



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 22, 2016 – 12:30 PM EST

PDB ID : 5LZT
EMDB ID: : EMD-4131
Title : Structure of the mammalian ribosomal termination complex with eRF1 and eRF3.
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.65 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

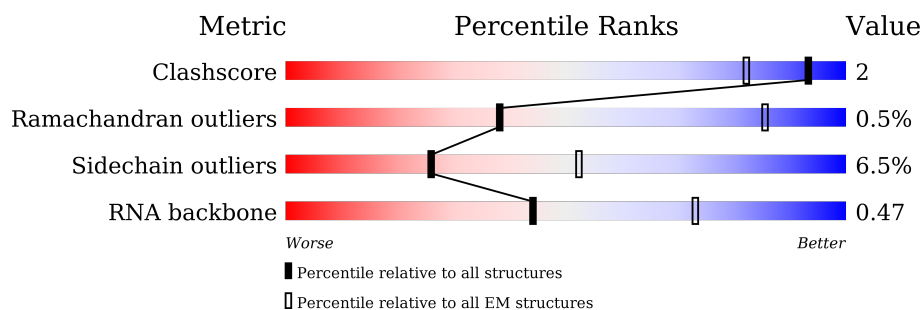
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 Å.

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




















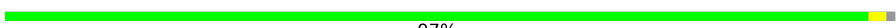







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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% 14% .
2	B	403	88% 10% .
3	C	425	78% 7% 15%
4	D	297	88% 10% .
5	E	291	66% 7% . 26%
6	F	247	81% 10% 9%
7	G	319	65% 8% . 27%
8	H	192	87% 12% .


























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Mol	Chain	Length	Quality of chain
9	I	214	 88% 7% . .
10	J	178	 86% 10% .
11	L	211	 91% 8%
12	M	218	 54% 8% . 37%
13	N	204	 92% 8%
14	O	203	 85% 12% . .
15	P	184	 76% 7% . 17%
16	Q	188	 91% 8% .
17	R	196	 83% 8% . 8%
18	S	176	 85% 14% .
19	T	160	 91% 8% .
20	U	128	 73% . 23%
21	V	140	 80% 13% . 6%
22	W	157	 65% . . 32%
23	X	156	 71% 5% 24%
24	Y	145	 86% 6% 8%
25	Z	136	 92% 7% .
26	a	148	 97% . .
27	b	245	 41% . 58%
28	c	115	 83% . 15%
29	d	125	 79% 6% 14%
30	e	135	 88% 7% 5%
31	f	110	 92% 7% .
32	g	117	 93% . .
33	h	123	 94% 5% .




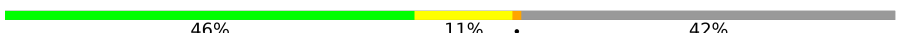



















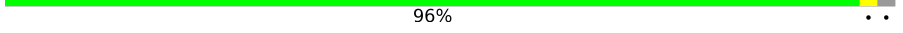

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Mol	Chain	Length	Quality of chain
34	i	105	95% 
35	j	97	84%  5% 11%
36	k	70	96% 
37	l	51	96% 
38	m	102	48%  49%
39	n	25	92% 
40	o	106	92%  6%
41	p	92	97% 
42	r	137	85%  5% 9%
43	s	318	59%  38%
44	t	165	88%  7%
45	1	15	87% 
46	2	76	78%  20%
47	3	75	68%  29%
48	5	3543	71%  26%
49	7	120	86%  13%
50	8	156	73%  21%
51	9	1869	63%  26% 9%
52	AA	295	66%  7% 26%
53	BB	264	67%  13% 19%
54	CC	293	66%  9% 25%
55	DD	243	82%  11% 6%
56	EE	263	85% 
57	FF	204	76%  13% 9%
58	GG	249	85%  9% 5%

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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	<div><div></div><div>95%</div><div></div><div>.</div><div>.</div></div>
85	hh	15	<div><div></div><div>47%</div><div></div><div>53%</div></div>
86	ii	459	<div><div></div><div>85%</div><div></div><div>6%</div><div>9%</div></div>
87	jj	637	<div><div></div><div>64%</div><div>.</div><div></div><div>33%</div></div>

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 222683 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	GLN	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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	117	LYS	-	insertion	UNP G1U945

- 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 (UGA stop codon).

Mol	Chain	Residues	Atoms					AltConf	Trace
85	hh	15	Total	C	N	O	P	0	0
			317	142	54	106	15		

- Molecule 86 is a protein called eRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	419	Total	C	N	O	S	0	0
			3307	2104	562	629	12		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	-21	MET	-	initiating methionine	UNP P62495
ii	-20	ARG	-	expression tag	UNP P62495
ii	-19	GLY	-	expression tag	UNP P62495
ii	-18	SER	-	expression tag	UNP P62495
ii	-17	HIS	-	expression tag	UNP P62495
ii	-16	HIS	-	expression tag	UNP P62495
ii	-15	HIS	-	expression tag	UNP P62495
ii	-14	HIS	-	expression tag	UNP P62495
ii	-13	HIS	-	expression tag	UNP P62495
ii	-12	HIS	-	expression tag	UNP P62495
ii	-11	GLY	-	expression tag	UNP P62495
ii	-10	MET	-	expression tag	UNP P62495
ii	-9	ALA	-	expression tag	UNP P62495
ii	-8	SER	-	expression tag	UNP P62495
ii	-7	GLU	-	expression tag	UNP P62495
ii	-6	ASN	-	expression tag	UNP P62495
ii	-5	LEU	-	expression tag	UNP P62495
ii	-4	TYR	-	expression tag	UNP P62495
ii	-3	PHE	-	expression tag	UNP P62495

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Chain	Residue	Modelled	Actual	Comment	Reference
ii	-2	GLN	-	expression tag	UNP P62495
ii	-1	GLY	-	expression tag	UNP P62495
ii	0	SER	-	expression tag	UNP P62495

- Molecule 87 is a protein called eRF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	428	Total	C	N	O	S	0	0
			3368	2144	580	623	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
jj	100	ALA	VAL	conflict	UNP P15170

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

Mol	Chain	Residues	Atoms		AltConf
88	P	3	Total	Mg	0
			3	3	
88	g	1	Total	Mg	0
			1	1	
88	j	1	Total	Mg	0
			1	1	
88	Q	1	Total	Mg	0
			1	1	
88	a	1	Total	Mg	0
			1	1	
88	jj	1	Total	Mg	0
			1	1	
88	B	1	Total	Mg	0
			1	1	
88	I	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	
88	7	5	Total	Mg	0
			5	5	
88	A	1	Total	Mg	0
			1	1	
88	5	185	Total	Mg	0
			185	185	

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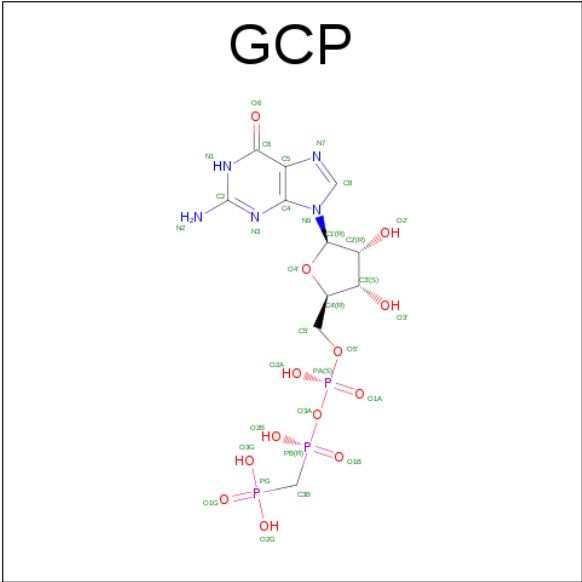
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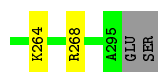
Mol	Chain	Residues	Atoms		AltConf
88	8	8	Total 8	Mg 8	0
88	9	71	Total 71	Mg 71	0
88	hh	1	Total 1	Mg 1	0

- 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

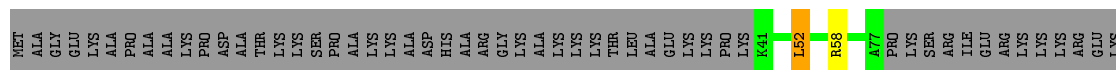
- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



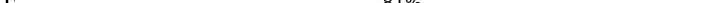


- Molecule 5: eL6

Chain E:  66% 7% 26%



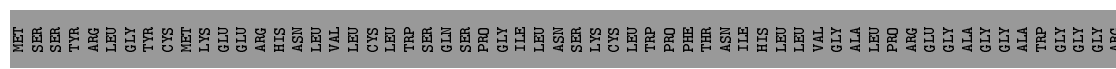
- Molecule 6: uL30

Chain F:  81% 10% 9%

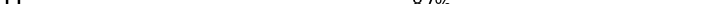


- Molecule 7: eL8

Chain G: 65% 8% 27%

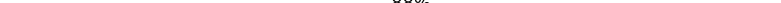


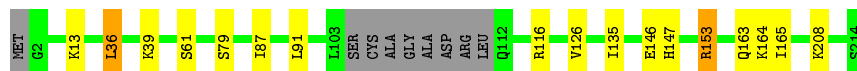
- Molecule 8: uL6

Chain H:  87% 12%

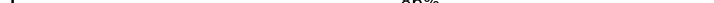


- Molecule 9: uL16

Chain I:  88% 7% ..



- Molecule 10: uL5

Chain J:  86% 10% .



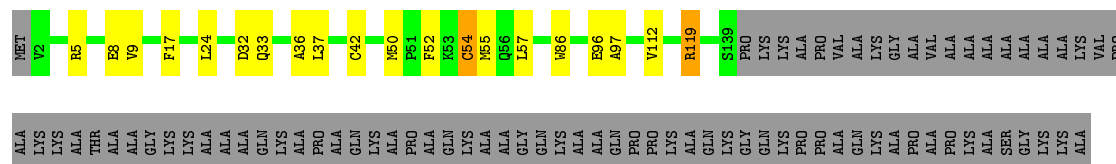
- Molecule 11: eL13

Chain L:  91% 8%



- Molecule 12: eL14

Chain M: 54% 8% 37%



- Molecule 13: eL15

Chain N:  92% 8%



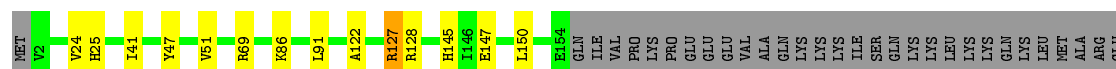
- Molecule 14: uL13

Chain 0:  85% 12% 3%



- Molecule 15: uL22

Chain P: 76% 7% 17%




- Molecule 16: eL18

Chain Q: 91% 8%




- Molecule 17: eL19

Chain R:  83% 8% 8%



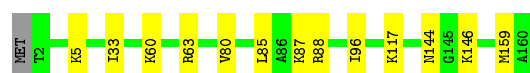
- Molecule 18: eL20

Chain S:  85% 14%



- Molecule 19: eL21

Chain T:  91% 8%




- Molecule 20: eL22

Chain U:  73% 23%



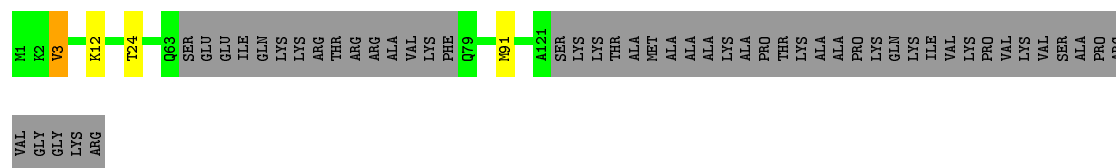
- Molecule 21: uL14

Chain V:  80% 13% 6%



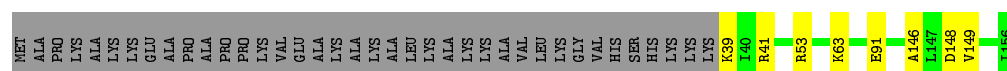
- Molecule 22: eL24

Chain W:  65% 32%




- Molecule 23: uL23

Chain X:  71% 5% 24%



- Molecule 24: uL24

Chain Y:  86% 6% 8%



- Molecule 25: eL27

Chain Z: 92% 7%



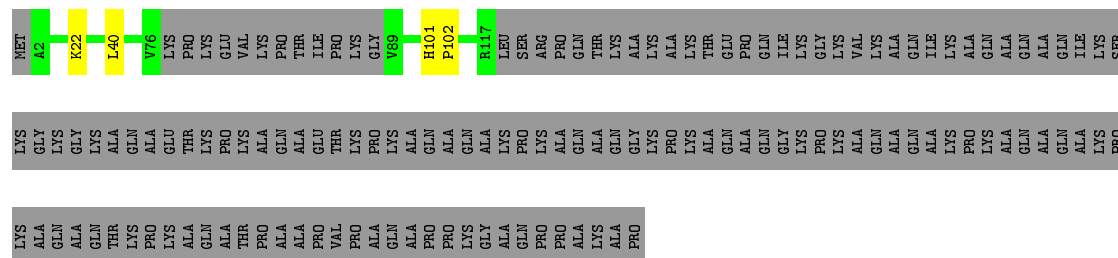
- Molecule 26: uL15

Chain a: 97%



- Molecule 27: eL29

Chain b: 41% 1% 58%



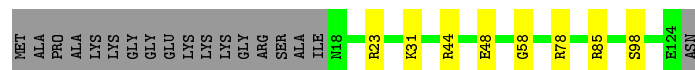
- Molecule 28: eL30

Chain c: 83% • 15%




- Molecule 29: eL31

Chain d: 79% 6% 14%




- Molecule 30: eL32

Chain e:  88% 7% 5%



- Molecule 31: eL33

Chain f:  92% 7%



- Molecule 32: eL34

Chain g:  93%



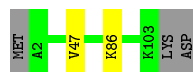
- Molecule 33: uL29

Chain h:  94% 5%




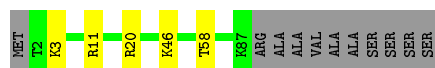
- Molecule 34: eL36

Chain i:  95%



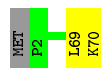
- Molecule 35: eL37

Chain j:  84% 5% 11%



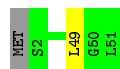
- Molecule 36: eL38

Chain k:  96%



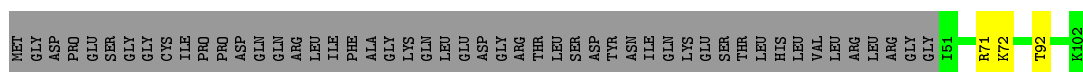
- Molecule 37: eL39

Chain l:  96%



- Molecule 38: eL40

Chain m:  48% 49%



- Molecule 39: eL41



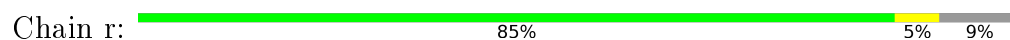
- Molecule 40: eL42



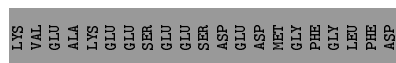
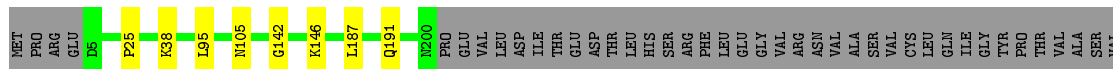
- Molecule 41: eL43



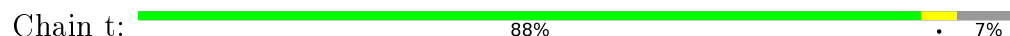
- Molecule 42: eL28



- Molecule 43: uL10



- Molecule 44: uL11



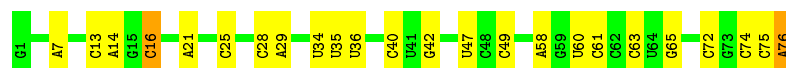
- Molecule 45: Nascent chain



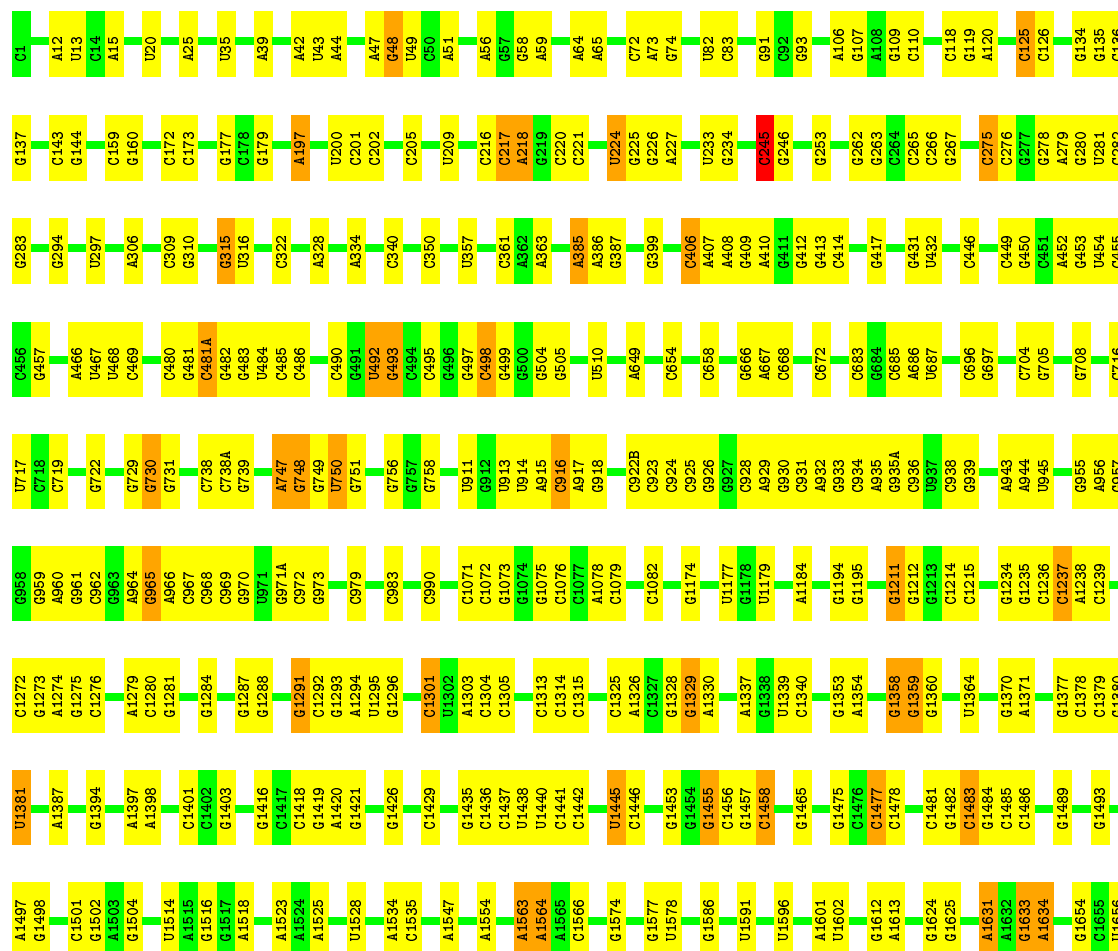
- Molecule 46: P-site tRNA



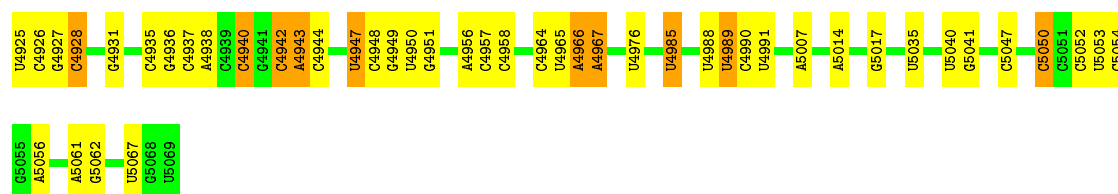
- Molecule 47: E-site tRNA



- Molecule 48: 28S ribosomal RNA



C4736	G4570	U4430	G3889	G3753	G2897	G2743	A2601	C2458	A2279	G2046	A1941	A1805	C1661
G4737	A4571	C4421	U3892	A3756	C3598	A2743	A2618	G2459	G2288	A2047	A1945	G1811	G1670
G4745	U4572	A4422	G3897	A3759	A3599	A2744	G2619	U2467	C2289	U2048	G1946	C1812	
	G4573	U4423	A3760	A3760	A3604	A2755	G2620	U2468	A2300	G2052	U1947	G1815	C1676
G4751	U4574	G4440	A3901	G3765	C3605	A2760	A2623	C2469	G2301	G2055	G1948	C1677	C1679
U4752	C4444	C4444	G3904	A3766	G3615	U2761	C2627	G2470	A2313	A2057	G1951	G1818	
U4753	G4448	G4448	A3905	U3773	U3616	G2763	C2627	G2471	G2314	G2062	G1952	G1819	C1678
G4754	U4449	A4449	A3906	U3774	G3617	A2764	G2638	G2474	G2342	C2063	G1959	U1820	C1679
C4756	U4450	G4450	G3907	A3775	G3620	A2769	U2639	G2475	G2322	G2064	A1960	U1822	G1691
C4757	U4585	C4453	U3914	G3776	G3625	U2769	G2640	G2479	G2331		G1961	G1823	G1724
U4758	G4586	G4457	U3915	G3777	G3626	C2772	A2647	G2483	A2332	C2068	A1962	C1828	U1726
C4759	U4590	U4457	G3916	U3778	G3626	C2772	A2647	U2484	A2333	A2069	C1963	G1833	G1733
G4760	G4618	U4459	A3917	A3783	A3635	A2787	U2661	G2485	C2340	U2070	A1964	U1834	G1734
G4761	U4460	U4460	C3919	A3784	U3644	U2788	G2662	U2486	G2340	U2084	C1965	G1835	U1735
G4765				A3785	U3644	U2789	G2663	C2488		G2085	A1967	G1836	
				U3786		U2790		C2489	G2348			A1837	C1740
C4771	U4627	U4464	U3927	U3798	A3653	C2794	C2669	U2489	C2351	A2088	G1976	G1741	G1742
C4772	U4636	A4467	A3928	A3799	A3656	A2795	C2670	U2490	G2357	C2089	C1977	G1842	
U4868	U4637	U4471	G3929	A3800		G2796	G2673	C2492	G2364	C2091	A1978	G1855	U1748
G4639	G4639		G3939	A3800	A3662	C2797	U2676	U2495		G2092	U1979	G1856	A1749
			A3943	G3809	G3671	A2798		U2495	A2367	G2093	U1980	A1867	G1750
G4475	U4218	U4067	U4067	G3810	G3672	A2806	G2681	A2502		C2094	G1981	A1868	
G4476	A4219	U4068	U4068	G3811	C3673	A2807	G2686	G2503	G2370	A2095	G1982	G1753	G1754
U4477	A4220	U4069	U4069	G3812	G3674	G2808	G2687	G2504	A2370	A1984	A1983	U1755	C1755
A4478	C4221	U4070	U4070	A3813		G2808	U2687	C2505	A2395	A2097	G1985	U1881	C1756
A4479	U4225	U4071	U4071	U3814	U3690	C2814	C2688	G2506	A2396	G2098	U1986	U1882	U1757
U4488	G4225	U4072	U4072	U3815	G3691		C2689		G2397	G2099	C1987	G1883	
G4489	U4229	U4073	U4073	A3817	A3692	U2826	G2693	A2513	U2398	G2100	A1990	A1888	G1761
G4495	U4232	G4076	G4076	U3818	G3696	G2827	G2694	G2521	A2101	G2102	A1991	C1762	C1763
U4500	A4233	G4084	G4084	G3819	U3696	U2828	A2695	U2530	A2103	A2103	U1992	C1893	G1764
A4510	G4237	A4085	A4085	U3822	U3696	U2829	A2696	U2537	G2402	A2104	C1993	C1894	C1768
U4511	G4249	G4086	G4086	U3831	G3710	G2835	U2707	A2537	U2408	A2105	U1997	G1895	
A4512	G4250	G4087	G4087	U3831	A3711	U2837	U2708	U2544	U2409	A2107	A1896	A1896	C1772
A4513	A4251	C4088	C4088	U3838	A3712	G2838	C2709	G2546	G2416	G2108	G2001	A1897	U1773
				G3838		U2839	C2710	G2547	A2417	A2109	G2002	A1907	
C4519	G4254	G4099	G4099	G3839	G3722	G2842	G2711	U2554	C2422	G2110	G2003	A1907	A1776
G4520	A4255	C4100	C4100	U3840	A3723	G2842	G2712	G2555	G2359	G2259	G2004	G1910	
	A4256	C4116	C4116	U3851	A3724	G2845	C2713	G2556	C2423	G2260	U2008	G1910	A1780
U4524	A4257	U4117	U4117	U3851	A3725	A2845	G2714	G2564	G2424	G2261	U2008	U1918	U1781
G4527	C4258	U4118	U4118	G3859	G3725	A2845	G2715	A2565	U2425	G2262	C2011	G1919	U1782
G4528	U4260	C4119	C4119	U3859	U3729	G2855	G2716	G2566		G2262	C2011	C1920	C1783
	C4261	U4120	U4120	A3867					A2428	G2265		C1921	
U4531	U4265	G4121	G4121	A3873	A3733	A2864	C2719	G2566	A2429	C2266	G2024	G1922	A1787
	A4266	C4122	C4122	G3873	G3740	G2875	C2720	C2571		U2267	A2025	A1923	
U4548	G4267	G4124	G4124	A3876	G3740	G2875	G2721	U2575	G2433	A2268	A2026	G1797	G1798
G4549	A4268	C4125	C4125	A3877	A3747	G2884	A2725	G2583	G2439	C2269	C2031	U1930	G1798
	A4271	A4127	A4127	C3878	A3748	G2891	G2726	C2586	U2440	G2270	U2032	C1931	G1799
C4560	G4272			G3879	C3749	U2891	G2726	C2586	G2441	G2275	U2044	A1932	U1800
G4567	A4273	G4150	G4150	G3888	G3750	G2896	U2740	G2586		G2278	U2044	G1933	G1803
							U2741	A2587	G2450			A1934	A1804



• Molecule 49: 5S ribosomal RNA

Chain 7: 86% 13%



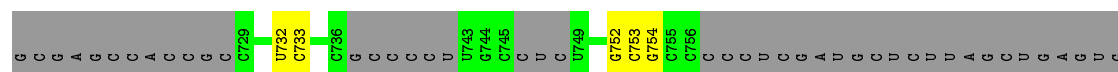
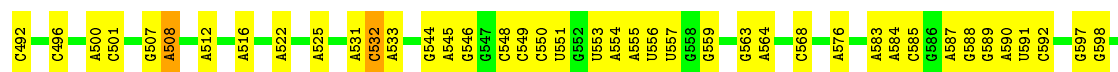
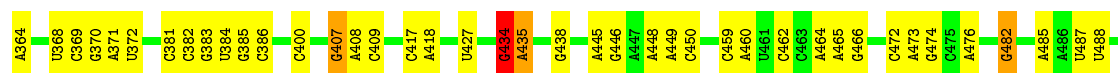
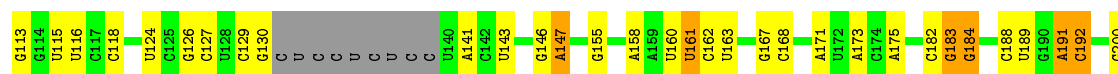
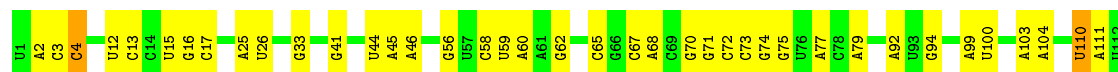
• Molecule 50: 5.8S ribosomal RNA

Chain 8: 73% 21%



• Molecule 51: 18S ribosomal RNA

Chain 9: 63% 26% 9%





- Molecule 59: eS7

Chain HH: 85% 11% 5%




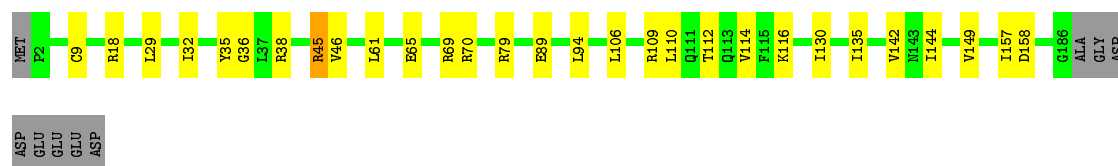
- Molecule 60: eS8

Chain II: 88% 10% ..



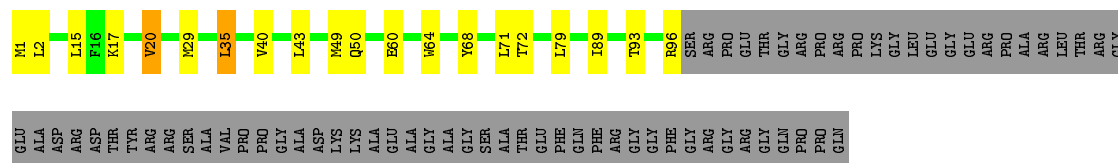
- Molecule 61: uS4

Chain JJ:  80% 14% 5%




- Molecule 62: eS10

Chain KK:  46% 11% . 42%

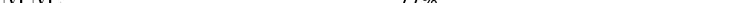


- Molecule 63: uS17

Chain LL:  80% 10% 9%

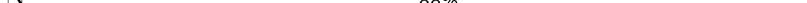


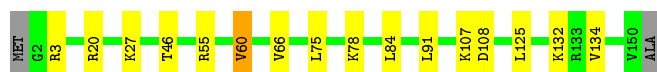
- Molecule 64: eS12

Chain MM:  77% 11% • 11%

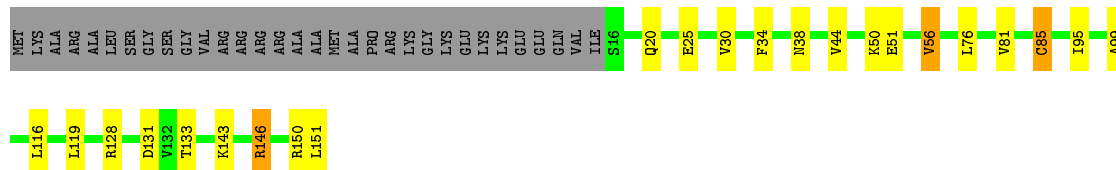


- Molecule 65: uS15

Chain NN:  88% 10% ..



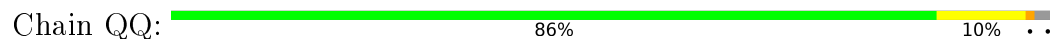
- Molecule 66: uS11



- Molecule 67: uS19



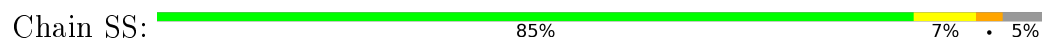
- Molecule 68: uS9



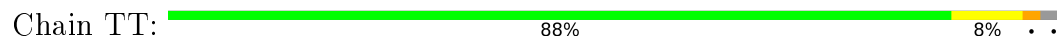
- Molecule 69: eS17



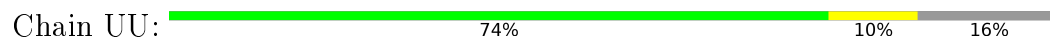
- Molecule 70: uS13



- Molecule 71: eS19



- Molecule 72: uS10





- Molecule 73: eS21

Chain VV: 88% 11% .



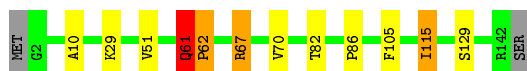
- Molecule 74: uS8

Chain WW: 81% 18% .



- Molecule 75: uS12

Chain XX: 90% 6% ...



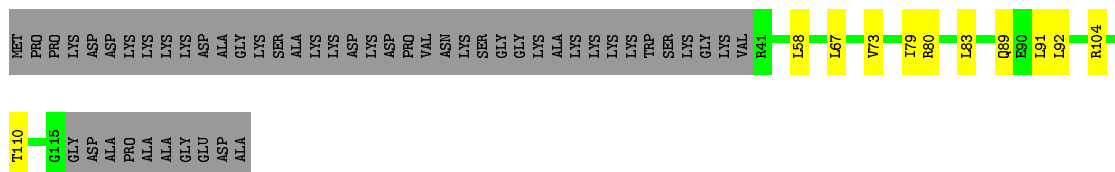
- Molecule 76: eS24

Chain YY: 82% 14% 5%



- Molecule 77: eS25

Chain ZZ: 51% 9% 40%



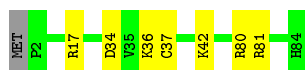
- Molecule 78: eS26

Chain aa: 81% 6% 12%



- Molecule 79: eS27

Chain bb: 90% 8% .



- Molecule 80: eS28

Chain cc: 83% 7% 10%



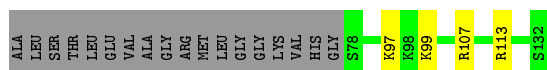
- Molecule 81: uS14

Chain dd: 96% ..



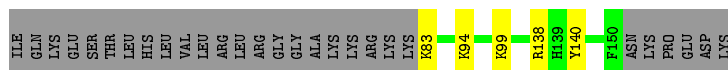
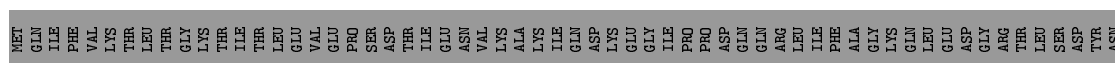
- Molecule 82: eS30

Chain ee: 38% . 59%



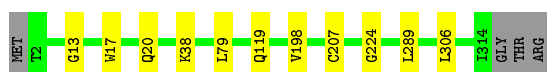
- Molecule 83: eS31

Chain ff: 40% . 56%



- Molecule 84: RACK1

Chain gg: 95% ..



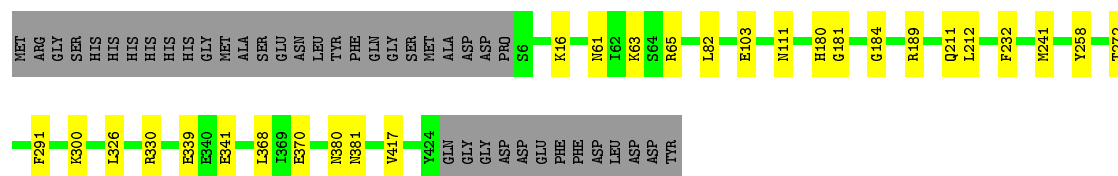
- Molecule 85: mRNA (UGA stop codon)

Chain hh: 47% 53%



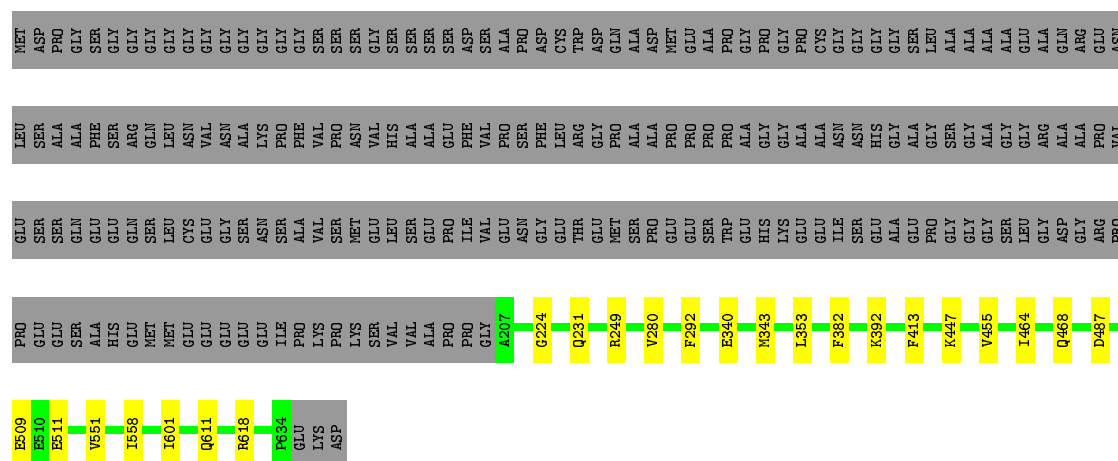
- Molecule 86: eRF1

Chain ii:



- Molecule 87: eRF3a

Chain jj:



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	61752	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	0.34	0/1936	0.69	0/2596
10	J	0.33	0/1385	0.61	0/1852
11	L	0.34	0/1733	0.67	0/2316
12	M	0.35	0/1158	0.65	0/1547
13	N	0.35	0/1746	0.67	0/2338
14	O	0.34	0/1662	0.66	0/2222
15	P	0.36	0/1268	0.64	0/1700
16	Q	0.35	0/1539	0.72	0/2054
17	R	0.34	0/1524	0.67	0/2013
18	S	0.37	0/1501	0.68	0/2012
19	T	0.33	0/1326	0.60	0/1770
2	B	0.33	0/3240	0.64	0/4339
20	U	0.35	0/823	0.55	0/1104
21	V	0.34	0/993	0.62	0/1332
22	W	0.34	0/873	0.56	0/1158
23	X	0.33	0/984	0.60	0/1323
24	Y	0.33	0/1132	0.62	0/1504
25	Z	0.34	0/1130	0.61	0/1507
26	a	0.32	0/1191	0.61	0/1590
27	b	0.34	0/861	0.58	0/1138
28	c	0.32	0/771	0.54	0/1034
29	d	0.34	0/903	0.66	0/1216
3	C	0.33	0/2937	0.66	0/3946
30	e	0.34	0/1071	0.66	0/1429
31	f	0.36	0/895	0.69	0/1198
32	g	0.33	0/916	0.67	0/1220
33	h	0.32	0/1021	0.61	0/1348
34	i	0.34	0/841	0.60	0/1112
35	j	0.36	0/720	0.72	0/952
36	k	0.32	0/575	0.55	0/761
37	l	0.35	0/459	0.63	0/608
38	m	0.34	0/435	0.61	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	n	0.34	0/240	0.67	0/305
4	D	0.34	0/2437	0.61	3/3264 (0.1%)
40	o	0.34	0/864	0.61	0/1140
41	p	0.32	0/718	0.62	0/953
42	r	0.35	0/1010	0.69	0/1354
43	s	0.36	0/1530	0.50	0/2064
44	t	0.36	0/1174	0.52	0/1582
45	1	0.41	0/129	0.61	0/173
46	2	0.22	0/1805	0.67	0/2809
47	3	0.21	0/1777	0.66	0/2763
48	5	0.27	0/84973	0.68	22/132508 (0.0%)
49	7	0.26	0/2858	0.67	0/4455
5	E	0.33	0/1762	0.63	0/2362
50	8	0.28	0/3581	0.67	0/5577
51	9	0.25	0/40524	0.69	10/63134 (0.0%)
52	AA	0.33	0/1747	0.60	0/2374
53	BB	0.33	0/1756	0.63	0/2350
54	CC	0.34	0/1753	0.62	0/2369
55	DD	0.35	0/1796	0.61	0/2417
56	EE	0.34	0/2118	0.64	0/2849
57	FF	0.33	0/1492	0.61	0/2005
58	GG	0.35	0/1946	0.67	0/2590
59	HH	0.35	0/1510	0.59	0/2022
6	F	0.36	0/1911	0.66	1/2549 (0.0%)
60	II	0.34	0/1715	0.63	0/2287
61	JJ	0.33	0/1550	0.68	0/2069
62	KK	0.34	0/834	0.59	0/1125
63	LL	0.35	0/1195	0.66	0/1597
64	MM	0.36	0/918	0.61	0/1233
65	NN	0.33	0/1226	0.62	0/1649
66	OO	0.34	0/1029	0.78	1/1380 (0.1%)
67	PP	0.34	0/1017	0.64	0/1358
68	QQ	0.32	0/1146	0.61	0/1534
69	RR	0.33	0/1082	0.60	0/1452
7	G	0.33	0/1910	0.62	0/2569
70	SS	0.34	0/1208	0.68	0/1618
71	TT	0.36	0/1115	0.63	1/1493 (0.1%)
72	UU	0.34	0/805	0.65	0/1081
73	VV	0.36	0/643	0.67	0/860
74	WW	0.34	0/1051	0.69	0/1406
75	XX	0.32	0/1116	0.64	0/1490
76	YY	0.35	0/1028	0.61	0/1366
77	ZZ	0.33	0/604	0.59	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	aa	0.35	0/828	0.74	0/1109
79	bb	0.33	0/665	0.59	0/891
8	H	0.31	0/1535	0.60	0/2063
80	cc	0.33	0/490	0.65	0/656
81	dd	0.37	0/470	0.62	0/623
82	ee	0.35	0/447	0.70	0/587
83	ff	0.36	0/567	0.56	0/753
84	gg	0.32	0/2493	0.55	0/3394
85	hh	0.31	0/353	0.77	0/547
86	ii	0.35	0/3361	0.54	0/4519
87	jj	0.35	0/3435	0.55	0/4633
9	I	0.33	0/1702	0.60	0/2272
All	All	0.30	0/238498	0.66	38/349206 (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	1
74	WW	0	1
75	XX	0	1
All	All	0	3

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1835	A	C2'-C3'-O3'	8.60	128.43	109.50
4	D	22	ARG	NE-CZ-NH1	8.45	124.52	120.30
51	9	1394	G	C2'-C3'-O3'	7.70	126.44	109.50
48	5	406	C	C2'-C3'-O3'	7.30	125.56	109.50
48	5	1477	C	C2'-C3'-O3'	6.95	124.81	113.70
48	5	3888	G	C2'-C3'-O3'	6.93	124.79	113.70
48	5	1211	G	C2'-C3'-O3'	6.79	124.57	113.70
48	5	275	C	C2'-C3'-O3'	6.74	124.49	113.70
66	OO	146	ARG	NE-CZ-NH1	6.70	123.65	120.30
51	9	1646	C	C2'-C3'-O3'	6.28	123.75	113.70
48	5	3697	U	C2'-C3'-O3'	6.24	123.67	113.70
48	5	1818	G	C2'-C3'-O3'	6.11	123.47	113.70
48	5	2046	G	C2'-C3'-O3'	6.08	123.43	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	2695	A	C2'-C3'-O3'	6.02	123.34	113.70
48	5	1834	U	C2'-C3'-O3'	6.00	123.29	113.70
48	5	1455	G	C2'-C3'-O3'	5.97	123.26	113.70
51	9	874	G	C2'-C3'-O3'	5.97	123.26	113.70
51	9	434	G	C2'-C3'-O3'	5.91	123.16	113.70
48	5	1291	G	C2'-C3'-O3'	5.77	122.93	113.70
48	5	4947	U	C2'-C3'-O3'	5.65	122.75	113.70
48	5	245	C	C2'-C3'-O3'	5.62	122.69	113.70
48	5	1329	G	C2'-C3'-O3'	5.57	122.60	113.70
51	9	110	U	C2'-C3'-O3'	5.56	122.59	113.70
6	F	88	LEU	CA-CB-CG	5.53	128.02	115.30
48	5	48	G	C2'-C3'-O3'	5.53	122.54	113.70
48	5	2068	C	C4'-C3'-O3'	5.50	124.01	113.00
48	5	4448	G	C4'-C3'-O3'	5.48	123.97	113.00
4	D	22	ARG	CG-CD-NE	5.44	123.22	111.80
48	5	385	A	C4'-C3'-O3'	5.34	123.68	113.00
51	9	1863	A	N9-C1'-C2'	5.23	120.81	114.00
51	9	532	C	C2'-C3'-O3'	5.21	122.04	113.70
48	5	125	C	C2'-C3'-O3'	5.18	122.00	113.70
48	5	1445	U	C2'-C3'-O3'	5.18	121.99	113.70
71	TT	110	LEU	CA-CB-CG	5.13	127.10	115.30
48	5	4884	G	C2'-C3'-O3'	5.09	121.84	113.70
51	9	1060	A	N9-C1'-C2'	5.08	120.61	114.00
4	D	22	ARG	NE-CZ-NH2	-5.02	117.79	120.30
51	9	1664	A	C4'-C3'-O3'	5.00	123.01	113.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	PHE	Peptide
74	WW	27	ILE	Peptide
75	XX	61	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	17	0
2	B	3172	0	3310	17	0
3	C	2883	0	3053	7	0
4	D	2391	0	2424	13	0
5	E	1729	0	1887	10	0
6	F	1875	0	1995	10	0
7	G	1879	0	2027	10	0
8	H	1516	0	1597	8	0
9	I	1664	0	1712	5	0
10	J	1362	0	1399	7	0
11	L	1702	0	1820	6	0
12	M	1137	0	1211	9	0
13	N	1701	0	1749	4	0
14	O	1630	0	1778	14	0
15	P	1242	0	1274	4	0
16	Q	1515	0	1634	5	0
17	R	1508	0	1664	5	0
18	S	1462	0	1508	12	0
19	T	1298	0	1366	4	0
20	U	809	0	833	1	0
21	V	979	0	1039	7	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	4	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	999	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
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	758	0	0
42	r	994	0	1051	0	0
43	s	1507	0	1564	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	t	1160	0	1218	0	0
45	1	125	0	117	1	0
46	2	1616	0	824	5	0
47	3	1593	0	811	3	0
48	5	75972	0	38393	128	0
49	7	2558	0	1296	2	0
50	8	3208	0	1629	6	0
51	9	36249	0	18316	98	0
52	AA	1710	0	1708	10	0
53	BB	1729	0	1803	11	0
54	CC	1716	0	1806	10	0
55	DD	1768	0	1866	9	0
56	EE	2076	0	2177	9	0
57	FF	1471	0	1522	11	0
58	GG	1923	0	2089	9	0
59	HH	1488	0	1582	4	0
60	II	1686	0	1772	6	0
61	JJ	1525	0	1640	12	0
62	KK	810	0	836	8	0
63	LL	1175	0	1249	4	0
64	MM	908	0	939	5	0
65	NN	1202	0	1289	2	0
66	OO	1016	0	1039	5	0
67	PP	997	0	1045	5	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	5	0
70	SS	1190	0	1249	3	0
71	TT	1097	0	1132	4	0
72	UU	795	0	862	3	0
73	VV	636	0	637	5	0
74	WW	1034	0	1080	8	0
75	XX	1098	0	1167	4	0
76	YY	1011	0	1083	1	0
77	ZZ	598	0	656	6	0
78	aa	814	0	864	0	0
79	bb	651	0	672	0	0
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	566	0	0
84	gg	2436	0	2393	0	0
85	hh	317	0	161	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	ii	3307	0	3346	0	0
87	jj	3368	0	3422	0	0
88	5	185	0	0	0	0
88	7	5	0	0	0	0
88	8	8	0	0	0	0
88	9	71	0	0	0	0
88	A	1	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	P	3	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	g	1	0	0	0	0
88	hh	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	jj	32	0	14	0	0
All	All	222683	0	167519	523	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 2.

All (523) 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)
48:5:2367:A:N1	48:5:2788:U:O4	1.66	1.25
51:9:1137:U:O4	51:9:1148:A:N1	1.68	1.23
51:9:1137:U:C4	51:9:1148:A:N1	2.11	1.18
51:9:1137:U:O4	51:9:1148:A:C2	2.17	0.98
51:9:1137:U:O4	51:9:1148:A:C6	2.32	0.82
48:5:2367:A:N1	48:5:2788:U:C4	2.49	0.81
57:FF:99:ILE:HG23	77:ZZ:67:LEU:HD21	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2367:A:N6	48:5:2788:U:N3	2.32	0.77
51:9:1137:U:C4	51:9:1148:A:C6	2.75	0.74
48:5:4579:U:H2'	48:5:4580:U:C6	2.23	0.72
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.71	0.72
48:5:3914:U:H3	48:5:4378:A:N6	1.87	0.71
62:KK:35:LEU:HD13	62:KK:40:VAL:HG21	1.72	0.70
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.90	0.69
48:5:3914:U:N3	48:5:4378:A:N6	2.40	0.69
48:5:4723:A:H2'	48:5:4724:A:C8	2.28	0.68
53:BB:66:VAL:HG22	53:BB:87:ILE:HG22	1.76	0.68
51:9:1407:U:H2'	51:9:1408:U:C6	2.29	0.68
67:PP:56:LEU:HD13	67:PP:78:THR:HG21	1.76	0.66
48:5:2031:C:O3'	48:5:2032:U:P	2.55	0.65
17:R:98:ARG:NH2	48:5:2262:G:OP2	170.93	0.65
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.79	0.65
51:9:1137:U:N3	51:9:1148:A:N6	2.45	0.64
1:A:126:LEU:HD13	1:A:150:LEU:HD21	1.79	0.64
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.80	0.63
48:5:747:A:H4'	48:5:748:G:OP1	1.97	0.63
60:II:36:THR:HG21	60:II:179:PRO:HB2	1.80	0.63
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.80	0.62
18:S:84:TYR:CE1	18:S:93:MET:HE2	2.34	0.62
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.33	0.62
55:DD:72:VAL:HG23	62:KK:20:VAL:HG21	1.82	0.62
51:9:1438:A:H2'	51:9:1439:A:C8	2.35	0.62
18:S:95:ARG:NH2	48:5:1951:G:O2'	2.33	0.62
53:BB:69:VAL:HG11	53:BB:74:LEU:HD13	1.80	0.61
14:O:72:HIS:N	48:5:4586:G:OP1	2.28	0.61
52:AA:33:GLN:HB3	52:AA:154:LEU:HD12	1.83	0.60
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.35	0.60
74:WW:75:ILE:HD11	74:WW:93:LEU:HD11	1.83	0.60
15:P:41:ILE:HD12	15:P:150:LEU:HD13	1.83	0.60
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.65	0.60
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.82	0.60
64:MM:33:ARG:NH2	64:MM:91:LEU:HD21	2.16	0.60
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.35	0.59
51:9:1130:G:N3	51:9:1130:G:H2'	2.17	0.59
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.85	0.59
48:5:217:C:O2'	48:5:218:A:OP2	2.12	0.59
1:A:199:VAL:HG21	48:5:1631:A:C8	2.38	0.59
14:O:160:ARG:NH2	48:5:4760:G:OP1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.85	0.58
64:MM:22:LEU:HD21	64:MM:89:VAL:HG23	1.86	0.58
51:9:980:A:H2'	51:9:981:A:C8	2.39	0.57
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.38	0.57
48:5:4942:C:H4'	48:5:4943:A:OP1	2.05	0.57
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.37	0.57
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.35	0.57
46:2:16:C:O4'	46:2:16:C:O2	2.24	0.56
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.56
64:MM:22:LEU:HD11	64:MM:89:VAL:HA	1.87	0.56
48:5:2395:A:O2'	48:5:2806:A:H1'	2.05	0.56
48:5:4510:A:O2'	48:5:4511:A:O4'	2.24	0.56
62:KK:15:LEU:HD22	62:KK:49:MET:HE1	1.87	0.56
48:5:3766:A:N1	51:9:1827:U:O2'	2.28	0.55
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.88	0.55
51:9:183:G:O2'	51:9:184:G:O5'	2.24	0.55
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.37	0.55
62:KK:15:LEU:HD22	62:KK:49:MET:CE	2.36	0.55
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	1.89	0.55
19:T:80:VAL:CG2	19:T:85:LEU:HD12	2.36	0.55
52:AA:60:LEU:HD13	52:AA:159:ILE:HD11	1.89	0.55
14:O:18:ARG:NH2	48:5:2057:A:OP1	2.38	0.55
2:B:174:ARG:NH1	48:5:4985:U:O2	2.40	0.55
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.88	0.55
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.89	0.55
5:E:159:ARG:NH1	48:5:4940:C:OP1	2.39	0.54
51:9:1274:G:N7	62:KK:43:LEU:HD13	2.22	0.54
3:C:130:ALA:HB3	3:C:246:VAL:HG12	1.89	0.54
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.41	0.54
51:9:945:U:H2'	51:9:946:U:C6	2.42	0.54
54:CC:176:LYS:O	54:CC:200:ARG:NH1	2.40	0.54
51:9:501:C:O2	51:9:501:C:H2'	2.06	0.54
48:5:245:C:O4'	48:5:245:C:O2	2.24	0.54
48:5:2505:C:O4'	48:5:2505:C:O2	2.24	0.54
8:H:88:PHE:CE1	8:H:151:ILE:HD12	2.43	0.54
51:9:1139:C:O4'	51:9:1139:C:O2	2.21	0.54
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.90	0.54
48:5:1483:C:O2	48:5:1483:C:O4'	2.23	0.53
51:9:1117:C:O2'	51:9:1118:C:O4'	2.27	0.53
51:9:434:G:H2'	51:9:435:A:C8	2.43	0.53
51:9:1315:U:O2	51:9:1315:U:O4'	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:165:VAL:HG11	5:E:178:VAL:HG13	1.89	0.53
57:FF:39:ILE:HG23	57:FF:68:ILE:HD13	1.89	0.53
48:5:3723:A:H2'	48:5:3724:A:C8	2.42	0.53
48:5:4989:U:O4'	48:5:4989:U:O2	2.27	0.53
6:F:88:LEU:HD22	6:F:89:ALA:N	2.23	0.53
62:KK:35:LEU:CD1	62:KK:40:VAL:HG21	2.37	0.53
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.90	0.53
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.90	0.53
18:S:3:ALA:O	18:S:111:ARG:NH1	2.41	0.53
21:V:82:ILE:HD12	21:V:104:VAL:HG13	1.90	0.53
25:Z:11:VAL:HG11	25:Z:80:LEU:HD22	1.91	0.53
74:WW:3:ARG:HD3	74:WW:6:VAL:HG22	1.91	0.53
5:E:165:VAL:HG13	5:E:180:GLY:N	2.24	0.53
71:TT:104:LEU:HD22	71:TT:121:ARG:HG2	1.90	0.53
48:5:3810:C:O4'	48:5:3810:C:O2	2.26	0.52
24:Y:49:ILE:HD13	24:Y:80:ILE:HD13	1.91	0.52
58:GG:18:VAL:HG21	58:GG:41:LEU:HD23	1.90	0.52
8:H:12:ILE:HG22	8:H:81:ILE:HD11	1.90	0.52
58:GG:63:MET:N	58:GG:63:MET:SD	2.83	0.52
48:5:498:C:O2	48:5:498:C:O4'	2.28	0.52
5:E:281:THR:OG1	48:5:4754:G:N7	2.42	0.52
51:9:4:C:O2'	61:JJ:18:ARG:NH1	2.42	0.52
51:9:1489:A:H4'	51:9:1490:G:OP2	2.10	0.51
48:5:224:U:O4'	48:5:224:U:O2	2.28	0.51
51:9:1284:A:C6	64:MM:91:LEU:HD22	2.44	0.51
51:9:1364:U:O4'	51:9:1364:U:O2	2.29	0.51
7:G:201:GLU:OE2	7:G:226:LEU:HD11	2.10	0.51
47:3:75:C:O4'	47:3:75:C:O2	2.28	0.51
48:5:2627:C:O4'	48:5:2627:C:O2	2.27	0.51
56:EE:31:PRO:HG2	56:EE:38:LEU:HD12	1.93	0.51
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.45	0.51
2:B:249:ARG:NH1	48:5:2837:U:OP1	2.43	0.51
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.93	0.51
50:8:125:C:O2	50:8:125:C:O4'	2.29	0.51
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	1.92	0.51
77:ZZ:73:VAL:HG12	77:ZZ:79:ILE:HD11	1.91	0.51
51:9:501:C:O2	51:9:501:C:C2'	2.57	0.51
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.92	0.51
56:EE:234:PRO:HG3	56:EE:238:LEU:HD11	1.92	0.50
48:5:2367:A:C2	48:5:2788:U:O4	2.53	0.50
1:A:179:ILE:O	48:5:3653:A:H4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LEU:O	3:C:152:LEU:N	2.43	0.50
11:L:58:ILE:HG23	11:L:70:VAL:CG1	2.42	0.50
21:V:39:ILE:HG23	21:V:61:VAL:CG2	2.41	0.50
48:5:2763:U:O2	48:5:2763:U:O4'	2.29	0.50
7:G:98:ILE:HG21	48:5:4125:C:H4'	1.92	0.50
6:F:75:ARG:NE	48:5:730:G:OP2	2.36	0.50
7:G:139:VAL:HG11	7:G:238:LYS:HG3	1.93	0.50
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.92	0.50
18:S:79:GLY:HA3	18:S:132:ILE:HD12	1.92	0.50
48:5:1237:C:O2	48:5:1237:C:O4'	2.29	0.50
51:9:1624:U:O4'	51:9:1624:U:O2	2.30	0.50
1:A:77:ILE:HD12	1:A:115:CYS:SG	2.51	0.50
54:CC:179:THR:HG23	54:CC:180:VAL:O	2.12	0.50
48:5:1426:G:N1	48:5:1458:C:OP2	2.35	0.50
5:E:185:ASN:ND2	5:E:274:LEU:O	2.44	0.50
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	1.94	0.50
57:FF:102:LEU:HD22	77:ZZ:110:THR:HG21	1.94	0.50
48:5:4378:A:O2'	48:5:4379:A:H2'	2.12	0.49
66:OO:99:ALA:H	66:OO:133:THR:HG22	1.77	0.49
21:V:99:GLU:HB3	22:W:24:THR:HG23	1.93	0.49
10:J:53:ALA:HB2	10:J:68:ILE:HD12	1.93	0.49
48:5:4758:U:O2	48:5:4758:U:O4'	2.30	0.49
51:9:853:C:O2	51:9:853:C:O4'	2.26	0.49
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.47	0.49
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.45	0.49
10:J:128:LEU:HD11	10:J:130:PHE:CE1	2.47	0.49
25:Z:11:VAL:CG1	25:Z:80:LEU:HD22	2.42	0.49
3:C:42:THR:HG21	48:5:2340:C:H5'	1.93	0.49
51:9:1374:C:H2'	51:9:1375:G:O4'	2.13	0.49
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.94	0.49
4:D:106:ALA:HB1	4:D:171:LEU:HD13	1.95	0.49
61:JJ:46:VAL:HG21	61:JJ:106:LEU:HD11	1.95	0.49
12:M:112:VAL:HG11	14:O:201:LEU:HD11	1.93	0.49
71:TT:39:LEU:HD11	71:TT:52:TRP:CZ3	2.47	0.49
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.94	0.49
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.60	0.49
48:5:1381:U:O2	48:5:1381:U:O4'	2.30	0.49
48:5:4579:U:O2	48:5:4580:U:C2	2.66	0.49
51:9:1137:U:H3	51:9:1148:A:N6	2.08	0.49
12:M:97:ALA:HB2	14:O:203:VAL:HB	1.94	0.49
77:ZZ:58:LEU:HD21	77:ZZ:91:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1149:A:N3	51:9:1149:A:H2'	2.28	0.49
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.48	0.48
74:WW:55:ASP:O	74:WW:57:ARG:N	2.46	0.48
48:5:3724:A:N6	48:5:3725:G:C6	2.81	0.48
48:5:4966:A:H2'	48:5:4967:A:C8	2.48	0.48
57:FF:87:LEU:CD2	68:QQ:47:LEU:HD13	2.43	0.48
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.48	0.48
16:Q:85:THR:HG22	16:Q:104:ARG:HB2	1.95	0.48
51:9:823:U:O2	51:9:823:U:O4'	2.30	0.48
8:H:12:ILE:HG22	8:H:81:ILE:CD1	2.43	0.48
55:DD:105:LEU:HD23	55:DD:184:ILE:HG23	1.94	0.48
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.42	0.48
17:R:42:ARG:HA	17:R:45:ILE:HD12	1.94	0.48
48:5:2097:A:OP1	48:5:2107:A:N6	2.46	0.48
48:5:4928:C:O2	48:5:4928:C:O4'	2.31	0.48
2:B:29:VAL:HG13	2:B:348:ARG:HD3	1.95	0.48
55:DD:24:PHE:CZ	55:DD:72:VAL:HG11	2.49	0.48
56:EE:100:ARG:HD2	56:EE:102:ILE:HD11	1.96	0.48
6:F:93:ARG:NH2	6:F:95:ARG:O	2.47	0.48
8:H:41:ILE:HG21	8:H:73:ILE:HD11	1.96	0.48
8:H:12:ILE:HG21	8:H:18:ILE:HD13	1.94	0.48
48:5:4305:G:N3	48:5:4305:G:C2'	2.76	0.48
67:PP:44:ARG:HD2	67:PP:84:ILE:HD13	1.96	0.48
18:S:80:ILE:HG12	18:S:129:VAL:HG13	1.95	0.48
21:V:50:ASN:ND2	48:5:4457:U:OP1	2.47	0.48
48:5:4478:G:H2'	48:5:4479:A:O4'	2.13	0.48
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.49	0.48
46:2:33:U:OP2	68:QQ:146:ARG:NH2	2.47	0.47
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.44	0.47
51:9:1834:A:C2	51:9:1836:G:C4	3.02	0.47
54:CC:210:PRO:HA	54:CC:240:THR:HG21	1.96	0.47
67:PP:37:TYR:OH	67:PP:45:LEU:HD11	2.14	0.47
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.49	0.47
57:FF:14:THR:HG23	57:FF:14:THR:O	2.14	0.47
16:Q:148:VAL:HG12	16:Q:152:PHE:CZ	2.49	0.47
50:8:34:U:HO2'	50:8:35:C:P	2.38	0.47
4:D:140:GLY:O	48:5:1819:G:O2'	2.24	0.47
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.47	0.47
48:5:4467:A:O2'	48:5:4510:A:N3	2.42	0.47
48:5:964:A:H2'	48:5:965:G:O4'	2.15	0.47
51:9:943:U:OP2	53:BB:216:LYS:NZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:139:VAL:HG11	7:G:238:LYS:CG	2.45	0.47
9:I:61:SER:HA	9:I:126:VAL:HG23	1.97	0.47
14:O:74:ARG:NH1	48:5:4586:G:OP 2	2.48	0.47
45:1:68:VAL:C	46:2:76:A:O3'	2.53	0.47
51:9:94:G:HO2'	51:9:508:A:HO2'	1.55	0.47
2:B:48:GLY:HA3	2:B:81:THR:HG22	1.95	0.47
57:FF:71:ARG:NH1	57:FF:148:ASN:OD1	2.45	0.47
13:N:193:ARG:O	13:N:197:THR:HG23	2.15	0.47
48:5:82:U:H2'	48:5:83:C:O4'	2.15	0.47
51:9:161:U:O2'	58:GG:87:ARG:NH1	2.48	0.47
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	1.96	0.47
48:5:3656:A:O2'	48:5:3747:A:O2'	2.32	0.47
51:9:1303:C:O2	51:9:1303:C:O4'	2.30	0.47
14:O:168:TYR:CE2	14:O:172:LYS:HD2	2.50	0.47
18:S:82:LEU:HB2	18:S:93:MET:HB2	1.97	0.47
48:5:1964:A:C6	48:5:4694:G:C6	3.03	0.47
48:5:1358:G:H4'	48:5:1359:G:OP 1	2.14	0.46
48:5:3617:G:O2'	48:5:3620:G:N7	2.48	0.46
48:5:1990:A:H3'	48:5:1991:A:H5''	1.97	0.46
51:9:183:G:N3	51:9:183:G:O2'	2.48	0.46
53:BB:39:PHE:CD1	53:BB:74:LEU:HD23	2.51	0.46
48:5:1358:G:O2'	48:5:1359:G:O5'	2.28	0.46
48:5:294:G:O6	48:5:315:G:H1'	2.16	0.46
48:5:4423:U:O4'	48:5:4423:U:O2	2.34	0.46
51:9:887:U:O2	51:9:887:U:O4'	2.31	0.46
53:BB:52:THR:HG23	53:BB:57:ILE:HA	1.97	0.46
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.50	0.46
11:L:71:ARG:NH2	48:5:74:G:O3'	2.49	0.46
16:Q:78:LYS:HG2	16:Q:137:VAL:HG23	1.97	0.46
63:LL:101:ARG:HB2	75:XX:10:ALA:HB2	1.97	0.46
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.45	0.46
48:5:2367:A:N6	48:5:2788:U:C4	2.80	0.46
4:D:53:VAL:HG11	4:D:159:VAL:HA	1.98	0.46
68:QQ:47:LEU:HB3	68:QQ:81:ILE:HD13	1.97	0.46
73:VV:55:ILE:HD11	73:VV:69:ILE:HG12	1.97	0.46
48:5:4723:A:C2	48:5:4724:A:C6	3.04	0.46
13:N:135:ILE:HD13	13:N:151:ILE:HD13	1.97	0.46
48:5:4305:G:N3	48:5:4305:G:H2'	2.31	0.46
48:5:716:C:H2'	48:5:717:U:O4'	2.16	0.46
48:5:3697:U:O2'	48:5:3698:G:OP 2	2.27	0.46
51:9:1130:G:O2'	51:9:1131:G:P	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:94:G:O2'	51:9:508:A:O2'	2.25	0.46
18:S:35:PRO:HD2	18:S:39:VAL:HG21	1.98	0.46
58:GG:162:LEU:HD11	58:GG:172:LYS:HB2	1.97	0.45
18:S:80:ILE:HG23	18:S:129:VAL:HG22	1.96	0.45
46:2:74:C:H2'	46:2:75:C:H5'	1.99	0.45
51:9:1653:U:H2'	51:9:1654:G:C8	2.52	0.45
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.46	0.45
15:P:127:ARG:NH2	48:5:2422:C:OP1	2.49	0.45
68:QQ:34:VAL:HG22	68:QQ:70:VAL:HB	1.98	0.45
48:5:4966:A:C2	48:5:5067:U:N3	2.85	0.45
51:9:92:A:C6	51:9:446:G:C6	3.04	0.45
57:FF:173:LEU:HD13	57:FF:177:LEU:HD12	1.98	0.45
48:5:1633:G:H5'	48:5:1634:A:OP1	2.15	0.45
51:9:183:G:N3	51:9:183:G:C2'	2.78	0.45
2:B:252:ALA:HB1	48:5:4524:G:N3	2.31	0.45
3:C:341:LEU:HD21	5:E:52:LEU:HD21	1.97	0.45
56:EE:136:ILE:HD12	56:EE:149:TYR:OH	2.16	0.45
48:5:1301:C:O2	48:5:1301:C:O4'	2.32	0.45
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.98	0.45
72:UU:24:LEU:CD2	72:UU:112:VAL:HG22	2.46	0.45
72:UU:50:VAL:HG23	72:UU:91:LEU:HD23	1.99	0.45
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.98	0.45
64:MM:22:LEU:HD13	64:MM:22:LEU:C	2.37	0.45
67:PP:56:LEU:HD13	67:PP:78:THR:CG2	2.43	0.45
6:F:158:TYR:CE2	6:F:167:ALA:HB2	2.52	0.45
51:9:146:G:O2'	51:9:147:A:O5'	2.33	0.45
68:QQ:34:VAL:HG21	68:QQ:84:ILE:HD12	1.97	0.45
48:5:3928:A:H2'	48:5:3929:G:O4'	2.17	0.45
2:B:29:VAL:HG11	2:B:32:PHE:CD1	2.52	0.45
14:O:79:ILE:HG21	14:O:138:LEU:HD11	1.97	0.45
54:CC:191:VAL:HG11	54:CC:236:PHE:HA	1.99	0.45
59:HH:51:ILE:HD11	59:HH:176:VAL:HG22	1.98	0.45
60:II:113:TYR:CE1	60:II:121:LEU:HD23	2.51	0.45
66:OO:56:VAL:HG12	66:OO:81:VAL:HG23	1.99	0.45
51:9:1207:G:C6	51:9:1837:G:C6	3.05	0.44
51:9:427:U:O4'	51:9:427:U:O2	2.31	0.44
4:D:64:ILE:HD12	4:D:109:LEU:HD22	1.99	0.44
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.99	0.44
12:M:17:PHE:CE1	12:M:54:CYS:HA	2.52	0.44
51:9:1144:A:C6	51:9:1145:A:C6	3.05	0.44
2:B:86:VAL:HG13	2:B:162:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:79:SER:HG	9:I:147:HIS:CE1	2.35	0.44
10:J:135:GLY:O	10:J:157:ILE:HD11	2.16	0.44
17:R:45:ILE:HG12	17:R:50:ILE:HD11	1.99	0.44
54:CC:251:LEU:HD23	73:VV:23:ILE:HG23	2.00	0.44
74:WW:11:LEU:HD22	74:WW:72:CYS:SG	2.58	0.44
9:I:91:LEU:HD12	9:I:135:ILE:HG23	1.99	0.44
68:QQ:51:LEU:HD22	68:QQ:84:ILE:HG13	1.99	0.44
69:RR:31:ASN:C	69:RR:31:ASN:HD22	2.20	0.44
51:9:12:U:H2'	51:9:13:C:C6	2.53	0.44
7:G:215:ASP:HB3	7:G:216:PRO:HD3	1.98	0.44
15:P:122:ALA:HB2	15:P:145:HIS:CD2	2.52	0.44
48:5:1961:G:O2'	48:5:2025:A:N6	2.50	0.44
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.80	0.44
5:E:153:LEU:HB3	5:E:197:VAL:HG13	1.99	0.44
53:BB:150:ILE:HD13	69:RR:129:LYS:HB2	1.99	0.44
48:5:106:A:H2'	48:5:107:G:O4'	2.17	0.44
50:8:94:G:H5'	50:8:94:G:C8	2.52	0.44
51:9:1351:G:O2'	51:9:1378:A:N1	2.34	0.44
51:9:929:G:H2'	51:9:930:C:O4'	2.18	0.44
3:C:27:VAL:CG2	3:C:264:TYR:HB2	2.47	0.44
57:FF:72:LEU:HD22	57:FF:112:LEU:HD11	1.99	0.44
56:EE:126:VAL:HG23	56:EE:156:VAL:O	2.18	0.44
62:KK:71:LEU:HD21	62:KK:79:LEU:HD12	2.00	0.44
48:5:2367:A:C6	48:5:2788:U:C4	3.06	0.44
51:9:980:A:C2	51:9:981:A:C6	3.05	0.44
55:DD:72:VAL:HG13	62:KK:68:TYR:CD1	2.52	0.44
51:9:1143:A:C2	51:9:1144:A:C2	3.06	0.43
51:9:15:U:H2'	51:9:16:G:O4'	2.18	0.43
3:C:208:CYS:SG	3:C:230:LEU:HD12	2.58	0.43
57:FF:89:THR:HA	57:FF:92:ILE:HD12	2.00	0.43
61:JJ:114:VAL:HG21	61:JJ:135:ILE:CD1	2.48	0.43
14:O:48:TYR:CD2	48:5:1930:U:C6	3.06	0.43
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.99	0.43
48:5:1748:U:C2	48:5:1783:C:C2	3.06	0.43
51:9:1130:G:O2'	51:9:1131:G:O5'	2.36	0.43
52:AA:33:GLN:CB	52:AA:154:LEU:HD12	2.47	0.43
7:G:189:LEU:HD22	7:G:255:VAL:HG12	2.00	0.43
51:9:1336:C:H2'	51:9:1337:C:O4'	2.19	0.43
52:AA:143:PRO:HA	73:VV:32:ILE:HD11	2.00	0.43
51:9:1129:G:C6	51:9:1130:G:O6	2.71	0.43
4:D:103:LEU:HD11	4:D:248:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:146:ALA:HA	23:X:149:VAL:HG12	2.00	0.43
48:5:481(A):C:O2	48:5:481(A):C:O4'	2.37	0.43
51:9:1238:U:H2'	51:9:1239:U:O4'	2.19	0.43
51:9:522:A:OP2	61:JJ:45:ARG:NH2	2.46	0.43
53:BB:123:ALA:HB2	53:BB:165:ARG:HG3	2.00	0.43
10:J:27:GLY:HA2	10:J:68:ILE:HG23	2.00	0.43
8:H:61:TRP:CZ3	12:M:33:GLN:HG2	2.53	0.43
74:WW:52:ILE:HG22	74:WW:61:ILE:HG23	2.01	0.43
51:9:1834:A:N3	51:9:1834:A:C2'	2.82	0.43
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.58	0.43
61:JJ:46:VAL:HG21	61:JJ:106:LEU:CD1	2.48	0.43
51:9:1674:G:N7	68:QQ:17:LYS:NZ	2.67	0.43
48:5:2088:A:O2'	48:5:2089:G:OP2	2.32	0.43
51:9:914:U:O4'	51:9:914:U:O2	2.36	0.43
60:II:3:ILE:O	60:II:3:ILE:HG23	2.18	0.43
72:UU:29:VAL:HG22	72:UU:85:HIS:CE1	2.54	0.43
57:FF:99:ILE:CG2	77:ZZ:67:LEU:HD21	2.41	0.43
48:5:2367:A:N6	48:5:2788:U:H3	2.12	0.43
52:AA:94:THR:HG23	52:AA:182:VAL:HG21	2.00	0.43
63:LL:68:ILE:HG21	63:LL:143:LEU:HD21	2.01	0.43
13:N:114:ARG:HD2	13:N:151:ILE:HG22	2.01	0.43
48:5:2094:C:O2	48:5:2094:C:O4'	2.34	0.43
48:5:750:U:H2'	48:5:751:G:O4'	2.18	0.43
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.48	0.43
14:O:193:THR:HG23	14:O:202:LEU:HD23	2.01	0.43
48:5:2458:C:H2'	48:5:2459:G:O4'	2.18	0.42
48:5:1963:C:N4	48:5:4694:G:O6	2.52	0.42
51:9:1228:A:H2'	51:9:1229:G:C8	2.54	0.42
7:G:210:ILE:HG12	7:G:254:THR:HG22	2.01	0.42
60:II:36:THR:HG23	60:II:96:LEU:HB2	2.00	0.42
10:J:139:PHE:CE1	10:J:151:ILE:HD13	2.54	0.42
15:P:47:TYR:O	15:P:51:VAL:HG23	2.18	0.42
18:S:13:VAL:HG23	18:S:62:VAL:HB	2.01	0.42
74:WW:52:ILE:HG22	74:WW:61:ILE:HG12	2.00	0.42
51:9:1596:U:H2'	51:9:1597:C:O4'	2.19	0.42
48:5:1787:A:N3	48:5:4210:U:O2'	2.53	0.42
48:5:2439:G:C6	48:5:2440:U:C4	3.06	0.42
51:9:1035:A:H2'	51:9:1036:A:O4'	2.20	0.42
66:OO:44:VAL:HG11	66:OO:85:CYS:SG	2.59	0.42
2:B:321:VAL:HA	48:5:5050:C:O2'	2.19	0.42
51:9:944:A:C5	51:9:945:U:C5	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PHE:CG	1:A:219:ILE:HG23	2.54	0.42
55:DD:156:LEU:HD12	55:DD:157:MET:N	2.35	0.42
6:F:90:PHE:CE2	6:F:92:ILE:HD11	2.55	0.42
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	2.00	0.42
48:5:1888:A:N6	48:5:3873:G:O2'	2.52	0.42
48:5:1895:G:O2'	48:5:1907:A:N3	2.46	0.42
48:5:686:A:H2'	48:5:686:A:N3	2.35	0.42
50:8:15:G:C6	50:8:16:G:N1	2.87	0.42
52:AA:134:LEU:CD2	52:AA:144:THR:HG21	2.48	0.42
52:AA:15:VAL:HG12	52:AA:19:LEU:HD12	2.00	0.42
6:F:89:ALA:CB	6:F:124:LEU:HD21	2.48	0.42
51:9:171:A:H5'	58:GG:177:GLN:HG2	2.02	0.42
60:II:194:GLU:HG2	63:LL:10:TYR:CD2	2.55	0.42
48:5:51:A:N3	48:5:1528:U:O2'	2.52	0.42
10:J:141:ILE:HD11	49:7:55:A:N3	2.35	0.42
51:9:958:G:N1	51:9:959:G:C6	2.88	0.42
56:EE:181:CYS:SG	56:EE:225:ILE:HG23	2.59	0.42
9:I:153:ARG:HA	9:I:165:ILE:HD11	2.02	0.42
12:M:50:MET:HE3	12:M:55:MET:HB3	2.02	0.42
66:OO:95:ILE:HD13	66:OO:116:LEU:HG	2.02	0.42
18:S:9:GLU:CG	18:S:33:PHE:CE1	3.02	0.42
51:9:1520:G:N3	51:9:1520:G:H2'	2.35	0.42
6:F:222:LYS:HE3	48:5:1907:A:H4'	2.01	0.42
7:G:131:PRO:HA	7:G:134:ASN:HB3	2.01	0.42
69:RR:119:VAL:O	69:RR:119:VAL:HG13	2.18	0.42
48:5:3656:A:O4'	48:5:3747:A:C2	2.72	0.42
48:5:4260:U:H2'	48:5:4261:C:C6	2.55	0.42
70:SS:59:LEU:HD12	70:SS:63:GLU:OE2	2.20	0.42
48:5:4724:A:C6	48:5:4725:C:C4	3.08	0.42
2:B:14:LEU:O	2:B:17:LEU:HG	2.20	0.42
22:W:3:VAL:O	22:W:3:VAL:HG23	2.20	0.42
48:5:1811:G:C2	48:5:1812:C:C2	3.08	0.41
51:9:356:C:O2	51:9:356:C:C2'	2.66	0.41
51:9:584:A:C6	51:9:585:C:C4	3.08	0.41
55:DD:35:SER:HG	55:DD:97:CYS:HG	1.68	0.41
57:FF:73:THR:HG22	57:FF:89:THR:HG23	2.01	0.41
10:J:53:ALA:HB2	10:J:68:ILE:CD1	2.50	0.41
11:L:58:ILE:HG23	11:L:70:VAL:HG11	2.00	0.41
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	2.02	0.41
77:ZZ:79:ILE:HB	77:ZZ:83:LEU:HD12	2.02	0.41
48:5:1932:A:C2'	48:5:1933:G:O5'	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3765:G:O2'	48:5:3766:A:N7	2.53	0.41
52:AA:134:LEU:HD21	52:AA:144:THR:HG21	2.01	0.41
48:5:1279:A:O2'	48:5:1281:G:N7	2.48	0.41
48:5:2408:U:O4'	48:5:2409:U:C5	2.74	0.41
51:9:1834:A:N1	51:9:1836:G:C2	2.88	0.41
2:B:299:ILE:N	2:B:299:ILE:HD12	2.36	0.41
56:EE:11:ARG:HH22	56:EE:24:THR:HG1	1.68	0.41
7:G:189:LEU:HD21	7:G:257:PHE:CE2	2.55	0.41
9:I:36:LEU:HD12	9:I:87:ILE:HB	2.02	0.41
60:II:117:TYR:CD1	60:II:156:ALA:HB2	2.56	0.41
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	2.01	0.41
67:PP:34:MET:HG2	67:PP:45:LEU:HD12	2.02	0.41
20:U:23:LEU:HD11	20:U:83:LEU:CD2	2.50	0.41
19:T:85:LEU:HD13	48:5:4305:G:C2	2.55	0.41
48:5:4459:U:H2'	48:5:4460:U:C6	2.55	0.41
51:9:482:G:N1	51:9:485:A:OP2	2.51	0.41
1:A:207:VAL:HG23	1:A:208:GLU:HG3	2.02	0.41
53:BB:87:ILE:HG23	53:BB:101:HIS:CG	2.56	0.41
61:JJ:35:TYR:CD2	61:JJ:106:LEU:HD23	2.55	0.41
11:L:116:ARG:NH1	11:L:155:MET:O	2.53	0.41
13:N:158:HIS:HB3	13:N:161:MET:HG2	2.02	0.41
48:5:916:C:O4'	48:5:916:C:O2	2.38	0.41
51:9:1243:U:O4	51:9:1257:G:N2	2.51	0.41
51:9:1707:U:H2'	51:9:1708:C:O4'	2.21	0.41
51:9:1700:C:C2	51:9:1834:A:N6	2.88	0.41
5:E:164:ARG:O	5:E:185:ASN:ND2	2.53	0.41
48:5:492:U:HO2'	48:5:493:G:P	2.43	0.41
51:9:1581:C:OP2	51:9:1582:C:N4	2.47	0.41
53:BB:189:ILE:HB	53:BB:190:PRO:HD3	2.02	0.41
4:D:50:ARG:NH2	4:D:72:ASP:OD2	2.53	0.41
61:JJ:149:VAL:HG11	61:JJ:157:ILE:HD11	2.02	0.41
65:NN:60:VAL:HG23	65:NN:66:VAL:HG21	2.02	0.41
48:5:4896:G:N2	48:5:4927:G:O6	2.50	0.41
52:AA:60:LEU:HD13	52:AA:159:ILE:CD1	2.51	0.41
2:B:164:ALA:HB3	2:B:183:ILE:HD12	2.03	0.41
2:B:29:VAL:HG23	2:B:346:THR:HG21	2.01	0.41
2:B:77:THR:HG21	2:B:337:VAL:HG22	2.02	0.41
4:D:64:ILE:CD1	4:D:109:LEU:HD22	2.49	0.41
21:V:20:LEU:HB2	21:V:55:ALA:O	2.21	0.41
48:5:1563:A:O2'	48:5:1564:A:O4'	2.38	0.41
48:5:197:A:N1	48:5:225:G:O2'	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:8:137:A:H2'	50:8:138:C:C6	2.55	0.41
51:9:118:C:H1'	51:9:445:A:C5	2.56	0.41
51:9:958:G:C6	51:9:959:G:C6	3.08	0.41
8:H:41:ILE:HD11	8:H:69:THR:HB	2.03	0.41
75:XX:67:ARG:HG2	75:XX:115:ILE:HG23	2.03	0.41
51:9:1530:U:H2'	51:9:1531:A:O4'	2.21	0.41
52:AA:25:LEU:HD11	52:AA:42:LYS:HZ2	1.84	0.41
53:BB:103:MET:CE	53:BB:212:VAL:HG23	2.51	0.41
54:CC:137:VAL:HG21	54:CC:217:ALA:HB2	2.03	0.41
66:OO:99:ALA:N	66:OO:133:THR:HG22	2.36	0.41
51:9:407:G:H3'	51:9:408:A:C5'	2.50	0.41
1:A:181:LYS:HB2	48:5:1577:G:C5	2.56	0.41
1:A:47:ASP:HA	1:A:84:THR:HG22	2.02	0.41
2:B:86:VAL:HG13	2:B:162:VAL:CG2	2.51	0.41
5:E:201:SER:N	5:E:291:PHE:O	2.54	0.41
71:TT:18:LEU:HB3	71:TT:58:ALA:HB1	2.03	0.41
47:3:75:C:H2'	47:3:76:A:H4'	2.04	0.41
51:9:1551:U:O2	51:9:1551:U:O4'	2.38	0.41
51:9:1650:A:H2'	51:9:1651:A:O4'	2.21	0.41
6:F:124:LEU:HD12	6:F:129:ILE:HG12	2.01	0.41
11:L:110:LEU:O	11:L:114:VAL:HG23	2.20	0.41
22:W:3:VAL:HG21	22:W:12:LYS:HE3	2.02	0.41
25:Z:75:TYR:CD2	25:Z:80:LEU:HD21	2.56	0.41
4:D:16:TYR:O	49:7:11:A:N6	2.54	0.40
2:B:29:VAL:HG11	2:B:32:PHE:CE1	2.55	0.40
53:BB:74:LEU:HD21	53:BB:86:LEU:HD11	2.03	0.40
59:HH:96:ALA:HB3	59:HH:98:ARG:NH1	2.36	0.40
14:O:58:LEU:HD11	14:O:145:VAL:HG22	2.02	0.40
17:R:11:ALA:HB1	17:R:50:ILE:HD13	2.02	0.40
69:RR:5:ARG:HB2	69:RR:10:LYS:HE2	2.03	0.40
73:VV:43:THR:HG22	73:VV:45:ARG:HG3	2.02	0.40
48:5:1325:C:O2	48:5:1325:C:O5'	2.39	0.40
51:9:1692:U:H2'	51:9:1693:G:C8	2.57	0.40
58:GG:32:MET:HE2	58:GG:63:MET:HG2	2.02	0.40
61:JJ:110:LEU:HD13	61:JJ:142:VAL:HG11	2.02	0.40
48:5:1314:C:C2	48:5:1315:C:C5	3.08	0.40
48:5:282:C:H2'	48:5:283:G:O4'	2.21	0.40
51:9:1045:U:H2'	51:9:1046:U:O4'	2.21	0.40
5:E:184:LEU:O	48:5:4883:C:N4	2.54	0.40
8:H:104:VAL:HG13	8:H:113:GLU:HB2	2.02	0.40
12:M:119:ARG:HH11	14:O:202:LEU:HD21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:22:VAL:HG23	21:V:53:PRO:O	2.21	0.40
48:5:1339:U:H2'	48:5:1340:C:C6	2.56	0.40
48:5:3690:U:H2'	48:5:3691:G:O4'	2.21	0.40
51:9:1130:G:HO2'	51:9:1131:G:C5'	2.34	0.40
51:9:1149:A:C4	51:9:1151:G:C8	3.10	0.40
51:9:1231:C:H2'	51:9:1232:U:O4'	2.21	0.40
51:9:1452:A:C6	51:9:1476:A:C6	3.09	0.40
51:9:191:A:C2'	51:9:192:C:OP1	2.70	0.40
51:9:953:C:H2'	51:9:954:U:O4'	2.21	0.40
1:A:117:GLU:HB2	1:A:162:ASN:HB2	2.03	0.40
1:A:199:VAL:HG21	48:5:1631:A:N7	2.37	0.40
58:GG:16:ILE:N	58:GG:16:ILE:HD12	2.36	0.40
61:JJ:32:ILE:O	61:JJ:36:GLY:N	2.53	0.40
48:5:2693:G:C6	48:5:2694:G:N1	2.90	0.40
48:5:3798:U:C2	48:5:3801:U:C5	3.09	0.40
48:5:1305:C:OP1	50:8:7:U:O2'	2.40	0.40
46:2:38:C:O2'	51:9:1058:A:OP1	2.36	0.40
51:9:1843:G:H2'	51:9:1844:U:O4'	2.21	0.40
51:9:488:U:O2	51:9:488:U:O4'	2.38	0.40
51:9:962:A:N1	51:9:1055:A:O2'	2.54	0.40
4:D:219:TYR:CE2	4:D:227:ILE:HD11	2.56	0.40
4:D:60:ILE:HD13	4:D:98:ALA:HB2	2.03	0.40
56:EE:44:LEU:HD21	56:EE:70:ILE:HG21	2.03	0.40
7:G:247:VAL:HG21	7:G:249:ARG:NH1	2.36	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%)	218 (89%)	26 (11%)	2 (1%)	24 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	392/403 (97%)	360 (92%)	29 (7%)	3 (1%)	24	70
3	C	360/425 (85%)	337 (94%)	21 (6%)	2 (1%)	30	74
4	D	291/297 (98%)	275 (94%)	15 (5%)	1 (0%)	46	83
5	E	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
6	F	223/247 (90%)	212 (95%)	10 (4%)	1 (0%)	39	80
7	G	229/319 (72%)	216 (94%)	11 (5%)	2 (1%)	21	68
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	201/214 (94%)	185 (92%)	16 (8%)	0	100	100
10	J	168/178 (94%)	161 (96%)	7 (4%)	0	100	100
11	L	208/211 (99%)	196 (94%)	11 (5%)	1 (0%)	34	77
12	M	136/218 (62%)	123 (90%)	12 (9%)	1 (1%)	26	72
13	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	34	77
14	O	197/203 (97%)	188 (95%)	8 (4%)	1 (0%)	34	77
15	P	151/184 (82%)	142 (94%)	9 (6%)	0	100	100
16	Q	185/188 (98%)	173 (94%)	12 (6%)	0	100	100
17	R	178/196 (91%)	173 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	30	74
19	T	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
20	U	97/128 (76%)	87 (90%)	10 (10%)	0	100	100
21	V	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
22	W	102/157 (65%)	97 (95%)	4 (4%)	1 (1%)	19	66
23	X	116/156 (74%)	107 (92%)	9 (8%)	0	100	100
24	Y	132/145 (91%)	122 (92%)	10 (8%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	5 (4%)	2 (2%)	13	59
26	a	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
27	b	100/245 (41%)	94 (94%)	5 (5%)	1 (1%)	19	66
28	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
29	d	105/125 (84%)	89 (85%)	15 (14%)	1 (1%)	19	66
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	10	55
32	g	112/117 (96%)	105 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	i	100/105 (95%)	94 (94%)	5 (5%)	1 (1%)	19	66
35	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
36	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
38	m	50/102 (49%)	47 (94%)	3 (6%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
41	p	89/92 (97%)	83 (93%)	5 (6%)	1 (1%)	17	65
42	r	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	24	70
43	s	194/318 (61%)	176 (91%)	16 (8%)	2 (1%)	19	66
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	15	61
45	l	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1	19
52	AA	215/295 (73%)	203 (94%)	11 (5%)	1 (0%)	34	77
53	BB	211/264 (80%)	198 (94%)	12 (6%)	1 (0%)	34	77
54	CC	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
55	DD	226/243 (93%)	213 (94%)	12 (5%)	1 (0%)	39	80
56	EE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
57	FF	181/204 (89%)	170 (94%)	9 (5%)	2 (1%)	17	65
58	GG	235/249 (94%)	224 (95%)	11 (5%)	0	100	100
59	HH	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
60	II	204/208 (98%)	192 (94%)	11 (5%)	1 (0%)	34	77
61	JJ	183/194 (94%)	177 (97%)	6 (3%)	0	100	100
62	KK	94/165 (57%)	89 (95%)	4 (4%)	1 (1%)	17	65
63	LL	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
64	MM	115/132 (87%)	103 (90%)	12 (10%)	0	100	100
65	NN	147/151 (97%)	142 (97%)	4 (3%)	1 (1%)	26	72
66	OO	134/168 (80%)	123 (92%)	9 (7%)	2 (2%)	13	59
67	PP	118/145 (81%)	105 (89%)	12 (10%)	1 (1%)	24	70
68	QQ	140/146 (96%)	132 (94%)	7 (5%)	1 (1%)	26	72
69	RR	130/135 (96%)	120 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	79 (98%)	2 (2%)	0	100	100
74	WW	127/130 (98%)	120 (94%)	5 (4%)	2 (2%)	12	58
75	XX	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	8	52
76	YY	122/130 (94%)	115 (94%)	7 (6%)	0	100	100
77	ZZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
78	aa	99/115 (86%)	93 (94%)	4 (4%)	2 (2%)	9	54
79	bb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
80	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
81	dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/156 (42%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/317 (98%)	285 (92%)	24 (8%)	2 (1%)	30	74
86	ii	417/459 (91%)	387 (93%)	24 (6%)	6 (1%)	14	60
87	jj	426/637 (67%)	371 (87%)	50 (12%)	5 (1%)	16	63
All	All	12375/14486 (85%)	11531 (93%)	780 (6%)	64 (0%)	38	77

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
75	XX	62	PRO
86	ii	258	TYR
86	ii	272	THR
87	jj	224	GLY
87	jj	280	VAL
13	N	89	VAL
42	r	11	ARG
43	s	142	GLY
65	NN	108	ASP
66	OO	20	GLN
66	OO	30	VAL
67	PP	80	LEU
68	QQ	30	GLY
75	XX	61	GLN

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Mol	Chain	Res	Type
75	XX	86	PRO
86	ii	181	GLY
1	A	14	SER
6	F	236	GLU
11	L	63	THR
18	S	155	PRO
25	Z	90	PRO
25	Z	91	LEU
27	b	102	PRO
31	f	107	PRO
44	t	125	LEU
55	DD	93	THR
60	II	3	ILE
62	KK	64	TRP
74	WW	56	HIS
86	ii	370	GLU
2	B	17	LEU
2	B	376	HIS
41	p	18	TYR
44	t	54	LYS
78	aa	15	ARG
86	ii	326	LEU
3	C	83	GLY
14	O	186	GLU
29	d	58	GLY
31	f	106	TYR
45	l	64	PRO
52	AA	159	ILE
57	FF	21	GLY
57	FF	80	GLY
74	WW	29	PRO
78	aa	47	ALA
86	ii	184	GLY
87	jj	487	ASP
1	A	195	CYS
7	G	221	VAL
43	s	25	PRO
84	gg	224	GLY
87	jj	464	ILE
87	jj	558	ILE
7	G	216	PRO
22	W	3	VAL

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Mol	Chain	Res	Type
53	BB	93	GLY
2	B	254	ILE
3	C	247	GLY
4	D	125	VAL
12	M	9	VAL
34	i	47	VAL
71	TT	109	GLY
84	gg	13	GLY

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%)	179 (94%)	11 (6%)	25	67
2	B	342/348 (98%)	325 (95%)	17 (5%)	30	71
3	C	302/347 (87%)	285 (94%)	17 (6%)	26	68
4	D	247/250 (99%)	235 (95%)	12 (5%)	31	71
5	E	190/251 (76%)	177 (93%)	13 (7%)	20	62
6	F	196/215 (91%)	184 (94%)	12 (6%)	23	66
7	G	200/272 (74%)	189 (94%)	11 (6%)	27	69
8	H	169/171 (99%)	157 (93%)	12 (7%)	18	60
9	I	175/181 (97%)	166 (95%)	9 (5%)	29	71
10	J	143/149 (96%)	136 (95%)	7 (5%)	31	71
11	L	175/176 (99%)	167 (95%)	8 (5%)	33	73
12	M	117/161 (73%)	108 (92%)	9 (8%)	16	57
13	N	171/172 (99%)	163 (95%)	8 (5%)	32	73
14	O	171/173 (99%)	160 (94%)	11 (6%)	22	64
15	P	134/163 (82%)	126 (94%)	8 (6%)	24	66
16	Q	164/165 (99%)	156 (95%)	8 (5%)	31	71
17	R	159/175 (91%)	147 (92%)	12 (8%)	17	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S	157/157 (100%)	146 (93%)	11 (7%)	19	61
19	T	139/140 (99%)	129 (93%)	10 (7%)	18	59
20	U	89/114 (78%)	86 (97%)	3 (3%)	44	79
21	V	101/107 (94%)	93 (92%)	8 (8%)	15	55
22	W	86/126 (68%)	85 (99%)	1 (1%)	78	91
23	X	106/134 (79%)	100 (94%)	6 (6%)	25	68
24	Y	124/135 (92%)	117 (94%)	7 (6%)	26	68
25	Z	117/118 (99%)	114 (97%)	3 (3%)	54	83
26	a	119/120 (99%)	116 (98%)	3 (2%)	55	83
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%)	91 (93%)	7 (7%)	18	60
30	e	114/121 (94%)	105 (92%)	9 (8%)	15	55
31	f	88/89 (99%)	82 (93%)	6 (7%)	20	62
32	g	98/100 (98%)	93 (95%)	5 (5%)	29	71
33	h	109/110 (99%)	103 (94%)	6 (6%)	27	69
34	i	86/89 (97%)	85 (99%)	1 (1%)	78	91
35	j	73/80 (91%)	68 (93%)	5 (7%)	20	62
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%)	45 (94%)	3 (6%)	22	65
39	n	24/24 (100%)	22 (92%)	2 (8%)	14	53
40	o	92/94 (98%)	86 (94%)	6 (6%)	21	64
41	p	74/75 (99%)	73 (99%)	1 (1%)	74	90
42	r	108/121 (89%)	102 (94%)	6 (6%)	26	68
43	s	164/258 (64%)	158 (96%)	6 (4%)	41	77
44	t	126/137 (92%)	121 (96%)	5 (4%)	38	76
45	1	13/13 (100%)	13 (100%)	0	100	100
52	AA	180/245 (74%)	168 (93%)	12 (7%)	20	63
53	BB	194/231 (84%)	176 (91%)	18 (9%)	11	49
54	CC	187/225 (83%)	175 (94%)	12 (6%)	22	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	DD	190/202 (94%)	174 (92%)	16 (8%)	14	53
56	EE	224/225 (100%)	202 (90%)	22 (10%)	10	45
57	FF	158/170 (93%)	144 (91%)	14 (9%)	12	51
58	GG	207/218 (95%)	192 (93%)	15 (7%)	18	59
59	HH	165/174 (95%)	152 (92%)	13 (8%)	15	55
60	II	178/180 (99%)	163 (92%)	15 (8%)	14	53
61	JJ	161/168 (96%)	146 (91%)	15 (9%)	11	49
62	KK	87/136 (64%)	75 (86%)	12 (14%)	4	29
63	LL	130/142 (92%)	120 (92%)	10 (8%)	16	57
64	MM	99/108 (92%)	85 (86%)	14 (14%)	4	28
65	NN	130/131 (99%)	118 (91%)	12 (9%)	11	49
66	OO	106/130 (82%)	91 (86%)	15 (14%)	4	28
67	PP	109/130 (84%)	98 (90%)	11 (10%)	9	44
68	QQ	117/121 (97%)	110 (94%)	7 (6%)	24	66
69	RR	119/121 (98%)	110 (92%)	9 (8%)	16	57
70	SS	125/132 (95%)	111 (89%)	14 (11%)	7	39
71	TT	111/115 (96%)	103 (93%)	8 (7%)	18	59
72	UU	92/107 (86%)	86 (94%)	6 (6%)	21	64
73	VV	67/67 (100%)	63 (94%)	4 (6%)	24	66
74	WW	112/113 (99%)	103 (92%)	9 (8%)	15	55
75	XX	113/115 (98%)	107 (95%)	6 (5%)	28	70
76	YY	107/112 (96%)	91 (85%)	16 (15%)	3	26
77	ZZ	66/103 (64%)	62 (94%)	4 (6%)	23	66
78	aa	88/98 (90%)	81 (92%)	7 (8%)	15	55
79	bb	75/76 (99%)	68 (91%)	7 (9%)	11	49
80	cc	55/62 (89%)	50 (91%)	5 (9%)	12	50
81	dd	48/49 (98%)	47 (98%)	1 (2%)	61	86
82	ee	46/106 (43%)	42 (91%)	4 (9%)	13	52
83	ff	61/140 (44%)	56 (92%)	5 (8%)	14	54
84	gg	272/275 (99%)	263 (97%)	9 (3%)	45	80
86	ii	361/394 (92%)	339 (94%)	22 (6%)	23	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
87	jj	372/520 (72%)	354 (95%)	18 (5%)	31	72
All	All	10789/12266 (88%)	10088 (94%)	701 (6%)	26	64

All (701) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	102	LEU
1	A	109	GLU
1	A	128	ARG
1	A	163	ARG
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	233	ARG
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	383	GLU
3	C	20	LYS
3	C	95	MET
3	C	113	ARG
3	C	122	TYR
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS

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Mol	Chain	Res	Type
3	C	175	LYS
3	C	188	ARG
3	C	193	LYS
3	C	213	GLU
3	C	232	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
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	225	GLN
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	286	PRO
5	E	289	LEU
5	E	291	PHE
6	F	30	LYS
6	F	41	LEU
6	F	46	ARG
6	F	65	ARG
6	F	67	GLU
6	F	88	LEU
6	F	134	ILE
6	F	151	GLU

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Mol	Chain	Res	Type
6	F	187	GLU
6	F	198	LYS
6	F	245	ARG
6	F	246	MET
7	G	126	ARG
7	G	163	LYS
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	242	ARG
7	G	273	GLU
7	G	293	ASN
8	H	1	MET
8	H	20	LEU
8	H	52	LYS
8	H	54	ARG
8	H	59	LYS
8	H	66	GLU
8	H	74	CYS
8	H	105	ILE
8	H	106	GLN
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	146	GLU
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	208	LYS
10	J	16	ARG
10	J	28	GLU
10	J	33	LEU
10	J	81	GLU
10	J	101	ASP
10	J	113	ILE

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Mol	Chain	Res	Type
10	J	175	LEU
11	L	10	LEU
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	5	ARG
12	M	8	GLU
12	M	32	ASP
12	M	37	LEU
12	M	42	CYS
12	M	54	CYS
12	M	57	LEU
12	M	96	GLU
12	M	119	ARG
13	N	9	GLU
13	N	26	ARG
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	87	HIS
13	N	162	ARG
13	N	182	HIS
14	O	49	ARG
14	O	67	SER
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	202	LEU
15	P	24	VAL
15	P	25	HIS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU

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Mol	Chain	Res	Type
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	61	LEU
16	Q	63	LEU
16	Q	75	ARG
16	Q	91	ARG
16	Q	97	LYS
16	Q	138	LEU
16	Q	143	ARG
16	Q	168	ARG
17	R	8	LYS
17	R	36	ASN
17	R	50	ILE
17	R	52	ARG
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	113	LYS
17	R	133	LYS
17	R	138	LEU
17	R	176	ARG
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	24	THR
18	S	43	ARG
18	S	70	LYS
18	S	83	ARG
18	S	84	TYR
18	S	135	SER
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	88	ARG
19	T	96	ILE
19	T	117	LYS
19	T	144	ASN

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Mol	Chain	Res	Type
19	T	146	LYS
19	T	159	MET
20	U	33	ILE
20	U	80	LYS
20	U	101	ARG
21	V	15	ARG
21	V	18	LEU
21	V	35	LYS
21	V	60	MET
21	V	91	LYS
21	V	99	GLU
21	V	109	LYS
21	V	123	LYS
22	W	91	MET
23	X	39	LYS
23	X	41	ARG
23	X	53	ARG
23	X	63	LYS
23	X	91	GLU
23	X	148	ASP
24	Y	2	LYS
24	Y	8	THR
24	Y	50	ARG
24	Y	52	ASP
24	Y	72	GLN
24	Y	74	TYR
24	Y	112	ASP
25	Z	33	THR
25	Z	42	LEU
25	Z	112	ARG
26	a	4	ARG
26	a	122	VAL
26	a	132	ARG
27	b	22	LYS
27	b	40	LEU
27	b	101	HIS
28	c	37	MET
28	c	65	MET
28	c	78	ASN
29	d	23	ARG
29	d	31	LYS
29	d	44	ARG

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Mol	Chain	Res	Type
29	d	48	GLU
29	d	78	ARG
29	d	85	ARG
29	d	98	SER
30	e	21	ILE
30	e	22	ARG
30	e	64	LYS
30	e	78	LEU
30	e	83	LYS
30	e	89	LEU
30	e	93	LYS
30	e	106	LYS
30	e	128	ARG
31	f	7	CYS
31	f	16	ARG
31	f	23	GLU
31	f	47	CYS
31	f	52	LYS
31	f	101	ILE
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	89	ASP
32	g	114	GLN
33	h	15	GLU
33	h	28	LEU
33	h	67	GLU
33	h	77	LYS
33	h	82	ASP
33	h	89	ARG
34	i	86	LYS
35	j	3	LYS
35	j	11	ARG
35	j	20	ARG
35	j	46	LYS
35	j	58	THR
36	k	69	LEU
36	k	70	LYS
37	l	49	LEU
38	m	71	ARG
38	m	72	LYS
38	m	92	THR

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Mol	Chain	Res	Type
39	n	1	MET
39	n	13	LEU
40	o	8	ARG
40	o	17	LYS
40	o	18	HIS
40	o	36	GLN
40	o	61	LYS
40	o	82	MET
41	p	8	VAL
42	r	8	MET
42	r	32	LEU
42	r	39	ARG
42	r	67	ARG
42	r	80	THR
42	r	103	HIS
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
44	t	137	GLN
44	t	144	ASP
52	AA	5	LEU
52	AA	12	GLU
52	AA	25	LEU
52	AA	56	GLU
52	AA	58	LEU
52	AA	59	LEU
52	AA	60	LEU
52	AA	111	GLN
52	AA	122	LEU
52	AA	132	GLN
52	AA	136	GLU
52	AA	178	LEU
53	BB	38	MET
53	BB	42	ARG
53	BB	71	LEU
53	BB	74	LEU

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Mol	Chain	Res	Type
53	BB	82	ARG
53	BB	92	GLN
53	BB	105	LEU
53	BB	125	VAL
53	BB	126	ASP
53	BB	157	GLN
53	BB	172	MET
53	BB	175	GLU
53	BB	181	LEU
53	BB	202	GLN
53	BB	207	LEU
53	BB	209	ASP
53	BB	213	ARG
53	BB	225	LEU
54	CC	72	ASP
54	CC	78	LEU
54	CC	114	LYS
54	CC	117	ARG
54	CC	121	ARG
54	CC	137	VAL
54	CC	167	ARG
54	CC	227	ARG
54	CC	235	ASN
54	CC	236	PHE
54	CC	252	THR
54	CC	254	ASP
55	DD	22	ASN
55	DD	28	GLU
55	DD	31	GLU
55	DD	35	SER
55	DD	45	ARG
55	DD	65	ARG
55	DD	76	ARG
55	DD	106	ARG
55	DD	120	TYR
55	DD	127	MET
55	DD	142	LEU
55	DD	156	LEU
55	DD	160	SER
55	DD	198	ILE
55	DD	215	ASP
55	DD	218	LEU

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Mol	Chain	Res	Type
56	EE	6	LYS
56	EE	17	HIS
56	EE	30	ARG
56	EE	42	LEU
56	EE	49	ARG
56	EE	51	ARG
56	EE	65	CYS
56	EE	66	MET
56	EE	67	GLN
56	EE	77	ARG
56	EE	88	ASP
56	EE	145	ARG
56	EE	159	THR
56	EE	162	ILE
56	EE	177	THR
56	EE	200	ARG
56	EE	205	PHE
56	EE	222	LEU
56	EE	232	ASN
56	EE	238	LEU
56	EE	240	ARG
56	EE	246	LEU
57	FF	29	GLN
57	FF	35	LEU
57	FF	36	GLN
57	FF	43	GLU
57	FF	63	LYS
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	91	ARG
57	FF	122	ARG
57	FF	168	THR
57	FF	169	ILE
57	FF	175	ASP
57	FF	204	ARG
58	GG	25	ARG
58	GG	41	LEU
58	GG	63	MET
58	GG	64	LYS
58	GG	67	VAL
58	GG	81	HIS

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Mol	Chain	Res	Type
58	GG	103	ASP
58	GG	116	LYS
58	GG	155	GLN
58	GG	159	ARG
58	GG	171	THR
58	GG	178	ARG
58	GG	190	ARG
58	GG	216	ARG
58	GG	230	LYS
59	HH	8	ILE
59	HH	36	LEU
59	HH	53	VAL
59	HH	76	GLN
59	HH	82	GLU
59	HH	100	ILE
59	HH	114	GLN
59	HH	127	ASP
59	HH	145	ARG
59	HH	151	SER
59	HH	160	LYS
59	HH	162	GLN
59	HH	194	LEU
60	II	12	ARG
60	II	23	LYS
60	II	26	LYS
60	II	56	ARG
60	II	74	ARG
60	II	79	ILE
60	II	100	CYS
60	II	121	LEU
60	II	130	THR
60	II	161	LEU
60	II	162	LEU
60	II	168	GLN
60	II	175	ILE
60	II	178	ARG
60	II	203	LYS
61	JJ	9	CYS
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	61	LEU

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Mol	Chain	Res	Type
61	JJ	65	GLU
61	JJ	69	ARG
61	JJ	70	ARG
61	JJ	79	ARG
61	JJ	89	GLU
61	JJ	94	LEU
61	JJ	109	ARG
61	JJ	112	THR
61	JJ	116	LYS
61	JJ	158	ASP
62	KK	1	MET
62	KK	2	LEU
62	KK	17	LYS
62	KK	20	VAL
62	KK	29	MET
62	KK	35	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	72	THR
62	KK	89	ILE
62	KK	93	THR
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	40	ILE
63	LL	42	LEU
63	LL	49	GLU
63	LL	56	ILE
63	LL	69	ARG
63	LL	111	VAL
63	LL	126	VAL
63	LL	134	LEU
64	MM	22	LEU
64	MM	31	LEU
64	MM	33	ARG
64	MM	36	ARG
64	MM	40	LYS
64	MM	42	LEU
64	MM	45	ARG
64	MM	49	LEU
64	MM	55	ASN
64	MM	83	LYS

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Mol	Chain	Res	Type
64	MM	85	LEU
64	MM	96	ARG
64	MM	101	ARG
64	MM	112	LYS
65	NN	3	ARG
65	NN	20	ARG
65	NN	27	LYS
65	NN	46	THR
65	NN	55	ARG
65	NN	60	VAL
65	NN	75	LEU
65	NN	78	LYS
65	NN	84	LEU
65	NN	107	LYS
65	NN	132	LYS
65	NN	134	VAL
66	OO	25	GLU
66	OO	34	PHE
66	OO	38	ASN
66	OO	50	LYS
66	OO	51	GLU
66	OO	56	VAL
66	OO	76	LEU
66	OO	85	CYS
66	OO	119	LEU
66	OO	128	ARG
66	OO	131	ASP
66	OO	143	LYS
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	27	ASP
67	PP	37	TYR
67	PP	42	ARG
67	PP	44	ARG
67	PP	83	MET
67	PP	108	LYS
67	PP	111	MET
67	PP	130	ARG

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Mol	Chain	Res	Type
68	QQ	31	LEU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	48	GLN
68	QQ	60	LYS
68	QQ	123	ASP
68	QQ	140	ARG
69	RR	3	ARG
69	RR	5	ARG
69	RR	30	THR
69	RR	31	ASN
69	RR	35	CYS
69	RR	44	LYS
69	RR	58	MET
69	RR	121	GLN
69	RR	132	ARG
70	SS	8	LYS
70	SS	23	ARG
70	SS	46	ARG
70	SS	52	LEU
70	SS	59	LEU
70	SS	62	ASP
70	SS	63	GLU
70	SS	69	THR
70	SS	75	ARG
70	SS	83	PHE
70	SS	110	ASP
70	SS	121	ARG
70	SS	132	ARG
70	SS	136	THR
71	TT	62	ARG
71	TT	75	MET
71	TT	102	ARG
71	TT	108	GLU
71	TT	110	LEU
71	TT	121	ARG
71	TT	124	THR
71	TT	142	LYS
72	UU	55	ARG
72	UU	56	MET
72	UU	79	ARG
72	UU	88	LEU

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Mol	Chain	Res	Type
72	UU	106	ILE
72	UU	111	GLU
73	VV	12	TYR
73	VV	32	ILE
73	VV	66	ASP
73	VV	68	SER
74	WW	12	LYS
74	WW	23	ARG
74	WW	28	ARG
74	WW	36	ARG
74	WW	51	GLU
74	WW	92	ASN
74	WW	103	VAL
74	WW	104	LEU
74	WW	117	ARG
75	XX	29	LYS
75	XX	67	ARG
75	XX	82	THR
75	XX	105	PHE
75	XX	115	ILE
75	XX	129	SER
76	YY	16	ARG
76	YY	17	LEU
76	YY	20	ARG
76	YY	32	LYS
76	YY	38	THR
76	YY	40	ILE
76	YY	47	MET
76	YY	50	THR
76	YY	61	ARG
76	YY	74	MET
76	YY	79	LEU
76	YY	88	LYS
76	YY	93	ARG
76	YY	100	LYS
76	YY	101	LYS
76	YY	115	LYS
77	ZZ	80	ARG
77	ZZ	89	GLN
77	ZZ	92	LEU
77	ZZ	104	ARG
78	aa	15	ARG

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Mol	Chain	Res	Type
78	aa	21	ILE
78	aa	34	LYS
78	aa	41	ILE
78	aa	44	ILE
78	aa	55	GLU
78	aa	100	ARG
79	bb	17	ARG
79	bb	34	ASP
79	bb	36	LYS
79	bb	37	CYS
79	bb	42	LYS
79	bb	80	ARG
79	bb	81	ARG
80	cc	27	CYS
80	cc	28	THR
80	cc	31	ARG
80	cc	40	ARG
80	cc	44	ARG
81	dd	20	SER
82	ee	97	LYS
82	ee	99	LYS
82	ee	107	ARG
82	ee	113	ARG
83	ff	83	LYS
83	ff	94	LYS
83	ff	99	LYS
83	ff	138	ARG
83	ff	140	TYR
84	gg	17	TRP
84	gg	20	GLN
84	gg	38	LYS
84	gg	79	LEU
84	gg	119	GLN
84	gg	198	VAL
84	gg	207	CYS
84	gg	289	LEU
84	gg	306	LEU
86	ii	16	LYS
86	ii	61	ASN
86	ii	63	LYS
86	ii	65	ARG
86	ii	82	LEU

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Mol	Chain	Res	Type
86	ii	103	GLU
86	ii	111	ASN
86	ii	180	HIS
86	ii	189	ARG
86	ii	211	GLN
86	ii	212	LEU
86	ii	232	PHE
86	ii	241	MET
86	ii	291	PHE
86	ii	300	LYS
86	ii	330	ARG
86	ii	339	GLU
86	ii	341	GLU
86	ii	368	LEU
86	ii	380	ASN
86	ii	381	ASN
86	ii	417	VAL
87	jj	231	GLN
87	jj	249	ARG
87	jj	292	PHE
87	jj	340	GLU
87	jj	343	MET
87	jj	353	LEU
87	jj	382	PHE
87	jj	392	LYS
87	jj	413	PHE
87	jj	447	LYS
87	jj	455	VAL
87	jj	468	GLN
87	jj	509	GLU
87	jj	511	GLU
87	jj	551	VAL
87	jj	601	ILE
87	jj	611	GLN
87	jj	618	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	191	ASN
7	G	135	GLN
8	H	78	GLN

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Mol	Chain	Res	Type
12	M	20	HIS
12	M	48	GLN
13	N	32	GLN
15	P	137	ASN
24	Y	14	ASN
24	Y	56	GLN
28	c	78	ASN
29	d	30	HIS
32	g	14	ASN
42	r	70	GLN
42	r	103	HIS
43	s	34	ASN
53	BB	158	HIS
54	CC	113	GLN
54	CC	235	ASN
56	EE	36	HIS
56	EE	142	HIS
56	EE	260	GLN
57	FF	118	ASN
58	GG	13	GLN
59	HH	114	GLN
59	HH	162	GLN
61	JJ	154	GLN
68	QQ	142	GLN
79	bb	49	HIS
80	cc	26	GLN
86	ii	67	ASN
86	ii	170	HIS
86	ii	380	ASN
87	jj	214	ASN
87	jj	313	GLN
87	jj	428	ASN
87	jj	499	ASN
87	jj	523	ASN
87	jj	555	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	13 (17%)	0
47	3	72/75 (96%)	22 (30%)	2 (2%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
48	5	3514/3543 (99%)	876 (24%)	169 (4%)
49	7	119/120 (99%)	14 (11%)	2 (1%)
50	8	149/156 (95%)	32 (21%)	6 (4%)
51	9	1679/1869 (89%)	422 (25%)	71 (4%)
85	hh	14/15 (93%)	8 (57%)	0
All	All	5621/5854 (96%)	1387 (24%)	250 (4%)

All (1387) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
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	46	G
46	2	47	U
46	2	49	C
46	2	58	A
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	58	A
47	3	60	U
47	3	61	C
47	3	63	C

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Mol	Chain	Res	Type
47	3	65	G
47	3	72	C
47	3	76	A
48	5	12	A
48	5	13	U
48	5	15	A
48	5	25	A
48	5	35	U
48	5	39	A
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	72	C
48	5	73	A
48	5	91	G
48	5	93	G
48	5	109	G
48	5	110	C
48	5	118	C
48	5	119	G
48	5	120	A
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	137	G
48	5	143	C
48	5	144	G
48	5	159	C
48	5	160	G
48	5	172	C
48	5	173	C
48	5	177	G
48	5	179	G
48	5	197	A

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Mol	Chain	Res	Type
48	5	200	U
48	5	201	C
48	5	202	C
48	5	205	C
48	5	209	U
48	5	216	C
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	263	G
48	5	266	C
48	5	267	G
48	5	276	C
48	5	279	A
48	5	280	G
48	5	281	U
48	5	297	U
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	322	C
48	5	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

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Mol	Chain	Res	Type
48	5	399	G
48	5	406	C
48	5	407	A
48	5	408	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	414	C
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	455	C
48	5	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	481	G
48	5	481(A)	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	649	A
48	5	654	C
48	5	658	C

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Mol	Chain	Res	Type
48	5	666	G
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
48	5	708	G
48	5	719	C
48	5	722	G
48	5	729	G
48	5	730	G
48	5	731	G
48	5	738	C
48	5	738(A)	C
48	5	739	G
48	5	747	A
48	5	748	G
48	5	749	G
48	5	750	U
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	915	A
48	5	916	C
48	5	917	A
48	5	918	G
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	928	C
48	5	929	A
48	5	931	C
48	5	932	A
48	5	933	G

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Mol	Chain	Res	Type
48	5	934	C
48	5	935	A
48	5	935(A)	G
48	5	936	C
48	5	938	C
48	5	939	G
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
48	5	962	C
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C
48	5	969	C
48	5	970	G
48	5	972	C
48	5	973	G
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	1194	G
48	5	1195	G
48	5	1211	G
48	5	1212	G

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Mol	Chain	Res	Type
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
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	1354	A
48	5	1359	G
48	5	1360	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1379	C
48	5	1380	G
48	5	1381	U
48	5	1387	A

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Mol	Chain	Res	Type
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1403	G
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
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	1477	C
48	5	1478	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1486	C
48	5	1489	G
48	5	1493	G
48	5	1497	A
48	5	1498	G
48	5	1501	C
48	5	1502	G
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A

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Mol	Chain	Res	Type
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	1574	G
48	5	1578	U
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1601	A
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
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	1691	G
48	5	1724	G
48	5	1726	U
48	5	1734	G
48	5	1735	U
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

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Mol	Chain	Res	Type
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	1780	A
48	5	1781	U
48	5	1787	A
48	5	1797	G
48	5	1799	G
48	5	1800	U
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1819	G
48	5	1820	U
48	5	1821	G
48	5	1822	U
48	5	1823	G
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	1867	A
48	5	1869	G
48	5	1882	U
48	5	1883	G
48	5	1893	C
48	5	1897	A
48	5	1910	G
48	5	1918	U
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A

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Mol	Chain	Res	Type
48	5	1931	C
48	5	1933	G
48	5	1941	A
48	5	1945	G
48	5	1948	G
48	5	1951	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	1979	A
48	5	1980	U
48	5	1981	G
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	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	2044	U
48	5	2046	G
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G

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Mol	Chain	Res	Type
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
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	2278	G
48	5	2279	A
48	5	2288	G
48	5	2289	C
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2322	G

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Mol	Chain	Res	Type
48	5	2331	G
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2357	G
48	5	2364	G
48	5	2370	A
48	5	2395	A
48	5	2396	A
48	5	2399	G
48	5	2402	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
48	5	2429	A
48	5	2433	G
48	5	2441	C
48	5	2450	G
48	5	2469	C
48	5	2470	C
48	5	2471	G
48	5	2475	G
48	5	2479	G
48	5	2483	G
48	5	2485	U
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	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

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Mol	Chain	Res	Type
48	5	2546	G
48	5	2547	G
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2571	C
48	5	2575	U
48	5	2583	C
48	5	2586	G
48	5	2587	A
48	5	2601	A
48	5	2618	G
48	5	2620	G
48	5	2623	A
48	5	2627	C
48	5	2638	G
48	5	2640	G
48	5	2647	A
48	5	2661	U
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2670	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

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Mol	Chain	Res	Type
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2740	U
48	5	2743	A
48	5	2744	A
48	5	2754	G
48	5	2755	A
48	5	2760	G
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2772	C
48	5	2787	A
48	5	2788	U
48	5	2789	A
48	5	2790	U
48	5	2794	C
48	5	2795	A
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2808	G
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	2845	A
48	5	2855	G
48	5	2864	A
48	5	2875	C
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C

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Mol	Chain	Res	Type
48	5	3599	A
48	5	3604	A
48	5	3605	C
48	5	3615	G
48	5	3625	G
48	5	3626	G
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3662	A
48	5	3671	G
48	5	3673	C
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	3750	G
48	5	3753	G
48	5	3756	A
48	5	3759	A
48	5	3760	A
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	3783	A
48	5	3784	A
48	5	3785	A
48	5	3786	U
48	5	3799	A
48	5	3810	C
48	5	3811	G

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Mol	Chain	Res	Type
48	5	3812	C
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	3851	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	3889	G
48	5	3892	U
48	5	3897	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
48	5	3927	U
48	5	3939	G
48	5	3943	A
48	5	4067	U
48	5	4069	U
48	5	4071	U
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U

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Mol	Chain	Res	Type
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	4168	G
48	5	4171	C
48	5	4183	G
48	5	4184	G
48	5	4190	U
48	5	4191	G
48	5	4203	A
48	5	4212	A
48	5	4213	A
48	5	4218	U
48	5	4219	A
48	5	4225	G
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

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Mol	Chain	Res	Type
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	4376	A
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4393	G
48	5	4394	A
48	5	4395	U
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	4464	A
48	5	4471	U
48	5	4475	G
48	5	4476	C
48	5	4488	A

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Mol	Chain	Res	Type
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	4519	C
48	5	4520	G
48	5	4524	G
48	5	4528	G
48	5	4531	U
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4578	G
48	5	4584	A
48	5	4586	G
48	5	4590	A
48	5	4618	G
48	5	4627	U
48	5	4636	U
48	5	4637	G
48	5	4639	G
48	5	4656	A
48	5	4657	U
48	5	4661	G
48	5	4667	C
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4678	G
48	5	4687	A
48	5	4694	G
48	5	4700	A
48	5	4701	A
48	5	4709	U
48	5	4719	G
48	5	4720	C

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Mol	Chain	Res	Type
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
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	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G
48	5	4918	C
48	5	4919	G
48	5	4921	C
48	5	4924	C
48	5	4925	U
48	5	4926	C

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Mol	Chain	Res	Type
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	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
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	5007	A
48	5	5014	A
48	5	5017	G
48	5	5035	U
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5052	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5061	A
48	5	5062	G
49	7	7	G
49	7	11	A
49	7	22	A

Continued on next page...

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Mol	Chain	Res	Type
49	7	33	U
49	7	42	A
49	7	53	U
49	7	54	A
49	7	64	G
49	7	97	G
49	7	100	A
49	7	106	G
49	7	110	G
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	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

Continued on next page...

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Mol	Chain	Res	Type
50	8	143	G
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	41	G
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	62	G
51	9	65	C
51	9	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	129	C
51	9	130	G
51	9	141	A

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Mol	Chain	Res	Type
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	173	A
51	9	175	A
51	9	182	C
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	191	A
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	289	G
51	9	292	A
51	9	293	C
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	314	U
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	340	C
51	9	347	G

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Mol	Chain	Res	Type
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	371	A
51	9	372	U
51	9	381	C
51	9	382	C
51	9	383	G
51	9	384	U
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G
51	9	409	C
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	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	507	G
51	9	508	A
51	9	512	A
51	9	516	A

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Mol	Chain	Res	Type
51	9	525	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
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	597	G
51	9	598	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	614	C
51	9	620	G
51	9	629	A
51	9	631	U
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	659	G

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Mol	Chain	Res	Type
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	684	G
51	9	688	U
51	9	689	U
51	9	732	U
51	9	733	C
51	9	752	G
51	9	753	C
51	9	754	G
51	9	810	A
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	834	C
51	9	847	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	913	A
51	9	914	U
51	9	920	A

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Mol	Chain	Res	Type
51	9	922	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	955	A
51	9	971	G
51	9	985	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1002	U
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1045	U
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1078	C
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1096	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	1133	A
51	9	1138	C
51	9	1139	C
51	9	1148	A
51	9	1149	A
51	9	1150	A
51	9	1153	C
51	9	1154	U

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Mol	Chain	Res	Type
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1197	G
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1213	C
51	9	1215	C
51	9	1216	C
51	9	1221	G
51	9	1223	A
51	9	1224	G
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	1259	A
51	9	1260	A
51	9	1265	A
51	9	1266	C
51	9	1270	G
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	1293	A
51	9	1298	G
51	9	1299	A
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1307	U
51	9	1308	U

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Mol	Chain	Res	Type
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1330	G
51	9	1331	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	1439	A
51	9	1449	G
51	9	1452	A
51	9	1454	A
51	9	1458	G
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	1490	G
51	9	1494	U
51	9	1497	G
51	9	1498	A
51	9	1507	G
51	9	1509	U
51	9	1510	G

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Mol	Chain	Res	Type
51	9	1519	U
51	9	1521	C
51	9	1522	A
51	9	1531	A
51	9	1533	A
51	9	1536	G
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	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	1582	C
51	9	1585	U
51	9	1586	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	1623	A
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1639	G
51	9	1641	A
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G

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Mol	Chain	Res	Type
51	9	1671	G
51	9	1680	G
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1700	C
51	9	1703	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	1737	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	1823	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	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A

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Mol	Chain	Res	Type
51	9	1867	U
51	9	1868	U
51	9	1869	A
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G
85	hh	49	U
85	hh	52	G
85	hh	54	U
85	hh	55	C

All (250) 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	125	C
48	5	134	G
48	5	143	C
48	5	159	C
48	5	217	C
48	5	226	G
48	5	234	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	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	480	C
48	5	481(A)	C

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Mol	Chain	Res	Type
48	5	482	G
48	5	484	U
48	5	485	C
48	5	492	U
48	5	497	G
48	5	498	C
48	5	504	G
48	5	696	C
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	748	G
48	5	915	A
48	5	916	C
48	5	922(B)	C
48	5	930	G
48	5	935(A)	G
48	5	936	C
48	5	955	G
48	5	956	A
48	5	959	G
48	5	965	G
48	5	966	A
48	5	969	C
48	5	971(A)	G
48	5	1071	C
48	5	1072	C
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	1294	A
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

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Mol	Chain	Res	Type
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1481	C
48	5	1484	G
48	5	1485	C
48	5	1497	A
48	5	1563	A
48	5	1633	G
48	5	1678	C
48	5	1733	G
48	5	1734	G
48	5	1740	C
48	5	1804	A
48	5	1815	G
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1881	C
48	5	1892	A
48	5	1921	C
48	5	1935	C
48	5	1947	U
48	5	1979	A
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2003	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	2398	U
48	5	2428	A

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Mol	Chain	Res	Type
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	2587	A
48	5	2661	U
48	5	2695	A
48	5	2741	U
48	5	2754	G
48	5	2794	C
48	5	2806	A
48	5	3625	G
48	5	3673	C
48	5	3697	U
48	5	3710	G
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	4116	C
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	4257	A
48	5	4266	G
48	5	4331	G
48	5	4378	A
48	5	4379	A
48	5	4395	U
48	5	4448	G
48	5	4449	A

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Mol	Chain	Res	Type
48	5	4510	A
48	5	4527	G
48	5	4572	U
48	5	4626	A
48	5	4699	U
48	5	4719	G
48	5	4753	U
48	5	4871	C
48	5	4872	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	4949	G
48	5	4965	U
48	5	4966	A
49	7	10	C
49	7	109	U
50	8	2	G
50	8	51	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	160	U
51	9	182	C
51	9	293	C
51	9	308	G
51	9	369	C
51	9	370	G
51	9	434	G
51	9	448	A
51	9	465	A
51	9	473	A

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Mol	Chain	Res	Type
51	9	487	U
51	9	500	A
51	9	532	C
51	9	550	C
51	9	553	U
51	9	555	A
51	9	563	G
51	9	591	U
51	9	606	G
51	9	620	G
51	9	642	U
51	9	656	G
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	1016	U
51	9	1114	U
51	9	1115	U
51	9	1120	U
51	9	1137	U
51	9	1165	G
51	9	1215	C
51	9	1253	A
51	9	1264	C
51	9	1284	A
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	1476	A
51	9	1489	A
51	9	1493	C
51	9	1519	U
51	9	1520	G
51	9	1535	U

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Mol	Chain	Res	Type
51	9	1585	U
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1664	A
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1826	G
51	9	1835	A
51	9	1867	U
51	9	1868	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 291 ligands modelled in this entry, 290 are monoatomic - leaving 1 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	jj	700	88	29,34,34	2.66	9 (31%)	31,54,54	1.17	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	jj	700	88	-	0/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C4-N9	-10.50	1.33	1.47
90	jj	700	GCP	C8-N9	-3.75	1.35	1.47
90	jj	700	GCP	PG-O3G	-2.66	1.48	1.54
90	jj	700	GCP	C5-C6	-2.15	1.49	1.53
90	jj	700	GCP	C2-N1	-2.03	1.35	1.44
90	jj	700	GCP	PB-O3A	2.12	1.60	1.58
90	jj	700	GCP	PG-O2G	2.72	1.61	1.54
90	jj	700	GCP	C1'-N9	3.57	1.48	1.42
90	jj	700	GCP	PG-O1G	5.06	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C4-C5-N7	2.57	106.68	102.67
90	jj	700	GCP	C8-N9-C4	3.63	108.92	104.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	30
51	9	7
47	3	2

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Mol	Chain	Number of breaks
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	41.06
1	5	1252:C	O3'	1271:G	P	35.64
1	5	1219:G	O3'	1233:G	P	22.79
1	5	3948:C	O3'	4065:G	P	19.75
1	5	1406(C):G	O3'	1411:C	P	18.65
1	5	990:C	O3'	1064:G	P	18.31
1	5	523:C	O3'	638:G	P	18.02
1	5	4138:C	O3'	4146:G	P	18.00
1	5	4101:C	O3'	4107:G	P	17.52
1	5	4777:C	O3'	4859:C	P	16.78
1	5	760:G	O3'	904:C	P	15.07
1	5	1696:C	O3'	1720:C	P	14.63
1	5	5022:U	O3'	5028:G	P	14.63
1	5	182:G	O3'	189:G	P	14.05
1	5	1364:U	O3'	1368:A	P	13.97
1	5	2901:G	O3'	3597:G	P	13.29
1	5	512:U	O3'	515:C	P	9.99
1	5	4729:A	O3'	4735:G	P	9.79
1	5	1180:C	O3'	1183:C	P	9.09
1	5	500:G	O3'	504:G	P	6.73
1	5	1100:U	O3'	1168:G	P	5.98
1	3	19:G	O3'	20:U	P	5.77
1	5	1239:C	O3'	1244:G	P	5.36
1	9	322:C	O3'	323:C	P	5.19
1	5	4740:G	O3'	4743:G	P	4.87
1	3	16:C	O3'	18:U	P	4.79
1	2	16:C	O3'	18:G	P	4.35
1	9	309:G	O3'	310:C	P	4.34
1	9	798:G	O3'	799:U	P	4.27
1	9	304:C	O3'	305:U	P	4.18
1	5	170:C	O3'	171:U	P	3.77
1	9	902:G	O3'	903:A	P	3.43
1	5	1438:U	O3'	1440:U	P	3.34
1	9	903:A	O3'	904:A	P	3.33
1	5	4899:G	O3'	4902:C	P	3.32
1	9	1295:A	O3'	1296:U	P	3.24
1	5	5020:G	O3'	5021:C	P	3.16
1	5	267:G	O3'	268:G	P	3.15

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	751:G	O3'	752:G	P	3.15
1	5	2031:C	O3'	2032:U	P	2.55