



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 22, 2016 – 12:43 PM EST

PDB ID : 5LZW
EMDB ID: : EMD-4134
Title : Structure of the mammalian rescue complex with Pelota and Hbs1l assembled on a truncated mRNA.
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.53 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)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

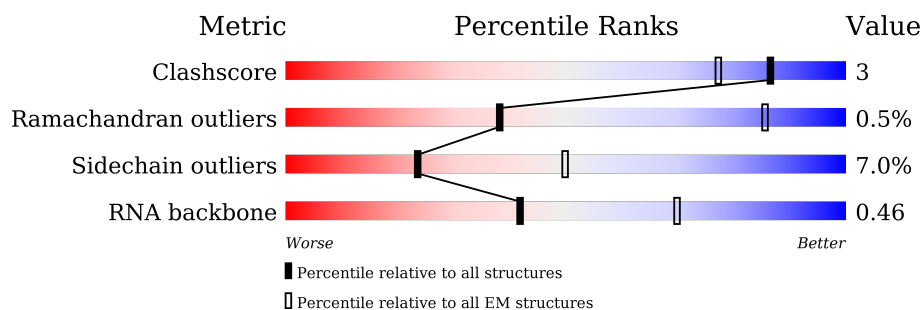
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 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.
















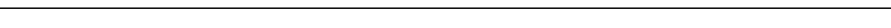




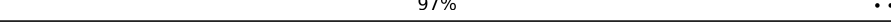




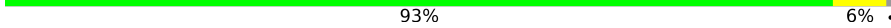
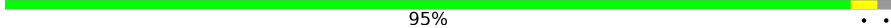
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	A	257	82% (green) 14% (yellow) .. (grey)
2	B	403	87% (green) 9% (yellow) .. (grey)
3	C	425	77% (green) 8% (yellow) . (orange) 15% (grey)
4	D	297	88% (green) 10% (yellow) . (orange)
5	E	291	65% (green) 8% (yellow) . (orange) 26% (grey)
6	F	247	80% (green) 10% (yellow) . (orange) 9% (grey)
7	G	319	67% (green) 6% (yellow) (orange) 27% (grey)
8	H	192	87% (green) 11% (yellow) .. (grey)

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Mol	Chain	Length	Quality of chain
9	I	214	 88% 7% .
10	J	178	 89% 6% .
11	L	211	 92% 7%
12	M	218	 54% 8% . 37%
13	N	204	 91% 8%
14	O	203	 83% 14% ..
15	P	184	 74% 8% . 17%
16	Q	188	 86% 14% .
17	R	196	 84% 8% 8%
18	S	176	 89% 11%
19	T	160	 88% 11% ..
20	U	128	 71% 6% 23%
21	V	140	 77% 16% . 6%
22	W	157	 62% 5% 32%
23	X	156	 71% . 24%
24	Y	145	 87% 6% 8%
25	Z	136	 91% 7% ..
26	a	148	 97% ..
27	b	245	 41% . 58%
28	c	115	 82% . 15%
29	d	125	 76% 10% 14%
30	e	135	 88% 7% 5%
31	f	110	 93% 6% .
32	g	116	 95% ..
33	h	123	 96% ..




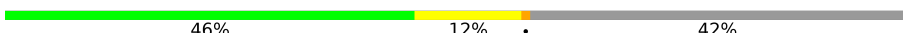





















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Mol	Chain	Length	Quality of chain
34	i	105	94%
35	j	97	85%
36	k	70	96%
37	l	51	96%
38	m	102	48%
39	n	25	92%
40	o	106	93%
41	p	92	97%
42	r	137	85%
43	s	318	59%
44	t	165	90%
45	1	15	93%
46	2	76	79%
47	3	75	64%
48	5	3543	70%
49	7	120	85%
50	8	156	70%
51	9	1869	60%
52	AA	295	62%
53	BB	264	70%
54	CC	293	62%
55	DD	243	80%
56	EE	263	86%
57	FF	204	81%
58	GG	249	84%

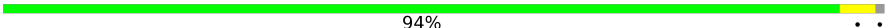



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Mol	Chain	Length	Quality of chain
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	

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Mol	Chain	Length	Quality of chain
84	gg	317	 94% . .
85	hh	8	 50% 50%
86	ii	403	 87% 5% 8%
87	jj	710	 56% . 40%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
90	GCP	9	1972	-	-	X	-

2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 222130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called uL4.

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

- Molecule 4 is a protein called uL18.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	LYS	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called eL6.

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

- Molecule 6 is a protein called uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called uL16.

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

- Molecule 10 is a protein called uL5.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	GLN	conflict	UNP G1SNY0

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called Nascent chain.

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

- Molecule 46 is a RNA chain called P-site tRNA.

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

- Molecule 47 is a RNA chain called E-site tRNA.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA (truncated).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	8	Total	C	N	O	P	0	0
			169	76	29	56	8		

- Molecule 86 is a protein called Pelota.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	372	Total	C	N	O	S	0	0
			2947	1844	528	559	16		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	221	MET	LEU	conflict	UNP Q9BRX2
ii	386	GLY	-	expression tag	UNP Q9BRX2
ii	387	SER	-	expression tag	UNP Q9BRX2
ii	388	GLU	-	expression tag	UNP Q9BRX2
ii	389	ASN	-	expression tag	UNP Q9BRX2
ii	390	LEU	-	expression tag	UNP Q9BRX2
ii	391	TYR	-	expression tag	UNP Q9BRX2
ii	392	PHE	-	expression tag	UNP Q9BRX2
ii	393	GLN	-	expression tag	UNP Q9BRX2
ii	394	GLY	-	expression tag	UNP Q9BRX2
ii	395	ALA	-	expression tag	UNP Q9BRX2
ii	396	HIS	-	expression tag	UNP Q9BRX2
ii	397	HIS	-	expression tag	UNP Q9BRX2
ii	398	HIS	-	expression tag	UNP Q9BRX2
ii	399	HIS	-	expression tag	UNP Q9BRX2
ii	400	HIS	-	expression tag	UNP Q9BRX2
ii	401	HIS	-	expression tag	UNP Q9BRX2
ii	402	SER	-	expression tag	UNP Q9BRX2
ii	403	THR	-	expression tag	UNP Q9BRX2

- Molecule 87 is a protein called Hbs1l.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	425	Total	C	N	O	S	0	0
			3292	2100	565	609	18		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
jj	-25	MET	-	initiating methionine	UNP Q9Y450
jj	-24	ASP	-	expression tag	UNP Q9Y450
jj	-23	TYR	-	expression tag	UNP Q9Y450
jj	-22	LYS	-	expression tag	UNP Q9Y450
jj	-21	ASP	-	expression tag	UNP Q9Y450
jj	-20	HIS	-	expression tag	UNP Q9Y450
jj	-19	ASP	-	expression tag	UNP Q9Y450
jj	-18	GLY	-	expression tag	UNP Q9Y450
jj	-17	ASP	-	expression tag	UNP Q9Y450
jj	-16	TYR	-	expression tag	UNP Q9Y450
jj	-15	LYS	-	expression tag	UNP Q9Y450
jj	-14	ASP	-	expression tag	UNP Q9Y450
jj	-13	HIS	-	expression tag	UNP Q9Y450
jj	-12	ASP	-	expression tag	UNP Q9Y450
jj	-11	ILE	-	expression tag	UNP Q9Y450
jj	-10	ASP	-	expression tag	UNP Q9Y450
jj	-9	TYR	-	expression tag	UNP Q9Y450
jj	-8	LYS	-	expression tag	UNP Q9Y450
jj	-7	ASP	-	expression tag	UNP Q9Y450
jj	-6	ASP	-	expression tag	UNP Q9Y450
jj	-5	ASP	-	expression tag	UNP Q9Y450
jj	-4	ASP	-	expression tag	UNP Q9Y450
jj	-3	LYS	-	expression tag	UNP Q9Y450
jj	-2	ALA	-	expression tag	UNP Q9Y450
jj	-1	GLY	-	expression tag	UNP Q9Y450
jj	0	SER	-	expression tag	UNP Q9Y450

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

Mol	Chain	Residues	Atoms	AltConf
88	P	2	Total Mg 2 2	0
88	g	1	Total Mg 1 1	0
88	j	1	Total Mg 1 1	0
88	Q	1	Total Mg 1 1	0
88	e	1	Total Mg 1 1	0
88	B	1	Total Mg 1 1	0

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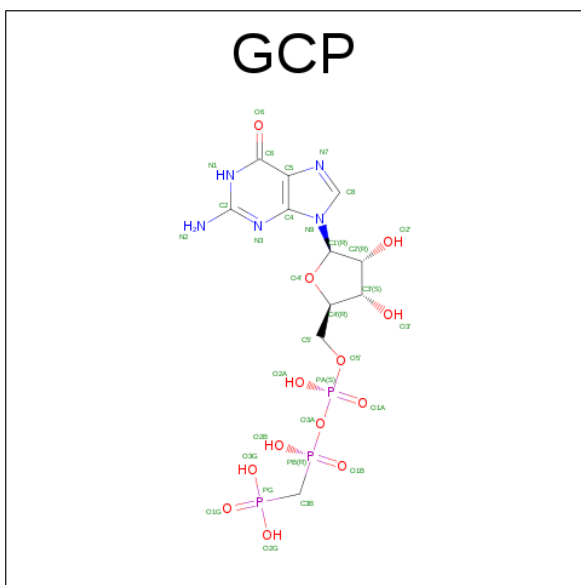
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Mol	Chain	Residues	Atoms		AltConf
88	I	1	Total 1	Mg 1	0
88	jj	1	Total 1	Mg 1	0
88	V	1	Total 1	Mg 1	0
88	7	5	Total 5	Mg 5	0
88	a	1	Total 1	Mg 1	0
88	5	188	Total 188	Mg 188	0
88	8	6	Total 6	Mg 6	0
88	9	71	Total 71	Mg 71	0

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

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

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

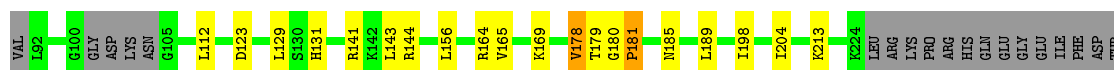
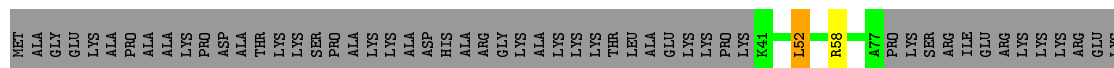


Mol	Chain	Residues	Atoms					AltConf
90	9	1	Total 32	C 11	N 5	O 13	P 3	0
90	jj	1	Total 32	C 11	N 5	O 13	P 3	0



• Molecule 5: eL6

Chain E: 65% 8% 26%



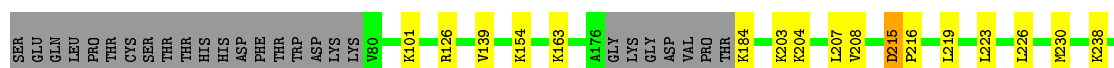
• Molecule 6: uL30

Chain F: 80% 10% 9%



• Molecule 7: eL8

Chain G: 67% 6% 27%



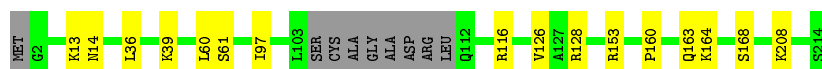
• Molecule 8: uL6

Chain H: 87% 11% 2%



• Molecule 9: uL16

Chain I: 88% 7% 5%



- Molecule 10: uL5

Chain J: 89% 6% .



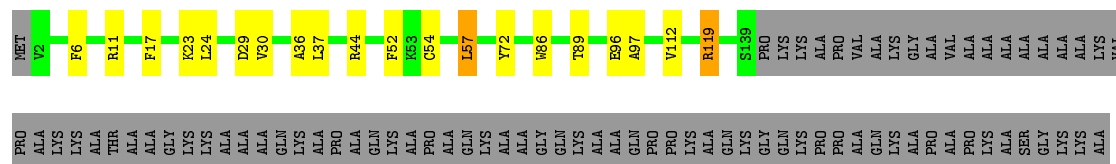
- Molecule 11: eL13

Chain L: 92% 7%



- Molecule 12: eL14

Chain M: 54% 8% 37%



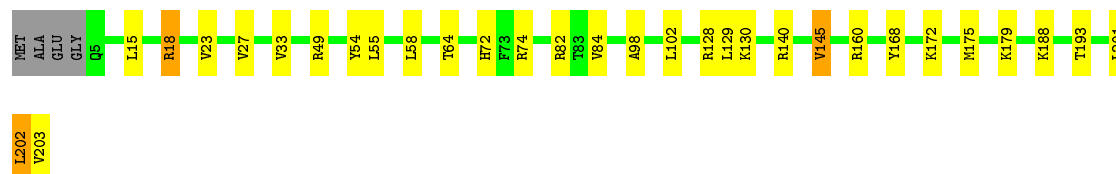
- Molecule 13: eL15

Chain N:  91% 8%



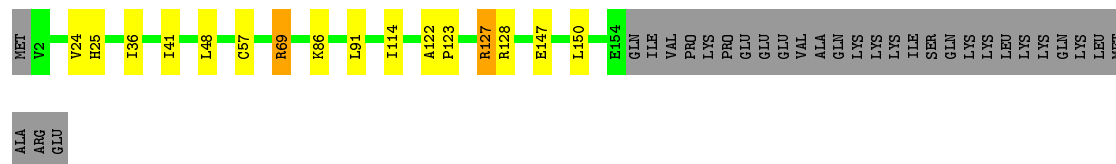
- Molecule 14: uL13

Chain O: 83% 14% 3%




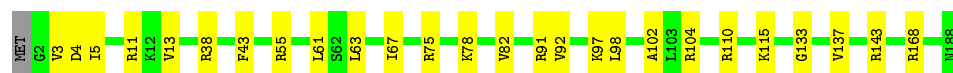
- Molecule 15: uL22

Chain P: 74% 8% 17%




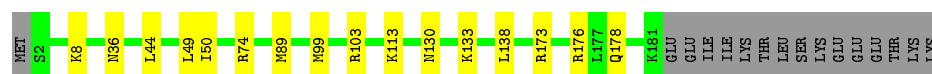
- Molecule 16: eL18

Chain Q:  86% 14% .




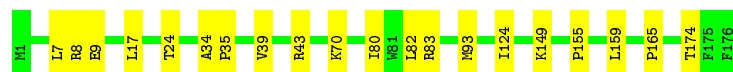
- Molecule 17: eL19

Chain R:  84% 8% 8%




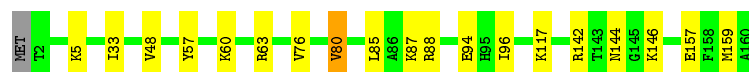
- Molecule 18: eL20

Chain S:  89% 11%



- Molecule 19: eL21

Chain T:  88% 11% ..

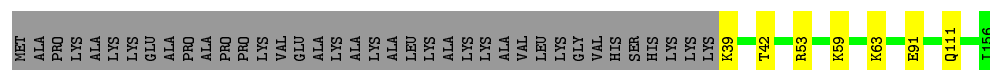


- Molecule 20: eL22


Chain U:  71% 6% 23%



Chain X:  71% . 24%



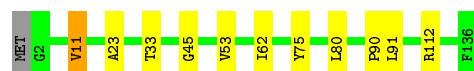
- Molecule 24: uL24

Chain Y:  87% 6% 8%



- Molecule 25: eL27

Chain Z: 91% 7%



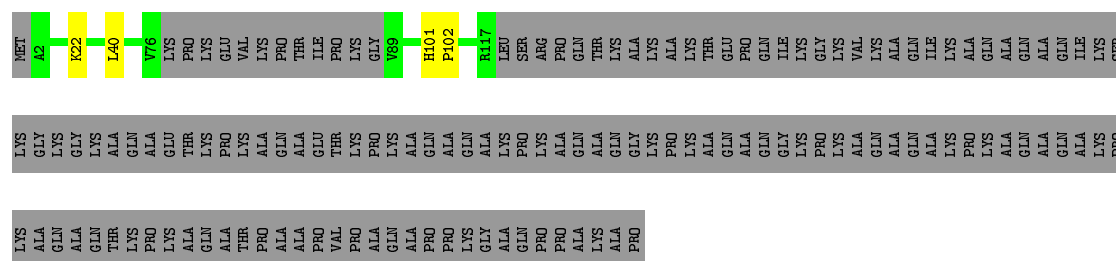
- Molecule 26: uL15

Chain a: 97%

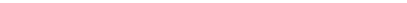


- Molecule 27: eL29

Chain b:  41% . 58%



- Molecule 28: eL30

Chain c:  82% • 15%




- Molecule 29: eL31

Chain d: 76% 10% 14%



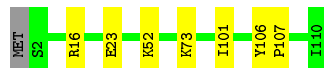
- Molecule 30: eL32

Chain e:  88% 7% 5%



- Molecule 31: eL33

Chain f:  93% 6% .



- Molecule 32: eL34

Chain g:  95% . .



- Molecule 33: uL29

Chain h:  96% . .




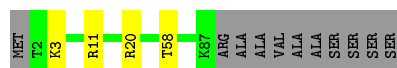
- Molecule 34: eL36

Chain i:  94% . .



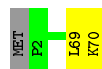
- Molecule 35: eL37

Chain j:  85% . 11%



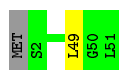
- Molecule 36: eL38

Chain k:  96% . .

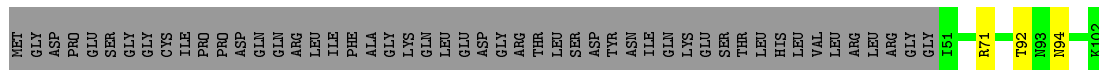


- Molecule 37: eL39

Chain l:  96% . .



- Molecule 38: eL40



- Molecule 39: eL41



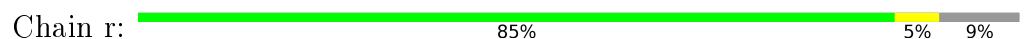
- Molecule 40: eL42



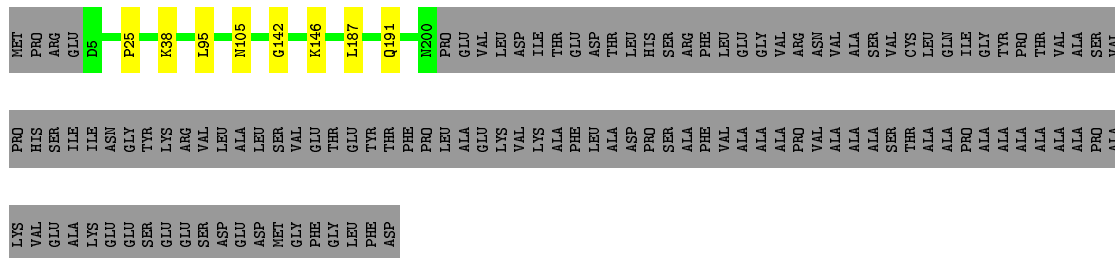
- Molecule 41: eL43




- Molecule 42: eL28



- Molecule 43: uL10



- Molecule 44: uL11

Chain t:  90% 7%




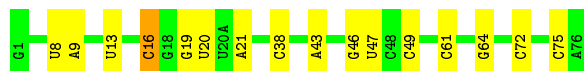
- Molecule 45: Nascent chain

Chain 1:  93% 7%



- Molecule 46: P-site tRNA

Chain 2:  79% 20%



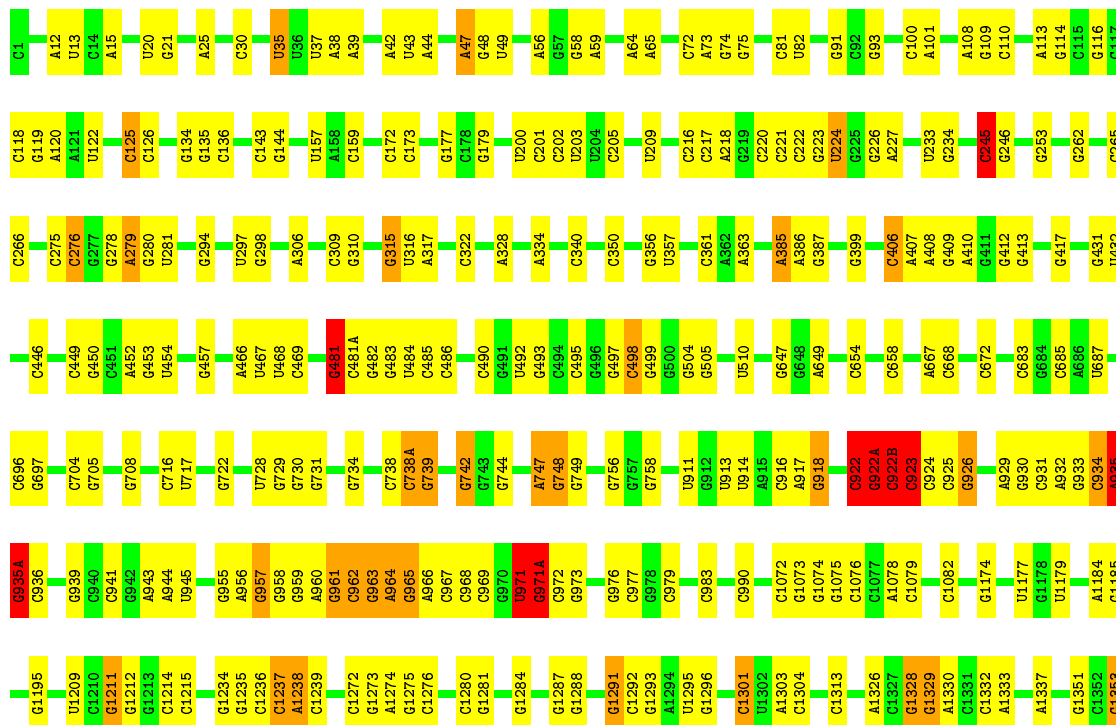
- Molecule 47: E-site tRNA

Chain 3:  64% 35%

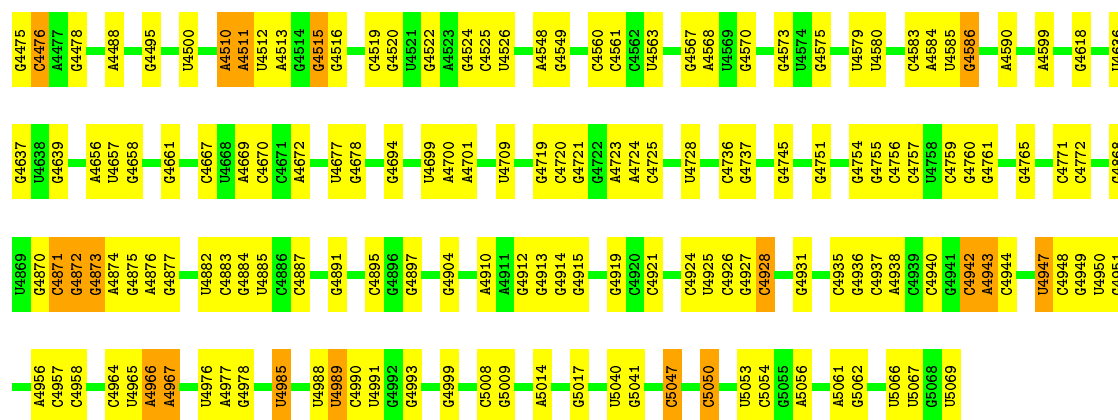


- Molecule 48: 28S ribosomal RNA

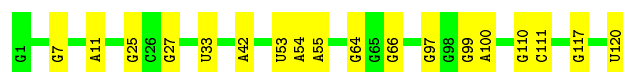
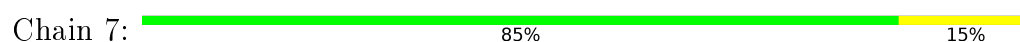
Chain 5:  70% 27%



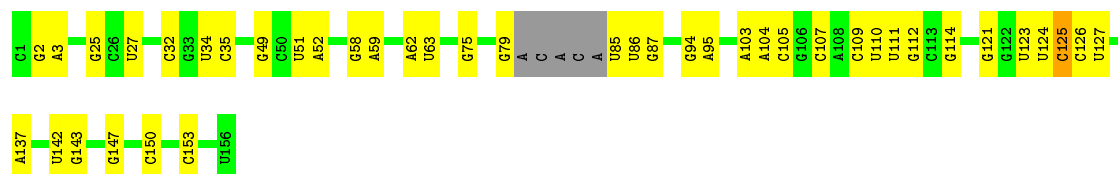
C4350	A4233	G4099	A3860	U3729	G2838	C2719	U2554	C2422	G2261	U2008	G1909	U1757	U1591	G1454	A1354
U4354	G4247	C4100	A3867	A3733	U2839	C2720	G2855	A2423	G2262	U2009	G1910	G1761	U1596	G1455	G1358
G4355	G4248	C4116	G3873	A3740	G2842	G2721	G2564	U2424	G2265	C2011	U1918	C1762	U1597	C1456	G1359
G4371	G4250	U4117	G3876	G3740	G2855	G2724	G2566	A2428	U2267	G2024	U1919	C1763	U1602	C1457	U1364
U4372	A4251	C4119	A3877	A3748	G2875	A2725	C2571	A2429	G2268	A2025	C1920	G1764	G1612	G1465	
G4373		U4120	C3878	G3753	G2884	G2726	C2572	A2433	G2270	A2026	C1921	C1768	A1613	G1475	G1370
G4377	G4254	C4122	G3879	G3756	U2891	C2735	U2575	G2439	G2275	C2031	A1923	U1772	G1624	C1476	A1371
A4378	A4255	G4124	G3888	A3759	G2896	U2740	G2583	U2440	G2278	A2032	C1931	U1773	G1625	C1477	G1377
A4379	A4256	C4126	A3890	A3760	G2897	U2743	A2587	C2441	A2279	G2033	A1932	A1776	G1626	C1478	C1378
A4380	A4257	A4127	U3891	C3761	G2897	U2744	A2587	C2441	A2280	G2034	G1933	U1781	G1632	G1482	G1380
	A4258	G4128	U3892	U3762	C3598	A2743	A2601	G2450	U2281	U2048	A1934	U1781	G1633	C1483	U1381
	A4259	A4129	G3997	G3765	G3603	G2751	G2620	G2459	G2289	G2052	G1940	C1785	C1635	C1485	A1387
	A4260	C4130	G3998	A3766	G3604	G2754	G2621	G2462	G2294	G2055	A1941	A1787	C1640	C1486	
	A4261	U4163	A3901	U3773	C3605	G2754	G2622	C2462	G2294	G2056	A1942	G1797	G1641	G1489	G1394
	A4262	C4164	G3904	A3774	G3615	G2760	G2638	U2467	G2301	A2057	G1948	G1798	G1654	A1497	A1397
	A4263	G4165	A3905	A3775	G3615	U2761	G2639	U2468	G2301	G2057	G1949	G1799	G1655	G1498	A1398
	A4264	C4166	A3906	G3776	C3622	G2762	U2639	G2469	A2313	G2062	G1952	U1800	U1656	C1502	C1401
	A4265	A4167	G3907	G3777	G3625	U2763	A2647	G2470	G2314	G2063	U1959	G1803	C1661	G1503	G1402
	A4266	A4170	A3908	U3778	G3626	A2764	A2647	G2471	G2314	G2064	A1960	A1804	C1665	G1504	G1403
	A4267	C4171	U3914	G3780	G3626	U2769	G2660	C2488	G2331	C2068	G1961	A1805	C1666	G1514	G1406
	A4268	A4172	G3915	A3784	A3630	U2782	G2661	G2489	G2332	A2069	A1962	G1818	A1667	A1515	C1406A
	A4269	C4173	G3916	A3785	A3635	U2787	G2662	U2490	G2333	U2070	C1963	G1819	C1670	G1516	C1406B
	A4270	U4188	G3917	U3786	U3644	U2788	G2663	G2491	G2333	G2084	G1964	U1820	G1670	G1517	C1406C
	A4271	C4183	G3918	U3787	A3648	U2789	G2664	G2492	G2334	G2085	A1965	G1821	C1671	G1518	C1411
	A4272	A4184	U3919	U3788	A3648	U2790	G2665	G2493	G2334	G2086	G1966	U1822	C1672	A1524	C1411A
	A4273	G4185	G3920	U3789	A3648	U2791	G2666	G2494	G2335	A2088	G1967	C1828	A1679	A1525	G1412
	A4274	C4186	A3921	U3801	A3653	C2794	A2676	G2495	A2360	U2090	C1977	G1833	A1684	G1416	G1416
	A4275	U4187	A3922	U3802	A3653	A2795	G2681	G2496	G2363	G2092	C1978	U1834	A1684	C1417	C1417
	A4276	C4188	G3923	C2802	A3653	A2796	G2682	G2497	A2364	G2093	A1979	G1835	A1684	C1418	C1418
	A4277	A4189	A3924	A2806	A3653	G2797	G2683	U2498	G2364	C2094	G1981	G1836	C1690	G1419	G1419
	A4278	U4190	A3925	A2807	A3653	A2798	G2684	G2502	A2367	A2095	G1982	A1837	G1691	C1535	A1420
	A4279	C4191	A3926	A2808	A3653	C2802	G2685	A2503	A2367	G2096	A1983	G1842	G1724	A1547	G1421
	A4280	U4192	A3927	A2809	A3653	A2809	G2686	G2504	A2367	G2097	A1984	G1842	G1724	A1547	G1421
	A4281	C4193	A3928	A2810	A3653	A2810	G2687	G2505	A2367	G2098	G1985	G1842	G1724	A1547	G1421
	A4282	U4194	A3929	A2811	A3653	A2811	G2688	G2506	A2367	G2099	U1986	G1842	G1724	A1547	G1421
	A4283	C4195	A3930	A2812	A3653	A2812	G2689	G2507	A2367	G2100	C1987	G1842	G1724	A1547	G1421
	A4284	U4196	A3931	A2813	A3653	A2813	G2690	G2508	A2367	G2101	U1988	G1842	G1724	A1547	G1421
	A4285	C4197	A3932	A2814	A3653	A2814	G2691	G2509	A2367	G2102	C1989	G1842	G1724	A1547	G1421
	A4286	U4198	A3933	A2815	A3653	A2815	G2692	G2510	A2367	G2103	U1990	G1842	G1724	A1547	G1421
	A4287	C4199	A3934	A2816	A3653	A2816	G2693	G2511	A2367	G2104	A1991	G1842	G1724	A1547	G1421
	A4288	U4200	A3935	A2817	A3653	A2817	G2694	G2512	A2367	G2105	U1991	G1842	G1724	A1547	G1421
	A4289	C4201	A3936	A2818	A3653	A2818	G2695	G2513	A2367	G2106	C1992	G1842	G1724	A1547	G1421
	A4290	U4202	A3937	A2819	A3653	A2819	G2696	G2514	A2367	G2107	U1992	G1842	G1724	A1547	G1421
	A4291	C4203	A3938	A2820	A3653	A2820	G2697	G2515	A2367	G2108	A1993	G1842	G1724	A1547	G1421
	A4292	U4204	A3939	A2821	A3653	A2821	G2698	G2516	A2367	G2109	U1993	G1842	G1724	A1547	G1421
	A4293	C4205	A3940	A2822	A3653	A2822	G2699	G2517	A2367	G2110	C1994	G1842	G1724	A1547	G1421
	A4294	U4206	A3941	A2823	A3653	A2823	G2700	G2518	A2367	G2111	U1994	G1842	G1724	A1547	G1421
	A4295	C4207	A3942	A2824	A3653	A2824	G2701	G2519	A2367	G2112	A1995	G1842	G1724	A1547	G1421
	A4296	U4208	A3943	A2825	A3653	A2825	G2702	G2520	A2367	G2113	U1996	G1842	G1724	A1547	G1421
	A4297	C4209	A3944	A2826	A3653	A2826	G2703	G2521	A2367	G2114	C1997	G1842	G1724	A1547	G1421
	A4298	U4210	A3945	A2827	A3653	A2827	G2704	G2522	A2367	G2115	U1997	G1842	G1724	A1547	G1421
	A4299	C4211	A3946	A2828	A3653	A2828	G2705	G2523	A2367	G2116	C2001	G1842	G1724	A1547	G1421
	A4300	U4212	A3947	A2829	A3653	A2829	G2706	G2524	A2367	G2117	A2002	G1842	G1724	A1547	G1421
	A4301	C4213	A3948	A2830	A3653	A2830	G2707	G2525	A2367	G2118	C2003	G1842	G1724	A1547	G1421
	A4302	U4214	A3949	A2831	A3653	A2831	G2708	G2526	A2367	G2119	U2004	G1842	G1724	A1547	G1421
	A4303	C4215	A3950	A2832	A3653	A2832	G2709	G2527	A2367	G2120	C2005	G1842	G1724	A1547	G1421
	A4304	U4216	A3951	A2833	A3653	A2833	G2710	G2528	A2367	G2121	U2006	G1842	G1724	A1547	G1421
	A4305	C4217	A3952	A2834	A3653	A2834	G2711	G2529	A2367	G2122	C2007	G1842	G1724	A1547	G1421
	A4306	U4218	A3953	A2835	A3653	A2835	G2712	G2530	A2367	G2123	U2008	G1842	G1724	A1547	G1421
	A4307	C4219	A3954	A2836	A3653	A2836	G2713	G2531	A2367	G2124	C2009	G1842	G1724	A1547	G1421
	A4308	U4220	A3955	A2837	A3653	A2837	G2714	G2532	A2367	G2125	U2010	G1842	G1724	A1547	G1421
	A4309	C4221	A3956	A2838	A3653	A2838	G2715	G2533	A2367	G2126	C2011	G1842	G1724	A1547	G1421
	A4310	U4222	A3957	A2839	A3653	A2839	G2716	G2534	A2367	G2127	A2009	G1842	G1724	A1547	G1421
	A4311	C4223	A3958	A2840	A3653	A2840	G2717	G2535	A2367	G2128	C2010	G1842	G1724	A1547	G1421
	A4312	U4224	A3959	A2841	A3653	A2841	G2718	G2536	A2367	G2129	U2011	G1842	G1724	A1547	G1421
	A4313	C4225	A3960	A2842	A3653	A2842	G2719	G2537	A2367	G2130	C2012	G1842	G1724	A1547	G1421
	A4314	U4226	A3961	A2843	A3653	A2843	G2720	G2538	A2367	G2131	U2013	G1842	G1724	A1547	G1421
	A4315	C4227	A3962	A2844	A3653	A2844	G2721	G2539	A2367	G2132	C2014	G1842	G1724	A1547	G1421
	A4316	U4228	A3963	A2845	A3653	A2845	G2722	G2540	A2367	G2133	U2015	G1842	G1724	A1547	G1421
	A4317	C4229	A3964	A2846	A3653	A2846	G2723	G2541	A2367	G2134	C2016	G1842	G1724	A1547	G1421
	A4318	U4230	A3965	A2847	A3653	A2847	G2724	G2542	A2367	G2135	U2017	G1842	G1724	A1547	G1421
	A4319	C4231	A3966	A2848	A3653	A2848	G2725	G2543	A2367	G2136	C2018	G1842	G1724	A1547	G1421
	A4320	U4232	A3967	A2849	A3653	A2849	G2726	G2544	A2367	G2137	U2019	G1842	G1724	A1547	G1421
	A4321	C4233	A3968	A2850	A3653	A2850	G2727	G2545	A2367	G2138	C2020	G1842	G1724	A1547	G1421
	A4322	U4234	A3969	A2851	A3653	A2851	G2728	G2546	A2367	G2139	U2021	G1842	G1724	A1547	G1421
	A4323	C4235	A3970	A2852	A3653	A2852	G2729	G2547	A2367	G2140	C2022	G1842	G1724	A1547	G1421
	A4324	U4236	A3971	A2853	A3653	A2853	G2730	G2548	A2367	G2141	U2023	G1842	G1724	A1547	G1421
	A4325	C4237	A3972	A2854	A3653	A2854	G2731	G2549	A2367	G2142	C2024	G1842	G1724	A1547	G1421
	A4326	U4238	A3973	A2855	A3653	A2855	G2732	G2550	A2367	G2143	U2025	G1842	G1724	A1547	G1421
	A4327	C4239	A3974	A2856	A3653	A2856	G2733	G2551	A2367	G2144	C2026	G1842	G1724	A1547	G1421
	A4328	U4240	A3975	A2857	A3653	A2857	G2734	G2552	A2367	G2145	U2027	G1842	G1724	A1547	G1421
	A4329	C4241	A3976	A2858	A3653	A2858	G2735	G2553	A2367	G2146	C2028	G1842	G1724	A1547	G1421
	A4330	U4242	A3977	A2859	A3653	A2859	G2736	G2554	A2367	G2147	U2029	G1842	G1724	A1547	G1421
	A4331	C4243	A3978	A2860	A3653	A2860	G2737	G2555	A2367	G2148	C2030	G1842	G1724	A1547	G1421
	A4332	U4244	A3979	A2861	A3653	A2861	G2738	G2556							



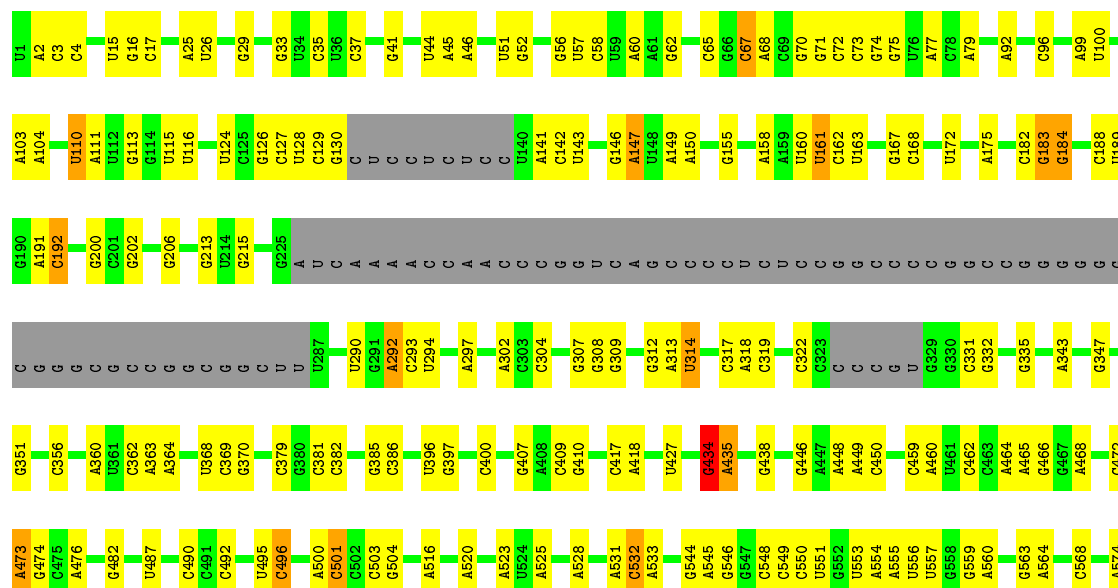
- Molecule 49: 5S ribosomal RNA



- Molecule 50: 5.8S ribosomal RNA



- Molecule 51: 18S ribosomal RNA

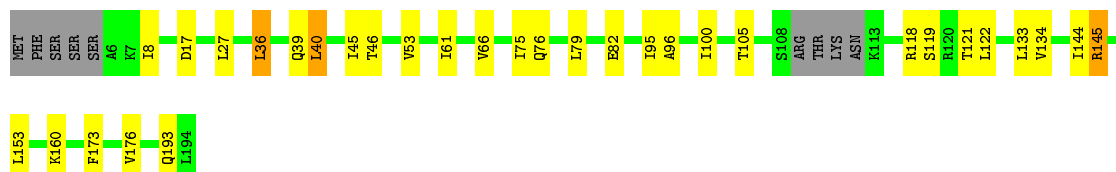







- Molecule 59: eS7

Chain HH: 79% 15% 5%



- Molecule 60: eS8

Chain II: 85% 14% 1%



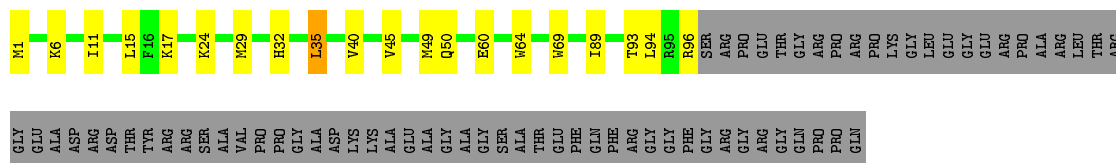
- Molecule 61: uS4

Chain JJ: 82% 13% 5%



- Molecule 62: eS10

Chain KK: 46% 12% 42%



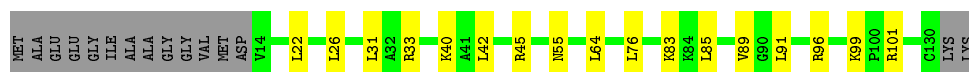
- Molecule 63: uS17

Chain LL: 77% 13% 9%




- Molecule 64: eS12

Chain MM: 76% 13% 11%



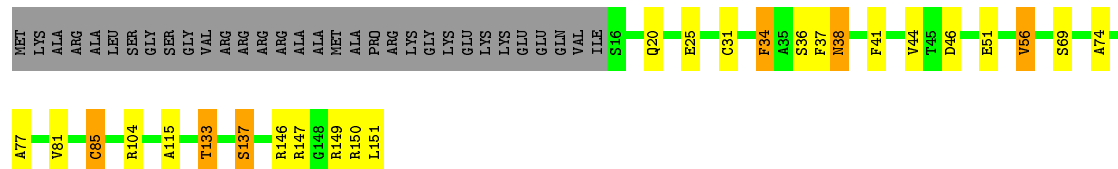
- Molecule 65: uS15

Chain NN:  83% 14% ..



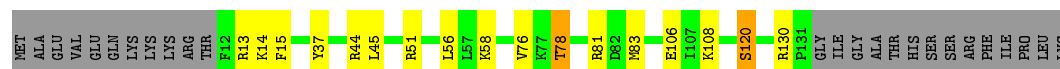
- Molecule 66: uS11

Chain 00: 65% 12% . 19%




- Molecule 67: uS19

Chain PP:  71% 10% • 17%

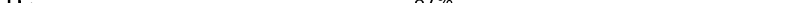


- Molecule 68: uS9

Chain QQ:  84% 14% .



- Molecule 69: eS17

Chain RR:  87% 10% ..



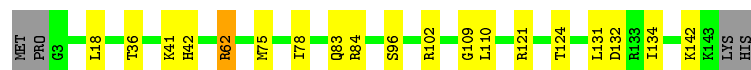
- Molecule 70: uS13

Chain SS: 81% 13% • 5%



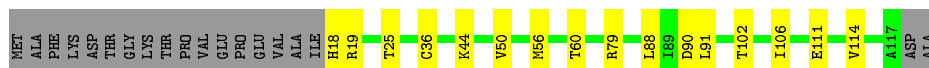
- Molecule 71: eS19

Chain TT: 84% 12% ..



- Molecule 72: uS10

Chain UU:  71% 13% 16%




- Molecule 73: eS21

Chain VV:  89% 10% .




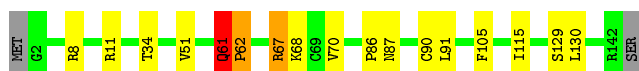
- Molecule 74: uS8

Chain WW:  85% 14% ..




- Molecule 75: uS12

Chain XX:  87% 10% ...



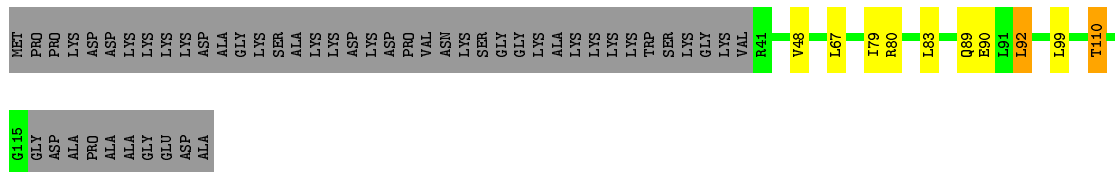
- Molecule 76: eS24

Chain YY:  81% 14% . 5%




- Molecule 77: eS25

Chain ZZ:  52% 6% . 40%



- Molecule 78: eS26

Chain aa:  78% 10% 12%



- Molecule 79: eS27

- Molecule 80: eS28

- Molecule 81: uS14

- Molecule 82: eS30

- Molecule 83: eS31

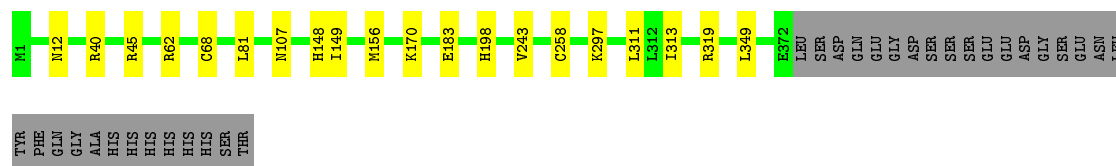
- Molecule 84: RACK1

- Molecule 85: mRNA (truncated)



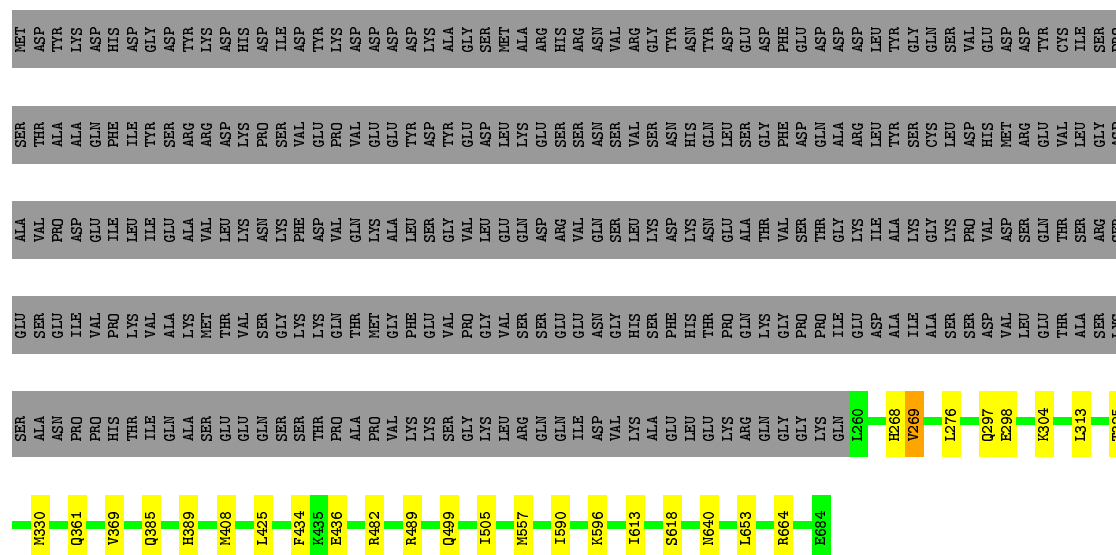

- Molecule 86: Pelota

Chain ii: 87% 5% 8%



- Molecule 87: Hbs11

Chain jj:  56% . 40%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	42011	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	104478	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: GCP, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.36	0/1936	0.71	0/2596
10	J	0.33	0/1385	0.60	0/1852
11	L	0.35	0/1733	0.66	0/2316
12	M	0.37	0/1158	0.68	0/1547
13	N	0.36	0/1746	0.69	0/2338
14	O	0.36	0/1662	0.67	0/2222
15	P	0.36	0/1268	0.65	0/1700
16	Q	0.36	0/1539	0.73	0/2054
17	R	0.35	0/1524	0.67	0/2013
18	S	0.35	0/1501	0.65	0/2012
19	T	0.37	0/1326	0.63	0/1770
2	B	0.34	0/3240	0.64	0/4339
20	U	0.36	0/823	0.56	0/1104
21	V	0.37	0/993	0.67	0/1332
22	W	0.35	0/873	0.57	0/1158
23	X	0.33	0/984	0.60	0/1323
24	Y	0.35	0/1132	0.64	0/1504
25	Z	0.35	0/1130	0.61	0/1507
26	a	0.34	0/1191	0.63	0/1590
27	b	0.33	0/861	0.58	0/1138
28	c	0.33	0/771	0.54	0/1034
29	d	0.35	0/903	0.67	0/1216
3	C	0.35	0/2937	0.67	0/3946
30	e	0.38	0/1071	0.68	0/1429
31	f	0.36	0/895	0.70	0/1198
32	g	0.34	0/916	0.70	0/1220
33	h	0.32	0/1021	0.59	0/1348
34	i	0.34	0/841	0.59	0/1112
35	j	0.35	0/720	0.70	0/952
36	k	0.32	0/575	0.54	0/761
37	l	0.34	0/459	0.62	0/608
38	m	0.35	0/435	0.63	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	n	0.35	0/240	0.68	0/305
4	D	0.34	0/2437	0.61	1/3264 (0.0%)
40	o	0.33	0/864	0.61	0/1140
41	p	0.33	0/718	0.60	0/953
42	r	0.36	0/1010	0.66	0/1354
43	s	0.36	0/1530	0.50	0/2064
44	t	0.36	0/1174	0.53	0/1582
45	1	0.44	0/129	0.61	0/173
46	2	0.21	0/1805	0.66	0/2809
47	3	0.21	0/1777	0.66	0/2763
48	5	0.74	31/84961 (0.0%)	0.78	72/132460 (0.1%)
49	7	0.26	0/2858	0.65	0/4455
5	E	0.34	0/1762	0.62	0/2362
50	8	0.26	0/3581	0.68	0/5577
51	9	0.27	0/40523	0.71	14/63130 (0.0%)
52	AA	0.36	0/1747	0.61	0/2374
53	BB	0.34	0/1756	0.59	0/2350
54	CC	0.36	0/1753	0.66	0/2369
55	DD	0.36	0/1796	0.63	0/2417
56	EE	0.36	0/2118	0.64	0/2849
57	FF	0.34	0/1492	0.60	0/2005
58	GG	0.36	0/1946	0.68	1/2590 (0.0%)
59	HH	0.36	0/1510	0.58	0/2022
6	F	0.36	0/1911	0.67	0/2549
60	II	0.36	0/1715	0.67	0/2287
61	JJ	0.35	0/1550	0.68	0/2069
62	KK	0.39	0/834	0.61	0/1125
63	LL	0.35	0/1195	0.68	0/1597
64	MM	0.37	0/918	0.59	0/1233
65	NN	0.36	0/1226	0.64	0/1649
66	OO	0.36	0/1029	0.73	0/1380
67	PP	0.38	0/1017	0.65	0/1358
68	QQ	0.35	0/1146	0.63	0/1534
69	RR	0.36	0/1082	0.61	0/1452
7	G	0.34	0/1910	0.61	0/2569
70	SS	0.37	0/1208	0.67	0/1618
71	TT	0.38	0/1115	0.65	0/1493
72	UU	0.35	0/805	0.65	0/1081
73	VV	0.38	0/643	0.66	0/860
74	WW	0.36	0/1051	0.71	0/1406
75	XX	0.33	0/1116	0.65	0/1490
76	YY	0.37	0/1028	0.64	0/1366
77	ZZ	0.36	0/604	0.60	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	aa	0.38	0/828	0.71	0/1109
79	bb	0.35	0/665	0.63	0/891
8	H	0.33	0/1535	0.62	0/2063
80	cc	0.38	0/490	0.73	1/656 (0.2%)
81	dd	0.39	0/470	0.65	0/623
82	ee	0.36	0/447	0.66	0/587
83	ff	0.38	0/567	0.55	0/753
84	gg	0.33	0/2493	0.55	0/3394
85	hh	0.29	0/188	0.82	0/290
86	ii	0.33	0/2996	0.56	0/4050
87	jj	0.34	0/3352	0.55	0/4523
9	I	0.35	0/1702	0.63	0/2272
All	All	0.52	31/237872 (0.0%)	0.71	89/348318 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
48	5	0	3
6	F	0	1
75	XX	0	1
86	ii	0	2
All	All	0	9

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	935	A	C6-N6	192.84	2.88	1.33
48	5	935	A	C5-C6	-20.65	1.22	1.41
48	5	922(A)	G	O3'-P	17.07	1.81	1.61
48	5	481	G	C2-N3	-13.50	1.22	1.32
48	5	971	U	C2-O2	-13.31	1.10	1.22
48	5	922	C	O3'-P	13.02	1.76	1.61
48	5	1411(C)	C	O5'-C5'	11.09	1.62	1.44
48	5	1411	C	P-O5'	10.73	1.70	1.59
48	5	935	A	C5-C4	-10.67	1.31	1.38
48	5	935	A	C6-N1	-10.62	1.28	1.35
48	5	935	A	N1-C2	-9.43	1.25	1.34
48	5	935	A	C2-N3	9.23	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	935	A	N3-C4	9.04	1.40	1.34
48	5	1411	C	P-OP1	-8.94	1.33	1.49
48	5	481	G	N1-C2	-8.66	1.30	1.37
48	5	971	U	N1-C2	-8.63	1.30	1.38
48	5	481	G	C5-C6	8.39	1.50	1.42
48	5	922(B)	C	O3'-P	7.49	1.70	1.61
48	5	1411	C	C5'-C4'	6.95	1.59	1.51
48	5	1411(C)	C	P-O5'	6.66	1.66	1.59
48	5	481	G	N9-C8	-6.64	1.33	1.37
48	5	922(A)	G	C3'-O3'	6.48	1.51	1.42
48	5	922	C	C3'-O3'	6.22	1.50	1.42
48	5	1411(C)	C	C5'-C4'	6.09	1.58	1.51
48	5	935(A)	G	P-O5'	5.99	1.65	1.59
48	5	922(B)	C	O5'-C5'	5.75	1.53	1.44
48	5	971	U	C2-N3	-5.72	1.33	1.37
48	5	1411(B)	C	O3'-P	5.59	1.67	1.61
48	5	1411	C	C4'-C3'	5.52	1.59	1.53
48	5	1406	G	P-O5'	5.47	1.65	1.59
48	5	922(B)	C	C5'-C4'	5.21	1.57	1.51

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	481	G	C8-N9-C1'	-61.05	47.63	127.00
48	5	935	A	C6-N1-C2	-39.97	94.62	118.60
48	5	935	A	C5-C6-N6	-39.04	92.47	123.70
48	5	481	G	N1-C2-N2	-38.45	81.59	116.20
48	5	481	G	N3-C2-N2	-37.53	93.63	119.90
48	5	935	A	C4-C5-C6	-36.79	98.61	117.00
48	5	481	G	C4-N9-C1'	-36.47	79.09	126.50
48	5	481	G	C2-N3-C4	-29.02	97.39	111.90
48	5	481	G	C6-N1-C2	-25.25	109.95	125.10
48	5	971	U	N3-C2-O2	-22.99	106.11	122.20
48	5	971	U	N1-C2-O2	-21.48	107.77	122.80
48	5	935	A	N1-C6-N6	-21.18	105.89	118.60
48	5	935	A	N3-C4-C5	-18.98	113.52	126.80
48	5	935	A	N1-C2-N3	-16.36	121.12	129.30
48	5	922	C	C2'-C3'-O3'	13.28	138.72	109.50
48	5	971	U	C2-N3-C4	-11.55	120.07	127.00
48	5	971	U	C6-N1-C2	-10.89	114.47	121.00
48	5	1411(C)	C	P-O5'-C5'	10.66	137.95	120.90
48	5	481	G	C5-C6-N1	-10.50	106.25	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	935	A	O5'-P-OP2	-10.33	96.40	105.70
48	5	935	A	C5-C6-N1	-10.03	112.69	117.70
51	9	1821	U	N1-C1'-C2'	-9.95	101.05	112.00
48	5	922	C	C4'-C3'-C2'	-9.39	93.21	102.60
48	5	922(B)	C	O4'-C1'-N1	9.27	115.62	108.20
48	5	922	C	C5'-C4'-O4'	9.13	120.06	109.10
48	5	481	G	N3-C4-C5	-8.85	124.17	128.60
48	5	922	C	N1-C1'-C2'	-8.53	102.62	112.00
51	9	1835	A	C2'-C3'-O3'	8.38	127.93	109.50
48	5	935	A	C1'-O4'-C4'	-8.17	103.37	109.90
48	5	481	G	N9-C1'-C2'	8.16	124.60	114.00
48	5	3888	G	C2'-C3'-O3'	8.09	127.30	109.50
51	9	1394	G	C2'-C3'-O3'	8.08	127.28	109.50
51	9	1820	G	N9-C1'-C2'	-7.83	103.38	112.00
48	5	922	C	O4'-C4'-C3'	-7.64	96.36	104.00
4	D	22	ARG	NE-CZ-NH1	7.45	124.02	120.30
48	5	481	G	N7-C8-N9	-7.17	109.52	113.10
48	5	922(A)	G	P-O3'-C3'	7.11	128.23	119.70
48	5	481	G	N9-C4-C5	-7.04	102.58	105.40
48	5	3761	C	N1-C1'-C2'	-6.83	104.48	112.00
48	5	3697	U	C2'-C3'-O3'	6.68	124.39	113.70
48	5	1477	C	C2'-C3'-O3'	6.64	124.33	113.70
48	5	922(A)	G	N9-C1'-C2'	6.62	122.61	114.00
48	5	922(B)	C	P-O5'-C5'	6.58	131.44	120.90
48	5	1411	C	C4'-C3'-O3'	6.58	126.17	113.00
48	5	935	A	C4-N9-C1'	-6.50	114.60	126.30
48	5	1329	G	C2'-C3'-O3'	6.44	124.00	113.70
48	5	406	C	C2'-C3'-O3'	6.39	123.92	113.70
48	5	1455	G	C2'-C3'-O3'	6.37	123.89	113.70
48	5	1411	C	C5'-C4'-O4'	6.36	116.73	109.10
48	5	2046	G	C2'-C3'-O3'	6.33	123.83	113.70
48	5	935	A	C8-N9-C1'	6.26	138.97	127.70
48	5	935	A	O4'-C1'-N9	6.24	113.19	108.20
48	5	1211	G	C2'-C3'-O3'	6.20	123.62	113.70
48	5	481	G	C8-N9-C4	6.19	108.88	106.40
48	5	1411	C	C5'-C4'-C3'	6.13	125.81	116.00
48	5	922(B)	C	C4'-C3'-O3'	6.09	125.19	113.00
48	5	47	A	C4'-C3'-O3'	5.99	124.98	113.00
48	5	385	A	C4'-C3'-O3'	5.99	124.97	113.00
48	5	2695	A	C2'-C3'-O3'	5.97	123.25	113.70
48	5	923	C	P-O5'-C5'	5.94	130.41	120.90
48	5	935(A)	G	C2'-C3'-O3'	5.93	123.19	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1646	C	C2'-C3'-O3'	5.89	123.12	113.70
48	5	1411	C	O4'-C1'-N1	5.86	112.88	108.20
48	5	4947	U	C2'-C3'-O3'	5.82	123.02	113.70
48	5	1411(C)	C	C5'-C4'-O4'	5.74	115.98	109.10
48	5	1291	G	C2'-C3'-O3'	5.66	122.75	113.70
48	5	1411	C	O4'-C4'-C3'	-5.63	98.37	104.00
48	5	245	C	C2'-C3'-O3'	5.61	122.68	113.70
48	5	922	C	O4'-C1'-N1	5.60	112.68	108.20
48	5	125	C	C2'-C3'-O3'	5.60	122.65	113.70
51	9	1820	G	C1'-C2'-O2'	-5.59	93.81	110.60
80	cc	66	ARG	NE-CZ-NH2	5.57	123.09	120.30
48	5	922(B)	C	C5'-C4'-C3'	5.54	124.86	116.00
48	5	922(B)	C	N1-C1'-C2'	5.51	121.17	114.00
51	9	1820	G	C4'-C3'-O3'	5.39	123.79	113.00
51	9	110	U	C2'-C3'-O3'	5.37	122.29	113.70
48	5	1445	U	C2'-C3'-O3'	5.27	122.13	113.70
48	5	4448	G	C4'-C3'-O3'	5.23	123.47	113.00
48	5	922(B)	C	C1'-C2'-O2'	-5.22	94.94	110.60
48	5	3603	G	C2'-C3'-O3'	5.19	122.00	113.70
51	9	1130	G	C4'-C3'-O3'	5.16	123.32	113.00
51	9	434	G	C2'-C3'-O3'	5.14	121.93	113.70
48	5	2474	G	C2'-C3'-O3'	5.10	121.86	113.70
51	9	1137	U	C2'-C3'-O3'	5.10	121.86	113.70
51	9	532	C	C2'-C3'-O3'	5.09	121.84	113.70
48	5	971(A)	G	C4'-C3'-O3'	5.09	123.17	113.00
51	9	1060	A	N9-C1'-C2'	5.06	120.57	114.00
58	GG	41	LEU	CA-CB-CG	5.05	126.91	115.30
51	9	1863	A	O4'-C1'-N9	5.02	112.22	108.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	481	G	Sidechain
48	5	935	A	Sidechain
48	5	971	U	Sidechain
2	B	16	PHE	Peptide
2	B	258	HIS	Peptide
6	F	235	ARG	Peptide
75	XX	61	GLN	Peptide
86	ii	45	ARG	Sidechain
86	ii	62	ARG	Sidechain

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	A	1898	0	1993	17	0
2	B	3172	0	3310	15	0
3	C	2883	0	3053	13	0
4	D	2391	0	2424	14	0
5	E	1729	0	1887	10	0
6	F	1875	0	1995	11	0
7	G	1879	0	2027	5	0
8	H	1516	0	1597	8	0
9	I	1664	0	1712	4	0
10	J	1362	0	1399	4	0
11	L	1702	0	1820	4	0
12	M	1137	0	1211	13	0
13	N	1701	0	1749	6	0
14	O	1630	0	1778	17	0
15	P	1242	0	1274	5	0
16	Q	1515	0	1634	10	0
17	R	1508	0	1664	3	0
18	S	1462	0	1508	7	0
19	T	1298	0	1366	6	0
20	U	809	0	833	5	0
21	V	979	0	1039	8	0
22	W	860	0	903	3	0
23	X	967	0	1040	1	0
24	Y	1115	0	1205	1	0
25	Z	1107	0	1182	5	0
26	a	1162	0	1209	0	0
27	b	848	0	920	0	0
28	c	761	0	794	0	0
29	d	888	0	930	0	0
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	1000	0	0
33	h	1013	0	1147	0	0
34	i	830	0	916	0	0
35	j	705	0	737	0	0
36	k	569	0	637	0	0
37	l	447	0	480	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	429	0	465	0	0
39	n	239	0	289	0	0
40	o	851	0	920	0	0
41	p	708	0	756	0	0
42	r	994	0	1051	0	0
43	s	1507	0	1564	0	0
44	t	1160	0	1218	0	0
45	1	125	0	117	1	0
46	2	1616	0	824	2	0
47	3	1593	0	811	1	0
48	5	75972	0	38402	283	0
49	7	2558	0	1296	3	0
50	8	3208	0	1629	5	0
51	9	36249	0	18314	186	0
52	AA	1710	0	1708	12	0
53	BB	1729	0	1803	8	0
54	CC	1716	0	1806	15	0
55	DD	1768	0	1866	26	0
56	EE	2076	0	2177	12	0
57	FF	1471	0	1522	7	0
58	GG	1923	0	2089	11	0
59	HH	1488	0	1582	12	0
60	II	1686	0	1772	10	0
61	JJ	1525	0	1640	7	0
62	KK	810	0	836	9	0
63	LL	1175	0	1249	3	0
64	MM	908	0	939	4	0
65	NN	1202	0	1289	6	0
66	OO	1016	0	1039	10	0
67	PP	997	0	1045	2	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	3	0
70	SS	1190	0	1249	4	0
71	TT	1097	0	1132	5	0
72	UU	795	0	862	2	0
73	VV	636	0	637	3	0
74	WW	1034	0	1080	8	0
75	XX	1098	0	1167	7	0
76	YY	1011	0	1083	5	0
77	ZZ	598	0	656	5	0
78	aa	814	0	865	0	0
79	bb	651	0	672	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	cc	488	0	514	0	0
81	dd	459	0	449	0	0
82	ee	443	0	492	0	0
83	ff	555	0	567	0	0
84	gg	2436	0	2393	0	0
85	hh	169	0	86	0	0
86	ii	2947	0	2957	0	0
87	jj	3292	0	3371	0	0
88	5	188	0	0	0	0
88	7	5	0	0	0	0
88	8	6	0	0	0	0
88	9	71	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	P	2	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	e	1	0	0	0	0
88	g	1	0	0	0	0
88	j	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	9	32	0	14	28	0
90	jj	32	0	14	0	0
All	All	222130	0	167026	791	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 3.

All (791) 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)
48:5:922:C:C5'	48:5:922(A):G:H3'	1.47	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:H5'	48:5:922(A):G:C3'	1.56	1.34
48:5:922:C:H2'	48:5:922(B):C:C2	1.62	1.33
51:9:1137:U:O4	51:9:1148:A:N1	1.64	1.29
51:9:614:C:C4'	51:9:626:G:H21	1.45	1.29
48:5:2367:A:N1	48:5:2788:U:O4	1.64	1.28
51:9:628:A:OP1	90:9:1972:GCP:N2	1.67	1.25
48:5:922:C:H2'	48:5:922(B):C:N1	1.52	1.25
48:5:935:A:C1'	48:5:935:A:H62	1.52	1.23
48:5:922:C:C5'	48:5:922(B):C:P	2.27	1.22
51:9:1137:U:C4	51:9:1148:A:N1	2.07	1.22
48:5:935:A:H1'	48:5:935:A:N6	1.53	1.21
48:5:922:C:H3'	48:5:922(B):C:C6	1.75	1.20
48:5:922:C:C3'	48:5:922(B):C:C6	2.26	1.19
48:5:922:C:H5''	48:5:922(B):C:P	1.72	1.18
48:5:922:C:O3'	48:5:922(B):C:C6	1.97	1.17
51:9:628:A:N6	51:9:1332:A:O4'	1.80	1.13
48:5:935:A:N6	48:5:935(A):G:OP1	1.82	1.11
48:5:922:C:O3'	48:5:922(B):C:O4'	1.67	1.11
90:9:1972:GCP:C3B	55:DD:179:GLN:HE22	1.64	1.09
48:5:922:C:C3'	48:5:922(B):C:O4'	2.00	1.09
55:DD:179:GLN:HE21	55:DD:179:GLN:HA	1.19	1.07
51:9:614:C:H4'	51:9:626:G:H21	1.18	1.06
51:9:614:C:C4'	51:9:626:G:N2	2.18	1.05
48:5:935:A:H62	48:5:935:A:C2'	1.68	1.05
48:5:935:A:C1'	48:5:935:A:N6	2.14	1.05
48:5:922(A):G:P	48:5:922(B):C:H6	1.79	1.05
48:5:922:C:O3'	48:5:922(B):C:H6	1.29	1.04
51:9:614:C:O4'	51:9:626:G:N2	1.91	1.04
48:5:922:C:C2'	48:5:922(B):C:N1	2.21	1.03
51:9:1137:U:O4	51:9:1148:A:C2	2.12	1.02
51:9:613:G:N2	51:9:629:A:OP2	1.93	1.02
48:5:922:C:C2'	48:5:922(B):C:C1'	2.38	1.01
51:9:613:G:H4'	51:9:615:C:C5	1.97	0.99
48:5:922:C:C3'	48:5:922(B):C:C1'	2.40	0.99
48:5:922:C:C2'	48:5:922(B):C:H1'	1.93	0.98
51:9:615:C:H2'	51:9:616:A:C8	1.99	0.97
48:5:922:C:O2'	48:5:922(B):C:H1'	1.65	0.97
51:9:614:C:H4'	51:9:626:G:N2	1.78	0.96
48:5:922:C:H5'	48:5:922(A):G:H3'	1.00	0.95
90:9:1972:GCP:C3B	55:DD:179:GLN:NE2	2.29	0.95
51:9:1711:U:N3	51:9:1822:A:N1	2.14	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:615:C:O2'	51:9:616:A:O4'	1.84	0.94
48:5:1411:C:O2'	48:5:1411(C):C:C3'	2.16	0.94
48:5:1411:C:O2'	48:5:1411(C):C:C6	2.22	0.91
51:9:628:A:P	90:9:1972:GCP:HN22	1.94	0.91
48:5:922:C:C5'	48:5:922(A):G:C3'	2.29	0.90
48:5:922:C:C3'	48:5:922(B):C:N1	2.35	0.89
48:5:922:C:P	48:5:922(A):G:OP2	2.30	0.89
48:5:922(A):G:P	48:5:922(B):C:C6	2.66	0.88
90:9:1972:GCP:H3B1	55:DD:179:GLN:NE2	1.87	0.88
48:5:3760:A:H2	51:9:1825:A:N3	1.72	0.87
51:9:1501:C:O2'	90:9:1972:GCP:H2'	1.75	0.87
51:9:628:A:H61	51:9:1332:A:C1'	1.86	0.87
48:5:922:C:O5'	48:5:922(A):G:H3'	1.74	0.86
48:5:922(B):C:O2'	48:5:923:C:OP1	1.94	0.86
48:5:1411:C:O4'	48:5:1411(B):C:H2'	1.75	0.86
51:9:1821:U:O2'	51:9:1822:A:O4'	1.95	0.85
51:9:1137:U:O4	51:9:1148:A:C6	2.30	0.85
51:9:1501:C:O2'	90:9:1972:GCP:N9	2.11	0.84
48:5:2367:A:N1	48:5:2788:U:C4	2.46	0.84
48:5:1411:C:O2'	48:5:1411(C):C:H3'	1.78	0.83
51:9:1824:A:N3	51:9:1824:A:H2'	1.92	0.83
48:5:1411:C:C5'	48:5:1411(C):C:H5'	2.08	0.83
48:5:1411:C:O2'	48:5:1411(C):C:O4'	1.96	0.82
48:5:922:C:C2'	48:5:922(B):C:C2	2.58	0.81
48:5:1411:C:O2'	48:5:1411(C):C:C4'	2.29	0.81
48:5:2367:A:N6	48:5:2788:U:N3	2.30	0.80
51:9:1823:A:H3'	51:9:1824:A:H5'	1.61	0.80
48:5:1406:G:O4'	48:5:1406(C):G:O2'	1.99	0.80
48:5:1411:C:O2'	48:5:1411(C):C:H6	1.62	0.80
48:5:1406:G:O4'	48:5:1406(C):G:C2'	2.30	0.79
48:5:922(B):C:O2'	48:5:923:C:P	2.38	0.79
48:5:3760:A:H2	51:9:1825:A:C4	2.00	0.79
51:9:612:U:O2	51:9:629:A:N6	2.15	0.79
48:5:3914:U:H3	48:5:4378:A:N6	1.80	0.78
48:5:1411:C:O2'	48:5:1411(C):C:C1'	2.32	0.78
55:DD:179:GLN:NE2	55:DD:179:GLN:HA	1.98	0.78
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.65	0.77
12:M:44:ARG:HB2	48:5:935:A:OP2	1.84	0.77
51:9:615:C:O2'	51:9:616:A:O5'	2.04	0.76
48:5:1411:C:C5'	48:5:1411(C):C:C5'	2.42	0.76
51:9:615:C:H2'	51:9:616:A:H8	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:738:C:O2'	48:5:738(A):C:O4'	2.01	0.75
90:9:1972:GCP:O2A	90:9:1972:GCP:O3G	2.05	0.75
48:5:1411:C:O4'	48:5:1411(B):C:C2'	2.35	0.74
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	1.69	0.74
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.68	0.74
51:9:628:A:C2	55:DD:145:GLN:OE1	2.41	0.74
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.52	0.74
51:9:615:C:O2'	51:9:616:A:C5'	2.36	0.73
51:9:1137:U:C4	51:9:1148:A:C6	2.77	0.73
51:9:1501:C:O2'	90:9:1972:GCP:C4	2.36	0.73
90:9:1972:GCP:H3B2	55:DD:179:GLN:HE22	1.52	0.73
51:9:1130:G:HO2'	51:9:1131:G:P	2.11	0.73
51:9:614:C:O4'	51:9:626:G:C2	2.41	0.73
48:5:1406:G:C8	48:5:1406(C):G:H2'	2.23	0.73
48:5:1406:G:O5'	48:5:1406(C):G:O3'	2.07	0.73
51:9:612:U:O2'	51:9:615:C:N3	2.19	0.73
48:5:922(A):G:OP1	48:5:922(B):C:C6	2.42	0.72
48:5:922:C:O5'	48:5:922(A):G:P	2.48	0.72
90:9:1972:GCP:O2B	55:DD:179:GLN:NE2	2.23	0.72
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.86	0.72
51:9:1500:G:N2	90:9:1972:GCP:O6	2.23	0.71
48:5:922:C:C6	48:5:922(A):G:C5	2.79	0.71
51:9:1501:C:H5''	90:9:1972:GCP:O1A	1.91	0.70
48:5:1411:C:O5'	48:5:1411(C):C:H5'	1.90	0.70
90:9:1972:GCP:O1G	55:DD:178:ARG:NH1	2.17	0.70
48:5:3914:U:N3	48:5:4378:A:N6	2.37	0.70
48:5:922:C:H2'	48:5:922(B):C:C6	2.27	0.70
51:9:1501:C:C5'	90:9:1972:GCP:O1A	2.40	0.70
51:9:96:C:O2	51:9:473:A:O2'	2.10	0.70
48:5:922:C:H5'	48:5:922(A):G:O3'	1.92	0.69
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.26	0.69
51:9:1501:C:HO2'	90:9:1972:GCP:H2'	1.55	0.69
48:5:922:C:H5'	48:5:922(A):G:C2'	2.20	0.69
51:9:1501:C:O2'	90:9:1972:GCP:C8	2.42	0.68
48:5:3760:A:C2	51:9:1825:A:N3	2.60	0.68
51:9:1130:G:H2'	51:9:1130:G:N3	2.08	0.68
51:9:613:G:H4'	51:9:615:C:C4	2.28	0.68
48:5:1411:C:HO2'	48:5:1411(C):C:H6	0.78	0.68
51:9:629:A:O2'	51:9:631:U:OP2	2.12	0.68
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.75	0.67
57:FF:102:LEU:HD22	77:ZZ:110:THR:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.77	0.67
48:5:935:A:O2'	48:5:935:A:N6	2.27	0.67
55:DD:179:GLN:HE21	55:DD:179:GLN:CA	2.00	0.67
48:5:1411:C:O5'	48:5:1411(C):C:C5'	2.43	0.67
48:5:922:C:O3'	48:5:922(B):C:C1'	2.40	0.67
48:5:1411:C:H1'	48:5:1411(C):C:O4'	1.95	0.66
64:MM:22:LEU:HD11	64:MM:89:VAL:HA	1.76	0.66
15:P:127:ARG:NH2	48:5:2422:C:OP1	2.29	0.66
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.78	0.66
12:M:23:LYS:NZ	48:5:935:A:O3'	2.25	0.66
48:5:4723:A:H2'	48:5:4724:A:C8	2.31	0.65
48:5:922:C:H5'	48:5:922(B):C:P	2.31	0.65
51:9:945:U:H2'	51:9:946:U:C6	2.31	0.65
48:5:2395:A:O2'	48:5:2806:A:N3	2.28	0.65
48:5:922:C:C2'	48:5:922(B):C:C6	2.76	0.65
48:5:1406(B):C:H2'	48:5:1406(C):G:O4'	1.95	0.65
48:5:971:U:N3	48:5:971(A):G:C4	2.65	0.64
51:9:628:A:C2	55:DD:145:GLN:CD	2.71	0.64
90:9:1972:GCP:PB	55:DD:179:GLN:HE22	2.20	0.64
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.30	0.64
51:9:613:G:C4'	51:9:615:C:C4	2.80	0.64
48:5:4579:U:H2'	48:5:4580:U:C6	2.32	0.64
48:5:922(B):C:H2'	48:5:923:C:H5''	1.79	0.64
48:5:922:C:C5'	48:5:922(A):G:O3'	2.44	0.64
48:5:1411:C:P	48:5:1411(C):C:OP1	2.56	0.64
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.77	0.64
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.80	0.63
48:5:481:G:O6	48:5:481(A):C:H3'	1.97	0.63
48:5:1406:G:O4'	48:5:1406(C):G:H2'	1.97	0.63
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.79	0.63
55:DD:176:LEU:N	55:DD:176:LEU:HD12	2.13	0.63
48:5:922:C:C5	48:5:922(A):G:C5	2.87	0.63
51:9:1589:A:N3	51:9:1653:U:O2'	2.27	0.63
48:5:935:A:C6	48:5:935(A):G:C8	2.87	0.62
51:9:1407:U:H2'	51:9:1408:U:C6	2.33	0.62
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.80	0.62
48:5:922:C:HO2'	48:5:922(B):C:H1'	1.61	0.62
48:5:922(B):C:N3	48:5:923:C:C5	2.67	0.62
48:5:1411(C):C:H2'	48:5:1412:G:O4'	1.98	0.62
48:5:922(A):G:OP1	48:5:922(B):C:C5	2.53	0.62
48:5:2367:A:C2	48:5:2788:U:O4	2.51	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3723:A:H2'	48:5:3724:A:C8	2.35	0.62
48:5:481:G:C6	48:5:481(A):C:H3'	2.35	0.62
3:C:101:MET:SD	3:C:104:PRO:HA	2.39	0.62
59:HH:27:LEU:HD13	59:HH:45:ILE:HD13	1.81	0.61
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.82	0.61
51:9:943:U:OP2	53:BB:216:LYS:NZ	2.32	0.61
51:9:1568:C:OP1	71:TT:96:SER:OG	2.17	0.61
6:F:152:LEU:HD21	6:F:243:ILE:HG23	1.83	0.61
20:U:87:THR:HG23	20:U:102:VAL:HG21	1.83	0.61
2:B:174:ARG:NH1	48:5:4985:U:O2	2.34	0.60
48:5:738(A):C:H5''	48:5:739:G:H5''	1.81	0.60
48:5:922:C:O5'	48:5:922(A):G:C3'	2.46	0.60
48:5:935:A:H61	48:5:935(A):G:P	2.22	0.60
51:9:1129:G:C6	51:9:1130:G:O6	2.54	0.60
51:9:183:G:O2'	51:9:184:G:O5'	2.19	0.60
48:5:922:C:C4'	48:5:922(B):C:O4'	2.49	0.60
51:9:980:A:H2'	51:9:981:A:C8	2.36	0.60
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.81	0.60
90:9:1972:GCP:PB	55:DD:179:GLN:NE2	2.74	0.60
48:5:922:C:O3'	48:5:922:C:O5'	2.20	0.60
51:9:1823:A:C3'	51:9:1824:A:H5'	2.32	0.60
48:5:4942:C:H4'	48:5:4943:A:OP1	2.01	0.60
48:5:934:C:O4'	48:5:935(A):G:O4'	2.19	0.59
48:5:1411:C:C1'	48:5:1411(C):C:O4'	2.50	0.59
48:5:1370:G:O2'	48:5:1371:A:OP2	2.12	0.59
48:5:738:C:O3'	48:5:738(A):C:H5'	2.02	0.59
48:5:922(B):C:H2'	48:5:923:C:C5'	2.33	0.59
48:5:3766:A:N1	51:9:1827:U:O2'	2.35	0.58
51:9:1501:C:O2'	90:9:1972:GCP:C2'	2.50	0.58
52:AA:38:ILE:HD11	52:AA:150:THR:HG22	1.84	0.58
48:5:922:C:C6	48:5:922(A):G:C4	2.91	0.58
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	1.84	0.58
48:5:738:C:O2'	48:5:738(A):C:C6	2.57	0.58
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	1.86	0.58
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	1.85	0.58
51:9:501:C:H2'	51:9:501:C:O2	2.03	0.58
48:5:922(B):C:HO2'	48:5:923:C:P	2.24	0.57
51:9:628:A:P	90:9:1972:GCP:N2	2.66	0.57
14:O:193:THR:HG23	14:O:202:LEU:HD23	1.84	0.57
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.87	0.57
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.87	0.57
48:5:3761:C:H2'	48:5:3762:U:C6	2.40	0.57
51:9:1130:G:O2'	51:9:1131:G:O5'	2.23	0.57
48:5:922(B):C:C2'	48:5:923:C:H5''	2.35	0.56
51:9:1117:C:O2'	51:9:1118:C:O4'	2.23	0.56
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.36	0.56
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.38	0.56
18:S:82:LEU:HB2	18:S:93:MET:HB2	1.88	0.56
20:U:23:LEU:HD11	20:U:83:LEU:CD2	2.35	0.56
51:9:615:C:O2'	51:9:616:A:C4'	2.54	0.56
46:2:16:C:O4'	46:2:16:C:O2	2.24	0.56
51:9:613:G:O4'	51:9:615:C:N4	2.38	0.56
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.87	0.56
48:5:922:C:OP2	48:5:922(A):G:OP2	2.23	0.56
2:B:249:ARG:NH1	48:5:2837:U:OP1	2.38	0.56
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.41	0.56
16:Q:11:ARG:NH2	48:5:1690:C:OP2	2.39	0.56
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.41	0.55
48:5:1411:C:O4'	48:5:1411(B):C:C3'	2.55	0.55
48:5:2395:A:O2'	48:5:2806:A:H1'	2.07	0.55
51:9:614:C:C1'	51:9:626:G:N2	2.69	0.55
56:EE:11:ARG:HH22	56:EE:24:THR:HG1	1.54	0.55
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.42	0.55
48:5:1411:C:O5'	48:5:1411(C):C:OP1	2.24	0.55
6:F:161:ILE:HD12	6:F:166:ILE:HB	1.89	0.55
60:II:36:THR:HG21	60:II:179:PRO:HB2	1.88	0.55
48:5:1411:C:C2'	48:5:1411(C):C:O4'	2.54	0.55
48:5:245:C:O2	48:5:245:C:O4'	2.24	0.55
48:5:742:G:C2	48:5:922(A):G:C6	2.94	0.55
13:N:76:PRO:O	13:N:79:ALA:HB3	2.06	0.55
48:5:2031:C:O3'	48:5:2032:U:P	2.65	0.54
51:9:1438:A:H2'	51:9:1439:A:C8	2.41	0.54
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.40	0.54
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.38	0.54
14:O:27:VAL:CG1	14:O:98:ALA:HB1	2.37	0.54
59:HH:36:LEU:HD23	59:HH:40:LEU:HD12	1.90	0.54
62:KK:35:LEU:HD13	62:KK:40:VAL:HG21	1.89	0.54
48:5:2627:C:O2	48:5:2627:C:O4'	2.26	0.54
51:9:614:C:C5	51:9:626:G:O2'	2.58	0.54
51:9:853:C:O4'	51:9:853:C:O2	2.25	0.54
54:CC:253:PRO:HA	54:CC:256:TRP:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1411:C:C2'	48:5:1411(C):C:C6	2.91	0.54
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.38	0.54
6:F:88:LEU:HD22	6:F:89:ALA:N	2.23	0.54
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.90	0.54
51:9:628:A:OP2	90:9:1972:GCP:N3	2.41	0.54
51:9:1502:C:H5'	90:9:1972:GCP:H2'	1.89	0.53
48:5:4459:U:H2'	48:5:4460:U:C6	2.43	0.53
8:H:41:ILE:HG21	8:H:73:ILE:HD11	1.90	0.53
12:M:112:VAL:HG11	14:O:201:LEU:HD11	1.90	0.53
48:5:2505:C:O4'	48:5:2505:C:O2	2.24	0.53
51:9:958:G:C6	51:9:959:G:C6	2.97	0.53
59:HH:118:ARG:O	59:HH:121:THR:HG22	2.08	0.53
14:O:58:LEU:HD11	14:O:145:VAL:HG22	1.89	0.53
48:5:114:G:N2	48:5:276:C:O2'	2.41	0.53
48:5:935:A:N6	48:5:935(A):G:P	2.81	0.53
59:HH:145:ARG:HA	74:WW:51:GLU:HB2	1.91	0.53
14:O:23:VAL:HG13	14:O:33:VAL:HG11	1.91	0.53
71:TT:75:MET:HA	71:TT:78:ILE:HG22	1.91	0.53
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.89	0.53
48:5:747:A:H4'	48:5:748:G:OP1	2.09	0.53
51:9:15:U:H2'	51:9:16:G:O4'	2.08	0.53
52:AA:134:LEU:HD21	52:AA:144:THR:HG21	1.91	0.53
48:5:294:G:O6	48:5:315:G:H1'	2.08	0.53
51:9:501:C:O2	51:9:501:C:C2'	2.57	0.53
71:TT:42:HIS:HB2	71:TT:83:GLN:HA	1.91	0.53
51:9:490:C:O2'	51:9:574:A:N1	2.37	0.53
48:5:922:C:H3'	48:5:922:C:C6	2.44	0.53
48:5:935:A:N6	48:5:935(A):G:H3'	2.23	0.53
48:5:1406:G:N9	48:5:1406(C):G:H2'	2.24	0.52
48:5:4989:U:O2	48:5:4989:U:O4'	2.27	0.52
51:9:1351:G:O2'	51:9:1378:A:N1	2.31	0.52
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.91	0.52
48:5:1411:C:O2'	48:5:1411(C):C:C2'	2.57	0.52
48:5:1483:C:O4'	48:5:1483:C:O2	2.25	0.52
51:9:1137:U:N3	51:9:1148:A:N6	2.57	0.52
51:9:1315:U:O2	51:9:1315:U:O4'	2.28	0.52
4:D:106:ALA:HB1	4:D:171:LEU:HD13	1.91	0.52
48:5:3810:C:O4'	48:5:3810:C:O2	2.26	0.52
19:T:85:LEU:HD13	48:5:4305:G:C2	2.45	0.52
51:9:1130:G:O2'	51:9:1131:G:P	2.65	0.52
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3760:A:C2	51:9:1825:A:C4	2.90	0.52
53:BB:139:CYS:SG	53:BB:140:VAL:N	2.83	0.52
48:5:224:U:O2	48:5:224:U:O4'	2.28	0.52
51:9:146:G:O2'	51:9:147:A:O5'	2.27	0.52
48:5:922:C:H5''	48:5:922(B):C:OP1	2.06	0.52
51:9:1012:A:H2'	51:9:1013:U:O4'	2.09	0.52
55:DD:176:LEU:N	55:DD:176:LEU:CD1	2.73	0.52
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	1.92	0.52
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.39	0.52
48:5:2097:A:OP1	48:5:2107:A:N6	2.43	0.52
51:9:1139:C:O4'	51:9:1139:C:O2	2.23	0.52
57:FF:72:LEU:HD22	57:FF:112:LEU:HD11	1.92	0.52
48:5:222:C:H2'	48:5:223:G:O4'	2.09	0.52
4:D:16:TYR:O	49:7:11:A:N6	2.43	0.52
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.42	0.52
17:R:44:LEU:HD22	17:R:49:LEU:HD12	1.91	0.51
48:5:5047:C:O2'	48:5:5050:C:OP2	2.28	0.51
8:H:18:ILE:HG22	8:H:27:VAL:HG22	1.92	0.51
51:9:1058:A:C6	51:9:1059:G:C6	2.98	0.51
48:5:113:A:H2'	48:5:114:G:O4'	2.11	0.51
48:5:1961:G:O2'	48:5:2025:A:N6	2.44	0.51
14:O:18:ARG:NH2	48:5:2057:A:OP1	2.43	0.51
51:9:1535:U:O2	51:9:1535:U:H2'	2.10	0.51
52:AA:183:LEU:HD22	52:AA:188:THR:HG21	1.92	0.51
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.51
58:GG:132:ARG:HB3	58:GG:133:LEU:HD12	1.92	0.51
66:OO:56:VAL:HG12	66:OO:81:VAL:HG23	1.92	0.51
51:9:1823:A:H2'	51:9:1824:A:H5''	1.93	0.51
52:AA:167:GLY:O	52:AA:171:VAL:HG23	2.11	0.51
56:EE:11:ARG:HA	56:EE:28:ALA:HB2	1.92	0.51
48:5:1872:G:O2'	48:5:4219:A:N3	2.38	0.51
50:8:125:C:O4'	50:8:125:C:O2	2.29	0.51
51:9:613:G:C4'	51:9:615:C:C5	2.83	0.51
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	1.93	0.51
51:9:1139:C:H2'	51:9:1140:G:O4'	2.11	0.51
51:9:92:A:O4'	56:EE:3:ARG:NH1	2.44	0.51
59:HH:144:ILE:HB	74:WW:52:ILE:HG12	1.93	0.51
68:QQ:49:TYR:O	68:QQ:53:GLU:N	2.43	0.51
51:9:1488:C:O2'	51:9:1490:G:OP2	2.28	0.51
55:DD:21:LEU:CD2	55:DD:48:ILE:HD11	2.41	0.51
18:S:34:ALA:HB1	18:S:39:VAL:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:101:LYS:HB3	23:X:42:THR:HG23	1.93	0.51
51:9:612:U:C2'	51:9:615:C:H42	2.25	0.50
55:DD:175:VAL:C	55:DD:176:LEU:HD12	2.32	0.50
57:FF:92:ILE:HD13	57:FF:169:ILE:HG21	1.93	0.50
51:9:919:A:C2	51:9:1020:A:C4	2.98	0.50
48:5:922(B):C:H2'	48:5:923:C:O5'	2.12	0.50
51:9:1824:A:N3	51:9:1824:A:C2'	2.72	0.50
48:5:922(B):C:C2	48:5:923:C:C6	2.99	0.50
10:J:63:ARG:NH2	50:8:58:G:N7	130.11	0.50
51:9:1489:A:H4'	51:9:1490:G:OP2	2.10	0.50
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.93	0.50
51:9:1162:C:H2'	51:9:1163:C:O4'	2.11	0.50
12:M:119:ARG:NH1	14:O:202:LEU:HD21	2.27	0.50
3:C:164:THR:HG21	48:5:223:G:H2'	1.94	0.49
48:5:4515:G:C2	48:5:4516:G:C8	3.00	0.49
51:9:1501:C:HO2'	90:9:1972:GCP:C4	2.25	0.49
21:V:80:VAL:HG23	21:V:106:VAL:HG21	1.94	0.49
24:Y:49:ILE:HD11	24:Y:55:VAL:HG21	1.92	0.49
48:5:1237:C:O2	48:5:1237:C:O4'	2.28	0.49
48:5:2094:C:O4'	48:5:2094:C:O2	2.30	0.49
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.94	0.49
9:I:97:ILE:HD13	9:I:126:VAL:HG11	1.94	0.49
63:LL:77:VAL:HG22	63:LL:86:ILE:HD12	1.95	0.49
22:W:45:ASN:HB3	22:W:48:GLN:HE21	1.78	0.49
48:5:922:C:P	48:5:922(A):G:P	3.10	0.49
3:C:33:ARG:HD2	3:C:36:ILE:HD12	1.94	0.49
51:9:67:C:C6	58:GG:162:LEU:HD23	2.47	0.49
8:H:92:MET:SD	8:H:161:ILE:HD11	2.52	0.49
48:5:2763:U:O2	48:5:2763:U:O4'	2.31	0.49
48:5:1328:G:O2'	48:5:2349:A:OP1	2.28	0.49
51:9:62:G:H4'	51:9:172:U:C5	2.48	0.49
53:BB:79:VAL:HG21	53:BB:81:PHE:CZ	2.48	0.49
66:OO:34:PHE:HB3	66:OO:41:PHE:HB2	1.93	0.49
12:M:72:TYR:CE1	48:5:918:G:H5'	2.47	0.49
56:EE:182:MET:CE	56:EE:192:ILE:HD11	2.42	0.49
62:KK:32:HIS:CD2	62:KK:45:VAL:HG21	2.47	0.49
12:M:72:TYR:CE1	48:5:738:C:H4'	2.48	0.49
76:YY:44:LEU:HB3	76:YY:55:ILE:HD13	1.94	0.49
48:5:1381:U:O4'	48:5:1381:U:O2	2.31	0.49
3:C:130:ALA:HB3	3:C:246:VAL:HG12	1.94	0.49
60:II:31:ARG:NH2	60:II:48:VAL:HG12	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:302:LEU:HD22	16:Q:38:ARG:HB3	1.95	0.49
6:F:97:ILE:HD11	16:Q:4:ASP:CG	2.33	0.49
48:5:1406:G:C1'	48:5:1406(C):G:HO2'	2.24	0.49
48:5:935:A:N6	48:5:935:A:C2'	2.53	0.49
51:9:830:A:OP2	51:9:846:G:N2	2.46	0.49
64:MM:22:LEU:HD21	64:MM:89:VAL:HG23	1.94	0.49
74:WW:26:LEU:HD11	74:WW:60:LYS:HB3	1.94	0.49
51:9:1624:U:O4'	51:9:1624:U:O2	2.31	0.48
51:9:1156:U:O4	54:CC:194:ARG:NH1	2.46	0.48
65:NN:125:LEU:HD22	65:NN:129:TYR:CE2	2.48	0.48
19:T:48:VAL:HG21	19:T:94:GLU:HG2	1.94	0.48
48:5:3839:G:N2	48:5:3843:C:O2'	2.47	0.48
48:5:4928:C:O2	48:5:4928:C:O4'	2.29	0.48
51:9:290:U:O2'	51:9:292:A:N7	2.44	0.48
51:9:396:U:O2'	60:II:14:THR:HG22	2.13	0.48
5:E:164:ARG:O	5:E:185:ASN:ND2	2.45	0.48
58:GG:63:MET:N	58:GG:63:MET:SD	2.86	0.48
16:Q:55:ARG:NH1	48:5:1351:G:N7	2.60	0.48
74:WW:55:ASP:O	74:WW:57:ARG:N	2.47	0.48
48:5:2268:A:H4'	48:5:2269:C:H5'	1.95	0.48
48:5:3724:A:N6	48:5:3725:G:C6	2.81	0.48
48:5:971:U:O4	48:5:971(A):G:C5	2.66	0.48
48:5:4305:G:N3	48:5:4305:G:C2'	2.76	0.48
48:5:922:C:H2'	48:5:922(B):C:C1'	2.18	0.48
48:5:1411:C:H4'	48:5:1411(C):C:C4'	1.98	0.48
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.49	0.48
62:KK:11:ILE:CD1	62:KK:45:VAL:HG22	2.43	0.48
51:9:1238:U:H2'	51:9:1239:U:O4'	2.14	0.48
51:9:1364:U:O4'	51:9:1364:U:O2	2.28	0.48
51:9:1823:A:N6	51:9:1824:A:N7	2.61	0.48
1:A:104:VAL:HG12	1:A:146:THR:HG21	1.96	0.48
51:9:612:U:H2'	51:9:615:C:H42	1.78	0.48
5:E:165:VAL:HG11	5:E:178:VAL:HG13	1.94	0.48
59:HH:66:VAL:HG22	59:HH:96:ALA:HB1	1.95	0.48
14:O:55:LEU:HD23	14:O:58:LEU:HD12	1.95	0.48
48:5:1665:C:H2'	48:5:1666:C:H6	1.78	0.48
51:9:823:U:O2	51:9:823:U:O4'	2.32	0.48
18:S:35:PRO:HD2	18:S:39:VAL:HG21	1.96	0.48
48:5:1411(A):G:C6	48:5:1411(B):C:C4	3.02	0.48
48:5:961:G:C6	48:5:971(A):G:C4	3.02	0.48
59:HH:39:GLN:HB3	59:HH:75:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:II:72:CYS:SG	60:II:72:CYS:O	2.71	0.48
77:ZZ:92:LEU:HD11	77:ZZ:99:LEU:HD12	1.96	0.48
1:A:242:ARG:HD2	48:5:3658:C:OP1	2.14	0.47
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.44	0.47
48:5:922(B):C:C2'	48:5:923:C:O5'	2.62	0.47
51:9:427:U:O4'	51:9:427:U:O2	2.33	0.47
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.96	0.47
48:5:1942:A:N3	48:5:4432:C:O2'	2.43	0.47
48:5:922(B):C:C2'	48:5:923:C:C5'	2.91	0.47
48:5:922(B):C:N3	48:5:923:C:C6	2.82	0.47
51:9:628:A:C6	90:9:1972:GCP:O6	2.67	0.47
52:AA:94:THR:HG23	52:AA:182:VAL:HG21	1.96	0.47
5:E:179:THR:OG1	5:E:189:LEU:HD23	2.13	0.47
17:R:173:ARG:NH2	51:9:910:G:OP2	2.47	0.47
22:W:9:SER:HG	22:W:36:CYS:HG	1.57	0.47
48:5:961:G:C6	48:5:962:C:C4	3.02	0.47
51:9:1599:U:H2'	57:FF:166:ILE:HD11	1.96	0.47
51:9:612:U:H3	51:9:629:A:H62	1.62	0.47
53:BB:134:LEU:CD2	53:BB:218:LEU:HD12	2.44	0.47
8:H:117:PHE:CE1	8:H:118:LEU:HD23	2.49	0.47
60:II:117:TYR:CD1	60:II:156:ALA:HB2	2.49	0.47
75:XX:51:VAL:HG22	75:XX:70:VAL:HG11	1.96	0.47
48:5:2367:A:N6	48:5:2788:U:C4	2.78	0.47
48:5:4723:A:C2	48:5:4724:A:C6	3.03	0.47
51:9:29:G:H4'	75:XX:129:SER:HB3	1.97	0.47
54:CC:88:ILE:HG21	54:CC:94:ILE:HD12	1.96	0.47
58:GG:52:ILE:O	58:GG:52:ILE:HG23	2.15	0.47
51:9:1543:U:OP1	68:QQ:37:ARG:NH1	2.46	0.47
51:9:887:U:O4'	51:9:887:U:O2	2.31	0.47
66:OO:56:VAL:HG13	66:OO:77:ALA:HB1	1.97	0.47
48:5:1332:C:H2'	48:5:1333:A:C8	2.49	0.47
21:V:87:SER:HA	21:V:97:TYR:HB3	1.97	0.47
48:5:4510:A:O2'	48:5:4511:A:O4'	2.31	0.47
48:5:498:C:O4'	48:5:498:C:O2	2.28	0.47
48:5:923:C:N4	48:5:926:G:C8	2.83	0.47
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.97	0.47
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.96	0.47
25:Z:11:VAL:HG11	25:Z:80:LEU:HD22	1.97	0.47
48:5:5008:C:H2'	48:5:5009:G:O4'	2.14	0.47
51:9:958:G:H2'	51:9:959:G:O4'	2.15	0.47
1:A:27:ALA:O	1:A:128:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.50	0.47
66:OO:74:ALA:HB1	66:OO:115:ALA:HB2	1.97	0.47
48:5:2459:G:N2	48:5:2462:C:OP2	2.47	0.47
51:9:1336:C:H2'	51:9:1337:C:O4'	2.15	0.47
48:5:2367:A:C6	48:5:2788:U:C4	3.04	0.46
48:5:4579:U:O2	48:5:4580:U:C2	2.67	0.46
11:L:116:ARG:NH1	11:L:155:MET:O	2.48	0.46
21:V:82:ILE:HD12	21:V:104:VAL:HG13	1.96	0.46
67:PP:56:LEU:HD13	67:PP:78:THR:HG21	1.97	0.46
21:V:117:ILE:HD11	21:V:132:ILE:HG23	1.97	0.46
57:FF:99:ILE:HG23	77:ZZ:67:LEU:HD21	1.97	0.46
10:J:141:ILE:HD11	49:7:55:A:N3	2.31	0.46
68:QQ:51:LEU:HD21	68:QQ:81:ILE:HG12	1.96	0.46
48:5:738:C:O3'	48:5:738(A):C:C5'	2.62	0.46
51:9:584:A:C6	51:9:585:C:C4	3.03	0.46
51:9:612:U:H2'	51:9:615:C:N4	2.31	0.46
58:GG:16:ILE:N	58:GG:16:ILE:HD12	2.31	0.46
51:9:1097:G:C6	51:9:1098:C:C4	3.04	0.46
51:9:1823:A:H2'	51:9:1824:A:C5'	2.45	0.46
60:II:162:LEU:HD11	60:II:191:GLU:HG2	1.97	0.46
76:YY:56:PHE:CE2	76:YY:82:ALA:HB1	2.50	0.46
48:5:2280:G:HO2'	48:5:2281:U:H6	1.62	0.46
48:5:4289:U:H2'	48:5:4290:U:C6	2.50	0.46
12:M:11:ARG:HD2	12:M:57:LEU:HD12	1.97	0.46
70:SS:40:TYR:O	70:SS:44:VAL:HG23	2.16	0.46
48:5:1665:C:H2'	48:5:1666:C:C6	2.50	0.46
48:5:2046:G:C2	48:5:2047:A:C2	3.03	0.46
48:5:4872:G:H4'	48:5:4873:G:H5''	1.97	0.46
48:5:4977:A:H2'	48:5:4978:G:O4'	2.16	0.46
48:5:935:A:N1	48:5:935(A):G:H2'	2.31	0.46
51:9:1499:U:H5'	55:DD:176:LEU:HD21	1.98	0.46
51:9:183:G:C2'	51:9:183:G:N3	2.77	0.46
18:S:80:ILE:HG22	18:S:82:LEU:HD22	1.98	0.46
48:5:1411:C:C2'	48:5:1411(C):C:C4'	2.93	0.46
48:5:4187:G:H2'	48:5:4188:U:O4'	2.16	0.46
51:9:1130:G:N3	51:9:1130:G:C2'	2.78	0.46
51:9:1228:A:O2'	51:9:1634:A:N3	2.34	0.46
60:II:27:TYR:CE1	60:II:28:GLU:HG3	2.51	0.46
62:KK:93:THR:HG23	62:KK:94:LEU:HD12	1.98	0.46
48:5:3723:A:C2	48:5:3724:A:C6	3.03	0.46
48:5:3928:A:H2'	48:5:3929:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4525:C:H2'	48:5:4526:U:O4'	2.16	0.46
48:5:1964:A:C6	48:5:4694:G:C6	3.03	0.46
51:9:1719:A:N6	51:9:1814:G:O2'	2.49	0.46
51:9:434:G:H2'	51:9:435:A:C8	2.51	0.46
51:9:92:A:H2'	51:9:446:G:N2	2.31	0.46
66:OO:44:VAL:HG11	66:OO:85:CYS:SG	2.56	0.46
67:PP:81:ARG:NH1	67:PP:120:SER:OG	2.48	0.46
48:5:356:G:O2'	50:8:25:G:N3	2.46	0.45
61:JJ:35:TYR:CD2	61:JJ:106:LEU:HD23	2.51	0.45
19:T:80:VAL:CG2	19:T:85:LEU:HD12	2.45	0.45
51:9:1823:A:C3'	51:9:1824:A:C5'	2.94	0.45
51:9:614:C:H5	51:9:626:G:O2'	1.97	0.45
55:DD:96:LEU:HD22	55:DD:198:ILE:HG13	1.98	0.45
10:J:103:GLY:O	10:J:134:LEU:HD12	2.16	0.45
61:JJ:94:LEU:HB2	61:JJ:97:ILE:HD12	1.98	0.45
51:9:1554:C:O2	62:KK:24:LYS:NZ	2.43	0.45
51:9:1303:C:O2	51:9:1303:C:O4'	2.33	0.45
52:AA:134:LEU:CD2	52:AA:144:THR:HG21	2.46	0.45
9:I:61:SER:HA	9:I:126:VAL:HG23	1.98	0.45
13:N:50:ARG:NH2	48:5:279:A:OP1	2.49	0.45
51:9:1284:A:C6	64:MM:91:LEU:HD22	2.52	0.45
53:BB:66:VAL:HG22	53:BB:87:ILE:HG22	1.98	0.45
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.80	0.45
48:5:1667:A:N1	48:5:2281:U:OP2	2.49	0.45
51:9:1551:U:O2	51:9:1551:U:O4'	2.35	0.45
8:H:118:LEU:HD21	8:H:177:ASP:HB2	1.98	0.45
53:BB:107:ARG:NH1	66:OO:133:THR:O	2.50	0.45
54:CC:191:VAL:HG11	54:CC:236:PHE:HA	1.99	0.45
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.62	0.45
4:D:4:VAL:HG11	48:5:4247:G:C5'	2.47	0.45
51:9:161:U:O2'	58:GG:87:ARG:NH1	2.50	0.45
51:9:1834:A:N3	51:9:1834:A:C2'	2.80	0.45
48:5:2816:G:N2	48:5:3622:C:O2	2.50	0.44
48:5:4476:C:O2'	48:5:4478:G:OP2	2.34	0.44
51:9:183:G:O2'	51:9:183:G:N3	2.50	0.44
51:9:933:G:H1'	51:9:1001:A:O4'	2.15	0.44
9:I:60:LEU:HD22	9:I:160:PRO:HD2	2.00	0.44
54:CC:251:LEU:HD23	73:VV:23:ILE:HG23	1.98	0.44
51:9:1035:A:H2'	51:9:1036:A:O4'	2.17	0.44
51:9:1374:C:H2'	51:9:1375:G:O4'	2.18	0.44
51:9:1520:G:H2'	51:9:1520:G:N3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:97:ALA:HB2	14:O:203:VAL:HB	1.99	0.44
3:C:95:MET:SD	3:C:95:MET:N	2.82	0.44
6:F:161:ILE:HB	6:F:166:ILE:HD12	1.99	0.44
8:H:41:ILE:CG2	8:H:73:ILE:HD11	2.48	0.44
48:5:922:C:C5	48:5:922(A):G:N7	2.85	0.44
75:XX:68:LYS:CG	75:XX:91:LEU:HD22	2.48	0.44
48:5:1990:A:H3'	48:5:1991:A:H5''	2.00	0.44
48:5:922(A):G:OP1	48:5:922(B):C:H6	1.85	0.44
51:9:1395:C:H2'	51:9:1396:A:N3	2.33	0.44
15:P:69:ARG:NH2	48:5:4568:A:N3	2.66	0.44
4:D:4:VAL:HG11	48:5:4247:G:H5'	1.99	0.44
3:C:341:LEU:HD21	5:E:52:LEU:HD21	2.00	0.44
3:C:334:THR:HG21	6:F:50:TYR:OH	2.17	0.44
48:5:5066:U:H2'	48:5:5067:U:C6	2.53	0.44
1:A:117:GLU:HB2	1:A:162:ASN:HB2	2.00	0.44
3:C:150:LEU:HB3	3:C:151:PRO:HD3	1.99	0.44
55:DD:105:LEU:HD23	55:DD:184:ILE:HG23	2.00	0.44
48:5:1634:A:C6	48:5:1635:C:C4	3.06	0.44
48:5:4305:G:H2'	48:5:4305:G:N3	2.33	0.44
48:5:922:C:O3'	48:5:922(B):C:N1	2.44	0.44
2:B:47:LEU:HD23	2:B:166:THR:HG23	1.99	0.44
56:EE:122:LYS:CG	56:EE:162:ILE:HD11	2.48	0.44
71:TT:18:LEU:HD13	71:TT:134:ILE:HD13	2.00	0.44
20:U:84:LYS:HA	20:U:87:THR:HG22	2.00	0.44
22:W:4:GLU:OE1	22:W:20:ARG:NH2	2.51	0.44
48:5:1888:A:N6	48:5:3873:G:O2'	2.50	0.43
48:5:2439:G:C6	48:5:2440:U:C4	3.06	0.43
51:9:1220:A:N6	51:9:1221:G:C6	2.86	0.43
54:CC:176:LYS:O	54:CC:200:ARG:NH1	2.51	0.43
51:9:297:A:H4'	56:EE:132:GLY:O	2.17	0.43
62:KK:49:MET:HB3	62:KK:69:TRP:CE2	2.53	0.43
48:5:4966:A:C2	48:5:4967:A:C2	3.06	0.43
51:9:149:A:H2'	51:9:150:A:C8	2.53	0.43
51:9:1667:U:H2'	51:9:1668:U:C6	2.52	0.43
3:C:152:LEU:HD23	3:C:251:ILE:HG12	2.00	0.43
11:L:47:ALA:HB3	11:L:48:PRO:HD3	2.01	0.43
12:M:29:ASP:OD1	12:M:30:VAL:N	2.51	0.43
51:9:1057:C:O2	51:9:1057:C:O4'	2.37	0.43
5:E:204:ILE:HD13	5:E:264:ILE:HG22	1.99	0.43
56:EE:192:ILE:HD13	56:EE:238:LEU:HD23	2.00	0.43
58:GG:41:LEU:O	58:GG:41:LEU:HD22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:II:190:LEU:HD12	60:II:194:GLU:HB3	2.00	0.43
48:5:4423:U:O2	48:5:4423:U:O4'	2.37	0.43
48:5:922:C:C3'	48:5:922:C:C6	3.02	0.43
51:9:1129:G:C6	51:9:1130:G:C6	3.06	0.43
51:9:314:U:H2'	51:9:314:U:O2	2.19	0.43
51:9:958:G:N1	51:9:959:G:C6	2.86	0.43
51:9:980:A:C2	51:9:981:A:C6	3.05	0.43
14:O:15:LEU:HD11	14:O:129:LEU:HD13	1.99	0.43
72:UU:50:VAL:HG23	72:UU:91:LEU:HD23	1.99	0.43
48:5:4467:A:O2'	48:5:4510:A:N3	2.45	0.43
48:5:739:G:H8	48:5:739:G:O5'	2.00	0.43
48:5:923:C:C5	48:5:926:G:O4'	2.71	0.43
51:9:928:G:H2'	51:9:929:G:C8	2.53	0.43
48:5:2265:G:O2'	48:5:2266:C:OP1	2.25	0.43
14:O:72:HIS:N	48:5:4586:G:OP1	2.47	0.43
48:5:738:C:HO2'	48:5:738(A):C:C1'	2.20	0.43
16:Q:67:ILE:HD13	16:Q:98:LEU:HD11	1.99	0.43
48:5:2729:C:H2'	48:5:2730:U:O4'	2.18	0.43
51:9:57:U:OP1	51:9:504:G:O2'	2.36	0.43
51:9:604:A:C6	51:9:605:A:N1	2.87	0.43
52:AA:161:ILE:HG22	52:AA:163:CYS:SG	2.59	0.43
64:MM:26:LEU:HD11	64:MM:89:VAL:O	2.18	0.43
66:OO:36:SER:OG	66:OO:37:PHE:N	2.50	0.43
48:5:100:C:O2	48:5:100:C:O4'	2.36	0.43
51:9:1345:G:OP1	51:9:1688:C:O2'	2.35	0.43
4:D:146:LEU:HD12	48:5:4323:A:C2	2.53	0.43
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	2.01	0.43
69:RR:5:ARG:HB2	69:RR:10:LYS:HE2	2.00	0.43
21:V:82:ILE:HG12	21:V:121:VAL:HG13	2.00	0.43
73:VV:11:LEU:HD12	73:VV:12:TYR:N	2.33	0.43
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	2.00	0.43
48:5:4966:A:H2'	48:5:4967:A:C8	2.53	0.43
65:NN:33:VAL:HG21	65:NN:66:VAL:HG11	2.00	0.43
18:S:82:LEU:HD12	18:S:124:ILE:HG23	2.01	0.43
25:Z:11:VAL:CG1	25:Z:80:LEU:HD22	2.49	0.43
48:5:1074:G:C2	48:5:1238:A:C2	3.06	0.43
48:5:3648:A:H1'	48:5:3785:A:N6	2.34	0.43
51:9:614:C:O4'	51:9:626:G:N3	2.52	0.43
6:F:89:ALA:CB	6:F:124:LEU:HD21	2.48	0.43
16:Q:78:LYS:HG2	16:Q:137:VAL:HG23	2.00	0.43
20:U:23:LEU:HD11	20:U:83:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:42:VAL:HG22	21:V:55:ALA:HB2	2.00	0.43
46:2:38:C:O2'	51:9:1058:A:OP1	2.37	0.42
51:9:1501:C:HO2'	90:9:1972:GCP:C2'	2.26	0.42
2:B:11:HIS:ND1	2:B:236:HIS:O	2.52	0.42
3:C:76:ILE:HG22	3:C:77:PRO:HD2	2.00	0.42
9:I:14:ASN:O	9:I:128:ARG:NH2	2.51	0.42
12:M:17:PHE:CE2	12:M:54:CYS:HA	2.54	0.42
69:RR:119:VAL:O	69:RR:119:VAL:HG13	2.18	0.42
48:5:1301:C:O2	48:5:1301:C:O4'	2.33	0.42
48:5:2693:G:C6	48:5:2694:G:N1	2.87	0.42
48:5:922(B):C:O2'	48:5:923:C:C5'	2.68	0.42
1:A:181:LYS:HB2	48:5:1577:G:C5	2.54	0.42
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	1.99	0.42
2:B:261:ARG:HB2	14:O:64:THR:HG21	2.01	0.42
16:Q:82:VAL:O	16:Q:102:ALA:HA	2.20	0.42
74:WW:52:ILE:HG22	74:WW:61:ILE:HG23	2.00	0.42
51:9:446:G:OP2	60:II:47:ARG:NH1	2.42	0.42
15:P:41:ILE:HD12	15:P:150:LEU:HD13	2.01	0.42
21:V:39:ILE:HG23	21:V:61:VAL:CG2	2.49	0.42
1:A:179:ILE:O	48:5:3653:A:H4'	2.19	0.42
65:NN:91:LEU:CD1	65:NN:125:LEU:HD12	2.50	0.42
48:5:100:C:H2'	48:5:101:A:O4'	2.19	0.42
48:5:1406:G:C2	48:5:1406(C):G:N2	2.87	0.42
48:5:962:C:C4	48:5:963:G:N7	2.87	0.42
51:9:363:A:N1	51:9:397:G:O2'	2.41	0.42
14:O:160:ARG:NH2	48:5:4760:G:OP1	2.52	0.42
51:9:943:U:H1'	66:OO:137:SER:HB3	2.01	0.42
68:QQ:34:VAL:HG21	68:QQ:84:ILE:HD12	2.00	0.42
76:YY:55:ILE:HG12	76:YY:75:ILE:HG23	2.02	0.42
48:5:1406(C):G:N2	48:5:1411(A):G:C2	2.87	0.42
48:5:2367:A:N6	48:5:2788:U:H3	2.10	0.42
48:5:81:C:H2'	48:5:82:U:O4'	2.19	0.42
48:5:935:A:H61	48:5:935(A):G:H3'	1.85	0.42
51:9:614:C:C2'	51:9:614:C:O2	2.68	0.42
1:A:96:LEU:HD22	1:A:166:VAL:HG21	2.01	0.42
52:AA:24:HIS:HB3	52:AA:51:LEU:HD21	2.02	0.42
55:DD:162:ASP:N	55:DD:163:PRO:HD2	2.34	0.42
57:FF:116:ILE:HD12	57:FF:151:ILE:HG13	2.00	0.42
48:5:2408:U:O4'	48:5:2409:U:C5	2.73	0.42
3:C:53:ALA:HB3	50:8:27:U:H4'	2.01	0.42
4:D:64:ILE:HG13	4:D:105:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:THR:HG22	49:7:27:G:OP2	2.20	0.42
62:KK:15:LEU:HD22	62:KK:49:MET:HE1	2.00	0.42
48:5:1633:G:H5'	48:5:1634:A:OP1	2.20	0.42
7:G:215:ASP:HB3	7:G:216:PRO:HD3	2.01	0.42
61:JJ:66:LYS:HA	61:JJ:71:LEU:HD11	2.01	0.42
62:KK:15:LEU:HD22	62:KK:49:MET:CE	2.50	0.42
25:Z:23:ALA:HA	25:Z:45:GLY:HA2	2.01	0.42
3:C:323:ARG:NH1	48:5:1281:G:C8	2.88	0.42
48:5:922(B):C:O2	48:5:923:C:O4'	2.38	0.42
1:A:82:ILE:HD11	1:A:99:GLY:CA	2.46	0.42
2:B:95:THR:HB	2:B:96:PRO:HD2	2.02	0.42
54:CC:252:THR:HG22	54:CC:253:PRO:HD2	2.01	0.42
54:CC:78:LEU:HD13	54:CC:82:TYR:CE2	2.55	0.42
5:E:156:LEU:HD11	5:E:198:ILE:HG13	2.01	0.42
7:G:219:LEU:HD23	13:N:7:ILE:CD1	2.50	0.42
48:5:1406:G:C1'	48:5:1406(C):G:H2'	2.50	0.41
48:5:3798:U:C2	48:5:3801:U:C5	3.08	0.41
48:5:957:G:N7	48:5:958:G:C6	2.88	0.41
51:9:1207:G:C6	51:9:1837:G:C6	3.07	0.41
2:B:317:LEU:HD21	2:B:381:THR:HA	2.01	0.41
53:BB:49:VAL:CG2	53:BB:62:LEU:HD13	2.49	0.41
7:G:139:VAL:HG11	7:G:238:LYS:HG3	2.02	0.41
12:M:6:PHE:O	12:M:11:ARG:NE	2.51	0.41
72:UU:102:THR:HG21	72:UU:114:VAL:HG21	2.02	0.41
25:Z:75:TYR:CD2	25:Z:80:LEU:HD21	2.55	0.41
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.47	0.41
51:9:628:A:C4	55:DD:145:GLN:NE2	2.89	0.41
48:5:964:A:H2'	48:5:965:G:O4'	2.19	0.41
59:HH:133:LEU:HD21	59:HH:176:VAL:HG11	2.01	0.41
14:O:168:TYR:CE2	14:O:172:LYS:HD2	2.56	0.41
15:P:122:ALA:HB1	15:P:123:PRO:HD2	2.02	0.41
16:Q:43:PHE:CD2	16:Q:133:GLY:HA3	2.56	0.41
48:5:37:U:H2'	48:5:38:A:O4'	2.20	0.41
13:N:38:ARG:NH1	50:8:142:U:OP2	2.43	0.41
2:B:29:VAL:HG13	2:B:348:ARG:HD3	2.03	0.41
59:HH:122:LEU:C	59:HH:122:LEU:HD13	2.40	0.41
11:L:58:ILE:HG12	11:L:157:ILE:HG23	2.02	0.41
45:1:66:LEU:HD12	48:5:3908:A:C2	2.55	0.41
51:9:1531:A:H2'	51:9:1532:C:C6	2.56	0.41
90:9:1972:GCP:O2A	90:9:1972:GCP:PG	2.79	0.41
52:AA:137:ALA:HB1	52:AA:142:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:53:ALA:HB2	10:J:68:ILE:CD1	2.50	0.41
61:JJ:136:ARG:NH1	61:JJ:159:PHE:O	2.53	0.41
14:O:84:VAL:HG11	14:O:102:LEU:HD22	2.02	0.41
51:9:944:A:C5	51:9:945:U:C5	3.08	0.41
51:9:981:A:H2'	51:9:982:G:O4'	2.20	0.41
6:F:242:LEU:O	6:F:246:MET:HG3	2.21	0.41
51:9:1666:C:H2'	51:9:1667:U:O4'	2.21	0.41
51:9:495:U:H2'	51:9:496:C:O4'	2.21	0.41
52:AA:122:LEU:HD13	52:AA:142:LEU:HD22	2.03	0.41
56:EE:31:PRO:HG2	56:EE:38:LEU:HD12	2.01	0.41
65:NN:87:ASP:OD2	65:NN:125:LEU:HD11	2.21	0.41
48:5:1632:A:H2'	48:5:1632:A:N3	2.35	0.41
48:5:4724:A:C6	48:5:4725:C:C4	3.08	0.41
51:9:35:C:O2	51:9:520:A:N1	2.54	0.41
52:AA:60:LEU:HD13	52:AA:159:ILE:HD11	2.03	0.41
2:B:14:LEU:HD23	2:B:17:LEU:CD2	2.51	0.41
55:DD:138:VAL:CG1	55:DD:182:LEU:HD23	2.51	0.41
7:G:207:LEU:HD23	7:G:208:VAL:N	2.35	0.41
8:H:12:ILE:HG22	8:H:81:ILE:CD1	2.50	0.41
59:HH:133:LEU:HD22	59:HH:173:PHE:CD1	2.56	0.41
13:N:48:ALA:HB1	13:N:53:TYR:CB	2.50	0.41
15:P:36:ILE:HD12	15:P:48:LEU:HD11	2.02	0.41
20:U:27:HIS:N	20:U:28:PRO:HD2	2.36	0.41
48:5:4966:A:C2	48:5:5067:U:N3	2.86	0.41
5:E:129:LEU:HD13	48:5:973:G:C8	2.56	0.41
51:9:1673:U:H2'	51:9:1674:G:O4'	2.20	0.41
52:AA:180:ARG:HG2	52:AA:195:TRP:CE3	2.56	0.41
4:D:83:LEU:N	4:D:84:PRO:CD	2.84	0.41
5:E:131:HIS:HB2	48:5:1281:G:C6	2.55	0.41
48:5:2396:A:N6	48:5:2814:C:O2	2.54	0.41
48:5:4310:A:H2'	48:5:4311:A:O4'	2.21	0.41
2:B:252:ALA:HB3	48:5:4457:U:H1'	2.03	0.41
2:B:86:VAL:HG13	2:B:162:VAL:HG22	2.02	0.41
54:CC:161:SER:O	54:CC:163:VAL:HG13	2.21	0.41
5:E:180:GLY:O	5:E:181:PRO:C	2.59	0.41
6:F:90:PHE:CD2	6:F:243:ILE:HD11	2.56	0.41
58:GG:76:LEU:HD22	58:GG:92:ARG:HB3	2.03	0.41
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.56	0.41
51:9:1855:G:OP2	66:OO:147:ARG:NH1	2.53	0.41
48:5:35:U:O2'	48:5:1525:A:N1	2.53	0.41
48:5:738:C:O3'	48:5:738(A):C:C4'	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922(B):C:C4	48:5:923:C:C5	3.09	0.41
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.50	0.41
51:9:356:C:O2	51:9:356:C:C2'	2.69	0.41
54:CC:180:VAL:HG22	54:CC:219:ILE:HD13	2.03	0.41
4:D:129:GLU:HB2	4:D:177:THR:HG21	2.03	0.41
58:GG:5:ILE:HD12	58:GG:16:ILE:CD1	2.46	0.41
60:II:194:GLU:HG2	63:LL:10:TYR:CD2	2.56	0.41
75:XX:90:CYS:SG	75:XX:130:LEU:HD21	2.61	0.41
48:5:1787:A:N3	48:5:4210:U:O2'	2.52	0.40
48:5:4170:A:HO2'	48:5:4171:C:P	2.44	0.40
5:E:286:PRO:HA	5:E:289:LEU:CD2	2.52	0.40
57:FF:88:MET:HE1	57:FF:92:ILE:HD11	2.03	0.40
8:H:7:ASN:N	8:H:7:ASN:OD1	2.54	0.40
13:N:158:HIS:HB3	13:N:161:MET:HG2	2.03	0.40
68:QQ:51:LEU:HD22	68:QQ:84:ILE:HD11	2.04	0.40
70:SS:23:ARG:HB3	77:ZZ:48:VAL:HG21	2.03	0.40
51:9:617:G:N7	75:XX:67:ARG:NH1	2.69	0.40
11:L:71:ARG:NH2	48:5:74:G:O3'	2.54	0.40
51:9:1100:A:H2'	51:9:1101:U:O4'	2.22	0.40
51:9:1485:U:H2'	51:9:1486:A:O4'	2.21	0.40
51:9:191:A:C2'	51:9:192:C:OP1	2.69	0.40
90:9:1972:GCP:PA	90:9:1972:GCP:O3G	2.79	0.40
51:9:625:G:O5'	51:9:626:G:OP2	2.39	0.40
2:B:299:ILE:N	2:B:299:ILE:HD12	2.36	0.40
54:CC:123:ARG:NH2	54:CC:143:CYS:SG	2.94	0.40
4:D:75:VAL:O	4:D:112:ARG:NH1	2.54	0.40
19:T:57:TYR:CD1	19:T:76:VAL:HG21	2.56	0.40
48:5:3891:A:H2'	48:5:3892:U:O4'	2.21	0.40
48:5:4371:G:O2'	48:5:4372:U:OP2	2.34	0.40
48:5:4871:C:O4'	48:5:4871:C:O2	2.38	0.40
48:5:976:G:C2	48:5:977:C:C5	3.09	0.40
2:B:92:TYR:CE1	2:B:101:THR:HB	2.57	0.40
56:EE:185:GLY:N	56:EE:189:LEU:HD13	2.36	0.40
68:QQ:70:VAL:HG11	68:QQ:84:ILE:HG22	2.03	0.40
76:YY:56:PHE:HE2	76:YY:82:ALA:HB1	1.86	0.40
51:9:1824:A:OP2	51:9:1824:A:H3'	2.20	0.40
51:9:613:G:N2	51:9:626:G:OP1	2.54	0.40
1:A:90:CYS:HB2	1:A:101:VAL:HG13	2.04	0.40
66:OO:38:ASN:C	66:OO:38:ASN:HD22	2.24	0.40
68:QQ:22:VAL:HG11	68:QQ:71:ARG:NH2	2.37	0.40
77:ZZ:79:ILE:HB	77:ZZ:83:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1411:C:C4	48:5:1411(B):C:C4	3.09	0.40
48:5:2363:A:C2	48:5:3860:A:C4	3.10	0.40
48:5:716:C:H2'	48:5:717:U:O4'	2.22	0.40
51:9:51:U:H2'	51:9:52:G:C8	2.56	0.40
2:B:36:ASP:N	2:B:36:ASP:OD1	2.54	0.40
53:BB:71:LEU:HD12	53:BB:82:ARG:HB3	2.04	0.40
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.55	0.40
56:EE:126:VAL:HG23	56:EE:156:VAL:O	2.22	0.40
56:EE:45:ILE:HD12	56:EE:80:ILE:HD12	2.04	0.40
16:Q:67:ILE:CD1	16:Q:98:LEU:HD11	2.51	0.40
74:WW:3:ARG:HD3	74:WW:6:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	222 (90%)	23 (9%)	1 (0%)	39	80
2	B	392/403 (97%)	363 (93%)	26 (7%)	3 (1%)	24	69
3	C	360/425 (85%)	339 (94%)	20 (6%)	1 (0%)	46	83
4	D	291/297 (98%)	276 (95%)	13 (4%)	2 (1%)	26	72
5	E	208/291 (72%)	190 (91%)	17 (8%)	1 (0%)	34	77
6	F	223/247 (90%)	209 (94%)	12 (5%)	2 (1%)	21	67
7	G	229/319 (72%)	222 (97%)	7 (3%)	0	100	100
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	201/214 (94%)	182 (90%)	19 (10%)	0	100	100
10	J	168/178 (94%)	162 (96%)	6 (4%)	0	100	100
11	L	208/211 (99%)	200 (96%)	7 (3%)	1 (0%)	34	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	136/218 (62%)	126 (93%)	10 (7%)	0	100	100
13	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	34	77
14	O	197/203 (97%)	188 (95%)	9 (5%)	0	100	100
15	P	151/184 (82%)	143 (95%)	7 (5%)	1 (1%)	26	72
16	Q	185/188 (98%)	169 (91%)	15 (8%)	1 (0%)	34	77
17	R	178/196 (91%)	172 (97%)	6 (3%)	0	100	100
18	S	174/176 (99%)	164 (94%)	8 (5%)	2 (1%)	17	63
19	T	157/160 (98%)	145 (92%)	12 (8%)	0	100	100
20	U	97/128 (76%)	85 (88%)	12 (12%)	0	100	100
21	V	129/140 (92%)	114 (88%)	15 (12%)	0	100	100
22	W	102/157 (65%)	96 (94%)	6 (6%)	0	100	100
23	X	116/156 (74%)	110 (95%)	6 (5%)	0	100	100
24	Y	132/145 (91%)	122 (92%)	10 (8%)	0	100	100
25	Z	133/136 (98%)	127 (96%)	4 (3%)	2 (2%)	13	56
26	a	145/148 (98%)	130 (90%)	15 (10%)	0	100	100
27	b	100/245 (41%)	92 (92%)	7 (7%)	1 (1%)	19	65
28	c	96/115 (84%)	90 (94%)	5 (5%)	1 (1%)	19	65
29	d	105/125 (84%)	89 (85%)	15 (14%)	1 (1%)	19	65
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	99 (92%)	6 (6%)	2 (2%)	10	51
32	g	112/116 (97%)	105 (94%)	7 (6%)	0	100	100
33	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	i	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
35	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
36	k	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
37	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
38	m	50/102 (49%)	49 (98%)	0	1 (2%)	9	50
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	96 (94%)	6 (6%)	0	100	100
41	p	89/92 (97%)	82 (92%)	6 (7%)	1 (1%)	17	63
42	r	122/137 (89%)	111 (91%)	10 (8%)	1 (1%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	s	194/318 (61%)	175 (90%)	17 (9%)	2 (1%)	19	65
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	15	59
45	1	13/15 (87%)	10 (77%)	3 (23%)	0	100	100
52	AA	215/295 (73%)	200 (93%)	13 (6%)	2 (1%)	21	67
53	BB	211/264 (80%)	197 (93%)	14 (7%)	0	100	100
54	CC	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
55	DD	226/243 (93%)	209 (92%)	14 (6%)	3 (1%)	15	59
56	EE	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
57	FF	181/204 (89%)	170 (94%)	11 (6%)	0	100	100
58	GG	235/249 (94%)	227 (97%)	7 (3%)	1 (0%)	39	80
59	HH	181/194 (93%)	170 (94%)	11 (6%)	0	100	100
60	II	204/208 (98%)	192 (94%)	12 (6%)	0	100	100
61	JJ	183/194 (94%)	173 (94%)	10 (6%)	0	100	100
62	KK	94/165 (57%)	85 (90%)	8 (8%)	1 (1%)	17	63
63	LL	139/158 (88%)	129 (93%)	10 (7%)	0	100	100
64	MM	115/132 (87%)	103 (90%)	12 (10%)	0	100	100
65	NN	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
66	OO	134/168 (80%)	122 (91%)	10 (8%)	2 (2%)	13	56
67	PP	118/145 (81%)	106 (90%)	12 (10%)	0	100	100
68	QQ	140/146 (96%)	131 (94%)	9 (6%)	0	100	100
69	RR	130/135 (96%)	122 (94%)	7 (5%)	1 (1%)	24	69
70	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
71	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	26	72
72	UU	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
73	VV	81/83 (98%)	78 (96%)	3 (4%)	0	100	100
74	WW	127/130 (98%)	118 (93%)	7 (6%)	2 (2%)	12	54
75	XX	139/143 (97%)	129 (93%)	7 (5%)	3 (2%)	8	48
76	YY	122/130 (94%)	112 (92%)	10 (8%)	0	100	100
77	ZZ	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
78	aa	99/115 (86%)	92 (93%)	6 (6%)	1 (1%)	19	65
79	bb	81/84 (96%)	74 (91%)	6 (7%)	1 (1%)	16	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
80	cc	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
81	dd	53/56 (95%)	47 (89%)	5 (9%)	1 (2%)	10	51
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/156 (42%)	60 (91%)	6 (9%)	0	100	100
84	gg	311/317 (98%)	285 (92%)	23 (7%)	3 (1%)	19	65
86	ii	370/403 (92%)	338 (91%)	31 (8%)	1 (0%)	46	83
87	jj	423/710 (60%)	387 (92%)	32 (8%)	4 (1%)	21	67
All	All	12325/14502 (85%)	11474 (93%)	794 (6%)	57 (0%)	38	77

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
75	XX	62	PRO
1	A	14	SER
3	C	83	GLY
11	L	63	THR
15	P	114	ILE
18	S	155	PRO
31	f	107	PRO
43	s	142	GLY
44	t	125	LEU
75	XX	86	PRO
13	N	89	VAL
27	b	102	PRO
28	c	92	CYS
29	d	58	GLY
31	f	106	TYR
38	m	94	ASN
62	KK	64	TRP
66	OO	20	GLN
66	OO	149	ARG
79	bb	6	ASP
86	ii	12	ASN
87	jj	618	SER
2	B	17	LEU
4	D	44	TYR
25	Z	90	PRO
25	Z	91	LEU
52	AA	102	ARG
52	AA	159	ILE

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Mol	Chain	Res	Type
55	DD	93	THR
81	dd	7	TYR
87	jj	268	HIS
87	jj	596	LYS
18	S	165	PRO
42	r	33	LYS
44	t	54	LYS
55	DD	44	THR
55	DD	48	ILE
58	GG	135	PRO
71	TT	109	GLY
78	aa	47	ALA
87	jj	269	VAL
2	B	258	HIS
6	F	196	VAL
74	WW	56	HIS
75	XX	61	GLN
16	Q	92	VAL
43	s	25	PRO
4	D	125	VAL
69	RR	119	VAL
84	gg	61	GLY
84	gg	224	GLY
5	E	181	PRO
6	F	99	GLY
41	p	9	GLY
84	gg	13	GLY
2	B	90	VAL
74	WW	29	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	A	190/199 (96%)	174 (92%)	16 (8%)	14 50
2	B	342/348 (98%)	324 (95%)	18 (5%)	28 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	302/347 (87%)	284 (94%)	18 (6%)	24	64
4	D	247/250 (99%)	235 (95%)	12 (5%)	31	70
5	E	190/251 (76%)	178 (94%)	12 (6%)	22	63
6	F	196/215 (91%)	183 (93%)	13 (7%)	21	61
7	G	200/272 (74%)	188 (94%)	12 (6%)	24	64
8	H	169/171 (99%)	157 (93%)	12 (7%)	18	58
9	I	175/181 (97%)	166 (95%)	9 (5%)	29	69
10	J	143/149 (96%)	138 (96%)	5 (4%)	43	78
11	L	175/176 (99%)	167 (95%)	8 (5%)	33	72
12	M	117/161 (73%)	112 (96%)	5 (4%)	35	74
13	N	171/172 (99%)	162 (95%)	9 (5%)	28	67
14	O	171/173 (99%)	159 (93%)	12 (7%)	19	59
15	P	134/163 (82%)	125 (93%)	9 (7%)	20	61
16	Q	164/165 (99%)	152 (93%)	12 (7%)	17	57
17	R	159/175 (91%)	147 (92%)	12 (8%)	17	56
18	S	157/157 (100%)	146 (93%)	11 (7%)	19	59
19	T	139/140 (99%)	126 (91%)	13 (9%)	11	45
20	U	89/114 (78%)	88 (99%)	1 (1%)	80	92
21	V	101/107 (94%)	92 (91%)	9 (9%)	12	48
22	W	86/126 (68%)	84 (98%)	2 (2%)	58	85
23	X	106/134 (79%)	100 (94%)	6 (6%)	25	66
24	Y	124/135 (92%)	118 (95%)	6 (5%)	31	71
25	Z	117/118 (99%)	114 (97%)	3 (3%)	54	83
26	a	119/120 (99%)	116 (98%)	3 (2%)	55	84
27	b	84/184 (46%)	81 (96%)	3 (4%)	42	78
28	c	84/98 (86%)	81 (96%)	3 (4%)	42	78
29	d	98/110 (89%)	87 (89%)	11 (11%)	7	35
30	e	114/121 (94%)	105 (92%)	9 (8%)	15	53
31	f	88/89 (99%)	83 (94%)	5 (6%)	25	66
32	g	98/99 (99%)	94 (96%)	4 (4%)	37	74
33	h	109/110 (99%)	105 (96%)	4 (4%)	41	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	i	86/89 (97%)	83 (96%)	3 (4%)	43	78
35	j	73/80 (91%)	69 (94%)	4 (6%)	27	67
36	k	64/65 (98%)	62 (97%)	2 (3%)	47	81
37	l	47/48 (98%)	46 (98%)	1 (2%)	61	86
38	m	48/90 (53%)	46 (96%)	2 (4%)	36	74
39	n	24/24 (100%)	22 (92%)	2 (8%)	14	50
40	o	92/94 (98%)	87 (95%)	5 (5%)	27	67
41	p	74/75 (99%)	73 (99%)	1 (1%)	74	91
42	r	108/121 (89%)	102 (94%)	6 (6%)	26	66
43	s	164/258 (64%)	158 (96%)	6 (4%)	41	76
44	t	126/137 (92%)	123 (98%)	3 (2%)	57	85
45	1	13/13 (100%)	13 (100%)	0	100	100
52	AA	180/245 (74%)	165 (92%)	15 (8%)	14	50
53	BB	194/231 (84%)	177 (91%)	17 (9%)	12	48
54	CC	187/225 (83%)	167 (89%)	20 (11%)	8	38
55	DD	190/202 (94%)	173 (91%)	17 (9%)	12	48
56	EE	224/225 (100%)	208 (93%)	16 (7%)	18	58
57	FF	158/170 (93%)	148 (94%)	10 (6%)	22	63
58	GG	207/218 (95%)	189 (91%)	18 (9%)	13	49
59	HH	165/174 (95%)	149 (90%)	16 (10%)	10	43
60	II	178/180 (99%)	164 (92%)	14 (8%)	15	53
61	JJ	161/168 (96%)	147 (91%)	14 (9%)	13	49
62	KK	87/136 (64%)	78 (90%)	9 (10%)	9	40
63	LL	130/142 (92%)	114 (88%)	16 (12%)	6	30
64	MM	99/108 (92%)	86 (87%)	13 (13%)	5	28
65	NN	130/131 (99%)	113 (87%)	17 (13%)	5	28
66	OO	106/130 (82%)	91 (86%)	15 (14%)	4	24
67	PP	109/130 (84%)	94 (86%)	15 (14%)	4	25
68	QQ	117/121 (97%)	108 (92%)	9 (8%)	16	55
69	RR	119/121 (98%)	108 (91%)	11 (9%)	11	46
70	SS	125/132 (95%)	108 (86%)	17 (14%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	TT	111/115 (96%)	100 (90%)	11 (10%)	10	42
72	UU	92/107 (86%)	80 (87%)	12 (13%)	5	28
73	VV	67/67 (100%)	62 (92%)	5 (8%)	17	56
74	WW	112/113 (99%)	105 (94%)	7 (6%)	22	63
75	XX	113/115 (98%)	106 (94%)	7 (6%)	23	63
76	YY	107/112 (96%)	94 (88%)	13 (12%)	6	31
77	ZZ	66/103 (64%)	61 (92%)	5 (8%)	16	55
78	aa	88/98 (90%)	78 (89%)	10 (11%)	7	34
79	bb	75/76 (99%)	69 (92%)	6 (8%)	15	53
80	cc	55/62 (89%)	50 (91%)	5 (9%)	12	46
81	dd	48/49 (98%)	46 (96%)	2 (4%)	36	74
82	ee	46/106 (43%)	41 (89%)	5 (11%)	8	37
83	ff	61/140 (44%)	55 (90%)	6 (10%)	10	42
84	gg	272/275 (99%)	261 (96%)	11 (4%)	38	75
86	ii	326/353 (92%)	309 (95%)	17 (5%)	29	68
87	jj	358/608 (59%)	332 (93%)	26 (7%)	17	57
All	All	10740/12312 (87%)	9991 (93%)	749 (7%)	23	59

All (749) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	64	ARG
1	A	102	LEU
1	A	109	GLU
1	A	115	CYS
1	A	125	LYS
1	A	128	ARG
1	A	142	GLU
1	A	163	ARG
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	226	ARG
1	A	233	ARG

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Mol	Chain	Res	Type
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	53	MET
2	B	62	ARG
2	B	66	LYS
2	B	97	ARG
2	B	135	LYS
2	B	248	LEU
2	B	261	ARG
2	B	262	VAL
2	B	279	GLU
2	B	294	LYS
2	B	309	LEU
2	B	314	ILE
2	B	333	LEU
2	B	356	LYS
2	B	381	THR
2	B	383	GLU
3	C	20	LYS
3	C	45	ARG
3	C	95	MET
3	C	113	ARG
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	188	ARG
3	C	193	LYS
3	C	208	CYS
3	C	232	VAL
3	C	246	VAL
3	C	281	MET
3	C	284	MET
3	C	307	LYS
3	C	312	ARG
4	D	22	ARG
4	D	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	56	THR

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Mol	Chain	Res	Type
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	128	ASP
4	D	234	ASP
4	D	264	LYS
4	D	268	ARG
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	123	ASP
5	E	141	ARG
5	E	143	LEU
5	E	144	ARG
5	E	169	LYS
5	E	178	VAL
5	E	213	LYS
5	E	289	LEU
5	E	291	PHE
6	F	30	LYS
6	F	38	GLN
6	F	46	ARG
6	F	65	ARG
6	F	88	LEU
6	F	134	ILE
6	F	151	GLU
6	F	187	GLU
6	F	198	LYS
6	F	211	LYS
6	F	231	ASP
6	F	245	ARG
6	F	246	MET
7	G	126	ARG
7	G	154	LYS
7	G	163	LYS
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	215	ASP
7	G	223	LEU
7	G	226	LEU
7	G	230	MET

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Mol	Chain	Res	Type
7	G	242	ARG
7	G	293	ASN
8	H	1	MET
8	H	20	LEU
8	H	23	ARG
8	H	52	LYS
8	H	54	ARG
8	H	59	LYS
8	H	66	GLU
8	H	105	ILE
8	H	108	ASN
8	H	128	MET
8	H	173	ARG
8	H	177	ASP
9	I	13	LYS
9	I	36	LEU
9	I	39	LYS
9	I	116	ARG
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	168	SER
9	I	208	LYS
10	J	16	ARG
10	J	28	GLU
10	J	81	GLU
10	J	113	ILE
10	J	175	LEU
11	L	35	ARG
11	L	63	THR
11	L	67	HIS
11	L	74	ARG
11	L	121	ARG
11	L	129	ARG
11	L	162	LYS
11	L	186	ARG
12	M	37	LEU
12	M	57	LEU
12	M	89	THR
12	M	96	GLU
12	M	119	ARG
13	N	9	GLU

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Mol	Chain	Res	Type
13	N	26	ARG
13	N	32	GLN
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	87	HIS
13	N	89	VAL
13	N	162	ARG
14	O	18	ARG
14	O	49	ARG
14	O	74	ARG
14	O	82	ARG
14	O	128	ARG
14	O	130	LYS
14	O	140	ARG
14	O	145	VAL
14	O	175	MET
14	O	179	LYS
14	O	188	LYS
14	O	202	LEU
15	P	24	VAL
15	P	25	HIS
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	5	ILE
16	Q	13	VAL
16	Q	61	LEU
16	Q	63	LEU
16	Q	75	ARG
16	Q	91	ARG
16	Q	97	LYS
16	Q	110	ARG
16	Q	115	LYS
16	Q	143	ARG
16	Q	168	ARG
17	R	8	LYS

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Mol	Chain	Res	Type
17	R	36	ASN
17	R	50	ILE
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	113	LYS
17	R	130	ASN
17	R	133	LYS
17	R	138	LEU
17	R	176	ARG
17	R	178	GLN
18	S	7	LEU
18	S	8	ARG
18	S	9	GLU
18	S	17	LEU
18	S	24	THR
18	S	43	ARG
18	S	70	LYS
18	S	83	ARG
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	33	ILE
19	T	60	LYS
19	T	63	ARG
19	T	80	VAL
19	T	88	ARG
19	T	96	ILE
19	T	117	LYS
19	T	142	ARG
19	T	144	ASN
19	T	146	LYS
19	T	157	GLU
19	T	159	MET
20	U	33	ILE
21	V	15	ARG
21	V	18	LEU
21	V	35	LYS
21	V	46	LYS
21	V	60	MET
21	V	82	ILE

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Mol	Chain	Res	Type
21	V	91	LYS
21	V	109	LYS
21	V	123	LYS
22	W	57	ARG
22	W	91	MET
23	X	39	LYS
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	91	GLU
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	50	ARG
24	Y	72	GLN
24	Y	74	TYR
24	Y	104	VAL
25	Z	11	VAL
25	Z	33	THR
25	Z	112	ARG
26	a	4	ARG
26	a	84	GLU
26	a	132	ARG
27	b	22	LYS
27	b	40	LEU
27	b	101	HIS
28	c	37	MET
28	c	52	CYS
28	c	78	ASN
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	44	ARG
29	d	48	GLU
29	d	78	ARG
29	d	79	ASN
29	d	83	ARG
29	d	85	ARG
29	d	98	SER
29	d	102	LEU
30	e	21	ILE
30	e	22	ARG

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Mol	Chain	Res	Type
30	e	48	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	89	LEU
30	e	106	LYS
30	e	128	ARG
31	f	16	ARG
31	f	23	GLU
31	f	52	LYS
31	f	73	LYS
31	f	101	ILE
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	114	GLN
33	h	16	GLU
33	h	67	GLU
33	h	77	LYS
33	h	89	ARG
34	i	48	CYS
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	11	ARG
35	j	20	ARG
35	j	58	THR
36	k	69	LEU
36	k	70	LYS
37	l	49	LEU
38	m	71	ARG
38	m	92	THR
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	36	GLN
40	o	61	LYS
40	o	82	MET
40	o	83	LEU
41	p	8	VAL
42	r	8	MET
42	r	20	ARG

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Mol	Chain	Res	Type
42	r	32	LEU
42	r	35	ARG
42	r	67	ARG
42	r	118	LEU
43	s	38	LYS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	98	ILE
44	t	133	LEU
52	AA	12	GLU
52	AA	23	THR
52	AA	25	LEU
52	AA	50	ASN
52	AA	56	GLU
52	AA	58	LEU
52	AA	59	LEU
52	AA	60	LEU
52	AA	111	GLN
52	AA	136	GLU
52	AA	142	LEU
52	AA	155	ARG
52	AA	169	HIS
52	AA	178	LEU
52	AA	200	ASP
53	BB	29	ASP
53	BB	38	MET
53	BB	71	LEU
53	BB	82	ARG
53	BB	96	CYS
53	BB	105	LEU
53	BB	125	VAL
53	BB	126	ASP
53	BB	157	GLN
53	BB	163	GLN
53	BB	175	GLU
53	BB	180	ASP
53	BB	181	LEU
53	BB	184	VAL

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Mol	Chain	Res	Type
53	BB	207	LEU
53	BB	209	ASP
53	BB	213	ARG
54	CC	78	LEU
54	CC	79	GLU
54	CC	105	GLU
54	CC	114	LYS
54	CC	117	ARG
54	CC	120	GLN
54	CC	121	ARG
54	CC	132	ASP
54	CC	144	SER
54	CC	167	ARG
54	CC	185	THR
54	CC	188	CYS
54	CC	192	LEU
54	CC	196	ILE
54	CC	236	PHE
54	CC	244	ILE
54	CC	248	TYR
54	CC	252	THR
54	CC	255	LEU
54	CC	271	ASP
55	DD	28	GLU
55	DD	31	GLU
55	DD	45	ARG
55	DD	72	VAL
55	DD	76	ARG
55	DD	127	MET
55	DD	134	CYS
55	DD	142	LEU
55	DD	145	GLN
55	DD	146	ARG
55	DD	168	VAL
55	DD	179	GLN
55	DD	182	LEU
55	DD	190	LEU
55	DD	218	LEU
55	DD	220	THR
55	DD	227	LYS
56	EE	17	HIS
56	EE	21	ASP

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Mol	Chain	Res	Type
56	EE	33	THR
56	EE	42	LEU
56	EE	51	ARG
56	EE	66	MET
56	EE	77	ARG
56	EE	145	ARG
56	EE	181	CYS
56	EE	200	ARG
56	EE	205	PHE
56	EE	222	LEU
56	EE	232	ASN
56	EE	245	ARG
56	EE	246	LEU
56	EE	247	THR
57	FF	63	LYS
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	95	HIS
57	FF	110	GLN
57	FF	127	ARG
57	FF	128	ILE
57	FF	146	ARG
57	FF	204	ARG
58	GG	34	THR
58	GG	41	LEU
58	GG	63	MET
58	GG	64	LYS
58	GG	67	VAL
58	GG	75	LEU
58	GG	95	LYS
58	GG	96	SER
58	GG	103	ASP
58	GG	116	LYS
58	GG	171	THR
58	GG	178	ARG
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	199	THR
58	GG	216	ARG
58	GG	230	LYS

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Mol	Chain	Res	Type
59	HH	8	ILE
59	HH	17	ASP
59	HH	36	LEU
59	HH	40	LEU
59	HH	46	THR
59	HH	53	VAL
59	HH	76	GLN
59	HH	79	LEU
59	HH	82	GLU
59	HH	100	ILE
59	HH	105	THR
59	HH	119	SER
59	HH	145	ARG
59	HH	153	LEU
59	HH	160	LYS
59	HH	193	GLN
60	II	12	ARG
60	II	23	LYS
60	II	26	LYS
60	II	49	ARG
60	II	66	SER
60	II	74	ARG
60	II	92	ARG
60	II	99	ASN
60	II	121	LEU
60	II	130	THR
60	II	161	LEU
60	II	168	GLN
60	II	178	ARG
60	II	203	LYS
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	70	ARG
61	JJ	79	ARG
61	JJ	80	ARG
61	JJ	89	GLU
61	JJ	95	ASP
61	JJ	109	ARG
61	JJ	116	LYS

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Mol	Chain	Res	Type
61	JJ	133	ARG
61	JJ	162	ARG
62	KK	1	MET
62	KK	6	LYS
62	KK	17	LYS
62	KK	29	MET
62	KK	35	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	89	ILE
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	39	ASN
63	LL	40	ILE
63	LL	42	LEU
63	LL	56	ILE
63	LL	69	ARG
63	LL	85	THR
63	LL	90	ARG
63	LL	91	ASP
63	LL	110	SER
63	LL	121	GLN
63	LL	126	VAL
63	LL	134	LEU
63	LL	135	SER
63	LL	144	LYS
64	MM	31	LEU
64	MM	33	ARG
64	MM	40	LYS
64	MM	42	LEU
64	MM	45	ARG
64	MM	55	ASN
64	MM	64	LEU
64	MM	76	LEU
64	MM	83	LYS
64	MM	85	LEU
64	MM	96	ARG
64	MM	99	LYS
64	MM	101	ARG
65	NN	3	ARG
65	NN	20	ARG

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Mol	Chain	Res	Type
65	NN	27	LYS
65	NN	29	THR
65	NN	36	GLN
65	NN	39	LYS
65	NN	55	ARG
65	NN	60	VAL
65	NN	75	LEU
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	94	LYS
65	NN	107	LYS
65	NN	110	ASP
65	NN	125	LEU
65	NN	132	LYS
66	OO	25	GLU
66	OO	31	CYS
66	OO	34	PHE
66	OO	38	ASN
66	OO	46	ASP
66	OO	51	GLU
66	OO	56	VAL
66	OO	69	SER
66	OO	85	CYS
66	OO	104	ARG
66	OO	133	THR
66	OO	137	SER
66	OO	146	ARG
66	OO	150	ARG
66	OO	151	LEU
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE
67	PP	37	TYR
67	PP	44	ARG
67	PP	45	LEU
67	PP	51	ARG
67	PP	58	LYS
67	PP	76	VAL
67	PP	78	THR
67	PP	83	MET
67	PP	106	GLU

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Mol	Chain	Res	Type
67	PP	108	LYS
67	PP	120	SER
67	PP	130	ARG
68	QQ	31	LEU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	60	LYS
68	QQ	67	ASP
68	QQ	90	LYS
68	QQ	100	VAL
68	QQ	127	CYS
68	QQ	140	ARG
69	RR	5	ARG
69	RR	22	THR
69	RR	31	ASN
69	RR	44	LYS
69	RR	62	GLN
69	RR	98	VAL
69	RR	99	ASP
69	RR	105	MET
69	RR	120	THR
69	RR	121	GLN
69	RR	132	ARG
70	SS	7	GLU
70	SS	8	LYS
70	SS	13	LEU
70	SS	21	ASP
70	SS	23	ARG
70	SS	46	ARG
70	SS	52	LEU
70	SS	59	LEU
70	SS	60	THR
70	SS	62	ASP
70	SS	63	GLU
70	SS	75	ARG
70	SS	81	ASP
70	SS	83	PHE
70	SS	104	ASP
70	SS	110	ASP
70	SS	132	ARG
71	TT	36	THR
71	TT	41	LYS

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Mol	Chain	Res	Type
71	TT	62	ARG
71	TT	84	ARG
71	TT	102	ARG
71	TT	110	LEU
71	TT	121	ARG
71	TT	124	THR
71	TT	131	LEU
71	TT	132	ASP
71	TT	142	LYS
72	UU	18	HIS
72	UU	19	ARG
72	UU	25	THR
72	UU	36	CYS
72	UU	44	LYS
72	UU	56	MET
72	UU	60	THR
72	UU	79	ARG
72	UU	88	LEU
72	UU	90	ASP
72	UU	106	ILE
72	UU	111	GLU
73	VV	7	GLU
73	VV	10	ASP
73	VV	12	TYR
73	VV	18	SER
73	VV	66	ASP
74	WW	23	ARG
74	WW	36	ARG
74	WW	51	GLU
74	WW	85	ASP
74	WW	92	ASN
74	WW	103	VAL
74	WW	104	LEU
75	XX	8	ARG
75	XX	11	ARG
75	XX	34	THR
75	XX	67	ARG
75	XX	87	ASN
75	XX	105	PHE
75	XX	115	ILE
76	YY	16	ARG
76	YY	17	LEU

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Mol	Chain	Res	Type
76	YY	20	ARG
76	YY	32	LYS
76	YY	40	ILE
76	YY	44	LEU
76	YY	46	LYS
76	YY	51	THR
76	YY	61	ARG
76	YY	74	MET
76	YY	88	LYS
76	YY	93	ARG
76	YY	101	LYS
77	ZZ	80	ARG
77	ZZ	89	GLN
77	ZZ	90	GLU
77	ZZ	92	LEU
77	ZZ	110	THR
78	aa	2	THR
78	aa	18	VAL
78	aa	19	GLN
78	aa	21	ILE
78	aa	23	CYS
78	aa	41	ILE
78	aa	42	ARG
78	aa	55	GLU
78	aa	74	CYS
78	aa	100	ARG
79	bb	17	ARG
79	bb	37	CYS
79	bb	42	LYS
79	bb	65	GLN
79	bb	80	ARG
79	bb	81	ARG
80	cc	31	ARG
80	cc	40	ARG
80	cc	44	ARG
80	cc	51	ARG
80	cc	68	LEU
81	dd	4	GLN
81	dd	22	ARG
82	ee	98	LYS
82	ee	99	LYS
82	ee	107	ARG

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Mol	Chain	Res	Type
82	ee	109	MET
82	ee	113	ARG
83	ff	83	LYS
83	ff	94	LYS
83	ff	99	LYS
83	ff	110	GLU
83	ff	138	ARG
83	ff	140	TYR
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	38	LYS
84	gg	113	PHE
84	gg	119	GLN
84	gg	198	VAL
84	gg	207	CYS
84	gg	273	GLU
84	gg	289	LEU
84	gg	306	LEU
86	ii	40	ARG
86	ii	68	CYS
86	ii	81	LEU
86	ii	107	ASN
86	ii	148	HIS
86	ii	149	ILE
86	ii	156	MET
86	ii	170	LYS
86	ii	183	GLU
86	ii	198	HIS
86	ii	243	VAL
86	ii	258	CYS
86	ii	297	LYS
86	ii	311	LEU
86	ii	313	ILE
86	ii	319	ARG
86	ii	349	LEU
87	jj	269	VAL
87	jj	276	LEU
87	jj	297	GLN
87	jj	298	GLU
87	jj	304	LYS
87	jj	313	LEU

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Mol	Chain	Res	Type
87	jj	325	THR
87	jj	330	MET
87	jj	361	GLN
87	jj	369	VAL
87	jj	385	GLN
87	jj	389	HIS
87	jj	408	MET
87	jj	425	LEU
87	jj	434	PHE
87	jj	436	GLU
87	jj	482	ARG
87	jj	489	ARG
87	jj	499	GLN
87	jj	505	ILE
87	jj	557	MET
87	jj	590	ILE
87	jj	613	ILE
87	jj	640	ASN
87	jj	653	LEU
87	jj	664	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
3	C	223	ASN
5	E	45	HIS
7	G	134	ASN
7	G	135	GLN
7	G	194	ASN
11	L	28	GLN
11	L	87	HIS
14	O	50	ASN
16	Q	188	ASN
17	R	130	ASN
22	W	48	GLN
23	X	105	ASN
24	Y	14	ASN
42	r	70	GLN
42	r	103	HIS
43	s	34	ASN
55	DD	4	GLN

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Mol	Chain	Res	Type
55	DD	179	GLN
56	EE	67	GLN
56	EE	260	GLN
59	HH	193	GLN
61	JJ	111	GLN
61	JJ	154	GLN
63	LL	100	ASN
66	OO	38	ASN
68	QQ	142	GLN
70	SS	10	GLN
71	TT	42	HIS
74	WW	92	ASN
86	ii	109	GLN
86	ii	166	ASN
87	jj	361	GLN
87	jj	385	GLN
87	jj	389	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	15 (20%)	0
47	3	72/75 (96%)	27 (37%)	2 (2%)
48	5	3506/3543 (98%)	868 (24%)	165 (4%)
49	7	119/120 (99%)	15 (12%)	0
50	8	150/156 (96%)	37 (24%)	7 (4%)
51	9	1680/1869 (89%)	434 (25%)	87 (5%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5608/5847 (95%)	1400 (24%)	261 (4%)

All (1400) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	8	U
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G
46	2	20	U
46	2	21	A
46	2	43	A

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Mol	Chain	Res	Type
46	2	46	G
46	2	47	U
46	2	49	C
46	2	61	C
46	2	64	G
46	2	72	C
46	2	75	C
47	3	7	A
47	3	13	C
47	3	14	A
47	3	16	C
47	3	21	A
47	3	25	C
47	3	28	C
47	3	29	A
47	3	34	U
47	3	35	U
47	3	36	U
47	3	40	C
47	3	42	G
47	3	47	U
47	3	49	C
47	3	51	G
47	3	53	G
47	3	58	A
47	3	60	U
47	3	61	C
47	3	63	C
47	3	65	G
47	3	71	G
47	3	72	C
47	3	74	C
47	3	75	C
47	3	76	A
48	5	12	A
48	5	13	U
48	5	15	A
48	5	21	G
48	5	25	A
48	5	30	C
48	5	35	U
48	5	39	A

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Mol	Chain	Res	Type
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	72	C
48	5	73	A
48	5	75	G
48	5	91	G
48	5	93	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	116	G
48	5	118	C
48	5	119	G
48	5	120	A
48	5	122	U
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	157	U
48	5	159	C
48	5	172	C
48	5	173	C
48	5	177	G
48	5	179	G
48	5	200	U
48	5	201	C
48	5	202	C
48	5	203	U
48	5	205	C
48	5	209	U
48	5	216	C

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Mol	Chain	Res	Type
48	5	217	C
48	5	218	A
48	5	220	C
48	5	221	C
48	5	224	U
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	245	C
48	5	246	G
48	5	253	G
48	5	262	G
48	5	265	C
48	5	266	C
48	5	276	C
48	5	279	A
48	5	280	G
48	5	281	U
48	5	297	U
48	5	298	G
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	317	A
48	5	322	C
48	5	328	A
48	5	334	A
48	5	340	C
48	5	350	C
48	5	357	U
48	5	361	C
48	5	363	A
48	5	386	A
48	5	387	G
48	5	399	G
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G

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Mol	Chain	Res	Type
48	5	413	G
48	5	431	G
48	5	432	U
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	482	G
48	5	483	G
48	5	484	U
48	5	485	C
48	5	486	C
48	5	490	C
48	5	492	U
48	5	493	G
48	5	495	C
48	5	497	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	510	U
48	5	647	G
48	5	649	A
48	5	654	C
48	5	658	C
48	5	667	A
48	5	668	C
48	5	672	C
48	5	683	C
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	704	C
48	5	705	G

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Mol	Chain	Res	Type
48	5	708	G
48	5	722	G
48	5	729	G
48	5	730	G
48	5	731	G
48	5	734	G
48	5	739	G
48	5	742	G
48	5	744	G
48	5	747	A
48	5	748	G
48	5	749	G
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	917	A
48	5	918	G
48	5	922(A)	G
48	5	922(B)	C
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	929	A
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	936	C
48	5	939	G
48	5	941	C
48	5	943	A
48	5	944	A
48	5	945	U
48	5	955	G
48	5	956	A
48	5	957	G
48	5	959	G
48	5	960	A
48	5	961	G

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Mol	Chain	Res	Type
48	5	962	C
48	5	963	G
48	5	964	A
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C
48	5	969	C
48	5	972	C
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1177	U
48	5	1179	U
48	5	1184	A
48	5	1185	G
48	5	1195	G
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1280	C
48	5	1284	G

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Mol	Chain	Res	Type
48	5	1287	G
48	5	1288	G
48	5	1291	G
48	5	1292	C
48	5	1293	G
48	5	1295	U
48	5	1296	G
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1328	G
48	5	1330	A
48	5	1337	A
48	5	1353	G
48	5	1354	A
48	5	1359	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1403	G
48	5	1411(B)	C
48	5	1411(C)	C
48	5	1416	G
48	5	1418	C
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1429	C
48	5	1435	G
48	5	1436	C
48	5	1437	C

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Mol	Chain	Res	Type
48	5	1438	U
48	5	1441	C
48	5	1442	C
48	5	1445	U
48	5	1446	C
48	5	1453	G
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1458	C
48	5	1465	G
48	5	1475	G
48	5	1478	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1525	A
48	5	1534	A
48	5	1535	C
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1568	C
48	5	1574	G
48	5	1578	U
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1602	U

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Mol	Chain	Res	Type
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1640	C
48	5	1641	G
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1670	G
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1684	A
48	5	1691	G
48	5	1724	G
48	5	1726	U
48	5	1733	G
48	5	1734	G
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1761	G
48	5	1763	C
48	5	1764	G
48	5	1768	C
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1781	U
48	5	1785	C
48	5	1787	A
48	5	1797	G
48	5	1799	G

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Mol	Chain	Res	Type
48	5	1800	U
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1819	G
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1869	G
48	5	1882	U
48	5	1890	G
48	5	1897	A
48	5	1909	G
48	5	1910	G
48	5	1918	U
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1932	A
48	5	1933	G
48	5	1940	G
48	5	1941	A
48	5	1948	G
48	5	1952	G
48	5	1959	U
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1966	C
48	5	1967	A
48	5	1976	G
48	5	1977	C
48	5	1978	C

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Mol	Chain	Res	Type
48	5	1980	U
48	5	1982	G
48	5	1983	A
48	5	1984	A
48	5	1986	U
48	5	1987	C
48	5	1991	A
48	5	1992	U
48	5	1993	C
48	5	1997	U
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2011	C
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2033	A
48	5	2046	G
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2069	A
48	5	2070	U
48	5	2084	U
48	5	2085	G
48	5	2089	G
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G

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Mol	Chain	Res	Type
48	5	2101	A
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2110	G
48	5	2259	G
48	5	2260	C
48	5	2262	G
48	5	2266	C
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2275	G
48	5	2279	A
48	5	2289	C
48	5	2294	G
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2331	G
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2352	U
48	5	2360	A
48	5	2364	G
48	5	2370	A
48	5	2380	G
48	5	2395	A
48	5	2396	A
48	5	2399	G
48	5	2416	G
48	5	2417	A
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2428	A

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Mol	Chain	Res	Type
48	5	2429	A
48	5	2433	G
48	5	2441	C
48	5	2447	U
48	5	2450	G
48	5	2467	U
48	5	2468	U
48	5	2469	C
48	5	2471	G
48	5	2475	G
48	5	2483	G
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2513	A
48	5	2521	G
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2553	A
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2571	C
48	5	2572	C
48	5	2575	U
48	5	2583	C
48	5	2587	A
48	5	2601	A
48	5	2620	G
48	5	2627	C
48	5	2638	G
48	5	2639	U

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Mol	Chain	Res	Type
48	5	2647	A
48	5	2660	A
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2673	G
48	5	2676	A
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2688	G
48	5	2689	C
48	5	2695	A
48	5	2696	A
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2735	G
48	5	2740	U
48	5	2743	A
48	5	2751	G
48	5	2754	G
48	5	2760	G
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2787	A
48	5	2789	A
48	5	2790	U
48	5	2795	A
48	5	2796	G
48	5	2798	A

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Mol	Chain	Res	Type
48	5	2802	C
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2835	A
48	5	2838	G
48	5	2839	U
48	5	2842	G
48	5	2855	G
48	5	2875	C
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3604	A
48	5	3605	C
48	5	3615	G
48	5	3625	G
48	5	3626	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3662	A
48	5	3674	G
48	5	3692	A
48	5	3696	C
48	5	3698	G
48	5	3711	A
48	5	3712	A
48	5	3722	G
48	5	3729	U
48	5	3733	A
48	5	3740	G
48	5	3748	A
48	5	3753	G
48	5	3756	A
48	5	3759	A

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Mol	Chain	Res	Type
48	5	3760	A
48	5	3761	C
48	5	3765	G
48	5	3766	A
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3784	A
48	5	3786	U
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3813	A
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3859	G
48	5	3867	A
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3888	G
48	5	3889	G
48	5	3892	U
48	5	3897	G
48	5	3898	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3915	U
48	5	3916	G
48	5	3917	A

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Mol	Chain	Res	Type
48	5	3927	U
48	5	3939	G
48	5	3943	A
48	5	4067	U
48	5	4069	U
48	5	4073	A
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4092	G
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4150	G
48	5	4158	C
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4166	G
48	5	4171	C
48	5	4177	C
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4201	G
48	5	4203	A
48	5	4212	A
48	5	4213	A
48	5	4215	C
48	5	4218	U
48	5	4219	A
48	5	4225	G

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Mol	Chain	Res	Type
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4249	G
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4297	G
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4326	G
48	5	4329	G
48	5	4330	G
48	5	4335	C
48	5	4336	A
48	5	4339	A
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4373	G
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4393	G
48	5	4394	A
48	5	4395	U

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Mol	Chain	Res	Type
48	5	4396	A
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4440	G
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4454	G
48	5	4464	A
48	5	4471	U
48	5	4475	G
48	5	4476	C
48	5	4488	A
48	5	4495	G
48	5	4500	U
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4522	G
48	5	4524	G
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4561	C
48	5	4563	U
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4584	A
48	5	4585	U
48	5	4586	G

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Mol	Chain	Res	Type
48	5	4590	A
48	5	4599	A
48	5	4618	G
48	5	4636	U
48	5	4637	G
48	5	4639	G
48	5	4656	A
48	5	4657	U
48	5	4658	G
48	5	4661	G
48	5	4667	C
48	5	4669	A
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4678	G
48	5	4700	A
48	5	4701	A
48	5	4709	U
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4728	U
48	5	4736	C
48	5	4737	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4755	G
48	5	4756	C
48	5	4757	C
48	5	4759	C
48	5	4761	G
48	5	4765	G
48	5	4771	C
48	5	4772	C
48	5	4868	G
48	5	4870	G
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A

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Mol	Chain	Res	Type
48	5	4875	G
48	5	4876	A
48	5	4877	G
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4887	C
48	5	4891	G
48	5	4895	C
48	5	4897	G
48	5	4904	G
48	5	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G
48	5	4919	G
48	5	4921	C
48	5	4924	C
48	5	4925	U
48	5	4926	C
48	5	4927	G
48	5	4928	C
48	5	4931	G
48	5	4935	C
48	5	4937	C
48	5	4938	A
48	5	4940	C
48	5	4942	C
48	5	4943	A
48	5	4944	C
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A
48	5	4957	C
48	5	4958	C
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A

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Mol	Chain	Res	Type
48	5	4976	U
48	5	4985	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4991	U
48	5	4993	G
48	5	4999	G
48	5	5014	A
48	5	5017	G
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5061	A
48	5	5062	G
48	5	5069	U
49	7	7	G
49	7	25	G
49	7	33	U
49	7	42	A
49	7	53	U
49	7	54	A
49	7	64	G
49	7	66	G
49	7	97	G
49	7	99	G
49	7	100	A
49	7	110	G
49	7	111	C
49	7	117	G
49	7	120	U
50	8	2	G
50	8	3	A
50	8	32	C
50	8	34	U
50	8	35	C
50	8	49	G
50	8	51	U

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Mol	Chain	Res	Type
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	G
50	8	79	G
50	8	86	U
50	8	87	G
50	8	94	G
50	8	95	A
50	8	103	A
50	8	104	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	114	G
50	8	121	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	147	G
50	8	150	C
50	8	153	C
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
51	9	41	G
51	9	44	U
51	9	45	A
51	9	46	A

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Mol	Chain	Res	Type
51	9	56	G
51	9	58	C
51	9	60	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	128	U
51	9	129	C
51	9	130	G
51	9	141	A
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C
51	9	175	A
51	9	182	C
51	9	183	G
51	9	184	G

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Mol	Chain	Res	Type
51	9	188	C
51	9	189	U
51	9	192	C
51	9	200	G
51	9	202	G
51	9	206	G
51	9	213	G
51	9	215	G
51	9	292	A
51	9	294	U
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	313	A
51	9	314	U
51	9	317	C
51	9	318	A
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	335	G
51	9	343	A
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	370	G
51	9	379	C
51	9	381	C
51	9	382	C
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G
51	9	409	C
51	9	410	G

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Mol	Chain	Res	Type
51	9	417	C
51	9	418	A
51	9	435	A
51	9	438	G
51	9	448	A
51	9	449	A
51	9	450	C
51	9	459	C
51	9	460	A
51	9	462	C
51	9	464	A
51	9	465	A
51	9	466	G
51	9	468	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	501	C
51	9	503	C
51	9	523	A
51	9	525	A
51	9	528	A
51	9	531	A
51	9	532	C
51	9	533	A
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	557	U
51	9	559	G

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Mol	Chain	Res	Type
51	9	560	A
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	595	U
51	9	597	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	613	G
51	9	614	C
51	9	615	C
51	9	616	A
51	9	617	G
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	630	U
51	9	632	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	659	G
51	9	660	C
51	9	663	C
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A

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Mol	Chain	Res	Type
51	9	683	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	732	U
51	9	752	G
51	9	753	C
51	9	754	G
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	834	C
51	9	847	A
51	9	849	A
51	9	861	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	885	U
51	9	887	U
51	9	890	U
51	9	892	U
51	9	911	C
51	9	913	A
51	9	914	U
51	9	920	A
51	9	922	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	971	G
51	9	985	G

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Mol	Chain	Res	Type
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1055	A
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1067	C
51	9	1078	C
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1099	G
51	9	1100	A
51	9	1113	A
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G
51	9	1131	G
51	9	1138	C
51	9	1139	C
51	9	1144	A
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1161	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1196	A
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1213	C

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Mol	Chain	Res	Type
51	9	1215	C
51	9	1221	G
51	9	1223	A
51	9	1224	G
51	9	1227	G
51	9	1230	C
51	9	1240	A
51	9	1242	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1258	A
51	9	1259	A
51	9	1265	A
51	9	1266	C
51	9	1268	C
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1281	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1287	A
51	9	1289	U
51	9	1291	A
51	9	1293	A
51	9	1298	G
51	9	1299	A
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1322	G
51	9	1330	G

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Mol	Chain	Res	Type
51	9	1331	C
51	9	1337	C
51	9	1342	U
51	9	1348	G
51	9	1354	G
51	9	1369	A
51	9	1371	U
51	9	1372	U
51	9	1378	A
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1401	A
51	9	1402	A
51	9	1404	U
51	9	1410	C
51	9	1412	C
51	9	1424	G
51	9	1428	G
51	9	1429	G
51	9	1439	A
51	9	1449	G
51	9	1454	A
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1466	G
51	9	1473	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1489	A
51	9	1490	G
51	9	1493	C
51	9	1494	U
51	9	1498	A
51	9	1507	G
51	9	1509	U
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1531	A

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Mol	Chain	Res	Type
51	9	1533	A
51	9	1536	G
51	9	1539	U
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1585	U
51	9	1587	G
51	9	1588	A
51	9	1589	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1624	U
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1641	A
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1682	C
51	9	1683	C

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Mol	Chain	Res	Type
51	9	1686	G
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1728	U
51	9	1729	U
51	9	1730	U
51	9	1732	G
51	9	1737	G
51	9	1744	G
51	9	1745	A
51	9	1753	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C
51	9	1800	A
51	9	1801	A
51	9	1805	G
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1850	A
51	9	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A
51	9	1867	U

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Mol	Chain	Res	Type
51	9	1868	U
51	9	1869	A
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G

All (261) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	7	A
47	3	74	C
48	5	12	A
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	119	G
48	5	125	C
48	5	134	G
48	5	143	C
48	5	159	C
48	5	217	C
48	5	226	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	G
48	5	315	G
48	5	385	A
48	5	387	G
48	5	406	C
48	5	408	A
48	5	409	G
48	5	417	G
48	5	449	C
48	5	484	U
48	5	485	C
48	5	492	U
48	5	497	G
48	5	498	C
48	5	504	G

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Mol	Chain	Res	Type
48	5	696	C
48	5	728	U
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	748	G
48	5	916	C
48	5	922	C
48	5	922(B)	C
48	5	930	G
48	5	933	G
48	5	935(A)	G
48	5	936	C
48	5	955	G
48	5	956	A
48	5	959	G
48	5	963	G
48	5	965	G
48	5	966	A
48	5	968	C
48	5	969	C
48	5	971(A)	G
48	5	1072	C
48	5	1209	U
48	5	1211	G
48	5	1214	C
48	5	1236	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1295	U
48	5	1329	G
48	5	1358	G
48	5	1359	G
48	5	1370	G
48	5	1378	C
48	5	1380	G
48	5	1420	A
48	5	1432	G
48	5	1440	U
48	5	1445	U
48	5	1455	G

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Mol	Chain	Res	Type
48	5	1477	C
48	5	1484	G
48	5	1485	C
48	5	1533	A
48	5	1563	A
48	5	1633	G
48	5	1678	C
48	5	1733	G
48	5	1740	C
48	5	1804	A
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1892	A
48	5	1919	G
48	5	1921	C
48	5	1935	C
48	5	1979	A
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2046	G
48	5	2068	C
48	5	2088	A
48	5	2089	G
48	5	2100	G
48	5	2265	G
48	5	2266	C
48	5	2278	G
48	5	2313	A
48	5	2396	A
48	5	2398	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	A
48	5	2546	G
48	5	2553	A

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Mol	Chain	Res	Type
48	5	2661	U
48	5	2695	A
48	5	2724	G
48	5	2754	G
48	5	2782	U
48	5	2789	A
48	5	2794	C
48	5	2806	A
48	5	3603	G
48	5	3625	G
48	5	3673	C
48	5	3697	U
48	5	3710	G
48	5	3759	A
48	5	3760	A
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4162	C
48	5	4170	A
48	5	4221	C
48	5	4232	U
48	5	4254	G
48	5	4266	G
48	5	4378	A
48	5	4395	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4488	A
48	5	4510	A
48	5	4583	C
48	5	4699	U
48	5	4719	G
48	5	4871	C

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Mol	Chain	Res	Type
48	5	4872	G
48	5	4873	G
48	5	4876	A
48	5	4884	G
48	5	4925	U
48	5	4936	G
48	5	4942	C
48	5	4947	U
48	5	4965	U
50	8	2	G
50	8	51	U
50	8	85	U
50	8	86	U
50	8	94	G
50	8	110	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	72	C
51	9	110	U
51	9	126	G
51	9	127	C
51	9	128	U
51	9	142	C
51	9	160	U
51	9	182	C
51	9	293	C
51	9	312	G
51	9	369	C
51	9	434	G
51	9	465	A
51	9	500	A
51	9	516	A
51	9	532	C
51	9	550	C
51	9	553	U
51	9	555	A
51	9	559	G
51	9	563	G
51	9	591	U
51	9	594	A
51	9	606	G

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Mol	Chain	Res	Type
51	9	607	U
51	9	613	G
51	9	614	C
51	9	615	C
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	642	U
51	9	670	A
51	9	688	U
51	9	752	G
51	9	821	G
51	9	869	A
51	9	870	A
51	9	872	A
51	9	874	G
51	9	932	G
51	9	990	A
51	9	1016	U
51	9	1087	A
51	9	1114	U
51	9	1115	U
51	9	1137	U
51	9	1165	G
51	9	1253	A
51	9	1264	C
51	9	1274	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1313	A
51	9	1330	G
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1438	A
51	9	1476	A
51	9	1489	A
51	9	1493	C
51	9	1519	U

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Mol	Chain	Res	Type
51	9	1520	G
51	9	1578	U
51	9	1581	C
51	9	1587	G
51	9	1621	U
51	9	1622	U
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1663	A
51	9	1664	A
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1825	A
51	9	1835	A
51	9	1867	U
51	9	1868	U

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 291 ligands modelled in this entry, 289 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
90	GCP	9	1972	-	29,34,34	2.57	8 (27%)	31,54,54	1.16	2 (6%)
90	GCP	jj	700	88	29,34,34	2.49	8 (27%)	31,54,54	1.12	2 (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
90	GCP	9	1972	-	-	0/18/38/38	0/3/3/3
90	GCP	jj	700	88	-	0/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	9	1972	GCP	C4-N9	-11.03	1.33	1.47
90	jj	700	GCP	C4-N9	-10.27	1.34	1.47
90	9	1972	GCP	C8-N9	-3.84	1.34	1.47
90	jj	700	GCP	C8-N9	-3.71	1.35	1.47
90	9	1972	GCP	C5-C6	-2.67	1.48	1.53
90	9	1972	GCP	C2-N1	-2.19	1.35	1.44
90	jj	700	GCP	C5-C6	-2.09	1.49	1.53
90	9	1972	GCP	PB-O2B	2.01	1.61	1.56
90	jj	700	GCP	PB-O2B	2.14	1.61	1.56
90	jj	700	GCP	PB-O3A	2.39	1.61	1.58
90	9	1972	GCP	PG-O3G	2.53	1.61	1.54
90	9	1972	GCP	PG-O2G	2.62	1.61	1.54
90	jj	700	GCP	PG-O2G	2.69	1.61	1.54
90	jj	700	GCP	PG-O3G	2.70	1.61	1.54
90	9	1972	GCP	C1'-N9	3.39	1.48	1.42
90	jj	700	GCP	C1'-N9	3.85	1.49	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C4-C5-N7	2.40	106.41	102.67
90	9	1972	GCP	C4-C5-N7	2.58	106.69	102.67
90	jj	700	GCP	C8-N9-C4	3.19	108.42	104.78
90	9	1972	GCP	C8-N9-C4	3.35	108.60	104.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
90	9	1972	GCP	28	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	44
51	9	8
47	3	2
46	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.78
1	5	1252:C	O3'	1271:G	P	35.85
1	5	1219:G	O3'	1233:G	P	22.84
1	5	1405:C	O3'	1406:G	P	22.78
1	5	3948:C	O3'	4065:G	P	19.74
1	5	1406:G	O3'	1406(A):G	P	19.63
1	5	4138:C	O3'	4146:G	P	18.06
1	5	990:C	O3'	1064:G	P	18.05
1	5	523:C	O3'	638:G	P	17.99
1	5	4101:C	O3'	4107:G	P	17.46
1	5	1406(C):G	O3'	1411:C	P	17.15
1	5	4777:C	O3'	4859:C	P	16.56
1	5	760:G	O3'	904:C	P	14.90
1	5	5022:U	O3'	5028:G	P	14.80
1	5	1696:C	O3'	1720:C	P	14.57
1	5	1364:U	O3'	1368:A	P	14.45
1	5	1411:C	O3'	1411(A):G	P	14.41
1	5	182:G	O3'	189:G	P	14.04

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	921:C	O3'	922:C	P	13.49
1	5	2901:G	O3'	3597:G	P	13.37
1	5	970:G	O3'	971:U	P	10.82
1	5	512:U	O3'	515:C	P	9.81
1	5	4729:A	O3'	4735:G	P	9.78
1	5	971:U	O3'	971(A):G	P	9.74
1	5	934:C	O3'	935:A	P	9.42
1	5	737:C	O3'	738:C	P	9.01
1	5	1180:C	O3'	1183:C	P	9.01
1	5	481:G	O3'	481(A):C	P	8.81
1	5	500:G	O3'	504:G	P	6.68
1	5	480:C	O3'	481:G	P	5.80
1	5	1100:U	O3'	1168:G	P	5.73
1	3	19:G	O3'	20:U	P	5.67
1	5	1239:C	O3'	1244:G	P	5.22
1	9	322:C	O3'	323:C	P	5.10
1	5	4740:G	O3'	4743:G	P	4.93
1	3	16:C	O3'	18:U	P	4.79
1	9	309:G	O3'	310:C	P	4.68
1	9	798:G	O3'	799:U	P	4.57
1	5	935:A	O3'	935(A):G	P	4.49
1	9	304:C	O3'	305:U	P	4.39
1	2	16:C	O3'	18:G	P	4.25
1	5	738:C	O3'	738(A):C	P	4.14
1	5	170:C	O3'	171:U	P	3.93
1	5	4899:G	O3'	4902:C	P	3.39
1	9	902:G	O3'	903:A	P	3.39
1	9	903:A	O3'	904:A	P	3.34
1	9	1295:A	O3'	1296:U	P	3.34
1	5	1438:U	O3'	1440:U	P	3.33
1	5	5020:G	O3'	5021:C	P	3.21
1	5	267:G	O3'	268:G	P	3.16
1	5	751:G	O3'	752:G	P	3.13
1	9	593:C	O3'	594:A	P	3.06
1	5	2031:C	O3'	2032:U	P	2.65
1	5	922(A):G	O3'	922(B):C	P	1.81
1	5	922:C	O3'	922(A):G	P	1.76