:4908:G:H21	37:52:4913:G:H1	1.57	0.53
1:A1:1299:A:N6	1:A1:1301:A:N7	2.57	0.53
5:E1:162:ASP:OD1	5:E1:165:ASN:ND2	2.42	0.53
18:R1:41:MET:N	18:R1:41:MET:SD	2.82	0.53
37:52:2430:C:H2'	37:52:2431:A:H8	1.74	0.52
5:E1:139:SER:OG	5:E1:140:GLY:N	2.42	0.52
5:E1:6:SER:OG	5:E1:7:LYS:N	2.42	0.52
37:52:2743:A:O2'	40:A3:21:LYS:NZ	2.43	0.52
44:F3:156:ARG:NH2	44:F3:211:LYS:O	2.42	0.52
37:52:2787:A:H2	37:52:2801:U:H3	1.56	0.52
3:C1:134:LEU:HD13	3:C1:219:LYS:HD2	1.91	0.52
37:52:4128:A:O2'	83:G3:88:ARG:NH1	2.43	0.52
8:H1:194:LEU:O	8:H1:198:ARG:NH2	2.42	0.52
52:R3:125:LEU:HA	52:R3:129:GLY:H	1.75	0.52
37:52:2081:C:O2'	51:Q3:10:ASP:O	2.27	0.52
11:K1:176:LYS:O	11:K1:180:LYS:N	2.41	0.52
12:L1:4:PRO:HD2	12:L1:7:ASN:HD22	1.73	0.52
37:52:1169:G:O6	37:52:1193:C:N4	2.42	0.52
41:B3:222:VAL:O	41:B3:343:ARG:NH1	2.43	0.52
37:52:119:G:N3	83:G3:185:ARG:CD	2.72	0.52
37:52:4039:G:H1'	37:52:4050:A:H1'	1.90	0.52
1:A1:1036:A:N3	1:A1:1844:U:O2'	2.43	0.52
37:52:3681:G:N3	40:A3:125:LYS:HD3	2.25	0.52
40:A3:57:PRO:HD2	40:A3:170:ALA:HB3	1.92	0.52
14:N1:93:LYS:HG2	14:N1:100:PRO:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Y3:26:ARG:NH1	59:Y3:75:ARG:O	2.42	0.52
37:52:1186:U:H2'	37:52:1187:G:C8	2.44	0.52
37:52:2631:U:C6	55:U3:49:VAL:CA	2.86	0.52
41:B3:283:LYS:HD3	41:B3:363:ILE:HD11	1.92	0.52
37:52:2533:C:OP1	58:X3:139:ARG:NH2	2.43	0.52
37:52:721:G:H1	37:52:947:C:H42	1.58	0.52
1:A1:1462:U:OP2	1:A1:1463:U:N3	2.42	0.52
41:B3:41:VAL:HG12	41:B3:187:GLY:HA3	1.91	0.52
82:J3:146:ARG:HG2	82:J3:147:ARG:HG2	1.90	0.52
13:M1:103:GLU:HB3	25:Y1:10:ALA:HB3	1.92	0.52
17:Q1:81:ARG:NH2	17:Q1:117:GLY:O	2.42	0.52
80:23:21:A:N6	80:23:48:C:OP2	2.42	0.51
1:A1:1082:A:O2'	1:A1:1842:C:O2'	2.24	0.51
1:A1:1328:G:N2	1:A1:1502:C:O2	2.43	0.51
3:C1:92:GLN:HB3	3:C1:95:ASN:HB2	1.91	0.51
80:23:30:G:H1	80:23:40:C:H42	1.57	0.51
37:52:1968:G:H22	37:52:2020:U:H3	1.59	0.51
1:A1:678:U:OP2	1:A1:1026:C:N4	2.43	0.51
4:D1:191:VAL:HG11	4:D1:236:PHE:HD1	1.74	0.51
13:M1:104:LYS:O	25:Y1:11:ARG:NH2	2.42	0.51
37:52:2631:U:C2	55:U3:49:VAL:N	2.78	0.51
56:V3:123:LYS:HB3	56:V3:140:ALA:HB2	1.92	0.51
37:52:4122:G:C2	60:Z3:135:ARG:HB3	2.45	0.51
44:F3:34:LYS:O	44:F3:38:GLN:NE2	2.43	0.51
1:A1:1679:A:OP1	7:G1:60:ARG:NH2	2.44	0.51
17:Q1:75:VAL:HG21	17:Q1:104:GLN:HE22	1.75	0.51
37:52:2659:A:N7	37:52:2675:G:N2	2.59	0.51
1:A1:681:U:H4'	25:Y1:9:THR:HG22	1.92	0.51
2:B1:183:LEU:HD22	2:B1:188:THR:HG21	1.93	0.51
41:B3:71:GLU:OE1	57:W3:1:MET:N	2.42	0.51
42:C3:169:LEU:HD12	42:C3:172:LYS:HG3	1.92	0.51
52:R3:95:TRP:HH2	52:R3:103:ARG:HH22	1.58	0.51
37:52:2452:G:N2	37:52:2508:U:O4	2.44	0.51
37:52:2822:G:H5'	52:R3:18:GLY:HA3	1.92	0.51
37:52:4680:G:N2	37:52:4711:C:O2	2.44	0.51
51:Q3:14:ARG:NE	51:Q3:14:ARG:CD	2.72	0.51
37:52:1952:G:H1	37:52:2031:C:H42	1.58	0.51
37:52:2460:A:O2'	48:N3:96:ARG:NH1	2.44	0.51
37:52:732:A:C8	37:52:733:A:H1'	2.46	0.51
1:A1:1286:G:N3	1:A1:1312:G:N2	2.59	0.51
1:A1:1741:U:OP1	10:J1:42:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N3:38:ARG:HG2	48:N3:62:TYR:HE1	1.76	0.51
37:52:2631:U:C5	55:U3:49:VAL:CB	2.93	0.51
3:C1:122:GLU:O	3:C1:165:ARG:NH2	2.43	0.51
37:52:423:G:OP1	50:P3:62:ARG:NH2	2.41	0.51
1:A1:190:G:O2'	1:A1:209:A:N6	2.43	0.51
4:D1:146:GLU:OE2	5:E1:120:TYR:OH	2.29	0.51
37:52:83:C:H1'	37:52:101:A:H61	1.76	0.51
37:52:125:C:O2	37:52:144:G:N2	2.40	0.51
37:52:1356:U:O2'	37:52:1505:C:O2	2.28	0.51
1:A1:970:G:N3	37:52:3712:A:N1	2.58	0.51
1:A1:1711:U:H2'	1:A1:1712:A:H8	1.74	0.51
47:M3:31:ILE:HG22	47:M3:32:ASP:HB2	1.92	0.51
37:52:2580:U:H3'	60:Z3:74:VAL:HA	1.93	0.51
37:52:450:G:H1	37:52:1297:U:H3	1.58	0.51
37:52:219:G:C2	42:C3:172:LYS:HD3	2.45	0.51
37:52:978:G:N2	37:52:1278:C:N3	2.57	0.51
59:Y3:89:LYS:HG2	59:Y3:90:ALA:H	1.76	0.51
1:A1:970:G:C2	37:52:3712:A:C6	2.98	0.50
14:N1:52:LEU:HB2	14:N1:76:LEU:HD13	1.94	0.50
42:C3:286:ASN:N	51:Q3:124:ASP:OD2	2.44	0.50
37:52:119:G:C5	83:G3:185:ARG:HD3	2.46	0.50
83:G3:314:LEU:O	83:G3:318:LEU:N	2.44	0.50
10:J1:139:LYS:O	10:J1:141:ARG:NH2	2.44	0.50
57:W3:96:GLN:HB3	57:W3:101:ARG:HH21	1.76	0.50
37:52:1991:A:N6	37:52:2003:G:OP1	2.44	0.50
37:52:4993:G:N2	37:52:5059:C:O2	2.42	0.50
8:H1:131:ARG:N	57:W3:85:ALA:O	2.45	0.50
37:52:2666:U:H5''	52:R3:107:ARG:HH21	1.75	0.50
37:52:2756:G:N1	37:52:2757:A:N3	2.60	0.50
43:E3:52:LEU:HD13	43:E3:53:VAL:HG23	1.93	0.50
60:Z3:46:ILE:HA	60:Z3:68:ILE:HG23	1.93	0.50
37:52:2088:A:OP1	51:Q3:38:ARG:NH2	2.40	0.50
37:52:3619:G:N2	37:52:3623:C:N3	2.60	0.50
1:A1:970:G:N1	37:52:3712:A:C6	2.79	0.50
41:B3:307:TYR:HD2	41:B3:366:LYS:HG2	1.76	0.50
84:D3:77:ALA:O	84:D3:108:ARG:NH2	2.45	0.50
84:D3:99:TYR:OH	84:D3:168:ASP:OD2	2.29	0.50
37:52:3942:A:O2'	37:52:3943:A:OP2	2.30	0.50
37:52:3971:G:H21	37:52:4050:A:H62	1.60	0.50
5:E1:40:ARG:HH12	5:E1:49:ILE:HD11	1.75	0.50
86:1:13:ALA:O	86:1:14:ALA:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:2738:C:O2'	37:52:2740:U:O2	2.29	0.50
37:52:4313:A:OP1	54:T3:92:ARG:NH2	2.44	0.50
1:A1:1296:U:O2	1:A1:1303:C:N4	2.44	0.50
3:C1:136:ARG:HE	3:C1:218:LEU:HD11	1.76	0.50
44:F3:156:ARG:HH22	44:F3:212:LEU:HA	1.77	0.50
37:52:4045:G:H22	37:52:4048:A:H5''	1.77	0.50
37:52:942:G:OP1	44:F3:244:ARG:NH1	2.40	0.50
1:A1:108:G:N2	1:A1:354:U:O2	2.45	0.50
10:J1:148:LYS:O	10:J1:152:ARG:N	2.45	0.50
52:R3:110:ARG:HD3	52:R3:111:GLU:HG3	1.94	0.50
37:52:2624:G:OP2	55:U3:97:ARG:NH2	2.45	0.50
60:Z3:40:HIS:O	60:Z3:77:TYR:OH	2.26	0.50
37:52:1398:A:H62	37:52:1419:G:H21	1.58	0.49
1:A1:559:G:HO2'	1:A1:560:A:H8	1.57	0.49
40:A3:45:VAL:HG22	40:A3:61:VAL:HG12	1.94	0.49
37:52:119:G:N2	83:G3:186:PRO:O	2.45	0.49
83:G3:315:ALA:HA	83:G3:318:LEU:HB2	1.94	0.49
37:52:1077:C:O2	37:52:1234:G:N2	2.45	0.49
37:52:709:C:H1'	37:52:4942:C:H5	1.77	0.49
1:A1:144:U:OP2	8:H1:139:SER:OG	2.31	0.49
1:A1:1498:A:OP2	5:E1:27:ARG:NH2	2.44	0.49
59:Y3:55:VAL:HG13	59:Y3:104:VAL:HG13	1.95	0.49
37:52:119:G:C4	83:G3:185:ARG:CD	2.95	0.49
1:A1:970:G:C5	37:52:3712:A:C4	3.01	0.49
37:52:91:G:H5'	37:52:92:C:H5''	1.92	0.49
37:52:1272:C:H3'	41:B3:117:ARG:HH21	135.02	0.49
42:C3:84:THR:HG23	42:C3:86:ARG:H	1.77	0.49
37:52:107:G:OP2	46:L3:42:ARG:NH1	2.45	0.49
8:H1:146:ASN:HB3	57:W3:101:ARG:HH12	1.77	0.49
57:W3:13:ILE:HG12	57:W3:32:LEU:HD13	1.94	0.49
24:X1:86:LEU:HD23	24:X1:117:ARG:HE	1.76	0.49
37:52:4091:G:N2	37:52:4159:C:O2	2.45	0.49
38:72:63:C:C4	85:I3:203:ARG:C	2.86	0.49
85:I3:35:ASP:OD1	85:I3:86:HIS:NE2	2.40	0.49
14:N1:52:LEU:HD23	14:N1:78:LYS:HG2	1.93	0.49
48:N3:110:CYS:HB3	48:N3:113:LEU:HD12	1.95	0.49
37:52:2891:U:OP2	52:R3:74:ARG:NH2	2.46	0.49
37:52:1397:A:HO2'	37:52:1467:C:HO2'	1.57	0.49
37:52:2468:U:N3	37:52:2471:G:O6	2.46	0.49
37:52:2897:G:N3	37:52:3603:G:N1	2.61	0.49
37:52:1964:A:N7	37:52:4694:G:N2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:65:C:H41	8:H1:136:LYS:HB2	1.75	0.49
43:E3:141:ARG:NH1	43:E3:172:SER:O	2.45	0.49
37:52:4165:C:OP1	83:G3:106:ARG:NH2	2.46	0.49
13:M1:40:ILE:HD11	13:M1:68:ILE:HG13	1.95	0.49
37:52:2422:C:O2'	37:52:3857:G:O2'	2.25	0.49
37:52:2479:G:H1	37:52:2499:C:H42	1.61	0.49
40:A3:8:GLN:NE2	40:A3:231:ALA:O	2.46	0.49
43:E3:216:THR:HG23	43:E3:218:ALA:H	1.77	0.49
26:Z1:55:ILE:HG12	26:Z1:75:ILE:HG12	1.95	0.49
37:52:517:C:H2'	37:52:518:G:H8	1.76	0.49
39:82:41:A:N6	39:82:102:G:O2'	2.46	0.49
37:52:2631:U:C4	55:U3:49:VAL:HB	2.48	0.49
1:A1:498:C:N4	1:A1:499:G:O6	2.46	0.49
83:G3:86:GLU:O	83:G3:88:ARG:NH1	2.46	0.49
8:H1:132:ARG:H	57:W3:82:ILE:HB	1.78	0.49
48:N3:58:GLY:HA3	48:N3:142:ILE:HD11	1.95	0.49
8:H1:132:ARG:N	57:W3:82:ILE:HB	2.28	0.49
37:52:1100:U:O2	37:52:1196:G:N2	2.46	0.49
37:52:962:C:H42	37:52:970:G:H1	1.60	0.49
1:A1:1692:U:H2'	1:A1:1693:G:C8	2.48	0.49
1:A1:677:G:H21	1:A1:1028:A:H62	1.61	0.49
5:E1:132:LYS:HG3	5:E1:156:LEU:HB3	1.95	0.49
8:H1:132:ARG:HG3	8:H1:133:LEU:HD12	1.95	0.49
21:U1:116:ASP:N	21:U1:120:GLY:O	2.46	0.49
26:Z1:85:ASN:N	26:Z1:85:ASN:OD1	2.46	0.49
37:52:1100:U:H3	37:52:1195:G:H22	1.61	0.48
37:52:1668:A:OP2	37:52:2280:G:N2	2.41	0.48
37:52:325:U:OP1	46:L3:103:ARG:NH1	2.46	0.48
1:A1:1355:C:O2	4:D1:235:ASN:ND2	2.46	0.48
1:A1:441:C:OP2	10:J1:2:GLY:N	2.46	0.48
37:52:1100:U:O2'	37:52:1101:C:O4'	2.31	0.48
37:52:1961:G:N2	37:52:2024:G:O2'	2.45	0.48
37:52:2599:G:N2	37:52:2747:U:O4	2.45	0.48
37:52:2444:U:HO2'	39:82:112:G:HO2'	1.60	0.48
1:A1:1401:A:N6	1:A1:1441:U:O2'	2.46	0.48
1:A1:1805:G:H2'	1:A1:1806:A:H8	1.77	0.48
37:52:3919:C:H4'	40:A3:207:VAL:HG12	1.94	0.48
41:B3:310:SER:OG	41:B3:311:ASP:N	2.45	0.48
82:J3:18:ARG:HG3	82:J3:135:GLY:HA3	1.95	0.48
14:N1:14:VAL:HG23	14:N1:18:LEU:HB2	1.94	0.48
16:P1:30:VAL:HG23	16:P1:94:HIS:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S3:168:THR:OG1	53:S3:169:THR:N	2.45	0.48
37:52:1982:G:N2	37:52:2009:A:O2'	2.41	0.48
37:52:2604:C:H42	37:52:2735:G:H1	1.60	0.48
37:52:4384:U:O2'	37:52:4386:C:OP1	2.30	0.48
38:72:6:C:H3'	38:72:7:G:H4'	1.95	0.48
1:A1:282:G:H5''	1:A1:891:G:H4'	1.95	0.48
1:A1:909:G:OP2	52:R3:176:ARG:NH1	2.43	0.48
37:52:3660:C:H2'	37:52:3682:A:H61	1.78	0.48
37:52:4910:A:H4'	41:B3:95:THR:HG22	1.96	0.48
4:D1:206:SER:OG	4:D1:207:ALA:N	2.46	0.48
23:W1:15:ARG:HH11	23:W1:33:GLN:HE21	1.61	0.48
37:52:1184:A:H2'	37:52:1185:G:C5	2.49	0.48
37:52:1487:G:H2'	37:52:1488:G:H8	1.77	0.48
37:52:156:G:N2	37:52:157:U:O4	2.47	0.48
37:52:164:G:N2	37:52:272:U:O2	2.46	0.48
37:52:4992:G:N2	37:52:5060:A:N3	2.62	0.48
6:F1:80:ILE:HG13	6:F1:81:THR:HG23	1.94	0.48
8:H1:7:PHE:HD1	8:H1:113:ILE:HB	1.78	0.48
37:52:1882:U:OP1	37:52:2280:G:O2'	2.29	0.48
41:B3:160:ILE:HD13	41:B3:194:LEU:HD13	1.95	0.48
55:U3:47:ILE:H	55:U3:56:LEU:HD22	1.79	0.48
37:52:2580:U:H5	60:Z3:38:TYR:CZ	2.30	0.48
37:52:1790:U:OP2	54:T3:13:TYR:OH	2.32	0.48
37:52:119:G:C5	83:G3:185:ARG:CD	2.97	0.48
37:52:2021:G:H2'	53:S3:83:ARG:H	54.12	0.48
37:52:1406(C):G:H1	37:52:1411:C:H42	1.61	0.48
37:52:1959:U:OP1	37:52:1960:A:O2'	2.28	0.48
37:52:2284:G:H2'	37:52:2285:A:H8	1.79	0.48
37:52:2389:A:H2'	37:52:2390:G:H8	1.78	0.48
1:A1:969:U:OP1	1:A1:970:G:O2'	2.28	0.48
5:E1:177:LEU:HD13	5:E1:182:LEU:HD13	1.96	0.48
5:E1:21:LEU:HD23	5:E1:37:VAL:HG21	1.96	0.48
51:Q3:22:ASP:OD1	51:Q3:22:ASP:N	2.46	0.48
37:52:1069:G:H2'	37:52:1070:G:H4'	1.96	0.48
37:52:2529:A:N6	37:52:2532:C:O2	2.47	0.48
37:52:5047:C:O2'	37:52:5050:C:OP2	2.32	0.48
38:72:47:G:H21	84:D3:222:GLN:HE22	1.61	0.48
16:P1:131:ASP:HB3	16:P1:133:THR:HG23	1.95	0.48
37:52:1237:C:N3	43:E3:61:ARG:NH2	2.61	0.48
37:52:1426:G:N1	37:52:1458:C:OP2	2.39	0.48
37:52:3605:C:OP1	52:R3:71:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:744:G:O2'	1:A1:746:C:N4	2.47	0.48
37:52:119:G:C6	83:G3:185:ARG:CZ	2.97	0.48
47:M3:6:PHE:O	47:M3:11:ARG:NE	2.46	0.48
50:P3:4:TYR:HE2	50:P3:16:LYS:HB3	1.78	0.48
37:52:1073:G:H2'	37:52:1074:G:H8	1.78	0.47
37:52:4045:G:H22	37:52:4047:A:H3'	1.79	0.47
39:82:131:G:H5''	58:X3:108:GLN:HE21	1.78	0.47
1:A1:1692:U:H2'	1:A1:1693:G:H8	1.79	0.47
40:A3:43:GLY:HA3	40:A3:88:VAL:H	1.79	0.47
37:52:1073:G:H2'	37:52:1074:G:C8	2.49	0.47
37:52:1691:G:OP1	51:Q3:15:ARG:NE	2.44	0.47
37:52:197:A:N1	37:52:225:G:O2'	2.39	0.47
37:52:5:A:O2'	83:G3:245:ARG:NH2	2.39	0.47
1:A1:1737:G:OP1	8:H1:94:ARG:NH2	2.47	0.47
1:A1:511:U:H2'	1:A1:512:A:H8	1.79	0.47
37:52:5057:C:O2'	84:D3:23:ARG:NH2	171.33	0.47
11:K1:19:PRO:O	11:K1:24:ARG:NH2	2.47	0.47
37:52:731:G:H21	53:S3:68:PHE:HE2	1.62	0.47
1:A1:1515:G:H2'	1:A1:1516:G:H8	1.78	0.47
40:A3:101:VAL:HB	40:A3:165:VAL:HG12	1.96	0.47
9:I1:61:ILE:HD11	9:I1:95:ILE:HD12	1.96	0.47
1:A1:677:G:OP1	15:O1:124:ARG:NH2	2.47	0.47
37:52:2084:U:C6	51:Q3:14:ARG:CD	2.98	0.47
37:52:3947:A:H61	37:52:4065:G:H22	1.62	0.47
37:52:488:G:N2	37:52:489:C:O2	2.47	0.47
37:52:95:G:H8	46:L3:11:LYS:HZ1	1.62	0.47
1:A1:1468:C:H2'	1:A1:1469:A:H8	1.79	0.47
1:A1:1616:U:OP2	17:Q1:43:ARG:NH2	2.46	0.47
1:A1:1662:U:O4	1:A1:1663:A:N6	2.47	0.47
37:52:2084:U:N3	51:Q3:14:ARG:HD3	2.29	0.47
37:52:3690:U:OP2	40:A3:200:ARG:NH1	2.47	0.47
37:52:68:U:OP1	48:N3:178:HIS:ND1	2.38	0.47
37:52:714:G:N3	37:52:955:G:N2	2.62	0.47
1:A1:970:G:N7	37:52:3712:A:H1'	2.30	0.47
3:C1:33:VAL:HA	3:C1:96:CYS:HB2	1.97	0.47
37:52:147:A:H1'	48:N3:57:GLN:HE21	1.80	0.47
50:P3:4:TYR:HE1	50:P3:18:ARG:HD3	1.79	0.47
37:52:235:A:O2'	37:52:237:G:OP2	2.28	0.47
37:52:4522:G:O2'	37:52:4525:C:OP2	2.26	0.47
38:72:120:U:H3'	84:D3:259:ARG:HH12	1.79	0.47
37:52:983:C:N3	43:E3:73:ARG:NE	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F1:125:LYS:H	6:F1:142:HIS:HD2	1.62	0.47
20:T1:14:ARG:HE	20:T1:17:ASN:HA	1.80	0.47
37:52:300:A:H2'	37:52:301:G:H8	1.80	0.47
37:52:2542:G:O2'	39:82:128:C:O2	2.24	0.47
84:D3:65:ALA:HB2	84:D3:74:ILE:HD13	1.96	0.47
37:52:119:G:H22	83:G3:186:PRO:HG2	1.79	0.47
9:I1:144:ILE:HD12	24:X1:52:ILE:HD11	1.97	0.47
46:L3:77:SER:OG	46:L3:78:LEU:N	2.47	0.47
23:W1:17:CYS:HB2	23:W1:56:CYS:HB3	1.96	0.47
57:W3:86:SER:OG	57:W3:89:ASP:N	2.48	0.47
37:52:3969:G:H1	37:52:4052:C:H42	1.62	0.47
1:A1:1808:U:H2'	1:A1:1809:A:H8	1.80	0.47
84:D3:90:VAL:HG21	84:D3:231:VAL:HG21	1.95	0.47
54:T3:31:MET:HG3	84:D3:69:ILE:HG22	1.96	0.47
49:O3:18:ARG:HH22	49:O3:128:ARG:CZ	2.28	0.47
18:R1:16:LYS:HG3	18:R1:17:LYS:H	1.79	0.47
19:S1:58:MET:O	19:S1:62:GLN:NE2	2.46	0.47
86:1:14:ALA:O	86:1:15:ALA:HB2	2.14	0.47
37:52:292:G:O6	48:N3:181:HIS:ND1	2.41	0.47
37:52:3920:U:O2	37:52:4382:G:N2	2.48	0.47
37:52:759:G:N2	37:52:760:G:O2'	2.47	0.47
3:C1:139:CYS:SG	3:C1:140:VAL:N	2.88	0.47
17:Q1:33:LEU:HG	17:Q1:37:TYR:HE1	1.79	0.47
24:X1:7:LEU:HD23	24:X1:34:ILE:HG12	1.97	0.47
37:52:106:A:OP1	46:L3:39:ARG:NH2	2.43	0.47
37:52:1549:G:H4'	52:R3:87:ALA:HA	1.97	0.47
37:52:4729:A:OP2	37:52:5068:G:N2	2.48	0.47
7:G1:86:LYS:HA	7:G1:89:THR:HG22	1.97	0.47
9:I1:31:GLU:HB2	9:I1:40:LEU:HB2	1.97	0.47
16:P1:98:ARG:NH1	16:P1:100:THR:O	2.48	0.47
16:P1:34:PHE:HD1	16:P1:98:ARG:HD2	1.79	0.47
18:R1:28:GLY:N	18:R1:65:GLY:O	2.40	0.47
57:W3:9:SER:OG	57:W3:36:CYS:SG	2.62	0.47
1:A1:149:A:H2'	1:A1:150:A:H8	1.80	0.47
2:B1:124:VAL:HG21	2:B1:134:LEU:HD21	1.97	0.47
41:B3:36:ASP:N	41:B3:36:ASP:OD1	2.63	0.47
83:G3:282:ARG:HG3	83:G3:283:TYR:H	1.80	0.47
8:H1:5:ILE:HG12	8:H1:111:LEU:HB2	1.96	0.47
37:52:2084:U:N1	51:Q3:14:ARG:CD	2.77	0.47
18:R1:146:ARG:HH22	80:23:33:U:H5	1.63	0.47
18:R1:116:ASP:HB3	18:R1:119:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:4300:U:H4'	54:T3:89:ILE:HG22	1.95	0.46
22:V1:41:ARG:HA	22:V1:44:LYS:HB2	1.96	0.46
1:A1:918:U:O2'	24:X1:56:HIS:O	2.33	0.46
37:52:4699:U:H1'	37:52:4700:A:H5''	1.98	0.46
37:52:469:C:OP2	37:52:684:G:N1	2.45	0.46
1:A1:1719:A:N6	1:A1:1814:G:O2'	2.48	0.46
42:C3:94:ASN:N	42:C3:94:ASN:OD1	2.47	0.46
84:D3:256:LYS:HD3	84:D3:257:PRO:HD2	1.97	0.46
83:G3:213:ASP:OD1	83:G3:213:ASP:N	2.45	0.46
1:A1:163:U:OP2	8:H1:87:ARG:NH2	2.47	0.46
37:52:1441:C:H42	37:52:2113:G:H1	1.63	0.46
37:52:729:G:C8	37:52:732:A:H4'	2.50	0.46
1:A1:316:G:H1	1:A1:334:C:H42	1.63	0.46
1:A1:317:C:H42	1:A1:333:G:H1	1.64	0.46
1:A1:667:U:O4	1:A1:1143:A:N6	2.48	0.46
37:52:1572:U:H4'	52:R3:95:TRP:CZ3	2.50	0.46
37:52:119:G:N1	83:G3:185:ARG:CD	2.79	0.46
37:52:119:G:N1	83:G3:185:ARG:HD2	2.30	0.46
37:52:1332:C:H2'	37:52:1333:A:C8	2.48	0.46
37:52:1976:G:O6	37:52:1990:A:N6	2.38	0.46
38:72:8:G:O6	38:72:111:C:N4	2.49	0.46
5:E1:72:VAL:HG22	12:L1:20:VAL:HG21	1.96	0.46
53:S3:68:PHE:HA	53:S3:68:PHE:C	2.32	0.46
55:U3:66:SER:HB2	55:U3:69:LYS:HB3	1.98	0.46
37:52:1395:U:OP1	46:L3:183:ARG:NH1	2.44	0.46
37:52:2848:G:O2'	37:52:3838:U:O4	2.29	0.46
40:A3:118:GLU:N	40:A3:162:ASN:HD22	2.08	0.46
4:D1:201:GLY:N	4:D1:221:ASP:OD2	2.48	0.46
9:I1:7:LYS:NZ	9:I1:40:LEU:O	2.38	0.46
15:O1:32:ASP:O	15:O1:36:GLN:N	2.46	0.46
55:U3:47:ILE:HB	55:U3:56:LEU:HD22	1.96	0.46
59:Y3:127:GLN:O	59:Y3:131:GLU:N	2.48	0.46
37:52:2583:C:C2	60:Z3:73:LYS:HG2	2.51	0.46
37:52:2749:C:H2'	37:52:2750:G:C8	2.50	0.46
37:52:351:C:N3	39:82:25:G:N2	2.63	0.46
13:M1:57:ASP:OD2	13:M1:60:CYS:N	2.49	0.46
19:S1:77:GLU:OE2	19:S1:81:ARG:NH1	2.46	0.46
53:S3:66:GLN:HG2	53:S3:68:PHE:HB3	1.97	0.46
25:Y1:107:ARG:HD3	25:Y1:112:VAL:HG22	1.98	0.46
37:52:280:G:N2	37:52:306:A:OP2	2.42	0.46
38:72:63:C:C6	85:I3:203:ARG:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:334:C:H5	8:H1:190:ARG:HH12	1.62	0.46
10:J1:70:GLU:OE1	10:J1:117:TYR:OH	2.30	0.46
37:52:2411:C:H2'	37:52:2412:A:H8	1.80	0.46
37:52:2581:A:P	60:Z3:75:TYR:H	2.38	0.46
1:A1:74:G:N2	1:A1:77:A:OP2	2.49	0.46
8:H1:2:LYS:HD3	8:H1:15:LEU:HD21	1.97	0.46
1:A1:446:G:OP2	10:J1:47:ARG:NH1	2.49	0.46
16:P1:20:GLN:HG2	16:P1:27:VAL:HG23	1.96	0.46
37:52:2084:U:C2	51:Q3:14:ARG:HD3	2.51	0.46
37:52:146:G:H2'	37:52:147:A:H8	1.81	0.46
37:52:3908:A:N6	86:1:20:ALA:HA	2.31	0.46
1:A1:1856:C:N4	1:A1:1857:G:O6	2.49	0.46
1:A1:210:U:H2'	1:A1:211:G:C8	2.51	0.46
5:E1:195:SER:HB2	5:E1:197:LYS:HE2	1.97	0.46
37:52:1209:U:O3'	44:F3:69:ARG:NH1	2.48	0.46
44:F3:93:ARG:NH2	44:F3:115:GLN:O	2.49	0.46
38:72:63:C:C2	85:I3:203:ARG:C	2.89	0.46
53:S3:154:LEU:HB3	53:S3:157:ARG:HD3	1.97	0.46
37:52:1868:A:N6	37:52:1870:C:O2	2.48	0.46
38:72:19:C:O2	38:72:60:G:N2	2.48	0.46
1:A1:1245:G:O2'	1:A1:1492:U:OP1	2.30	0.46
1:A1:77:A:O2'	8:H1:174:PRO:O	2.33	0.46
40:A3:125:LYS:HZ2	40:A3:126:LEU:HD22	1.81	0.46
7:G1:39:ILE:HG23	7:G1:68:ILE:HG21	1.98	0.46
85:I3:150:GLU:OE2	85:I3:153:ARG:NH1	2.49	0.46
14:N1:45:ARG:NH1	14:N1:71:GLU:OE2	2.49	0.46
53:S3:80:ILE:HG12	53:S3:129:VAL:HG22	1.97	0.46
21:U1:6:VAL:O	21:U1:11:GLN:NE2	2.42	0.46
60:Z3:42:LEU:HD21	60:Z3:101:PHE:HZ	1.82	0.46
37:52:4740:G:H22	37:52:4959:U:H3	1.63	0.45
1:A1:375:U:H2'	1:A1:376:A:H8	1.81	0.45
1:A1:532:C:H2'	1:A1:533:A:C8	2.51	0.45
3:C1:32:ASP:OD1	3:C1:46:LYS:NZ	2.37	0.45
18:R1:53:GLU:OE1	18:R1:85:ARG:NH2	2.49	0.45
51:Q3:167:VAL:HG12	51:Q3:169:SER:H	1.80	0.45
55:U3:31:ASP:OD2	55:U3:114:TYR:OH	2.31	0.45
8:H1:147:LEU:HD11	8:H1:156:TYR:HD2	1.82	0.45
37:52:303:C:OP2	48:N3:68:ARG:NH2	2.49	0.45
26:Z1:35:VAL:HG21	26:Z1:40:ILE:HD11	1.98	0.45
37:52:1215:C:OP2	44:F3:58:LYS:NZ	2.40	0.45
37:52:1477:C:O2	37:52:1489:G:N2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:1664:U:O2	37:52:2286:G:N2	2.50	0.45
37:52:4896:G:N2	37:52:4925:U:O2	2.50	0.45
1:A1:97:U:H2'	1:A1:98:C:H6	1.81	0.45
2:B1:126:ASP:OD1	2:B1:165:ASN:ND2	2.49	0.45
6:F1:85:GLY:N	6:F1:88:ASP:OD2	2.50	0.45
45:H3:41:ILE:HG12	45:H3:73:ILE:HD11	1.99	0.45
85:I3:29:ALA:HB3	85:I3:32:ARG:HH22	1.81	0.45
37:52:2631:U:C4	55:U3:49:VAL:C	2.90	0.45
37:52:2631:U:C5	55:U3:49:VAL:CA	2.88	0.45
37:52:4471:U:OP2	45:H3:168:LYS:NZ	2.47	0.45
37:52:732:A:N1	53:S3:68:PHE:CA	2.69	0.45
37:52:907:C:H2'	37:52:908:G:C8	2.52	0.45
1:A1:1575:G:H2'	1:A1:1576:G:H8	1.81	0.45
3:C1:88:THR:HG22	3:C1:98:THR:HG22	1.98	0.45
11:K1:179:LYS:HA	11:K1:182:GLN:HB2	1.98	0.45
37:52:151:G:OP2	48:N3:4:TYR:OH	2.34	0.45
37:52:2411:C:H2'	37:52:2412:A:C8	2.52	0.45
37:52:719:C:H42	37:52:949:G:H1	1.65	0.45
52:R3:83:GLY:H	52:R3:88:ARG:HH21	1.63	0.45
60:Z3:27:LYS:HG2	60:Z3:93:LYS:HD3	1.99	0.45
37:52:115:C:O2'	37:52:276:C:OP1	2.33	0.45
1:A1:970:G:C4	37:52:3712:A:N1	2.85	0.45
37:52:4156:G:H5''	37:52:4157:A:H3'	1.97	0.45
37:52:4633:G:N2	37:52:4664:A:OP2	2.38	0.45
1:A1:1816:G:HO2'	37:52:3807:A:HO2'	1.53	0.45
49:O3:18:ARG:HH12	49:O3:128:ARG:HH11	1.65	0.45
51:Q3:61:LEU:HD21	51:Q3:66:MET:HB2	1.97	0.45
37:52:2484:A:N1	37:52:2495:U:N3	2.65	0.45
37:52:2581:A:OP2	60:Z3:73:LYS:N	2.33	0.45
37:52:3853:U:O2'	37:52:4979:A:N3	2.49	0.45
43:E3:153:LEU:HD13	43:E3:197:VAL:HG11	1.98	0.45
52:R3:174:GLU:O	52:R3:178:GLN:NE2	2.49	0.45
37:52:2084:U:C4	51:Q3:14:ARG:CZ	3.00	0.45
37:52:280:G:OP2	48:N3:44:ARG:NH2	2.38	0.45
37:52:4704:C:H2'	37:52:4705:A:C8	2.52	0.45
1:A1:1216:C:H5''	1:A1:1217:A:H5''	1.97	0.45
1:A1:613:G:N2	1:A1:626:G:OP1	2.41	0.45
8:H1:148:SER:OG	57:W3:105:ARG:NH2	2.45	0.45
53:S3:15:ARG:HH21	54:T3:141:VAL:HG22	1.82	0.45
5:E1:40:ARG:HG2	22:V1:108:PRO:HG3	1.99	0.45
37:52:1931:C:N4	37:52:2040:A:O2'	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1234:C:H4'	1:A1:1246:A:H61	1.82	0.45
1:A1:551:U:H2'	1:A1:552:G:H8	1.82	0.45
5:E1:59:LEU:HB2	5:E1:63:GLY:HA2	1.99	0.45
37:52:1411:C:H2'	37:52:1411(A):G:C8	2.52	0.44
1:A1:1100:A:O5'	19:S1:132:ARG:NH2	2.50	0.44
1:A1:1215:C:H42	1:A1:1220:A:H61	1.65	0.44
40:A3:227:ARG:HG3	40:A3:239:ALA:HB2	1.98	0.44
38:72:49:A:H5''	84:D3:224:SER:HB3	2.00	0.44
5:E1:10:LYS:NZ	5:E1:14:ASP:OD2	2.50	0.44
7:G1:194:ASP:OD2	7:G1:198:ARG:NH2	2.50	0.44
45:H3:121:LYS:HB2	45:H3:121:LYS:HE2	1.79	0.44
3:C1:67:PHE:HE1	16:P1:48:SER:HB2	1.81	0.44
37:52:4898:G:N2	37:52:4923:U:O2'	2.50	0.44
83:G3:126:ARG:HH12	83:G3:296:GLY:N	2.15	0.44
83:G3:149:LEU:HD13	83:G3:242:ARG:HH11	1.82	0.44
13:M1:126:VAL:HG23	13:M1:145:VAL:HG22	1.99	0.44
14:N1:28:HIS:CG	14:N1:114:TYR:HB3	2.52	0.44
37:52:423:G:H21	50:P3:118:GLN:HE22	1.65	0.44
37:52:3893:C:H5''	50:P3:66:GLY:HA2	2.00	0.44
1:A1:1648:G:N2	1:A1:1675:A:OP2	2.48	0.44
40:A3:54:ARG:HG3	40:A3:56:ALA:H	1.82	0.44
56:V3:13:LYS:HD2	56:V3:128:LEU:HD22	1.99	0.44
37:52:2084:U:C5	51:Q3:14:ARG:CD	3.01	0.44
37:52:2759:G:H21	37:52:2765:A:H2	1.63	0.44
1:A1:1867:U:H4'	1:A1:1868:U:H5'	1.99	0.44
38:72:59:G:O2'	84:D3:267:ASN:ND2	2.51	0.44
8:H1:57:ASP:OD2	8:H1:72:ARG:NH1	2.50	0.44
9:I1:10:LYS:NZ	9:I1:15:LYS:O	2.50	0.44
37:52:2062:C:O2'	53:S3:111:ARG:NH1	2.50	0.44
37:52:1068:G:H2'	37:52:1069:G:H8	1.82	0.44
37:52:440:U:H2'	37:52:441:G:H8	1.82	0.44
1:A1:1549:U:OP1	5:E1:34:TYR:OH	30.03	0.44
41:B3:261:ARG:HE	49:O3:64:THR:HG21	1.82	0.44
6:F1:31:PRO:HG3	6:F1:43:PRO:HG3	1.99	0.44
37:52:966:A:C8	44:F3:24:PHE:HB2	2.53	0.44
85:I3:54:SER:HB2	85:I3:135:ILE:HD11	1.99	0.44
13:M1:80:MET:HG2	13:M1:86:ILE:HG22	1.98	0.44
52:R3:94:THR:HG23	52:R3:98:ARG:HH22	1.82	0.44
55:U3:34:MET:HB2	55:U3:38:ASN:HD22	1.81	0.44
86:1:7:ALA:O	86:1:8:ALA:HB3	2.17	0.44
37:52:1109:C:N4	37:52:1161:G:O6	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:4275:G:N2	37:52:4334:U:O2	2.51	0.44
39:82:28:C:H2'	39:82:29:G:H8	1.83	0.44
22:V1:98:VAL:HA	22:V1:101:ILE:HB	2.00	0.44
60:Z3:38:TYR:O	60:Z3:40:HIS:ND1	2.51	0.44
60:Z3:99:ASP:O	60:Z3:103:ASP:N	2.42	0.44
37:52:1912:G:H1	37:52:2051:C:H42	1.66	0.44
37:52:5043:A:OP2	41:B3:393:LYS:NZ	2.39	0.44
37:52:648:G:H2'	37:52:649:A:H8	1.82	0.44
40:A3:154:SER:OG	40:A3:155:LYS:N	2.46	0.44
40:A3:79:ALA:HB1	40:A3:167:GLY:HA3	2.00	0.44
37:52:1577:G:N7	40:A3:181:LYS:HE3	2.33	0.44
83:G3:214:VAL:HG13	83:G3:217:ILE:HA	1.99	0.44
37:52:74:G:O3'	46:L3:71:ARG:NH2	2.50	0.44
37:52:1199:G:H2'	37:52:1200:G:C8	2.52	0.44
37:52:19:G:OP2	45:H3:93:ARG:NH2	168.90	0.44
37:52:89:C:O2'	37:52:293:G:OP1	2.35	0.44
37:52:3758:U:H3	37:52:3767:C:H42	1.64	0.44
44:F3:93:ARG:NH1	44:F3:96:GLY:O	2.50	0.44
11:K1:136:ARG:NE	11:K1:158:ASP:OD1	2.47	0.44
37:52:1094:G:H2'	37:52:1095:A:C8	2.52	0.44
37:52:176:G:N2	37:52:260:C:O2	2.51	0.44
37:52:350:C:OP1	37:52:2294:G:O2'	2.34	0.44
37:52:2622:G:OP2	55:U3:104:ALA:HB3	2.18	0.44
3:C1:131:ASP:N	3:C1:131:ASP:OD1	2.48	0.44
42:C3:266:THR:OG1	42:C3:267:TRP:N	2.50	0.44
37:52:1244:G:O6	41:B3:117:ARG:N	138.10	0.43
37:52:1304:C:H2'	37:52:1305:C:H6	1.83	0.43
40:A3:70:LYS:HD3	40:A3:72:ARG:HH12	1.83	0.43
3:C1:144:LYS:HB2	3:C1:208:HIS:HB3	1.99	0.43
37:52:101:A:H2'	37:52:102:G:H8	1.81	0.43
37:52:4906:C:H2'	37:52:4907:G:C8	2.53	0.43
1:A1:183:G:O2'	1:A1:184:G:O4'	2.35	0.43
1:A1:547:G:H21	1:A1:548:C:H5	1.64	0.43
1:A1:640:A:H2'	1:A1:641:A:C8	2.53	0.43
3:C1:143:THR:HB	3:C1:205:TYR:HE2	1.83	0.43
84:D3:25:GLU:OE1	84:D3:27:LYS:NZ	2.38	0.43
8:H1:121:ILE:HG23	8:H1:124:LEU:HB2	1.99	0.43
38:72:63:C:C6	85:I3:204:GLY:HA2	2.53	0.43
41:B3:261:ARG:HB2	49:O3:64:THR:HG21	1.99	0.43
37:52:2608:G:P	52:R3:100:ARG:HH22	2.40	0.43
49:O3:22:ILE:HG23	53:S3:166:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:2656:U:H3'	37:52:2657:G:C8	2.53	0.43
37:52:489:C:N3	37:52:664:G:N1	2.62	0.43
1:A1:106:C:OP1	1:A1:431:G:O2'	2.36	0.43
1:A1:1103:C:N4	1:A1:1104:G:O6	2.52	0.43
41:B3:329:ASP:N	41:B3:329:ASP:OD1	2.51	0.43
84:D3:56:THR:OG1	84:D3:59:ASP:O	2.36	0.43
55:U3:28:PRO:HB2	55:U3:34:MET:HG2	2.00	0.43
37:52:3716:C:H3'	37:52:3735:G:H22	1.83	0.43
37:52:4620:U:OP2	37:52:4670:C:N4	2.51	0.43
40:A3:79:ALA:HA	40:A3:169:VAL:HA	2.01	0.43
47:M3:38:VAL:HG21	47:M3:50:MET:HE2	1.99	0.43
14:N1:60:MET:O	14:N1:64:LEU:N	2.48	0.43
17:Q1:108:LYS:HD2	20:T1:117:ILE:HG22	1.99	0.43
52:R3:44:LEU:HD22	52:R3:49:LEU:HD12	2.00	0.43
19:S1:120:THR:OG1	19:S1:121:GLN:N	2.51	0.43
37:52:1285:U:H2'	37:52:1286:C:H6	1.83	0.43
37:52:1391:A:P	51:Q3:181:ARG:HH12	2.42	0.43
37:52:2761:U:O5'	37:52:2762:G:N2	2.52	0.43
37:52:4237:C:O2	37:52:4321:U:O2'	2.36	0.43
1:A1:1384:C:H2'	1:A1:1385:G:H8	1.83	0.43
37:52:2084:U:N1	51:Q3:14:ARG:HD2	2.33	0.43
37:52:2492:C:H2'	37:52:2493:G:H4'	2.00	0.43
37:52:2664:G:H4'	37:52:2677:G:H4'	1.99	0.43
37:52:4114:C:H2'	37:52:4115:G:H8	1.83	0.43
1:A1:429:C:OP1	6:F1:10:LYS:NZ	2.35	0.43
41:B3:37:PRO:HA	41:B3:188:GLY:HA2	2.00	0.43
42:C3:341:LEU:O	42:C3:345:ARG:NH1	2.51	0.43
38:72:7:G:OP1	84:D3:33:ARG:NH2	2.51	0.43
10:J1:6:ASP:OD2	10:J1:8:TRP:NE1	2.52	0.43
37:52:1341:U:O3'	48:N3:204:ARG:NH1	2.51	0.43
52:R3:100:ARG:HH21	52:R3:104:ARG:NH2	2.17	0.43
37:52:732:A:C5	53:S3:68:PHE:CG	3.07	0.43
20:T1:112:GLU:O	20:T1:116:LYS:N	2.47	0.43
37:52:2261:G:N7	37:52:2262:G:N1	2.67	0.43
1:A1:544:G:H2'	1:A1:545:A:H8	1.84	0.43
41:B3:217:ILE:HD13	41:B3:284:ILE:HD11	2.01	0.43
41:B3:44:THR:HG21	41:B3:186:ASN:HD22	1.83	0.43
85:I3:66:GLU:OE2	85:I3:69:ARG:NH1	2.52	0.43
14:N1:56:CYS:SG	14:N1:82:ASN:ND2	2.92	0.43
37:52:2631:U:N1	55:U3:49:VAL:N	2.66	0.43
37:52:1687:U:H2'	37:52:1688:G:H8	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1114:U:H3	1:A1:1119:A:H61	1.67	0.43
2:B1:59:LEU:O	2:B1:63:ARG:N	2.50	0.43
11:K1:65:GLU:HG3	11:K1:66:LYS:HD2	2.01	0.43
16:P1:150:ARG:HD3	16:P1:150:ARG:H	1.84	0.43
37:52:1573:G:OP1	52:R3:95:TRP:NE1	2.51	0.43
37:52:1996:C:H42	37:52:2000:G:H22	1.67	0.43
37:52:732:A:H3'	37:52:733:A:H4'	2.01	0.43
1:A1:1008:A:H2'	1:A1:1009:A:H8	1.84	0.43
19:S1:71:ILE:HG22	19:S1:73:LEU:H	1.83	0.43
56:V3:26:ILE:HG22	56:V3:101:ASN:HB3	2.00	0.43
24:X1:83:LEU:HD13	24:X1:83:LEU:HA	1.92	0.43
37:52:4099:G:H22	37:52:4108:G:H1	1.67	0.43
37:52:755:C:H2'	37:52:756:G:H8	1.83	0.43
5:E1:119:CYS:HB2	5:E1:152:PHE:HE2	1.84	0.43
10:J1:137:LEU:O	10:J1:141:ARG:NH1	2.35	0.43
82:J3:112:HIS:CE1	82:J3:126:TYR:H	2.37	0.43
82:J3:80:GLU:OE2	82:J3:170:TYR:OH	2.32	0.43
37:52:935:A:H1'	47:M3:44:ARG:HB3	2.00	0.43
19:S1:98:VAL:HG21	19:S1:117:LEU:HD22	2.01	0.43
57:W3:98:PRO:HA	57:W3:101:ARG:HB2	2.00	0.43
37:52:2753:G:C3'	60:Z3:51:ARG:HE	2.29	0.43
37:52:1802:A:H5''	37:52:1803:G:H5'	2.01	0.42
37:52:4476:C:O2'	37:52:4478:G:OP2	2.30	0.42
4:D1:123:ARG:NH2	4:D1:143:CYS:SG	2.92	0.42
5:E1:135:GLU:HG3	5:E1:153:VAL:HG22	2.01	0.42
5:E1:64:ARG:HH21	12:L1:94:LEU:HD11	1.84	0.42
37:52:3839:G:N2	37:52:3843:C:O2	2.37	0.42
37:52:78:U:H5''	48:N3:185:GLY:HA2	2.00	0.42
1:A1:385:G:O2'	10:J1:10:LYS:NZ	2.49	0.42
41:B3:119:TYR:OH	41:B3:129:ALA:N	2.51	0.42
37:52:2591:A:N6	60:Z3:51:ARG:HH22	2.16	0.42
1:A1:1339:U:H2'	1:A1:1340:U:H6	1.84	0.42
2:B1:159:ILE:HD12	2:B1:159:ILE:HA	1.90	0.42
41:B3:13:SER:OG	41:B3:14:LEU:N	2.52	0.42
4:D1:154:ALA:O	4:D1:158:ALA:N	2.50	0.42
84:D3:103:LEU:HD11	84:D3:248:ARG:HH21	1.84	0.42
46:L3:56:ARG:O	46:L3:116:ARG:NH2	2.52	0.42
37:52:4302:U:H4'	54:T3:5:LYS:HD2	2.01	0.42
56:V3:48:ARG:HB3	56:V3:51:ARG:HG3	2.00	0.42
37:52:1109:C:O2	37:52:1162:G:N2	2.52	0.42
37:52:1405:C:H2'	37:52:1406:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:3870:C:H2'	37:52:3871:A:C8	2.54	0.42
38:72:75:G:O2'	38:72:99:G:O6	2.35	0.42
1:A1:1550:G:H3'	1:A1:1579:A:H61	1.84	0.42
1:A1:1847:G:O6	1:A1:1852:C:N4	2.48	0.42
40:A3:196:TRP:O	40:A3:198:ARG:N	2.53	0.42
10:J1:142:SER:OG	10:J1:143:LYS:N	2.52	0.42
37:52:3667:C:O2	37:52:3675:G:N2	2.43	0.42
1:A1:1332:A:H62	1:A1:1493:C:H42	1.66	0.42
2:B1:214:GLU:OE2	19:S1:81:ARG:NH1	2.53	0.42
37:52:4868:G:O3'	47:M3:90:ARG:NH1	2.52	0.42
51:Q3:38:ARG:HA	51:Q3:38:ARG:HD3	1.92	0.42
37:52:732:A:C2	53:S3:69:GLU:N	2.88	0.42
56:V3:43:LYS:HD3	56:V3:60:MET:HG2	2.02	0.42
37:52:152:U:OP2	48:N3:49:ARG:NH2	2.38	0.42
37:52:114:G:H22	37:52:158:A:H61	1.66	0.42
37:52:4301:U:H4'	54:T3:54:HIS:CD2	2.54	0.42
37:52:4489:G:N1	37:52:4708:A:N7	2.67	0.42
43:E3:167:PHE:HE1	43:E3:176:LEU:HD22	1.85	0.42
16:P1:34:PHE:CD1	16:P1:98:ARG:HD2	2.55	0.42
56:V3:82:ILE:HG23	56:V3:121:VAL:HG13	2.01	0.42
37:52:1403:G:O6	37:52:1414:C:N4	2.52	0.42
37:52:3661:G:H1'	40:A3:125:LYS:HZ1	1.85	0.42
37:52:4123:C:O4'	60:Z3:135:ARG:HG3	2.19	0.42
37:52:4325:A:N3	84:D3:36:LEU:HB3	2.35	0.42
7:G1:144:LEU:O	7:G1:148:ASN:ND2	2.52	0.42
85:I3:168:SER:OG	85:I3:169:LYS:N	2.52	0.42
37:52:4895:C:H1'	47:M3:132:ARG:HH22	1.83	0.42
15:O1:136:PRO:HA	15:O1:137:PRO:HD3	1.89	0.42
49:O3:142:ALA:HA	49:O3:145:VAL:HG12	2.00	0.42
1:A1:1453:C:OP2	19:S1:45:LYS:NZ	2.52	0.42
56:V3:33:GLY:HA3	56:V3:69:LYS:HD2	2.01	0.42
37:52:1071:C:H41	43:E3:48:ARG:HH22	1.68	0.42
37:52:3777:G:O2'	37:52:3815:G:O6	2.31	0.42
1:A1:1337:C:H2'	1:A1:1338:G:C8	2.54	0.42
1:A1:1734:G:O2'	1:A1:1800:A:N6	2.48	0.42
37:52:5058:A:H4'	84:D3:23:ARG:HH12	170.26	0.42
37:52:1239:C:C4	43:E3:65:TYR:CE1	3.08	0.42
23:W1:21:ASN:HB3	24:X1:67:GLY:HA3	2.01	0.42
58:X3:143:ASP:N	58:X3:143:ASP:OD1	2.53	0.42
37:52:4122:G:N3	60:Z3:135:ARG:HB3	2.35	0.42
80:23:29:C:H2'	80:23:30:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:52:168:C:H1'	37:52:268:G:H1	1.83	0.42
37:52:2703:G:H1	37:52:2713:C:H42	1.67	0.42
1:A1:970:G:C5	37:52:3712:A:N1	2.88	0.42
37:52:3965:A:H61	37:52:4045:G:N2	2.17	0.42
38:72:63:C:C5	85:I3:203:ARG:O	2.72	0.42
1:A1:521:A:H5''	11:K1:45:ARG:HH12	1.85	0.42
41:B3:301:ASN:HB2	41:B3:304:SER:HB2	2.02	0.42
83:G3:275:ILE:HG22	83:G3:276:ARG:H	1.85	0.42
16:P1:147:ARG:HH21	16:P1:150:ARG:NH1	2.18	0.42
51:Q3:67:ILE:HD12	51:Q3:96:PRO:HD2	2.02	0.42
37:52:1472:C:O2	37:52:1493:G:N1	2.53	0.42
37:52:4277:G:N2	37:52:4332:C:N3	2.67	0.42
37:52:4930:C:H5'	43:E3:269:GLN:HG2	2.00	0.42
1:A1:126:G:OP2	8:H1:195:LYS:NZ	2.53	0.42
40:A3:103:PRO:HG3	40:A3:163:ARG:CZ	2.50	0.42
3:C1:208:HIS:CD2	3:C1:209:ASP:HB2	2.54	0.42
84:D3:129:GLU:OE1	84:D3:175:HIS:NE2	2.53	0.42
11:K1:109:ARG:HG2	11:K1:111:GLN:H	1.85	0.42
37:52:1346:C:H2'	37:52:1347:G:C8	2.55	0.41
1:A1:1268:C:O2	17:Q1:97:TYR:OH	2.36	0.41
1:A1:65:C:C4	8:H1:133:LEU:HD23	2.54	0.41
1:A1:695:C:H2'	1:A1:696:G:C8	2.54	0.41
41:B3:46:PHE:HE2	41:B3:81:THR:HB	1.84	0.41
37:52:1378:C:N4	46:L3:159:ASN:O	2.48	0.41
49:O3:18:ARG:HH22	49:O3:128:ARG:NH1	2.17	0.41
49:O3:195:VAL:HG23	49:O3:196:LEU:HD12	2.02	0.41
21:U1:124:THR:HG23	21:U1:126:GLN:H	1.84	0.41
55:U3:49:VAL:HG11	55:U3:49:VAL:CG2	2.05	0.41
37:52:1073:G:H22	37:52:1239:C:H1'	1.83	0.41
37:52:1890:G:N2	37:52:1939:A:H61	2.18	0.41
37:52:2395:A:H1'	37:52:2806:A:H1'	2.02	0.41
37:52:3654:G:O6	37:52:3691:G:N2	2.53	0.41
37:52:4291:G:H8	37:52:4328:G:H2'	1.85	0.41
1:A1:982:G:N2	1:A1:1045:U:O2	2.44	0.41
40:A3:62:VAL:HG12	40:A3:73:THR:HG22	2.02	0.41
37:52:4459:U:H5'	41:B3:10:ARG:HG2	2.01	0.41
3:C1:107:ARG:HA	3:C1:110:MET:HB3	2.01	0.41
37:52:2581:A:C5	60:Z3:74:VAL:HB	2.55	0.41
37:52:2753:G:H3'	60:Z3:51:ARG:NE	2.32	0.41
1:A1:970:G:C5	37:52:3712:A:H1'	2.55	0.41
38:72:3:C:O2	38:72:116:G:N2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:130:G:O6	1:A1:181:A:N6	2.53	0.41
1:A1:744:G:H2'	1:A1:745:C:C2	2.55	0.41
2:B1:50:ASN:HD21	19:S1:109:LEU:HD11	1.85	0.41
37:52:1069:G:N2	37:52:1070:G:HO2'	2.18	0.41
37:52:1687:U:H2'	37:52:1688:G:C8	2.56	0.41
37:52:3947:A:N6	37:52:3948:C:O3'	2.53	0.41
1:A1:544:G:H2'	1:A1:545:A:C8	2.56	0.41
40:A3:237:LEU:HD23	40:A3:237:LEU:H	1.86	0.41
41:B3:43:LEU:HD23	41:B3:183:ILE:HG21	2.03	0.41
41:B3:249:ARG:HH11	41:B3:249:ARG:HD3	1.74	0.41
44:F3:97:ILE:HD12	44:F3:97:ILE:HA	1.84	0.41
48:N3:119:TYR:CZ	48:N3:131:GLU:HG3	2.56	0.41
49:O3:196:LEU:HB3	49:O3:202:LEU:HD13	2.02	0.41
19:S1:111:PHE:HB3	19:S1:114:LEU:HD21	2.02	0.41
59:Y3:80:ILE:HG23	59:Y3:101:PRO:HG3	2.02	0.41
37:52:983:C:OP1	43:E3:75:TYR:OH	2.38	0.41
1:A1:390:C:O2'	13:M1:8:ARG:NH2	2.54	0.41
1:A1:747:U:O2'	1:A1:751:G:N1	2.53	0.41
37:52:1237:C:H5''	44:F3:50:TYR:CE2	2.55	0.41
82:J3:15:LEU:HD22	82:J3:165:TRP:CG	2.55	0.41
57:W3:17:HIS:HB3	57:W3:18:GLY:H	1.67	0.41
1:A1:920:A:OP1	24:X1:57:ARG:NH2	2.53	0.41
37:52:1072:C:N3	43:E3:71:TYR:HB3	2.36	0.41
37:52:2378:G:N2	37:52:2381:A:OP2	2.46	0.41
37:52:3957:U:N3	37:52:3964:U:H5'	2.35	0.41
1:A1:1140:G:H2'	1:A1:1141:G:C8	2.55	0.41
1:A1:1221:G:H2'	1:A1:1222:G:C8	2.55	0.41
37:52:3651:A:OP1	40:A3:200:ARG:HG2	2.20	0.41
40:A3:33:ASP:OD1	40:A3:33:ASP:N	2.54	0.41
7:G1:59:LYS:HG2	7:G1:60:ARG:H	1.85	0.41
9:I1:154:ILE:HB	9:I1:185:VAL:HG22	2.02	0.41
54:T3:30:TYR:HE1	54:T3:94:GLU:HG3	1.85	0.41
1:A1:407:G:C2	25:Y1:36:LEU:HD23	2.56	0.41
37:52:2754:G:O5'	60:Z3:51:ARG:HB3	2.21	0.41
37:52:2766:A:C5	37:52:2767:U:H1'	2.56	0.41
1:A1:677:G:N1	1:A1:1027:A:OP2	2.45	0.41
41:B3:317:LEU:HB2	41:B3:372:SER:HB2	2.03	0.41
5:E1:51:LEU:HG	5:E1:91:VAL:HG22	2.03	0.41
48:N3:84:PRO:HA	48:N3:87:HIS:ND1	2.35	0.41
37:52:2055:G:C5	49:O3:130:LYS:HG2	2.56	0.41
50:P3:129:THR:OG1	50:P3:130:TYR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U1:105:GLN:O	21:U1:109:GLY:N	2.53	0.41
37:52:1956:A:N6	37:52:1957:U:O4	2.53	0.41
37:52:2084:U:N3	51:Q3:14:ARG:CZ	2.83	0.41
37:52:2706:G:H21	37:52:2709:C:H5	1.68	0.41
1:A1:220:U:H2'	1:A1:221:A:H8	1.86	0.41
1:A1:886:A:N6	1:A1:900:C:N3	2.69	0.41
1:A1:955:A:N7	1:A1:972:A:N6	2.69	0.41
84:D3:31:TYR:O	84:D3:35:ARG:NH1	2.53	0.41
6:F1:68:ARG:HG3	6:F1:76:VAL:HG11	2.02	0.41
8:H1:126:ASP:O	8:H1:128:THR:N	3.09	0.41
11:K1:67:ASP:HB3	11:K1:70:ARG:HB3	2.03	0.41
37:52:1549:G:O2'	52:R3:86:ASN:OD1	2.38	0.41
22:V1:55:ARG:HG2	22:V1:87:ARG:HG3	2.02	0.41
57:W3:25:ASP:N	57:W3:25:ASP:OD1	2.54	0.41
37:52:2754:G:C8	60:Z3:51:ARG:HB2	2.56	0.41
37:52:1924:C:H42	37:52:2060:G:H1	1.67	0.41
37:52:2897:G:OP1	52:R3:135:LYS:HG2	2.21	0.41
37:52:4034:G:H2'	37:52:4035:G:C8	2.56	0.41
1:A1:1275:G:N2	1:A1:1506:A:OP2	2.47	0.41
2:B1:33:GLN:HB3	2:B1:154:LEU:HD12	2.03	0.41
2:B1:213:GLU:O	2:B1:217:ALA:N	2.52	0.41
37:52:965:G:H5'	44:F3:24:PHE:CE1	2.55	0.41
83:G3:191:ALA:O	83:G3:195:THR:OG1	2.39	0.41
46:L3:200:LYS:HB2	46:L3:200:LYS:HE3	1.92	0.41
37:52:1924:C:H5'	47:M3:34:ASN:HD21	1.86	0.41
14:N1:106:CYS:SG	14:N1:107:SER:N	2.94	0.41
37:52:1480:C:O2'	37:52:1482:G:OP2	2.39	0.41
4:D1:77:SER:OG	4:D1:78:LEU:N	2.54	0.41
52:R3:122:SER:HA	52:R3:125:LEU:HB2	2.03	0.41
54:T3:39:ILE:HD12	54:T3:102:ARG:HB2	2.02	0.41
37:52:1676:C:O2	37:52:4191:G:O2'	2.30	0.41
37:52:2722:G:N2	37:52:2723:U:O2	2.53	0.41
37:52:407:A:O2'	37:52:410:A:OP1	2.31	0.41
40:A3:175:ILE:HG13	40:A3:175:ILE:H	1.77	0.41
42:C3:275:SER:OG	42:C3:276:ASN:N	2.54	0.41
46:L3:46:ILE:HB	46:L3:49:ARG:HB2	2.03	0.41
37:52:2896:G:O6	37:52:3604:A:N6	2.54	0.40
37:52:4492:U:O2'	37:52:4512:U:O2	2.32	0.40
37:52:942:G:P	44:F3:244:ARG:HH12	2.44	0.40
8:H1:121:ILE:HD12	8:H1:122:PRO:HD2	2.03	0.40
8:H1:4:ASN:O	8:H1:111:LEU:N	2.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:J3:72:CYS:SG	82:J3:73:THR:N	2.94	0.40
26:Z1:7:ILE:HG12	26:Z1:27:VAL:HG22	2.03	0.40
37:52:1996:C:N4	37:52:2000:G:H22	2.19	0.40
37:52:3681:G:OP2	40:A3:128:ARG:NH2	2.54	0.40
37:52:4223:C:H2'	37:52:4224:A:H8	1.86	0.40
1:A1:925:G:OP1	15:O1:121:ARG:NH2	2.54	0.40
40:A3:116:LEU:HB3	40:A3:117:GLU:H	1.72	0.40
40:A3:245:ARG:HD3	40:A3:247:ARG:HH12	1.86	0.40
2:B1:206:ASP:HB3	2:B1:209:GLU:HB2	2.03	0.40
13:M1:5:GLN:HG2	13:M1:11:GLN:HB2	2.03	0.40
3:C1:46:LYS:HE3	16:P1:19:PRO:HG2	2.03	0.40
8:H1:146:ASN:HB3	57:W3:101:ARG:HH22	1.87	0.40
37:52:1390:G:N2	37:52:1393:G:OP2	2.54	0.40
37:52:153:G:OP2	48:N3:54:LYS:NZ	2.49	0.40
1:A1:1740:C:OP1	10:J1:44:HIS:ND1	2.42	0.40
37:52:4124:G:H5''	40:A3:69:PHE:HE1	1.86	0.40
40:A3:42:LYS:HD2	40:A3:89:TYR:HE1	1.85	0.40
41:B3:161:ARG:HD3	41:B3:182:GLU:HB3	2.03	0.40
41:B3:293:ILE:HG12	41:B3:298:LEU:HB3	2.02	0.40
41:B3:35:ASP:OD1	41:B3:35:ASP:N	2.51	0.40
38:72:63:C:N1	85:I3:203:ARG:C	2.74	0.40
10:J1:132:GLU:HG3	10:J1:135:GLU:HB3	2.03	0.40
17:Q1:43:ARG:NH1	17:Q1:47:ARG:HH21	2.19	0.40
1:A1:1542:C:O2'	18:R1:43:GLU:OE2	2.39	0.40
24:X1:8:ALA:HA	24:X1:74:VAL:HG11	2.03	0.40
60:Z3:49:TYR:CD2	60:Z3:133:LYS:HA	2.56	0.40
37:52:1573:G:N7	37:52:1574:G:N1	2.70	0.40
37:52:4034:G:H2'	37:52:4035:G:H8	1.87	0.40
37:52:4305:G:H22	54:T3:87:LYS:NZ	2.20	0.40
1:A1:1039:C:H42	1:A1:1076:G:H1	1.68	0.40
4:D1:178:HIS:HB2	4:D1:220:ASP:HB3	2.03	0.40
54:T3:33:ILE:HG13	54:T3:33:ILE:H	1.74	0.40
58:X3:89:LYS:HD3	58:X3:93:ASN:HD22	1.85	0.40
37:52:2590:G:N2	60:Z3:65:ARG:HH21	2.18	0.40
37:52:1734:G:O2'	37:52:1793:A:N6	2.55	0.40
37:52:2267:U:H2'	37:52:2267:U:H6	1.72	0.40
37:52:228:C:H2'	37:52:229:G:H8	1.86	0.40
37:52:2610:G:H2'	37:52:2611:A:H8	1.85	0.40
37:52:4061:G:H2'	37:52:4062:A:H8	1.87	0.40
37:52:729:G:OP1	53:S3:63:TYR:OH	2.40	0.40
37:52:740:G:H1	37:52:922(B):C:H42	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:649:U:H2'	1:A1:650:A:C8	2.56	0.40
4:D1:144:SER:OG	4:D1:145:LYS:N	2.55	0.40
8:H1:131:ARG:HA	57:W3:82:ILE:H	1.85	0.40
82:J3:44:THR:OG1	82:J3:45:GLY:N	2.54	0.40
13:M1:39:ASN:OD1	13:M1:39:ASN:N	2.54	0.40
37:52:738(A):C:H4'	47:M3:69:ARG:HH21	1.85	0.40
48:N3:197:THR:OG1	48:N3:199:GLN:NE2	2.54	0.40
52:R3:106:LEU:HA	52:R3:106:LEU:HD13	3.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B1	215/295 (73%)	199 (93%)	16 (7%)	0	100	100
3	C1	211/264 (80%)	191 (90%)	20 (10%)	0	100	100
4	D1	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
5	E1	226/243 (93%)	211 (93%)	15 (7%)	0	100	100
6	F1	260/263 (99%)	226 (87%)	34 (13%)	0	100	100
7	G1	181/204 (89%)	167 (92%)	14 (8%)	0	100	100
8	H1	235/249 (94%)	218 (93%)	17 (7%)	0	100	100
9	I1	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
10	J1	204/208 (98%)	184 (90%)	20 (10%)	0	100	100
11	K1	183/194 (94%)	173 (94%)	10 (6%)	0	100	100
12	L1	94/165 (57%)	83 (88%)	11 (12%)	0	100	100
13	M1	139/158 (88%)	128 (92%)	11 (8%)	0	100	100
14	N1	115/132 (87%)	101 (88%)	14 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O1	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
16	P1	134/168 (80%)	123 (92%)	11 (8%)	0	100	100
17	Q1	118/145 (81%)	106 (90%)	12 (10%)	0	100	100
18	R1	140/146 (96%)	126 (90%)	14 (10%)	0	100	100
19	S1	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
20	T1	142/152 (93%)	129 (91%)	13 (9%)	0	100	100
21	U1	139/145 (96%)	128 (92%)	11 (8%)	0	100	100
22	V1	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
23	W1	81/83 (98%)	72 (89%)	9 (11%)	0	100	100
24	X1	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
25	Y1	139/143 (97%)	124 (89%)	14 (10%)	1 (1%)	24	64
26	Z1	122/130 (94%)	109 (89%)	13 (11%)	0	100	100
27	a1	73/125 (58%)	65 (89%)	8 (11%)	0	100	100
28	b1	99/115 (86%)	92 (93%)	7 (7%)	0	100	100
29	c1	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
30	d1	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
31	e1	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
32	f1	53/133 (40%)	49 (92%)	4 (8%)	0	100	100
33	g1	66/156 (42%)	58 (88%)	8 (12%)	0	100	100
34	h1	311/317 (98%)	268 (86%)	43 (14%)	0	100	100
35	j1	417/439 (95%)	388 (93%)	29 (7%)	0	100	100
36	k1	571/599 (95%)	517 (90%)	54 (10%)	0	100	100
40	A3	246/257 (96%)	185 (75%)	54 (22%)	7 (3%)	5	39
41	B3	392/403 (97%)	355 (91%)	37 (9%)	0	100	100
42	C3	360/425 (85%)	325 (90%)	35 (10%)	0	100	100
43	E3	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
44	F3	223/247 (90%)	204 (92%)	19 (8%)	0	100	100
45	H3	188/192 (98%)	174 (93%)	13 (7%)	1 (0%)	31	71
46	L3	208/211 (99%)	194 (93%)	12 (6%)	2 (1%)	17	57
47	M3	136/218 (62%)	121 (89%)	15 (11%)	0	100	100
48	N3	201/204 (98%)	181 (90%)	20 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	O3	197/203 (97%)	185 (94%)	12 (6%)	0	100	100
50	P3	151/184 (82%)	143 (95%)	8 (5%)	0	100	100
51	Q3	185/188 (98%)	167 (90%)	18 (10%)	0	100	100
52	R3	178/196 (91%)	161 (90%)	17 (10%)	0	100	100
53	S3	174/176 (99%)	154 (88%)	20 (12%)	0	100	100
54	T3	157/160 (98%)	144 (92%)	12 (8%)	1 (1%)	27	67
55	U3	97/128 (76%)	79 (81%)	18 (19%)	0	100	100
56	V3	129/140 (92%)	119 (92%)	10 (8%)	0	100	100
57	W3	102/157 (65%)	92 (90%)	10 (10%)	0	100	100
58	X3	116/156 (74%)	109 (94%)	7 (6%)	0	100	100
59	Y3	132/145 (91%)	120 (91%)	12 (9%)	0	100	100
60	Z3	133/136 (98%)	105 (79%)	25 (19%)	3 (2%)	7	43
61	a3	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
62	b3	100/226 (44%)	94 (94%)	6 (6%)	0	100	100
63	c3	96/115 (84%)	82 (85%)	14 (15%)	0	100	100
64	d3	105/125 (84%)	90 (86%)	15 (14%)	0	100	100
65	e3	126/135 (93%)	115 (91%)	11 (9%)	0	100	100
66	f3	107/110 (97%)	96 (90%)	11 (10%)	0	100	100
67	g3	112/117 (96%)	98 (88%)	13 (12%)	1 (1%)	19	59
68	h3	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
69	i3	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
70	j3	84/97 (87%)	75 (89%)	9 (11%)	0	100	100
71	k3	67/70 (96%)	59 (88%)	8 (12%)	0	100	100
72	l3	48/51 (94%)	41 (85%)	7 (15%)	0	100	100
73	m3	50/102 (49%)	48 (96%)	2 (4%)	0	100	100
74	n3	23/25 (92%)	23 (100%)	0	0	100	100
75	o3	102/106 (96%)	96 (94%)	6 (6%)	0	100	100
76	p3	89/92 (97%)	77 (86%)	12 (14%)	0	100	100
77	r3	122/137 (89%)	110 (90%)	12 (10%)	0	100	100
78	s3	194/318 (61%)	156 (80%)	37 (19%)	1 (0%)	31	71
79	t3	151/165 (92%)	126 (83%)	25 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
82	J3	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
83	G3	229/319 (72%)	195 (85%)	34 (15%)	0	100	100
84	D3	291/297 (98%)	253 (87%)	38 (13%)	0	100	100
85	I3	201/214 (94%)	167 (83%)	33 (16%)	1 (0%)	31	71
86	1	20/22 (91%)	11 (55%)	4 (20%)	5 (25%)	0	1
87	u3	215/217 (99%)	183 (85%)	30 (14%)	2 (1%)	19	59
All	All	12742/14633 (87%)	11465 (90%)	1252 (10%)	25 (0%)	53	83

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
40	A3	116	LEU
40	A3	118	GLU
40	A3	126	LEU
46	L3	64	VAL
60	Z3	73	LYS
86	1	15	ALA
87	u3	101	LYS
40	A3	169	VAL
78	s3	34	ASN
86	1	7	ALA
87	u3	210	MET
46	L3	63	THR
60	Z3	75	TYR
67	g3	44	SER
86	1	13	ALA
86	1	14	ALA
40	A3	117	GLU
86	1	8	ALA
40	A3	125	LYS
45	H3	108	ASN
40	A3	150	LEU
25	Y1	62	PRO
85	I3	205	PRO
54	T3	82	GLY
60	Z3	90	PRO

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	
2	B1	180/245 (74%)	177 (98%)	3 (2%)	63	83
3	C1	194/231 (84%)	191 (98%)	3 (2%)	67	85
4	D1	187/225 (83%)	186 (100%)	1 (0%)	90	95
5	E1	190/202 (94%)	186 (98%)	4 (2%)	56	79
6	F1	224/225 (100%)	223 (100%)	1 (0%)	92	96
7	G1	158/170 (93%)	156 (99%)	2 (1%)	71	86
8	H1	207/218 (95%)	205 (99%)	2 (1%)	78	89
9	I1	165/174 (95%)	165 (100%)	0	100	100
10	J1	178/180 (99%)	174 (98%)	4 (2%)	55	78
11	K1	161/168 (96%)	157 (98%)	4 (2%)	50	75
12	L1	87/136 (64%)	85 (98%)	2 (2%)	53	77
13	M1	130/142 (92%)	128 (98%)	2 (2%)	67	85
14	N1	99/108 (92%)	98 (99%)	1 (1%)	78	89
15	O1	130/131 (99%)	128 (98%)	2 (2%)	67	85
16	P1	106/130 (82%)	104 (98%)	2 (2%)	60	81
17	Q1	109/130 (84%)	108 (99%)	1 (1%)	81	90
18	R1	117/121 (97%)	115 (98%)	2 (2%)	63	83
19	S1	119/121 (98%)	119 (100%)	0	100	100
20	T1	125/132 (95%)	124 (99%)	1 (1%)	83	91
21	U1	111/115 (96%)	110 (99%)	1 (1%)	81	90
22	V1	92/107 (86%)	90 (98%)	2 (2%)	55	78
23	W1	67/67 (100%)	66 (98%)	1 (2%)	67	85
24	X1	112/113 (99%)	112 (100%)	0	100	100
25	Y1	113/115 (98%)	113 (100%)	0	100	100
26	Z1	107/112 (96%)	106 (99%)	1 (1%)	81	90
27	a1	66/103 (64%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	b1	88/98 (90%)	88 (100%)	0	100	100
29	c1	75/76 (99%)	74 (99%)	1 (1%)	71	86
30	d1	55/62 (89%)	55 (100%)	0	100	100
31	e1	48/49 (98%)	48 (100%)	0	100	100
32	f1	46/106 (43%)	44 (96%)	2 (4%)	32	64
33	g1	61/140 (44%)	60 (98%)	1 (2%)	65	84
34	h1	272/275 (99%)	269 (99%)	3 (1%)	76	88
35	j1	361/377 (96%)	356 (99%)	5 (1%)	69	86
36	k1	509/526 (97%)	505 (99%)	4 (1%)	83	91
40	A3	190/199 (96%)	185 (97%)	5 (3%)	49	75
41	B3	342/348 (98%)	340 (99%)	2 (1%)	87	94
42	C3	302/347 (87%)	295 (98%)	7 (2%)	53	77
43	E3	190/251 (76%)	188 (99%)	2 (1%)	76	88
44	F3	196/215 (91%)	194 (99%)	2 (1%)	78	89
45	H3	169/171 (99%)	164 (97%)	5 (3%)	44	71
46	L3	175/176 (99%)	174 (99%)	1 (1%)	87	94
47	M3	117/161 (73%)	117 (100%)	0	100	100
48	N3	171/172 (99%)	168 (98%)	3 (2%)	62	83
49	O3	171/173 (99%)	169 (99%)	2 (1%)	74	87
50	P3	134/163 (82%)	133 (99%)	1 (1%)	85	93
51	Q3	164/165 (99%)	161 (98%)	3 (2%)	62	83
52	R3	159/175 (91%)	154 (97%)	5 (3%)	43	71
53	S3	157/157 (100%)	157 (100%)	0	100	100
54	T3	139/140 (99%)	137 (99%)	2 (1%)	69	86
55	U3	89/114 (78%)	87 (98%)	2 (2%)	55	78
56	V3	101/107 (94%)	99 (98%)	2 (2%)	58	80
57	W3	86/126 (68%)	85 (99%)	1 (1%)	74	87
58	X3	106/134 (79%)	106 (100%)	0	100	100
59	Y3	124/135 (92%)	122 (98%)	2 (2%)	65	84
60	Z3	117/118 (99%)	115 (98%)	2 (2%)	63	83
61	a3	119/120 (99%)	118 (99%)	1 (1%)	83	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	b3	84/172 (49%)	83 (99%)	1 (1%)	74	87
63	c3	84/98 (86%)	84 (100%)	0	100	100
64	d3	98/110 (89%)	96 (98%)	2 (2%)	58	80
65	e3	114/121 (94%)	114 (100%)	0	100	100
66	f3	88/89 (99%)	88 (100%)	0	100	100
67	g3	98/100 (98%)	96 (98%)	2 (2%)	58	80
68	h3	109/110 (99%)	109 (100%)	0	100	100
69	i3	86/89 (97%)	85 (99%)	1 (1%)	74	87
70	j3	73/80 (91%)	72 (99%)	1 (1%)	69	86
71	k3	64/65 (98%)	63 (98%)	1 (2%)	65	84
72	l3	47/48 (98%)	47 (100%)	0	100	100
73	m3	48/90 (53%)	47 (98%)	1 (2%)	56	79
74	n3	24/24 (100%)	24 (100%)	0	100	100
75	o3	92/94 (98%)	91 (99%)	1 (1%)	76	88
76	p3	74/75 (99%)	73 (99%)	1 (1%)	69	86
77	r3	108/121 (89%)	106 (98%)	2 (2%)	60	81
78	s3	164/258 (64%)	162 (99%)	2 (1%)	74	87
79	t3	126/137 (92%)	126 (100%)	0	100	100
82	J3	143/149 (96%)	143 (100%)	0	100	100
83	G3	200/272 (74%)	191 (96%)	9 (4%)	30	63
84	D3	247/250 (99%)	240 (97%)	7 (3%)	47	73
85	I3	175/181 (97%)	167 (95%)	8 (5%)	29	62
87	u3	195/196 (100%)	191 (98%)	4 (2%)	56	79
All	All	11108/12426 (89%)	10957 (99%)	151 (1%)	71	86

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B1	50	ASN
2	B1	117	ARG
2	B1	186	ARG
3	C1	40	ASN
3	C1	147	ASN
3	C1	213	ARG

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Mol	Chain	Res	Type
4	D1	167	ARG
5	E1	22	ASN
5	E1	76	ARG
5	E1	94	ARG
5	E1	227	LYS
6	F1	232	ASN
7	G1	81	ARG
7	G1	91	ARG
8	H1	31	ARG
8	H1	63	MET
10	J1	47	ARG
10	J1	84	ASN
10	J1	87	ASN
10	J1	99	ASN
11	K1	45	ARG
11	K1	70	ARG
11	K1	79	ARG
11	K1	136	ARG
12	L1	55	ARG
12	L1	96	ARG
13	M1	20	LYS
13	M1	97	ARG
14	N1	33	ARG
15	O1	19	ARG
15	O1	27	LYS
16	P1	146	ARG
16	P1	150	ARG
17	Q1	13	ARG
18	R1	41	MET
18	R1	85	ARG
20	T1	8	LYS
21	U1	62	ARG
22	V1	47	ASN
22	V1	79	ARG
23	W1	82	ASN
26	Z1	101	LYS
29	c1	81	ARG
32	f1	99	LYS
32	f1	104	ARG
33	g1	138	ARG
34	h1	5	MET
34	h1	159	ASN

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Mol	Chain	Res	Type
34	h1	178	ASN
35	j1	67	ASN
35	j1	121	ASN
35	j1	245	ARG
35	j1	265	ASN
35	j1	289	ARG
36	k1	190	ARG
36	k1	250	LYS
36	k1	321	ASN
36	k1	385	LYS
40	A3	101	VAL
40	A3	155	LYS
40	A3	193	ARG
40	A3	194	ASN
40	A3	242	ARG
41	B3	24	ARG
41	B3	261	ARG
42	C3	38	ASN
42	C3	95	MET
42	C3	100	ARG
42	C3	188	ARG
42	C3	223	ASN
42	C3	312	ARG
42	C3	321	ASN
43	E3	58	ARG
43	E3	164	ARG
44	F3	165	ARG
44	F3	205	ASN
45	H3	1	MET
45	H3	15	ASN
45	H3	102	ASN
45	H3	128	MET
45	H3	173	ARG
46	L3	42	ARG
48	N3	50	ARG
48	N3	96	ARG
48	N3	162	ARG
49	O3	117	ARG
49	O3	140	ARG
50	P3	128	ARG
51	Q3	14	ARG
51	Q3	91	ARG

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Mol	Chain	Res	Type
51	Q3	97	LYS
52	R3	36	ASN
52	R3	105	LEU
52	R3	110	ARG
52	R3	130	ASN
52	R3	133	LYS
54	T3	136	ARG
54	T3	146	LYS
55	U3	80	LYS
55	U3	81	ARG
56	V3	48	ARG
56	V3	85	ARG
57	W3	82	ILE
59	Y3	2	LYS
59	Y3	77	LYS
60	Z3	75	TYR
60	Z3	84	ARG
61	a3	4	ARG
62	b3	60	ASN
64	d3	18	ASN
64	d3	31	LYS
67	g3	14	ASN
67	g3	18	ASN
69	i3	29	ARG
70	j3	20	ARG
71	k3	36	VAL
73	m3	96	ARG
75	o3	82	MET
76	p3	84	ARG
77	r3	12	ASN
77	r3	67	ARG
78	s3	6	ARG
78	s3	200	ASN
83	G3	88	ARG
83	G3	106	ARG
83	G3	117	GLN
83	G3	134	ASN
83	G3	166	ARG
83	G3	228	ARG
83	G3	280	ASN
83	G3	293	ASN
83	G3	308	LYS

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Mol	Chain	Res	Type
84	D3	23	ARG
84	D3	33	ARG
84	D3	50	ARG
84	D3	143	THR
84	D3	220	LYS
84	D3	242	LYS
84	D3	293	ARG
85	I3	3	ARG
85	I3	10	ARG
85	I3	39	LYS
85	I3	100	ASN
85	I3	102	MET
85	I3	162	ARG
85	I3	164	LYS
85	I3	175	LYS
87	u3	156	LYS
87	u3	159	MET
87	u3	188	ASN
87	u3	212	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
2	B1	141	ASN
3	C1	40	ASN
3	C1	147	ASN
4	D1	113	GLN
5	E1	22	ASN
5	E1	165	ASN
6	F1	138	HIS
6	F1	142	HIS
6	F1	209	HIS
6	F1	232	ASN
7	G1	82	ASN
7	G1	114	ASN
8	H1	81	HIS
8	H1	186	GLN
8	H1	202	ASN
9	I1	33	ASN
9	I1	186	ASN
10	J1	84	ASN
10	J1	87	ASN

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Mol	Chain	Res	Type
10	J1	99	ASN
12	L1	7	ASN
13	M1	19	ASN
13	M1	106	HIS
14	N1	28	HIS
14	N1	82	ASN
15	O1	5	HIS
15	O1	105	ASN
16	P1	94	HIS
17	Q1	104	GLN
18	R1	97	GLN
20	T1	120	HIS
20	T1	135	HIS
22	V1	47	ASN
23	W1	33	GLN
24	X1	113	HIS
26	Z1	15	ASN
30	d1	26	GLN
30	d1	29	GLN
33	g1	111	ASN
33	g1	135	HIS
34	h1	133	ASN
34	h1	159	ASN
34	h1	178	ASN
35	j1	11	ASN
35	j1	67	ASN
35	j1	121	ASN
35	j1	380	ASN
36	k1	171	GLN
36	k1	251	GLN
36	k1	321	ASN
36	k1	381	ASN
36	k1	440	GLN
36	k1	520	HIS
40	A3	194	ASN
41	B3	179	HIS
41	B3	245	HIS
42	C3	38	ASN
42	C3	245	HIS
42	C3	321	ASN
44	F3	38	GLN
44	F3	79	ASN

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Mol	Chain	Res	Type
44	F3	205	ASN
45	H3	8	GLN
45	H3	15	ASN
45	H3	102	ASN
48	N3	199	GLN
49	O3	5	GLN
50	P3	25	HIS
50	P3	80	GLN
50	P3	120	ASN
52	R3	36	ASN
52	R3	130	ASN
52	R3	143	HIS
52	R3	178	GLN
53	S3	156	HIS
53	S3	163	HIS
54	T3	95	HIS
58	X3	93	ASN
58	X3	105	ASN
58	X3	111	GLN
64	d3	18	ASN
66	f3	65	ASN
66	f3	99	HIS
67	g3	14	ASN
67	g3	114	GLN
70	j3	76	HIS
77	r3	12	ASN
82	J3	104	ASN
83	G3	134	ASN
83	G3	280	ASN
83	G3	293	ASN
84	D3	195	HIS
84	D3	202	GLN
84	D3	222	GLN
84	D3	275	GLN
85	I3	95	HIS
85	I3	100	ASN
87	u3	40	ASN
87	u3	188	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1709/1869 (91%)	474 (27%)	23 (1%)
37	52	3591/3634 (98%)	1136 (31%)	45 (1%)
38	72	119/120 (99%)	34 (28%)	0
39	82	149/156 (95%)	43 (28%)	0
80	23	74/76 (97%)	18 (24%)	0
81	w3	22/23 (95%)	10 (45%)	0
All	All	5664/5878 (96%)	1715 (30%)	68 (1%)

All (1715) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	2	A
1	A1	3	C
1	A1	5	U
1	A1	16	G
1	A1	17	C
1	A1	26	U
1	A1	33	G
1	A1	39	A
1	A1	41	G
1	A1	42	A
1	A1	44	U
1	A1	45	A
1	A1	46	A
1	A1	56	G
1	A1	58	C
1	A1	65	C
1	A1	67	C
1	A1	68	A
1	A1	72	C
1	A1	73	C
1	A1	74	G
1	A1	76	U
1	A1	79	A
1	A1	89	C
1	A1	91	A
1	A1	95	G
1	A1	100	U
1	A1	101	U
1	A1	103	A
1	A1	111	A
1	A1	113	G
1	A1	115	U

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Mol	Chain	Res	Type
1	A1	116	U
1	A1	124	U
1	A1	126	G
1	A1	127	C
1	A1	129	C
1	A1	130	G
1	A1	141	A
1	A1	143	U
1	A1	147	A
1	A1	153	G
1	A1	155	G
1	A1	162	C
1	A1	163	U
1	A1	167	G
1	A1	168	C
1	A1	170	A
1	A1	172	U
1	A1	178	C
1	A1	182	C
1	A1	183	G
1	A1	184	G
1	A1	187	G
1	A1	188	C
1	A1	189	U
1	A1	190	G
1	A1	191	A
1	A1	192	C
1	A1	202	G
1	A1	206	G
1	A1	209	A
1	A1	211	G
1	A1	213	G
1	A1	222	U
1	A1	227	U
1	A1	228	C
1	A1	229	A
1	A1	230	A
1	A1	231	A
1	A1	233	C
1	A1	236	A
1	A1	238	C
1	A1	239	C

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Mol	Chain	Res	Type
1	A1	240	G
1	A1	241	G
1	A1	242	U
1	A1	243	C
1	A1	281	C
1	A1	285	U
1	A1	292	A
1	A1	297	A
1	A1	306	C
1	A1	307	G
1	A1	308	G
1	A1	309	G
1	A1	312	G
1	A1	313	A
1	A1	314	U
1	A1	317	C
1	A1	318	A
1	A1	319	C
1	A1	322	C
1	A1	335	G
1	A1	339	A
1	A1	347	G
1	A1	350	C
1	A1	351	G
1	A1	354	U
1	A1	360	A
1	A1	361	U
1	A1	362	C
1	A1	364	A
1	A1	368	U
1	A1	382	C
1	A1	384	U
1	A1	385	G
1	A1	386	C
1	A1	400	C
1	A1	407	G
1	A1	408	A
1	A1	409	C
1	A1	413	G
1	A1	417	C
1	A1	418	A
1	A1	422	U

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Mol	Chain	Res	Type
1	A1	435	A
1	A1	441	C
1	A1	448	A
1	A1	449	A
1	A1	450	C
1	A1	452	G
1	A1	464	A
1	A1	465	A
1	A1	466	G
1	A1	472	C
1	A1	473	A
1	A1	474	G
1	A1	482	G
1	A1	485	A
1	A1	487	U
1	A1	492	C
1	A1	493	A
1	A1	495	U
1	A1	496	C
1	A1	501	C
1	A1	503	C
1	A1	516	A
1	A1	522	A
1	A1	525	A
1	A1	531	A
1	A1	532	C
1	A1	533	A
1	A1	536	A
1	A1	542	U
1	A1	544	G
1	A1	547	G
1	A1	548	C
1	A1	549	C
1	A1	550	C
1	A1	551	U
1	A1	554	A
1	A1	555	A
1	A1	559	G
1	A1	560	A
1	A1	562	U
1	A1	563	G
1	A1	564	A

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Mol	Chain	Res	Type
1	A1	565	G
1	A1	568	C
1	A1	582	U
1	A1	583	A
1	A1	588	G
1	A1	589	G
1	A1	590	A
1	A1	591	U
1	A1	593	C
1	A1	606	G
1	A1	608	C
1	A1	614	C
1	A1	615	C
1	A1	621	C
1	A1	622	C
1	A1	628	A
1	A1	629	A
1	A1	631	U
1	A1	637	U
1	A1	642	U
1	A1	643	A
1	A1	644	G
1	A1	658	U
1	A1	660	C
1	A1	664	A
1	A1	668	A
1	A1	669	A
1	A1	671	A
1	A1	672	A
1	A1	673	G
1	A1	675	U
1	A1	684	G
1	A1	688	U
1	A1	689	U
1	A1	690	G
1	A1	747	U
1	A1	750	C
1	A1	752	G
1	A1	753	C
1	A1	790	C
1	A1	793	G
1	A1	797	C

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Mol	Chain	Res	Type
1	A1	798	G
1	A1	799	U
1	A1	800	U
1	A1	811	A
1	A1	820	U
1	A1	821	G
1	A1	830	A
1	A1	834	C
1	A1	844	U
1	A1	847	A
1	A1	852	G
1	A1	867	G
1	A1	869	A
1	A1	870	A
1	A1	871	U
1	A1	872	A
1	A1	873	G
1	A1	874	G
1	A1	875	A
1	A1	876	C
1	A1	878	G
1	A1	879	C
1	A1	881	G
1	A1	886	A
1	A1	887	U
1	A1	888	U
1	A1	889	U
1	A1	890	U
1	A1	891	G
1	A1	892	U
1	A1	893	U
1	A1	895	G
1	A1	913	A
1	A1	914	U
1	A1	917	U
1	A1	919	A
1	A1	920	A
1	A1	930	C
1	A1	933	G
1	A1	934	G
1	A1	943	U
1	A1	960	U

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Mol	Chain	Res	Type
1	A1	966	U
1	A1	970	G
1	A1	971	G
1	A1	979	C
1	A1	985	G
1	A1	989	C
1	A1	990	A
1	A1	992	A
1	A1	997	A
1	A1	999	G
1	A1	1002	U
1	A1	1005	G
1	A1	1013	U
1	A1	1017	U
1	A1	1021	U
1	A1	1023	A
1	A1	1028	A
1	A1	1041	G
1	A1	1047	C
1	A1	1058	A
1	A1	1060	A
1	A1	1067	C
1	A1	1071	G
1	A1	1083	A
1	A1	1085	C
1	A1	1087	A
1	A1	1089	G
1	A1	1097	G
1	A1	1099	G
1	A1	1100	A
1	A1	1101	U
1	A1	1106	C
1	A1	1115	U
1	A1	1116	C
1	A1	1117	C
1	A1	1118	C
1	A1	1123	C
1	A1	1126	G
1	A1	1131	G
1	A1	1138	C
1	A1	1139	C
1	A1	1144	A

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Mol	Chain	Res	Type
1	A1	1145	A
1	A1	1149	A
1	A1	1150	A
1	A1	1153	C
1	A1	1154	U
1	A1	1155	U
1	A1	1170	A
1	A1	1171	G
1	A1	1175	G
1	A1	1178	U
1	A1	1194	A
1	A1	1195	A
1	A1	1200	A
1	A1	1207	G
1	A1	1212	G
1	A1	1215	C
1	A1	1216	C
1	A1	1221	G
1	A1	1230	C
1	A1	1241	A
1	A1	1242	U
1	A1	1246	A
1	A1	1251	A
1	A1	1253	A
1	A1	1254	C
1	A1	1256	G
1	A1	1257	G
1	A1	1258	A
1	A1	1266	C
1	A1	1274	G
1	A1	1275	G
1	A1	1282	A
1	A1	1284	A
1	A1	1285	G
1	A1	1286	G
1	A1	1287	A
1	A1	1291	A
1	A1	1293	A
1	A1	1295	A
1	A1	1299	A
1	A1	1300	U
1	A1	1301	A

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Mol	Chain	Res	Type
1	A1	1302	G
1	A1	1303	C
1	A1	1308	U
1	A1	1311	C
1	A1	1314	U
1	A1	1319	U
1	A1	1330	G
1	A1	1336	C
1	A1	1342	U
1	A1	1344	A
1	A1	1345	G
1	A1	1355	C
1	A1	1371	U
1	A1	1372	U
1	A1	1375	G
1	A1	1378	A
1	A1	1395	C
1	A1	1396	A
1	A1	1397	U
1	A1	1402	A
1	A1	1412	C
1	A1	1413	G
1	A1	1417	C
1	A1	1427	C
1	A1	1428	G
1	A1	1429	G
1	A1	1430	C
1	A1	1439	A
1	A1	1440	C
1	A1	1447	G
1	A1	1450	G
1	A1	1452	A
1	A1	1453	C
1	A1	1454	A
1	A1	1461	G
1	A1	1462	U
1	A1	1463	U
1	A1	1464	C
1	A1	1466	G
1	A1	1471	C
1	A1	1476	A
1	A1	1477	U

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Mol	Chain	Res	Type
1	A1	1480	A
1	A1	1486	A
1	A1	1487	A
1	A1	1489	A
1	A1	1490	G
1	A1	1496	U
1	A1	1498	A
1	A1	1501	C
1	A1	1502	C
1	A1	1521	C
1	A1	1522	A
1	A1	1523	C
1	A1	1532	C
1	A1	1533	A
1	A1	1535	U
1	A1	1536	G
1	A1	1545	A
1	A1	1548	G
1	A1	1552	G
1	A1	1553	C
1	A1	1554	C
1	A1	1555	U
1	A1	1556	A
1	A1	1557	C
1	A1	1558	C
1	A1	1567	G
1	A1	1570	G
1	A1	1574	C
1	A1	1579	A
1	A1	1580	A
1	A1	1585	U
1	A1	1586	U
1	A1	1588	A
1	A1	1591	C
1	A1	1596	U
1	A1	1597	C
1	A1	1599	U
1	A1	1601	A
1	A1	1602	U
1	A1	1603	G
1	A1	1604	G
1	A1	1621	U

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Mol	Chain	Res	Type
1	A1	1623	A
1	A1	1637	A
1	A1	1638	G
1	A1	1640	A
1	A1	1641	A
1	A1	1646	C
1	A1	1648	G
1	A1	1654	G
1	A1	1665	G
1	A1	1666	C
1	A1	1668	U
1	A1	1670	C
1	A1	1671	G
1	A1	1674	G
1	A1	1678	A
1	A1	1683	C
1	A1	1695	A
1	A1	1698	C
1	A1	1699	A
1	A1	1700	C
1	A1	1701	C
1	A1	1702	G
1	A1	1715	A
1	A1	1721	U
1	A1	1722	G
1	A1	1729	U
1	A1	1732	G
1	A1	1735	A
1	A1	1746	U
1	A1	1748	G
1	A1	1753	C
1	A1	1756	C
1	A1	1757	G
1	A1	1758	G
1	A1	1759	G
1	A1	1777	G
1	A1	1778	C
1	A1	1781	A
1	A1	1783	C
1	A1	1792	G
1	A1	1800	A
1	A1	1816	G

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Mol	Chain	Res	Type
1	A1	1821	U
1	A1	1823	A
1	A1	1824	A
1	A1	1825	A
1	A1	1826	G
1	A1	1831	A
1	A1	1834	A
1	A1	1836	G
1	A1	1838	U
1	A1	1839	U
1	A1	1840	U
1	A1	1844	U
1	A1	1845	A
1	A1	1849	G
1	A1	1851	A
1	A1	1852	C
1	A1	1861	G
1	A1	1862	G
1	A1	1863	A
1	A1	1864	U
1	A1	1865	C
1	A1	1869	A
37	52	5	A
37	52	6	C
37	52	8	U
37	52	9	C
37	52	10	A
37	52	13	U
37	52	18	C
37	52	21	G
37	52	25	A
37	52	30	C
37	52	39	A
37	52	42	A
37	52	44	A
37	52	48	G
37	52	49	U
37	52	58	G
37	52	59	A
37	52	64	A
37	52	65	A
37	52	67	C

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Mol	Chain	Res	Type
37	52	70	A
37	52	71	C
37	52	72	C
37	52	76	A
37	52	82	U
37	52	84	A
37	52	87	A
37	52	91	G
37	52	93	G
37	52	96	U
37	52	104	G
37	52	108	A
37	52	109	G
37	52	119	G
37	52	120	A
37	52	122	U
37	52	126	C
37	52	133	C
37	52	135	G
37	52	136	C
37	52	137	G
37	52	142	G
37	52	144	G
37	52	149	A
37	52	151	G
37	52	153	G
37	52	156	G
37	52	157	U
37	52	159	C
37	52	160	G
37	52	161	G
37	52	164	G
37	52	168	C
37	52	170	C
37	52	172	C
37	52	173	C
37	52	174	C
37	52	179	G
37	52	181	C
37	52	182	G
37	52	197	A
37	52	200	U

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Mol	Chain	Res	Type
37	52	201	C
37	52	214	G
37	52	216	C
37	52	217	C
37	52	220	C
37	52	224	U
37	52	225	G
37	52	232	G
37	52	233	U
37	52	234	G
37	52	236	G
37	52	246	G
37	52	262	G
37	52	265	C
37	52	266	C
37	52	276	C
37	52	277	G
37	52	280	G
37	52	294	G
37	52	297	U
37	52	306	A
37	52	308	G
37	52	309	C
37	52	310	G
37	52	315	G
37	52	316	U
37	52	321	U
37	52	322	C
37	52	323	C
37	52	334	A
37	52	340	C
37	52	341	G
37	52	345	C
37	52	346	G
37	52	349	A
37	52	367	C
37	52	379	G
37	52	383	A
37	52	384	A
37	52	387	G
37	52	390	C
37	52	395	A

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Mol	Chain	Res	Type
37	52	396	A
37	52	410	A
37	52	412	G
37	52	413	G
37	52	417	G
37	52	440	U
37	52	446	C
37	52	448	G
37	52	449	C
37	52	450	G
37	52	452	A
37	52	453	G
37	52	454	U
37	52	455	C
37	52	463	A
37	52	465	G
37	52	467	U
37	52	468	U
37	52	474	C
37	52	475	G
37	52	481	G
37	52	481(A)	C
37	52	482	G
37	52	483	G
37	52	484	U
37	52	485	C
37	52	486	C
37	52	487	G
37	52	490	C
37	52	491	G
37	52	492	U
37	52	493	G
37	52	495	C
37	52	498	C
37	52	499	G
37	52	505	G
37	52	506	C
37	52	510	U
37	52	516	C
37	52	641	G
37	52	642	G
37	52	661	C

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Mol	Chain	Res	Type
37	52	666	G
37	52	667	A
37	52	669	C
37	52	670	G
37	52	674	G
37	52	676	C
37	52	685	C
37	52	686	A
37	52	688	U
37	52	691	C
37	52	696	C
37	52	697	G
37	52	700	G
37	52	704	C
37	52	705	G
37	52	719	C
37	52	722	G
37	52	729	G
37	52	730	G
37	52	731	G
37	52	733	A
37	52	738	C
37	52	743	G
37	52	747	A
37	52	749	G
37	52	750	U
37	52	751	G
37	52	758	G
37	52	760	G
37	52	905	C
37	52	908	G
37	52	913	U
37	52	914	U
37	52	915	A
37	52	917	A
37	52	922(B)	C
37	52	923	C
37	52	925	C
37	52	926	G
37	52	929	A
37	52	930	G
37	52	931	C

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Mol	Chain	Res	Type
37	52	932	A
37	52	933	G
37	52	934	C
37	52	935	A
37	52	935(A)	G
37	52	941	C
37	52	944	A
37	52	945	U
37	52	946	C
37	52	951	G
37	52	955	G
37	52	956	A
37	52	959	G
37	52	960	A
37	52	961	G
37	52	962	C
37	52	965	G
37	52	966	A
37	52	967	C
37	52	968	C
37	52	969	C
37	52	972	C
37	52	978	G
37	52	983	C
37	52	985	C
37	52	990	C
37	52	1070	G
37	52	1071	C
37	52	1072	C
37	52	1073	G
37	52	1074	G
37	52	1077	C
37	52	1082	C
37	52	1090	G
37	52	1101	C
37	52	1104	C
37	52	1107	C
37	52	1108	C
37	52	1163	G
37	52	1164	G
37	52	1165	G
37	52	1166	G

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Mol	Chain	Res	Type
37	52	1167	C
37	52	1181	C
37	52	1183	C
37	52	1196	G
37	52	1199	G
37	52	1201	U
37	52	1203	G
37	52	1205	G
37	52	1211	G
37	52	1212	G
37	52	1214	C
37	52	1215	C
37	52	1216	C
37	52	1219	G
37	52	1221	G
37	52	1235	G
37	52	1236	C
37	52	1237	C
37	52	1238	A
37	52	1239	C
37	52	1246	G
37	52	1272	C
37	52	1273	G
37	52	1276	C
37	52	1279	A
37	52	1281	G
37	52	1284	G
37	52	1287	G
37	52	1292	C
37	52	1293	G
37	52	1295	U
37	52	1296	G
37	52	1299	G
37	52	1300	G
37	52	1301	C
37	52	1303	A
37	52	1309	C
37	52	1318	C
37	52	1321	G
37	52	1326	A
37	52	1330	A
37	52	1338	G

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Mol	Chain	Res	Type
37	52	1341	U
37	52	1352	C
37	52	1353	G
37	52	1354	A
37	52	1356	U
37	52	1358	G
37	52	1359	G
37	52	1360	G
37	52	1361	G
37	52	1362	G
37	52	1371	A
37	52	1372	A
37	52	1373	A
37	52	1377	G
37	52	1378	C
37	52	1379	C
37	52	1387	A
37	52	1389	U
37	52	1391	A
37	52	1394	G
37	52	1396	G
37	52	1397	A
37	52	1398	A
37	52	1399	G
37	52	1400	G
37	52	1405	C
37	52	1406	G
37	52	1420	A
37	52	1425	G
37	52	1429	C
37	52	1434	G
37	52	1436	C
37	52	1437	C
37	52	1438	U
37	52	1445	U
37	52	1446	C
37	52	1453	G
37	52	1454	G
37	52	1456	C
37	52	1457	G
37	52	1459	A
37	52	1466	G

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Mol	Chain	Res	Type
37	52	1468	C
37	52	1475	G
37	52	1478	C
37	52	1481	C
37	52	1482	G
37	52	1483	C
37	52	1484	G
37	52	1491	A
37	52	1493	G
37	52	1497	A
37	52	1498	G
37	52	1501	C
37	52	1502	G
37	52	1514	U
37	52	1517	G
37	52	1518	A
37	52	1521	C
37	52	1523	A
37	52	1524	A
37	52	1531	U
37	52	1534	A
37	52	1535	C
37	52	1538	U
37	52	1540	C
37	52	1543	G
37	52	1547	A
37	52	1549	G
37	52	1553	A
37	52	1558	A
37	52	1566	C
37	52	1571	G
37	52	1573	G
37	52	1578	U
37	52	1585	C
37	52	1590	C
37	52	1591	U
37	52	1592	G
37	52	1596	U
37	52	1597	G
37	52	1602	U
37	52	1605	G
37	52	1609	U

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Mol	Chain	Res	Type
37	52	1612	G
37	52	1613	A
37	52	1614	C
37	52	1624	G
37	52	1625	G
37	52	1626	G
37	52	1627	G
37	52	1631	A
37	52	1632	A
37	52	1633	G
37	52	1634	A
37	52	1638	A
37	52	1643	A
37	52	1650	A
37	52	1651	G
37	52	1652	U
37	52	1654	G
37	52	1658	G
37	52	1660	U
37	52	1661	C
37	52	1663	C
37	52	1673	U
37	52	1676	C
37	52	1677	U
37	52	1679	A
37	52	1684	A
37	52	1724	G
37	52	1725	U
37	52	1729	A
37	52	1730	U
37	52	1731	C
37	52	1734	G
37	52	1735	U
37	52	1740	C
37	52	1741	G
37	52	1742	A
37	52	1746	A
37	52	1750	G
37	52	1753	G
37	52	1754	U
37	52	1755	C
37	52	1756	U

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Mol	Chain	Res	Type
37	52	1757	U
37	52	1763	C
37	52	1764	G
37	52	1768	C
37	52	1772	C
37	52	1775	A
37	52	1776	A
37	52	1777	C
37	52	1787	A
37	52	1792	U
37	52	1796	U
37	52	1800	U
37	52	1804	A
37	52	1805	A
37	52	1806	G
37	52	1807	C
37	52	1808	C
37	52	1810	G
37	52	1812	C
37	52	1815	G
37	52	1818	G
37	52	1820	U
37	52	1821	G
37	52	1822	U
37	52	1824	G
37	52	1828	C
37	52	1834	U
37	52	1836	G
37	52	1837	A
37	52	1842	G
37	52	1843	A
37	52	1844	G
37	52	1855	G
37	52	1861	U
37	52	1866	U
37	52	1867	A
37	52	1869	G
37	52	1870	C
37	52	1889	U
37	52	1892	A
37	52	1893	C
37	52	1897	A

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Mol	Chain	Res	Type
37	52	1910	G
37	52	1915	C
37	52	1918	U
37	52	1920	C
37	52	1921	C
37	52	1922	G
37	52	1924	C
37	52	1928	C
37	52	1930	U
37	52	1931	C
37	52	1932	A
37	52	1934	A
37	52	1935	C
37	52	1940	G
37	52	1942	A
37	52	1944	A
37	52	1948	G
37	52	1951	G
37	52	1958	A
37	52	1959	U
37	52	1960	A
37	52	1961	G
37	52	1969	G
37	52	1971	U
37	52	1976	G
37	52	1977	C
37	52	1979	A
37	52	1980	U
37	52	1981	G
37	52	1983	A
37	52	1984	A
37	52	1991	A
37	52	1993	C
37	52	1994	C
37	52	1995	G
37	52	1998	A
37	52	2001	G
37	52	2002	A
37	52	2003	G
37	52	2005	G
37	52	2007	G
37	52	2010	A

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Mol	Chain	Res	Type
37	52	2011	C
37	52	2014	C
37	52	2020	U
37	52	2021	G
37	52	2022	C
37	52	2023	C
37	52	2024	G
37	52	2025	A
37	52	2026	A
37	52	2042	A
37	52	2043	A
37	52	2046	G
37	52	2047	A
37	52	2048	U
37	52	2052	G
37	52	2054	U
37	52	2055	G
37	52	2056	G
37	52	2057	A
37	52	2062	C
37	52	2063	G
37	52	2064	G
37	52	2069	A
37	52	2078	C
37	52	2084	U
37	52	2085	G
37	52	2088	A
37	52	2089	G
37	52	2090	U
37	52	2092	G
37	52	2093	G
37	52	2094	C
37	52	2097	A
37	52	2098	G
37	52	2099	C
37	52	2101	A
37	52	2102	G
37	52	2105	A
37	52	2108	G
37	52	2112	G
37	52	2259	G
37	52	2260	C

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Mol	Chain	Res	Type
37	52	2261	G
37	52	2263	A
37	52	2268	A
37	52	2269	C
37	52	2270	G
37	52	2274	C
37	52	2275	G
37	52	2277	C
37	52	2279	A
37	52	2281	U
37	52	2289	C
37	52	2295	C
37	52	2300	A
37	52	2301	G
37	52	2306	G
37	52	2308	A
37	52	2313	A
37	52	2314	G
37	52	2328	G
37	52	2333	G
37	52	2335	C
37	52	2345	G
37	52	2346	C
37	52	2348	G
37	52	2351	C
37	52	2353	U
37	52	2360	A
37	52	2363	A
37	52	2364	G
37	52	2374	A
37	52	2380	G
37	52	2385	U
37	52	2395	A
37	52	2396	A
37	52	2397	G
37	52	2399	G
37	52	2414	G
37	52	2415	U
37	52	2416	G
37	52	2421	G
37	52	2422	C
37	52	2426	U

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Mol	Chain	Res	Type
37	52	2428	A
37	52	2433	G
37	52	2437	C
37	52	2438	A
37	52	2439	G
37	52	2440	U
37	52	2441	C
37	52	2447	U
37	52	2450	G
37	52	2451	A
37	52	2454	U
37	52	2456	G
37	52	2458	C
37	52	2460	A
37	52	2461	G
37	52	2471	G
37	52	2473	A
37	52	2475	G
37	52	2480	G
37	52	2481	G
37	52	2485	U
37	52	2488	C
37	52	2489	C
37	52	2490	U
37	52	2491	C
37	52	2492	C
37	52	2493	G
37	52	2494	U
37	52	2496	G
37	52	2501	C
37	52	2503	G
37	52	2505	C
37	52	2506	G
37	52	2511	A
37	52	2512	A
37	52	2513	A
37	52	2516	G
37	52	2521	G
37	52	2529	A
37	52	2532	C
37	52	2535	G
37	52	2536	A

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Mol	Chain	Res	Type
37	52	2537	A
37	52	2538	U
37	52	2542	G
37	52	2544	G
37	52	2546	G
37	52	2549	G
37	52	2551	A
37	52	2555	G
37	52	2556	G
37	52	2561	C
37	52	2562	G
37	52	2563	C
37	52	2566	G
37	52	2570	U
37	52	2575	U
37	52	2576	G
37	52	2577	C
37	52	2580	U
37	52	2581	A
37	52	2587	A
37	52	2588	C
37	52	2589	C
37	52	2593	C
37	52	2597	G
37	52	2599	G
37	52	2600	A
37	52	2601	A
37	52	2604	C
37	52	2607	C
37	52	2620	G
37	52	2621	A
37	52	2622	G
37	52	2624	G
37	52	2627	C
37	52	2631	U
37	52	2639	U
37	52	2653	C
37	52	2655	C
37	52	2656	U
37	52	2658	G
37	52	2662	G
37	52	2663	G

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Mol	Chain	Res	Type
37	52	2668	G
37	52	2669	C
37	52	2670	C
37	52	2674	A
37	52	2675	G
37	52	2683	C
37	52	2685	C
37	52	2686	G
37	52	2687	U
37	52	2689	C
37	52	2693	G
37	52	2695	A
37	52	2696	A
37	52	2697	A
37	52	2701	U
37	52	2706	G
37	52	2707	U
37	52	2708	U
37	52	2709	C
37	52	2710	C
37	52	2711	G
37	52	2712	G
37	52	2714	G
37	52	2716	C
37	52	2719	C
37	52	2725	A
37	52	2726	G
37	52	2732	G
37	52	2739	C
37	52	2740	U
37	52	2741	U
37	52	2743	A
37	52	2744	A
37	52	2750	G
37	52	2752	G
37	52	2754	G
37	52	2756	G
37	52	2757	A
37	52	2760	G
37	52	2761	U
37	52	2763	U
37	52	2764	A

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Mol	Chain	Res	Type
37	52	2766	A
37	52	2767	U
37	52	2768	C
37	52	2769	U
37	52	2778	G
37	52	2787	A
37	52	2788	U
37	52	2789	A
37	52	2790	U
37	52	2794	C
37	52	2796	G
37	52	2798	A
37	52	2799	G
37	52	2807	A
37	52	2809	G
37	52	2811	G
37	52	2812	A
37	52	2813	A
37	52	2817	C
37	52	2821	U
37	52	2822	G
37	52	2823	G
37	52	2826	U
37	52	2827	G
37	52	2842	G
37	52	2847	G
37	52	2849	A
37	52	2850	A
37	52	2854	G
37	52	2855	G
37	52	2856	C
37	52	2858	A
37	52	2862	G
37	52	2864	A
37	52	2872	C
37	52	2873	U
37	52	2875	C
37	52	2876	G
37	52	2889	G
37	52	2895	A
37	52	2897	G
37	52	2898	G

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Mol	Chain	Res	Type
37	52	3598	C
37	52	3599	A
37	52	3600	G
37	52	3604	A
37	52	3605	C
37	52	3606	U
37	52	3615	G
37	52	3616	U
37	52	3618	C
37	52	3620	G
37	52	3622	C
37	52	3625	G
37	52	3626	G
37	52	3635	A
37	52	3638	G
37	52	3642	A
37	52	3643	A
37	52	3644	U
37	52	3646	A
37	52	3662	A
37	52	3664	G
37	52	3668	C
37	52	3673	C
37	52	3674	G
37	52	3678	G
37	52	3680	U
37	52	3682	A
37	52	3683	C
37	52	3685	C
37	52	3690	U
37	52	3692	A
37	52	3696	C
37	52	3705	G
37	52	3707	U
37	52	3712	A
37	52	3713	U
37	52	3714	G
37	52	3729	U
37	52	3731	C
37	52	3732	A
37	52	3734	U
37	52	3743	G

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Mol	Chain	Res	Type
37	52	3744	G
37	52	3753	G
37	52	3760	A
37	52	3763	A
37	52	3766	A
37	52	3773	U
37	52	3775	A
37	52	3776	G
37	52	3777	G
37	52	3783	A
37	52	3784	A
37	52	3793	U
37	52	3796	U
37	52	3798	U
37	52	3802	U
37	52	3807	A
37	52	3810	C
37	52	3811	G
37	52	3812	C
37	52	3814	U
37	52	3817	A
37	52	3819	G
37	52	3822	U
37	52	3825	A
37	52	3834	C
37	52	3837	C
37	52	3838	U
37	52	3840	U
37	52	3843	C
37	52	3858	C
37	52	3865	A
37	52	3867	A
37	52	3868	G
37	52	3876	A
37	52	3877	A
37	52	3878	C
37	52	3879	G
37	52	3881	G
37	52	3882	C
37	52	3889	G
37	52	3895	G
37	52	3897	G

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Mol	Chain	Res	Type
37	52	3901	A
37	52	3902	A
37	52	3905	A
37	52	3906	A
37	52	3907	G
37	52	3909	C
37	52	3915	U
37	52	3921	U
37	52	3925	U
37	52	3926	C
37	52	3937	C
37	52	3940	U
37	52	3941	G
37	52	3942	A
37	52	3944	G
37	52	3947	A
37	52	3957	U
37	52	3959	U
37	52	3960	A
37	52	3962	A
37	52	3963	A
37	52	3964	U
37	52	3965	A
37	52	3966	A
37	52	3967	G
37	52	3969	G
37	52	3970	G
37	52	3973	G
37	52	4037	C
37	52	4038	C
37	52	4044	U
37	52	4047	A
37	52	4048	A
37	52	4049	U
37	52	4053	A
37	52	4065	G
37	52	4066	U
37	52	4067	U
37	52	4069	U
37	52	4071	U
37	52	4076	G
37	52	4084	G

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Mol	Chain	Res	Type
37	52	4085	A
37	52	4086	G
37	52	4091	G
37	52	4093	G
37	52	4094	G
37	52	4100	C
37	52	4111	U
37	52	4112	C
37	52	4116	C
37	52	4117	U
37	52	4118	U
37	52	4119	C
37	52	4120	U
37	52	4121	G
37	52	4122	G
37	52	4124	G
37	52	4127	A
37	52	4129	G
37	52	4131	G
37	52	4133	C
37	52	4157	A
37	52	4158	C
37	52	4159	C
37	52	4162	C
37	52	4163	U
37	52	4166	G
37	52	4170	A
37	52	4171	C
37	52	4172	A
37	52	4173	G
37	52	4180	G
37	52	4183	G
37	52	4184	G
37	52	4191	G
37	52	4194	U
37	52	4195	G
37	52	4203	A
37	52	4205	A
37	52	4206	C
37	52	4207	C
37	52	4209	G
37	52	4212	A

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Mol	Chain	Res	Type
37	52	4215	C
37	52	4229	U
37	52	4233	A
37	52	4234	A
37	52	4251	A
37	52	4254	G
37	52	4255	A
37	52	4257	A
37	52	4265	U
37	52	4266	G
37	52	4268	A
37	52	4271	A
37	52	4273	A
37	52	4275	G
37	52	4280	A
37	52	4281	A
37	52	4282	A
37	52	4285	U
37	52	4290	U
37	52	4291	G
37	52	4293	U
37	52	4305	G
37	52	4306	U
37	52	4317	A
37	52	4318	C
37	52	4322	G
37	52	4329	G
37	52	4330	G
37	52	4335	C
37	52	4336	A
37	52	4339	A
37	52	4348	A
37	52	4349	C
37	52	4350	C
37	52	4351	U
37	52	4355	G
37	52	4359	U
37	52	4366	A
37	52	4374	U
37	52	4377	G
37	52	4378	A
37	52	4379	A

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Mol	Chain	Res	Type
37	52	4380	A
37	52	4386	C
37	52	4387	C
37	52	4393	G
37	52	4394	A
37	52	4395	U
37	52	4396	A
37	52	4398	C
37	52	4405	G
37	52	4417	C
37	52	4419	U
37	52	4420	U
37	52	4422	A
37	52	4424	A
37	52	4426	C
37	52	4430	G
37	52	4431	U
37	52	4433	G
37	52	4435	U
37	52	4437	U
37	52	4440	G
37	52	4444	C
37	52	4448	G
37	52	4449	A
37	52	4450	U
37	52	4452	U
37	52	4453	C
37	52	4464	A
37	52	4466	C
37	52	4472	G
37	52	4475	G
37	52	4476	C
37	52	4477	A
37	52	4480	A
37	52	4481	U
37	52	4482	U
37	52	4497	U
37	52	4499	G
37	52	4500	U
37	52	4501	U
37	52	4507	A
37	52	4511	A

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Mol	Chain	Res	Type
37	52	4512	U
37	52	4513	A
37	52	4519	C
37	52	4522	G
37	52	4524	G
37	52	4530	U
37	52	4531	U
37	52	4532	U
37	52	4548	A
37	52	4549	G
37	52	4552	U
37	52	4553	A
37	52	4554	G
37	52	4567	G
37	52	4570	G
37	52	4573	G
37	52	4575	G
37	52	4589	A
37	52	4590	A
37	52	4599	A
37	52	4604	G
37	52	4606	G
37	52	4634	U
37	52	4635	A
37	52	4636	U
37	52	4637	G
37	52	4639	G
37	52	4652	G
37	52	4654	C
37	52	4656	A
37	52	4657	U
37	52	4662	C
37	52	4670	C
37	52	4672	A
37	52	4673	U
37	52	4677	U
37	52	4693	C
37	52	4694	G
37	52	4695	C
37	52	4700	A
37	52	4709	U
37	52	4716	C

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Mol	Chain	Res	Type
37	52	4719	G
37	52	4720	C
37	52	4721	G
37	52	4726	G
37	52	4728	U
37	52	4738	C
37	52	4739	C
37	52	4740	G
37	52	4750	G
37	52	4751	G
37	52	4753	U
37	52	4754	G
37	52	4757	C
37	52	4759	C
37	52	4761	G
37	52	4764	A
37	52	4765	G
37	52	4766	C
37	52	4771	C
37	52	4772	C
37	52	4860	G
37	52	4862	G
37	52	4868	G
37	52	4870	G
37	52	4871	C
37	52	4872	G
37	52	4873	G
37	52	4874	A
37	52	4875	G
37	52	4876	A
37	52	4877	G
37	52	4882	U
37	52	4883	C
37	52	4885	U
37	52	4893	A
37	52	4894	A
37	52	4895	C
37	52	4898	G
37	52	4904	G
37	52	4905	C
37	52	4906	C
37	52	4907	G

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Mol	Chain	Res	Type
37	52	4908	G
37	52	4909	A
37	52	4910	A
37	52	4911	A
37	52	4912	G
37	52	4913	G
37	52	4914	G
37	52	4915	G
37	52	4918	C
37	52	4920	C
37	52	4921	C
37	52	4922	C
37	52	4923	U
37	52	4924	C
37	52	4926	C
37	52	4927	G
37	52	4928	C
37	52	4930	C
37	52	4931	G
37	52	4933	C
37	52	4935	C
37	52	4937	C
37	52	4938	A
37	52	4940	C
37	52	4943	A
37	52	4944	C
37	52	4945	G
37	52	4947	U
37	52	4949	G
37	52	4950	U
37	52	4951	G
37	52	4955	A
37	52	4956	A
37	52	4958	C
37	52	4959	U
37	52	4964	C
37	52	4965	U
37	52	4966	A
37	52	4967	A
37	52	4976	U
37	52	4980	C
37	52	4988	U

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Mol	Chain	Res	Type
37	52	4989	U
37	52	4990	C
37	52	5005	G
37	52	5009	G
37	52	5017	G
37	52	5018	C
37	52	5019	A
37	52	5022	U
37	52	5035	U
37	52	5040	U
37	52	5041	G
37	52	5043	A
37	52	5047	C
37	52	5048	A
37	52	5050	C
37	52	5053	U
37	52	5054	C
37	52	5055	G
37	52	5056	A
37	52	5058	A
37	52	5059	C
37	52	5061	A
37	52	5062	G
37	52	5069	U
38	72	2	U
38	72	3	C
38	72	6	C
38	72	7	G
38	72	11	A
38	72	17	C
38	72	21	G
38	72	22	A
38	72	23	A
38	72	24	C
38	72	25	G
38	72	28	C
38	72	30	C
38	72	42	A
38	72	45	U
38	72	48	G
38	72	50	A
38	72	53	U

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Mol	Chain	Res	Type
38	72	54	A
38	72	55	A
38	72	60	G
38	72	61	G
38	72	63	C
38	72	64	G
38	72	78	C
38	72	90	A
38	72	97	G
38	72	100	A
38	72	102	U
38	72	103	A
38	72	106	G
38	72	110	G
38	72	117	G
38	72	120	U
39	82	8	U
39	82	23	C
39	82	34	U
39	82	35	C
39	82	37	A
39	82	39	G
39	82	45	C
39	82	49	G
39	82	50	C
39	82	51	U
39	82	59	A
39	82	62	A
39	82	63	U
39	82	87	G
39	82	90	C
39	82	92	U
39	82	94	G
39	82	95	A
39	82	96	C
39	82	102	G
39	82	103	A
39	82	105	C
39	82	109	C
39	82	110	U
39	82	111	U
39	82	114	G

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Mol	Chain	Res	Type
39	82	117	C
39	82	118	C
39	82	119	C
39	82	120	G
39	82	121	G
39	82	122	G
39	82	123	U
39	82	124	U
39	82	125	C
39	82	126	C
39	82	127	U
39	82	128	C
39	82	137	A
39	82	143	G
39	82	150	C
39	82	153	C
39	82	156	U
80	23	7	G
80	23	8	U
80	23	9	A
80	23	13	U
80	23	14	A
80	23	20	U
80	23	21	A
80	23	31	C
80	23	32	C
80	23	37	A
80	23	46	G
80	23	47	U
80	23	49	C
80	23	53	G
80	23	59	A
80	23	61	C
80	23	65	G
80	23	67	G
81	w3	38	A
81	w3	39	A
81	w3	42	C
81	w3	43	A
81	w3	45	A
81	w3	46	G
81	w3	49	U

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Mol	Chain	Res	Type
81	w3	56	A
81	w3	58	A
81	w3	59	A

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	110	U
1	A1	182	C
1	A1	228	C
1	A1	241	G
1	A1	434	G
1	A1	465	A
1	A1	532	C
1	A1	553	U
1	A1	642	U
1	A1	688	U
1	A1	751	G
1	A1	870	A
1	A1	874	G
1	A1	1137	U
1	A1	1253	A
1	A1	1394	G
1	A1	1395	C
1	A1	1396	A
1	A1	1489	A
1	A1	1520	G
1	A1	1637	A
1	A1	1664	A
1	A1	1824	A
37	52	48	G
37	52	125	C
37	52	265	C
37	52	275	C
37	52	449	C
37	52	480	C
37	52	498	C
37	52	504	G
37	52	930	G
37	52	959	G
37	52	966	A
37	52	971(A)	G

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Mol	Chain	Res	Type
37	52	1106	A
37	52	1211	G
37	52	1238	A
37	52	1291	G
37	52	1329	G
37	52	1370	G
37	52	1445	U
37	52	1455	G
37	52	1979	A
37	52	1994	C
37	52	2046	G
37	52	2089	G
37	52	2502	A
37	52	2536	A
37	52	2875	C
37	52	3625	G
37	52	3876	A
37	52	3888	G
37	52	3939	G
37	52	3940	U
37	52	3959	U
37	52	3965	A
37	52	3968	U
37	52	4036	G
37	52	4157	A
37	52	4232	U
37	52	4448	G
37	52	4699	U
37	52	4719	G
37	52	4859	C
37	52	4884	G
37	52	4925	U
37	52	4936	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 310 ligands modelled in this entry, 308 are monoatomic - leaving 2 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	k1	600	-	0,12,12	0.00	-	0,24,24	0.00	-
90	SF4	k1	601	-	0,12,12	0.00	-	0,24,24	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	SF4	k1	600	-	-	0/0/48/48	0/6/5/5
90	SF4	k1	601	-	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	52	37
1	A1	12
78	s3	1
80	23	1
85	I3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	52	2113:G	O3'	2258:C	P	42.99
1	52	1252:C	O3'	1271:G	P	36.84
1	52	1406(C):G	O3'	1411:C	P	19.25
1	52	1109:C	O3'	1161:G	P	17.69
1	52	3977:C	O3'	4034:G	P	16.37
1	52	1696:C	O3'	1720:C	P	16.22
1	52	4101:C	O3'	4107:G	P	15.99
1	52	990:C	O3'	1064:G	P	15.06
1	52	5022:U	O3'	5028:G	P	14.93
1	52	4777:C	O3'	4859:C	P	14.91
1	52	523:C	O3'	638:G	P	14.66
1	52	1364:U	O3'	1368:A	P	14.61
1	52	2901:G	O3'	3597:G	P	13.74
1	52	4138:C	O3'	4146:G	P	13.54
1	52	760:G	O3'	904:C	P	12.47
1	52	4729:A	O3'	4735:G	P	9.89
1	52	182:G	O3'	189:G	P	9.08
1	52	500:G	O3'	504:G	P	7.93
1	A1	745:C	O3'	746:C	P	7.34
1	52	512:U	O3'	515:C	P	7.27
1	52	3938:G	O3'	3939:G	P	6.79
1	52	3937:C	O3'	3938:G	P	6.76
1	52	4740:G	O3'	4743:G	P	6.72
1	A1	787:G	O3'	788:G	P	6.11
1	52	3948:C	O3'	3949:A	P	5.77
1	52	4899:G	O3'	4902:C	P	5.75
1	52	1222:A	O3'	1223:G	P	5.52
1	23	16:C	O3'	18:G	P	5.52
1	52	3942:A	O3'	3943:A	P	5.07
1	52	1219:G	O3'	1220:G	P	4.89
1	A1	225:G	O3'	226:A	P	4.57
1	52	1221:G	O3'	1222:A	P	4.50
1	52	3947:A	O3'	3948:C	P	4.39
1	52	170:C	O3'	171:U	P	4.17
1	52	5020:G	O3'	5021:C	P	4.08

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	748:C	O3'	749:U	P	4.02
1	A1	322:C	O3'	323:C	P	3.93
1	A1	747:U	O3'	748:C	P	3.87
1	A1	286:U	O3'	287:U	P	3.86
1	A1	304:C	O3'	305:U	P	3.66
1	A1	903:A	O3'	904:A	P	3.65
1	52	1239:C	O3'	1244:G	P	3.53
1	52	1088:C	O3'	1089:G	P	3.45
1	A1	309:G	O3'	310:C	P	3.43
1	A1	902:G	O3'	903:A	P	3.29
1	52	1438:U	O3'	1440:U	P	3.24
1	52	751:G	O3'	752:G	P	3.23
1	A1	1295:A	O3'	1296:U	P	3.20
1	52	267:G	O3'	268:G	P	3.20
1	52	4076:G	O3'	4077:A	P	3.11
1	I3	203:ARG	C	204:GLY	N	1.96
1	s3	186:GLY	C	187:LEU	N	1.66