



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 10, 2017 – 07:25 PM EST

PDB ID : 5M1J
EMDB ID: : EMD-4140
Title : Nonstop ribosomal complex bound with Dom34 and Hbs1
Authors : Hilal, T.; Yamamoto, H.; Loerke, J.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on : 2016-10-07
Resolution : 3.30 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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

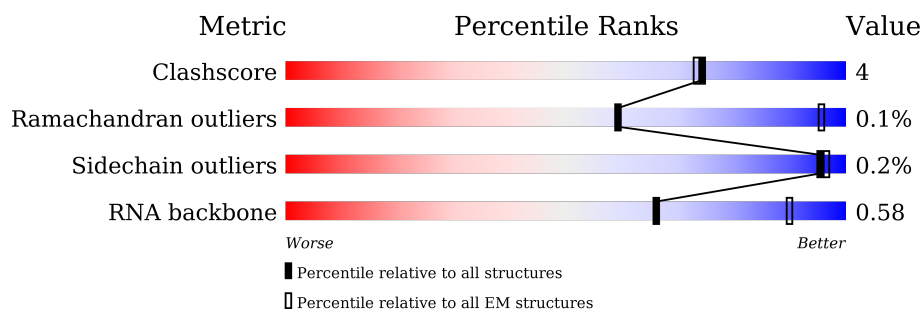
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A1	381	83% 17%
2	A2	207	86% 14%
3	a2	98	99% .
4	B2	214	89% 11%
5	b2	81	100%
6	C2	217	90% 10%
7	c2	63	98% .
8	D2	223	88% 12%


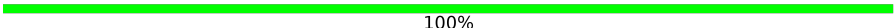



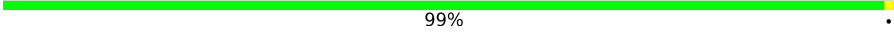



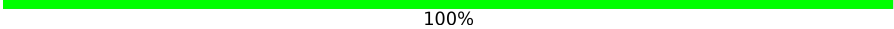




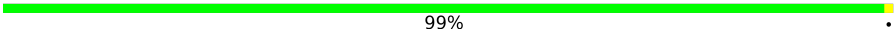

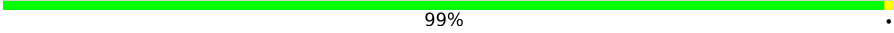

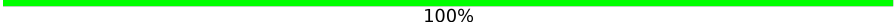

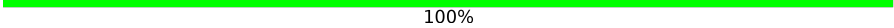


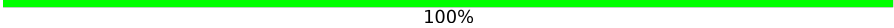
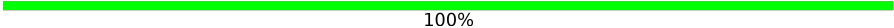
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Mol	Chain	Length	Quality of chain
9	d2	53	100%
10	E2	260	88% 12%
11	e2	60	100%
12	F2	206	83% 17%
13	G2	226	89% 11%
14	g2	318	100%
15	H2	184	82% 18%
16	I2	199	74% 21% 6%
17	J2	185	89% 10% .
18	K2	96	99% .
19	L2	155	90% 10%
20	M2	124	87% 13%
21	N2	150	90% 10%
22	O2	127	85% 15%
23	P2	124	80% 19% .
24	Q2	141	85% 15%
25	R2	125	86% 14%
26	S2	145	82% 17% .
27	T2	143	91% 9%
28	U2	107	86% 14%
29	V2	87	91% 9%
30	W2	129	83% 17%
31	X2	144	74% 26%
32	Y2	134	87% 13%
33	Z2	70	80% 20%

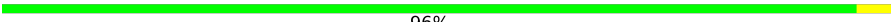









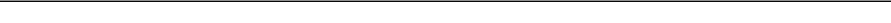

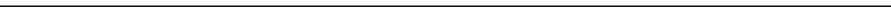


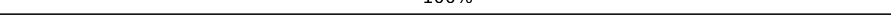





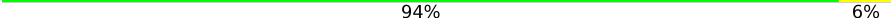


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Mol	Chain	Length	Quality of chain
34	22	1798	 67% 27% 5%
35	f2	71	 100%
36	14	3396	 72% 21% . .
37	34	121	 80% 18% .
38	44	158	 66% 29% .
39	a5	148	 99% .
40	A5	252	 85% 15%
41	b5	58	 100%
42	B5	386	 83% 17%
43	c5	97	 100%
44	C5	361	 86% 14%
45	D5	296	 92% 8%
46	d5	109	 100%
47	e5	127	 100%
48	f5	106	 99% .
49	F5	222	 90% 10%
50	g5	112	 99% .
51	G5	233	 88% 12%
52	h5	119	 100%
53	H5	191	 84% 16%
54	i5	99	 100%
55	I5	220	 87% 9% .
56	J5	169	 83% 17%
57	j5	87	 100%
58	k5	77	 100%

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Mol	Chain	Length	Quality of chain
59	l5	50	 96% .
60	L5	193	 93% 7%
61	m5	52	 100%
62	M5	136	 85% 15%
63	N5	203	 77% 23%
64	o5	105	 99% .
65	p5	91	 100%
66	P5	183	 83% 17%
67	Q5	185	 92% 8%
68	S5	172	 88% 12%
69	U5	100	 98% .
70	V5	136	 84% 16%
71	Z5	135	 90% 10%
72	K5	197	 91% 9%
73	n5	25	 100%
74	R5	188	 92% 8%
75	X5	121	 87% 13%
76	Y5	126	 90% 10%
77	T5	159	 90% 10%
78	E5	175	 76% 14% 10%
79	W5	98	 94% 6%
80	A6	611	 74% 14% 12%
81	X7	20	 20% 30% 10% 40%
82	A3	76	 54% 36% 9% .

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 212865 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein DOM34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	381	Total	C	N	O	S	0	0
			3058	1976	478	589	15		

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	207	Total	C	N	O	S	0	0
			1621	1039	286	294	2		

- Molecule 3 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a2	98	Total	C	N	O	S	0	0
			778	480	162	131	5		

- Molecule 4 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B2	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 5 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b2	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 6 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C2	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 7 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c2	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 8 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D2	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 9 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d2	53	Total	C	N	O	S	0	0
			443	275	92	72	4		

- Molecule 10 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E2	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 11 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e2	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 12 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F2	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 13 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G2	226	Total	C	N	O	S	0	0
			1820	1142	350	325	3		

- Molecule 14 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	g2	318	Total	C	N	O	S	0	0
			2445	1546	419	472	8		

- Molecule 15 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H2	184	Total	C	N	O	S	0	0
			1481	951	265	265			

- Molecule 16 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I2	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 17 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J2	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 18 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K2	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 19 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L2	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 20 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M2	124	Total	C	N	O	S	0	0
			934	587	165	180	2		

- Molecule 21 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N2	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 22 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O2	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 23 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P2	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 24 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q2	141	Total	C	N	O		0	0
			1105	708	203	194			

- Molecule 25 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R2	125	Total	C	N	O	S	0	0
			1000	625	188	185	2		

- Molecule 26 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S2	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 27 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T2	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 28 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U2	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 29 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V2	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 30 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W2	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 31 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X2	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 32 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y2	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 33 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z2	70	Total	C	N	O	0	0
			563	360	104	99		

- Molecule 34 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	22	1781	Total	C	N	O	P	0	0
			37948	16965	6715	12487	1781		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f2	71	Total	C	N	O	S	0	0
			497	309	93	91	4		

- Molecule 36 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	14	3295	Total	C	N	O	P	0	0
			70476	31477	12696	23008	3295		

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	34	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	44	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 39 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	a5	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 40 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A5	252	Total	C	N	O	S	0	0
			1918	1193	389	335	1		

- Molecule 41 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	b5	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 42 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B5	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 43 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	c5	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 44 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	C5	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 45 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	D5	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 46 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	d5	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 47 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	e5	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 48 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	f5	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 49 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	F5	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 50 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	g5	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 51 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	G5	233	Total	C	N	O	S	0	0
			1817	1159	326	329	3		

- Molecule 52 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	h5	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 53 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	H5	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 54 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	i5	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 55 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	I5	211	Total	C	N	O	S	0	0
			1717	1089	325	297	6		

- Molecule 56 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	J5	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 57 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	j5	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 58 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	k5	77	Total	C	N	O	S	0	0
			612	391	115	106			

- Molecule 59 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	l5	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 60 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	L5	193	Total	C	N	O	S	0	0
			1543	962	315	266			

- Molecule 61 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	m5	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 62 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	M5	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 63 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	N5	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 64 is a protein called 60S ribosomal protein L42-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	o5	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 65 is a protein called 60S ribosomal protein L43-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	p5	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 66 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	P5	183	Total	C	N	O	S	0	0
			1442	896	287	259			

- Molecule 67 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Q5	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 68 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	S5	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 69 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	U5	100	Total	C	N	O	S	0	0
			796	516	131	149			

- Molecule 70 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	V5	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 71 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Z5	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 72 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	K5	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 73 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	n5	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 74 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	R5	188	Total	C	N	O		0	0
			1521	935	326	260			

- Molecule 75 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	X5	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 76 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Y5	126	Total	C	N	O		0	0
			993	625	192	176			

- Molecule 77 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	T5	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 78 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	E5	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 79 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	W5	98	Total	C	N	O	S	0	0
			800	508	159	132	1		

- Molecule 80 is a protein called Protein HBS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	A6	539	Total	C	N	O	S	0	0
			4279	2712	723	827	17		

- Molecule 81 is a RNA chain called nonstop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	X7	12	Total	C	N	O	P	0	0
			259	116	49	82	12		

- Molecule 82 is a RNA chain called yeast Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	A3	76	Total	C	N	O	P	0	0
			1651	745	294	536	76		

- Molecule 83 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
83	m5	1	Total	Zn	0
			1	1	
83	j5	1	Total	Zn	0
			1	1	
83	f2	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
83	d2	1	Total 1	Zn 1	0
83	b2	1	Total 1	Zn 1	0
83	o5	1	Total 1	Zn 1	0
83	a2	1	Total 1	Zn 1	0
83	p5	1	Total 1	Zn 1	0

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	I2	2	Total 2	Mg 2	0
84	f5	1	Total 1	Mg 1	0
84	J5	2	Total 2	Mg 2	0
84	C5	8	Total 8	Mg 8	0
84	L2	1	Total 1	Mg 1	0
84	N5	7	Total 7	Mg 7	0
84	F2	2	Total 2	Mg 2	0
84	A6	2	Total 2	Mg 2	0
84	Y5	2	Total 2	Mg 2	0
84	d5	3	Total 3	Mg 3	0
84	o5	3	Total 3	Mg 3	0
84	J2	1	Total 1	Mg 1	0
84	E5	1	Total 1	Mg 1	0
84	I5	4	Total 4	Mg 4	0

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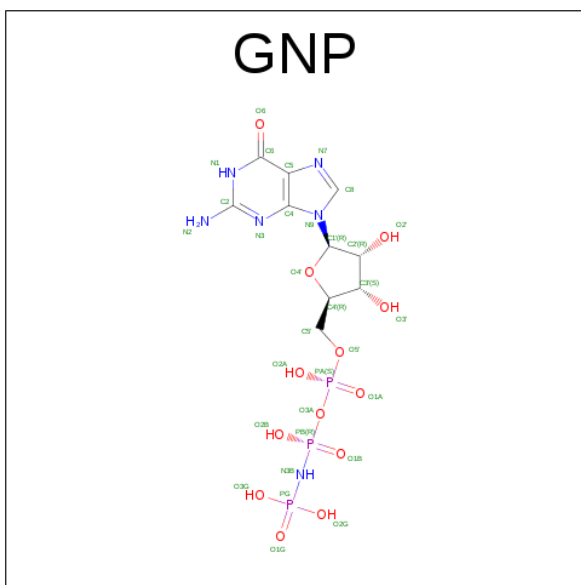
Mol	Chain	Residues	Atoms		AltConf
84	B5	5	Total 5	Mg 5	0
84	T5	1	Total 1	Mg 1	0
84	M5	1	Total 1	Mg 1	0
84	E2	2	Total 2	Mg 2	0
84	S2	4	Total 4	Mg 4	0
84	D5	1	Total 1	Mg 1	0
84	d2	1	Total 1	Mg 1	0
84	B2	1	Total 1	Mg 1	0
84	N2	2	Total 2	Mg 2	0
84	34	16	Total 16	Mg 16	0
84	A5	6	Total 6	Mg 6	0
84	S5	4	Total 4	Mg 4	0
84	L5	4	Total 4	Mg 4	0
84	T2	1	Total 1	Mg 1	0
84	b5	1	Total 1	Mg 1	0
84	22	177	Total 177	Mg 177	0
84	m5	3	Total 3	Mg 3	0
84	Q2	1	Total 1	Mg 1	0
84	R5	3	Total 3	Mg 3	0
84	K5	5	Total 5	Mg 5	0
84	V5	3	Total 3	Mg 3	0

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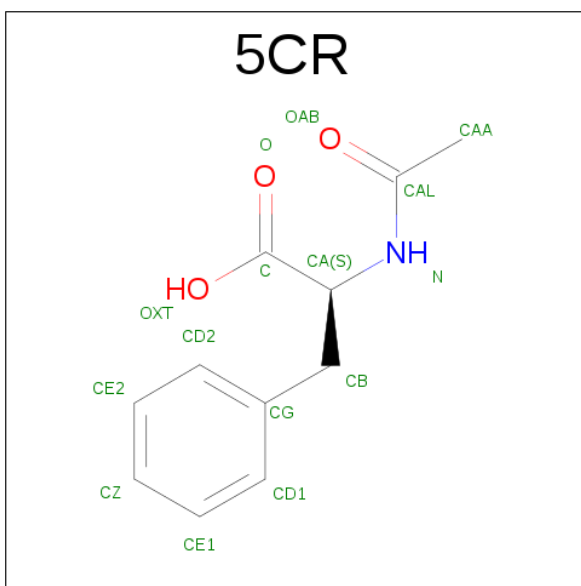
Mol	Chain	Residues	Atoms		AltConf
84	U2	1	Total 1	Mg 1	0
84	a5	3	Total 3	Mg 3	0
84	F5	4	Total 4	Mg 4	0
84	l5	1	Total 1	Mg 1	0
84	X2	3	Total 3	Mg 3	0
84	14	701	Total 701	Mg 701	0
84	44	34	Total 34	Mg 34	0
84	Q5	4	Total 4	Mg 4	0
84	j5	7	Total 7	Mg 7	0
84	Y2	1	Total 1	Mg 1	0
84	C2	2	Total 2	Mg 2	0
84	e5	3	Total 3	Mg 3	0
84	A3	6	Total 6	Mg 6	0
84	P5	7	Total 7	Mg 7	0

- Molecule 85 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
85	A6	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 86 is N-acetyl-L-phenylalanine (three-letter code: 5CR) (formula: $C_{11}H_{13}NO_3$).



Mol	Chain	Residues	Atoms				AltConf
86	A3	1	Total	C	N	O	0
			14	11	1	2	

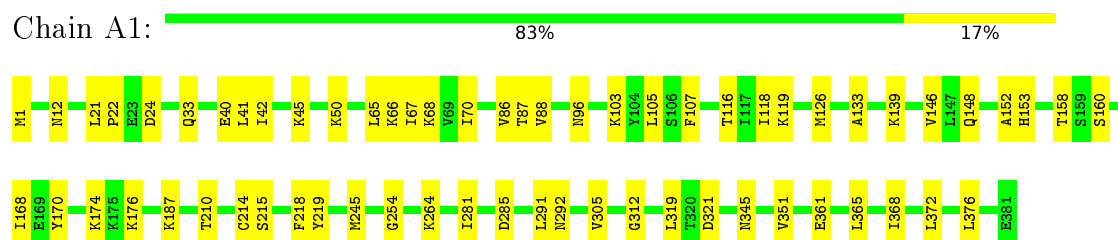
- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
87	A1	7	Total 7	O 7	0
87	A6	6	Total 6	O 6	0

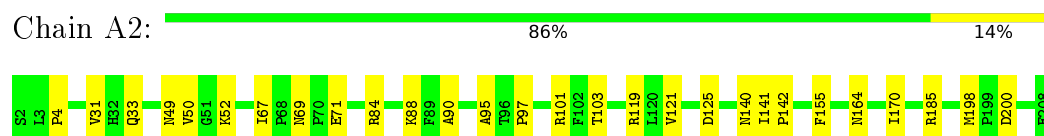
3 Residue-property plots [i](#)

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

- Molecule 1: Protein DOM34



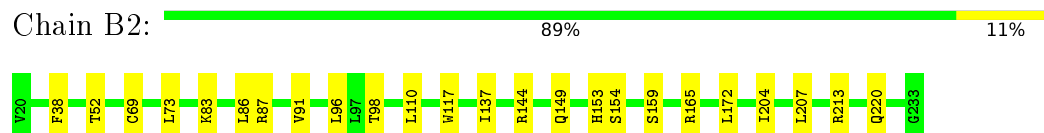
- Molecule 2: 40S ribosomal protein S0-A



- Molecule 3: 40S ribosomal protein S26-B



- Molecule 4: 40S ribosomal protein S1-A



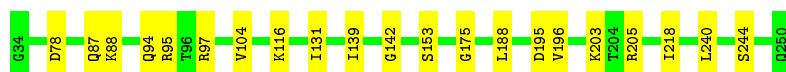
- Molecule 5: 40S ribosomal protein S27-A



There are no outlier residues recorded for this chain.

- Molecule 6: 40S ribosomal protein S2





- Molecule 7: 40S ribosomal protein S28-B

Chain c2: 98%



- Molecule 8: 40S ribosomal protein S3

Chain D2: 88%



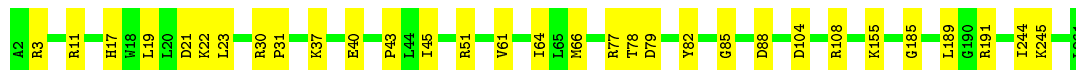
- Molecule 9: 40S ribosomal protein S29-A

Chain d2: 100%

There are no outlier residues recorded for this chain.

- Molecule 10: 40S ribosomal protein S4-A

Chain E2: 88%



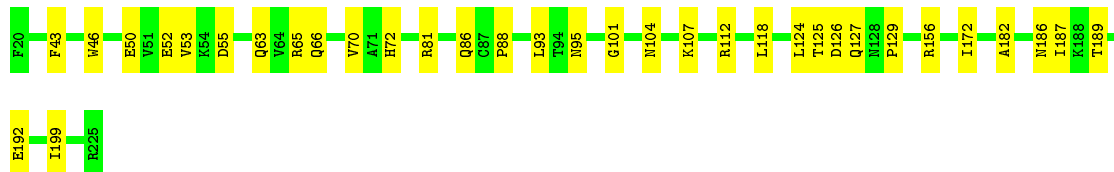
- Molecule 11: 40S ribosomal protein S30-A

Chain e2: 100%

There are no outlier residues recorded for this chain.

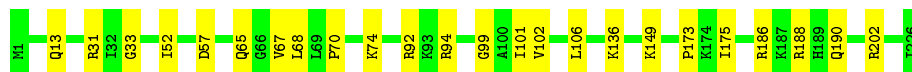
- Molecule 12: 40S ribosomal protein S5

Chain F2: 83%



- Molecule 13: 40S ribosomal protein S6-A

Chain G2: 89%




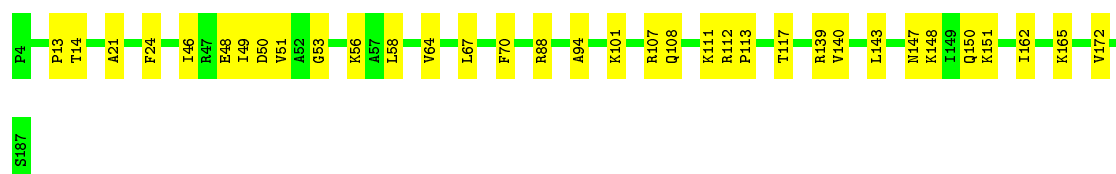
- Molecule 14: Guanine nucleotide-binding protein subunit beta-like protein

Chain g2:  100%

There are no outlier residues recorded for this chain.

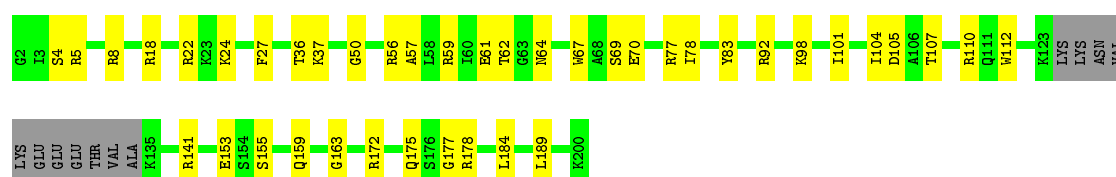
- Molecule 15: 40S ribosomal protein S7-A

Chain H2:  82%



- Molecule 16: 40S ribosomal protein S8-A

Chain I2:  74%



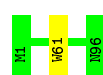
- Molecule 17: 40S ribosomal protein S9-A

Chain J2:  89%



- Molecule 18: 40S ribosomal protein S10-A

Chain K2:  99%



- Molecule 19: 40S ribosomal protein S11-A

Chain L2:  90%



- Molecule 20: 40S ribosomal protein S12

Chain M2:  87%



- Molecule 21: 40S ribosomal protein S13

Chain N2: 90% 10%



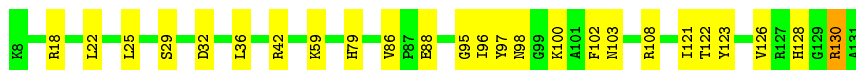
- Molecule 22: 40S ribosomal protein S14-A

Chain O2: 85% 15%



- Molecule 23: 40S ribosomal protein S15

Chain P2: 80% 19%



- Molecule 24: 40S ribosomal protein S16-A

Chain Q2: 85% 15%



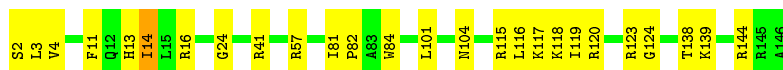
- Molecule 25: 40S ribosomal protein S17-B

Chain R2: 86% 14%



- Molecule 26: 40S ribosomal protein S18-A

Chain S2: 82% 17%

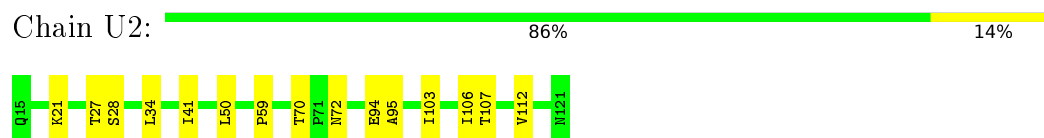


- Molecule 27: 40S ribosomal protein S19-A

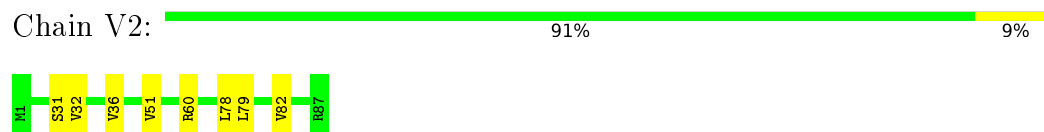
Chain T2: 91% 9%



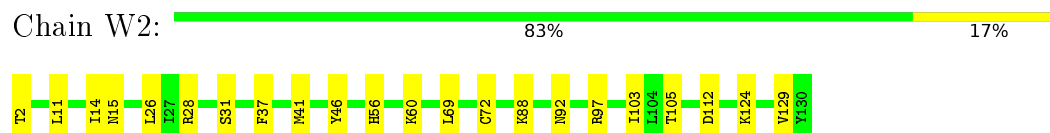
- Molecule 28: 40S ribosomal protein S20



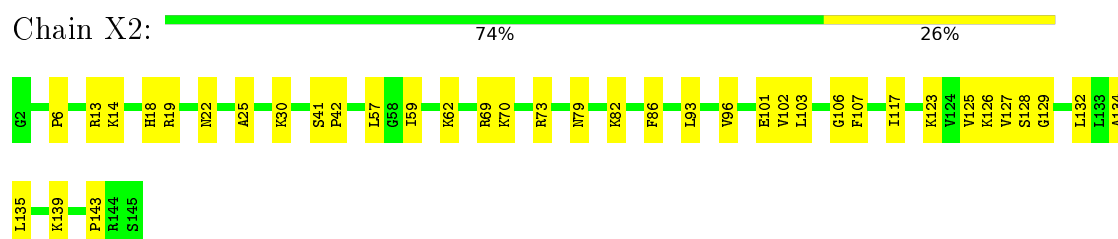
- Molecule 29: 40S ribosomal protein S21-A



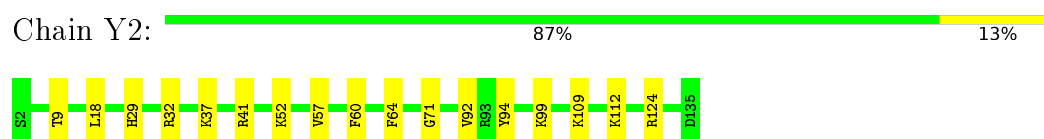
- Molecule 30: 40S ribosomal protein S22-A



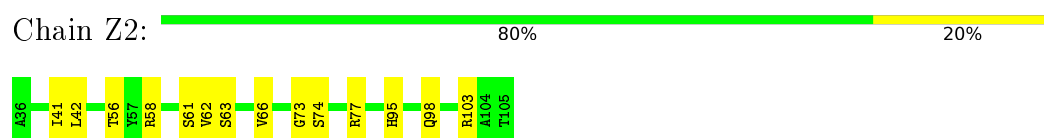
- Molecule 31: 40S ribosomal protein S23-A



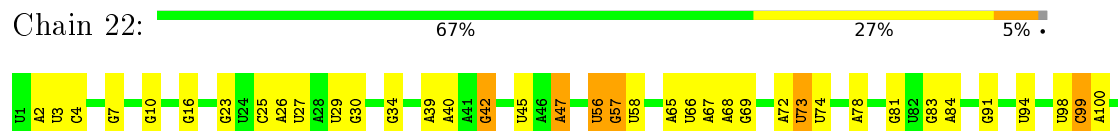
- Molecule 32: 40S ribosomal protein S24-A



- Molecule 33: 40S ribosomal protein S25-A

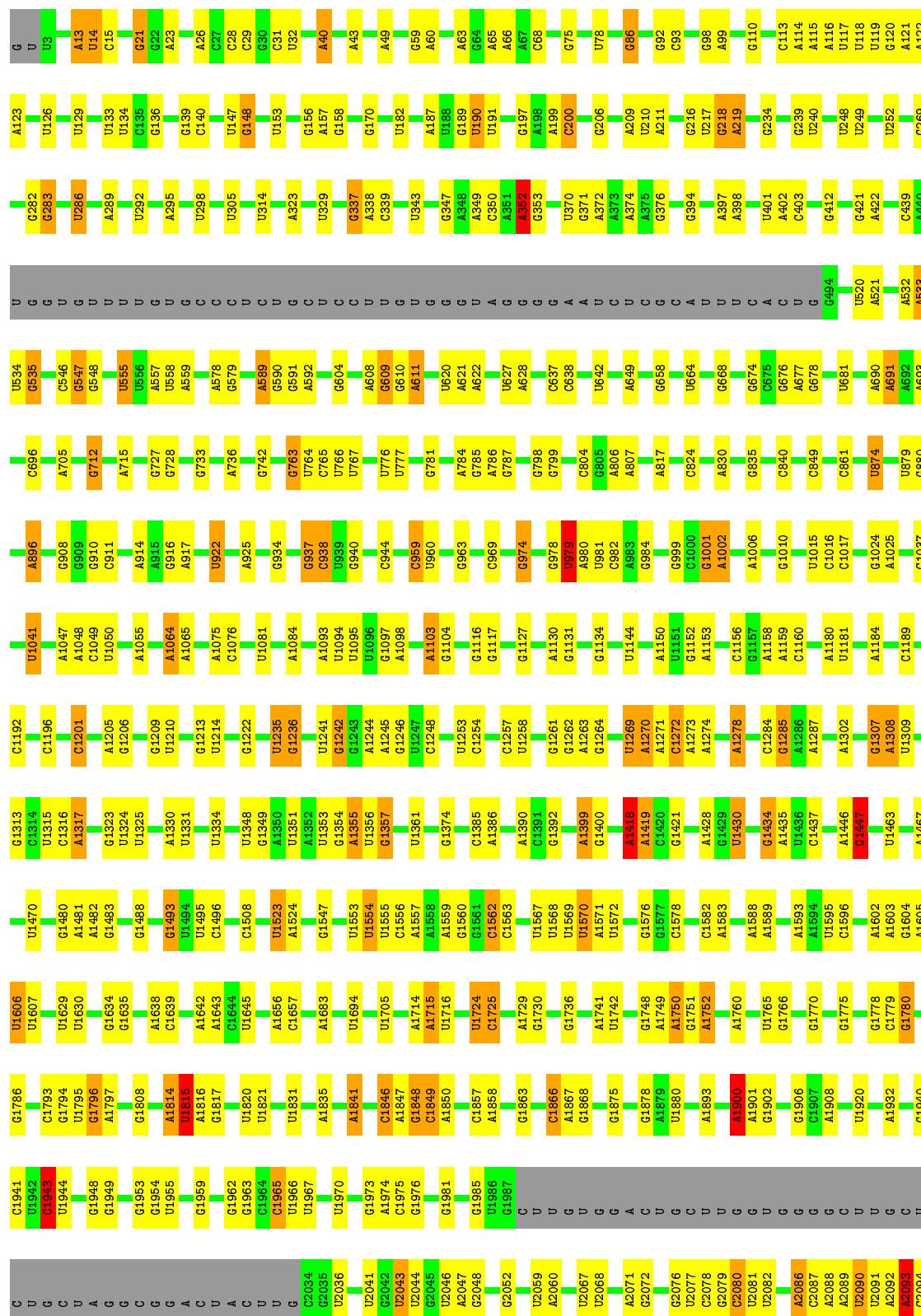


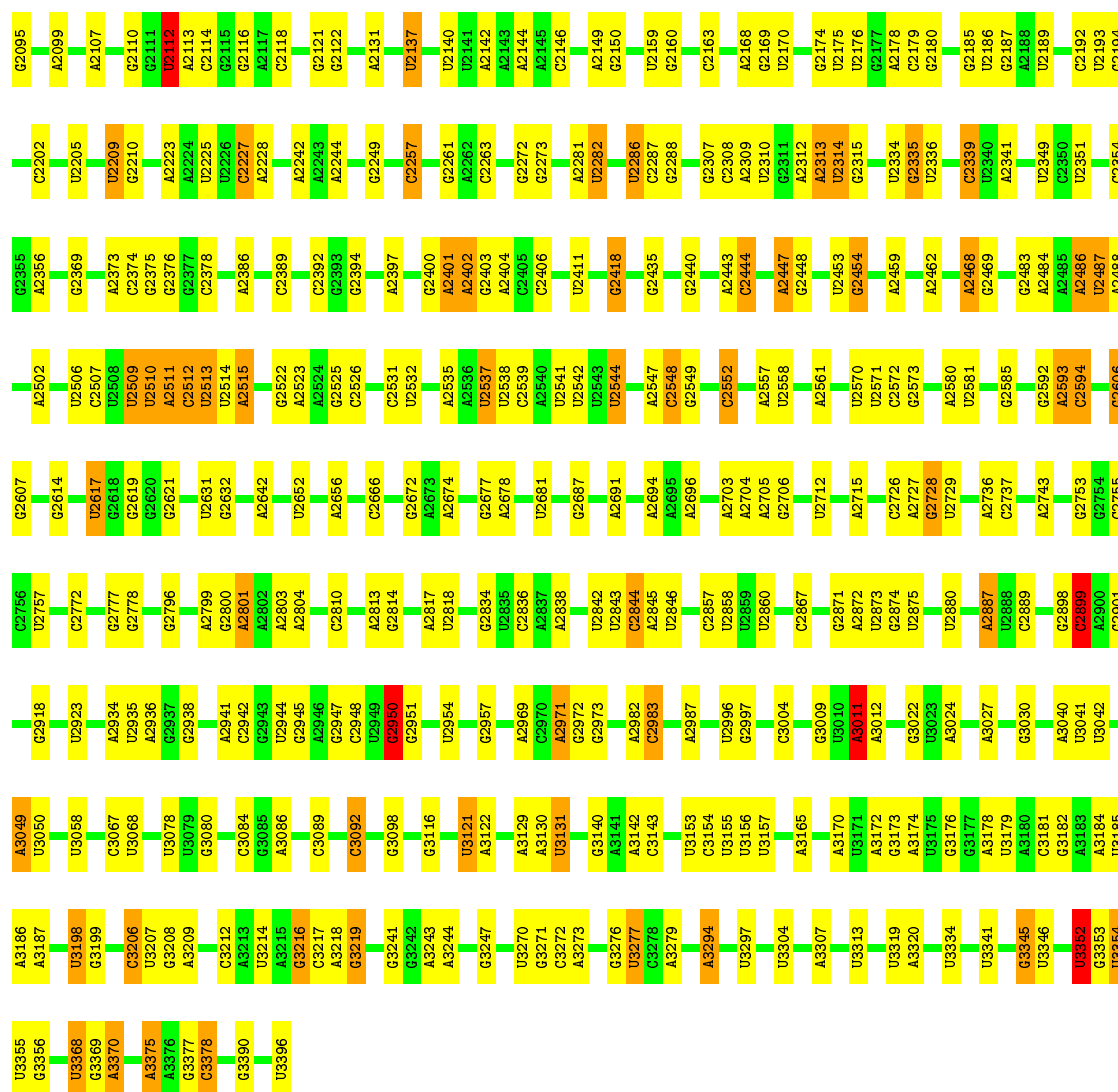
- Molecule 34: 18S ribosomal RNA





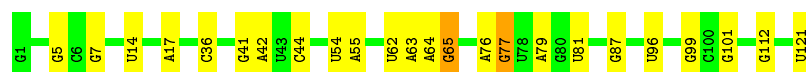
Chain 14:  72% 21% . .





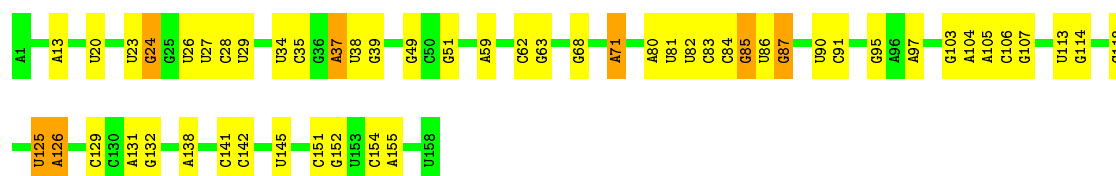
- Molecule 37: 5S ribosomal RNA

Chain 34: 80% 18% .



- Molecule 38: 5.8S ribosomal RNA

Chain 44: 66% 29% .




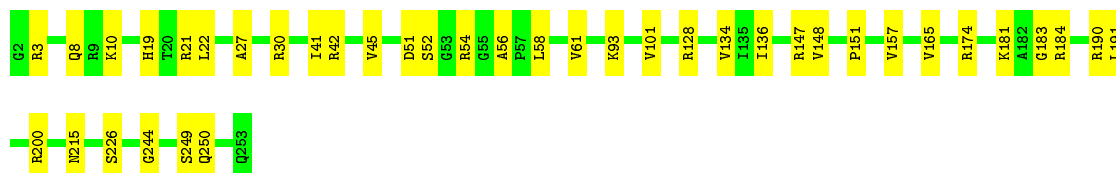
- Molecule 39: 60S ribosomal protein L28

Chain a5:  99%



- Molecule 40: 60S ribosomal protein L2-A

Chain A5:  85% 15%




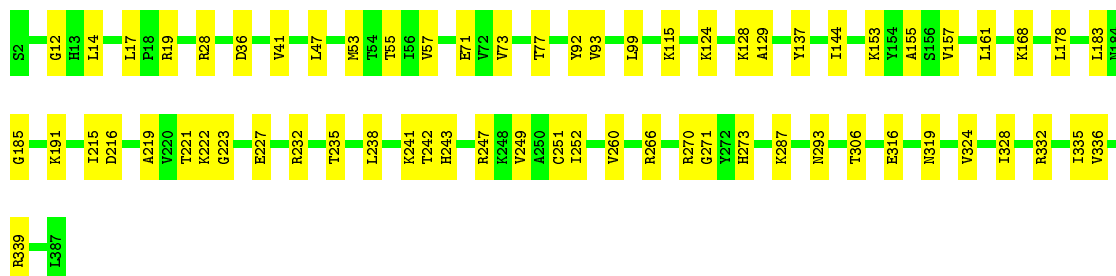
- Molecule 41: 60S ribosomal protein L29

Chain b5:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 60S ribosomal protein L3

Chain B5:  83% 17%




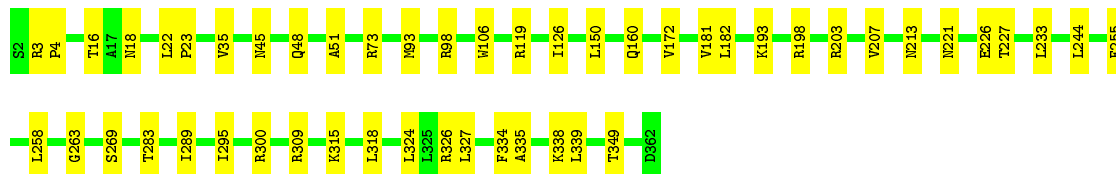
- Molecule 43: 60S ribosomal protein L30

Chain c5:  100%

There are no outlier residues recorded for this chain.

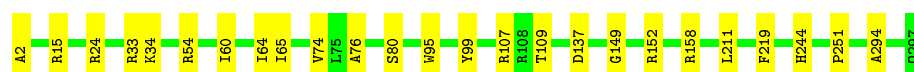
- Molecule 44: 60S ribosomal protein L4-A

Chain C5:  86% 14%



- Molecule 45: 60S ribosomal protein L5

Chain D5:  92% 8%



- Molecule 46: 60S ribosomal protein L31-A

Chain d5:  100%

There are no outlier residues recorded for this chain.

- Molecule 47: 60S ribosomal protein L32

Chain e5:  100%

There are no outlier residues recorded for this chain.

- Molecule 48: 60S ribosomal protein L33-A

Chain f5:  99%



- Molecule 49: 60S ribosomal protein L7-A

Chain F5:  90% 10%



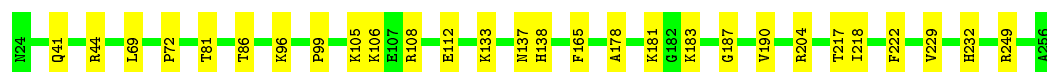
- Molecule 50: 60S ribosomal protein L34-A

Chain g5:  99%



- Molecule 51: 60S ribosomal protein L8-A

Chain G5:  88% 12%

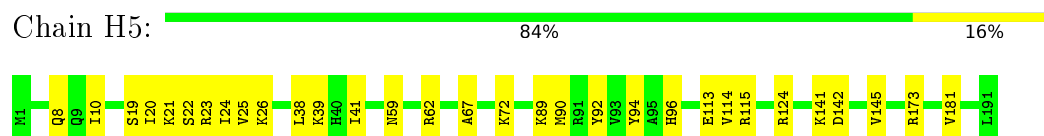


- Molecule 52: 60S ribosomal protein L35-A

Chain h5:  100%

There are no outlier residues recorded for this chain.

- Molecule 53: 60S ribosomal protein L9-A

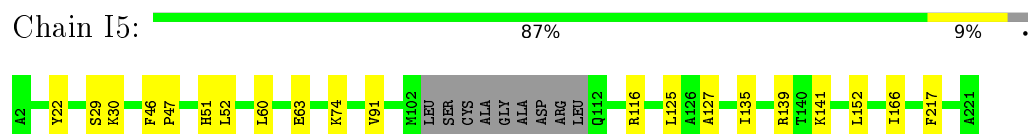


- Molecule 54: 60S ribosomal protein L36-A

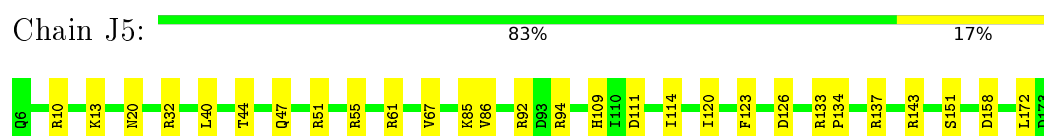


There are no outlier residues recorded for this chain.

- Molecule 55: 60S ribosomal protein L10



- Molecule 56: 60S ribosomal protein L11-A



- Molecule 57: 60S ribosomal protein L37-A



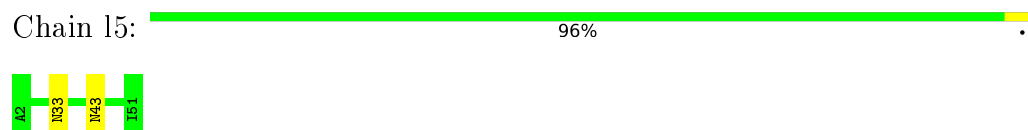
There are no outlier residues recorded for this chain.

- Molecule 58: 60S ribosomal protein L38

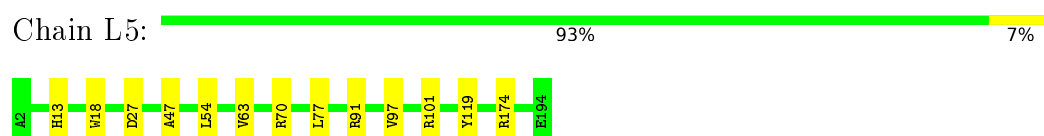


There are no outlier residues recorded for this chain.

- Molecule 59: 60S ribosomal protein L39



- Molecule 60: 60S ribosomal protein L13-A




- Molecule 61: Ubiquitin-60S ribosomal protein L40

Chain m5:  100%


There are no outlier residues recorded for this chain.

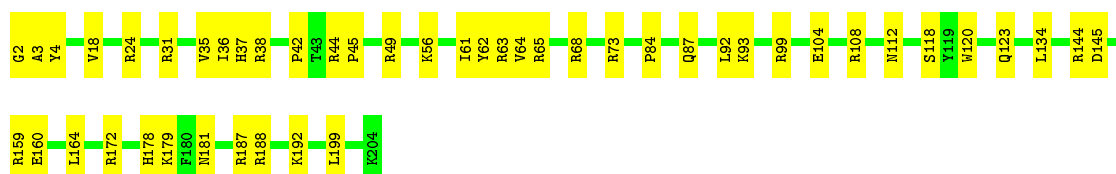
- Molecule 62: 60S ribosomal protein L14-A

Chain M5:  85% 15%



- Molecule 63: 60S ribosomal protein L15-A

Chain N5:  77% 23%



- Molecule 64: 60S ribosomal protein L42-B

Chain o5:  99%




- Molecule 65: 60S ribosomal protein L43-B

Chain p5:  100%

There are no outlier residues recorded for this chain.

- Molecule 66: 60S ribosomal protein L17-A

Chain P5:  83% 17%



- Molecule 67: 60S ribosomal protein L18-A

Chain Q5:  92% 8%



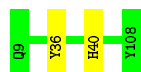
- Molecule 68: 60S ribosomal protein L20-A

Chain S5:  88% 12%



- Molecule 69: 60S ribosomal protein L22-A

Chain U5: 98%



- Molecule 70: 60S ribosomal protein L23-A

Chain V5: 84% 16%



- Molecule 71: 60S ribosomal protein L27-A

Chain Z5: 90% 10%



- Molecule 72: 60S ribosomal protein L16-A

Chain K5: 91% 9%



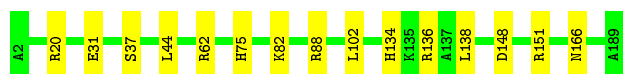
- Molecule 73: 60S ribosomal protein L41-B

Chain n5: 100%

There are no outlier residues recorded for this chain.

- Molecule 74: 60S ribosomal protein L19-A

Chain R5: 92% 8%



- Molecule 75: 60S ribosomal protein L25

Chain X5: 87% 13%



- Molecule 76: 60S ribosomal protein L26-A

Chain Y5:  90% 10%




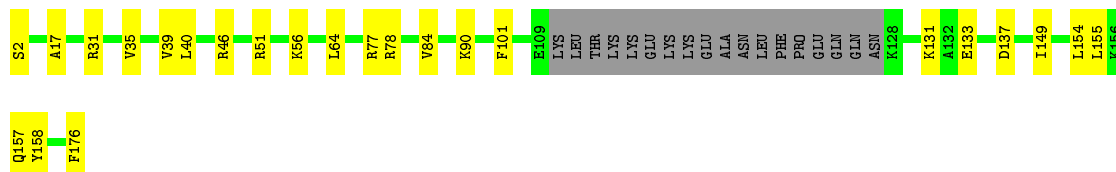
- Molecule 77: 60S ribosomal protein L21-A

Chain T5:  90% 10%



- Molecule 78: 60S ribosomal protein L6-A

Chain E5:  76% 14% 10%



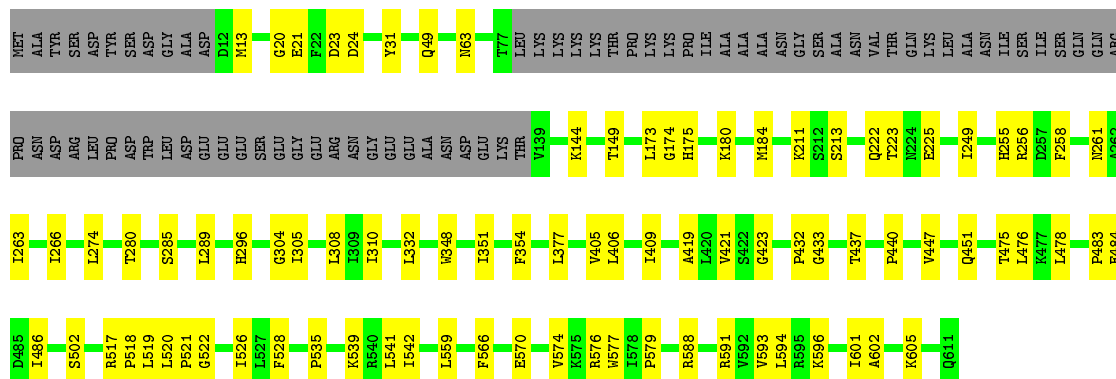
- Molecule 79: 60S ribosomal protein L24-A

Chain W5:  94% 6%



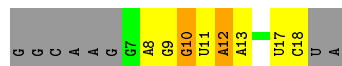
- Molecule 80: Protein HBS1

Chain A6:  74% 14% 12%

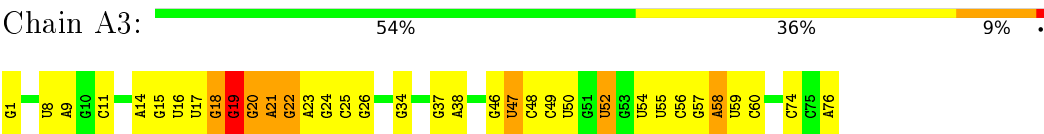


- Molecule 81: nonstop mRNA

Chain X7:  20% 30% 10% 40%



● Molecule 82: yeast Phe-tRNA-Phe



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	73391	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	80645	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MU, ZN, OMG, 5CR, H2U, MG, GNP, YYG, 2MG, 5MC, 1MA, M2G, 7MG, PSU

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	0.25	0/3110	0.51	0/4179
10	E2	0.26	0/2109	0.53	0/2839
11	e2	0.24	0/483	0.47	0/643
12	F2	0.24	0/1629	0.50	0/2202
13	G2	0.25	0/1844	0.51	0/2464
14	g2	0.25	0/2498	0.50	0/3398
15	H2	0.27	0/1506	0.52	0/2028
16	I2	0.26	0/1514	0.52	0/2021
17	J2	0.26	0/1519	0.51	1/2035 (0.0%)
18	K2	0.25	0/837	0.51	0/1131
19	L2	0.27	0/1272	0.50	0/1712
2	A2	0.26	0/1662	0.51	0/2273
20	M2	0.26	0/942	0.65	0/1274
21	N2	0.25	0/1215	0.50	0/1638
22	O2	0.26	0/952	0.54	0/1279
23	P2	0.31	0/1012	0.53	0/1356
24	Q2	0.25	0/1125	0.52	0/1510
25	R2	0.24	0/1010	0.53	0/1355
26	S2	0.26	0/1211	0.55	0/1628
27	T2	0.25	0/1130	0.50	0/1517
28	U2	0.25	0/865	0.49	0/1169
29	V2	0.25	0/693	0.54	0/935
3	a2	0.24	0/791	0.51	0/1059
30	W2	0.25	0/1038	0.53	0/1395
31	X2	0.26	0/1139	0.53	0/1518
32	Y2	0.25	0/1087	0.46	0/1449
33	Z2	0.24	0/571	0.51	0/768
34	22	0.21	0/42444	0.85	83/66138 (0.1%)
35	f2	0.25	0/504	0.51	0/682
36	14	0.21	0/78885	0.82	76/122992 (0.1%)
37	34	0.18	0/2883	0.79	0/4491
38	44	0.19	0/3746	0.82	1/5832 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	a5	0.24	0/1204	0.50	0/1612
4	B2	0.26	0/1735	0.55	0/2335
40	A5	0.26	0/1952	0.52	0/2622
41	b5	0.25	0/473	0.44	0/629
42	B5	0.25	0/3152	0.49	0/4239
43	c5	0.25	0/751	0.46	0/1008
44	C5	0.26	0/2801	0.53	0/3792
45	D5	0.25	0/2425	0.50	1/3271 (0.0%)
46	d5	0.26	0/904	0.48	0/1213
47	e5	0.24	0/1041	0.47	0/1394
48	f5	0.26	0/868	0.46	0/1168
49	F5	0.26	0/1821	0.49	0/2451
5	b2	0.25	0/620	0.53	0/838
50	g5	0.25	0/891	0.50	0/1191
51	G5	0.26	0/1849	0.52	0/2495
52	h5	0.24	0/978	0.49	0/1301
53	H5	0.26	0/1539	0.51	1/2073 (0.0%)
54	i5	0.25	0/778	0.50	0/1034
55	I5	0.25	0/1753	0.47	0/2350
56	J5	0.25	0/1374	0.55	1/1842 (0.1%)
57	j5	0.26	0/696	0.50	0/923
58	k5	0.25	0/618	0.51	0/826
59	l5	0.24	0/443	0.49	0/588
6	C2	0.26	0/1665	0.50	0/2263
60	L5	0.26	0/1568	0.52	0/2106
61	m5	0.25	0/423	0.50	0/562
62	M5	0.24	0/1068	0.48	0/1438
63	N5	0.24	0/1757	0.46	0/2354
64	o5	0.25	0/860	0.49	0/1136
65	p5	0.24	0/701	0.47	0/934
66	P5	0.26	0/1465	0.52	0/1968
67	Q5	0.25	0/1465	0.50	0/1965
68	S5	0.26	0/1481	0.47	0/1990
69	U5	0.28	0/812	0.51	0/1099
7	c2	0.25	0/499	0.44	0/670
70	V5	0.26	0/1018	0.48	0/1369
71	Z5	0.26	0/1118	0.48	0/1497
72	K5	0.26	0/1585	0.45	0/2128
73	n5	0.20	0/234	0.45	0/300
74	R5	0.23	0/1538	0.46	0/2050
75	X5	0.26	0/983	0.50	0/1325
76	Y5	0.24	0/1004	0.51	1/1341 (0.1%)
77	T5	0.25	0/1300	0.47	0/1743

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	E5	0.26	0/1269	0.46	0/1705
79	W5	0.28	0/814	0.54	0/1081
8	D2	0.27	0/1759	0.51	1/2368 (0.0%)
80	A6	0.26	0/4364	0.51	0/5898
81	X7	0.66	0/290	1.00	0/450
82	A3	0.85	1/1487 (0.1%)	1.13	7/2315 (0.3%)
9	d2	0.27	0/453	0.50	0/602
All	All	0.24	1/226872 (0.0%)	0.73	173/332762 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	F2	0	1
17	J2	0	2
20	M2	0	1
26	S2	0	1
31	X2	0	1
49	F5	0	1
60	L5	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	A3	1	G	OP3-P	-11.07	1.47	1.61

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	22	1389	C	N1-C2-O2	15.99	128.50	118.90
34	22	1389	C	N3-C2-O2	-13.77	112.26	121.90
34	22	1389	C	C2-N1-C1'	12.13	132.14	118.80
34	22	1389	C	C6-N1-C2	-9.87	116.35	120.30
36	14	922	U	C2-N1-C1'	9.16	128.69	117.70
36	14	922	U	N1-C2-O2	8.15	128.51	122.80
34	22	965	U	C2-N1-C1'	8.03	127.33	117.70
34	22	767	U	N1-C2-O2	7.97	128.38	122.80
34	22	1389	C	C6-N1-C1'	-7.81	111.43	120.80
34	22	767	U	C2-N1-C1'	7.79	127.05	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	22	767	U	N3-C2-O2	-7.65	116.85	122.20
34	22	965	U	N1-C2-O2	7.44	128.01	122.80
82	A3	19	G	P-O3'-C3'	7.41	128.59	119.70
34	22	1560	U	C2-N1-C1'	7.28	126.43	117.70
82	A3	19	G	C4-N9-C1'	-7.28	117.04	126.50
36	14	922	U	N3-C2-O2	-7.26	117.12	122.20
36	14	3277	U	C2-N1-C1'	7.26	126.41	117.70
34	22	1560	U	N3-C2-O2	-7.23	117.14	122.20
34	22	1560	U	N1-C2-O2	7.21	127.85	122.80
36	14	979	U	P-O3'-C3'	7.13	128.25	119.70
76	Y5	126	LEU	CA-CB-CG	7.13	131.70	115.30
34	22	1246	C	N1-C2-O2	7.12	123.17	118.90
36	14	1715	A	P-O3'-C3'	7.11	128.23	119.70
36	14	2468	A	P-O3'-C3'	7.05	128.16	119.70
34	22	578	U	P-O3'-C3'	7.02	128.12	119.70
34	22	686	C	P-O3'-C3'	7.00	128.11	119.70
34	22	965	U	N3-C2-O2	-6.99	117.31	122.20
36	14	1815	U	P-O3'-C3'	6.98	128.08	119.70
34	22	1761	U	P-O3'-C3'	6.95	128.04	119.70
36	14	2112	U	OP2-P-O3'	6.95	120.49	105.20
36	14	3277	U	N1-C2-O2	6.95	127.66	122.80
34	22	1246	C	C2-N1-C1'	6.90	126.39	118.80
36	14	2447	A	P-O3'-C3'	6.89	127.97	119.70
34	22	139	C	P-O3'-C3'	6.87	127.94	119.70
34	22	497	G	P-O3'-C3'	6.87	127.94	119.70
36	14	2093	A	P-O3'-C3'	6.81	127.87	119.70
34	22	610	G	C4-N9-C1'	6.79	135.32	126.50
34	22	934	C	C2-N1-C1'	6.77	126.25	118.80
82	A3	19	G	C8-N9-C1'	6.76	135.78	127.00
36	14	2112	U	P-O3'-C3'	6.73	127.77	119.70
34	22	1473	U	N1-C2-O2	6.71	127.50	122.80
34	22	1257	U	C2-N1-C1'	6.63	125.66	117.70
34	22	812	A	P-O3'-C3'	6.55	127.56	119.70
34	22	73	U	P-O3'-C3'	6.54	127.55	119.70
34	22	1573	A	OP2-P-O3'	6.47	119.44	105.20
36	14	2487	U	P-O3'-C3'	6.46	127.46	119.70
34	22	1573	A	P-O3'-C3'	6.46	127.45	119.70
34	22	720	G	P-O3'-C3'	6.45	127.44	119.70
34	22	1458	G	C4-N9-C1'	6.44	134.87	126.50
36	14	3277	U	N3-C2-O2	-6.44	117.69	122.20
36	14	2257	C	N1-C2-O2	6.39	122.73	118.90
34	22	657	U	P-O3'-C3'	6.35	127.32	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	22	315	A	P-O3'-C3'	6.35	127.32	119.70
36	14	547	G	P-O3'-C3'	6.35	127.32	119.70
36	14	2537	U	P-O3'-C3'	6.34	127.31	119.70
36	14	2950	G	P-O3'-C3'	6.34	127.31	119.70
36	14	3058	U	C2-N1-C1'	6.33	125.30	117.70
34	22	934	C	N1-C2-O2	6.32	122.69	118.90
36	14	1103	A	P-O3'-C3'	6.30	127.26	119.70
36	14	2086	A	P-O3'-C3'	6.29	127.25	119.70
34	22	1000	C	C2-N1-C1'	6.29	125.72	118.80
34	22	622	A	P-O3'-C3'	6.27	127.22	119.70
34	22	1456	C	C2-N1-C1'	6.27	125.69	118.80
36	14	2257	C	C2-N1-C1'	6.21	125.64	118.80
36	14	2513	U	P-O3'-C3'	6.21	127.16	119.70
36	14	2090	U	P-O3'-C3'	6.21	127.15	119.70
34	22	1491	U	P-O3'-C3'	6.18	127.11	119.70
36	14	1064	A	P-O3'-C3'	6.13	127.06	119.70
36	14	3352	U	N1-C2-O2	6.13	127.09	122.80
34	22	99	C	P-O3'-C3'	6.12	127.04	119.70
36	14	2286	U	P-O3'-C3'	6.12	127.04	119.70
34	22	1473	U	N3-C2-O2	-6.11	117.93	122.20
36	14	1900	A	P-O3'-C3'	6.09	127.01	119.70
34	22	1473	U	C2-N1-C1'	6.05	124.96	117.70
36	14	3011	A	P-O3'-C3'	6.00	126.90	119.70
36	14	283	G	N3-C4-N9	5.98	129.59	126.00
34	22	1389	C	C5-C6-N1	5.97	123.99	121.00
36	14	922	U	C6-N1-C1'	-5.97	112.83	121.20
34	22	782	U	P-O3'-C3'	5.94	126.83	119.70
34	22	1596	C	C2-N1-C1'	5.93	125.32	118.80
36	14	2447	A	OP1-P-O3'	5.88	118.13	105.20
36	14	2899	C	C2-N1-C1'	5.85	125.23	118.80
36	14	2726	C	C2-N1-C1'	5.84	125.23	118.80
34	22	1113	A	P-O3'-C3'	5.84	126.71	119.70
36	14	2836	C	C2-N1-C1'	5.82	125.20	118.80
34	22	1137	A	P-O3'-C3'	5.81	126.68	119.70
82	A3	52	U	N3-C2-O2	-5.81	118.14	122.20
34	22	657	U	OP1-P-O3'	5.81	117.97	105.20
34	22	1489	U	C2-N1-C1'	5.80	124.67	117.70
36	14	2209	U	P-O3'-C3'	5.80	126.66	119.70
34	22	1246	C	N3-C2-O2	-5.79	117.85	121.90
34	22	721	U	P-O3'-C3'	5.78	126.63	119.70
36	14	1317	A	O4'-C1'-N9	5.75	112.80	108.20
34	22	610	G	C8-N9-C1'	-5.74	119.54	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	14	1795	U	N1-C1'-C2'	5.74	121.46	114.00
36	14	2971	A	P-O3'-C3'	5.74	126.58	119.70
34	22	581	U	C2-N1-C1'	5.69	124.53	117.70
53	H5	38	LEU	CA-CB-CG	5.69	128.38	115.30
36	14	2593	A	P-O3'-C3'	5.69	126.52	119.70
34	22	1082	C	C2-N1-C1'	5.68	125.04	118.80
36	14	922	U	C5-C6-N1	5.67	125.53	122.70
34	22	1456	C	N1-C2-O2	5.67	122.30	118.90
36	14	2983	C	C2-N1-C1'	5.66	125.03	118.80
36	14	283	G	C4-N9-C1'	5.66	133.85	126.50
36	14	2509	U	O4'-C1'-N1	5.62	112.70	108.20
34	22	1752	U	C2-N1-C1'	5.61	124.43	117.70
34	22	610	G	N3-C4-N9	5.60	129.36	126.00
34	22	1257	U	N3-C2-O2	-5.59	118.28	122.20
34	22	543	C	C2-N1-C1'	5.57	124.93	118.80
36	14	283	G	N3-C4-C5	-5.57	125.81	128.60
36	14	2552	C	C2-N1-C1'	5.56	124.91	118.80
34	22	1458	G	C8-N9-C1'	-5.53	119.81	127.00
36	14	352	A	P-O3'-C3'	5.53	126.33	119.70
36	14	2509	U	C2'-C3'-O3'	5.53	122.55	113.70
36	14	2227	C	P-O3'-C3'	5.52	126.32	119.70
34	22	959	U	N1-C2-O2	5.50	126.65	122.80
34	22	959	U	C2-N1-C1'	5.50	124.30	117.70
36	14	1278	A	O4'-C1'-N9	5.49	112.59	108.20
36	14	2552	C	N1-C2-O2	5.49	122.19	118.90
34	22	131	C	P-O3'-C3'	5.49	126.28	119.70
36	14	3058	U	N1-C2-O2	5.49	126.64	122.80
34	22	1696	G	P-O3'-C3'	5.47	126.27	119.70
36	14	2043	U	P-O3'-C3'	5.47	126.27	119.70
34	22	1458	G	N3-C4-N9	5.46	129.28	126.00
36	14	1562	C	P-O3'-C3'	5.45	126.25	119.70
34	22	959	U	N3-C2-O2	-5.42	118.41	122.20
34	22	507	U	C2-N1-C1'	5.39	124.17	117.70
34	22	1344	A	P-O3'-C3'	5.39	126.17	119.70
36	14	1103	A	OP2-P-O3'	5.39	117.05	105.20
36	14	2846	U	C2-N1-C1'	5.38	124.16	117.70
34	22	216	U	P-O3'-C3'	5.37	126.15	119.70
36	14	3214	U	C2-N1-C1'	5.37	124.14	117.70
36	14	1418	A	P-O3'-C3'	5.37	126.14	119.70
34	22	1000	C	N1-C2-O2	5.36	122.12	118.90
34	22	610	G	N3-C4-C5	-5.36	125.92	128.60
36	14	2899	C	N1-C2-O2	5.34	122.11	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	14	3352	U	N3-C2-O2	-5.33	118.47	122.20
38	44	125	U	C2-N1-C1'	5.33	124.09	117.70
45	D5	137	ASP	CB-CG-OD1	5.33	123.09	118.30
34	22	1458	G	N3-C4-C5	-5.32	125.94	128.60
34	22	830	U	C2-N1-C1'	5.31	124.07	117.70
36	14	1570	U	P-O3'-C3'	5.31	126.07	119.70
82	A3	19	G	N1-C6-O6	-5.30	116.72	119.90
34	22	1113	A	OP1-P-O3'	5.29	116.84	105.20
36	14	1965	C	P-O3'-C3'	5.29	126.05	119.70
36	14	2617	U	C2-N1-C1'	5.28	124.04	117.70
82	A3	19	G	N3-C4-N9	-5.28	122.83	126.00
36	14	2772	C	N1-C2-O2	5.28	122.07	118.90
36	14	3121	U	P-O3'-C3'	5.27	126.03	119.70
36	14	1943	C	P-O3'-C3'	5.26	126.02	119.70
34	22	1257	U	N1-C2-O2	5.26	126.48	122.80
8	D2	214	GLU	C-N-CA	5.25	134.82	121.70
36	14	2137	U	C2-N1-C1'	5.24	123.99	117.70
34	22	1796	C	C2-N1-C1'	5.24	124.56	118.80
36	14	2836	C	N1-C2-O2	5.22	122.03	118.90
36	14	3058	U	N3-C2-O2	-5.20	118.56	122.20
56	J5	172	LEU	CA-CB-CG	5.20	127.26	115.30
34	22	1456	C	N3-C2-O2	-5.18	118.28	121.90
34	22	1060	U	C2-N1-C1'	5.17	123.90	117.70
36	14	1355	A	P-O3'-C3'	5.16	125.90	119.70
34	22	1596	C	N1-C2-O2	5.15	121.99	118.90
34	22	497	G	OP1-P-O3'	5.13	116.49	105.20
34	22	1388	A	P-O3'-C3'	5.13	125.86	119.70
36	14	1269	U	C2-N1-C1'	5.13	123.86	117.70
17	J2	93	LEU	CA-CB-CG	5.10	127.04	115.30
34	22	1398	U	C2-N1-C1'	5.09	123.81	117.70
34	22	965	U	C6-N1-C1'	-5.08	114.09	121.20
34	22	417	A	P-O3'-C3'	5.07	125.79	119.70
82	A3	52	U	N1-C2-O2	5.07	126.35	122.80
36	14	1604	G	C4-N9-C1'	5.06	133.08	126.50
36	14	2257	C	N3-C2-O2	-5.05	118.36	121.90
36	14	1447	G	OP2-P-O3'	5.01	116.23	105.20
36	14	763	G	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	F2	126	ASP	Peptide
49	F5	156	ILE	Peptide
17	J2	133	HIS	Peptide
17	J2	163	PRO	Peptide
60	L5	47	ALA	Peptide
20	M2	90	LYS	Peptide
26	S2	13	HIS	Peptide
31	X2	41	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	3058	0	3134	56	0
2	A2	1621	0	1629	20	0
3	a2	778	0	823	0	0
4	B2	1709	0	1784	14	0
5	b2	610	0	631	0	0
6	C2	1635	0	1723	15	0
7	c2	497	0	535	0	0
8	D2	1734	0	1817	21	0
9	d2	443	0	434	0	0
10	E2	2068	0	2154	22	0
11	e2	475	0	525	0	0
12	F2	1609	0	1674	38	0
13	G2	1820	0	1918	17	0
14	g2	2445	0	2401	0	0
15	H2	1481	0	1572	22	0
16	I2	1489	0	1525	29	0
17	J2	1494	0	1573	13	0
18	K2	817	0	804	1	0
19	L2	1244	0	1314	11	0
20	M2	934	0	975	10	0
21	N2	1192	0	1255	11	0
22	O2	941	0	979	14	0
23	P2	991	0	1035	28	0
24	Q2	1105	0	1166	12	0
25	R2	1000	0	1063	11	0
26	S2	1192	0	1222	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	T2	1112	0	1124	11	0
28	U2	855	0	917	11	0
29	V2	684	0	672	7	0
30	W2	1021	0	1060	15	0
31	X2	1121	0	1196	25	0
32	Y2	1073	0	1132	12	0
33	Z2	563	0	602	68	0
34	22	37948	0	19089	221	0
35	f2	497	0	439	0	0
36	14	70476	0	35381	281	0
37	34	2579	0	1304	15	0
38	44	3353	0	1693	20	0
39	a5	1173	0	1214	0	0
40	A5	1918	0	1986	30	0
41	b5	462	0	491	0	0
42	B5	3081	0	3165	45	0
43	c5	743	0	797	0	0
44	C5	2749	0	2863	38	0
45	D5	2375	0	2324	16	0
46	d5	890	0	938	0	0
47	e5	1020	0	1090	0	0
48	f5	850	0	880	0	0
49	F5	1784	0	1862	14	0
50	g5	881	0	949	0	0
51	G5	1817	0	1908	19	0
52	h5	969	0	1078	0	0
53	H5	1518	0	1587	26	0
54	i5	771	0	849	0	0
55	I5	1717	0	1753	12	0
56	J5	1353	0	1383	42	0
57	j5	681	0	683	0	0
58	k5	612	0	682	0	0
59	l5	436	0	475	0	0
60	L5	1543	0	1608	8	0
61	m5	417	0	455	0	0
62	M5	1053	0	1149	13	0
63	N5	1720	0	1778	36	0
64	o5	847	0	915	0	0
65	p5	694	0	735	0	0
66	P5	1442	0	1485	22	0
67	Q5	1441	0	1542	11	0
68	S5	1445	0	1487	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	U5	796	0	812	1	0
70	V5	1003	0	1048	16	0
71	Z5	1092	0	1155	8	0
72	K5	1555	0	1659	11	0
73	n5	233	0	284	0	0
74	R5	1521	0	1617	13	0
75	X5	968	0	1036	10	0
76	Y5	993	0	1081	8	0
77	T5	1276	0	1323	15	0
78	E5	1248	0	1339	13	0
79	W5	800	0	865	5	0
80	A6	4279	0	4232	80	0
81	X7	259	0	130	4	0
82	A3	1651	0	856	39	0
83	a2	1	0	0	0	0
83	b2	1	0	0	0	0
83	d2	1	0	0	0	0
83	f2	1	0	0	0	0
83	j5	1	0	0	0	0
83	m5	1	0	0	0	0
83	o5	1	0	0	0	0
83	p5	1	0	0	0	0
84	14	701	0	0	0	0
84	22	177	0	0	0	0
84	34	16	0	0	0	0
84	44	34	0	0	0	0
84	A3	6	0	0	0	0
84	A5	6	0	0	0	0
84	A6	2	0	0	0	0
84	B2	1	0	0	0	0
84	B5	5	0	0	0	0
84	C2	2	0	0	0	0
84	C5	8	0	0	0	0
84	D5	1	0	0	0	0
84	E2	2	0	0	0	0
84	E5	1	0	0	0	0
84	F2	2	0	0	0	0
84	F5	4	0	0	0	0
84	I2	2	0	0	0	0
84	I5	4	0	0	0	0
84	J2	1	0	0	0	0
84	J5	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	K5	5	0	0	0	0
84	L2	1	0	0	0	0
84	L5	4	0	0	0	0
84	M5	1	0	0	0	0
84	N2	2	0	0	0	0
84	N5	7	0	0	0	0
84	P5	7	0	0	0	0
84	Q2	1	0	0	0	0
84	Q5	4	0	0	0	0
84	R5	3	0	0	0	0
84	S2	4	0	0	0	0
84	S5	4	0	0	0	0
84	T2	1	0	0	0	0
84	T5	1	0	0	0	0
84	U2	1	0	0	0	0
84	V5	3	0	0	0	0
84	X2	3	0	0	0	0
84	Y2	1	0	0	0	0
84	Y5	2	0	0	0	0
84	a5	3	0	0	0	0
84	b5	1	0	0	0	0
84	d2	1	0	0	0	0
84	d5	3	0	0	0	0
84	e5	3	0	0	0	0
84	f5	1	0	0	0	0
84	j5	7	0	0	0	0
84	l5	1	0	0	0	0
84	m5	3	0	0	0	0
84	o5	3	0	0	0	0
85	A6	32	0	13	1	0
86	A3	14	0	0	3	0
87	A1	7	0	0	0	0
87	A6	6	0	0	0	0
All	All	212865	0	157835	1199	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 4.

All (1199) 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)
26:S2:4:VAL:CG1	33:Z2:42:LEU:HD22	1.12	1.52
56:J5:55:ARG:CD	82:A3:20:G:H22	1.25	1.47
12:F2:125:THR:N	33:Z2:58:ARG:NH2	1.64	1.45
26:S2:4:VAL:HG11	33:Z2:42:LEU:CD2	0.99	1.44
1:A1:218:PHE:CD2	80:A6:225:GLU:OE2	1.75	1.40
56:J5:55:ARG:HD3	82:A3:20:G:N2	1.03	1.32
56:J5:55:ARG:CD	82:A3:20:G:H1	1.41	1.31
26:S2:4:VAL:HG11	33:Z2:42:LEU:CG	1.68	1.24
56:J5:55:ARG:CD	82:A3:20:G:N2	1.87	1.23
56:J5:55:ARG:CD	82:A3:20:G:N1	2.01	1.23
23:P2:128:HIS:NE2	34:22:1459:C:O2'	1.68	1.22
1:A1:218:PHE:CE2	80:A6:225:GLU:OE1	1.95	1.18
56:J5:55:ARG:CD	82:A3:20:G:C2	2.27	1.17
33:Z2:73:GLY:N	34:22:1534:G:O2'	1.75	1.17
33:Z2:77:ARG:NH1	34:22:1533:C:C5	2.12	1.15
56:J5:55:ARG:HD2	82:A3:20:G:N1	1.62	1.14
53:H5:96:HIS:CD2	80:A6:280:THR:HG23	1.83	1.13
56:J5:55:ARG:NE	82:A3:20:G:H1	1.48	1.12
26:S2:4:VAL:HG13	33:Z2:42:LEU:HD13	1.22	1.12
33:Z2:77:ARG:CZ	34:22:1533:C:H5	1.62	1.11
56:J5:55:ARG:HD3	82:A3:20:G:C2	1.85	1.10
33:Z2:77:ARG:NH1	34:22:1534:G:N7	2.00	1.09
12:F2:112:ARG:NH1	33:Z2:95:HIS:CD2	2.20	1.09
33:Z2:77:ARG:CZ	34:22:1533:C:C5	2.38	1.06
56:J5:55:ARG:NE	82:A3:20:G:N1	2.03	1.05
56:J5:55:ARG:HD2	82:A3:20:G:H1	1.08	1.05
23:P2:130:ARG:H	23:P2:130:ARG:HD3	1.21	1.03
12:F2:112:ARG:NH1	33:Z2:95:HIS:NE2	2.07	1.02
33:Z2:73:GLY:CA	34:22:1534:G:O2'	2.07	1.02
12:F2:112:ARG:HH11	33:Z2:95:HIS:CD2	1.77	1.01
1:A1:218:PHE:CD2	80:A6:225:GLU:CD	2.33	0.99
1:A1:218:PHE:CE2	80:A6:225:GLU:CD	2.35	0.98
26:S2:4:VAL:CB	33:Z2:42:LEU:HD22	1.93	0.98
26:S2:4:VAL:CG1	33:Z2:42:LEU:HD13	1.95	0.96
36:14:2954:U:C1'	86:A3:101:5CR:OAB	2.15	0.94
33:Z2:73:GLY:HA3	34:22:1534:G:O2'	1.68	0.93
36:14:2954:U:O4'	86:A3:101:5CR:OAB	1.91	0.89
26:S2:4:VAL:CG1	33:Z2:42:LEU:CD2	1.94	0.88
26:S2:4:VAL:CG1	33:Z2:42:LEU:CD1	2.52	0.88
1:A1:176:LYS:HD2	80:A6:222:GLN:HG3	1.54	0.88
36:14:2954:U:H1'	86:A3:101:5CR:OAB	1.72	0.87
30:W2:2:THR:N	34:22:1034:C:HO2'	1.71	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z2:74:SER:OG	34:22:1534:G:OP2	1.90	0.87
1:A1:174:LYS:HD3	80:A6:409:ILE:HG12	1.57	0.87
26:S2:4:VAL:HG13	33:Z2:42:LEU:CD1	2.04	0.86
23:P2:128:HIS:CE1	34:22:1459:C:O2'	2.29	0.85
1:A1:291:LEU:CB	80:A6:518:PRO:HG2	2.07	0.84
1:A1:291:LEU:HB2	80:A6:518:PRO:HG2	1.60	0.84
23:P2:128:HIS:CE1	34:22:1459:C:HO2'	1.97	0.81
1:A1:285:ASP:OD1	80:A6:517:ARG:NH2	2.14	0.81
56:J5:55:ARG:NH1	82:A3:19:G:H1'	1.97	0.80
1:A1:176:LYS:NZ	80:A6:223:THR:OG1	2.13	0.80
26:S2:4:VAL:CG1	33:Z2:42:LEU:CG	2.45	0.79
12:F2:112:ARG:NH1	33:Z2:95:HIS:HE2	1.78	0.78
22:O2:137:LEU:HD13	81:X7:12:A:O2'	1.83	0.77
1:A1:218:PHE:HE2	80:A6:225:GLU:OE1	1.63	0.76
56:J5:55:ARG:NE	82:A3:20:G:C2	2.50	0.76
23:P2:97:TYR:HB2	23:P2:102:PHE:CD1	2.21	0.75
56:J5:55:ARG:NH2	82:A3:20:G:N2	2.34	0.75
36:14:412:G:H5''	66:P5:30:ARG:HE	1.52	0.74
12:F2:124:LEU:HA	33:Z2:58:ARG:HE	1.51	0.74
1:A1:218:PHE:CG	80:A6:225:GLU:OE2	2.38	0.73
26:S2:4:VAL:HG12	33:Z2:42:LEU:HD22	1.57	0.73
33:Z2:73:GLY:HA3	34:22:1534:G:C2'	2.18	0.73
33:Z2:73:GLY:H	34:22:1534:G:C2'	2.01	0.72
1:A1:218:PHE:HD2	80:A6:225:GLU:OE2	1.62	0.72
56:J5:55:ARG:NE	82:A3:20:G:N2	2.38	0.72
56:J5:55:ARG:HH21	82:A3:20:G:N2	1.87	0.71
12:F2:125:THR:CA	33:Z2:58:ARG:NH2	2.53	0.71
36:14:1158:A:N7	49:F5:93:ASN:ND2	2.38	0.71
26:S2:4:VAL:HG21	33:Z2:42:LEU:HD21	1.72	0.70
1:A1:176:LYS:HZ1	80:A6:223:THR:HG1	1.36	0.70
53:H5:96:HIS:NE2	80:A6:280:THR:HG23	2.07	0.70
12:F2:187:ILE:HG12	33:Z2:66:VAL:HG11	1.73	0.69
23:P2:122:THR:HG21	34:22:1454:G:O3'	1.93	0.69
33:Z2:77:ARG:NH1	34:22:1533:C:H5	1.66	0.69
36:14:1981:G:H1	36:14:2041:U:H3	1.40	0.68
8:D2:56:GLN:N	80:A6:31:TYR:OH	2.25	0.68
12:F2:125:THR:N	33:Z2:58:ARG:HH22	1.81	0.68
33:Z2:73:GLY:C	34:22:1534:G:C8	2.67	0.67
36:14:1385:C:H42	36:14:1421:G:H1	1.42	0.67
23:P2:100:LYS:HD3	34:22:1183:A:C4	2.29	0.67
33:Z2:77:ARG:NH2	34:22:1533:C:C6	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O2:85:ALA:H	22:O2:119:THR:HG22	1.60	0.66
23:P2:100:LYS:HD3	34:22:1183:A:N9	2.11	0.66
42:B5:227:GLU:HG2	42:B5:270:ARG:HE	1.61	0.66
26:S2:4:VAL:HG11	33:Z2:42:LEU:CD1	2.19	0.65
12:F2:81:ARG:HD2	34:22:1615:C:H2'	1.78	0.65
13:G2:202:ARG:HH22	34:22:179:A:H61	1.44	0.65
33:Z2:77:ARG:NH2	34:22:1533:C:OP2	2.29	0.65
1:A1:176:LYS:HE3	80:A6:222:GLN:H	1.62	0.64
56:J5:55:ARG:CZ	82:A3:20:G:N2	2.60	0.64
23:P2:79:HIS:CD2	23:P2:102:PHE:HE1	2.15	0.64
12:F2:112:ARG:HH12	33:Z2:95:HIS:HE2	1.46	0.64
33:Z2:73:GLY:CA	34:22:1534:G:C2'	2.76	0.63
12:F2:53:VAL:HG12	12:F2:55:ASP:H	1.64	0.63
36:14:1634:G:N7	71:Z5:17:ARG:NH1	2.46	0.63
44:C5:318:LEU:H	44:C5:324:LEU:HD13	1.64	0.63
1:A1:176:LYS:HD2	80:A6:222:GLN:CG	2.27	0.62
8:D2:94:ARG:HD3	80:A6:24:ASP:HB3	1.80	0.62
33:Z2:74:SER:HG	34:22:1534:G:P	2.20	0.62
34:22:1220:C:H42	34:22:1263:G:H1	1.47	0.62
22:O2:20:TYR:HB3	22:O2:27:PHE:HB2	1.80	0.62
36:14:170:G:H1	36:14:248:U:H3	1.48	0.62
49:F5:60:ARG:NH1	66:P5:169:THR:OG1	67.34	0.62
63:N5:36:ILE:HG12	63:N5:64:VAL:HG23	1.82	0.62
63:N5:42:PRO:HG3	63:N5:61:ILE:HG13	1.81	0.61
12:F2:112:ARG:HH12	33:Z2:95:HIS:CD2	2.16	0.61
26:S2:116:LEU:HD21	26:S2:123:ARG:HE	1.63	0.61
36:14:676:G:HO2'	36:14:678:G:HO2'	1.44	0.61
36:14:1841:A:H1'	36:14:1848:G:H1'	1.82	0.61
78:E5:56:LYS:HB3	78:E5:64:LEU:HD12	1.82	0.61
15:H2:140:VAL:HG22	15:H2:150:GLN:HG2	1.82	0.61
24:Q2:50:GLU:OE1	24:Q2:82:ARG:NH2	2.33	0.61
30:W2:31:SER:HB2	34:22:636:A:H5''	1.82	0.61
34:22:1680:G:O2'	34:22:1721:A:N6	2.33	0.61
53:H5:96:HIS:CG	80:A6:280:THR:HG23	2.35	0.60
42:B5:235:THR:HG21	42:B5:249:VAL:HG22	1.83	0.60
36:14:2193:U:H5'	36:14:2194:G:H5'	1.82	0.60
56:J5:40:LEU:HD13	56:J5:114:ILE:HD11	1.83	0.60
26:S2:4:VAL:CB	33:Z2:42:LEU:CD2	2.68	0.60
44:C5:106:TRP:HB2	63:N5:199:LEU:HD22	1.83	0.60
53:H5:96:HIS:NE2	80:A6:280:THR:CG2	2.65	0.60
16:I2:57:ALA:HB2	16:I2:177:GLY:HA2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:R5:102:LEU:HD22	74:R5:138:LEU:HD13	1.84	0.60
1:A1:291:LEU:CD1	80:A6:520:LEU:HD21	2.32	0.60
1:A1:291:LEU:HD13	80:A6:520:LEU:HD21	1.83	0.60
23:P2:95:GLY:HA2	23:P2:103:ASN:O	2.02	0.59
26:S2:14:ILE:HD12	26:S2:24:GLY:H	1.66	0.59
31:X2:70:LYS:HB3	31:X2:93:LEU:HD22	1.83	0.59
26:S2:4:VAL:CG1	33:Z2:42:LEU:HB2	2.31	0.59
33:Z2:77:ARG:NH2	34:22:1533:C:H6	2.00	0.59
20:M2:22:VAL:HG12	20:M2:23:THR:HG23	1.84	0.59
53:H5:92:TYR:HB2	53:H5:142:ASP:HB3	1.83	0.59
16:I2:172:ARG:HE	16:I2:175:GLN:HG3	1.65	0.59
33:Z2:73:GLY:N	34:22:1534:G:C2'	2.64	0.59
36:14:2944:U:HO2'	42:B5:251:CYS:HG	1.50	0.59
16:I2:61:GLU:HG3	16:I2:62:THR:HG23	1.85	0.59
23:P2:130:ARG:N	23:P2:130:ARG:HD3	2.02	0.59
36:14:2557:A:H5'	71:Z5:135:ARG:HE	1.67	0.59
8:D2:137:VAL:HB	8:D2:185:LYS:HB2	1.84	0.59
36:14:2402:A:N7	44:C5:73:ARG:NH2	2.50	0.59
36:14:117:U:OP2	63:N5:2:GLY:N	2.36	0.58
27:T2:102:ARG:NH2	34:22:1502:G:N7	2.50	0.58
31:X2:125:VAL:HG12	31:X2:126:LYS:HG3	1.85	0.58
33:Z2:74:SER:OG	34:22:1533:C:H3'	2.03	0.58
19:L2:71:LEU:HB3	19:L2:88:ARG:HH12	1.69	0.58
60:L5:91:ARG:HH21	60:L5:97:VAL:HB	1.68	0.58
27:T2:89:ARG:NH2	34:22:1562:G:OP1	2.37	0.58
31:X2:102:VAL:HG12	31:X2:127:VAL:HG12	1.86	0.58
22:O2:137:LEU:CD1	81:X7:12:A:O2'	2.52	0.58
10:E2:191:ARG:HH11	10:E2:245:LYS:HB3	1.68	0.58
16:I2:5:ARG:NH2	34:22:334:G:O6	2.37	0.58
36:14:2858:U:O2'	36:14:2887:A:N6	2.36	0.58
56:J5:20:ASN:HB3	56:J5:126:ASP:HB2	1.86	0.58
56:J5:47:GLN:HG2	56:J5:67:VAL:HG12	1.85	0.58
19:L2:17:PRO:HG2	34:22:249:U:H3	1.69	0.58
20:M2:42:ALA:HB3	20:M2:122:VAL:HB	1.85	0.58
36:14:2137:U:OP2	36:14:2142:A:N6	2.37	0.58
36:14:2736:A:OP1	77:T5:92:ARG:NH1	2.37	0.58
29:V2:36:VAL:HB	29:V2:51:VAL:HB	1.86	0.58
23:P2:128:HIS:CD2	34:22:1459:C:HO2'	2.07	0.57
2:A2:67:ILE:O	2:A2:185:ARG:NH1	2.37	0.57
56:J5:55:ARG:NE	82:A3:20:G:H22	1.92	0.57
19:L2:128:CYS:SG	19:L2:129:ARG:N	2.76	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z2:77:ARG:CZ	34:22:1533:C:C6	2.87	0.57
36:14:2440:G:N2	36:14:2507:C:N3	2.52	0.57
26:S2:144:ARG:HH12	34:22:1570:A:H4'	1.69	0.57
36:14:2898:G:OP2	53:H5:173:ARG:NH2	2.38	0.57
36:14:804:C:OP1	44:C5:98:ARG:NH2	2.38	0.57
79:W5:6:ASP:HB3	79:W5:10:GLY:H	1.69	0.57
67:Q5:86:THR:HG22	67:Q5:105:ARG:HB3	1.85	0.57
81:X7:9:G:O2'	81:X7:10:G:N2	2.37	0.57
31:X2:30:LYS:NZ	34:22:1132:A:OP1	2.37	0.57
1:A1:176:LYS:CD	80:A6:222:GLN:HG3	2.29	0.57
42:B5:238:LEU:HB3	42:B5:242:THR:HG21	1.86	0.57
36:14:1523:U:H5'	75:X5:113:LEU:HB3	1.87	0.57
23:P2:97:TYR:HB2	23:P2:102:PHE:CE1	2.39	0.57
2:A2:88:LYS:NZ	25:R2:82:ASP:OD2	2.34	0.57
1:A1:152:ALA:HB3	1:A1:168:ILE:HB	1.87	0.56
36:14:2799:A:O2'	40:A5:42:ARG:NH1	103.71	0.56
36:14:712:G:OP1	60:L5:174:ARG:NH1	2.38	0.56
34:22:1588:G:H1	34:22:1608:U:H3	1.52	0.56
10:E2:79:ASP:HB3	10:E2:82:TYR:HB2	1.86	0.56
16:I2:37:LYS:HB2	16:I2:59:ARG:HG2	1.86	0.56
38:44:141:C:O2	63:N5:112:ASN:ND2	2.38	0.56
21:N2:4:MET:SD	21:N2:124:ARG:NH1	2.78	0.56
36:14:129:U:OP1	75:X5:45:LYS:NZ	2.37	0.56
36:14:1796:G:H5'	40:A5:22:LEU:HD21	1.88	0.56
56:J5:133:ARG:NH2	56:J5:158:ASP:OD2	2.39	0.56
36:14:1447:G:N2	36:14:2356:A:OP2	2.38	0.56
36:14:3041:U:OP1	70:V5:12:ARG:NH1	2.38	0.56
12:F2:63:GLN:NE2	12:F2:86:GLN:O	2.38	0.56
2:A2:125:ASP:OD1	2:A2:164:ASN:ND2	2.39	0.56
53:H5:96:HIS:CD2	80:A6:280:THR:CG2	2.74	0.56
22:O2:82:LYS:NZ	22:O2:116:GLU:OE2	2.38	0.56
36:14:200:C:N4	36:14:219:A:OP2	2.39	0.56
70:V5:81:GLN:O	70:V5:98:ASN:ND2	2.38	0.56
36:14:1302:A:N7	36:14:2857:C:O2'	2.38	0.56
37:34:7:G:OP1	45:D5:33:ARG:NH1	2.38	0.56
80:A6:591:ARG:HG2	80:A6:605:LYS:HG2	1.88	0.56
70:V5:21:ALA:HB3	70:V5:36:ILE:HD12	1.88	0.56
36:14:1390:A:O4'	36:14:1418:A:N6	2.38	0.56
6:C2:94:GLN:NE2	34:22:10:G:O2'	2.38	0.56
17:J2:133:HIS:HD2	17:J2:162:SER:HB2	1.70	0.56
36:14:1428:A:O2'	36:14:1430:U:OP2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:52:LYS:HG2	29:V2:82:VAL:HG22	1.88	0.55
42:B5:137:TYR:HA	42:B5:144:ILE:HD11	1.87	0.55
12:F2:112:ARG:HE	24:Q2:43:ILE:HD11	1.71	0.55
6:C2:88:LYS:HA	34:22:10:G:H21	1.72	0.55
34:22:152:U:H3	34:22:162:A:H61	1.54	0.55
1:A1:291:LEU:HB3	80:A6:518:PRO:HG2	1.84	0.55
45:D5:65:ILE:HG12	45:D5:74:VAL:HG22	1.87	0.55
1:A1:42:ILE:HB	1:A1:116:THR:HB	1.88	0.55
42:B5:168:LYS:O	42:B5:319:ASN:ND2	2.40	0.55
63:N5:73:ARG:HH21	63:N5:92:LEU:HD21	1.71	0.55
25:R2:79:GLU:O	25:R2:83:GLN:NE2	2.39	0.55
80:A6:440:PRO:HD3	80:A6:579:PRO:HD3	1.88	0.55
66:P5:109:ALA:HA	66:P5:112:LEU:HD13	1.87	0.55
36:14:216:G:OP1	76:Y5:16:ARG:NH1	2.40	0.55
16:I2:98:LYS:HB3	34:22:329:G:H5''	1.88	0.55
28:U2:21:LYS:HG2	28:U2:94:GLU:HG2	1.87	0.55
36:14:1374:G:O6	40:A5:10:LYS:NZ	83.05	0.55
36:14:2116:G:OP1	36:14:2118:C:N4	2.39	0.55
27:T2:7:ARG:NH1	34:22:1366:U:O2'	2.40	0.55
80:A6:519:LEU:HD12	80:A6:559:LEU:HD23	1.87	0.55
36:14:140:C:OP1	51:G5:106:LYS:NZ	2.38	0.55
34:22:1584:G:N2	34:22:1611:A:OP2	2.39	0.55
42:B5:53:MET:HG2	42:B5:77:THR:HG22	1.89	0.55
36:14:1334:U:H5''	49:F5:206:LYS:HB3	1.89	0.55
36:14:2950:G:OP2	36:14:2950:G:N2	2.39	0.55
37:34:41:G:O2'	37:34:44:C:N4	2.40	0.55
1:A1:361:GLU:HG3	80:A6:522:GLY:O	2.07	0.55
53:H5:113:GLU:OE2	53:H5:115:ARG:NH2	2.39	0.55
72:K5:22:VAL:HG21	72:K5:120:VAL:HG11	1.89	0.55
36:14:2341:A:OP2	42:B5:247:ARG:NH1	2.40	0.55
36:14:2535:A:H61	36:14:2544:U:H3	1.54	0.55
34:22:434:G:N1	34:22:437:A:OP2	2.38	0.55
34:22:1191:U:O2	82:A3:34:OMG:H5'	2.07	0.55
51:G5:72:PRO:HG3	63:N5:18:VAL:HA	1.89	0.55
36:14:668:G:O2'	67:Q5:164:ARG:NH1	2.40	0.55
36:14:3140:G:N7	42:B5:28:ARG:NH2	2.55	0.54
38:44:71:A:N6	38:44:87:G:O2'	2.40	0.54
4:B2:69:CYS:HA	4:B2:83:LYS:HA	1.88	0.54
36:14:959:C:H41	36:14:2801:A:H5''	1.72	0.54
15:H2:113:PRO:HD3	34:22:811:A:H61	1.71	0.54
6:C2:88:LYS:HE2	6:C2:95:ARG:HE	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:190:U:OP1	76:Y5:40:ARG:NH1	2.40	0.54
34:22:67:A:N6	34:22:83:G:O2'	2.40	0.54
36:14:3297:U:O4	42:B5:124:LYS:NZ	2.40	0.54
19:L2:67:ARG:NH1	34:22:112:A:O2'	2.41	0.54
13:G2:136:LYS:NZ	34:22:66:U:OP2	2.40	0.54
66:P5:23:ARG:HH22	66:P5:125:GLN:HG3	1.72	0.54
36:14:126:U:OP1	63:N5:144:ARG:NH1	2.41	0.54
36:14:75:G:OP1	60:L5:101:ARG:NH2	2.41	0.54
55:I5:47:PRO:HD2	55:I5:141:LYS:HA	1.89	0.54
36:14:98:G:N7	60:L5:13:HIS:NE2	2.55	0.54
36:14:1084:A:H5"	77:T5:35:LYS:HE3	1.90	0.54
30:W2:103:ILE:HA	30:W2:112:ASP:HA	1.89	0.54
31:X2:132:LEU:HD23	31:X2:135:LEU:HD12	1.89	0.54
12:F2:104:ASN:ND2	34:22:1587:A:O2'	2.39	0.54
34:22:156:A:O2'	34:22:416:A:N6	2.41	0.54
1:A1:88:VAL:O	1:A1:96:ASN:ND2	2.41	0.54
24:Q2:44:LEU:HB3	24:Q2:78:VAL:HG11	1.88	0.54
36:14:2899:C:N3	53:H5:173:ARG:NH1	2.53	0.54
10:E2:191:ARG:NH1	10:E2:244:ILE:O	2.41	0.54
33:Z2:77:ARG:HH22	34:22:1533:C:H6	1.56	0.54
10:E2:108:ARG:NH1	34:22:788:A:OP2	2.41	0.54
36:14:2202:C:H5"	40:A5:226:SER:HB2	1.90	0.54
40:A5:30:ARG:HH12	40:A5:41:ILE:HD13	1.73	0.54
12:F2:125:THR:CA	33:Z2:58:ARG:HH22	2.18	0.54
36:14:1150:A:N6	36:14:2369:G:O2'	2.41	0.53
36:14:3182:G:OP1	72:K5:117:ARG:NH2	2.40	0.53
21:N2:121:ARG:NH1	34:22:868:G:OP1	2.41	0.53
80:A6:451:GLN:HB2	80:A6:475:THR:HB	1.90	0.53
66:P5:129:THR:HG23	66:P5:139:TYR:HB2	1.90	0.53
71:Z5:14:VAL:HG13	71:Z5:15:ARG:HG2	1.89	0.53
36:14:664:U:H3	36:14:798:G:H1	1.55	0.53
1:A1:40:GLU:HB2	1:A1:118:ILE:HB	1.90	0.53
80:A6:539:LYS:HD2	80:A6:570:GLU:HB2	1.88	0.53
56:J5:51:ARG:O	56:J5:61:ARG:NH2	2.41	0.53
20:M2:43:ARG:NH1	20:M2:102:GLY:O	2.41	0.53
42:B5:221:THR:HB	42:B5:273:HIS:H	1.72	0.53
68:S5:154:HIS:HE1	72:K5:126:VAL:HG22	1.73	0.53
63:N5:56:LYS:NZ	63:N5:145:ASP:OD2	2.41	0.53
27:T2:122:ARG:NH1	34:22:1499:G:OP1	2.41	0.53
34:22:716:C:H41	34:22:723:G:H21	1.55	0.53
80:A6:526:ILE:HA	80:A6:535:PRO:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:590:G:O2'	44:C5:309:ARG:NH1	2.41	0.53
51:G5:86:THR:HG21	51:G5:217:THR:HG21	1.90	0.53
31:X2:42:PRO:O	31:X2:79:ASN:ND2	2.41	0.53
1:A1:41:LEU:HD12	1:A1:67:ILE:HD11	1.90	0.53
15:H2:64:VAL:HB	34:22:856:A:H1'	1.89	0.53
63:N5:44:ARG:NH1	63:N5:120:TRP:O	2.42	0.53
36:14:3206:C:H1'	68:S5:155:ARG:HH12	1.73	0.53
23:P2:128:HIS:CD2	34:22:1459:C:O2'	2.55	0.53
56:J5:55:ARG:NH2	82:A3:19:G:O2'	2.41	0.53
40:A5:21:ARG:HH21	40:A5:22:LEU:HD12	1.73	0.53
80:A6:304:GLY:O	80:A6:588:ARG:NH1	2.42	0.53
34:22:1202:A:N6	34:22:1457:C:OP1	2.35	0.53
80:A6:173:LEU:HD13	80:A6:296:HIS:HB3	1.90	0.53
42:B5:287:LYS:O	42:B5:293:ASN:ND2	2.41	0.53
44:C5:3:ARG:HE	44:C5:22:LEU:HB2	1.72	0.53
36:14:3040:A:H5''	70:V5:12:ARG:HB2	1.91	0.53
6:C2:203:LYS:NZ	34:22:16:G:O6	2.42	0.53
37:34:5:G:OP1	56:J5:143:ARG:NH2	2.42	0.53
6:C2:87:GLN:OE1	6:C2:94:GLN:NE2	2.42	0.53
45:D5:64:ILE:HD13	45:D5:109:THR:HG21	1.90	0.53
13:G2:65:GLN:NE2	34:22:1682:U:O2'	2.42	0.53
26:S2:4:VAL:CG1	33:Z2:42:LEU:CB	2.85	0.53
68:S5:22:PRO:O	77:T5:146:ASN:ND2	2.39	0.53
36:14:1900:A:H61	36:14:1908:A:H61	1.57	0.52
36:14:2880:U:OP1	70:V5:47:ASN:ND2	2.41	0.52
17:J2:77:ILE:HD11	17:J2:93:LEU:HB2	1.92	0.52
36:14:2548:C:OP2	40:A5:93:LYS:NZ	2.42	0.52
36:14:3011:A:N6	42:B5:12:GLY:O	2.42	0.52
38:44:24:G:O6	76:Y5:13:ARG:NH2	2.43	0.52
10:E2:104:ASP:HB2	10:E2:108:ARG:H	1.73	0.52
67:Q5:75:GLY:O	67:Q5:79:LYS:NZ	2.42	0.52
36:14:1214:U:OP2	68:S5:137:ARG:NH2	2.42	0.52
36:14:3049:A:N3	42:B5:55:THR:OG1	2.39	0.52
34:22:42:G:H1	34:22:433:C:H42	1.55	0.52
1:A1:264:LYS:HD2	80:A6:517:ARG:HH12	1.73	0.52
1:A1:312:GLY:HA3	1:A1:345:ASN:HD22	1.75	0.52
1:A1:67:ILE:HA	1:A1:87:THR:HA	1.90	0.52
36:14:3027:A:H1'	80:A6:256:ARG:NH2	2.24	0.52
4:B2:86:LEU:HD23	4:B2:98:THR:HG21	1.91	0.52
63:N5:37:HIS:HE1	63:N5:63:ARG:HH11	1.55	0.52
12:F2:156:ARG:NH1	22:O2:53:ASP:OD2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:2969:A:N7	40:A5:215:ASN:ND2	2.57	0.52
1:A1:103:LYS:NZ	34:22:578:U:OP2	2.41	0.52
72:K5:61:ALA:HA	72:K5:70:PRO:HD2	1.91	0.52
66:P5:30:ARG:HH12	66:P5:62:ARG:HH11	1.56	0.52
36:14:1189:C:N4	36:14:1315:U:O2'	2.43	0.52
36:14:1900:A:O2'	36:14:1902:G:N7	2.41	0.52
34:22:1594:G:OP2	34:22:1596:C:N4	2.42	0.52
37:34:44:C:OP2	56:J5:137:ARG:NH2	2.41	0.52
38:44:29:U:H5''	60:L5:27:ASP:HB3	1.92	0.52
42:B5:219:ALA:HB2	42:B5:336:VAL:HG23	1.92	0.52
36:14:1245:A:N6	36:14:1272:C:O2'	2.38	0.52
12:F2:63:GLN:HG2	12:F2:88:PRO:HB3	1.92	0.52
25:R2:5:ARG:NH2	34:22:1390:U:OP1	2.43	0.52
56:J5:55:ARG:HE	82:A3:20:G:H1	1.46	0.52
80:A6:274:LEU:HB3	80:A6:310:ILE:HG23	1.92	0.52
49:F5:66:LYS:NZ	49:F5:78:GLU:OE2	2.43	0.52
36:14:1603:A:H61	75:X5:71:THR:HG21	1.74	0.52
33:Z2:56:THR:O	33:Z2:103:ARG:NH1	2.42	0.52
36:14:116:A:OP2	63:N5:2:GLY:N	2.42	0.52
4:B2:204:ILE:O	34:22:1064:G:O2'	2.28	0.52
12:F2:125:THR:HA	33:Z2:58:ARG:HH22	1.75	0.52
15:H2:46:ILE:HD11	15:H2:58:LEU:HB3	1.90	0.52
26:S2:117:LYS:O	26:S2:120:ARG:NH2	2.43	0.52
36:14:119:U:H4'	36:14:120:G:H3'	1.91	0.52
36:14:2727:A:OP2	36:14:2728:G:N2	2.43	0.52
34:22:16:G:H21	34:22:1138:A:H62	1.58	0.52
34:22:815:G:OP2	74:R5:166:ASN:ND2	2.43	0.52
36:14:1160:C:OP1	67:Q5:2:GLY:N	2.43	0.51
36:14:13:A:H61	38:44:145:U:H3	1.58	0.51
36:14:374:A:OP1	76:Y5:77:LYS:NZ	2.44	0.51
36:14:608:A:O2'	44:C5:326:ARG:NH1	2.43	0.51
36:14:784:A:H2'	67:Q5:69:ARG:HE	1.75	0.51
45:D5:54:ARG:HH12	45:D5:149:GLY:HA3	1.75	0.51
36:14:1361:U:O2	49:F5:159:GLN:NE2	2.44	0.51
51:G5:137:ASN:HD21	63:N5:4:TYR:HE2	1.58	0.51
75:X5:100:LYS:NZ	75:X5:106:ASP:OD1	2.43	0.51
36:14:2335:G:N2	36:14:2339:C:O2'	2.43	0.51
36:14:394:G:N1	36:14:397:A:OP2	2.43	0.51
8:D2:27:ARG:NH2	34:22:1436:A:OP2	2.43	0.51
44:C5:16:THR:HG22	44:C5:18:ASN:H	1.75	0.51
44:C5:300:ARG:O	67:Q5:39:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:1324:U:H5''	68:S5:1:MET:HA	1.91	0.51
36:14:874:U:OP2	42:B5:241:LYS:NZ	2.40	0.51
38:44:103:G:OP2	38:44:105:A:O2'	2.29	0.51
40:A5:181:LYS:HG3	40:A5:184:ARG:H	1.75	0.51
12:F2:52:GLU:OE2	12:F2:65:ARG:NH1	2.43	0.51
19:L2:123:VAL:HG23	19:L2:142:VAL:HG22	1.93	0.51
68:S5:38:LYS:HD3	68:S5:58:ILE:HG21	1.93	0.51
30:W2:15:ASN:HD21	30:W2:72:CYS:H	1.57	0.51
36:14:2712:U:O2'	36:14:2743:A:O2'	2.28	0.51
16:I2:67:TRP:NE1	16:I2:69:SER:OG	2.44	0.51
36:14:1547:G:OP1	63:N5:108:ARG:NH2	2.43	0.51
36:14:1481:A:O2'	36:14:1858:A:N3	2.42	0.51
34:22:91:G:OP1	34:22:397:A:N6	2.42	0.51
1:A1:158:THR:HG22	1:A1:160:SER:H	1.76	0.51
82:A3:47:U:O2'	82:A3:50:U:OP1	2.27	0.51
80:A6:502:SER:HB3	80:A6:577:TRP:HB3	1.91	0.51
36:14:3198:U:H1'	53:H5:21:LYS:HB2	1.92	0.51
53:H5:8:GLN:HB3	53:H5:72:LYS:HD2	1.93	0.51
34:22:472:U:O2'	34:22:769:A:N3	2.42	0.51
12:F2:95:ASN:OD1	12:F2:107:LYS:NZ	2.43	0.51
51:G5:108:ARG:NH2	51:G5:112:GLU:OE2	2.44	0.51
36:14:32:U:O4	63:N5:188:ARG:NH2	2.43	0.51
31:X2:14:LYS:NZ	34:22:1105:C:OP2	2.43	0.51
4:B2:149:GLN:HE22	4:B2:154:SER:HB2	1.75	0.51
44:C5:4:PRO:HD2	44:C5:22:LEU:HD12	1.93	0.51
16:I2:105:ASP:OD2	16:I2:107:THR:OG1	2.26	0.51
23:P2:86:VAL:HG13	23:P2:88:GLU:H	1.76	0.51
36:14:86:G:N2	36:14:99:A:OP2	2.44	0.51
15:H2:111:LYS:HB3	34:22:811:A:H62	1.74	0.51
8:D2:191:ASP:HB3	8:D2:194:LYS:HG2	1.93	0.51
13:G2:70:PRO:HD3	13:G2:101:ILE:HD12	1.93	0.51
15:H2:143:LEU:HB2	15:H2:147:ASN:HB2	1.93	0.51
16:I2:56:ARG:NH2	34:22:332:U:OP1	2.44	0.51
37:34:101:G:OP2	68:S5:52:LYS:NZ	2.44	0.51
70:V5:102:ILE:HG23	70:V5:110:LYS:HB3	1.92	0.51
40:A5:54:ARG:HG2	40:A5:56:ALA:H	1.76	0.51
2:A2:119:ARG:HH22	6:C2:240:LEU:HB3	1.76	0.51
6:C2:78:ASP:HA	6:C2:104:VAL:HG12	1.93	0.51
53:H5:24:ILE:HD11	53:H5:39:LYS:HE2	1.92	0.51
21:N2:99:ARG:NH2	21:N2:119:GLU:OE2	2.43	0.51
22:O2:18:ARG:NH1	34:22:918:U:O2'	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:1724:U:O2'	36:14:1725:C:O4'	2.29	0.51
36:14:68:C:N4	36:14:314:U:O2'	2.44	0.51
17:J2:3:ARG:NH2	34:22:39:A:OP1	2.44	0.51
34:22:65:A:H2	34:22:84:A:H62	1.59	0.51
36:14:911:C:H42	40:A5:3:ARG:HD3	1.75	0.51
36:14:292:U:OP2	63:N5:68:ARG:NH2	2.44	0.51
67:Q5:8:LYS:HB3	67:Q5:11:LYS:HD3	1.92	0.51
28:U2:28:SER:HB3	28:U2:34:LEU:HD12	1.93	0.51
32:Y2:41:ARG:NH2	32:Y2:52:LYS:O	2.41	0.51
36:14:1354:G:N7	36:14:1357:G:O2'	2.44	0.50
16:I2:77:ARG:NH2	36:14:3354:U:O2'	2.44	0.50
34:22:936:G:OP1	34:22:1074:G:N2	2.42	0.50
36:14:1213:G:OP2	68:S5:137:ARG:NH1	2.44	0.50
16:I2:92:ARG:HE	36:14:3345:G:H4'	1.76	0.50
36:14:347:G:N2	36:14:352:A:O2'	2.42	0.50
36:14:2549:G:OP2	36:14:2549:G:N2	2.44	0.50
34:22:142:G:H22	34:22:173:A:H2	1.59	0.50
49:F5:88:ARG:NH1	49:F5:108:LEU:O	2.44	0.50
56:J5:109:HIS:HD2	56:J5:123:PHE:H	1.60	0.50
24:Q2:36:ILE:HD13	24:Q2:52:LEU:HD11	1.94	0.50
68:S5:6:GLU:OE2	68:S5:28:ARG:NH1	2.43	0.50
36:14:218:G:H1'	36:14:372:A:H1'	1.93	0.50
34:22:58:U:O2'	34:22:451:A:N3	2.44	0.50
2:A2:142:PRO:HG3	29:V2:32:VAL:HG13	1.93	0.50
36:14:3377:G:H21	42:B5:332:ARG:HH21	1.59	0.50
26:S2:4:VAL:HG11	33:Z2:42:LEU:CB	2.35	0.50
77:T5:50:LYS:HB3	77:T5:92:ARG:HH11	1.77	0.50
36:14:3178:A:H2'	72:K5:115:LYS:HD2	1.93	0.50
21:N2:64:ARG:NH2	34:22:861:U:OP2	2.45	0.50
34:22:1026:A:N7	34:22:1772:C:O2'	2.42	0.50
45:D5:76:ALA:HB3	45:D5:109:THR:HG22	1.94	0.50
36:14:1985:G:H1	36:14:2036:U:H3	1.59	0.50
26:S2:41:ARG:NH1	34:22:1565:C:OP1	2.45	0.50
44:C5:160:GLN:NE2	44:C5:213:ASN:O	2.45	0.50
63:N5:4:TYR:HE1	63:N5:45:PRO:HB2	1.77	0.50
27:T2:130:ARG:HH12	27:T2:134:ARG:HD3	1.77	0.50
31:X2:19:ARG:HH12	34:22:610:G:H21	1.60	0.50
44:C5:334:PHE:HA	44:C5:339:LEU:HD12	1.93	0.50
69:U5:36:TYR:O	69:U5:40:HIS:ND1	2.44	0.50
4:B2:110:LEU:HD21	4:B2:213:ARG:HD2	1.93	0.49
53:H5:114:VAL:HB	53:H5:124:ARG:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:A6:432:PRO:HA	80:A6:447:VAL:HG13	1.94	0.49
10:E2:104:ASP:N	10:E2:108:ARG:O	2.46	0.49
10:E2:19:LEU:HD11	10:E2:108:ARG:HD2	1.94	0.49
13:G2:67:VAL:HG23	13:G2:99:GLY:HA2	1.93	0.49
22:O2:18:ARG:HA	22:O2:82:LYS:HB2	1.94	0.49
31:X2:134:ALA:HB1	31:X2:139:LYS:HB2	1.92	0.49
36:14:197:G:N2	36:14:218:G:O2'	2.46	0.49
2:A2:155:PHE:HA	29:V2:60:ARG:HB3	1.93	0.49
17:J2:134:ILE:HG22	17:J2:158:PHE:HA	1.95	0.49
36:14:286:U:O2'	63:N5:179:LYS:O	2.29	0.49
26:S2:138:THR:OG1	34:22:1459:C:OP2	2.30	0.49
27:T2:16:ASN:OD1	27:T2:56:LYS:NZ	2.45	0.49
31:X2:96:VAL:HG12	31:X2:127:VAL:HG21	1.94	0.49
36:14:217:U:O2	76:Y5:103:LYS:NZ	2.44	0.49
34:22:1022:C:O2'	34:22:1125:A:N1	2.45	0.49
16:I2:141:ARG:NH2	34:22:196:G:O6	2.44	0.49
40:A5:52:SER:HB3	40:A5:191:LEU:HD23	1.94	0.49
16:I2:153:GLU:HG2	16:I2:155:SER:H	1.78	0.49
62:M5:85:TRP:NE1	62:M5:91:CYS:SG	2.85	0.49
28:U2:106:ILE:HG23	28:U2:107:THR:HG23	1.93	0.49
76:Y5:87:LYS:HB2	76:Y5:97:ILE:HD11	1.94	0.49
36:14:1307:G:OP1	72:K5:60:LYS:NZ	2.41	0.49
36:14:2945:G:O2'	36:14:2948:C:OP2	2.31	0.49
1:A1:146:VAL:HA	1:A1:214:CYS:HB2	1.95	0.49
82:A3:8:U:O2'	82:A3:21:A:N1	2.38	0.49
82:A3:22:G:H2'	82:A3:23:A:H8	1.78	0.49
42:B5:14:LEU:HA	42:B5:17:LEU:HD13	1.94	0.49
36:14:3067:C:H3'	74:R5:62:ARG:HH12	1.78	0.49
28:U2:72:ASN:ND2	34:22:1429:G:N3	2.59	0.49
16:I2:5:ARG:NH1	34:22:332:U:O2'	2.43	0.49
34:22:368:U:O2'	34:22:603:U:O2'	2.29	0.49
44:C5:327:LEU:HD23	49:F5:181:ILE:HG21	1.95	0.49
17:J2:52:ILE:HG23	17:J2:76:LEU:HD11	1.94	0.49
72:K5:34:VAL:HG12	72:K5:103:LYS:HB2	1.95	0.49
36:14:1048:A:HO2'	36:14:2632:G:HO2'	1.54	0.49
36:14:3092:C:H2'	70:V5:12:ARG:HH21	1.75	0.49
34:22:1488:G:H3'	34:22:1515:A:H61	1.77	0.49
34:22:396:G:N2	34:22:399:A:OP2	2.43	0.49
32:Y2:112:LYS:NZ	34:22:57:G:OP1	2.42	0.49
80:A6:308:LEU:HD12	80:A6:310:ILE:HD11	1.93	0.49
36:14:1794:G:O2'	36:14:1796:G:N2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:2631:U:OP2	77:T5:4:SER:OG	2.30	0.49
34:22:393:C:H41	34:22:400:A:H1'	1.77	0.49
34:22:514:G:H2'	34:22:515:A:H8	1.78	0.49
15:H2:112:ARG:NH1	34:22:638:U:O2'	2.46	0.49
8:D2:54:ARG:HD3	80:A6:20:GLY:HA2	1.93	0.49
36:14:2349:U:O2'	36:14:3307:A:N3	2.46	0.49
36:14:2947:G:OP1	36:14:2982:A:N6	2.44	0.49
34:22:701:U:O2	34:22:738:G:N2	2.46	0.49
1:A1:24:ASP:OD2	1:A1:139:LYS:NZ	2.42	0.49
62:M5:19:ARG:HB3	62:M5:35:ILE:HD12	1.94	0.49
74:R5:148:ASP:OD1	74:R5:151:ARG:NH1	2.46	0.49
71:Z5:23:VAL:HG12	71:Z5:45:GLY:HA3	1.95	0.49
34:22:1191:U:C2	82:A3:34:OMG:H5'	2.48	0.48
8:D2:132:LYS:HG3	8:D2:156:PHE:HB3	1.95	0.48
28:U2:59:PRO:HG3	34:22:1381:U:H4'	1.94	0.48
36:14:1385:C:O2	78:E5:2:SER:N	2.46	0.48
32:Y2:109:LYS:NZ	34:22:458:G:OP1	2.44	0.48
27:T2:105:LEU:HD13	27:T2:122:ARG:HD2	1.95	0.48
34:22:1640:C:N4	81:X7:18:C:OP1	2.46	0.48
1:A1:1:MET:N	1:A1:133:ALA:O	2.46	0.48
36:14:1419:A:H3'	44:C5:193:LYS:HZ2	1.78	0.48
16:I2:5:ARG:NH2	16:I2:27:PHE:O	2.46	0.48
36:14:2617:U:O2'	55:I5:116:ARG:NH2	2.46	0.48
34:22:542:A:O2'	34:22:543:C:O2	2.32	0.48
37:34:36:C:H42	37:34:41:G:H1	1.60	0.48
82:A3:23:A:H2'	82:A3:24:G:C8	2.49	0.48
42:B5:93:VAL:HG22	42:B5:155:ALA:H	1.78	0.48
44:C5:203:ARG:NH2	44:C5:226:GLU:OE1	2.45	0.48
78:E5:131:LYS:HG3	78:E5:133:GLU:H	1.78	0.48
12:F2:187:ILE:HG21	33:Z2:66:VAL:HB	1.96	0.48
62:M5:123:LEU:HD22	72:K5:190:VAL:HG23	1.95	0.48
38:44:13:A:O2'	66:P5:121:GLN:O	2.32	0.48
2:A2:84:ARG:NH2	25:R2:82:ASP:O	2.47	0.48
13:G2:31:ARG:HE	13:G2:68:LEU:HD21	1.77	0.48
53:H5:41:ILE:HD11	53:H5:67:ALA:HB1	1.94	0.48
16:I2:83:TYR:HB3	16:I2:101:ILE:HB	1.94	0.48
36:14:1447:G:OP1	66:P5:65:SER:OG	2.27	0.48
36:14:21:G:O2'	38:44:37:A:N6	2.47	0.48
38:44:27:U:H4'	44:C5:51:ALA:HB3	1.95	0.48
24:Q2:12:LYS:HG2	24:Q2:17:THR:HG22	1.95	0.48
24:Q2:39:VAL:HG12	24:Q2:41:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:22:104:A:OP2	34:22:308:C:N4	2.43	0.48
34:22:1122:G:N2	34:22:1125:A:OP2	2.44	0.48
40:A5:249:SER:OG	40:A5:250:GLN:N	2.46	0.48
13:G2:57:ASP:HB3	13:G2:106:LEU:HD23	1.96	0.48
26:S2:16:ARG:NH2	56:J5:111:ASP:OD1	2.33	0.48
63:N5:99:ARG:NH2	63:N5:118:SER:O	2.45	0.48
30:W2:105:THR:N	30:W2:124:LYS:O	2.47	0.48
36:14:1635:G:N2	36:14:1638:A:OP2	2.42	0.48
34:22:1362:U:O2	34:22:1363:U:N3	2.45	0.48
34:22:322:G:N2	34:22:325:G:O6	2.42	0.48
80:A6:574:VAL:HG22	80:A6:576:ARG:H	1.79	0.48
36:14:289:A:O2'	63:N5:93:LYS:O	2.27	0.48
68:S5:1:MET:HG2	68:S5:3:HIS:H	1.79	0.48
33:Z2:77:ARG:NH2	34:22:1533:C:C5	2.76	0.48
15:H2:108:GLN:NE2	34:22:743:U:O4'	2.47	0.48
21:N2:104:ARG:NH1	34:22:950:C:O2'	2.46	0.48
1:A1:65:LEU:HD13	1:A1:105:LEU:HD21	1.96	0.48
40:A5:51:ASP:HB2	40:A5:58:LEU:HG	1.95	0.48
70:V5:14:SER:O	70:V5:81:GLN:NE2	2.47	0.48
30:W2:28:ARG:HD3	30:W2:60:LYS:HE2	1.95	0.48
31:X2:101:GLU:O	31:X2:128:SER:N	2.46	0.48
4:B2:165:ARG:HH12	34:22:946:U:H5''	1.79	0.48
10:E2:31:PRO:HG3	10:E2:43:PRO:HG3	1.94	0.48
17:J2:59:LEU:HD22	17:J2:69:ARG:HA	1.96	0.48
63:N5:159:ARG:NH2	63:N5:164:LEU:O	2.47	0.48
36:14:29:C:O3'	63:N5:172:ARG:NH2	2.46	0.48
23:P2:18:ARG:HB2	23:P2:36:LEU:HD13	1.94	0.48
26:S2:115:ARG:HA	26:S2:118:LYS:HE2	1.95	0.48
36:14:2987:A:H5''	72:K5:68:ARG:HH12	1.79	0.47
2:A2:90:ALA:HB2	2:A2:97:PRO:HD3	1.96	0.47
15:H2:48:GLU:OE2	15:H2:88:ARG:NH2	2.47	0.47
36:14:1940:G:OP1	74:R5:75:HIS:ND1	2.47	0.47
68:S5:83:SER:OG	68:S5:86:GLY:O	2.29	0.47
36:14:114:A:H4'	63:N5:49:ARG:HG2	1.96	0.47
36:14:2261:G:O2'	36:14:2263:C:N4	2.47	0.47
27:T2:102:ARG:NH1	34:22:1501:C:OP2	2.47	0.47
80:A6:354:PHE:HE2	85:A6:701:GNP:H2'	1.79	0.47
12:F2:124:LEU:HA	33:Z2:58:ARG:NE	2.25	0.47
13:G2:188:ARG:HD3	34:22:283:U:H5''	1.96	0.47
56:J5:10:ARG:NH1	56:J5:151:SER:O	2.48	0.47
36:14:2351:U:H5''	66:P5:82:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:2406:C:O2'	36:14:2619:G:N2	2.43	0.47
36:14:3027:A:H1'	80:A6:256:ARG:HH22	1.79	0.47
34:22:987:G:N2	34:22:1013:A:OP1	2.47	0.47
1:A1:70:ILE:HD11	1:A1:86:VAL:HG23	1.95	0.47
10:E2:155:LYS:NZ	34:22:244:A:OP1	2.48	0.47
36:14:1156:C:OP2	49:F5:94:LYS:NZ	2.37	0.47
17:J2:17:ARG:NH1	34:22:4:C:O2'	2.38	0.47
2:A2:198:MET:HG2	2:A2:200:ASP:H	1.79	0.47
6:C2:188:LEU:HD13	6:C2:196:VAL:HG11	1.96	0.47
15:H2:13:PRO:HA	15:H2:14:THR:HA	1.56	0.47
32:Y2:60:PHE:H	32:Y2:71:GLY:HA2	1.79	0.47
34:22:1537:C:O2'	34:22:1540:G:O6	2.33	0.47
16:I2:64:ASN:ND2	34:22:257:A:N3	2.62	0.47
34:22:766:U:H5'	34:22:767:U:H5''	1.97	0.47
2:A2:31:VAL:HG12	2:A2:33:GLN:H	1.78	0.47
70:V5:15:LEU:HD23	70:V5:53:SER:HB3	1.96	0.47
12:F2:192:GLU:OE1	33:Z2:63:SER:HB2	2.14	0.47
36:14:910:G:O6	40:A5:3:ARG:NH1	2.48	0.47
1:A1:176:LYS:HE3	80:A6:222:GLN:N	2.29	0.47
4:B2:144:ARG:NH2	4:B2:207:LEU:O	2.48	0.47
4:B2:87:ARG:NH1	4:B2:220:GLN:OE1	2.47	0.47
49:F5:186:HIS:O	49:F5:190:THR:OG1	2.29	0.47
23:P2:126:VAL:HG21	34:22:1459:C:C4'	2.44	0.47
36:14:118:U:O4	36:14:148:G:N2	2.45	0.47
44:C5:181:VAL:HG12	44:C5:182:LEU:HD12	1.96	0.47
23:P2:79:HIS:HD2	23:P2:102:PHE:HE1	1.61	0.47
2:A2:52:LYS:HE2	29:V2:82:VAL:HA	1.96	0.47
71:Z5:22:LYS:NZ	71:Z5:129:TRP:O	2.43	0.47
36:14:1694:U:H3	36:14:1752:A:H61	1.62	0.47
34:22:632:U:O2'	34:22:1103:U:OP1	2.32	0.47
23:P2:59:LYS:NZ	34:22:1242:A:OP1	2.42	0.47
80:A6:332:LEU:HD22	80:A6:348:TRP:HH2	1.80	0.47
12:F2:127:GLN:HE22	12:F2:199:ILE:HG12	1.80	0.47
38:44:154:C:H5''	51:G5:181:LYS:HE2	1.95	0.47
53:H5:19:SER:HB2	53:H5:26:LYS:HB3	1.95	0.47
17:J2:61:THR:HA	30:W2:97:ARG:HH22	1.80	0.47
44:C5:295:ILE:HD11	67:Q5:129:VAL:HA	1.96	0.47
36:14:2400:G:O6	36:14:2401:A:N6	2.48	0.47
36:14:1943:C:H5'	36:14:3346:U:H4'	1.96	0.47
1:A1:67:ILE:HG22	1:A1:87:THR:HG22	1.97	0.47
36:14:3004:C:O2'	42:B5:99:LEU:O	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:H5:96:HIS:CE1	80:A6:280:THR:CG2	2.97	0.47
16:I2:70:GLU:HG2	16:I2:112:TRP:HH2	1.79	0.47
36:14:1793:C:O2	40:A5:174:ARG:NH1	2.48	0.47
36:14:2163:C:H4'	40:A5:8:GLN:HA	1.97	0.47
36:14:3042:U:OP2	36:14:3092:C:N4	2.48	0.47
34:22:1482:C:OP2	34:22:1521:G:N2	2.40	0.47
33:Z2:74:SER:N	34:22:1534:G:C8	2.83	0.47
16:I2:178:ARG:NH1	34:22:207:U:O2	2.42	0.47
42:B5:71:GLU:OE2	79:W5:1:MET:N	2.48	0.47
44:C5:150:LEU:HD21	44:C5:172:VAL:HG11	1.96	0.47
49:F5:151:ARG:NH1	49:F5:206:LYS:O	2.48	0.47
71:Z5:95:VAL:HG21	71:Z5:113:VAL:HG11	1.97	0.47
36:14:2510:U:H2'	36:14:2511:A:H8	1.80	0.47
36:14:3089:C:OP1	42:B5:222:LYS:NZ	2.41	0.47
36:14:3273:A:OP2	78:E5:77:ARG:NH2	2.48	0.47
78:E5:40:LEU:HD13	78:E5:84:VAL:HG11	1.96	0.47
12:F2:43:PHE:HB3	12:F2:46:TRP:HB2	1.97	0.47
17:J2:139:GLN:NE2	32:Y2:64:PHE:O	2.48	0.47
19:L2:113:PRO:O	19:L2:116:ARG:NH2	2.45	0.47
22:O2:16:VAL:HG12	22:O2:80:HIS:HB2	1.97	0.47
23:P2:98:ASN:ND2	23:P2:121:ILE:O	2.48	0.47
27:T2:63:ARG:NH2	34:22:1480:G:OP1	2.48	0.47
44:C5:35:VAL:HG11	44:C5:244:LEU:HD21	1.96	0.46
8:D2:71:LEU:HD22	8:D2:75:LYS:HE3	1.97	0.46
62:M5:113:THR:OG1	78:E5:176:PHE:O	2.33	0.46
55:I5:46:PHE:HB2	55:I5:139:ARG:HH11	1.79	0.46
36:14:1863:G:N1	36:14:1866:C:OP2	2.44	0.46
34:22:992:A:O2'	34:22:1785:U:O2	2.32	0.46
38:44:126:A:O2'	38:44:129:C:N4	2.48	0.46
80:A6:305:ILE:HD13	80:A6:588:ARG:HH12	1.80	0.46
6:C2:175:GLY:N	6:C2:195:ASP:OD2	2.47	0.46
10:E2:66:MET:SD	10:E2:78:THR:OG1	2.74	0.46
66:P5:177:ALA:HA	66:P5:180:LYS:HE3	1.96	0.46
36:14:2666:C:OP2	36:14:2687:G:N1	2.47	0.46
34:22:1657:U:H5''	34:22:1658:G:H5''	1.96	0.46
34:22:40:A:H62	34:22:467:G:H21	1.62	0.46
45:D5:15:ARG:HA	77:T5:20:ARG:HD3	1.98	0.46
10:E2:185:GLY:H	10:E2:189:LEU:HD13	1.79	0.46
31:X2:18:HIS:O	31:X2:22:ASN:ND2	2.49	0.46
34:22:1191:U:C2	82:A3:34:OMG:C5'	2.98	0.46
40:A5:136:ILE:HG13	40:A5:148:VAL:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:658:G:N2	44:C5:93:MET:O	2.42	0.46
36:14:591:G:O2'	78:E5:17:ALA:O	2.31	0.46
24:Q2:90:VAL:HG11	24:Q2:117:LEU:HD21	1.98	0.46
25:R2:18:GLU:HA	25:R2:71:PHE:HA	1.97	0.46
74:R5:31:GLU:HG3	74:R5:44:LEU:HD21	1.97	0.46
36:14:1863:G:H4'	74:R5:82:LYS:HD3	1.97	0.46
36:14:2889:C:HO2'	36:14:2934:A:HO2'	1.63	0.46
36:14:807:A:H61	36:14:934:G:H22	1.64	0.46
20:M2:46:ARG:HH22	34:22:1253:U:H3'	1.81	0.46
34:22:1533:C:N4	34:22:1534:G:O6	2.48	0.46
37:34:62:U:O4	37:34:63:A:N6	2.49	0.46
80:A6:175:HIS:O	80:A6:180:LYS:NZ	2.40	0.46
80:A6:149:THR:OG1	80:A6:433:GLY:O	2.32	0.46
44:C5:207:VAL:HB	44:C5:227:THR:HG22	1.98	0.46
53:H5:94:TYR:OH	53:H5:141:LYS:NZ	2.49	0.46
21:N2:86:GLU:OE2	34:22:961:U:O2'	2.30	0.46
63:N5:35:VAL:HA	63:N5:65:ARG:HD3	1.98	0.46
63:N5:84:PRO:HA	63:N5:87:GLN:HB2	1.97	0.46
25:R2:7:LYS:HE2	25:R2:11:ARG:HE	1.80	0.46
36:14:1493:G:N2	36:14:1493:G:OP2	2.47	0.46
36:14:1963:G:H1	36:14:2059:U:H3	1.62	0.46
36:14:896:A:H5'	40:A5:183:GLY:HA2	1.97	0.46
56:J5:32:ARG:NH1	56:J5:120:ILE:O	2.42	0.46
72:K5:109:PRO:HG2	72:K5:112:TYR:HB2	1.98	0.46
19:L2:83:THR:HG21	34:22:325:G:H4'	1.97	0.46
4:B2:52:THR:OG1	21:N2:56:ASP:OD2	87.67	0.46
36:14:2945:G:OP1	36:14:2945:G:N2	2.48	0.46
36:14:2901:G:O2'	36:14:3024:A:N1	2.47	0.46
32:Y2:124:ARG:NH2	34:22:151:G:O6	2.49	0.46
30:W2:56:HIS:O	34:22:861:U:O2'	2.33	0.46
80:A6:351:ILE:HD13	80:A6:377:LEU:HD22	1.98	0.46
36:14:693:A:OP1	44:C5:45:ASN:ND2	2.48	0.46
49:F5:135:ALA:HB2	49:F5:229:PHE:HA	1.98	0.46
55:I5:52:LEU:HB2	55:I5:152:LEU:HD23	1.97	0.46
26:S2:101:LEU:H	26:S2:104:ASN:HB3	1.81	0.46
70:V5:58:VAL:O	70:V5:76:ALA:N	2.49	0.46
36:14:3334:U:O2	36:14:3368:U:O2'	2.34	0.46
36:14:974:G:OP1	67:Q5:16:ARG:NE	2.42	0.46
56:J5:55:ARG:CZ	82:A3:20:G:H22	2.27	0.46
6:C2:116:LYS:HB2	6:C2:131:ILE:HD12	1.98	0.46
36:14:590:G:H4'	44:C5:309:ARG:HH12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I2:50:GLY:HA2	34:22:397:A:H4'	1.98	0.46
56:J5:55:ARG:CZ	82:A3:20:G:C2	2.99	0.46
45:D5:60:ILE:HB	45:D5:80:SER:HB3	1.98	0.46
78:E5:35:VAL:HG21	78:E5:90:LYS:HE2	1.98	0.46
15:H2:162:ILE:HG22	15:H2:165:LYS:HD2	1.98	0.46
20:M2:52:LEU:HD11	20:M2:60:VAL:HG11	1.96	0.46
20:M2:97:LEU:HD22	20:M2:119:SER:H	1.81	0.46
66:P5:41:LEU:HD12	66:P5:150:VAL:HG11	1.98	0.46
12:F2:189:THR:OG1	33:Z2:98:GLN:NE2	2.49	0.46
36:14:2483:G:N2	36:14:2486:A:OP2	2.40	0.46
36:14:3004:C:H4'	42:B5:99:LEU:HB2	1.97	0.46
4:B2:137:ILE:HD11	4:B2:172:LEU:HB3	1.97	0.46
6:C2:142:GLY:N	6:C2:153:SER:O	2.44	0.46
24:Q2:17:THR:OG1	24:Q2:70:THR:OG1	2.33	0.46
26:S2:82:PRO:HB2	26:S2:84:TRP:CD1	2.51	0.46
31:X2:73:ARG:HH21	31:X2:82:LYS:HB3	1.81	0.46
36:14:727:G:OP2	36:14:742:G:N2	2.47	0.45
34:22:1352:G:N2	34:22:1373:C:O2	2.41	0.45
42:B5:77:THR:HG21	42:B5:328:ILE:HG22	1.97	0.45
44:C5:23:PRO:HG2	44:C5:258:LEU:HD23	1.98	0.45
13:G2:175:ILE:HD13	34:22:78:A:H1'	1.98	0.45
20:M2:60:VAL:HG22	20:M2:122:VAL:HG22	1.98	0.45
70:V5:18:PRO:HA	70:V5:51:ALA:HA	1.96	0.45
31:X2:69:ARG:HG3	31:X2:117:ILE:HG12	1.98	0.45
31:X2:143:PRO:HG3	80:A6:484:GLU:HB2	1.98	0.45
36:14:1778:G:O2'	36:14:1780:G:OP2	2.33	0.45
36:14:2843:U:H5''	36:14:2844:C:H5	1.81	0.45
36:14:728:G:H5''	67:Q5:43:PRO:HB2	1.97	0.45
8:D2:34:TYR:OH	34:22:1487:A:OP1	28.47	0.45
8:D2:23:GLU:HB3	18:K2:61:TRP:HE1	1.81	0.45
62:M5:38:ILE:HG13	62:M5:44:VAL:HG12	1.98	0.45
31:X2:6:PRO:HG3	31:X2:14:LYS:HD3	1.97	0.45
31:X2:25:ALA:HB1	34:22:1108:G:H2'	1.99	0.45
31:X2:69:ARG:HB3	31:X2:86:PHE:HE1	1.82	0.45
36:14:2631:U:OP1	36:14:2757:U:O2'	2.33	0.45
34:22:47:A:N7	34:22:98:U:O2'	2.47	0.45
80:A6:447:VAL:HG21	80:A6:476:LEU:HD22	1.96	0.45
8:D2:42:THR:OG1	8:D2:45:LYS:O	2.29	0.45
66:P5:61:ARG:HG2	66:P5:78:VAL:HG21	1.97	0.45
36:14:2389:C:H5''	66:P5:66:SER:HA	1.98	0.45
30:W2:41:MET:HG2	30:W2:129:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:1962:G:H1'	36:14:2080:C:H42	1.80	0.45
36:14:3129:A:N6	36:14:3131:U:O2	2.49	0.45
33:Z2:74:SER:CB	34:22:1534:G:OP2	2.63	0.45
45:D5:99:TYR:HE2	45:D5:244:HIS:HE1	1.63	0.45
10:E2:85:GLY:N	10:E2:88:ASP:OD2	2.44	0.45
15:H2:51:VAL:HG23	15:H2:53:GLY:H	1.80	0.45
26:S2:116:LEU:HB3	26:S2:124:GLY:HA3	1.98	0.45
36:14:129:U:H3	36:14:139:G:H1	1.65	0.45
36:14:609:G:OP2	44:C5:315:LYS:NZ	2.40	0.45
34:22:720:G:OP2	34:22:720:G:N2	2.49	0.45
10:E2:45:ILE:HG13	10:E2:61:VAL:HG21	1.98	0.45
15:H2:64:VAL:HG22	15:H2:94:ALA:HB1	1.98	0.45
16:I2:159:GLN:HE22	16:I2:189:LEU:HD11	1.81	0.45
24:Q2:16:ALA:HB2	24:Q2:72:GLY:HA3	1.98	0.45
36:14:1846:C:OP1	36:14:1849:C:N4	2.44	0.45
36:14:3184:A:O2'	53:H5:23:ARG:NH1	2.48	0.45
36:14:3212:C:OP2	62:M5:124:ARG:NH2	2.50	0.45
36:14:337:G:H1	38:44:26:U:H3	1.65	0.45
36:14:371:G:N1	36:14:374:A:OP2	2.46	0.45
31:X2:62:LYS:NZ	34:22:1136:U:OP1	2.45	0.45
34:22:895:G:H1	34:22:917:U:H3	1.63	0.45
36:14:1831:U:O2'	38:44:114:G:OP1	2.30	0.45
42:B5:183:LEU:O	42:B5:191:LYS:NZ	2.45	0.45
37:34:14:U:OP1	45:D5:24:ARG:NH1	2.50	0.45
15:H2:148:LYS:NZ	34:22:640:U:O2'	2.50	0.45
53:H5:23:ARG:HD2	53:H5:39:LYS:HA	1.98	0.45
55:I5:30:LYS:HG3	55:I5:63:GLU:HG3	1.99	0.45
23:P2:108:ARG:HH21	26:S2:119:ILE:HA	1.81	0.45
33:Z2:73:GLY:HA3	34:22:1534:G:N9	2.31	0.45
36:14:1257:C:H42	36:14:1261:G:H22	1.64	0.45
34:22:1208:A:O2'	34:22:1270:G:OP2	2.34	0.45
2:A2:50:VAL:H	25:R2:109:LEU:HD21	1.80	0.45
36:14:2737:C:O2'	42:B5:36:ASP:OD1	137.22	0.45
37:34:17:A:OP1	45:D5:2:ALA:N	2.49	0.45
13:G2:102:VAL:HG13	13:G2:106:LEU:HD12	1.98	0.45
53:H5:90:MET:HG2	53:H5:181:VAL:HA	1.98	0.45
16:I2:78:ILE:HG12	16:I2:104:ILE:HG22	1.99	0.45
77:T5:92:ARG:HB3	77:T5:95:HIS:HD2	1.81	0.45
36:14:1235:U:H4'	36:14:1236:G:H5'	1.99	0.45
36:14:1705:U:O2	36:14:1786:G:O2'	2.34	0.45
36:14:1201:C:N4	36:14:2857:C:OP1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:3272:C:H5'	78:E5:78:ARG:HB2	1.99	0.45
12:F2:101:GLY:H	34:22:1166:A:H5''	1.82	0.45
1:A1:33:GLN:NE2	1:A1:321:ASP:OD2	2.50	0.45
80:A6:258:PHE:HD1	80:A6:261:ASN:HD22	1.63	0.45
13:G2:190:GLN:NE2	34:22:265:A:N7	2.64	0.45
16:I2:4:SER:HB2	16:I2:24:LYS:HE2	1.98	0.45
31:X2:107:PHE:HE1	31:X2:123:LYS:HB3	1.81	0.45
75:X5:75:LYS:HB3	75:X5:81:ILE:HB	1.98	0.45
36:14:1210:U:H5''	53:H5:62:ARG:HD3	1.99	0.45
36:14:2149:A:N6	36:14:2187:G:O2'	2.47	0.45
34:22:996:U:H3	34:22:1008:G:H1	1.65	0.45
1:A1:68:LYS:N	1:A1:86:VAL:O	2.50	0.45
19:L2:102:LYS:O	31:X2:13:ARG:NH2	2.46	0.45
71:Z5:33:SER:HB2	71:Z5:40:HIS:HE1	1.82	0.45
36:14:999:G:N3	36:14:1002:A:N6	2.65	0.45
36:14:1242:G:N2	36:14:1270:A:O2'	2.50	0.45
36:14:1553:U:H5''	36:14:1554:U:H5'	1.99	0.45
10:E2:77:ARG:NH2	34:22:122:U:O3'	2.50	0.45
34:22:473:A:H5'	34:22:769:A:H1'	1.98	0.45
34:22:898:A:N6	34:22:914:G:O2'	2.46	0.45
42:B5:232:ARG:NH1	42:B5:266:ARG:O	2.49	0.45
42:B5:47:LEU:HB3	42:B5:335:ILE:HD11	1.99	0.45
42:B5:57:VAL:HG22	42:B5:73:VAL:HG12	1.98	0.45
36:14:696:C:OP2	44:C5:119:ARG:NH2	2.50	0.45
78:E5:39:VAL:HG11	78:E5:158:TYR:HE2	1.83	0.45
68:S5:66:GLU:HB3	68:S5:69:PRO:HG3	1.98	0.45
36:14:1048:A:H2'	55:I5:22:TYR:HE2	1.82	0.44
36:14:63:A:N3	36:14:78:U:O2'	2.43	0.44
36:14:733:G:N2	36:14:736:A:OP2	2.42	0.44
34:22:163:G:N2	34:22:163:G:OP2	2.47	0.44
12:F2:182:ALA:O	12:F2:186:ASN:ND2	2.39	0.44
53:H5:20:ILE:HG13	53:H5:25:VAL:HA	1.99	0.44
55:I5:29:SER:HB2	55:I5:125:LEU:HD12	1.98	0.44
10:E2:23:LEU:HD21	17:J2:6:ARG:HH12	1.81	0.44
10:E2:64:ILE:HD11	32:Y2:18:LEU:HD11	1.99	0.44
36:14:532:A:N6	36:14:555:U:O2	2.50	0.44
34:22:1085:G:N2	34:22:1088:A:OP2	2.43	0.44
8:D2:108:LYS:NZ	80:A6:21:GLU:OE2	2.30	0.44
49:F5:96:PRO:HB2	49:F5:99:PRO:HD2	2.00	0.44
17:J2:78:ARG:NH1	34:22:763:G:OP1	2.50	0.44
62:M5:20:VAL:HB	62:M5:70:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:X5:96:LYS:HG3	75:X5:107:VAL:HB	2.00	0.44
36:14:2144:A:H1'	36:14:2281:A:H61	1.82	0.44
36:14:3116:G:N2	36:14:3116:G:OP1	2.41	0.44
36:14:3277:U:O4	66:P5:172:GLN:NE2	2.50	0.44
36:14:674:G:O6	67:Q5:56:LYS:NZ	2.49	0.44
6:C2:97:ARG:NH2	34:22:1301:U:OP2	2.50	0.44
12:F2:112:ARG:NH1	34:22:1529:C:OP1	2.49	0.44
8:D2:54:ARG:CD	80:A6:23:ASP:OD2	2.65	0.44
20:M2:51:ALA:HB1	20:M2:57:ALA:HB2	2.00	0.44
63:N5:120:TRP:HE1	63:N5:123:GLN:HB3	1.82	0.44
25:R2:102:VAL:HG21	25:R2:119:LEU:HG	1.99	0.44
70:V5:93:LEU:HB3	79:W5:20:LEU:HB3	1.99	0.44
36:14:1055:A:N3	37:34:81:U:O2'	2.44	0.44
36:14:1184:A:H5''	62:M5:59:ASN:HD22	1.82	0.44
36:14:1419:A:OP1	38:44:20:U:O2'	2.32	0.44
34:22:538:A:O2'	34:22:539:G:O4'	2.36	0.44
1:A1:146:VAL:HG23	1:A1:153:HIS:HB2	1.99	0.44
44:C5:283:THR:HB	44:C5:289:ILE:HD11	2.00	0.44
13:G2:74:LYS:HB3	13:G2:94:ARG:HG2	1.98	0.44
51:G5:133:LYS:HD2	51:G5:138:HIS:HE1	1.83	0.44
36:14:1875:G:N7	74:R5:20:ARG:NH2	2.65	0.44
1:A1:264:LYS:HB3	1:A1:281:ILE:HG12	1.99	0.44
44:C5:263:GLY:HA3	44:C5:269:SER:HA	1.98	0.44
10:E2:22:LYS:NZ	34:22:758:U:OP1	2.50	0.44
51:G5:187:GLY:HA2	51:G5:190:VAL:HG12	2.00	0.44
19:L2:2:SER:HA	19:L2:113:PRO:HB3	1.98	0.44
22:O2:30:VAL:HG13	22:O2:39:ILE:HG13	2.00	0.44
36:14:2898:G:N7	62:M5:125:LYS:NZ	98.06	0.44
8:D2:160:SER:OG	34:22:1329:A:OP2	2.31	0.44
42:B5:19:ARG:HB2	42:B5:232:ARG:HH21	1.81	0.44
8:D2:24:PHE:HZ	8:D2:72:LEU:HD13	1.82	0.44
21:N2:66:ILE:HG23	21:N2:67:THR:HG23	2.00	0.44
23:P2:96:ILE:O	23:P2:102:PHE:HA	2.17	0.44
25:R2:24:LEU:HD21	25:R2:34:LEU:HD22	1.99	0.44
36:14:2454:G:O6	36:14:2484:A:N6	2.41	0.44
36:14:627:U:H4'	36:14:1399:A:H1'	1.99	0.44
36:14:691:A:N1	38:44:28:C:O2'	2.44	0.44
36:14:40:A:O2'	36:14:937:G:O6	2.28	0.44
34:22:286:C:N4	34:22:287:G:O6	2.50	0.44
10:E2:3:ARG:NH2	34:22:94:U:OP2	2.50	0.44
23:P2:22:LEU:HD23	23:P2:25:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:14:1447:G:N7	66:P5:25:SER:OG	2.50	0.44
34:22:1151:A:O3'	34:22:1766:A:N6	2.51	0.44
34:22:1793:G:H1'	34:22:1794:A:H2'	2.00	0.44
34:22:417:A:O2'	34:22:418:G:OP2	2.32	0.44
15:H2:101:LYS:HD2	34:22:639:U:H5''	2.00	0.44
1:A1:119:LYS:NZ	1:A1:126:MET:SD	2.90	0.44
1:A1:66:LYS:HB3	1:A1:96:ASN:HD21	1.83	0.44
80:A6:521:PRO:HG3	80:A6:541:LEU:HD13	2.00	0.44
78:E5:149:ILE:HG12	78:E5:155:LEU:HD12	2.00	0.44
23:P2:123:TYR:CD2	23:P2:123:TYR:O	2.70	0.44
30:W2:2:THR:N	34:22:1034:C:O2'	2.44	0.44
75:X5:77:GLU:HG2	75:X5:133:LEU:HD12	2.00	0.44
36:14:147:U:O4	51:G5:183:LYS:NZ	2.45	0.44
36:14:2515:A:O3'	63:N5:31:ARG:NH2	2.51	0.44
1:A1:170:TYR:HB3	1:A1:187:LYS:HE2	1.99	0.44
45:D5:95:TRP:HD1	45:D5:158:ARG:HA	1.82	0.44
78:E5:101:PHE:HZ	78:E5:137:ASP:HB3	1.83	0.44
53:H5:20:ILE:HG22	53:H5:22:SER:H	1.82	0.44
36:14:1779:C:N4	74:R5:88:ARG:O	2.51	0.44
75:X5:111:ASN:HB2	75:X5:123:TYR:HB2	2.00	0.44
36:14:1050:U:OP2	77:T5:13:TYR:OH	2.26	0.43
36:14:28:C:OP1	63:N5:192:LYS:NZ	2.38	0.43
36:14:3241:G:OP2	42:B5:153:LYS:NZ	2.47	0.43
23:P2:126:VAL:HG21	34:22:1459:C:O4'	2.18	0.43
80:A6:174:GLY:HA2	80:A6:274:LEU:HD12	1.99	0.43
45:D5:107:ARG:HG3	45:D5:251:PRO:HG3	2.00	0.43
12:F2:93:LEU:HD23	12:F2:172:ILE:HG23	1.99	0.43
12:F2:50:GLU:HA	12:F2:65:ARG:HH22	1.83	0.43
70:V5:15:LEU:HD13	70:V5:51:ALA:HB3	2.00	0.43
31:X2:126:LYS:HE2	31:X2:129:GLY:HA2	2.00	0.43
36:14:1001:G:O2'	36:14:1041:U:OP2	2.36	0.43
36:14:840:C:H5'	36:14:1724:U:H5	1.83	0.43
36:14:3084:C:OP1	79:W5:38:SER:OG	2.32	0.43
56:J5:55:ARG:HH21	82:A3:20:G:H22	1.53	0.43
2:A2:69:ASN:OD1	6:C2:244:SER:OG	2.36	0.43
8:D2:54:ARG:HD2	80:A6:23:ASP:OD2	2.18	0.43
78:E5:154:LEU:HD23	78:E5:157:GLN:HE21	1.83	0.43
30:W2:11:LEU:HD23	30:W2:14:ILE:HD12	2.00	0.43
34:22:1267:G:O2'	34:22:1448:G:O2'	2.35	0.43
37:34:96:U:OP1	68:S5:43:TYR:OH	2.33	0.43
42:B5:252:ILE:HG21	42:B5:260:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E2:37:LYS:HB2	10:E2:40:GLU:HG2	2.00	0.43
55:I5:51:HIS:HB2	55:I5:166:ILE:HD11	1.99	0.43
56:J5:86:VAL:HG21	56:J5:111:ASP:HB3	2.00	0.43
28:U2:70:THR:OG1	28:U2:72:ASN:OD1	2.36	0.43
34:22:1693:A:H61	34:22:1709:C:H42	1.67	0.43
34:22:56:U:O2'	34:22:57:G:O4'	2.33	0.43
40:A5:190:ARG:HG3	40:A5:191:LEU:HD12	1.99	0.43
8:D2:69:LEU:HD23	8:D2:72:LEU:HD12	1.99	0.43
36:14:2838:A:H4'	55:I5:74:LYS:HD2	2.00	0.43
62:M5:20:VAL:O	62:M5:66:THR:OG1	2.32	0.43
32:Y2:57:VAL:O	32:Y2:94:TYR:OH	2.36	0.43
36:14:1127:G:N2	36:14:1130:A:OP2	2.41	0.43
36:14:1868:G:N2	36:14:2118:C:O2	2.51	0.43
36:14:1959:G:H1	36:14:2082:U:H3	1.65	0.43
36:14:75:G:O3'	60:L5:70:ARG:NH2	2.49	0.43
34:22:460:A:H3'	34:22:461:G:H8	1.83	0.43
40:A5:45:VAL:HB	40:A5:61:VAL:HG22	2.01	0.43
80:A6:255:HIS:HB2	80:A6:258:PHE:HD2	1.83	0.43
68:S5:80:ARG:HE	77:T5:156:TYR:HB2	1.83	0.43
36:14:3368:U:H1'	36:14:3370:A:H1'	2.01	0.43
15:H2:107:ARG:NH1	34:22:741:C:O2	2.45	0.43
51:G5:99:PRO:HG2	51:G5:190:VAL:HG23	1.99	0.43
24:Q2:21:HIS:CE1	24:Q2:68:ARG:HH12	2.37	0.43
25:R2:44:LYS:HG3	25:R2:47:ARG:HH21	1.83	0.43
36:14:14:U:O2'	75:X5:42:ARG:NE	2.51	0.43
34:22:1001:A:OP1	82:A3:38:A:O2'	2.36	0.43
34:22:1158:C:H1'	34:22:1161:C:H41	1.83	0.43
53:H5:89:LYS:HG2	53:H5:145:VAL:HG22	2.00	0.43
63:N5:104:GLU:HA	63:N5:160:GLU:HG3	2.01	0.43
63:N5:62:TYR:HD2	63:N5:134:LEU:HD13	1.83	0.43
76:Y5:119:ILE:HG22	76:Y5:124:GLY:HA3	2.00	0.43
36:14:2512:C:OP1	51:G5:249:ARG:NH1	2.46	0.43
36:14:590:G:N1	36:14:611:A:OP2	2.51	0.43
34:22:1533:C:H4'	34:22:1539:G:C6	2.54	0.43
22:O2:123:SER:HB2	34:22:885:G:H21	1.83	0.43
2:A2:49:ASN:HD22	2:A2:52:LYS:HD2	1.83	0.43
26:S2:2:SER:OG	26:S2:3:LEU:N	2.51	0.43
36:14:938:C:O2	36:14:2813:A:O2'	2.37	0.43
34:22:1542:G:N2	34:22:1568:C:O2'	2.47	0.43
40:A5:134:VAL:HG12	40:A5:151:PRO:HD3	2.00	0.43
51:G5:165:PHE:HZ	63:N5:3:ALA:HB1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:V5:38:ALA:HB3	70:V5:59:MET:HB2	2.00	0.43
30:W2:26:LEU:HD21	30:W2:60:LYS:HD3	2.01	0.43
31:X2:103:LEU:N	31:X2:126:LYS:O	2.51	0.43
32:Y2:37:LYS:HG3	34:22:522:U:H5''	2.01	0.43
36:14:3050:U:H4'	79:W5:17:ARG:HG3	2.01	0.43
80:A6:419:ALA:HB3	80:A6:478:LEU:HB2	2.00	0.43
42:B5:306:THR:HG21	42:B5:316:GLU:HG2	2.00	0.43
53:H5:10:ILE:HG12	53:H5:72:LYS:HG3	2.00	0.43
77:T5:99:SER:HG	77:T5:101:CYS:HG	1.60	0.43
36:14:1796:G:H4'	40:A5:22:LEU:HD11	2.00	0.42
36:14:2948:C:H5''	42:B5:243:HIS:HB3	1.99	0.42
23:P2:42:ARG:NH2	34:22:1550:A:OP2	2.50	0.42
31:X2:106:GLY:H	34:22:599:A:H4'	1.84	0.42
32:Y2:9:THR:N	34:22:780:A:O2'	2.47	0.42
36:14:1152:G:N2	36:14:1152:G:OP2	2.49	0.42
37:34:44:C:O2'	45:D5:152:ARG:NH1	2.52	0.42
28:U2:50:LEU:HD21	28:U2:95:ALA:HB2	2.01	0.42
29:V2:78:LEU:HD12	29:V2:79:LEU:HD12	2.01	0.42
36:14:1595:U:O2'	36:14:1606:U:O2	2.33	0.42
36:14:638:C:O2'	36:14:1434:G:N2	2.50	0.42
34:22:1523:G:N2	34:22:1523:G:OP2	2.48	0.42
34:22:23:G:O2'	34:22:368:U:OP1	2.37	0.42
1:A1:21:LEU:HD12	1:A1:22:PRO:HD2	2.01	0.42
82:A3:58:1MA:O2'	82:A3:60:C:OP2	2.29	0.42
80:A6:542:ILE:HB	80:A6:566:PHE:HB2	2.00	0.42
44:C5:126:ILE:HD11	44:C5:233:LEU:HD11	2.00	0.42
44:C5:22:LEU:HD23	44:C5:255:PHE:HZ	1.84	0.42
45:D5:294:ALA:HA	55:I5:217:PHE:HB3	2.02	0.42
36:14:2418:G:OP2	36:14:2606:G:N2	2.53	0.42
34:22:495:C:H3'	34:22:496:G:H4'	2.01	0.42
34:22:901:G:N2	34:22:901:G:OP2	2.43	0.42
37:34:77:G:HO2'	37:34:101:G:H1	1.67	0.42
40:A5:101:VAL:HA	40:A5:165:VAL:HA	2.01	0.42
42:B5:223:GLY:HA2	42:B5:271:GLY:HA3	2.00	0.42
49:F5:178:ILE:HD11	49:F5:187:GLU:HG3	2.00	0.42
22:O2:24:ASN:ND2	34:22:902:G:N7	2.67	0.42
36:14:2146:C:OP1	40:A5:200:ARG:NH1	2.50	0.42
42:B5:115:LYS:NZ	42:B5:129:ALA:O	2.51	0.42
42:B5:168:LYS:HB3	42:B5:319:ASN:HD21	1.84	0.42
6:C2:139:ILE:HG12	6:C2:218:ILE:HB	2.01	0.42
10:E2:11:ARG:NH1	10:E2:21:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:C5:318:LEU:HD21	49:F5:145:ARG:HH12	1.83	0.42
33:Z2:61:SER:OG	33:Z2:62:VAL:N	2.52	0.42
36:14:1307:G:O2'	36:14:1308:A:O5'	2.35	0.42
36:14:520:U:O4	44:C5:349:THR:OG1	2.34	0.42
36:14:533:A:N6	36:14:535:G:N3	2.67	0.42
34:22:1191:U:O2	82:A3:34:OMG:C5'	2.66	0.42
6:C2:205:ARG:NH1	34:22:7:G:N7	2.67	0.42
82:A3:18:G:O2'	82:A3:60:C:N4	2.52	0.42
51:G5:229:VAL:HA	51:G5:232:HIS:HD2	1.85	0.42
15:H2:67:LEU:HD12	15:H2:70:PHE:HB2	2.02	0.42
20:M2:63:VAL:HG11	20:M2:94:ALA:HB2	2.02	0.42
26:S2:139:LYS:HD3	34:22:1177:C:H41	1.84	0.42
26:S2:57:ARG:HH22	33:Z2:74:SER:HB2	1.83	0.42
36:14:589:A:N6	36:14:610:G:O2'	2.45	0.42
34:22:628:G:H21	34:22:971:A:H62	1.66	0.42
38:44:68:G:OP2	56:J5:85:LYS:NZ	187.78	0.42
1:A1:372:LEU:HD22	1:A1:376:LEU:HD12	2.00	0.42
2:A2:101:ARG:HG2	2:A2:103:THR:H	1.85	0.42
40:A5:27:ALA:HB3	40:A5:128:ARG:HH21	1.85	0.42
1:A1:365:LEU:HD21	80:A6:521:PRO:HD2	2.01	0.42
42:B5:41:VAL:HA	42:B5:185:GLY:HA3	2.01	0.42
13:G2:92:ARG:O	34:22:405:C:O2'	2.34	0.42
15:H2:49:ILE:HD11	15:H2:172:VAL:HG22	2.01	0.42
16:I2:22:ARG:HB3	34:22:385:A:H5''	2.01	0.42
34:22:593:U:H4'	34:22:595:G:H4'	2.00	0.42
21:N2:20:ARG:HH22	34:22:861:U:H4'	1.85	0.42
1:A1:210:THR:HA	1:A1:245:MET:HB3	2.02	0.42
44:C5:326:ARG:HG3	44:C5:327:LEU:HD12	2.01	0.42
15:H2:139:ARG:HB2	15:H2:151:LYS:HB2	2.02	0.42
16:I2:184:LEU:HD23	16:I2:189:LEU:HA	2.02	0.42
21:N2:97:SER:HA	21:N2:100:LYS:HE2	2.01	0.42
26:S2:81:ILE:HA	26:S2:82:PRO:HD3	1.89	0.42
2:A2:140:ASN:ND2	29:V2:31:SER:O	2.42	0.42
30:W2:46:TYR:HB3	30:W2:69:LEU:HD13	2.01	0.42
36:14:1463:U:H3	36:14:1467:A:H62	1.66	0.42
36:14:1920:U:O2'	36:14:1932:A:N7	2.46	0.42
19:L2:106:ASN:ND2	34:22:349:U:OP2	2.51	0.42
82:A3:37:YYG:H2'	82:A3:37:YYG:H31	2.02	0.42
80:A6:406:LEU:HD12	80:A6:423:GLY:HA2	2.02	0.42
80:A6:451:GLN:O	80:A6:475:THR:N	2.50	0.42
10:E2:17:HIS:O	10:E2:51:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G2:70:PRO:HA	13:G2:99:GLY:HA3	2.02	0.42
16:I2:110:ARG:HH22	36:14:3352:U:H3	1.68	0.42
23:P2:130:ARG:CD	23:P2:130:ARG:H	2.11	0.42
32:Y2:29:HIS:ND1	32:Y2:32:ARG:O	2.47	0.42
26:S2:4:VAL:CG2	33:Z2:42:LEU:CD2	2.98	0.42
36:14:2185:G:O2'	36:14:2314:U:OP2	2.29	0.42
36:14:3022:G:N7	80:A6:211:LYS:NZ	2.47	0.42
36:14:691:A:N7	44:C5:48:GLN:NE2	2.67	0.42
34:22:1291:G:H1	34:22:1324:G:H22	1.66	0.42
37:34:64:A:H5'	37:34:65:G:H5''	2.02	0.42
56:J5:55:ARG:CZ	82:A3:19:G:O2'	2.68	0.42
40:A5:147:ARG:HA	40:A5:157:VAL:HA	2.02	0.42
80:A6:405:VAL:HG13	80:A6:421:VAL:HG13	2.02	0.42
12:F2:187:ILE:HG22	33:Z2:63:SER:HA	2.02	0.42
62:M5:28:SER:HB3	62:M5:31:LYS:HB2	2.01	0.42
22:O2:47:LYS:NZ	22:O2:62:LEU:O	2.53	0.42
66:P5:179:GLN:HA	66:P5:182:ILE:HD12	2.02	0.42
77:T5:92:ARG:HB3	77:T5:95:HIS:CD2	2.54	0.42
30:W2:11:LEU:HD21	30:W2:37:PHE:HE2	1.85	0.42
30:W2:88:LYS:O	30:W2:92:ASN:ND2	2.53	0.42
36:14:2110:G:O2'	36:14:2112:U:OP2	2.37	0.41
36:14:2192:C:O2'	36:14:2312:A:N1	2.49	0.41
36:14:824:C:H5''	40:A5:21:ARG:HG3	2.01	0.41
36:14:978:G:O2'	36:14:979:U:O2	2.38	0.41
27:T2:60:SER:HB2	34:22:1479:A:H5''	2.02	0.41
38:44:142:C:OP1	63:N5:38:ARG:NH1	2.51	0.41
63:N5:35:VAL:HG12	63:N5:36:ILE:HG13	2.01	0.41
36:14:2168:A:N6	36:14:2170:U:O2	2.53	0.41
36:14:2392:C:H1'	42:B5:266:ARG:HH21	1.84	0.41
36:14:2621:G:N2	82:A3:74:C:C4	2.88	0.41
34:22:646:C:H42	34:22:688:G:H1	1.68	0.41
38:44:83:C:O2'	38:44:85:G:N2	2.53	0.41
2:A2:121:VAL:HG23	2:A2:141:ILE:HG21	2.02	0.41
80:A6:594:LEU:HB2	80:A6:602:ALA:HB3	2.02	0.41
45:D5:34:LYS:HG2	77:T5:27:LEU:HD21	2.02	0.41
22:O2:61:MET:HG3	22:O2:100:ALA:HB1	2.02	0.41
36:14:2592:G:H4'	36:14:2594:C:C2	2.55	0.41
36:14:1134:G:O2'	36:14:2642:A:N3	2.48	0.41
36:14:3375:A:O2'	36:14:3378:C:OP2	2.32	0.41
1:A1:148:GLN:HB2	1:A1:254:GLY:HA3	2.01	0.41
80:A6:285:SER:HA	80:A6:289:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R2:27:ASP:O	25:R2:31:ASN:ND2	2.53	0.41
74:R5:134:HIS:HE1	74:R5:136:ARG:HB3	1.85	0.41
36:14:969:C:OP1	77:T5:82:ASN:ND2	2.53	0.41
71:Z5:27:LYS:HB3	71:Z5:42:LEU:HB2	2.01	0.41
36:14:2354:C:O2'	66:P5:139:TYR:OH	2.32	0.41
13:G2:186:ARG:NH2	34:22:269:G:OP2	2.44	0.41
19:L2:57:LYS:NZ	34:22:326:G:OP1	2.49	0.41
1:A1:319:LEU:HB2	1:A1:351:VAL:HG22	2.01	0.41
1:A1:45:LYS:HD2	1:A1:107:PHE:HD1	1.85	0.41
42:B5:161:LEU:HB3	42:B5:178:LEU:HD11	2.02	0.41
42:B5:216:ASP:HB2	42:B5:339:ARG:HB3	2.02	0.41
51:G5:178:ALA:HB2	51:G5:218:ILE:HD13	2.02	0.41
66:P5:122:ALA:HB3	66:P5:143:PRO:HG2	2.01	0.41
77:T5:66:ASN:O	77:T5:73:GLY:N	2.53	0.41
36:14:1750:A:O2'	36:14:1752:A:OP2	2.35	0.41
36:14:2178:A:H1'	36:14:2180:G:C6	2.56	0.41
36:14:2150:G:O2'	36:14:2189:U:OP1	2.35	0.41
36:14:3022:G:O5'	80:A6:213:SER:OG	2.33	0.41
38:44:97:A:O2'	53:H5:59:ASN:ND2	151.21	0.41
56:J5:13:LYS:HE3	56:J5:134:PRO:HG3	2.03	0.41
66:P5:67:ILE:HB	66:P5:80:LYS:HE2	2.02	0.41
36:14:799:G:HO2'	60:L5:18:TRP:HE1	1.68	0.41
34:22:1502:G:N2	34:22:1505:A:OP2	2.50	0.41
1:A1:176:LYS:HE3	80:A6:222:GLN:C	2.41	0.41
36:14:3009:G:O2'	42:B5:14:LEU:O	2.34	0.41
42:B5:215:ILE:HD11	42:B5:324:VAL:HG21	2.02	0.41
36:14:209:A:N3	44:C5:221:ASN:ND2	2.69	0.41
8:D2:56:GLN:H	80:A6:31:TYR:HH	1.62	0.41
21:N2:108:ASP:OD1	34:22:878:G:O2'	2.34	0.41
70:V5:104:ASN:OD1	70:V5:108:GLU:N	2.54	0.41
31:X2:57:LEU:HB3	31:X2:59:ILE:HG12	2.02	0.41
75:X5:105:VAL:HG21	75:X5:135:ILE:HD12	2.03	0.41
33:Z2:77:ARG:NH1	34:22:1533:C:C6	2.78	0.41
36:14:123:A:OP1	51:G5:105:LYS:NZ	2.40	0.41
36:14:1857:C:N4	36:14:1858:A:N1	2.69	0.41
36:14:3216:G:O2'	36:14:3219:G:O2'	2.25	0.41
34:22:1472:C:O2'	34:22:1534:G:N2	2.54	0.41
44:C5:193:LYS:HA	44:C5:198:ARG:HA	2.03	0.41
8:D2:7:LYS:HE2	28:U2:27:THR:HG21	2.03	0.41
12:F2:118:LEU:HD22	12:F2:129:PRO:HB2	2.01	0.41
51:G5:69:LEU:HD21	63:N5:24:ARG:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:G5:81:THR:HA	51:G5:222:PHE:HZ	1.85	0.41
23:P2:29:SER:HB2	23:P2:32:ASP:HB2	2.02	0.41
28:U2:41:ILE:HG23	28:U2:103:ILE:HD11	2.01	0.41
28:U2:28:SER:HB2	28:U2:112:VAL:HG22	2.02	0.41
33:Z2:73:GLY:HA3	34:22:1534:G:C1'	2.51	0.41
36:14:2186:U:O2'	36:14:2313:A:N3	2.47	0.41
1:A1:210:THR:OG1	1:A1:245:MET:O	2.35	0.41
36:14:2242:A:H5''	40:A5:244:GLY:HA3	2.02	0.41
4:B2:91:VAL:HA	4:B2:96:LEU:HA	2.03	0.41
44:C5:335:ALA:HA	44:C5:338:LYS:HA	2.02	0.41
12:F2:65:ARG:HA	12:F2:66:GLN:HA	1.86	0.41
12:F2:72:HIS:ND1	24:Q2:79:TYR:OH	2.39	0.41
13:G2:33:GLY:N	13:G2:52:ILE:O	2.53	0.41
15:H2:21:ALA:HA	15:H2:24:PHE:HD2	1.85	0.41
16:I2:159:GLN:O	16:I2:163:GLY:N	2.54	0.41
55:I5:91:VAL:HG23	55:I5:135:ILE:HA	2.02	0.41
68:S5:124:LEU:HA	77:T5:153:PRO:HG2	2.02	0.41
36:14:1953:G:N1	36:14:2093:A:N7	2.68	0.41
13:G2:13:GLN:NE2	34:22:151:G:N3	2.68	0.41
2:A2:164:ASN:HA	2:A2:170:ILE:HD11	2.03	0.41
80:A6:184:MET:HG2	80:A6:249:ILE:HD11	2.03	0.41
4:B2:117:TRP:HE3	4:B2:153:HIS:HB3	1.85	0.41
56:J5:55:ARG:HD2	82:A3:20:G:C2	2.24	0.41
74:R5:134:HIS:CE1	74:R5:136:ARG:HB3	2.56	0.41
68:S5:80:ARG:HB3	68:S5:122:HIS:HB2	2.02	0.41
76:Y5:68:GLY:HA2	76:Y5:84:LYS:HD2	2.03	0.41
36:14:2282:U:OP1	36:14:2973:G:O2'	2.38	0.41
36:14:3294:A:H5'	42:B5:128:LYS:HD3	2.03	0.41
34:22:1297:G:N2	34:22:1300:A:OP2	2.41	0.41
10:E2:30:ARG:NH2	34:22:298:C:O2'	2.46	0.41
37:34:79:A:H62	37:34:101:G:H21	1.67	0.41
42:B5:92:TYR:HB2	42:B5:157:VAL:HG23	2.03	0.41
8:D2:113:LEU:HD11	8:D2:117:ARG:HD2	2.03	0.41
8:D2:39:VAL:HG23	8:D2:48:VAL:HG22	2.02	0.41
12:F2:70:VAL:HG23	12:F2:72:HIS:H	1.85	0.41
55:I5:60:LEU:O	55:I5:127:ALA:N	2.52	0.41
70:V5:79:VAL:HB	70:V5:118:VAL:HG22	2.03	0.41
36:14:1970:U:H3	36:14:2052:G:H1	1.69	0.41
36:14:3068:U:OP2	74:R5:62:ARG:NH1	2.50	0.41
80:A6:263:ILE:HA	80:A6:266:ILE:HG12	2.01	0.41
17:J2:143:ILE:HA	17:J2:144:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q2:13:LYS:HG3	24:Q2:14:LYS:H	1.85	0.41
26:S2:4:VAL:HG21	33:Z2:42:LEU:CD2	2.45	0.41
36:14:1814:A:H4'	36:14:1815:U:H5'	2.03	0.40
34:22:648:G:H22	34:22:687:G:H1'	1.87	0.40
34:22:732:G:O2'	34:22:733:A:O4'	2.39	0.40
34:22:907:A:N3	34:22:997:G:O2'	2.45	0.40
1:A1:305:VAL:HG21	1:A1:368:ILE:HG22	2.02	0.40
80:A6:528:PHE:HB2	80:A6:593:VAL:HB	2.02	0.40
56:J5:92:ARG:HH12	56:J5:94:ARG:HD2	1.85	0.40
62:M5:25:LYS:HE2	62:M5:62:GLN:HG2	2.03	0.40
36:14:627:U:H2'	36:14:628:A:C8	2.57	0.40
34:22:1561:U:H2'	34:22:1562:G:H8	1.85	0.40
16:I2:36:THR:OG1	16:I2:59:ARG:N	2.54	0.40
17:J2:113:VAL:HG13	17:J2:118:LEU:HB2	2.04	0.40
72:K5:77:SER:HB2	72:K5:104:VAL:HG12	2.02	0.40
66:P5:114:VAL:HA	66:P5:150:VAL:HA	2.02	0.40
66:P5:64:ASN:O	66:P5:80:LYS:NZ	2.39	0.40
68:S5:8:GLN:HB3	68:S5:64:ILE:HD11	2.03	0.40
32:Y2:92:VAL:HG21	32:Y2:99:LYS:HD3	2.04	0.40
36:14:1284:C:O2'	36:14:1285:G:O4'	2.40	0.40
38:44:131:A:H2'	38:44:132:G:H8	1.87	0.40
56:J5:55:ARG:NH2	82:A3:20:G:H22	2.06	0.40
40:A5:19:HIS:ND1	40:A5:190:ARG:O	2.42	0.40
80:A6:483:PRO:HA	80:A6:486:ILE:HD12	2.03	0.40
51:G5:41:GLN:HB3	51:G5:44:ARG:HH12	1.86	0.40
15:H2:50:ASP:HA	15:H2:56:LYS:HA	2.03	0.40
62:M5:23:ILE:HA	62:M5:63:VAL:HG23	2.03	0.40
66:P5:50:GLN:HB3	66:P5:55:GLN:HB3	2.03	0.40
27:T2:37:VAL:HG11	27:T2:100:ILE:HD11	2.03	0.40
36:14:153:U:H4'	36:14:158:G:H4'	2.03	0.40
36:14:2444:C:H42	36:14:2502:A:H61	1.69	0.40
36:14:31:C:OP2	63:N5:187:ARG:NH2	2.47	0.40
34:22:29:U:H2'	34:22:30:G:H8	1.86	0.40
15:H2:117:THR:OG1	34:22:638:U:O3'	2.35	0.40
4:B2:159:SER:OG	34:22:874:C:OP1	2.33	0.40
80:A6:144:LYS:HE2	80:A6:437:THR:HG21	2.03	0.40
45:D5:211:LEU:HB3	45:D5:219:PHE:HB2	2.03	0.40
51:G5:96:LYS:HB3	51:G5:204:ARG:HH12	1.86	0.40
16:I2:8:ARG:HA	16:I2:18:ARG:HE	1.85	0.40
60:L5:54:LEU:HD11	60:L5:119:TYR:CG	2.55	0.40
20:M2:97:LEU:HD13	20:M2:119:SER:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:U2:103:ILE:HA	28:U2:106:ILE:HG22	2.03	0.40
36:14:23:A:OP1	56:J5:44:THR:N	127.32	0.40
1:A1:215:SER:HB2	1:A1:219:TYR:HB2	2.02	0.40
2:A2:71:GLU:HA	2:A2:95:ALA:H	1.87	0.40
80:A6:596:LYS:HG2	80:A6:601:ILE:HD13	2.02	0.40
4:B2:38:PHE:CG	4:B2:73:LEU:HD13	2.57	0.40
63:N5:178:HIS:O	63:N5:181:ASN:ND2	2.55	0.40
36:14:1602:A:H5'	74:R5:37:SER:HA	2.04	0.40
26:S2:11:PHE:CE1	33:Z2:41:ILE:HG13	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	379/381 (100%)	352 (93%)	27 (7%)	0	100	100
2	A2	205/207 (99%)	185 (90%)	19 (9%)	1 (0%)	34	71
3	a2	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
4	B2	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
5	b2	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
6	C2	215/217 (99%)	206 (96%)	9 (4%)	0	100	100
7	c2	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
8	D2	221/223 (99%)	210 (95%)	11 (5%)	0	100	100
9	d2	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
10	E2	258/260 (99%)	233 (90%)	25 (10%)	0	100	100
11	e2	58/60 (97%)	55 (95%)	3 (5%)	0	100	100
12	F2	204/206 (99%)	182 (89%)	22 (11%)	0	100	100
13	G2	224/226 (99%)	204 (91%)	18 (8%)	2 (1%)	21	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	g2	316/318 (99%)	299 (95%)	17 (5%)	0	100	100
15	H2	182/184 (99%)	166 (91%)	16 (9%)	0	100	100
16	I2	184/199 (92%)	163 (89%)	21 (11%)	0	100	100
17	J2	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
18	K2	94/96 (98%)	82 (87%)	12 (13%)	0	100	100
19	L2	153/155 (99%)	140 (92%)	13 (8%)	0	100	100
20	M2	122/124 (98%)	95 (78%)	27 (22%)	0	100	100
21	N2	148/150 (99%)	140 (95%)	8 (5%)	0	100	100
22	O2	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
23	P2	122/124 (98%)	113 (93%)	9 (7%)	0	100	100
24	Q2	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
25	R2	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
26	S2	143/145 (99%)	128 (90%)	14 (10%)	1 (1%)	26	66
27	T2	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
28	U2	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
29	V2	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
30	W2	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
31	X2	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
32	Y2	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
33	Z2	68/70 (97%)	68 (100%)	0	0	100	100
35	f2	69/71 (97%)	56 (81%)	13 (19%)	0	100	100
39	a5	146/148 (99%)	129 (88%)	16 (11%)	1 (1%)	26	66
40	A5	250/252 (99%)	235 (94%)	15 (6%)	0	100	100
41	b5	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
42	B5	384/386 (100%)	368 (96%)	16 (4%)	0	100	100
43	c5	95/97 (98%)	95 (100%)	0	0	100	100
44	C5	359/361 (99%)	330 (92%)	29 (8%)	0	100	100
45	D5	294/296 (99%)	281 (96%)	13 (4%)	0	100	100
46	d5	107/109 (98%)	99 (92%)	8 (8%)	0	100	100
47	e5	125/127 (98%)	118 (94%)	7 (6%)	0	100	100
48	f5	104/106 (98%)	99 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	F5	220/222 (99%)	211 (96%)	7 (3%)	2 (1%)	21	60
50	g5	110/112 (98%)	108 (98%)	2 (2%)	0	100	100
51	G5	231/233 (99%)	219 (95%)	12 (5%)	0	100	100
52	h5	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
53	H5	189/191 (99%)	173 (92%)	16 (8%)	0	100	100
54	i5	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
55	I5	207/220 (94%)	201 (97%)	6 (3%)	0	100	100
56	J5	167/169 (99%)	155 (93%)	12 (7%)	0	100	100
57	j5	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
58	k5	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
59	l5	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
60	L5	191/193 (99%)	174 (91%)	15 (8%)	2 (1%)	19	58
61	m5	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
62	M5	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
63	N5	201/203 (99%)	187 (93%)	14 (7%)	0	100	100
64	o5	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
65	p5	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
66	P5	181/183 (99%)	175 (97%)	6 (3%)	0	100	100
67	Q5	183/185 (99%)	175 (96%)	8 (4%)	0	100	100
68	S5	170/172 (99%)	158 (93%)	12 (7%)	0	100	100
69	U5	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
70	V5	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
71	Z5	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
72	K5	195/197 (99%)	191 (98%)	4 (2%)	0	100	100
73	n5	23/25 (92%)	23 (100%)	0	0	100	100
74	R5	186/188 (99%)	177 (95%)	9 (5%)	0	100	100
75	X5	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
76	Y5	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
77	T5	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
78	E5	153/175 (87%)	144 (94%)	9 (6%)	0	100	100
79	W5	96/98 (98%)	83 (86%)	13 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	A6	535/611 (88%)	496 (93%)	39 (7%)	0	100	100
All	All	11887/12157 (98%)	11117 (94%)	761 (6%)	9 (0%)	59	89

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	S2	14	ILE
13	G2	149	LYS
60	L5	77	LEU
49	F5	234	GLU
39	a5	46	ASP
49	F5	157	ASN
60	L5	63	VAL
13	G2	173	PRO
2	A2	4	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	
1	A1	344/344 (100%)	341 (99%)	3 (1%)	84	92
2	A2	174/174 (100%)	174 (100%)	0	100	100
3	a2	84/84 (100%)	83 (99%)	1 (1%)	78	90
4	B2	191/191 (100%)	191 (100%)	0	100	100
5	b2	70/70 (100%)	70 (100%)	0	100	100
6	C2	176/176 (100%)	176 (100%)	0	100	100
7	c2	56/56 (100%)	55 (98%)	1 (2%)	66	85
8	D2	182/182 (100%)	182 (100%)	0	100	100
9	d2	47/47 (100%)	47 (100%)	0	100	100
10	E2	221/221 (100%)	221 (100%)	0	100	100
11	e2	51/51 (100%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	F2	173/173 (100%)	173 (100%)	0	100	100
13	G2	193/193 (100%)	193 (100%)	0	100	100
14	g2	261/261 (100%)	261 (100%)	0	100	100
15	H2	165/165 (100%)	165 (100%)	0	100	100
16	I2	150/160 (94%)	150 (100%)	0	100	100
17	J2	158/158 (100%)	158 (100%)	0	100	100
18	K2	89/89 (100%)	89 (100%)	0	100	100
19	L2	136/136 (100%)	136 (100%)	0	100	100
20	M2	100/100 (100%)	100 (100%)	0	100	100
21	N2	127/127 (100%)	127 (100%)	0	100	100
22	O2	96/96 (100%)	96 (100%)	0	100	100
23	P2	104/104 (100%)	103 (99%)	1 (1%)	82	91
24	Q2	117/117 (100%)	117 (100%)	0	100	100
25	R2	113/113 (100%)	112 (99%)	1 (1%)	84	92
26	S2	128/128 (100%)	128 (100%)	0	100	100
27	T2	115/115 (100%)	115 (100%)	0	100	100
28	U2	100/100 (100%)	100 (100%)	0	100	100
29	V2	74/74 (100%)	74 (100%)	0	100	100
30	W2	110/110 (100%)	110 (100%)	0	100	100
31	X2	119/119 (100%)	119 (100%)	0	100	100
32	Y2	112/112 (100%)	112 (100%)	0	100	100
33	Z2	61/61 (100%)	61 (100%)	0	100	100
35	f2	43/62 (69%)	43 (100%)	0	100	100
39	a5	118/118 (100%)	118 (100%)	0	100	100
40	A5	194/194 (100%)	194 (100%)	0	100	100
41	b5	46/46 (100%)	46 (100%)	0	100	100
42	B5	322/322 (100%)	322 (100%)	0	100	100
43	c5	81/81 (100%)	81 (100%)	0	100	100
44	C5	288/288 (100%)	288 (100%)	0	100	100
45	D5	244/244 (100%)	244 (100%)	0	100	100
46	d5	96/96 (100%)	96 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	e5	109/109 (100%)	109 (100%)	0	100	100
48	f5	90/90 (100%)	89 (99%)	1 (1%)	80	90
49	F5	186/186 (100%)	186 (100%)	0	100	100
50	g5	95/95 (100%)	94 (99%)	1 (1%)	80	90
51	G5	191/191 (100%)	191 (100%)	0	100	100
52	h5	104/104 (100%)	104 (100%)	0	100	100
53	H5	171/171 (100%)	171 (100%)	0	100	100
54	i5	81/81 (100%)	81 (100%)	0	100	100
55	I5	180/186 (97%)	180 (100%)	0	100	100
56	J5	147/147 (100%)	147 (100%)	0	100	100
57	j5	70/70 (100%)	70 (100%)	0	100	100
58	k5	68/68 (100%)	68 (100%)	0	100	100
59	l5	45/45 (100%)	43 (96%)	2 (4%)	35	72
60	L5	154/154 (100%)	154 (100%)	0	100	100
61	m5	47/47 (100%)	47 (100%)	0	100	100
62	M5	107/107 (100%)	107 (100%)	0	100	100
63	N5	175/175 (100%)	175 (100%)	0	100	100
64	o5	90/90 (100%)	89 (99%)	1 (1%)	80	90
65	p5	71/71 (100%)	71 (100%)	0	100	100
66	P5	145/145 (100%)	145 (100%)	0	100	100
67	Q5	150/150 (100%)	150 (100%)	0	100	100
68	S5	156/156 (100%)	156 (100%)	0	100	100
69	U5	87/87 (100%)	87 (100%)	0	100	100
70	V5	104/104 (100%)	104 (100%)	0	100	100
71	Z5	115/115 (100%)	115 (100%)	0	100	100
72	K5	160/160 (100%)	159 (99%)	1 (1%)	90	95
73	n5	23/23 (100%)	23 (100%)	0	100	100
74	R5	153/153 (100%)	153 (100%)	0	100	100
75	X5	105/105 (100%)	105 (100%)	0	100	100
76	Y5	109/109 (100%)	109 (100%)	0	100	100
77	T5	136/136 (100%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	E5	135/152 (89%)	132 (98%)	3 (2%)	60	84
79	W5	86/86 (100%)	86 (100%)	0	100	100
80	A6	478/538 (89%)	475 (99%)	3 (1%)	90	95
All	All	10152/10264 (99%)	10133 (100%)	19 (0%)	95	98

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	12	ASN
1	A1	50	LYS
1	A1	292	ASN
3	a2	11	ASN
7	c2	67	ARG
23	P2	130	ARG
25	R2	123	ASN
48	f5	70	LYS
50	g5	14	ASN
59	l5	33	ASN
59	l5	43	ASN
64	o5	98	LYS
72	K5	160	ARG
78	E5	31	ARG
78	E5	46	ARG
78	E5	51	ARG
80	A6	13	MET
80	A6	49	GLN
80	A6	63	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	12	ASN
1	A1	96	ASN
1	A1	153	HIS
1	A1	292	ASN
1	A1	325	HIS
1	A1	345	ASN
2	A2	23	HIS
2	A2	92	HIS
3	a2	11	ASN

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Mol	Chain	Res	Type
4	B2	101	HIS
4	B2	118	GLN
4	B2	149	GLN
6	C2	94	GLN
6	C2	220	ASN
7	c2	27	GLN
9	d2	37	ASN
10	E2	36	HIS
10	E2	98	ASN
12	F2	104	ASN
12	F2	127	GLN
13	G2	65	GLN
13	G2	190	GLN
13	G2	201	GLN
14	g2	174	ASN
14	g2	198	ASN
14	g2	268	GLN
16	I2	9	HIS
16	I2	103	GLN
16	I2	159	GLN
21	N2	5	HIS
24	Q2	62	ASN
25	R2	123	ASN
30	W2	15	ASN
30	W2	16	ASN
30	W2	80	ASN
30	W2	92	ASN
31	X2	18	HIS
31	X2	79	ASN
31	X2	94	ASN
33	Z2	38	HIS
33	Z2	98	GLN
39	a5	40	HIS
39	a5	64	GLN
39	a5	74	ASN
40	A5	209	HIS
41	b5	12	GLN
42	B5	109	HIS
44	C5	114	ASN
45	D5	45	ASN
45	D5	63	GLN
45	D5	244	HIS

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Mol	Chain	Res	Type
47	e5	52	GLN
48	f5	42	GLN
49	F5	166	ASN
50	g5	14	ASN
50	g5	52	GLN
51	G5	138	HIS
51	G5	192	GLN
51	G5	232	HIS
52	h5	59	ASN
53	H5	77	ASN
53	H5	96	HIS
55	I5	14	ASN
56	J5	109	HIS
59	l5	4	GLN
59	l5	33	ASN
59	l5	43	ASN
61	m5	90	ASN
63	N5	37	HIS
63	N5	181	ASN
63	N5	182	ASN
64	o5	82	GLN
68	S5	154	HIS
70	V5	98	ASN
71	Z5	40	HIS
71	Z5	57	HIS
74	R5	134	HIS
78	E5	157	GLN
80	A6	63	ASN
80	A6	239	HIS
80	A6	261	ASN
80	A6	281	ASN
80	A6	345	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	22	1779/1798 (98%)	367 (20%)	42 (2%)
36	14	3292/3396 (96%)	562 (17%)	74 (2%)
37	34	120/121 (99%)	10 (8%)	0
38	44	157/158 (99%)	34 (21%)	0
81	X7	11/20 (55%)	6 (54%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
82	A3	75/76 (98%)	24 (32%)	2 (2%)
All	All	5434/5569 (97%)	1003 (18%)	118 (2%)

All (1003) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	22	2	A
34	22	3	U
34	22	25	C
34	22	26	A
34	22	27	U
34	22	34	G
34	22	42	G
34	22	45	U
34	22	47	A
34	22	57	G
34	22	68	A
34	22	69	G
34	22	72	A
34	22	73	U
34	22	74	U
34	22	81	G
34	22	100	A
34	22	104	A
34	22	111	U
34	22	114	C
34	22	115	G
34	22	116	U
34	22	131	C
34	22	132	U
34	22	133	U
34	22	134	U
34	22	135	A
34	22	136	C
34	22	137	U
34	22	138	A
34	22	140	A
34	22	141	U
34	22	144	U
34	22	145	A
34	22	153	G
34	22	158	U

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Mol	Chain	Res	Type
34	22	166	C
34	22	178	U
34	22	185	U
34	22	192	U
34	22	193	U
34	22	195	G
34	22	197	A
34	22	200	A
34	22	217	A
34	22	219	A
34	22	232	U
34	22	233	C
34	22	242	U
34	22	250	C
34	22	261	U
34	22	265	A
34	22	272	U
34	22	278	U
34	22	279	G
34	22	280	U
34	22	281	G
34	22	288	A
34	22	290	G
34	22	299	A
34	22	302	U
34	22	313	U
34	22	316	A
34	22	321	C
34	22	322	G
34	22	323	A
34	22	337	G
34	22	338	C
34	22	352	A
34	22	359	A
34	22	360	A
34	22	361	C
34	22	399	A
34	22	400	A
34	22	402	C
34	22	404	G
34	22	416	A
34	22	417	A

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Mol	Chain	Res	Type
34	22	418	G
34	22	423	G
34	22	424	C
34	22	425	A
34	22	426	G
34	22	428	A
34	22	434	G
34	22	439	U
34	22	445	A
34	22	452	A
34	22	453	U
34	22	456	A
34	22	475	A
34	22	477	A
34	22	484	C
34	22	488	G
34	22	492	A
34	22	493	U
34	22	494	U
34	22	495	C
34	22	496	G
34	22	497	G
34	22	498	G
34	22	499	U
34	22	501	U
34	22	502	U
34	22	504	U
34	22	505	A
34	22	506	A
34	22	507	U
34	22	508	U
34	22	510	G
34	22	511	A
34	22	513	U
34	22	519	C
34	22	539	G
34	22	541	A
34	22	544	A
34	22	555	A
34	22	556	A
34	22	557	G
34	22	558	U

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Mol	Chain	Res	Type
34	22	559	C
34	22	565	C
34	22	568	G
34	22	578	U
34	22	579	A
34	22	581	U
34	22	582	U
34	22	594	A
34	22	595	G
34	22	611	U
34	22	619	A
34	22	620	A
34	22	623	A
34	22	624	G
34	22	629	U
34	22	639	U
34	22	650	U
34	22	654	C
34	22	655	G
34	22	656	G
34	22	658	C
34	22	677	G
34	22	684	A
34	22	686	C
34	22	687	G
34	22	689	G
34	22	694	U
34	22	696	C
34	22	698	U
34	22	700	C
34	22	705	U
34	22	706	A
34	22	708	C
34	22	709	C
34	22	710	U
34	22	712	G
34	22	717	C
34	22	718	U
34	22	719	U
34	22	721	U
34	22	722	G
34	22	723	G

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Mol	Chain	Res	Type
34	22	725	U
34	22	727	U
34	22	731	C
34	22	732	G
34	22	733	A
34	22	734	A
34	22	735	C
34	22	736	C
34	22	741	C
34	22	742	U
34	22	743	U
34	22	754	A
34	22	755	A
34	22	756	A
34	22	765	G
34	22	766	U
34	22	774	A
34	22	775	G
34	22	781	U
34	22	783	G
34	22	787	G
34	22	789	A
34	22	794	U
34	22	811	A
34	22	813	U
34	22	814	A
34	22	816	G
34	22	818	C
34	22	820	U
34	22	821	U
34	22	823	G
34	22	824	G
34	22	826	U
34	22	829	A
34	22	833	U
34	22	840	U
34	22	841	U
34	22	846	G
34	22	849	C
34	22	850	A
34	22	857	U
34	22	860	U

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Mol	Chain	Res	Type
34	22	863	A
34	22	876	G
34	22	898	A
34	22	912	U
34	22	913	G
34	22	914	G
34	22	915	A
34	22	925	G
34	22	933	A
34	22	934	C
34	22	935	U
34	22	942	G
34	22	944	A
34	22	951	A
34	22	960	U
34	22	966	A
34	22	988	A
34	22	992	A
34	22	993	A
34	22	1003	A
34	22	1004	U
34	22	1005	A
34	22	1012	U
34	22	1024	U
34	22	1026	A
34	22	1028	C
34	22	1039	A
34	22	1040	G
34	22	1051	G
34	22	1052	U
34	22	1053	G
34	22	1058	U
34	22	1061	A
34	22	1074	G
34	22	1076	A
34	22	1082	C
34	22	1091	A
34	22	1092	A
34	22	1096	C
34	22	1097	U
34	22	1098	U
34	22	1099	U

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Mol	Chain	Res	Type
34	22	1100	G
34	22	1113	A
34	22	1114	G
34	22	1138	A
34	22	1158	C
34	22	1160	A
34	22	1167	G
34	22	1185	U
34	22	1194	A
34	22	1196	A
34	22	1197	C
34	22	1199	G
34	22	1200	G
34	22	1207	C
34	22	1208	A
34	22	1217	A
34	22	1218	G
34	22	1227	A
34	22	1228	G
34	22	1229	G
34	22	1232	U
34	22	1243	G
34	22	1244	A
34	22	1245	G
34	22	1246	C
34	22	1251	U
34	22	1254	U
34	22	1258	U
34	22	1284	C
34	22	1285	U
34	22	1290	U
34	22	1314	U
34	22	1315	U
34	22	1316	G
34	22	1321	A
34	22	1327	C
34	22	1337	A
34	22	1339	C
34	22	1340	U
34	22	1344	A
34	22	1345	A
34	22	1362	U

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Mol	Chain	Res	Type
34	22	1363	U
34	22	1364	G
34	22	1370	U
34	22	1371	A
34	22	1372	U
34	22	1373	C
34	22	1389	C
34	22	1390	U
34	22	1399	C
34	22	1413	U
34	22	1415	U
34	22	1427	A
34	22	1428	G
34	22	1431	C
34	22	1432	U
34	22	1436	A
34	22	1445	G
34	22	1446	A
34	22	1448	G
34	22	1457	C
34	22	1459	C
34	22	1460	A
34	22	1471	A
34	22	1473	U
34	22	1474	G
34	22	1482	C
34	22	1486	G
34	22	1490	C
34	22	1492	A
34	22	1506	G
34	22	1516	A
34	22	1521	G
34	22	1523	G
34	22	1524	A
34	22	1535	U
34	22	1536	G
34	22	1537	C
34	22	1538	U
34	22	1540	G
34	22	1542	G
34	22	1557	U
34	22	1559	A

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Mol	Chain	Res	Type
34	22	1568	C
34	22	1569	A
34	22	1574	G
34	22	1584	G
34	22	1600	A
34	22	1601	G
34	22	1616	G
34	22	1626	U
34	22	1631	A
34	22	1634	C
34	22	1646	C
34	22	1657	U
34	22	1658	G
34	22	1680	G
34	22	1682	U
34	22	1684	U
34	22	1689	A
34	22	1696	G
34	22	1697	G
34	22	1700	C
34	22	1702	A
34	22	1704	U
34	22	1713	G
34	22	1756	A
34	22	1760	G
34	22	1762	A
34	22	1769	U
34	22	1770	U
34	22	1780	G
34	22	1782	A
34	22	1783	C
34	22	1792	G
34	22	1793	G
34	22	1794	A
34	22	1796	C
34	22	1797	A
34	22	1798	U
36	14	13	A
36	14	14	U
36	14	15	C
36	14	21	G
36	14	26	A

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Mol	Chain	Res	Type
36	14	40	A
36	14	43	A
36	14	49	A
36	14	59	G
36	14	60	A
36	14	65	A
36	14	66	A
36	14	86	G
36	14	92	G
36	14	93	C
36	14	110	G
36	14	113	C
36	14	115	A
36	14	121	A
36	14	122	A
36	14	133	U
36	14	134	U
36	14	136	G
36	14	148	G
36	14	156	G
36	14	157	A
36	14	182	U
36	14	187	A
36	14	189	G
36	14	190	U
36	14	191	U
36	14	200	C
36	14	206	G
36	14	210	U
36	14	211	A
36	14	218	G
36	14	219	A
36	14	234	G
36	14	240	U
36	14	249	U
36	14	252	U
36	14	269	G
36	14	283	G
36	14	286	U
36	14	295	A
36	14	298	U
36	14	305	U

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Mol	Chain	Res	Type
36	14	323	A
36	14	329	U
36	14	338	A
36	14	339	C
36	14	343	U
36	14	349	A
36	14	350	C
36	14	352	A
36	14	353	G
36	14	370	U
36	14	376	G
36	14	398	A
36	14	401	U
36	14	402	A
36	14	403	C
36	14	421	G
36	14	422	A
36	14	439	C
36	14	521	A
36	14	534	U
36	14	535	G
36	14	546	C
36	14	547	G
36	14	548	G
36	14	555	U
36	14	557	A
36	14	558	U
36	14	559	A
36	14	578	A
36	14	579	G
36	14	589	A
36	14	592	A
36	14	604	G
36	14	609	G
36	14	611	A
36	14	620	U
36	14	621	A
36	14	622	A
36	14	637	C
36	14	642	U
36	14	649	A
36	14	677	A

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Mol	Chain	Res	Type
36	14	681	U
36	14	690	A
36	14	691	A
36	14	705	A
36	14	712	G
36	14	715	A
36	14	764	U
36	14	765	C
36	14	766	U
36	14	767	U
36	14	776	U
36	14	777	U
36	14	781	G
36	14	785	G
36	14	786	A
36	14	787	G
36	14	806	A
36	14	817	A
36	14	830	A
36	14	835	G
36	14	849	C
36	14	861	C
36	14	874	U
36	14	879	U
36	14	880	G
36	14	896	A
36	14	908	G
36	14	914	A
36	14	916	G
36	14	917	A
36	14	922	U
36	14	925	A
36	14	937	G
36	14	938	C
36	14	940	G
36	14	944	C
36	14	959	C
36	14	960	U
36	14	963	G
36	14	974	G
36	14	979	U
36	14	980	A

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Mol	Chain	Res	Type
36	14	981	U
36	14	982	C
36	14	984	G
36	14	1001	G
36	14	1002	A
36	14	1006	A
36	14	1010	G
36	14	1015	U
36	14	1016	C
36	14	1017	C
36	14	1024	G
36	14	1025	A
36	14	1037	C
36	14	1041	U
36	14	1047	A
36	14	1049	C
36	14	1064	A
36	14	1065	A
36	14	1075	A
36	14	1076	C
36	14	1081	U
36	14	1093	A
36	14	1094	U
36	14	1095	U
36	14	1098	A
36	14	1103	A
36	14	1104	G
36	14	1117	G
36	14	1131	G
36	14	1144	U
36	14	1153	A
36	14	1159	A
36	14	1180	A
36	14	1181	U
36	14	1192	C
36	14	1196	C
36	14	1201	C
36	14	1205	A
36	14	1206	G
36	14	1209	G
36	14	1222	G
36	14	1235	U

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Mol	Chain	Res	Type
36	14	1236	G
36	14	1241	U
36	14	1242	G
36	14	1244	A
36	14	1246	G
36	14	1248	C
36	14	1253	U
36	14	1254	C
36	14	1258	U
36	14	1262	G
36	14	1263	A
36	14	1264	G
36	14	1269	U
36	14	1270	A
36	14	1271	A
36	14	1272	C
36	14	1273	A
36	14	1274	A
36	14	1278	A
36	14	1285	G
36	14	1287	A
36	14	1308	A
36	14	1309	U
36	14	1313	G
36	14	1316	C
36	14	1317	A
36	14	1323	G
36	14	1325	U
36	14	1330	A
36	14	1331	U
36	14	1348	U
36	14	1349	G
36	14	1351	U
36	14	1353	U
36	14	1355	A
36	14	1356	U
36	14	1357	G
36	14	1386	A
36	14	1392	G
36	14	1399	A
36	14	1400	G
36	14	1419	A

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Mol	Chain	Res	Type
36	14	1430	U
36	14	1434	G
36	14	1435	A
36	14	1437	C
36	14	1446	A
36	14	1447	G
36	14	1470	U
36	14	1480	G
36	14	1482	A
36	14	1483	G
36	14	1488	G
36	14	1493	G
36	14	1495	U
36	14	1496	C
36	14	1508	C
36	14	1523	U
36	14	1524	A
36	14	1554	U
36	14	1555	U
36	14	1556	C
36	14	1557	A
36	14	1560	G
36	14	1562	C
36	14	1563	C
36	14	1567	U
36	14	1568	U
36	14	1569	U
36	14	1570	U
36	14	1571	A
36	14	1572	U
36	14	1576	G
36	14	1578	C
36	14	1582	C
36	14	1583	A
36	14	1588	A
36	14	1589	A
36	14	1593	A
36	14	1596	C
36	14	1605	A
36	14	1606	U
36	14	1607	U
36	14	1629	U

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Mol	Chain	Res	Type
36	14	1630	U
36	14	1639	C
36	14	1642	A
36	14	1643	A
36	14	1645	U
36	14	1656	A
36	14	1657	C
36	14	1683	A
36	14	1714	A
36	14	1715	A
36	14	1716	U
36	14	1724	U
36	14	1725	C
36	14	1730	G
36	14	1736	G
36	14	1741	A
36	14	1742	U
36	14	1749	A
36	14	1751	G
36	14	1752	A
36	14	1760	A
36	14	1765	U
36	14	1766	G
36	14	1770	G
36	14	1775	G
36	14	1780	G
36	14	1796	G
36	14	1797	A
36	14	1808	G
36	14	1814	A
36	14	1816	A
36	14	1817	G
36	14	1820	U
36	14	1821	U
36	14	1835	A
36	14	1841	A
36	14	1847	A
36	14	1849	C
36	14	1850	A
36	14	1866	C
36	14	1867	A
36	14	1878	G

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Mol	Chain	Res	Type
36	14	1880	U
36	14	1893	A
36	14	1901	A
36	14	1906	G
36	14	1941	C
36	14	1944	U
36	14	1948	G
36	14	1949	G
36	14	1954	G
36	14	1955	U
36	14	1966	U
36	14	1967	U
36	14	1973	G
36	14	1974	A
36	14	1975	C
36	14	1976	G
36	14	2044	U
36	14	2047	A
36	14	2048	G
36	14	2060	A
36	14	2067	U
36	14	2068	U
36	14	2071	A
36	14	2072	G
36	14	2076	G
36	14	2077	U
36	14	2078	C
36	14	2079	G
36	14	2080	C
36	14	2081	U
36	14	2087	C
36	14	2088	A
36	14	2089	A
36	14	2090	U
36	14	2091	U
36	14	2092	A
36	14	2094	C
36	14	2095	G
36	14	2099	A
36	14	2107	A
36	14	2112	U
36	14	2113	A

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Mol	Chain	Res	Type
36	14	2114	C
36	14	2121	G
36	14	2122	G
36	14	2131	A
36	14	2140	U
36	14	2159	U
36	14	2160	G
36	14	2169	G
36	14	2174	G
36	14	2175	U
36	14	2176	U
36	14	2179	C
36	14	2205	U
36	14	2209	U
36	14	2210	G
36	14	2223	A
36	14	2225	U
36	14	2228	A
36	14	2244	A
36	14	2249	G
36	14	2257	C
36	14	2272	G
36	14	2273	G
36	14	2282	U
36	14	2286	U
36	14	2287	C
36	14	2288	G
36	14	2307	G
36	14	2308	C
36	14	2309	A
36	14	2310	U
36	14	2313	A
36	14	2314	U
36	14	2315	G
36	14	2334	U
36	14	2336	U
36	14	2339	C
36	14	2373	A
36	14	2374	C
36	14	2375	G
36	14	2376	G
36	14	2378	C

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Mol	Chain	Res	Type
36	14	2386	A
36	14	2394	G
36	14	2397	A
36	14	2401	A
36	14	2402	A
36	14	2403	G
36	14	2404	A
36	14	2411	U
36	14	2418	G
36	14	2435	G
36	14	2443	A
36	14	2444	C
36	14	2447	A
36	14	2448	G
36	14	2453	U
36	14	2454	G
36	14	2459	A
36	14	2462	A
36	14	2468	A
36	14	2469	G
36	14	2486	A
36	14	2487	U
36	14	2488	A
36	14	2506	U
36	14	2510	U
36	14	2511	A
36	14	2512	C
36	14	2514	U
36	14	2515	A
36	14	2522	G
36	14	2523	A
36	14	2526	C
36	14	2531	C
36	14	2532	U
36	14	2537	U
36	14	2538	U
36	14	2539	C
36	14	2541	U
36	14	2542	U
36	14	2544	U
36	14	2547	A
36	14	2548	C

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Mol	Chain	Res	Type
36	14	2552	C
36	14	2558	U
36	14	2561	A
36	14	2571	U
36	14	2572	C
36	14	2573	G
36	14	2580	A
36	14	2581	U
36	14	2585	G
36	14	2593	A
36	14	2594	C
36	14	2606	G
36	14	2607	G
36	14	2614	G
36	14	2652	U
36	14	2656	A
36	14	2672	G
36	14	2674	A
36	14	2677	G
36	14	2678	A
36	14	2681	U
36	14	2691	A
36	14	2694	A
36	14	2696	A
36	14	2703	A
36	14	2704	A
36	14	2705	A
36	14	2706	G
36	14	2715	A
36	14	2728	G
36	14	2729	U
36	14	2753	G
36	14	2755	C
36	14	2777	G
36	14	2778	G
36	14	2796	G
36	14	2800	G
36	14	2801	A
36	14	2803	A
36	14	2804	A
36	14	2810	C
36	14	2814	G

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Mol	Chain	Res	Type
36	14	2817	A
36	14	2818	U
36	14	2834	G
36	14	2842	U
36	14	2844	C
36	14	2845	A
36	14	2860	U
36	14	2867	C
36	14	2871	G
36	14	2872	A
36	14	2873	U
36	14	2874	G
36	14	2875	U
36	14	2887	A
36	14	2899	C
36	14	2918	G
36	14	2923	U
36	14	2935	U
36	14	2936	A
36	14	2938	G
36	14	2941	A
36	14	2942	C
36	14	2951	G
36	14	2957	G
36	14	2971	A
36	14	2972	G
36	14	2983	C
36	14	2996	U
36	14	2997	G
36	14	3011	A
36	14	3012	A
36	14	3030	G
36	14	3049	A
36	14	3078	U
36	14	3080	G
36	14	3086	A
36	14	3092	C
36	14	3098	G
36	14	3121	U
36	14	3122	A
36	14	3130	A
36	14	3131	U

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Mol	Chain	Res	Type
36	14	3142	A
36	14	3143	C
36	14	3153	U
36	14	3154	C
36	14	3155	U
36	14	3156	U
36	14	3157	U
36	14	3165	A
36	14	3170	A
36	14	3172	A
36	14	3173	G
36	14	3174	A
36	14	3176	G
36	14	3179	U
36	14	3181	C
36	14	3185	U
36	14	3186	A
36	14	3187	A
36	14	3199	G
36	14	3206	C
36	14	3207	U
36	14	3208	G
36	14	3209	A
36	14	3216	G
36	14	3217	C
36	14	3218	A
36	14	3219	G
36	14	3243	A
36	14	3244	A
36	14	3247	G
36	14	3270	U
36	14	3271	G
36	14	3276	G
36	14	3279	A
36	14	3294	A
36	14	3304	U
36	14	3313	U
36	14	3319	U
36	14	3320	A
36	14	3341	U
36	14	3345	G
36	14	3352	U

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Mol	Chain	Res	Type
36	14	3353	G
36	14	3354	U
36	14	3355	U
36	14	3356	G
36	14	3368	U
36	14	3369	G
36	14	3370	A
36	14	3375	A
36	14	3378	C
36	14	3390	G
36	14	3396	U
37	34	42	A
37	34	54	U
37	34	55	A
37	34	65	G
37	34	76	A
37	34	77	G
37	34	87	G
37	34	99	G
37	34	112	G
37	34	121	U
38	44	23	U
38	44	24	G
38	44	34	U
38	44	35	C
38	44	37	A
38	44	38	U
38	44	39	G
38	44	49	G
38	44	51	G
38	44	59	A
38	44	62	C
38	44	63	G
38	44	71	A
38	44	80	A
38	44	81	U
38	44	82	U
38	44	84	C
38	44	85	G
38	44	86	U
38	44	87	G
38	44	90	U

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Mol	Chain	Res	Type
38	44	91	C
38	44	95	G
38	44	104	A
38	44	106	C
38	44	107	G
38	44	113	U
38	44	118	C
38	44	125	U
38	44	126	A
38	44	138	A
38	44	151	C
38	44	152	G
38	44	155	A
81	X7	8	A
81	X7	10	G
81	X7	11	U
81	X7	12	A
81	X7	13	A
81	X7	17	U
82	A3	9	A
82	A3	11	C
82	A3	14	A
82	A3	15	G
82	A3	16	H2U
82	A3	17	H2U
82	A3	18	G
82	A3	20	G
82	A3	21	A
82	A3	22	G
82	A3	25	C
82	A3	26	M2G
82	A3	46	7MG
82	A3	47	U
82	A3	48	C
82	A3	49	5MC
82	A3	52	U
82	A3	54	5MU
82	A3	55	PSU
82	A3	56	C
82	A3	57	G
82	A3	58	1MA
82	A3	59	U

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Mol	Chain	Res	Type
82	A3	76	A

All (118) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	22	56	U
34	22	73	U
34	22	99	C
34	22	131	C
34	22	133	U
34	22	139	C
34	22	216	U
34	22	280	U
34	22	315	A
34	22	322	G
34	22	417	A
34	22	444	C
34	22	497	G
34	22	503	G
34	22	538	A
34	22	555	A
34	22	578	U
34	22	580	A
34	22	622	A
34	22	657	U
34	22	686	C
34	22	720	G
34	22	721	U
34	22	782	U
34	22	812	A
34	22	819	G
34	22	1113	A
34	22	1137	A
34	22	1157	A
34	22	1207	C
34	22	1250	U
34	22	1344	A
34	22	1388	A
34	22	1447	C
34	22	1481	C
34	22	1491	U
34	22	1568	C

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Mol	Chain	Res	Type
34	22	1573	A
34	22	1600	A
34	22	1696	G
34	22	1761	U
34	22	1769	U
36	14	13	A
36	14	199	A
36	14	210	U
36	14	239	G
36	14	282	G
36	14	337	G
36	14	338	A
36	14	352	A
36	14	533	A
36	14	547	G
36	14	763	G
36	14	764	U
36	14	786	A
36	14	916	G
36	14	979	U
36	14	1015	U
36	14	1064	A
36	14	1094	U
36	14	1097	G
36	14	1103	A
36	14	1116	G
36	14	1253	U
36	14	1307	G
36	14	1317	A
36	14	1355	A
36	14	1418	A
36	14	1493	G
36	14	1554	U
36	14	1559	A
36	14	1562	C
36	14	1570	U
36	14	1656	A
36	14	1715	A
36	14	1729	A
36	14	1748	G
36	14	1750	A
36	14	1815	U

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Mol	Chain	Res	Type
36	14	1816	A
36	14	1846	C
36	14	1848	G
36	14	1866	C
36	14	1900	A
36	14	1943	C
36	14	1965	C
36	14	2043	U
36	14	2046	U
36	14	2080	C
36	14	2086	A
36	14	2090	U
36	14	2093	A
36	14	2112	U
36	14	2209	U
36	14	2227	C
36	14	2286	U
36	14	2307	G
36	14	2309	A
36	14	2335	G
36	14	2447	A
36	14	2468	A
36	14	2487	U
36	14	2509	U
36	14	2513	U
36	14	2525	G
36	14	2537	U
36	14	2541	U
36	14	2570	U
36	14	2580	A
36	14	2593	A
36	14	2705	A
36	14	2950	G
36	14	2971	A
36	14	3011	A
36	14	3121	U
36	14	3198	U
82	A3	19	G
82	A3	58	1MA

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

14 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
82	2MG	A3	10	82	18,26,27	3.46	4 (22%)	21,38,41	2.32	7 (33%)
82	H2U	A3	16	82	17,21,22	1.20	2 (11%)	23,30,33	1.82	5 (21%)
82	H2U	A3	17	82	17,21,22	1.15	2 (11%)	23,30,33	1.62	4 (17%)
82	M2G	A3	26	82,84	18,27,28	1.97	4 (22%)	22,40,43	2.72	7 (31%)
82	OMC	A3	32	82	15,22,23	1.03	2 (13%)	20,31,34	2.38	4 (20%)
82	OMG	A3	34	82,81	17,25,27	2.62	5 (29%)	19,37,41	2.25	4 (21%)
82	YYG	A3	37	82	28,42,43	2.12	9 (32%)	28,62,65	2.80	8 (28%)
82	PSU	A3	39	82	15,21,22	4.28	5 (33%)	16,30,33	1.92	2 (12%)
82	5MC	A3	40	82	14,22,23	1.04	2 (14%)	17,32,35	1.17	2 (11%)
82	7MG	A3	46	82	20,26,27	3.11	7 (35%)	23,39,42	2.38	8 (34%)
82	5MC	A3	49	82	14,22,23	0.85	0	17,32,35	1.00	1 (5%)
82	5MU	A3	54	82	13,22,23	1.92	2 (15%)	16,32,35	3.54	2 (12%)
82	PSU	A3	55	82	15,21,22	4.39	6 (40%)	16,30,33	1.94	2 (12%)
82	1MA	A3	58	82	15,25,26	1.37	2 (13%)	15,37,40	1.61	1 (6%)

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
82	2MG	A3	10	82	-	0/5/27/28	0/3/3/3
82	H2U	A3	16	82	-	0/7/38/39	0/2/2/2
82	H2U	A3	17	82	-	0/7/38/39	0/2/2/2
82	M2G	A3	26	82,84	-	0/7/29/30	0/3/3/3
82	OMC	A3	32	82	-	0/5/27/28	0/2/2/2
82	OMG	A3	34	82,81	-	0/3/25/28	0/3/3/3
82	YYG	A3	37	82	-	2/20/42/43	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	PSU	A3	39	82	-	0/7/25/26	0/2/2/2
82	5MC	A3	40	82	-	0/3/25/26	0/2/2/2
82	7MG	A3	46	82	-	0/7/37/38	0/3/3/3
82	5MC	A3	49	82	-	0/3/25/26	0/2/2/2
82	5MU	A3	54	82	-	0/3/25/26	0/2/2/2
82	PSU	A3	55	82	-	0/7/25/26	0/2/2/2
82	1MA	A3	58	82	-	0/3/25/26	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	A3	55	PSU	O4'-C1'	-2.70	1.40	1.44
82	A3	54	5MU	C5M-C5	-2.43	1.46	1.51
82	A3	39	PSU	O4'-C1'	-2.42	1.40	1.44
82	A3	40	5MC	C4-N3	-2.29	1.31	1.35
82	A3	40	5MC	CM5-C5	-2.15	1.46	1.51
82	A3	55	PSU	C2-N1	2.03	1.42	1.38
82	A3	10	2MG	CM2-N2	2.07	1.49	1.45
82	A3	37	YYG	C14-C15	2.21	1.58	1.53
82	A3	37	YYG	C15-C16	2.23	1.58	1.52
82	A3	37	YYG	O18-C16	2.24	1.39	1.33
82	A3	37	YYG	C4-N3	2.35	1.41	1.39
82	A3	37	YYG	C15-N20	2.49	1.51	1.45
82	A3	32	OMC	C2-N3	2.53	1.43	1.38
82	A3	32	OMC	C4-N4	2.62	1.42	1.35
82	A3	39	PSU	C2-N3	2.79	1.44	1.38
82	A3	55	PSU	C2-N3	2.80	1.44	1.38
82	A3	46	7MG	C2-N1	2.84	1.40	1.35
82	A3	34	OMG	C2-N1	2.92	1.40	1.35
82	A3	37	YYG	C21-N20	2.94	1.42	1.34
82	A3	17	H2U	C2-N1	2.97	1.40	1.35
82	A3	34	OMG	C6-C5	3.13	1.47	1.41
82	A3	16	H2U	C2-N3	3.15	1.43	1.38
82	A3	16	H2U	C2-N1	3.15	1.40	1.35
82	A3	17	H2U	C2-N3	3.24	1.44	1.38
82	A3	26	M2G	C4-N3	3.24	1.40	1.35
82	A3	58	1MA	C4-N3	3.35	1.40	1.35
82	A3	46	7MG	C2-N3	3.39	1.41	1.35
82	A3	34	OMG	C4-N3	3.46	1.41	1.35
82	A3	58	1MA	C6-C5	3.48	1.47	1.40
82	A3	26	M2G	C2-N1	3.50	1.40	1.34
82	A3	37	YYG	C6-C5	3.61	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	A3	26	M2G	C6-N1	4.13	1.40	1.33
82	A3	10	2MG	C4-N3	4.49	1.42	1.35
82	A3	46	7MG	C8-N9	4.49	1.51	1.45
82	A3	39	PSU	C6-N1	4.57	1.44	1.34
82	A3	55	PSU	C6-N1	4.58	1.44	1.34
82	A3	46	7MG	C6-C5	4.96	1.48	1.41
82	A3	46	7MG	C2-N2	4.98	1.44	1.34
82	A3	26	M2G	C2-N2	5.11	1.43	1.34
82	A3	37	YYG	O23-C21	5.51	1.41	1.34
82	A3	34	OMG	C2-N2	5.55	1.45	1.34
82	A3	37	YYG	C6-N1	6.23	1.48	1.37
82	A3	54	5MU	C4-N3	6.23	1.44	1.33
82	A3	46	7MG	C4-N3	6.94	1.43	1.34
82	A3	34	OMG	C6-N1	7.11	1.45	1.33
82	A3	46	7MG	C6-N1	7.11	1.45	1.33
82	A3	39	PSU	C4-N3	7.69	1.46	1.33
82	A3	55	PSU	C4-N3	7.78	1.47	1.33
82	A3	10	2MG	C6-N1	7.96	1.47	1.33
82	A3	10	2MG	C2-N2	10.95	1.46	1.34
82	A3	39	PSU	C5-C1'	13.10	1.63	1.52
82	A3	55	PSU	C5-C1'	13.59	1.64	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	A3	54	5MU	C5-C4-N3	-10.62	116.44	125.35
82	A3	37	YYG	C13-C12-C11	-9.70	117.37	131.05
82	A3	26	M2G	C5-C6-N1	-6.74	114.72	123.52
82	A3	37	YYG	O23-C21-O22	-5.86	116.38	124.61
82	A3	46	7MG	C5-C4-N3	-5.10	121.55	126.74
82	A3	34	OMG	N3-C2-N1	-5.06	120.67	127.56
82	A3	46	7MG	N1-C2-N3	-4.67	117.88	125.51
82	A3	34	OMG	C5-C6-N1	-4.45	117.71	123.52
82	A3	10	2MG	N3-C2-N1	-3.74	120.60	126.19
82	A3	46	7MG	C5-C6-N1	-3.59	118.04	123.39
82	A3	10	2MG	C5-C6-N1	-3.58	118.84	123.52
82	A3	32	OMC	C5-C4-N3	-3.57	117.27	121.79
82	A3	32	OMC	C6-N1-C2	-3.44	115.71	121.33
82	A3	37	YYG	O18-C16-O17	-3.33	116.77	123.77
82	A3	26	M2G	N1-C2-N2	-2.75	114.13	117.14
82	A3	40	5MC	CM5-C5-C4	-2.65	118.66	121.47
82	A3	16	H2U	O2-C2-N3	-2.58	116.38	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	A3	10	2MG	C6-C5-C4	-2.54	117.95	120.86
82	A3	17	H2U	O2-C2-N3	-2.43	116.68	121.44
82	A3	37	YYG	O22-C21-N20	-2.16	121.14	124.89
82	A3	26	M2G	N3-C2-N1	-2.10	122.78	126.35
82	A3	55	PSU	O4'-C1'-C2'	2.07	106.92	104.69
82	A3	10	2MG	CM2-N2-C2	2.12	125.42	123.03
82	A3	26	M2G	CM2-N2-C2	2.13	123.47	121.34
82	A3	46	7MG	N3-C4-N9	2.21	129.84	126.98
82	A3	49	5MC	CM5-C5-C6	2.24	123.16	118.63
82	A3	17	H2U	O2-C2-N1	2.42	126.35	123.17
82	A3	39	PSU	O4'-C1'-C2'	2.49	107.38	104.69
82	A3	37	YYG	C24-O23-C21	2.53	118.80	115.65
82	A3	46	7MG	C2-N3-C4	2.60	121.91	114.50
82	A3	26	M2G	CM1-N2-C2	2.67	124.01	121.34
82	A3	40	5MC	CM5-C5-C6	2.69	124.07	118.63
82	A3	46	7MG	C4-N9-C1'	2.69	133.02	126.65
82	A3	17	H2U	C5-C4-N3	2.72	119.49	116.62
82	A3	16	H2U	O2-C2-N1	2.74	126.77	123.17
82	A3	10	2MG	C6-N1-C2	2.75	119.18	115.24
82	A3	16	H2U	C1'-N1-C2	2.88	122.22	118.19
82	A3	16	H2U	C5-C4-N3	3.05	119.84	116.62
82	A3	46	7MG	N2-C2-N3	3.10	122.31	117.20
82	A3	34	OMG	C6-N1-C2	3.29	119.73	115.88
82	A3	37	YYG	C6-C5-C4	3.29	122.27	119.93
82	A3	32	OMC	N4-C4-N3	3.62	122.82	116.50
82	A3	37	YYG	O18-C16-C15	3.76	121.21	111.41
82	A3	26	M2G	N3-C2-N2	5.40	123.09	117.14
82	A3	34	OMG	C1'-N9-C4	5.54	132.98	126.81
82	A3	58	1MA	C6-C5-C4	5.62	121.31	116.80
82	A3	10	2MG	N2-C2-N3	5.64	123.49	116.94
82	A3	10	2MG	C2-N3-C4	5.66	121.20	114.99
82	A3	46	7MG	C6-N1-C2	5.71	122.57	115.88
82	A3	17	H2U	C5-C6-N1	5.75	117.06	110.76
82	A3	37	YYG	O23-C21-N20	5.76	122.48	110.84
82	A3	16	H2U	C5-C6-N1	6.20	117.55	110.76
82	A3	39	PSU	C4-N3-C2	6.71	120.76	115.16
82	A3	55	PSU	C4-N3-C2	6.85	120.87	115.16
82	A3	26	M2G	C1'-N9-C4	7.63	135.32	126.81
82	A3	32	OMC	C6-C5-C4	8.31	120.69	117.44
82	A3	54	5MU	C4-N3-C2	9.01	122.67	115.16

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	A3	37	YYG	C24-O23-C21-O22
82	A3	37	YYG	C24-O23-C21-N20

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	A3	34	OMG	4	0
82	A3	37	YYG	1	0
82	A3	58	1MA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1068 ligands modelled in this entry, 1066 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	$\# Z > 2$
86	5CR	A3	101	82	12,14,15	0.51	0	14,17,19	1.02	1 (7%)
85	GNP	A6	701	84	29,34,34	2.68	10 (34%)	28,54,54	1.96	7 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	5CR	A3	101	82	-	0/8/10/12	0/1/1/1
85	GNP	A6	701	84	-	0/16/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	A6	701	GNP	C4-N9	-7.13	1.38	1.47
85	A6	701	GNP	C5-C6	-6.08	1.42	1.53
85	A6	701	GNP	PB-O3A	-5.25	1.52	1.59
85	A6	701	GNP	PB-O2B	-3.16	1.48	1.56
85	A6	701	GNP	C8-N9	-2.92	1.37	1.47
85	A6	701	GNP	C2-N3	-2.49	1.33	1.43
85	A6	701	GNP	PB-O1B	2.06	1.48	1.46
85	A6	701	GNP	C1'-N9	2.31	1.46	1.42
85	A6	701	GNP	C6-N1	3.84	1.39	1.33
85	A6	701	GNP	PG-O1G	4.87	1.51	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	A6	701	GNP	O3G-PG-O1G	-3.23	105.08	113.58
86	A3	101	5CR	O-C-CA	-3.07	117.31	125.69
85	A6	701	GNP	PA-O3A-PB	-2.87	122.28	132.71
85	A6	701	GNP	O6-C6-N1	-2.19	119.92	122.80
85	A6	701	GNP	O3G-PG-O2G	2.70	115.51	107.67
85	A6	701	GNP	O2B-PB-O1B	4.35	118.59	110.02
85	A6	701	GNP	O6-C6-C5	4.52	128.34	119.69
85	A6	701	GNP	C4-C5-N7	5.23	110.83	102.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
86	A3	101	5CR	3	0
85	A6	701	GNP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.