



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 17, 2017 – 01:38 PM EDT

PDB ID : 5LZZ  
EMDB ID: : EMD-4137  
Title : Structure of the mammalian rescue complex with Pelota and Hbs1l (combined)  
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.  
Deposited on : unknown  
Resolution : 3.47 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](mailto: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 : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

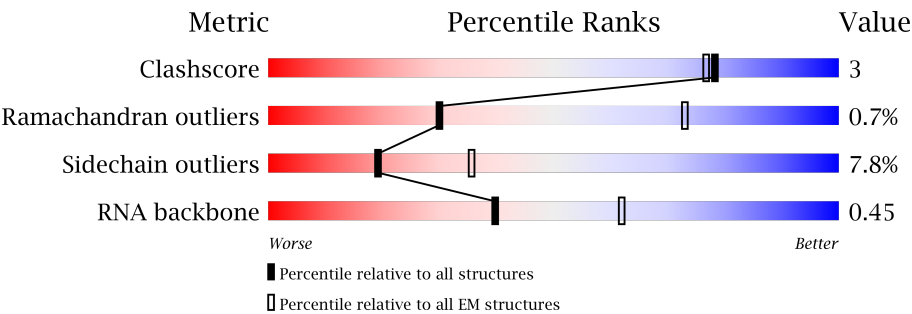


# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.47 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335


















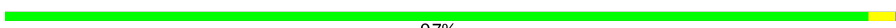







The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of 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	<div><div>79%</div><div>16%</div><div>.</div><div>.</div></div>
2	B	403	<div><div>80%</div><div>17%</div><div>.</div><div>.</div></div>
3	C	425	<div><div>69%</div><div>15%</div><div>.</div><div>15%</div></div>
4	D	297	<div><div>88%</div><div>9%</div><div>.</div><div>.</div></div>
5	E	291	<div><div>68%</div><div>.</div><div>.</div><div>26%</div></div>
6	F	247	<div><div>74%</div><div>17%</div><div>.</div><div>9%</div></div>
7	G	319	<div><div>64%</div><div>8%</div><div>.</div><div>27%</div></div>
8	H	192	<div><div>82%</div><div>16%</div><div>.</div><div>.</div></div>

Continued on next page...









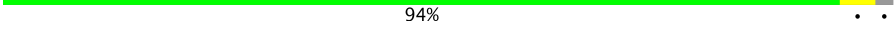




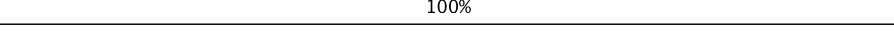







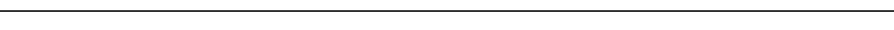

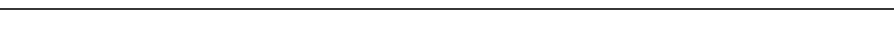
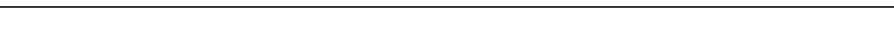


Continued from previous page...

Mol	Chain	Length	Quality of chain
9	I	214	 84% 11% . .
10	J	178	 82% 12% . .
11	L	211	 91% 8%
12	M	218	 54% 8% . 37%
13	N	204	 85% 13% .
14	O	203	 79% 16% . .
15	P	184	 72% 9% . 17%
16	Q	188	 84% 15% .
17	R	196	 77% 15% . 8%
18	S	176	 81% 18% .
19	T	160	 83% 16% ..
20	U	128	 66% 10% . 23%
21	V	140	 78% 15% . 6%
22	W	157	 61% 7% 32%
23	X	156	 71% 5% 24%
24	Y	145	 81% 11% . 8%
25	Z	136	 86% 13% .
26	a	148	 97% . .
27	b	245	 40% . 58%
28	c	115	 79% 6% 15%
29	d	125	 74% 11% 14%
30	e	135	 89% 6% 5%
31	f	110	 90% 9% .
32	g	117	 91% 6% .
33	h	123	 95% . .

Continued on next page...




























Continued from previous page...

Mol	Chain	Length	Quality of chain
34	i	105	 93% . .
35	j	97	 82% 6% 11%
36	k	70	 93% 6% .
37	l	51	 94% . .
38	m	102	 47% . 49%
39	n	25	 92% 8%
40	o	106	 94% . .
41	p	92	 92% 7% .
42	r	137	 80% 11% 9%
43	s	318	 59% . 38%
44	t	165	 89% . 7%
45	1	7	 100%
46	2	76	 79% 20% .
47	3	75	 68% 29% .
48	5	3543	 67% 28% 5%
49	7	120	 81% 19%
50	8	156	 63% 30% . .
51	9	1869	 58% 28% . 9%
52	AA	295	 58% 15% . 26%
53	BB	264	 67% 13% . 19%
54	CC	293	 63% 12% 25%
55	DD	243	 82% 11% . 6%
56	EE	263	 84% 16%
57	FF	204	 80% 9% . 9%
58	GG	249	 81% 14% 5%

Continued on next page...



Continued from previous page...

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	

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
84	gg	317	<div><div></div><div>93%</div><div>6% •</div></div>
85	hh	8	<div><div></div><div>50%</div><div>50%</div></div>
86	ii	403	<div><div></div><div>88%</div><div>• 8%</div></div>
87	jj	710	<div><div></div><div>56%</div><div>• 40%</div></div>



## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 222005 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called uL4.

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

- Molecule 4 is a protein called 60S ribosomal protein L5.

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	-	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called 60S ribosomal protein L6.



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 Uncharacterized protein.

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 60S ribosomal protein L7a,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 Ribosomal protein L10 (Predicted).

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 Ribosomal protein L15.

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 60S ribosomal protein L27.

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

- Molecule 26 is a protein called uL15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.



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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called 60S ribosomal protein L36.

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 Ribosomal protein L37.

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	7	Total	C	N	O	0	0
			49	31	8	10		

- 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 40S ribosomal protein S3a.

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 Uncharacterized protein.

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 40S ribosomal protein S6.



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 40S ribosomal protein S8.

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 Ribosomal protein S9 (Predicted).

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 Uncharacterized protein.

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 Uncharacterized protein.

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 40S ribosomal protein S12.



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 40S ribosomal protein S24.

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 40S ribosomal protein S27.

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.

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

- Molecule 86 is a protein called Protein pelota homolog.

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

There are 19 discrepancies between the modelled and reference sequences:

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

- Molecule 87 is a protein called HBS1-like protein.

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



There are 26 discrepancies between the modelled and reference sequences:

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

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

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

*Continued on next page...*



*Continued from previous page...*

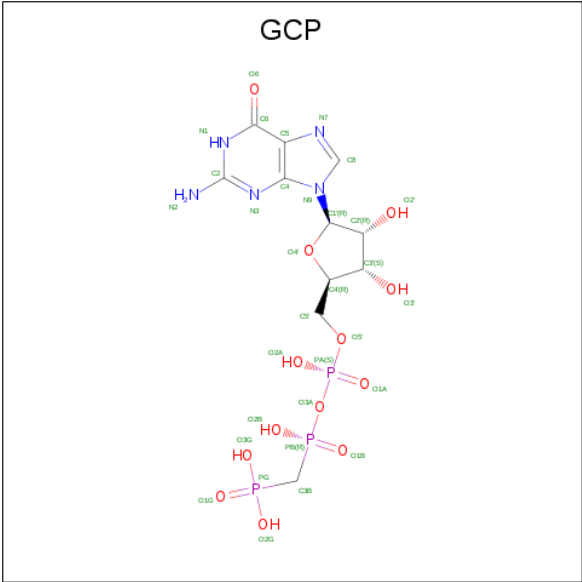
Mol	Chain	Residues	Atoms		AltConf
88	jj	1	Total 1	Mg 1	0
88	V	1	Total 1	Mg 1	0
88	7	5	Total 5	Mg 5	0
88	a	1	Total 1	Mg 1	0
88	5	178	Total 178	Mg 178	0
88	8	5	Total 5	Mg 5	0
88	9	66	Total 66	Mg 66	0
88	L	1	Total 1	Mg 1	0

- 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: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).





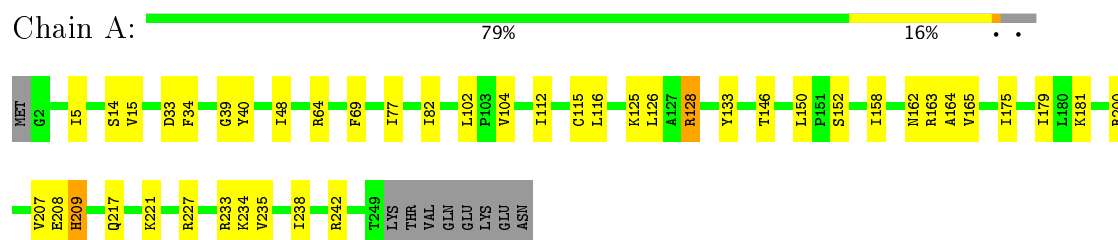
Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	



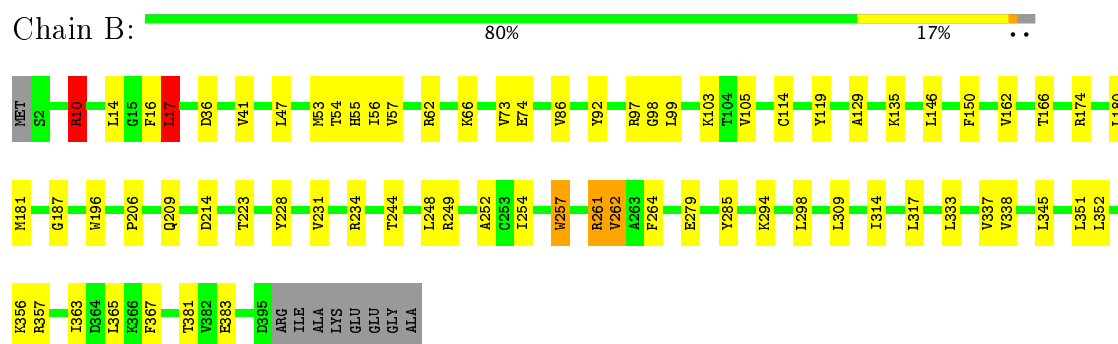
### 3 Residue-property plots

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

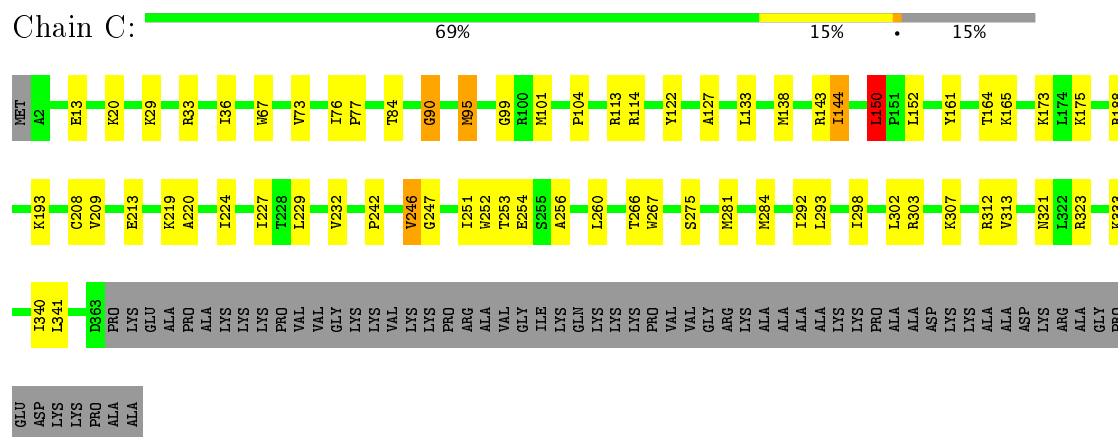
#### • Molecule 1: uL2



#### • Molecule 2: uL3



#### • Molecule 3: uL4



#### • Molecule 4: 60S ribosomal protein L5



- Molecule 5: 60S ribosomal protein L6


- Molecule 6: Uncharacterized protein

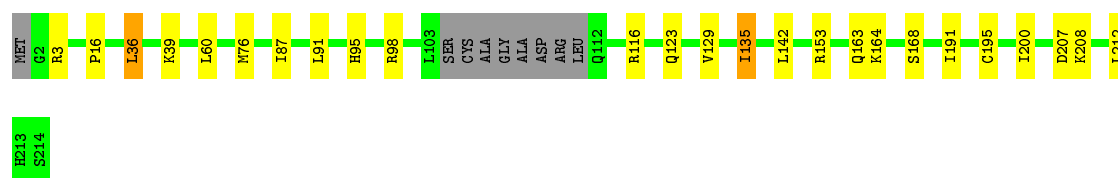
- Molecule 7: 60S ribosomal protein L7a,eL8

- Molecule 8: uL6


- Molecule 9: Ribosomal protein L10 (Predicted)



Chain I:  84% 11% . .



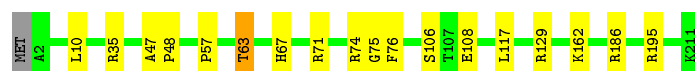
- Molecule 10: uL5

Chain J:  82% 12% . .



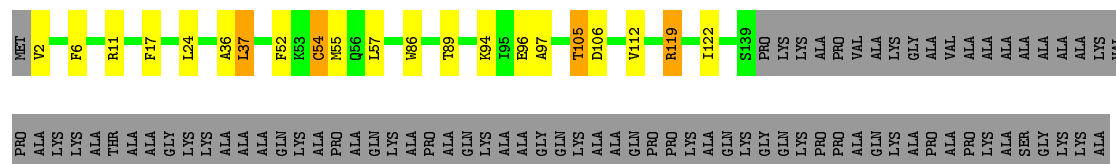
- Molecule 11: eL13

Chain L:  91% 8%




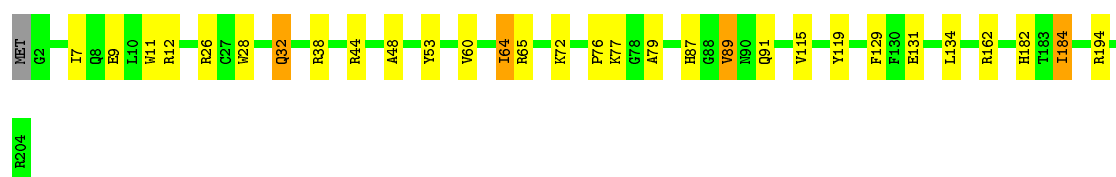
- Molecule 12: eL14

Chain M:  54% 8% 37%




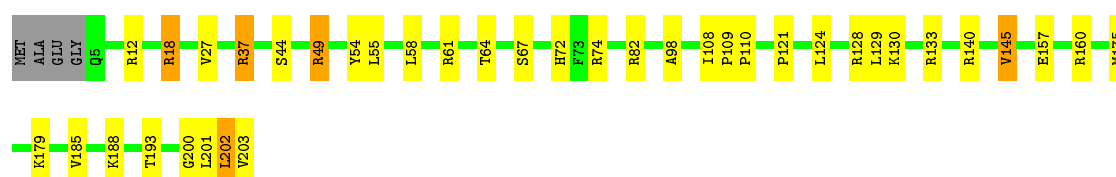
- Molecule 13: Ribosomal protein L15

Chain N:  85% 13% .



- Molecule 14: uL13

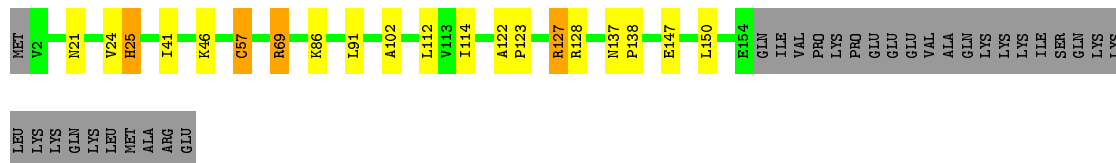
Chain O:  79% 16% . .






- Molecule 15: uL22

Chain P:  72% 9% 17%



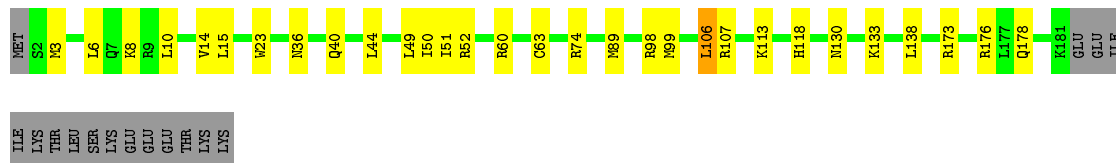
- Molecule 16: eL18

Chain Q:  84% 15%




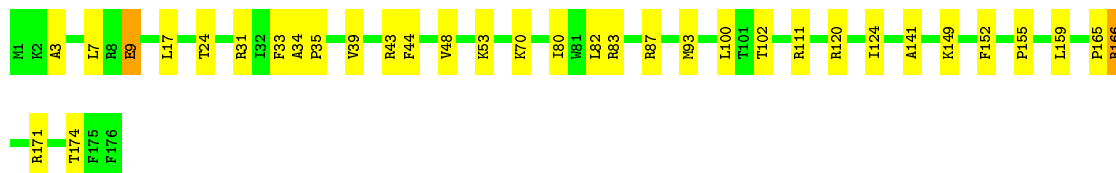
- Molecule 17: eL19

Chain R:  77% 15% 8%




- Molecule 18: eL20

Chain S:  81% 18%



- Molecule 19: eL21

Chain T:  83% 16%



- Molecule 20: eL22

Chain U:  66% 10% 23%

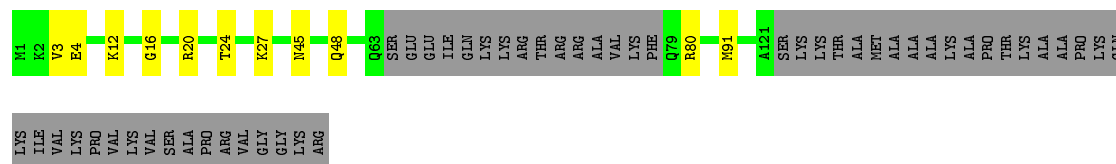


- Molecule 21: uL14

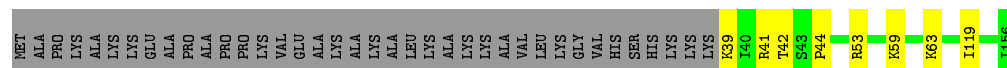





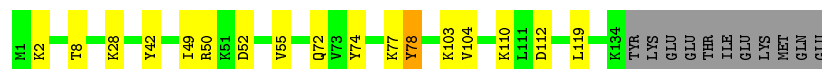
- Chain W:  61% 7% 32%

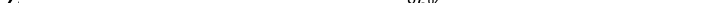


- Chain X:  71% 5% 24%



- Chain Y:  81% 11% 8%



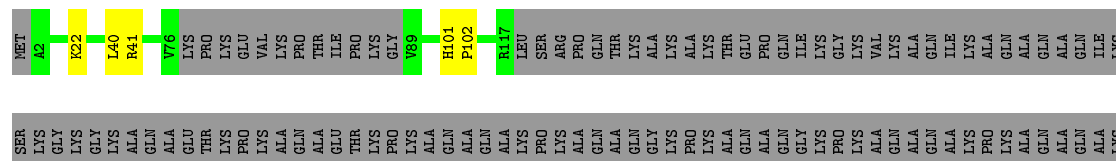
- Chain Z:  86% 13%



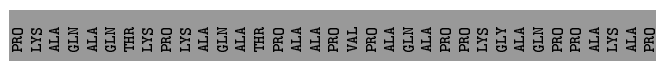
- Chain a:  97%



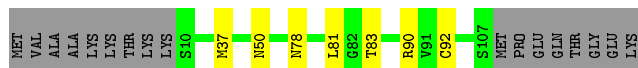
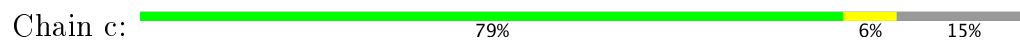
- Chain b:  40% . 58%







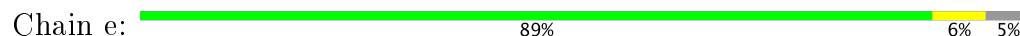
• Molecule 28: eL30



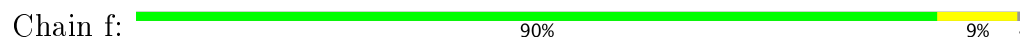
• Molecule 29: eL31



• Molecule 30: eL32



• Molecule 31: eL33



• Molecule 32: eL34



• Molecule 33: uL29




• Molecule 34: 60S ribosomal protein L36





- Molecule 35: Ribosomal protein L37

Chain j:  82% 6% 11%



- Molecule 36: eL38

Chain k:  93% 6% .



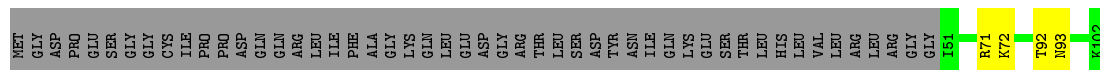
- Molecule 37: eL39

Chain l:  94% . .



- Molecule 38: eL40

Chain m:  47% . 49%



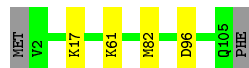
- Molecule 39: eL41

Chain n:  92% 8%



- Molecule 40: eL42

Chain o:  94% . .



- Molecule 41: eL43

Chain p:  92% 7% .



- Molecule 42: eL28

Chain r:  80% 11% 9%

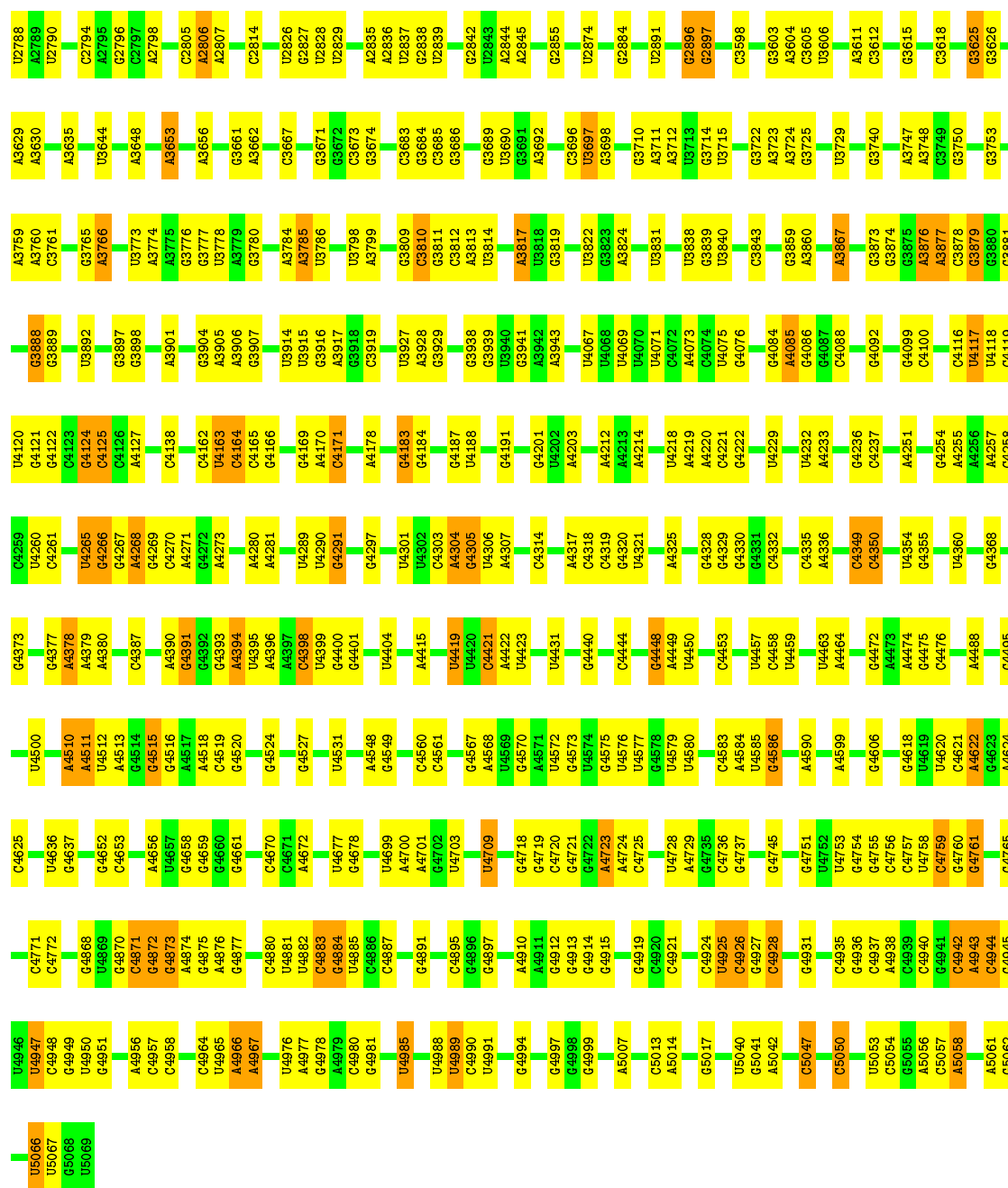






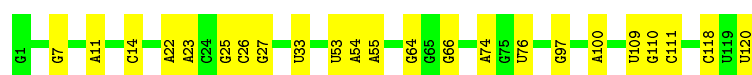
G2686	G2687	A2513	G2514	G2399	G2262	C2031	A1923	G1799	C1676	C1546	G1432	A1326	G1075	A917	G497	G387	G234
G2693	G2694	U2519	G2520	U2409	G2266	A2032	C1928	G1803	C1678	A1547	G1433	C1327	G1076	G918	C498	G399	A235
G2695	A2695	G2521	G2522	G2416	U2267	G2034	C1931	A1804	A1679	A1554	G1435	G1328	A1077	C922	G499	A400	G236
A2696	A2696	G2523	G2524	A2417	C2269	G2044	A1932	A1805	C1686	A1563	C1437	A1330	C1079	C922B	G504	G401	C245
C2704	U2707	U2524	A2529	G2421	G2270	G2045	C1935	G1813	C1686	A1564	U1438	A1337	C1082	C923	G647	U404	G246
U2708	C2709	A2530	G2422	C2423	G2274	G2046	C1938	G1819	C1686	A1565	U1440	G1338	G1174	C924	G648	U405	G253
C2710	G2711	U2537	G2424	U2425	G2275	A2047	C1939	U1820	C1686	A1566	U1441	G1339	G1177	C925	A406	A407	G262
G2712	G2713	C2540	A2428	G2433	C2278	U2048	U1939	U1821	C1694	U1567	C1442	C1340	U1177	G926	A649	A408	G265
G2714	G2715	G2546	G2429	U2441	G2279	G2052	U1947	U1822	G1724	U1577	U1445	G1353	G1178	A929	C654	A409	C266
G2716	G2717	G2547	G2430	U2442	A2279	G2055	G1948	C1828	A1729	U1578	C1446	A1354	U1179	C930	C658	A410	G267
C2719	C2720	U2548	U2549	G2439	G2280	G2056	G1951	G1833	C1733	G1586	G1453	G1358	G1195	C931	G666	G412	C275
G2721	G2722	C2540	G2540	U2441	U2281	A2057	G1952	U1834	G1733	G1591	G1454	G1359	U1209	C934	A667	A413	C276
G2723	G2724	G2546	G2547	G2439	C2289	C2062	G1961	G1835	G1734	U1591	G1455	U1364	C1210	A935	C668	G417	G277
G2725	G2726	G2548	G2549	U2441	C2292	G2063	A1962	G1836	C1740	U1596	G1456	G1370	G1212	C936	C672	G423	G278
C2729	U2730	U2553	U2554	U2447	U2293	G2064	A1963	U1837	G1741	A1600	G1457	G1371	G1213	U937	C683	G424	A279
G2724	A2725	G2555	G2555	G2450	G2294	C2068	C1966	G1842	A1742	A1601	G1458	G1377	C1214	C938	G684	U432	U281
G2726	G2727	G2556	G2556	G2451	G2297	A2069	A1967	G1846	U1744	U1602	C1477	G1378	C1215	C940	C685	U433	U297
G2729	U2730	U2557	U2557	G2452	G2300	C2072	G1976	G1847	A1746	U1613	C1478	G1380	G1234	C941	A686	A433	A306
A2725	G2726	G2558	G2558	G2453	G2301	C2081	C1977	G1848	U1747	A1613	C1479	G1381	G1235	A943	C696	G441	A307
G2730	G2731	G2559	G2559	G2454	A2307	G2082	C1978	G1849	G1748	A1630	G1481	G1385	C1236	U945	G697	G444	C309
G2732	G2733	G2560	G2560	U2467	G2313	C2083	U1980	G1854	A1749	G1624	G1482	G1386	C1237	U945	G704	U445	G310
G2734	G2735	G2561	G2561	U2468	G2314	U2084	G1981	G1855	G1750	G1625	G1483	G1387	C1239	G955	C705	U454	U321
G2736	G2737	G2562	G2562	U2469	G2325	G2085	G1982	G1856	G1753	G1626	G1484	G1388	C1280	A956	G705	U454	C322
G2738	G2739	G2563	G2563	U2470	G2326	A2088	A1983	G1857	U1754	G1627	G1485	G1390	G1272	A957	G706	U455	G315
G2740	G2741	G2564	G2564	U2471	G2327	G2089	A1984	G1858	C1755	G1628	G1486	G1391	G1273	A958	G707	U456	U316
G2742	G2743	G2565	G2565	U2472	G2328	G2090	A1985	G1859	U1756	G1629	G1487	G1392	G1274	A959	G708	U457	A317
G2744	G2745	G2566	G2566	U2473	G2329	G2091	C1986	G1860	U1757	G1630	G1488	G1393	G1275	A960	G709	U458	A318
G2746	G2747	G2567	G2567	U2474	G2330	C2092	C1987	G1861	G1761	G1631	G1489	G1394	G1276	A961	G710	U459	U321
G2748	G2749	G2568	G2568	U2475	G2331	G2093	A1988	G1862	C1762	G1632	G1490	G1395	G1277	A962	G711	U460	C322
G2750	G2751	G2569	G2569	U2476	G2332	G2094	A1989	G1863	G1763	G1633	G1491	G1396	G1278	A963	G712	U461	A334
G2752	G2753	G2570	G2570	U2477	G2333	C2095	C1990	G1864	G1764	G1634	G1492	G1397	G1279	A964	G713	U462	A335
G2754	G2755	G2571	G2571	U2478	G2334	G2096	C1991	G1865	G1765	G1635	G1493	G1398	G1280	A965	G714	U463	A336
G2756	G2757	G2572	G2572	U2479	G2335	G2097	C1992	G1866	G1766	G1636	G1494	G1399	G1281	A966	G715	U464	C340
G2758	G2759	G2573	G2573	U2480	G2336	G2098	C1993	G1867	G1767	G1637	G1495	G1400	G1282	A967	G716	U465	A347
G2760	G2761	G2574	G2574	U2481	G2337	G2099	C1994	G1868	G1768	G1638	G1496	G1401	G1283	A968	G717	U466	G350
G2762	G2763	G2575	G2575	U2482	G2338	G2100	C1995	G1869	G1769	G1639	G1497	G1402	G1284	A969	G718	U467	G356
G2764	G2765	G2576	G2576	U2483	G2339	G2101	C1996	G1870	G1770	G1640	G1498	G1403	G1285	A970	G719	U468	U357
G2766	G2767	G2577	G2577	U2484	G2340	G2102	C1997	G1871	G1771	G1641	G1499	G1404	G1286	A971	G720	U469	C361
G2768	G2769	G2578	G2578	U2485	G2341	G2103	C1998	G1872	G1772	G1642	G1500	G1405	G1287	A972	G721	U470	A362
G2770	G2771	G2579	G2579	U2486	G2342	G2104	C1999	G1873	G1773	G1643	G1501	G1406	G1288	A973	G722	U471	A363
G2772	G2773	G2580	G2580	U2487	G2343	G2105	C2000	G1874	G1774	G1644	G1502	G1407	G1289	A974	G723	U472	U365
G2774	G2775	G2581	G2581	U2488	G2344	G2106	C2001	G1875	G1775	G1645	G1503	G1408	G1290	A975	G724	U473	A385
G2776	G2777	G2582	G2582	U2489	G2345	G2107	C2002	G1876	G1776	G1646	G1504	G1409	G1291	A976	G725	U474	A386
G2778	G2779	G2583	G2583	U2490	G2346	G2108	C2003	G1877	G1777	G1647	G1505	G1410	G1292	A977	G726	U475	
G2780	G2781	G2584	G2584	U2491	G2347	G2109	C2004	G1878	G1778	G1648	G1506	G1411	G1293	A978	G727	U476	
G2782	G2783	G2585	G2585	U2492	G2348	G2110	C2005	G1879	G1779	G1649	G1507	G1412	G1294	A979	G728	U477	
G2784	G2785	G2586	G2586	U2493	G2349	G2111	C2006	G1880	G1780	G1650	G1508	G1413	G1295	A980	G729	U478	
G2786	G2787	G2587	G2587	U2494	G2350	G2112	C2007	G1881	G1781	G1651	G1509	G1414	G1296	A981	G730	U479	
G2788	G2789	G2588	G2588	U2495	G2351	G2113	C2008	G1882	G1782	G1652	G1510	G1415	G1297	A982	G731	U480	
G2790	G2791	G2589	G2589	U2496	G2352	G2114	C2009	G1883	G1783	G1653	G1511	G1416	G1298	A983	G732	U481	
G2792	G2793	G2590	G2590	U2497	G2353	G2115	C2010	G1884	G1784	G1654	G1512	G1417	G1299	A984	G733	U482	
G2794	G2795	G2591	G2591	U2498	G2354	G2116	C2011	G1885	G1785	G1655	G1513	G1418	G1300	A985	G734	U483	
G2796	G2797	G2592	G2592	U2499	G2355	G2117	C2012	G1886	G1786	G1656	G1514	G1419	G1301	A986	G735	U484	
G2798	G2799	G2593	G2593	U2500	G2356	G2118	C2013	G1887	G1787	G1657	G1515	G1420	G1302	A987	G736	U485	
G2800	G2801	G2594	G2594	U2501	G2357	G2119	C2014	G1888	G1788	G1658	G1516	G1421	G1303	A988	G737	U486	
G2802	G2803	G2595	G2595	U2502	G2358	G2120	C2015	G1889	G1789	G1659	G1517	G1422	G1304	A989	G738	U487	
G2804	G2805	G2596	G2596	U2503	G2359	G2121	C2016	G1890	G1790	G1660	G1518	G1423	G1305	A990	G739	U488	
G2806	G2807	G2597	G2597	U2504	G2360	G2122	C2017	G1891	G1791	G1661	G1519	G1424	G1306	A991	G740	U489	
G2808	G2809	G2598	G2598	U2505	G2361	G2123	C2018	G1892	G1792	G1662	G1520	G1425	G1307	A992	G741	U490	
G2810	G2811	G2599	G2599	U2506	G2362	G2124	C2019	G1893	G1793	G1663	G1521	G1426	G1308	A993	G742	U491	
G2812	G2813	G2600	G2600	U2507	G2363	G2125	C2020	G1894	G1794	G1664	G1522	G1427	G1309	A994	G743	U492	
G2814	G2815	G2601	G2601	U2508	G2364	G2126	C2021	G1895	G1795	G1665	G1523	G1428	G1310	A995	G744	U493	
G2816	G2817	G2602	G2602	U2509	G2365	G2127	C2022	G1896	G1796	G1666	G1524	G1429	G1311	A996	G745	U494	
G2818	G2819	G2603	G2603	U2510	G2366	G2128	C2023	G1897	G1797	G1667	G1525	G1430	G1312	A997	G746	U495	
G2820	G2821	G2604	G2604	U2511	G2367	G2129	C2024	G1898	G1798	G1668	G1526	G1431	G1313	A998	G747	U496	
G2822	G2823	G2605	G2605	U2512	G2368	G2130	C2025	G1899	G1799	G1669	G1527	G1432	G1314	A999	G748	U497	
G2824	G2825	G2606	G2606	U2513	G2369	G2131	C2026	G1900	G1800	G1670	G1528	G1433	G1315	A1000	G749	U498	
G2826	G2827	G2607	G2607	U2514	G2370	G2132	C2027	G1901	G1801	G1671	G1529	G1434	G1316	A1001	G750	U499	
G2828	G2829	G2608	G2608	U2515	G2371	G2133	C2028	G1902	G1802	G1672	G1530	G1435	G1317	A1002	G751	U500	
G2830	G2831	G2609	G2609	U2516	G2372	G2134	C2029	G1903	G1803	G1673	G1531	G1436	G1318	A1003	G752	U501	
G2832	G2833	G2610	G2610	U2517	G2373	G2135	C2030	G1904	G1804	G1674	G1532	G1437	G1319	A1004	G753	U502	
G2834	G2835	G2611	G2611	U2518	G2374	G2136	C2031	G1905	G1805	G1675	G1533	G1438	G1320	A1005	G754	U503	
G2836	G2837	G2612	G2612	U2519	G2375	G2137	C2032	G1906	G1806	G1676	G1534	G1439	G1321	A1006	G755	U504	
G2838	G2839	G2613	G2613	U2520	G2376	G2138	C2033	G1907	G1807	G1677	G1535	G1440	G1322	A1007	G756	U505	
G2840	G2841	G2614	G2614	U2521	G2377	G2139	C2034	G1908	G1808	G1678	G1536	G1441	G1323	A1008	G757	U506	
G2842	G2843	G2615	G2615	U2													





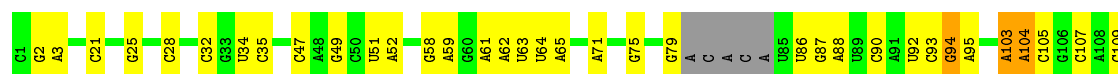
- Molecule 49: 5S ribosomal RNA

Chain 7: 81% 19%



- Molecule 50: 5.8S ribosomal RNA

Chain 8: 63% 30%

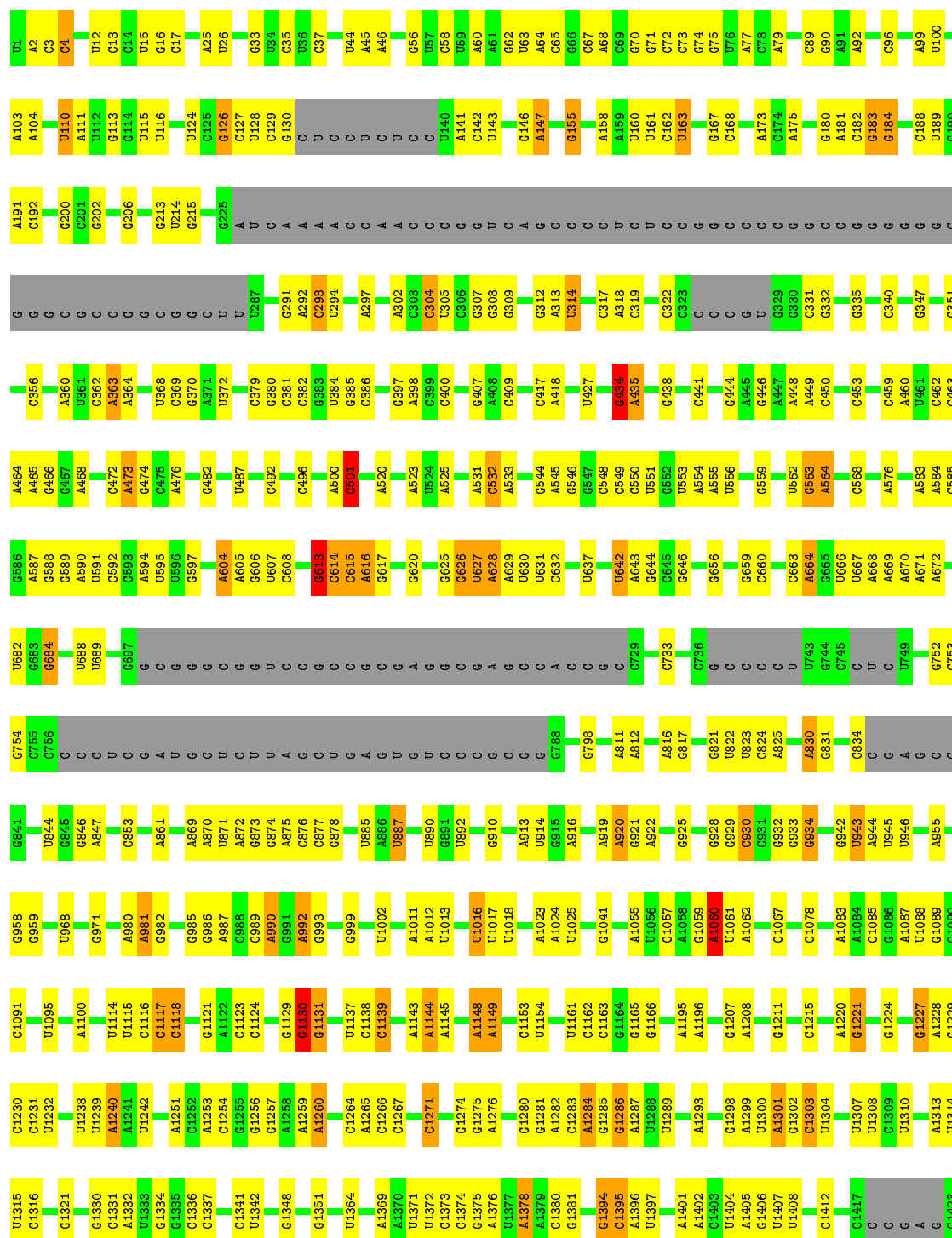






● Molecule 51: 18S ribosomal RNA

Chain 9: 58% 28% 9%

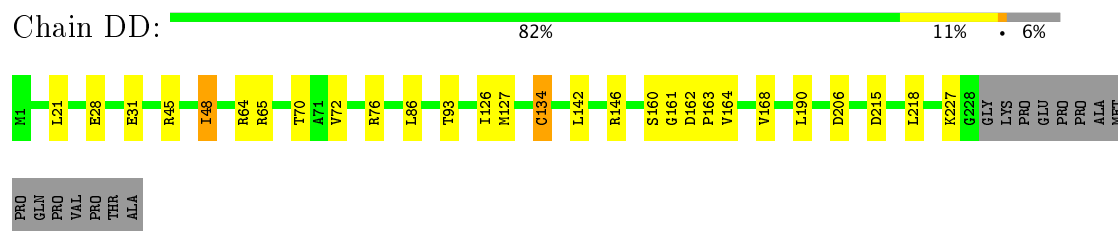




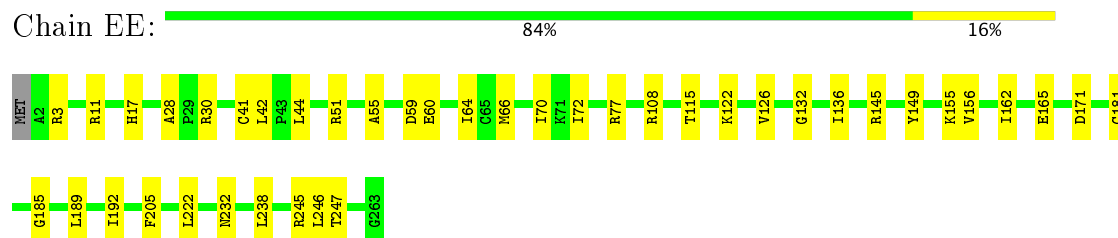




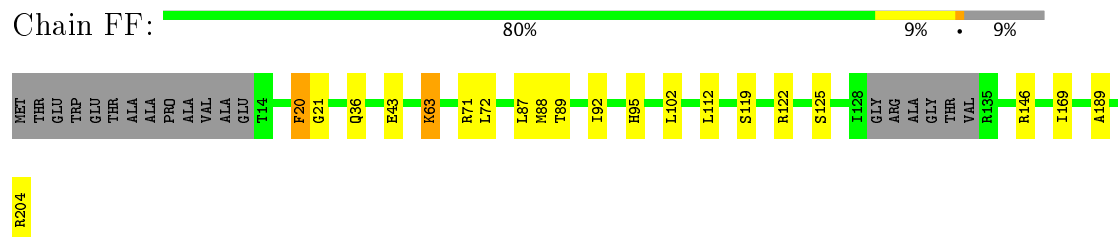
- Molecule 55: Uncharacterized protein



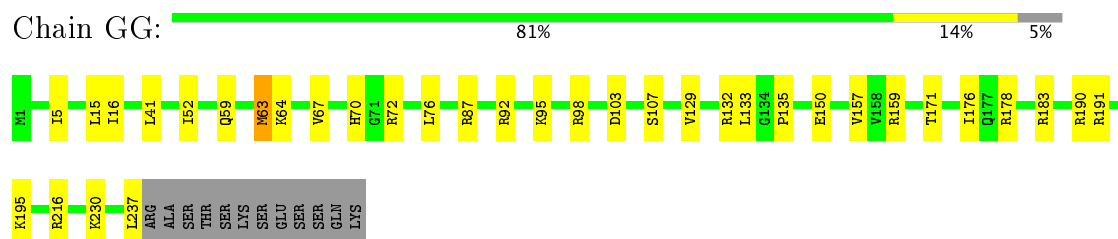
- Molecule 56: eS4



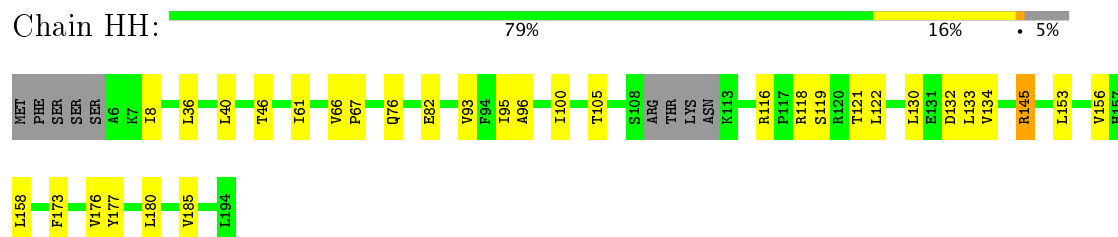
- Molecule 57: uS7



- Molecule 58: 40S ribosomal protein S6

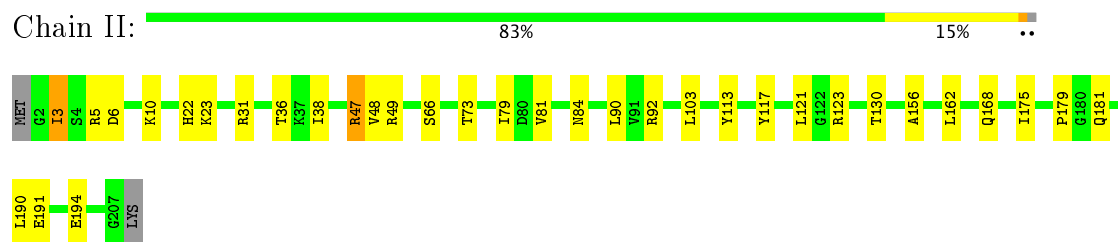


- Molecule 59: eS7

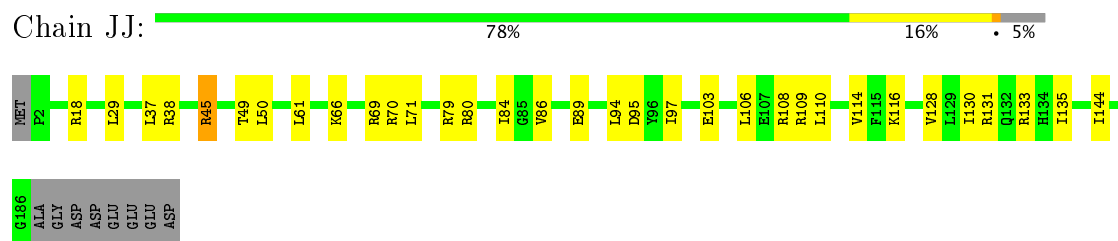


- Molecule 60: 40S ribosomal protein S8

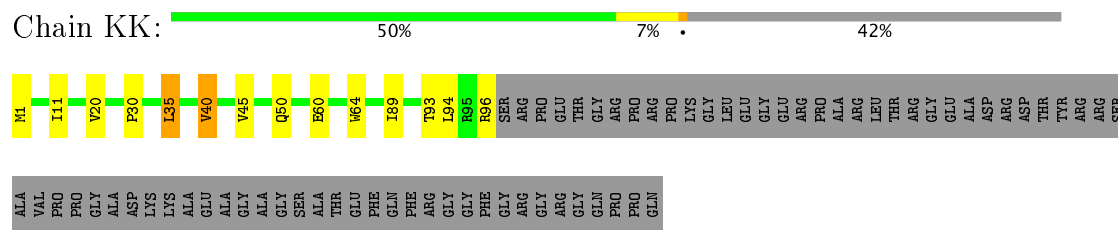




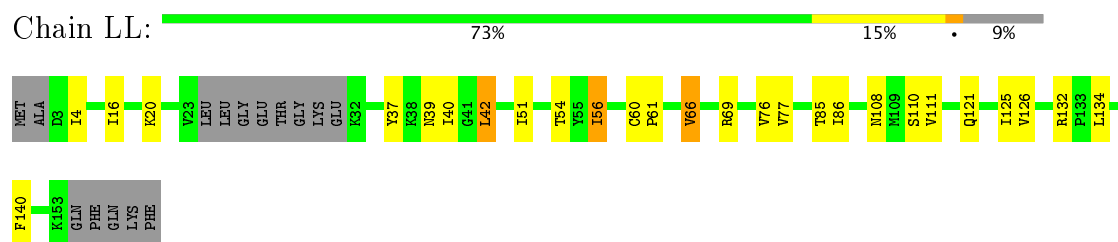
- Molecule 61: Ribosomal protein S9 (Predicted)



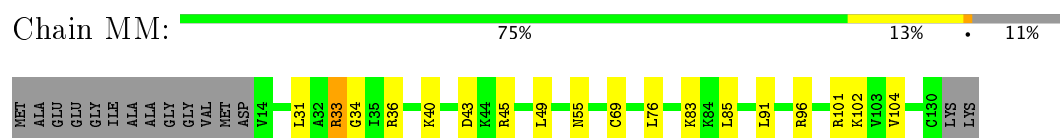
- Molecule 62: Uncharacterized protein



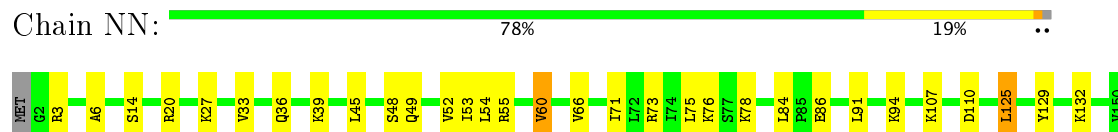
- Molecule 63: Uncharacterized protein



- Molecule 64: 40S ribosomal protein S12



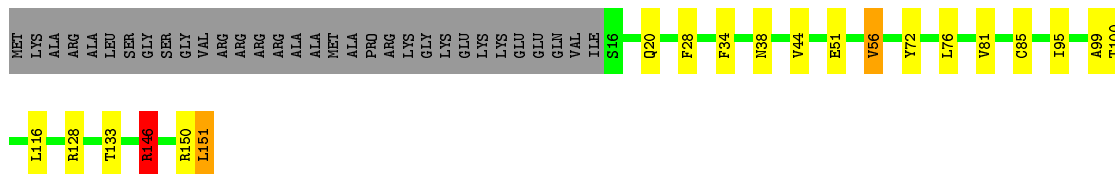
- Molecule 65: uS15



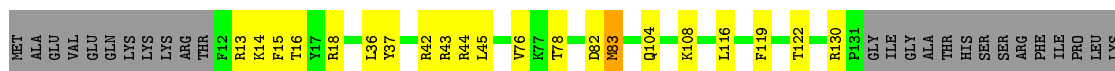


ALA


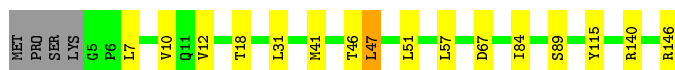
- Molecule 66: uS11

Chain OO:  69% 10% .. 19%


- Molecule 67: uS19

Chain PP:  68% 14% . 17%

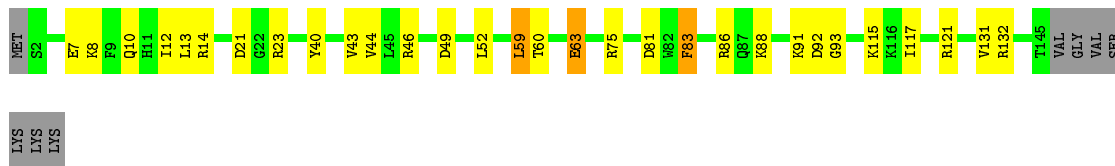
- Molecule 68: uS9

Chain QQ:  86% 10% ..

- Molecule 69: eS17

Chain RR:  83% 13% ..

- Molecule 70: uS13

Chain SS:  75% 18% . 5%

- Molecule 71: eS19

Chain TT:  88% 8% ..


- Molecule 72: uS10



Chain UU:  71% 13% 16%




- Molecule 73: eS21

Chain VV:  86% 13%




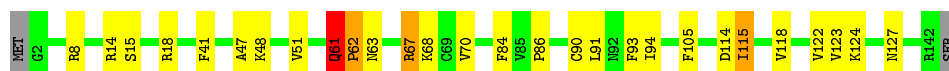
- Molecule 74: uS8

Chain WW:  76% 22%




- Molecule 75: uS12

Chain XX:  79% 17%



- Molecule 76: 40S ribosomal protein S24

Chain YY:  81% 15% 5%




- Molecule 77: eS25

Chain ZZ:  50% 10% 40%




- Molecule 78: eS26

Chain aa:  75% 12% 12%




- Molecule 79: 40S ribosomal protein S27



Chain bb:  87% 12%



- Molecule 80: eS28

Chain cc:  77% 10% 10%




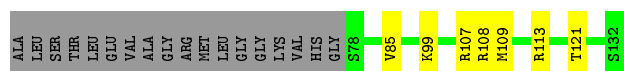
- Molecule 81: uS14

Chain dd:  91% 7%



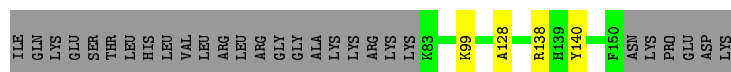
- Molecule 82: eS30

Chain ee:  36% 5% 59%



- Molecule 83: eS31

Chain ff:  41% 1% 56%



- Molecule 84: RACK1

Chain gg:  93% 6%



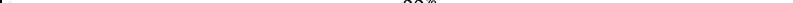
- Molecule 85: mRNA

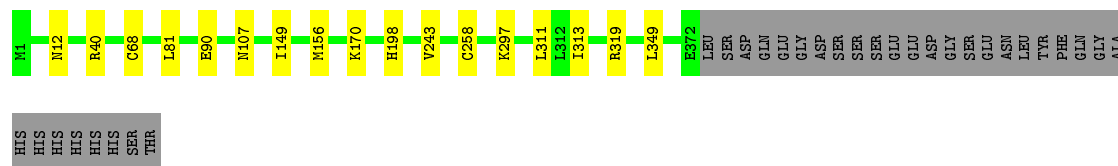
Chain hh:  50% 50%





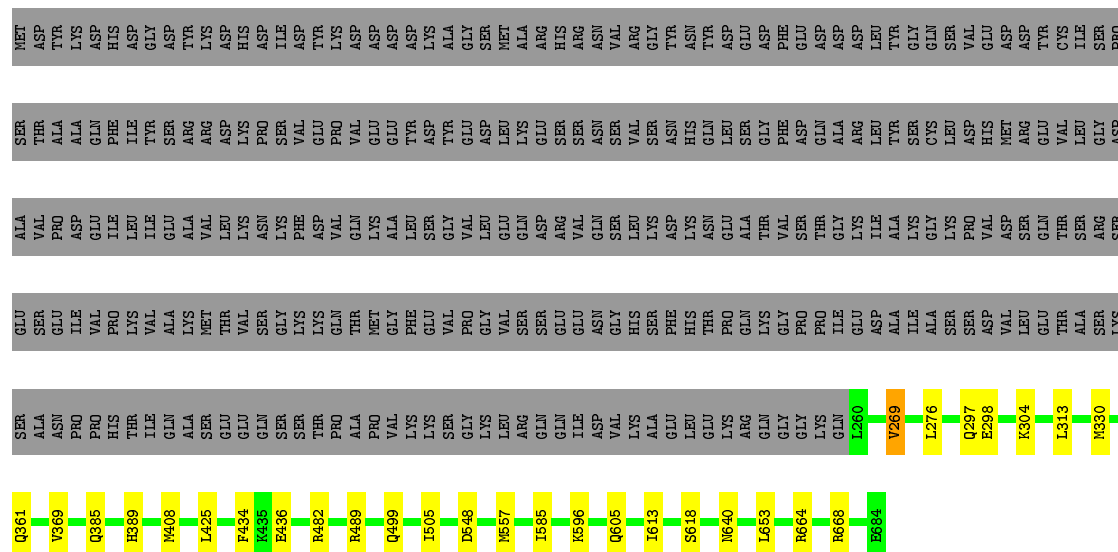
- Molecule 86: Protein pelota homolog

Chain ii:  88% • 8%



- Molecule 87: HBS1-like protein

Chain jj:  56% . 40%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58773	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/1936	0.79	0/2596
10	J	0.40	0/1385	0.70	0/1852
11	L	0.41	0/1733	0.74	0/2316
12	M	0.44	0/1158	0.72	0/1547
13	N	0.43	0/1746	0.78	0/2338
14	O	0.44	0/1662	0.73	0/2222
15	P	0.49	0/1268	0.73	0/1700
16	Q	0.44	0/1539	0.82	0/2054
17	R	0.41	0/1524	0.74	1/2013 (0.0%)
18	S	0.54	0/1501	0.79	1/2012 (0.0%)
19	T	0.42	0/1326	0.70	0/1770
2	B	0.48	0/3240	0.75	1/4339 (0.0%)
20	U	0.39	0/823	0.64	0/1104
21	V	0.45	0/993	0.72	0/1332
22	W	0.45	0/873	0.62	0/1158
23	X	0.37	0/984	0.66	0/1323
24	Y	0.42	0/1132	0.72	0/1504
25	Z	0.44	0/1130	0.70	0/1507
26	a	0.44	0/1191	0.72	0/1590
27	b	0.37	0/861	0.63	0/1138
28	c	0.40	0/771	0.60	0/1034
29	d	0.44	0/903	0.75	0/1216
3	C	0.46	0/2937	0.77	2/3946 (0.1%)
30	e	0.45	0/1071	0.74	0/1429
31	f	0.48	0/895	0.78	0/1198
32	g	0.42	0/916	0.74	0/1220
33	h	0.36	0/1021	0.66	0/1348
34	i	0.43	0/841	0.69	0/1112
35	j	0.45	0/720	0.77	0/952
36	k	0.35	0/575	0.60	0/761
37	l	0.43	0/459	0.70	0/608
38	m	0.47	0/435	0.72	0/575



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	n	0.39	0/240	0.77	0/305
4	D	0.39	0/2437	0.69	2/3264 (0.1%)
40	o	0.44	0/864	0.70	0/1140
41	p	0.47	0/718	0.70	0/953
42	r	0.47	0/1010	0.76	0/1354
43	s	0.37	0/1530	0.49	0/2064
44	t	0.36	0/1174	0.52	0/1582
45	1	0.48	0/49	0.59	0/65
46	2	0.26	0/1805	0.66	0/2809
47	3	0.23	0/1777	0.66	0/2763
48	5	0.41	15/84961 (0.0%)	0.78	53/132460 (0.0%)
49	7	0.37	0/2858	0.67	0/4455
5	E	0.38	0/1762	0.69	0/2362
50	8	0.38	0/3581	0.70	0/5577
51	9	0.37	3/40523 (0.0%)	0.73	14/63130 (0.0%)
52	AA	0.40	0/1747	0.67	0/2374
53	BB	0.38	0/1756	0.64	0/2350
54	CC	0.40	0/1753	0.70	0/2369
55	DD	0.37	0/1796	0.65	0/2417
56	EE	0.37	0/2118	0.69	0/2849
57	FF	0.35	0/1492	0.66	0/2005
58	GG	0.37	0/1946	0.69	0/2590
59	HH	0.36	0/1510	0.61	0/2022
6	F	0.54	0/1911	0.79	0/2549
60	II	0.40	0/1715	0.72	0/2287
61	JJ	0.40	0/1550	0.76	0/2069
62	KK	0.39	0/834	0.61	0/1125
63	LL	0.41	0/1195	0.73	0/1597
64	MM	0.37	0/918	0.62	0/1233
65	NN	0.40	0/1226	0.74	0/1649
66	OO	0.42	0/1029	0.83	1/1380 (0.1%)
67	PP	0.40	0/1017	0.71	0/1358
68	QQ	0.36	0/1146	0.66	0/1534
69	RR	0.37	0/1082	0.65	0/1452
7	G	0.40	0/1910	0.68	0/2569
70	SS	0.37	0/1208	0.70	0/1618
71	TT	0.37	0/1115	0.66	0/1493
72	UU	0.37	0/805	0.68	0/1081
73	VV	0.41	0/643	0.73	0/860
74	WW	0.45	0/1051	0.79	2/1406 (0.1%)
75	XX	0.43	0/1116	0.75	1/1490 (0.1%)
76	YY	0.37	0/1028	0.67	0/1366
77	ZZ	0.36	0/604	0.66	0/810



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
78	aa	0.42	0/828	0.80	0/1109
79	bb	0.37	0/665	0.65	0/891
8	H	0.42	0/1535	0.69	0/2063
80	cc	0.37	0/490	0.73	0/656
81	dd	0.43	0/470	0.72	0/623
82	ee	0.38	0/447	0.70	0/587
83	ff	0.37	0/567	0.53	0/753
84	gg	0.34	0/2493	0.59	0/3394
85	hh	0.28	0/188	0.79	0/290
86	ii	0.34	0/2996	0.58	0/4050
87	jj	0.34	0/3352	0.57	0/4523
9	I	0.43	0/1702	0.69	0/2272
All	All	0.40	18/237792 (0.0%)	0.73	78/348210 (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
11	L	0	1
13	N	0	1
2	B	0	2
3	C	0	1
31	f	0	1
48	5	0	2
56	EE	0	1
74	WW	0	1
75	XX	0	1
78	aa	0	1
80	cc	0	1
All	All	0	13

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	935	A	C5-C6	-15.99	1.26	1.41
48	5	935	A	C6-N1	-12.18	1.27	1.35
48	5	935	A	C2-N3	10.23	1.42	1.33
48	5	481	G	N1-C2	-9.91	1.29	1.37
48	5	922(A)	G	O3'-P	9.08	1.72	1.61
48	5	481	G	C5-C6	8.94	1.51	1.42

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	481	G	C2-N2	-8.56	1.25	1.34
48	5	935	A	N3-C4	7.10	1.39	1.34
48	5	1411(B)	C	O3'-P	7.03	1.69	1.61
48	5	481	G	C2-N3	-6.41	1.27	1.32
48	5	935	A	C6-N6	-6.09	1.29	1.33
48	5	922	C	O3'-P	5.78	1.68	1.61
51	9	613	G	O3'-P	-5.73	1.54	1.61
48	5	441	G	O3'-P	-5.60	1.54	1.61
48	5	4622	A	O3'-P	-5.42	1.54	1.61
51	9	1658	G	O3'-P	-5.20	1.54	1.61
48	5	2836	A	O3'-P	-5.12	1.55	1.61
51	9	1095	U	O3'-P	-5.09	1.55	1.61

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	481	G	N1-C2-N2	-52.63	68.83	116.20
48	5	935	A	C5-C6-N6	-48.73	84.72	123.70
48	5	935	A	N1-C6-N6	-35.80	97.12	118.60
48	5	935	A	C6-N1-C2	-31.95	99.43	118.60
48	5	481	G	N3-C2-N2	-29.88	98.98	119.90
48	5	935	A	C4-C5-C6	-26.98	103.51	117.00
48	5	481	G	C6-N1-C2	-21.12	112.42	125.10
48	5	481	G	C2-N3-C4	-17.67	103.06	111.90
48	5	922	C	C2'-C3'-O3'	12.68	137.40	109.50
48	5	935	A	N3-C4-C5	-11.67	118.63	126.80
48	5	935	A	N1-C2-N3	-10.89	123.86	129.30
51	9	1835	A	C2'-C3'-O3'	9.70	130.85	109.50
4	D	22	ARG	NE-CZ-NH1	8.98	124.79	120.30
48	5	922	C	N1-C1'-C2'	-8.89	102.22	112.00
48	5	922	C	O4'-C4'-C3'	-8.40	95.60	104.00
48	5	3697	U	C2'-C3'-O3'	8.21	127.57	109.50
51	9	1394	G	C2'-C3'-O3'	8.13	127.38	109.50
48	5	1455	G	C2'-C3'-O3'	8.08	127.27	109.50
48	5	3888	G	C2'-C3'-O3'	7.92	126.94	109.50
48	5	2046	G	C2'-C3'-O3'	7.86	126.80	109.50
48	5	1211	G	C2'-C3'-O3'	7.44	125.86	109.50
51	9	434	G	C2'-C3'-O3'	7.40	125.78	109.50
48	5	922	C	C4'-C3'-C2'	-7.20	95.41	102.60
48	5	1834	U	C2'-C3'-O3'	7.16	125.24	109.50
48	5	406	C	C2'-C3'-O3'	7.14	125.21	109.50
48	5	481	G	N3-C4-C5	-7.10	125.05	128.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1477	C	C2'-C3'-O3'	7.10	125.11	109.50
48	5	1411	C	C2'-C3'-O3'	-7.04	94.00	109.50
51	9	110	U	C2'-C3'-O3'	6.99	124.88	113.70
48	5	1411	C	C4'-C3'-O3'	6.92	126.84	113.00
48	5	922	C	C5'-C4'-O4'	6.77	117.23	109.10
48	5	125	C	C2'-C3'-O3'	6.64	124.32	113.70
48	5	1428	U	C2'-C3'-O3'	6.62	124.29	113.70
48	5	4947	U	C2'-C3'-O3'	6.61	124.28	113.70
4	D	22	ARG	NE-CZ-NH2	-6.41	117.09	120.30
51	9	1520	G	C4'-C3'-O3'	6.24	125.48	113.00
48	5	922(A)	G	N9-C1'-C2'	6.15	122.00	114.00
2	B	10	ARG	NE-CZ-NH2	6.05	123.32	120.30
48	5	1329	G	C2'-C3'-O3'	6.04	123.37	113.70
48	5	4884	G	C2'-C3'-O3'	6.00	123.30	113.70
48	5	4723	A	N9-C1'-C2'	5.92	121.70	114.00
51	9	1130	G	C4'-C3'-O3'	5.92	124.83	113.00
48	5	1291	G	C2'-C3'-O3'	5.88	123.10	113.70
48	5	2474	G	C2'-C3'-O3'	5.81	123.00	113.70
48	5	481	G	C5-C6-N1	-5.80	108.60	111.50
48	5	47	A	C4'-C3'-O3'	5.76	124.52	113.00
48	5	90	G	C2'-C3'-O3'	5.74	122.88	113.70
48	5	2695	A	C2'-C3'-O3'	5.73	122.87	113.70
51	9	1489	A	C4'-C3'-O3'	5.70	124.39	113.00
48	5	275	C	C2'-C3'-O3'	5.69	122.80	113.70
48	5	385	A	C4'-C3'-O3'	5.62	124.23	113.00
51	9	642	U	C2'-C3'-O3'	5.60	122.65	113.70
51	9	1060	A	N9-C1'-C2'	5.58	121.26	114.00
48	5	922	C	O4'-C1'-N1	5.53	112.62	108.20
48	5	1411(C)	C	C5'-C4'-O4'	5.52	115.72	109.10
48	5	1445	U	C2'-C3'-O3'	5.49	122.49	113.70
17	R	60	ARG	NE-CZ-NH1	5.49	123.05	120.30
48	5	4448	G	C4'-C3'-O3'	5.48	123.95	113.00
51	9	1863	A	O4'-C1'-C2'	-5.42	100.38	105.80
51	9	1664	A	C4'-C3'-O3'	5.41	123.83	113.00
48	5	922(A)	G	P-O3'-C3'	5.39	126.17	119.70
48	5	1818	G	C2'-C3'-O3'	5.37	122.29	113.70
48	5	971(A)	G	C4'-C3'-O3'	5.29	123.58	113.00
48	5	922(B)	C	C5'-C4'-O4'	5.28	115.44	109.10
48	5	3625	G	C2'-C3'-O3'	5.27	122.13	113.70
48	5	48	G	C2'-C3'-O3'	5.20	122.02	113.70
48	5	4653	C	O5'-P-OP2	-5.17	101.05	105.70
74	WW	3	ARG	NE-CZ-NH1	5.17	122.88	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	150	LEU	CB-CG-CD2	5.16	119.77	111.00
51	9	532	C	C2'-C3'-O3'	5.14	121.93	113.70
51	9	1395	C	C4'-C3'-O3'	5.14	123.28	113.00
51	9	501	C	N1-C1'-C2'	5.12	120.65	114.00
66	OO	146	ARG	NE-CZ-NH1	5.11	122.86	120.30
75	XX	14	ARG	NE-CZ-NH1	5.10	122.85	120.30
48	5	1411	C	O4'-C4'-C3'	-5.07	98.93	104.00
18	S	87	ARG	NE-CZ-NH1	5.01	122.80	120.30
3	C	114	ARG	NE-CZ-NH1	5.01	122.80	120.30
74	WW	3	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	481	G	Sidechain
48	5	935	A	Sidechain
2	B	16	PHE	Peptide
2	B	257	TRP	Peptide
3	C	90	GLY	Peptide
56	EE	155	LYS	Peptide
11	L	71	ARG	Peptide
13	N	184	ILE	Peptide
74	WW	27	ILE	Peptide
75	XX	61	GLN	Peptide
78	aa	26	CYS	Peptide
80	cc	20	ARG	Sidechain
31	f	105	LEU	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	23	0
2	B	3172	0	3310	29	0
3	C	2883	0	3053	34	0
4	D	2391	0	2424	16	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1729	0	1887	8	0
6	F	1875	0	1995	16	0
7	G	1879	0	2027	14	0
8	H	1516	0	1597	19	0
9	I	1664	0	1712	9	0
10	J	1362	0	1399	10	0
11	L	1702	0	1820	4	0
12	M	1137	0	1211	13	0
13	N	1701	0	1749	16	0
14	O	1630	0	1778	23	0
15	P	1242	0	1274	8	0
16	Q	1515	0	1634	12	0
17	R	1508	0	1664	10	0
18	S	1462	0	1508	19	0
19	T	1298	0	1366	11	0
20	U	809	0	833	7	0
21	V	979	0	1039	7	0
22	W	860	0	903	9	0
23	X	967	0	1040	2	0
24	Y	1115	0	1205	5	0
25	Z	1107	0	1182	9	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	1002	0	0
33	h	1013	0	1147	0	0
34	i	830	0	916	0	0
35	j	705	0	738	0	0
36	k	569	0	637	0	0
37	l	447	0	480	0	0
38	m	429	0	466	0	0
39	n	239	0	289	0	0
40	o	851	0	920	0	0
41	p	708	0	756	0	0
42	r	994	0	1051	0	0
43	s	1507	0	1564	0	0
44	t	1160	0	1218	0	0
45	1	49	0	51	0	0
46	2	1616	0	824	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	3	1593	0	811	3	0
48	5	75972	0	38398	321	0
49	7	2558	0	1296	7	0
50	8	3208	0	1629	14	0
51	9	36249	0	18317	196	0
52	AA	1710	0	1708	18	0
53	BB	1729	0	1803	14	0
54	CC	1716	0	1806	11	0
55	DD	1768	0	1866	9	0
56	EE	2076	0	2177	13	0
57	FF	1471	0	1522	7	0
58	GG	1923	0	2089	12	0
59	HH	1488	0	1582	15	0
60	II	1686	0	1772	14	0
61	JJ	1525	0	1640	10	0
62	KK	810	0	836	7	0
63	LL	1175	0	1249	8	0
64	MM	908	0	939	16	0
65	NN	1202	0	1289	11	0
66	OO	1016	0	1039	11	0
67	PP	997	0	1045	19	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	7	0
70	SS	1190	0	1249	22	0
71	TT	1097	0	1132	3	0
72	UU	795	0	862	4	0
73	VV	636	0	637	5	0
74	WW	1034	0	1080	13	0
75	XX	1098	0	1167	13	0
76	YY	1011	0	1083	3	0
77	ZZ	598	0	656	3	0
78	aa	814	0	863	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	565	0	0
84	gg	2436	0	2393	0	0
85	hh	169	0	86	0	0
86	ii	2947	0	2957	0	0
87	jj	3292	0	3371	0	0
88	5	178	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	7	5	0	0	0	0
88	8	5	0	0	0	0
88	9	66	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	L	1	0	0	0	0
88	P	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	e	1	0	0	0	0
88	g	1	0	0	0	0
88	j	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	32	0	14	0	0
All	All	222005	0	166945	992	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (992) 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)
48:5:3914:U:O4	48:5:4378:A:N1	1.58	1.35
48:5:922:C:C5'	48:5:922(A):G:H3'	1.59	1.31
48:5:922:C:H5''	48:5:922(B):C:O5'	1.38	1.23
51:9:1283:C:N4	64:MM:102:LYS:HE3	1.52	1.21
48:5:1411:C:H4'	48:5:1411(C):C:O4'	1.41	1.16
51:9:1283:C:H41	64:MM:102:LYS:HE3	1.00	1.08
51:9:1284:A:N1	64:MM:91:LEU:HD22	1.69	1.07
48:5:922:C:H5'	48:5:922(A):G:C3'	1.85	1.07
48:5:922:C:H5''	48:5:922(B):C:P	2.03	0.97
51:9:1282:A:N7	64:MM:102:LYS:NZ	2.12	0.97
51:9:1283:C:H41	64:MM:102:LYS:CE	1.78	0.96

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:C5'	48:5:922(B):C:O5'	2.15	0.95
48:5:922:C:H5'	48:5:922(A):G:H3'	0.95	0.93
48:5:922:C:P	48:5:922(B):C:O5'	2.31	0.89
48:5:1411:C:O3'	48:5:1411(C):C:C5'	2.21	0.88
51:9:1283:C:N4	64:MM:102:LYS:CE	2.36	0.87
51:9:615:C:H2'	51:9:616:A:C8	2.09	0.87
48:5:2031:C:O3'	48:5:2032:U:P	2.33	0.86
52:AA:60:LEU:HD13	52:AA:159:ILE:HD11	1.59	0.84
51:9:1284:A:C4	64:MM:91:LEU:HD13	2.12	0.84
48:5:1524:A:N1	48:5:1652:U:O4	2.10	0.84
48:5:922:C:C2'	48:5:922(B):C:C2	2.62	0.82
48:5:922:C:C5'	48:5:922(A):G:C3'	2.50	0.82
51:9:628:A:H61	51:9:1332:A:C1'	1.92	0.81
48:5:922:C:H2'	48:5:922(B):C:N3	1.96	0.81
48:5:922:C:H2'	48:5:922(B):C:C2	2.16	0.81
51:9:615:C:O2'	51:9:616:A:O4'	1.97	0.80
51:9:628:A:N6	51:9:1332:A:O4'	2.14	0.80
8:H:12:ILE:HG21	8:H:18:ILE:HD13	1.63	0.80
48:5:2395:A:O2'	48:5:2806:A:H1'	1.80	0.80
51:9:1284:A:C2	64:MM:91:LEU:HD22	2.17	0.80
48:5:922:C:O3'	48:5:922(B):C:C6	2.34	0.79
74:WW:75:ILE:HD11	74:WW:93:LEU:HD11	1.65	0.79
48:5:1411:C:O3'	48:5:1411(C):C:O5'	2.02	0.78
67:PP:18:ARG:CD	70:SS:88:LYS:HG2	2.14	0.77
48:5:922:C:C5'	48:5:922(B):C:P	2.72	0.77
48:5:3914:U:C4	48:5:4378:A:N1	2.52	0.77
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.67	0.77
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.65	0.76
3:C:76:ILE:HG22	3:C:77:PRO:HD2	1.68	0.76
48:5:1411:C:C3'	48:5:1411(C):C:O5'	2.34	0.76
51:9:615:C:H2'	51:9:616:A:H8	1.48	0.75
53:BB:139:CYS:SG	53:BB:140:VAL:N	2.58	0.75
1:A:126:LEU:HD13	1:A:150:LEU:HD21	1.68	0.75
3:C:101:MET:SD	3:C:104:PRO:HA	2.26	0.75
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.68	0.74
48:5:1411:C:O3'	48:5:1411(C):C:H5''	1.88	0.73
51:9:1130:G:H2'	51:9:1130:G:N3	2.01	0.73
9:I:191:ILE:HD11	9:I:212:LEU:HD11	1.70	0.73
48:5:3914:U:O4	48:5:4378:A:C2	2.42	0.73
51:9:980:A:H2'	51:9:981:A:C8	2.24	0.71
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.37	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:O2'	48:5:922(B):C:C2	2.42	0.71
48:5:1411:C:C4'	48:5:1411(C):C:O4'	2.32	0.70
48:5:4510:A:O2'	48:5:4511:A:O4'	2.10	0.70
48:5:1411:C:H3'	48:5:1411(B):C:H3'	1.72	0.69
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.74	0.69
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.75	0.69
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	1.75	0.69
48:5:922:C:O5'	48:5:922(A):G:H3'	1.93	0.69
51:9:628:A:H61	51:9:1332:A:H1'	1.57	0.68
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	1.76	0.68
1:A:77:ILE:HD12	1:A:115:CYS:SG	2.33	0.68
48:5:738:C:O2'	48:5:738(A):C:O4'	2.10	0.67
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.76	0.67
48:5:3914:U:H3	48:5:4378:A:N6	1.93	0.66
51:9:92:A:O4'	56:EE:3:ARG:NH1	2.28	0.66
51:9:615:C:O2'	51:9:616:A:O5'	2.14	0.66
52:AA:104:THR:O	52:AA:107:THR:HG23	1.97	0.65
48:5:742:G:C2	48:5:922(A):G:C6	2.84	0.65
48:5:4579:U:H2'	48:5:4580:U:C6	2.31	0.65
48:5:747:A:H4'	48:5:748:G:OP1	1.96	0.65
51:9:1284:A:C2	64:MM:91:LEU:CD2	2.79	0.65
48:5:1818:G:O2'	48:5:1819:G:OP1	2.12	0.65
48:5:3914:U:N3	48:5:4378:A:N6	2.45	0.65
48:5:1411:C:H3'	48:5:1411(B):C:C3'	2.26	0.64
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.31	0.64
51:9:1407:U:H2'	51:9:1408:U:C6	2.32	0.64
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.32	0.64
48:5:4942:C:H4'	48:5:4943:A:OP1	1.97	0.64
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.80	0.64
48:5:1411:C:C5'	48:5:1411(B):C:H2'	2.28	0.64
3:C:341:LEU:HD21	5:E:52:LEU:HD21	1.80	0.63
2:B:174:ARG:NH1	48:5:4985:U:O2	2.31	0.63
2:B:92:TYR:HB3	2:B:99:LEU:HD21	1.81	0.63
14:O:72:HIS:N	48:5:4586:G:OP1	2.32	0.63
51:9:446:G:OP2	60:II:47:ARG:NH1	2.32	0.63
18:S:82:LEU:HB2	18:S:93:MET:HB2	1.80	0.62
48:5:922(B):C:O2'	48:5:923:C:O5'	2.17	0.62
48:5:922:C:C6	48:5:922(A):G:C6	2.86	0.62
51:9:183:G:O2'	51:9:184:G:O5'	2.17	0.62
52:AA:60:LEU:HD13	52:AA:159:ILE:CD1	2.29	0.62
8:H:41:ILE:HG21	8:H:73:ILE:HD11	1.81	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:43:PHE:CD2	16:Q:133:GLY:HA3	2.35	0.62
48:5:2033:A:O2'	48:5:2034:G:O5'	2.10	0.61
8:H:4:ILE:HD11	18:S:152:PHE:CD2	2.34	0.61
51:9:146:G:O2'	51:9:147:A:O5'	2.17	0.61
48:5:922:C:C6	48:5:922(A):G:C5	2.88	0.61
8:H:18:ILE:HG22	8:H:27:VAL:HG22	1.81	0.61
67:PP:18:ARG:NE	70:SS:88:LYS:HD3	2.15	0.61
73:VV:1:MET:SD	73:VV:1:MET:N	2.72	0.61
51:9:1286:G:O6	64:MM:34:GLY:HA3	2.00	0.61
63:LL:37:TYR:CE2	63:LL:51:ILE:HG23	2.34	0.61
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	1.83	0.61
57:FF:92:ILE:HD13	57:FF:169:ILE:HG21	1.83	0.61
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.82	0.61
51:9:1589:A:N3	51:9:1653:U:O2'	2.33	0.61
48:5:1370:G:O2'	48:5:1371:A:OP2	2.17	0.60
5:E:52:LEU:HD23	5:E:58:ARG:HA	1.81	0.60
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.83	0.60
48:5:4723:A:H2'	48:5:4724:A:C8	2.36	0.60
51:9:1130:G:O2'	51:9:1131:G:O5'	2.19	0.60
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.82	0.60
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.83	0.60
48:5:922:C:O5'	48:5:922(A):G:P	2.60	0.60
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.37	0.60
48:5:1411:C:O2'	48:5:1411(C):C:C6	2.45	0.60
14:O:18:ARG:NH2	48:5:2057:A:OP1	2.34	0.60
48:5:922:C:O5'	48:5:922(A):G:O5'	2.19	0.60
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.84	0.60
51:9:1284:A:C8	64:MM:104:VAL:HG21	2.37	0.60
51:9:614:C:H1'	51:9:626:G:H21	1.66	0.59
19:T:48:VAL:HG21	19:T:94:GLU:HG2	1.84	0.59
15:P:69:ARG:NH2	48:5:4568:A:N3	2.49	0.59
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.41	0.59
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.37	0.59
4:D:106:ALA:HB1	4:D:171:LEU:HD13	1.83	0.59
7:G:101:LYS:HB3	23:X:42:THR:HG23	1.84	0.59
51:9:1130:G:HO2'	51:9:1131:G:P	2.25	0.59
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.35	0.59
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.35	0.58
4:D:33:ARG:NH1	4:D:72:ASP:OD2	2.36	0.58
14:O:193:THR:HG23	14:O:202:LEU:HD23	1.85	0.58
48:5:3766:A:N1	51:9:1827:U:O2'	2.30	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:141:ILE:HD11	49:7:55:A:N3	2.17	0.58
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.36	0.58
16:Q:85:THR:HG22	16:Q:104:ARG:HB2	1.84	0.58
48:5:113:A:H2'	48:5:114:G:O4'	2.03	0.58
48:5:964:A:H2'	48:5:965:G:O4'	2.03	0.58
51:9:1129:G:C6	51:9:1130:G:O6	2.56	0.58
59:HH:93:VAL:HG21	59:HH:133:LEU:HD23	1.84	0.58
48:5:922:C:O3'	48:5:922:C:O5'	2.22	0.58
1:A:48:ILE:HD11	1:A:82:ILE:HG22	1.84	0.58
12:M:119:ARG:NH1	14:O:202:LEU:HD21	2.19	0.58
17:R:98:ARG:NH2	48:5:2262:G:OP2	171.11	0.58
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	1.85	0.58
51:9:614:C:H4'	51:9:615:C:H5''	1.86	0.58
12:M:112:VAL:HG11	14:O:201:LEU:HD11	1.85	0.58
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.84	0.58
48:5:4266:G:H2'	48:5:4266:G:N3	2.19	0.57
51:9:1091:C:HO2'	74:WW:2:VAL:N	2.02	0.57
2:B:337:VAL:HG21	2:B:345:LEU:HD21	1.85	0.57
51:9:4:C:O2'	61:JJ:18:ARG:NH1	2.37	0.57
48:5:1381:U:O2	48:5:1381:U:H5''	2.03	0.57
6:F:154:TYR:CE1	6:F:186:MET:HG2	2.39	0.57
67:PP:18:ARG:HE	70:SS:88:LYS:HD3	1.69	0.57
72:UU:48:LEU:HD11	72:UU:91:LEU:HD22	1.86	0.57
48:5:922:C:H3'	48:5:922:C:C6	2.39	0.57
51:9:1310:U:OP1	64:MM:36:ARG:NH1	2.38	0.57
18:S:9:GLU:CG	18:S:33:PHE:CE1	2.88	0.57
6:F:161:ILE:HD12	6:F:166:ILE:HB	1.87	0.57
18:S:80:ILE:HG22	18:S:82:LEU:CD2	2.34	0.57
48:5:2439:G:C6	48:5:2440:U:C4	2.93	0.57
9:I:91:LEU:HD11	9:I:135:ILE:HG12	1.86	0.57
48:5:2268:A:H4'	48:5:2269:C:H5'	1.87	0.57
5:E:185:ASN:ND2	5:E:274:LEU:O	2.38	0.57
51:9:628:A:N6	51:9:1332:A:C1'	2.67	0.56
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.56
48:5:3723:A:H2'	48:5:3724:A:C8	2.40	0.56
46:2:16:C:O4'	46:2:16:C:O2	2.24	0.56
48:5:245:C:O2	48:5:245:C:O4'	2.24	0.56
65:NN:125:LEU:HD22	65:NN:129:TYR:CE2	2.41	0.56
48:5:1961:G:O2'	48:5:2025:A:N6	2.38	0.56
51:9:1130:G:O2'	51:9:1131:G:P	2.63	0.56
51:9:1284:A:C5	64:MM:91:LEU:HD13	2.40	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:RR:28:PHE:HA	69:RR:55:THR:HG21	1.87	0.56
74:WW:102:ILE:O	74:WW:102:ILE:HG22	2.05	0.56
48:5:4977:A:H2'	48:5:4978:G:O4'	2.05	0.56
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.87	0.56
48:5:4515:G:C2	48:5:4516:G:C8	2.94	0.56
48:5:747:A:O2'	48:5:748:G:H3'	2.06	0.56
51:9:1351:G:O2'	51:9:1378:A:N1	2.31	0.56
51:9:615:C:O2'	51:9:616:A:C5'	2.54	0.55
2:B:57:VAL:HG22	2:B:73:VAL:HG12	1.88	0.55
18:S:53:LYS:NZ	49:7:74:A:O2'	2.39	0.55
51:9:1719:A:N6	51:9:1814:G:O2'	2.39	0.55
4:D:35:ARG:HB2	48:5:4325:A:C2	2.41	0.55
5:E:165:VAL:HG12	5:E:178:VAL:HG22	1.88	0.55
66:OO:99:ALA:N	66:OO:133:THR:HG22	2.22	0.55
48:5:1411:C:O3'	48:5:1411(C):C:P	2.65	0.55
54:CC:253:PRO:HA	54:CC:256:TRP:CD1	2.42	0.55
48:5:1074:G:C2	48:5:1238:A:C2	2.95	0.55
3:C:323:ARG:NH1	48:5:1281:G:C8	2.75	0.55
48:5:922:C:P	48:5:922(B):C:C5'	2.95	0.55
52:AA:18:PHE:CD1	52:AA:173:LEU:HD11	2.42	0.55
48:5:5066:U:H2'	48:5:5067:U:C6	2.42	0.55
48:5:2097:A:OP1	48:5:2107:A:N6	2.40	0.55
48:5:1872:G:O2'	48:5:4219:A:N3	2.36	0.55
46:2:33:U:OP2	68:QQ:146:ARG:NH2	2.40	0.55
51:9:1139:C:O4'	51:9:1139:C:O2	2.19	0.55
63:LL:4:ILE:HD12	63:LL:56:ILE:HD11	1.87	0.55
14:O:27:VAL:CG1	14:O:98:ALA:HB1	2.37	0.55
48:5:1325:C:O2	48:5:1325:C:O5'	2.25	0.54
4:D:16:TYR:O	49:7:11:A:N6	2.40	0.54
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.89	0.54
15:P:127:ARG:NH2	48:5:2422:C:OP1	2.40	0.54
48:5:1411:C:C3'	48:5:1411(C):C:P	2.95	0.54
6:F:90:PHE:CD2	6:F:243:ILE:HD11	2.42	0.54
51:9:1238:U:H2'	51:9:1239:U:O4'	2.08	0.54
7:G:219:LEU:HD23	13:N:7:ILE:HD11	1.88	0.54
25:Z:41:ALA:HB2	25:Z:77:TYR:CE1	2.43	0.54
48:5:923:C:C5	48:5:926:G:O4'	2.61	0.54
51:9:1622:U:H3	67:PP:122:THR:HG1	1.55	0.54
10:J:15:LEU:HD21	10:J:134:LEU:HD13	1.90	0.54
67:PP:18:ARG:NE	70:SS:88:LYS:HG2	2.22	0.54
25:Z:41:ALA:HB2	25:Z:77:TYR:HE1	1.73	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:945:U:H2'	51:9:946:U:C6	2.42	0.54
2:B:252:ALA:HB3	48:5:4457:U:O2	2.08	0.54
51:9:584:A:C6	51:9:585:C:C4	2.95	0.54
14:O:12:ARG:O	18:S:171:ARG:NH2	2.40	0.54
48:5:106:A:H2'	48:5:107:G:O4'	2.08	0.54
62:KK:35:LEU:CD1	62:KK:40:VAL:HG21	2.38	0.54
51:9:1667:U:H2'	51:9:1668:U:C6	2.43	0.54
12:M:54:CYS:SG	12:M:55:MET:N	2.80	0.54
48:5:1411:C:H3'	48:5:1411(C):C:P	2.48	0.54
48:5:2505:C:O2	48:5:2505:C:O4'	2.23	0.54
51:9:666:U:C2	51:9:667:U:C5	2.96	0.54
53:BB:136:ARG:HB2	53:BB:218:LEU:HD11	1.90	0.54
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.72	0.54
22:W:4:GLU:OE1	22:W:20:ARG:NH2	2.41	0.53
48:5:4260:U:H2'	48:5:4261:C:C6	2.43	0.53
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.89	0.53
55:DD:126:ILE:HD11	55:DD:134:CYS:SG	2.49	0.53
62:KK:35:LEU:HD12	62:KK:40:VAL:HG21	1.90	0.53
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	1.90	0.53
73:VV:20:SER:HB3	73:VV:59:ILE:HD11	1.90	0.53
75:XX:94:ILE:HD11	75:XX:122:VAL:HG11	1.90	0.53
48:5:922(B):C:N3	48:5:923:C:C5	2.77	0.53
51:9:958:G:C6	51:9:959:G:C6	2.96	0.53
59:HH:133:LEU:HD22	59:HH:173:PHE:CD1	2.43	0.53
67:PP:18:ARG:NE	70:SS:88:LYS:CD	2.72	0.53
4:D:22:ARG:HH11	4:D:22:ARG:HG3	1.73	0.53
59:HH:118:ARG:O	59:HH:121:THR:HG22	2.07	0.53
3:C:292:ILE:HG22	3:C:298:ILE:HD12	1.91	0.53
56:EE:192:ILE:HD13	56:EE:238:LEU:HD23	1.89	0.53
51:9:929:G:H2'	51:9:930:C:O4'	2.08	0.53
51:9:943:U:H2'	51:9:944:A:O4'	2.09	0.53
55:DD:72:VAL:HG23	62:KK:20:VAL:HG21	1.89	0.53
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.90	0.53
22:W:3:VAL:HG21	22:W:12:LYS:CE	2.38	0.53
48:5:1483:C:O4'	48:5:1483:C:O2	2.25	0.53
48:5:4871:C:O4'	48:5:4871:C:O2	2.25	0.53
8:H:12:ILE:HG22	8:H:81:ILE:HD11	1.91	0.53
18:S:9:GLU:HG2	18:S:33:PHE:CE1	2.44	0.53
25:Z:75:TYR:CD2	25:Z:80:LEU:HD21	2.44	0.53
50:8:47:C:H1'	50:8:61:A:H2'	1.90	0.53
51:9:613:G:H2'	51:9:627:U:C6	2.44	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:136:ILE:HG23	56:EE:149:TYR:CE1	2.43	0.53
22:W:3:VAL:HG21	22:W:12:LYS:HE2	1.91	0.53
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.44	0.52
13:N:76:PRO:O	13:N:79:ALA:HB3	2.09	0.52
8:H:1:MET:HG3	18:S:141:ALA:HB2	1.91	0.52
24:Y:49:ILE:HD11	24:Y:55:VAL:HG21	1.91	0.52
51:9:1117:C:O2'	51:9:1118:C:O4'	2.26	0.52
11:L:108:GLU:OE1	11:L:108:GLU:N	2.42	0.52
57:FF:102:LEU:HD22	77:ZZ:110:THR:HG21	1.91	0.52
48:5:1888:A:N6	48:5:3873:G:O2'	2.43	0.52
51:9:1550:G:O2'	51:9:1558:C:O2	2.26	0.52
51:9:830:A:OP2	51:9:846:G:N2	2.42	0.52
58:GG:157:VAL:HB	58:GG:176:ILE:HD11	1.91	0.52
48:5:4305:G:N3	48:5:4305:G:C2'	2.73	0.52
18:S:80:ILE:HG22	18:S:82:LEU:HD22	1.91	0.52
20:U:33:ILE:HD12	20:U:96:LEU:HD22	1.91	0.52
53:BB:129:THR:OG1	53:BB:131:ASP:O	2.25	0.52
6:F:121:PHE:HB2	6:F:204:ASN:OD1	2.10	0.52
48:5:1411:C:H5'	48:5:1411(B):C:C2'	2.40	0.52
51:9:1624:U:O2	51:9:1624:U:O4'	2.27	0.52
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.90	0.52
18:S:82:LEU:HD12	18:S:124:ILE:HG23	1.90	0.52
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.40	0.52
48:5:3810:C:O4'	48:5:3810:C:O2	2.28	0.52
53:BB:66:VAL:HG22	53:BB:87:ILE:HG22	1.92	0.52
66:OO:99:ALA:H	66:OO:133:THR:HG22	1.75	0.52
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.90	0.52
51:9:1143:A:H2'	51:9:1144:A:C8	2.45	0.52
51:9:1373:C:O2'	69:RR:10:LYS:NZ	2.42	0.52
51:9:1438:A:H2'	51:9:1439:A:C8	2.45	0.52
2:B:254:ILE:HG21	2:B:262:VAL:HB	1.92	0.52
14:O:49:ARG:NH2	48:5:1932:A:OP2	2.43	0.52
1:A:104:VAL:HG12	1:A:146:THR:HG21	1.91	0.52
48:5:4989:U:O4'	48:5:4989:U:O2	2.27	0.51
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.40	0.51
56:EE:55:ALA:HB1	56:EE:60:GLU:HB2	1.91	0.51
61:JJ:45:ARG:O	61:JJ:49:THR:HG23	2.10	0.51
48:5:4579:U:O2	48:5:4580:U:C2	2.64	0.51
18:S:3:ALA:O	18:S:111:ARG:NH1	2.43	0.51
51:9:1315:U:O2	51:9:1315:U:O4'	2.28	0.51
51:9:501:C:O2	51:9:501:C:C2'	2.59	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD13	1:A:164:ALA:HB2	1.93	0.51
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.45	0.51
3:C:76:ILE:HG22	3:C:77:PRO:CD	2.40	0.51
2:B:261:ARG:HB2	14:O:64:THR:HG21	1.91	0.51
25:Z:53:VAL:CG2	25:Z:62:ILE:HG12	2.41	0.51
24:Y:103:LYS:HE3	48:5:231:U:O2'	2.09	0.51
51:9:1130:G:N3	51:9:1130:G:C2'	2.72	0.51
53:BB:134:LEU:CD2	53:BB:218:LEU:HD12	2.41	0.51
48:5:1528:U:H2'	48:5:1529:G:O4'	2.11	0.51
52:AA:180:ARG:HG2	52:AA:195:TRP:CE3	2.46	0.51
3:C:302:LEU:HD22	16:Q:38:ARG:HB3	1.93	0.51
48:5:4723:A:C2	48:5:4724:A:C6	2.99	0.51
13:N:28:TRP:O	13:N:32:GLN:NE2	2.42	0.51
19:T:17:ARG:CD	19:T:47:THR:HG23	2.41	0.51
16:Q:186:TYR:CD2	48:5:4307:A:H4'	2.45	0.51
19:T:62:GLY:HA3	19:T:76:VAL:HG12	1.93	0.51
48:5:100:C:O2	48:5:100:C:O4'	2.27	0.50
48:5:2627:C:O2	48:5:2627:C:O4'	2.28	0.50
51:9:501:C:H2'	51:9:501:C:O2	2.10	0.50
3:C:164:THR:HG22	3:C:220:ALA:O	2.12	0.50
50:8:137:A:H2'	50:8:138:C:C6	2.46	0.50
51:9:1834:A:H2	51:9:1837:G:N1	2.10	0.50
51:9:314:U:H2'	51:9:314:U:O2	2.11	0.50
51:9:96:C:O2	51:9:473:A:O2'	2.29	0.50
59:HH:176:VAL:HG12	59:HH:180:LEU:HD12	1.93	0.50
3:C:303:ARG:O	16:Q:38:ARG:NH1	2.44	0.50
20:U:82:TYR:CZ	20:U:86:LEU:HD11	2.46	0.50
51:9:615:C:HO2'	51:9:616:A:C4'	2.20	0.50
51:9:928:G:H2'	51:9:929:G:C8	2.46	0.50
2:B:223:THR:HA	2:B:338:VAL:HG22	1.92	0.50
16:Q:70:MET:HE3	16:Q:137:VAL:HG21	1.92	0.50
48:5:2094:C:O2	48:5:2094:C:O4'	2.29	0.50
48:5:4291:G:H5''	48:5:4291:G:N3	2.26	0.50
2:B:54:THR:OG1	2:B:55:HIS:N	2.45	0.50
6:F:242:LEU:HD23	6:F:246:MET:HG3	1.93	0.50
67:PP:83:MET:HB3	67:PP:116:LEU:HD12	1.93	0.50
24:Y:77:LYS:O	24:Y:78:TYR:C	2.48	0.50
48:5:922:C:P	48:5:922(B):C:P	3.10	0.50
50:8:94:G:H5'	50:8:94:G:C8	2.47	0.50
14:O:160:ARG:NH2	48:5:4760:G:OP1	2.44	0.50
51:9:1616:U:OP2	67:PP:43:ARG:NH2	2.45	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ILE:O	48:5:3653:A:H4'	2.11	0.50
48:5:4966:A:C2	48:5:4967:A:C2	3.00	0.50
8:H:117:PHE:CZ	8:H:118:LEU:HD23	2.46	0.50
17:R:44:LEU:HD22	17:R:49:LEU:HD12	1.93	0.50
53:BB:136:ARG:HD2	53:BB:138:PHE:CZ	2.47	0.50
57:FF:72:LEU:HD22	57:FF:112:LEU:HD11	1.94	0.50
48:5:1411:C:HO2'	48:5:1411(C):C:H6	1.42	0.49
6:F:119:GLY:O	6:F:120:THR:HG23	2.11	0.49
9:I:191:ILE:CD1	9:I:212:LEU:HD11	2.42	0.49
48:5:1665:C:H2'	48:5:1666:C:C6	2.47	0.49
48:5:4723:A:C2	48:5:4724:A:C5	3.00	0.49
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.42	0.49
72:UU:50:VAL:HG23	72:UU:91:LEU:HD23	1.92	0.49
48:5:1524:A:H61	48:5:1652:U:H3	1.58	0.49
55:DD:21:LEU:CD2	55:DD:48:ILE:HD11	2.42	0.49
57:FF:119:SER:OG	57:FF:189:ALA:HB1	2.11	0.49
8:H:5:LEU:HD22	8:H:60:TRP:CH2	2.47	0.49
59:HH:116:ARG:NH2	59:HH:121:THR:OG1	2.46	0.49
6:F:111:LEU:O	6:F:120:THR:HG21	2.12	0.49
48:5:1237:C:O2	48:5:1237:C:O4'	2.30	0.49
48:5:1786:A:H2'	48:5:1789:C:C5	2.47	0.49
8:H:69:THR:HA	8:H:72:THR:HG22	1.95	0.49
9:I:3:ARG:NH2	48:5:4431:U:OP2	2.44	0.49
51:9:1012:A:H2'	51:9:1013:U:O4'	2.12	0.49
51:9:853:C:O2	51:9:853:C:O4'	2.26	0.49
65:NN:52:VAL:O	65:NN:53:ILE:C	2.50	0.49
2:B:249:ARG:NH1	48:5:2837:U:OP1	2.43	0.49
7:G:215:ASP:HB3	7:G:216:PRO:HD3	1.93	0.49
48:5:224:U:O2	48:5:224:U:O4'	2.27	0.49
59:HH:145:ARG:HA	74:WW:51:GLU:HB2	1.93	0.49
51:9:291:G:N3	63:LL:42:LEU:HD13	2.28	0.49
51:9:1489:A:H4'	51:9:1490:G:OP2	2.12	0.49
9:I:91:LEU:HD12	9:I:135:ILE:HG23	1.95	0.49
14:O:55:LEU:HD23	14:O:58:LEU:HD12	1.95	0.49
47:3:75:C:H2'	47:3:76:A:H4'	1.94	0.49
48:5:5047:C:O2'	48:5:5050:C:OP2	2.31	0.49
51:9:434:G:H2'	51:9:435:A:C8	2.47	0.49
51:9:887:U:O4'	51:9:887:U:O2	2.31	0.48
7:G:219:LEU:HA	13:N:7:ILE:HD11	1.94	0.48
48:5:1411:C:H1'	48:5:1411(C):C:C5	2.48	0.48
48:5:2439:G:C5	48:5:2440:U:C5	3.01	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:SER:OG	48:5:3661:G:N7	2.29	0.48
51:9:1614:A:P	67:PP:42:ARG:HH11	2.36	0.48
59:HH:133:LEU:HD21	59:HH:176:VAL:HG11	1.95	0.48
11:L:57:PRO:HG3	11:L:75:GLY:O	2.13	0.48
48:5:99:A:H2'	48:5:100:C:O2	2.12	0.48
3:C:224:ILE:HG22	3:C:227:ILE:HD13	1.95	0.48
3:C:224:ILE:CG2	3:C:227:ILE:HD13	2.43	0.48
58:GG:52:ILE:O	58:GG:52:ILE:HG23	2.13	0.48
8:H:3:THR:HB	8:H:67:LEU:HD11	1.95	0.48
51:9:823:U:O2	51:9:823:U:O4'	2.32	0.48
51:9:958:G:N1	51:9:959:G:C6	2.81	0.48
2:B:86:VAL:HG13	2:B:162:VAL:HG22	1.95	0.48
7:G:139:VAL:HG11	7:G:238:LYS:CG	2.43	0.48
8:H:118:LEU:HD21	8:H:177:ASP:HB2	1.96	0.48
61:JJ:94:LEU:HB2	61:JJ:97:ILE:HD12	1.95	0.48
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.48	0.48
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.95	0.48
48:5:1667:A:N1	48:5:2281:U:OP2	2.47	0.48
51:9:1144:A:H2'	51:9:1145:A:C8	2.49	0.48
52:AA:62:ALA:O	52:AA:66:VAL:HG23	2.13	0.48
52:AA:68:ILE:HG21	52:AA:74:VAL:HG23	1.96	0.48
10:J:27:GLY:HA2	10:J:68:ILE:HG23	1.96	0.48
74:WW:26:LEU:HD11	74:WW:60:LYS:HB3	1.94	0.48
48:5:1523:A:C8	48:5:1652:U:O4	2.66	0.48
50:8:125:C:O4'	50:8:125:C:O2	2.32	0.48
52:AA:134:LEU:CD2	52:AA:144:THR:HG21	2.44	0.48
17:R:10:LEU:O	17:R:14:VAL:HG23	2.14	0.48
1:A:40:TYR:CE2	48:5:4117:U:C4	3.02	0.48
13:N:119:TYR:CZ	13:N:131:GLU:HB2	2.48	0.48
51:9:1834:A:N3	51:9:1834:A:C2'	2.77	0.48
56:EE:126:VAL:HG23	56:EE:156:VAL:O	2.14	0.48
48:5:1411:C:C5'	48:5:1411(C):C:O5'	2.62	0.48
70:SS:121:ARG:HG3	70:SS:131:VAL:CG2	2.43	0.48
74:WW:92:ASN:HD22	74:WW:92:ASN:C	2.17	0.48
48:5:1411:C:C5'	48:5:1411(B):C:C2'	2.91	0.48
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.44	0.48
51:9:664:A:N1	51:9:1163:C:O2	2.47	0.48
2:B:47:LEU:HD23	2:B:166:THR:HG23	1.94	0.48
51:9:1124:C:H5"	53:BB:150:ILE:HD12	1.96	0.48
51:9:925:G:N2	65:NN:48:SER:OG	2.46	0.48
17:R:23:TRP:CZ3	17:R:51:ILE:HD12	2.49	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1746:A:C2	48:5:1785:C:C2	3.02	0.47
48:5:4724:A:C6	48:5:4725:C:C4	3.02	0.47
56:EE:55:ALA:HB2	56:EE:64:ILE:HD12	1.95	0.47
60:II:3:ILE:HG23	60:II:3:ILE:O	2.14	0.47
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.43	0.47
51:9:15:U:H2'	51:9:16:G:O4'	2.14	0.47
2:B:317:LEU:HD21	2:B:381:THR:HA	1.96	0.47
56:EE:122:LYS:HG2	56:EE:162:ILE:HD11	1.95	0.47
51:9:1700:C:C2	51:9:1834:A:N6	2.82	0.47
51:9:604:A:C6	51:9:605:A:N1	2.83	0.47
51:9:980:A:C2	51:9:981:A:C6	3.02	0.47
4:D:39:GLN:HG2	4:D:48:LYS:HB2	1.96	0.47
3:C:313:VAL:CG1	6:F:169:THR:HG21	2.43	0.47
14:O:37:ARG:NH2	48:5:4761:G:OP2	2.47	0.47
48:5:2307:A:C8	48:5:2332:A:C6	3.03	0.47
48:5:4390:A:H2'	48:5:4391:G:O4'	2.14	0.47
48:5:1854:G:N2	48:5:4394:A:O4'	2.48	0.47
48:5:961:G:C6	48:5:962:C:C4	3.02	0.47
51:9:830:A:C2	51:9:831:G:C8	3.02	0.47
15:P:137:ASN:HB3	15:P:138:PRO:HD2	1.96	0.47
48:5:3928:A:H2'	48:5:3929:G:O4'	2.15	0.47
1:A:209:HIS:CE1	1:A:235:VAL:HG11	2.50	0.47
14:O:109:PRO:HB2	14:O:110:PRO:HD2	1.96	0.47
48:5:2363:A:C2	48:5:3860:A:C4	3.03	0.47
48:5:4966:A:H2'	48:5:4967:A:C8	2.49	0.47
51:9:1364:U:O4'	51:9:1364:U:O2	2.30	0.47
7:G:111:PRO:HD2	7:G:114:ILE:HD12	1.97	0.47
7:G:210:ILE:HG23	7:G:220:VAL:HG11	1.96	0.47
61:JJ:114:VAL:HG21	61:JJ:135:ILE:CD1	2.44	0.47
5:E:131:HIS:HB2	48:5:1281:G:C6	2.50	0.47
48:5:3648:A:C4	48:5:3785:A:C6	3.02	0.47
48:5:4289:U:H2'	48:5:4290:U:C6	2.49	0.47
51:9:183:G:C2'	51:9:183:G:N3	2.76	0.47
51:9:824:C:H2'	51:9:825:A:O4'	2.14	0.47
52:AA:131:HIS:O	52:AA:135:THR:HG23	2.15	0.47
2:B:119:TYR:OH	2:B:129:ALA:N	2.48	0.47
62:KK:93:THR:HG23	62:KK:94:LEU:HD12	1.97	0.47
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.50	0.47
16:Q:4:ASP:N	16:Q:4:ASP:OD1	2.47	0.47
68:QQ:51:LEU:HD22	68:QQ:84:ILE:HG13	1.96	0.47
10:J:119:TYR:CD2	70:SS:12:ILE:HD12	2.50	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4658:G:C5	48:5:4659:G:N7	2.83	0.47
48:5:740:G:O6	48:5:922:C:N3	2.48	0.47
1:A:207:VAL:HG23	1:A:208:GLU:HG3	1.97	0.47
4:D:64:ILE:HG13	4:D:105:LEU:HD21	1.97	0.47
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.78	0.47
51:9:163:U:OP2	58:GG:87:ARG:NH2	2.48	0.47
10:J:26:VAL:HG21	10:J:33:LEU:HA	1.97	0.47
75:XX:67:ARG:NH2	75:XX:114:ASP:OD2	2.48	0.47
6:F:92:ILE:HA	6:F:118:ASN:O	2.15	0.47
12:M:17:PHE:CE2	12:M:54:CYS:HA	2.50	0.47
48:5:1665:C:H2'	48:5:1666:C:H6	1.80	0.47
74:WW:104:LEU:HD12	74:WW:104:LEU:O	2.15	0.47
74:WW:55:ASP:O	74:WW:57:ARG:N	2.48	0.47
24:Y:42:TYR:CG	24:Y:119:LEU:HD23	2.50	0.47
51:9:1011:A:H2'	51:9:1012:A:O4'	2.15	0.46
51:9:942:G:H2'	51:9:943:U:C6	2.50	0.46
3:C:95:MET:N	3:C:95:MET:SD	2.85	0.46
9:I:16:PRO:HA	9:I:95:HIS:CD2	2.49	0.46
61:JJ:66:LYS:HA	61:JJ:71:LEU:HD11	1.96	0.46
66:OO:95:ILE:HD13	66:OO:116:LEU:HG	1.96	0.46
18:S:35:PRO:HD2	18:S:39:VAL:HG21	1.97	0.46
48:5:1411:C:C4'	48:5:1411(C):C:O5'	2.64	0.46
10:J:63:ARG:NH2	50:8:58:G:N7	130.26	0.46
58:GG:132:ARG:HB3	58:GG:133:LEU:HD12	1.96	0.46
61:JJ:37:LEU:HD21	61:JJ:106:LEU:HD21	1.96	0.46
17:R:6:LEU:HD22	17:R:6:LEU:O	2.15	0.46
7:G:108:VAL:HA	23:X:44:PRO:O	2.15	0.46
48:5:1328:G:O2'	48:5:2349:A:OP1	2.32	0.46
48:5:3747:A:C2	48:5:3817:A:C5	3.03	0.46
48:5:922:C:O5'	48:5:922(A):G:C3'	2.59	0.46
51:9:1162:C:H2'	51:9:1163:C:O4'	2.15	0.46
51:9:183:G:O2'	51:9:184:G:O4'	2.33	0.46
51:9:584:A:N6	51:9:585:C:N4	2.62	0.46
22:W:45:ASN:HB3	22:W:48:GLN:HE21	1.80	0.46
48:5:4944:C:O4'	48:5:4944:C:O2	2.30	0.46
51:9:1220:A:N6	51:9:1221:G:C6	2.83	0.46
68:QQ:10:VAL:HG12	68:QQ:12:VAL:HG23	1.96	0.46
51:9:12:U:H2'	51:9:13:C:C6	2.51	0.46
51:9:1834:A:C2	51:9:1837:G:N1	2.83	0.46
67:PP:16:THR:OG1	70:SS:91:LYS:O	2.22	0.46
48:5:3689:G:C5	48:5:3690:U:C5	3.03	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1148:A:H4'	51:9:1149:A:O4'	2.15	0.46
51:9:1517:G:C6	51:9:1518:C:C5	3.03	0.46
9:I:98:ARG:NH1	48:5:1864:G:OP1	2.49	0.46
60:II:162:LEU:HD11	60:II:191:GLU:HG2	1.98	0.46
67:PP:18:ARG:HD3	70:SS:88:LYS:HG2	1.93	0.46
48:5:2763:U:O2	48:5:2763:U:O4'	2.33	0.46
70:SS:121:ARG:HG3	70:SS:131:VAL:HG21	1.98	0.46
73:VV:24:ILE:HG23	73:VV:31:SER:OG	2.16	0.46
2:B:285:TYR:CD1	2:B:363:ILE:HG12	2.51	0.46
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.46	0.46
51:9:1857:G:C8	66:OO:146:ARG:NH2	2.84	0.46
48:5:1411:C:C4'	48:5:1411(B):C:H2'	2.46	0.46
48:5:1545:G:H2'	48:5:1546:C:C6	2.51	0.46
48:5:1804:A:N6	48:5:1833:G:O4'	2.49	0.46
48:5:2409:U:C4	48:5:2783:A:N1	2.84	0.46
48:5:976:G:N2	48:5:977:C:C2	2.84	0.46
8:H:41:ILE:HG12	8:H:73:ILE:HD11	1.97	0.46
48:5:36:U:OP1	48:5:1652:U:O2	2.34	0.46
51:9:614:C:C4'	51:9:615:C:H5''	2.45	0.46
52:AA:167:GLY:O	52:AA:171:VAL:HG23	2.16	0.46
55:DD:161:GLY:O	55:DD:164:VAL:HG12	2.16	0.46
14:O:121:PRO:HD2	18:S:166:ARG:O	2.16	0.46
73:VV:55:ILE:HD11	73:VV:69:ILE:HG12	1.97	0.46
52:AA:30:LEU:HD13	52:AA:38:ILE:CD1	2.46	0.45
51:9:297:A:H4'	56:EE:132:GLY:O	2.16	0.45
12:M:122:ILE:HG22	14:O:185:VAL:HG11	1.98	0.45
15:P:102:ALA:CB	15:P:112:LEU:HD11	2.46	0.45
48:5:922:C:C3'	48:5:922:C:C6	2.98	0.45
51:9:1057:C:O2	51:9:1057:C:O4'	2.33	0.45
51:9:304:C:H3'	51:9:305:U:P	2.56	0.45
66:OO:72:TYR:CE2	66:OO:76:LEU:HD11	2.52	0.45
67:PP:18:ARG:CD	70:SS:88:LYS:CG	2.88	0.45
48:5:2292:C:H2'	48:5:2293:U:C6	2.52	0.45
2:B:206:PRO:HD2	2:B:209:GLN:HG3	1.98	0.45
3:C:252:TRP:CH2	3:C:260:LEU:HD11	2.51	0.45
58:GG:63:MET:N	58:GG:63:MET:SD	2.89	0.45
75:XX:90:CYS:HG	75:XX:93:PHE:HE2	1.62	0.45
48:5:1600:A:C6	48:5:1638:A:C5	3.05	0.45
48:5:404:U:C4	48:5:405:U:C4	3.05	0.45
51:9:684:G:C8	51:9:920:A:N6	2.84	0.45
3:C:127:ALA:HA	3:C:246:VAL:HG12	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:60:VAL:HG21	50:8:141:C:H5''	1.99	0.45
14:O:121:PRO:HA	14:O:124:LEU:HB2	1.97	0.45
74:WW:11:LEU:HD22	74:WW:72:CYS:SG	2.57	0.45
48:5:1651:G:C2	48:5:1652:U:N3	2.85	0.45
48:5:2468:U:C2	48:5:2506:G:N7	2.84	0.45
48:5:4872:G:H4'	48:5:4873:G:H5''	1.98	0.45
51:9:1276:A:N6	51:9:1321:G:O2'	2.49	0.45
51:9:62:G:C6	51:9:63:U:C5	3.04	0.45
1:A:208:GLU:HG2	48:5:1629:G:H1	1.81	0.45
3:C:209:VAL:HB	3:C:229:LEU:CD1	2.46	0.45
7:G:219:LEU:HD23	13:N:7:ILE:CD1	2.46	0.45
48:5:2268:A:C4'	48:5:2269:C:H5'	2.46	0.45
51:9:1240:A:C8	51:9:1267:C:O2'	2.66	0.45
53:BB:79:VAL:HG21	53:BB:81:PHE:CZ	2.52	0.45
60:II:117:TYR:CD1	60:II:156:ALA:HB2	2.52	0.45
25:Z:73:LYS:HG2	25:Z:75:TYR:CZ	2.51	0.45
48:5:1523:A:N7	48:5:1652:U:C4	2.85	0.45
51:9:1535:U:O2	51:9:1535:U:H2'	2.16	0.45
51:9:427:U:O4'	51:9:427:U:O2	2.34	0.45
60:II:190:LEU:HD12	60:II:194:GLU:HB3	1.99	0.45
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	1.99	0.45
13:N:184:ILE:O	13:N:194:ARG:NH1	2.49	0.45
69:RR:38:ILE:HD12	69:RR:39:ALA:HB2	1.99	0.45
48:5:2758:G:O2'	48:5:2765:A:N3	2.35	0.45
51:9:1551:U:O2	51:9:1551:U:O4'	2.33	0.45
8:H:112:VAL:HG21	8:H:128:MET:HE1	1.99	0.45
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.98	0.45
21:V:82:ILE:HG12	21:V:121:VAL:HG13	1.98	0.45
48:5:100:C:H2'	48:5:101:A:O4'	2.16	0.45
48:5:1733:G:C4	48:5:4214:A:C2	3.05	0.45
48:5:423:G:H2'	48:5:424:U:O4'	2.16	0.45
51:9:183:G:O2'	51:9:183:G:N3	2.49	0.45
4:D:56:THR:HG22	49:7:27:G:P	2.57	0.45
63:LL:111:VAL:HG22	63:LL:140:PHE:HB2	1.99	0.45
20:U:84:LYS:HG3	20:U:102:VAL:HG11	1.99	0.45
48:5:1406(B):C:H2'	48:5:1406(C):G:O4'	2.17	0.45
51:9:626:G:OP2	51:9:626:G:C8	2.70	0.45
7:G:139:VAL:HG11	7:G:238:LYS:HG3	1.99	0.45
60:II:84:ASN:OD1	60:II:90:LEU:HD12	2.16	0.45
66:OO:56:VAL:HG12	66:OO:81:VAL:HG23	1.98	0.45
68:QQ:57:LEU:HD11	68:QQ:115:TYR:CD2	2.52	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1524:A:N1	48:5:1652:U:C4	2.84	0.44
48:5:82:U:H2'	48:5:83:C:O4'	2.17	0.44
51:9:1823:A:H3'	51:9:1824:A:H5'	1.99	0.44
65:NN:33:VAL:HG21	65:NN:66:VAL:HG11	1.98	0.44
48:5:4219:A:H2'	48:5:4220:A:C8	2.53	0.44
48:5:4576:U:C4	48:5:4577:U:C4	3.06	0.44
51:9:1303:C:O2	51:9:1303:C:O4'	2.33	0.44
51:9:992:A:C2	51:9:993:G:C8	3.05	0.44
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.52	0.44
2:B:41:VAL:HG21	2:B:196:TRP:CG	2.52	0.44
3:C:302:LEU:HD22	16:Q:38:ARG:CB	2.46	0.44
48:5:1358:G:H4'	48:5:1359:G:OP1	2.18	0.44
48:5:1381:U:O4'	48:5:1381:U:O2	2.34	0.44
48:5:1632:A:H2'	48:5:1632:A:N3	2.32	0.44
48:5:498:C:O4'	48:5:498:C:O2	2.34	0.44
51:9:1604:G:C6	51:9:1605:G:C4	3.05	0.44
52:AA:24:HIS:HB3	52:AA:51:LEU:HD21	1.98	0.44
59:HH:130:LEU:HD21	59:HH:156:VAL:HG21	1.98	0.44
48:5:33:A:C6	48:5:34:A:C6	3.05	0.44
48:5:4269:G:C6	48:5:4270:C:C4	3.05	0.44
48:5:5057:C:H2'	48:5:5058:A:C8	2.52	0.44
51:9:944:A:C5	51:9:945:U:C5	3.04	0.44
2:B:105:VAL:HG11	2:B:150:PHE:CZ	2.53	0.44
3:C:133:LEU:HD12	3:C:133:LEU:N	2.32	0.44
56:EE:192:ILE:CD1	56:EE:238:LEU:HD23	2.48	0.44
10:J:128:LEU:HD11	10:J:130:PHE:CE1	2.52	0.44
66:OO:151:LEU:N	66:OO:151:LEU:HD13	2.32	0.44
48:5:1411:C:C4	48:5:1411(B):C:C4	3.05	0.44
48:5:1990:A:H3'	48:5:1991:A:H5''	2.00	0.44
48:5:3724:A:N6	48:5:3725:G:C6	2.85	0.44
48:5:4423:U:O2	48:5:4423:U:O4'	2.36	0.44
3:C:13:GLU:HB2	3:C:161:TYR:OH	2.18	0.44
7:G:214:VAL:HG11	7:G:220:VAL:HG23	1.99	0.44
10:J:151:ILE:HD11	10:J:156:ARG:HG2	1.98	0.44
62:KK:11:ILE:CD1	62:KK:45:VAL:HG22	2.48	0.44
71:TT:39:LEU:HD11	71:TT:52:TRP:CH2	2.51	0.44
75:XX:84:PHE:HB2	75:XX:118:VAL:HG11	1.98	0.44
48:5:1523:A:C2	48:5:1524:A:N7	2.86	0.44
48:5:3648:A:H1'	48:5:3785:A:N6	2.32	0.44
48:5:4510:A:C6	48:5:4511:A:C2	3.06	0.44
48:5:4759:C:O2	48:5:4759:C:O4'	2.34	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:914:U:O4	48:5:918:G:N7	2.50	0.44
51:9:1227:G:C2	51:9:1228:A:C8	3.05	0.44
51:9:1735:A:C4	51:9:1800:A:C2	3.05	0.44
70:SS:59:LEU:HD12	70:SS:63:GLU:OE2	2.18	0.44
48:5:1848:C:H2'	48:5:1849:U:O4'	2.18	0.44
48:5:223:G:H4'	48:5:225:G:C8	2.53	0.44
48:5:3685:C:H2'	48:5:3686:G:O4'	2.18	0.44
60:II:66:SER:HA	60:II:73:THR:HA	2.00	0.44
2:B:55:HIS:CE1	22:W:16:GLY:HA3	2.53	0.44
77:ZZ:73:VAL:HG12	77:ZZ:79:ILE:HD11	2.00	0.44
48:5:4928:C:O2	48:5:4928:C:O4'	2.34	0.44
48:5:922(B):C:C4	48:5:923:C:C5	3.06	0.44
51:9:1260:A:C6	51:9:1619:A:C6	3.06	0.44
19:T:108:ARG:HH12	48:5:1836:G:HO2'	1.60	0.44
51:9:1438:A:C2	51:9:1439:A:C6	3.05	0.44
9:I:36:LEU:HD12	9:I:87:ILE:HB	1.99	0.44
48:5:1339:U:H2'	48:5:1340:C:C6	2.52	0.43
48:5:4658:G:C6	48:5:4659:G:C5	3.05	0.43
48:5:356:G:O2'	50:8:25:G:N3	2.51	0.43
60:II:31:ARG:NH2	60:II:48:VAL:HG12	2.32	0.43
75:XX:123:VAL:HG12	75:XX:124:LYS:HG3	2.00	0.43
48:5:1411:C:H1'	48:5:1411(C):C:C6	2.52	0.43
48:5:1889:U:O4	48:5:1939:A:N6	2.51	0.43
48:5:2539:C:H2'	48:5:2540:C:O4'	2.18	0.43
48:5:4583:C:O2'	48:5:4718:G:N2	2.49	0.43
48:5:922:C:O3'	48:5:922(B):C:C5	2.69	0.43
49:7:23:A:N3	49:7:118:C:O2'	2.45	0.43
54:CC:195:LEU:HD23	54:CC:224:THR:HG22	1.99	0.43
56:EE:11:ARG:HA	56:EE:28:ALA:HB2	1.99	0.43
19:T:12:ARG:NH2	48:5:1789:C:OP2	2.52	0.43
19:T:17:ARG:HD3	19:T:47:THR:HG23	1.98	0.43
21:V:89:ARG:HD2	21:V:95:PHE:CZ	2.54	0.43
22:W:3:VAL:O	22:W:3:VAL:HG23	2.18	0.43
48:5:1354:A:N1	48:5:1385:G:O2'	2.41	0.43
48:5:2395:A:O2'	48:5:2806:A:C1'	2.58	0.43
48:5:4169:G:H4'	48:5:4171:C:C2	2.54	0.43
48:5:4268:A:H2'	48:5:4269:G:O4'	2.19	0.43
48:5:481(A):C:O4'	48:5:481(A):C:O2	2.36	0.43
51:9:1485:U:H2'	51:9:1486:A:O4'	2.18	0.43
51:9:1823:A:C3'	51:9:1824:A:H5'	2.49	0.43
51:9:981:A:H2'	51:9:982:G:O4'	2.18	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:CC:124:PHE:O	54:CC:143:CYS:HA	2.19	0.43
4:D:75:VAL:O	4:D:112:ARG:NH1	2.52	0.43
13:N:48:ALA:HB1	13:N:53:TYR:HB3	1.99	0.43
51:9:916:A:C5	65:NN:73:ARG:HD3	2.52	0.43
69:RR:16:ILE:HG12	69:RR:38:ILE:HD11	1.99	0.43
18:S:44:PHE:CZ	18:S:48:VAL:HG21	2.53	0.43
1:A:69:PHE:HB2	48:5:4125:C:H1'	2.01	0.43
2:B:257:TRP:HB3	48:5:4518:A:OP1	2.19	0.43
51:9:1271:C:H4'	51:9:1301:A:C8	2.54	0.43
51:9:563:G:O2'	51:9:564:A:O4'	2.35	0.43
18:S:34:ALA:HB1	18:S:39:VAL:CG2	2.48	0.43
47:3:71:G:N3	48:5:3715:U:O2'	2.49	0.43
48:5:1390:G:N2	48:5:1393:G:OP2	2.52	0.43
48:5:1411:C:HO3'	48:5:1411(C):C:P	2.40	0.43
48:5:1634:A:C6	48:5:1635:C:C4	3.07	0.43
3:C:138:MET:HG2	3:C:144:ILE:HG22	2.00	0.43
67:PP:36:LEU:O	70:SS:88:LYS:HD3	2.19	0.43
48:5:3656:A:O4'	48:5:3747:A:C2	2.71	0.43
48:5:4758:U:O4'	48:5:4758:U:O2	2.36	0.43
48:5:976:G:N2	48:5:977:C:N3	2.66	0.43
51:9:1334:G:C4	51:9:1498:A:C2	3.06	0.43
5:E:286:PRO:HA	5:E:289:LEU:CD2	2.49	0.43
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	2.01	0.43
12:M:97:ALA:HB2	14:O:203:VAL:HB	2.00	0.43
48:5:43:U:H2'	48:5:44:A:O5'	2.18	0.43
52:AA:161:ILE:HG22	52:AA:163:CYS:SG	2.59	0.43
54:CC:108:LYS:HB2	54:CC:233:LEU:HD23	2.00	0.43
60:II:36:THR:HG21	60:II:179:PRO:HB2	2.01	0.43
48:5:2002:A:N3	48:5:2002:A:H2'	2.33	0.43
48:5:2465:C:H2'	48:5:2466:G:O4'	2.19	0.43
48:5:4966:A:C2	48:5:4967:A:C6	3.07	0.43
50:8:103:A:C8	50:8:104:A:C8	3.07	0.43
51:9:1129:G:C6	51:9:1130:G:C6	3.07	0.43
51:9:1646:C:C2'	51:9:1647:A:OP2	2.66	0.43
2:B:254:ILE:CG2	2:B:262:VAL:HB	2.49	0.43
3:C:253:THR:O	3:C:256:ALA:N	2.52	0.43
13:N:64:ILE:HD12	13:N:65:ARG:N	2.33	0.43
51:9:1016:U:OP2	65:NN:14:SER:HA	2.19	0.43
65:NN:45:LEU:HG	65:NN:49:GLN:HB2	2.01	0.43
67:PP:119:PHE:CE1	70:SS:117:ILE:HD12	2.54	0.43
48:5:1236:C:O2'	48:5:1238:A:OP1	2.37	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:35:U:O2'	48:5:1525:A:N1	2.52	0.43
48:5:4305:G:N3	48:5:4305:G:H2'	2.33	0.43
51:9:1123:C:C4	51:9:1124:C:C5	3.07	0.43
51:9:126:G:O4'	58:GG:195:LYS:HB3	2.18	0.43
51:9:35:C:O2	51:9:520:A:N1	2.52	0.43
52:AA:24:HIS:CB	52:AA:51:LEU:HD21	2.49	0.43
2:B:47:LEU:HD13	2:B:181:MET:SD	2.59	0.43
53:BB:141:GLY:C	53:BB:142:PHE:CD1	2.92	0.43
56:EE:44:LEU:HD21	56:EE:70:ILE:HG21	2.01	0.43
12:M:37:LEU:HD23	18:S:100:LEU:HD21	2.00	0.43
48:5:3876:A:HO2'	48:5:3877:A:P	2.41	0.42
48:5:740:G:N1	48:5:922:C:O2	2.52	0.42
4:D:56:THR:HG21	49:7:26:C:H5''	2.01	0.42
57:FF:87:LEU:HD21	68:QQ:47:LEU:HD22	2.00	0.42
59:HH:134:VAL:HG12	59:HH:173:PHE:CD2	2.54	0.42
59:HH:66:VAL:HG22	59:HH:96:ALA:HB1	2.00	0.42
15:P:69:ARG:NH1	48:5:4980:C:N3	2.66	0.42
20:U:84:LYS:HA	20:U:87:THR:HG22	1.99	0.42
21:V:117:ILE:HD11	21:V:132:ILE:HG23	2.00	0.42
13:N:115:VAL:HG22	13:N:134:LEU:HD21	2.00	0.42
65:NN:3:ARG:HB2	65:NN:6:ALA:HB3	2.01	0.42
51:9:1018:U:H5''	65:NN:71:ILE:HD12	2.01	0.42
66:OO:99:ALA:O	66:OO:100:THR:C	2.57	0.42
66:OO:44:VAL:HG11	66:OO:85:CYS:SG	2.59	0.42
69:RR:119:VAL:O	69:RR:119:VAL:HG13	2.19	0.42
24:Y:52:ASP:HB2	24:Y:110:LYS:HG3	2.01	0.42
48:5:3723:A:C2	48:5:3724:A:C6	3.07	0.42
51:9:363:A:N1	51:9:397:G:O2'	2.36	0.42
67:PP:18:ARG:HA	70:SS:93:GLY:CA	2.49	0.42
70:SS:40:TYR:O	70:SS:44:VAL:HG23	2.19	0.42
25:Z:12:LEU:HB2	25:Z:81:MET:HB3	2.01	0.42
48:5:1818:G:H2'	48:5:1820:U:OP2	2.18	0.42
48:5:2395:A:C2'	48:5:2806:A:HO2'	2.32	0.42
48:5:5007:A:N7	48:5:5042:A:O2'	2.35	0.42
49:7:14:C:C4	49:7:66:G:N2	2.88	0.42
50:8:152:U:H2'	50:8:153:C:O4'	2.19	0.42
50:8:92:U:H2'	50:8:93:C:O4'	2.20	0.42
51:9:1231:C:H2'	51:9:1232:U:O4'	2.19	0.42
51:9:1533:A:C2	51:9:1604:G:H4'	2.55	0.42
58:GG:63:MET:HA	58:GG:98:ARG:O	2.20	0.42
61:JJ:84:ILE:O	61:JJ:108:ARG:NH1	2.52	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:106:LEU:O	17:R:107:ARG:C	2.94	0.42
76:YY:62:THR:HA	76:YY:69:THR:HG22	2.01	0.42
25:Z:42:LEU:HD23	25:Z:43:VAL:N	2.34	0.42
25:Z:75:TYR:CG	25:Z:80:LEU:HD21	2.54	0.42
48:5:113:A:C2	48:5:278:G:C4	3.08	0.42
51:9:1228:A:H2'	51:9:1229:G:C8	2.54	0.42
51:9:1406:G:O2'	51:9:1443:C:N3	2.53	0.42
51:9:293:C:O2'	51:9:294:U:H3'	2.19	0.42
51:9:380:G:OP2	60:II:181:GLN:NE2	2.51	0.42
1:A:181:LYS:HB2	48:5:1577:G:C5	2.55	0.42
58:GG:5:ILE:CD1	58:GG:16:ILE:HD13	2.48	0.42
63:LL:77:VAL:HG22	63:LL:86:ILE:HD12	2.02	0.42
21:V:87:SER:HA	21:V:97:TYR:HB3	2.01	0.42
48:5:2729:C:H2'	48:5:2730:U:O4'	2.19	0.42
51:9:384:U:O4	60:II:5:ARG:NH2	2.51	0.42
51:9:444:G:N2	51:9:446:G:H3'	2.34	0.42
52:AA:94:THR:HG23	52:AA:182:VAL:HG21	2.01	0.42
2:B:14:LEU:HD23	2:B:17:LEU:HD23	2.00	0.42
3:C:323:ARG:NE	48:5:976:G:H21	2.16	0.42
59:HH:122:LEU:HD13	59:HH:122:LEU:C	2.40	0.42
60:II:38:ILE:HD11	60:II:81:VAL:HG23	2.01	0.42
48:5:1371:A:N1	50:8:28:C:O2'	2.47	0.42
48:5:1337:A:C2	48:5:2349:A:C2	3.08	0.42
48:5:4349:C:H3'	48:5:4350:C:H5'	2.01	0.42
48:5:4621:C:C2	48:5:4622:A:C8	3.08	0.42
48:5:4709:U:O2	48:5:4709:U:H2'	2.20	0.42
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.50	0.42
69:RR:111:PHE:HB3	69:RR:114:LEU:HD21	2.02	0.42
74:WW:79:PHE:O	74:WW:125:ILE:HG22	2.19	0.42
75:XX:61:GLN:O	75:XX:63:ASN:N	2.53	0.42
48:5:4398:C:C4	48:5:4399:U:C5	3.08	0.42
48:5:492:U:O2'	48:5:493:G:P	2.78	0.42
48:5:686:A:N3	48:5:686:A:H2'	2.35	0.42
51:9:1374:C:H2'	51:9:1375:G:O4'	2.20	0.42
51:9:1452:A:C6	51:9:1476:A:C6	3.08	0.42
52:AA:5:LEU:CD2	52:AA:8:LEU:HD12	2.48	0.42
55:DD:48:ILE:HG23	55:DD:86:LEU:HD12	2.01	0.42
8:H:94:SER:HB3	8:H:142:ASP:HB3	2.00	0.42
64:MM:33:ARG:NH2	64:MM:91:LEU:HD21	2.35	0.42
15:P:41:ILE:HD12	15:P:150:LEU:CD1	2.49	0.42
72:UU:102:THR:HG21	72:UU:114:VAL:HG21	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1895:G:C6	48:5:1896:A:C4	3.08	0.42
48:5:3611:A:C6	48:5:3612:C:C4	3.08	0.42
48:5:4320:G:H2'	48:5:4321:U:O4'	2.19	0.42
48:5:433:A:C2	48:5:3867:A:H4'	2.55	0.42
48:5:916:C:O4'	48:5:916:C:O2	2.36	0.42
51:9:1024:A:H2'	51:9:1025:U:O4'	2.19	0.42
54:CC:260:VAL:HG23	54:CC:260:VAL:O	2.19	0.42
59:HH:177:TYR:CD2	59:HH:185:VAL:HG21	2.55	0.42
60:II:79:ILE:HG22	60:II:103:LEU:HB2	2.01	0.42
13:N:65:ARG:HG3	13:N:129:PHE:CE1	2.55	0.42
48:5:1633:G:H5'	48:5:1634:A:OP1	2.20	0.42
48:5:1748:U:C2	48:5:1783:C:C2	3.07	0.42
48:5:1846:G:H2'	48:5:1847:C:C6	2.55	0.42
48:5:1905:U:H2'	48:5:1906:U:O4'	2.20	0.42
51:9:666:U:O4'	51:9:1088:U:C2	2.73	0.42
51:9:1088:U:H4'	51:9:1089:G:OP2	2.20	0.42
51:9:1604:G:C6	51:9:1605:G:C5	3.08	0.42
51:9:682:U:OP2	75:XX:8:ARG:HD3	2.20	0.42
2:B:41:VAL:HA	2:B:187:GLY:HA3	2.01	0.42
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.53	0.42
22:W:80:ARG:NH2	58:GG:129:VAL:O	2.53	0.42
8:H:189:GLN:OE1	8:H:189:GLN:N	2.53	0.42
13:N:12:ARG:NH1	48:5:308:G:O6	2.53	0.42
72:UU:24:LEU:HB3	72:UU:32:LEU:HD11	2.02	0.42
74:WW:102:ILE:HB	74:WW:113:HIS:HB3	2.02	0.42
48:5:3683:C:H4'	48:5:3684:G:OP2	2.20	0.41
48:5:4236:G:H4'	48:5:4328:G:O2'	2.20	0.41
51:9:1680:G:H2'	51:9:1681:U:C6	2.55	0.41
51:9:89:C:H2'	51:9:90:G:O4'	2.20	0.41
51:9:955:A:N1	51:9:968:U:O2'	2.45	0.41
51:9:981:A:H2'	51:9:982:G:C8	2.55	0.41
53:BB:87:ILE:HG23	53:BB:101:HIS:CG	2.55	0.41
3:C:101:MET:CE	48:5:2343:G:C4	3.03	0.41
7:G:189:LEU:HD22	7:G:255:VAL:HG12	2.02	0.41
14:O:108:ILE:HG22	14:O:157:GLU:OE1	2.20	0.41
57:FF:87:LEU:HD22	68:QQ:46:THR:OG1	2.19	0.41
75:XX:68:LYS:CG	75:XX:91:LEU:HD22	2.50	0.41
14:O:133:ARG:CZ	48:5:1928:C:C4	3.03	0.41
48:5:2693:G:C6	48:5:2694:G:N1	2.88	0.41
6:F:75:ARG:NE	48:5:730:G:OP2	2.44	0.41
51:9:1657:G:C6	51:9:1658:G:C5	3.07	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:180:G:C6	51:9:181:A:N1	2.88	0.41
14:O:44:SER:HB3	14:O:129:LEU:HD11	2.02	0.41
15:P:122:ALA:HB1	15:P:123:PRO:HD2	2.02	0.41
15:P:46:LYS:O	15:P:57:CYS:HA	9.95	0.41
16:Q:106:THR:HG21	48:5:1353:G:H3'	2.01	0.41
67:PP:18:ARG:C	70:SS:92:ASP:O	2.59	0.41
20:U:39:PHE:CZ	20:U:43:LEU:HD11	2.55	0.41
22:W:3:VAL:HG21	22:W:12:LYS:HE3	2.02	0.41
75:XX:51:VAL:HG13	75:XX:70:VAL:CG1	2.50	0.41
48:5:1301:C:O2	48:5:1301:C:O4'	2.34	0.41
48:5:1546:C:N3	48:5:1612:G:O6	2.54	0.41
48:5:2370:A:N1	48:5:2390:G:O2'	2.39	0.41
48:5:318:A:C2	48:5:4360:U:C2	3.09	0.41
51:9:1336:C:H2'	51:9:1337:C:O4'	2.20	0.41
51:9:1380:C:H2'	51:9:1381:G:O4'	2.20	0.41
51:9:1545:A:H2'	51:9:1546:G:C8	2.55	0.41
51:9:155:G:H4'	58:GG:15:LEU:HD12	2.02	0.41
51:9:1653:U:H2'	51:9:1654:G:C8	2.55	0.41
51:9:932:G:H2'	51:9:934:G:OP2	2.20	0.41
56:EE:185:GLY:N	56:EE:189:LEU:HD13	2.36	0.41
11:L:76:PHE:CD2	11:L:117:LEU:HD11	2.55	0.41
63:LL:76:VAL:HB	63:LL:125:ILE:HD13	2.01	0.41
13:N:11:TRP:CE3	13:N:44:ARG:NH2	2.88	0.41
69:RR:5:ARG:HG2	69:RR:9:VAL:HG11	2.02	0.41
19:T:17:ARG:HD2	19:T:47:THR:HG23	2.02	0.41
20:U:27:HIS:N	20:U:28:PRO:HD2	2.34	0.41
3:C:340:ILE:HG21	5:E:52:LEU:HD12	2.02	0.41
54:CC:70:VAL:HG22	54:CC:75:ILE:CG2	2.50	0.41
9:I:60:LEU:HG	9:I:129:VAL:HG21	2.02	0.41
48:5:1846:G:O2'	48:5:1847:C:O5'	2.35	0.41
48:5:2896:G:H5''	48:5:2897:G:OP2	2.21	0.41
48:5:3714:G:H2'	48:5:3715:U:O4'	2.21	0.41
51:9:1539:U:OP1	71:TT:44:GLU:N	2.44	0.41
48:5:3629:A:O2'	51:9:1721:U:O2	2.29	0.41
3:C:67:TRP:CE3	3:C:73:VAL:HG21	2.56	0.41
12:M:105:THR:HG22	12:M:106:ASP:H	1.85	0.41
51:9:1857:G:OP2	66:OO:146:ARG:HG3	2.19	0.41
75:XX:67:ARG:HG2	75:XX:115:ILE:HG23	2.03	0.41
48:5:1524:A:N6	48:5:1652:U:N3	2.59	0.41
48:5:2750:G:H2'	48:5:2751:G:O4'	2.20	0.41
48:5:2409:U:C5	48:5:2783:A:N1	2.89	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4183:G:N3	48:5:4183:G:H2'	2.36	0.41
48:5:444:G:N2	48:5:1304:C:C2	2.89	0.41
48:5:4880:C:O4'	48:5:4880:C:O2	2.39	0.41
13:N:38:ARG:NH1	50:8:142:U:OP2	2.44	0.41
51:9:1834:A:N3	51:9:1834:A:H2'	2.36	0.41
51:9:92:A:C6	51:9:446:G:C6	3.08	0.41
8:H:12:ILE:HG22	8:H:81:ILE:CD1	2.50	0.41
10:J:103:GLY:O	10:J:134:LEU:HD12	2.20	0.41
10:J:24:ILE:HG21	10:J:36:ALA:HB1	2.02	0.41
21:V:99:GLU:HB3	22:W:24:THR:HG23	2.03	0.41
48:5:4303:C:O2'	48:5:4304:A:H2'	2.21	0.41
48:5:68:U:H2'	48:5:69:A:O4'	2.21	0.41
50:8:64:U:C2	50:8:65:A:C8	3.08	0.41
51:9:1059:G:C6	51:9:1060:A:C2	3.09	0.41
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.49	0.41
51:9:1673:U:H2'	51:9:1674:G:O4'	2.21	0.41
51:9:1857:G:C2'	51:9:1858:G:O5'	2.68	0.41
51:9:356:C:O2	51:9:356:C:C2'	2.68	0.41
53:BB:74:LEU:HD21	53:BB:86:LEU:HD11	2.02	0.41
17:R:173:ARG:NH2	51:9:910:G:OP2	2.54	0.41
48:5:2313:A:O2'	48:5:2314:G:OP1	2.28	0.41
48:5:2523:G:C6	48:5:2524:U:C4	3.08	0.41
48:5:4085:A:C6	48:5:4164:C:C5	3.08	0.41
48:5:4458:C:H2'	48:5:4459:U:C6	2.55	0.41
51:9:666:U:N3	51:9:667:U:C5	2.88	0.41
3:C:152:LEU:HD23	3:C:251:ILE:HG12	2.01	0.41
8:H:117:PHE:CE2	8:H:118:LEU:HD23	2.56	0.41
60:II:113:TYR:OH	60:II:156:ALA:O	2.33	0.41
51:9:1284:A:N3	64:MM:91:LEU:HD13	2.34	0.41
76:YY:29:HIS:CG	76:YY:29:HIS:O	2.74	0.41
48:5:2519:U:H1'	48:5:2520:C:C6	2.55	0.41
48:5:4518:A:H8	48:5:4518:A:OP2	2.04	0.41
48:5:934:C:O4'	48:5:935(A):G:O4'	2.38	0.41
50:8:71:A:C2	50:8:88:A:H1'	2.55	0.41
51:9:816:A:C6	51:9:817:G:C4	3.09	0.41
1:A:158:ILE:HG23	1:A:162:ASN:ND2	2.36	0.41
2:B:10:ARG:NH1	2:B:14:LEU:HG	2.36	0.41
3:C:313:VAL:HG11	6:F:169:THR:HG21	2.03	0.41
6:F:167:ALA:O	6:F:169:THR:HG23	2.21	0.41
75:XX:41:PHE:CE1	75:XX:47:ALA:HB3	2.56	0.41
51:9:1692:U:H2'	51:9:1693:G:C8	2.56	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:989:C:O4'	51:9:990:A:C2	2.74	0.41
4:D:17:GLN:O	48:5:4265:U:N3	2.53	0.41
6:F:93:ARG:NH2	6:F:97:ILE:HD12	2.36	0.41
1:A:39:GLY:HA3	7:G:94:ILE:HG21	2.02	0.41
8:H:5:LEU:HD22	8:H:60:TRP:CZ3	2.56	0.41
67:PP:18:ARG:NE	70:SS:88:LYS:CG	2.84	0.41
48:5:106:A:H1'	48:5:336:A:N3	2.36	0.41
48:5:1744:U:H2'	48:5:1745:G:O4'	2.21	0.41
48:5:2088:A:O2'	48:5:2089:G:OP2	2.31	0.41
48:5:4303:C:O2	48:5:4303:C:O4'	2.39	0.41
48:5:4624:A:H2'	48:5:4625:C:O4'	2.21	0.41
51:9:398:A:C8	51:9:398:A:H5'	2.56	0.41
2:B:56:ILE:CG1	2:B:365:LEU:HD22	2.51	0.41
3:C:150:LEU:O	3:C:152:LEU:N	2.54	0.41
3:C:266:THR:OG1	3:C:267:TRP:N	2.54	0.41
58:GG:16:ILE:N	58:GG:16:ILE:HD12	2.35	0.41
8:H:41:ILE:CG2	8:H:73:ILE:HD11	2.50	0.41
48:5:2805:C:N4	48:5:2806:A:N6	2.69	0.40
48:5:4419:U:OP1	48:5:4421:C:N4	2.54	0.40
48:5:4925:U:H4'	48:5:4926:C:H5'	2.03	0.40
48:5:750:U:H2'	48:5:751:G:O4'	2.21	0.40
48:5:914:U:O4	48:5:918:G:C8	2.74	0.40
51:9:1536:G:H2'	51:9:1537:A:C8	2.56	0.40
1:A:15:VAL:HG21	48:5:1628:C:H5''	2.03	0.40
2:B:36:ASP:N	2:B:36:ASP:OD1	2.53	0.40
6:F:161:ILE:HB	6:F:166:ILE:HD12	2.03	0.40
7:G:122:ILE:HD13	48:5:4163:U:H1'	2.03	0.40
12:M:6:PHE:O	12:M:11:ARG:NE	2.52	0.40
18:S:9:GLU:OE2	18:S:31:ARG:NH2	2.54	0.40
19:T:83:LYS:HD2	19:T:85:LEU:HD21	2.04	0.40
77:ZZ:102:LYS:HB2	77:ZZ:107:VAL:HG12	2.03	0.40
17:R:118:HIS:ND1	48:5:2663:G:OP1	2.52	0.40
48:5:3879:G:O2'	48:5:3881:G:OP2	2.35	0.40
12:M:94:LYS:NZ	48:5:4872:G:OP2	2.50	0.40
48:5:4966:A:C2	48:5:4967:A:N1	2.89	0.40
51:9:958:G:H2'	51:9:959:G:O4'	2.22	0.40
2:B:57:VAL:HB	2:B:367:PHE:HB3	2.04	0.40
53:BB:66:VAL:HG22	53:BB:87:ILE:CG2	2.51	0.40
4:D:106:ALA:CB	4:D:171:LEU:HD13	2.51	0.40
55:DD:72:VAL:HG23	62:KK:20:VAL:CG2	2.51	0.40
59:HH:66:VAL:N	59:HH:67:PRO:CD	2.84	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:23:TRP:CE3	17:R:51:ILE:HD12	2.56	0.40
67:PP:18:ARG:HD2	70:SS:88:LYS:CG	2.51	0.40
48:5:1411:C:H5'	48:5:1411(B):C:O3'	2.21	0.40
48:5:2473:A:C2	48:5:2506:G:C2	3.09	0.40
48:5:4187:G:H2'	48:5:4188:U:O4'	2.21	0.40
48:5:4399:U:H2'	48:5:4400:G:O4'	2.21	0.40
51:9:614:C:C2'	51:9:614:C:O2	2.69	0.40
51:9:986:G:H2'	51:9:987:A:O4'	2.21	0.40
1:A:33:ASP:O	1:A:34:PHE:C	2.60	0.40
3:C:242:PRO:HB2	48:5:2297:G:H4'	2.03	0.40
52:AA:69:GLU:HB3	54:CC:270:THR:HG21	2.03	0.40
51:9:1614:A:OP2	67:PP:42:ARG:NH1	2.53	0.40
19:T:64:VAL:HG13	19:T:72:VAL:HB	2.04	0.40
20:U:80:LYS:HD3	20:U:110:TYR:CE2	2.57	0.40
48:5:1685:G:C5	48:5:1686:C:C4	3.09	0.40
48:5:2268:A:C3'	48:5:2269:C:H5'	2.52	0.40
48:5:922:C:N1	48:5:922(A):G:C6	2.90	0.40
51:9:1546:G:H5'	68:QQ:18:THR:HG21	2.04	0.40
51:9:1646:C:O2'	51:9:1647:A:OP2	2.36	0.40
51:9:1664:A:H4'	51:9:1665:G:OP1	2.21	0.40
52:AA:5:LEU:HD23	52:AA:8:LEU:HD12	2.03	0.40
53:BB:38:MET:HE3	53:BB:185:VAL:HG21	2.02	0.40
3:C:209:VAL:HB	3:C:229:LEU:HD13	2.04	0.40
3:C:321:ASN:OD1	48:5:1280:C:O2'	2.40	0.40
3:C:33:ARG:HD2	3:C:36:ILE:HD12	2.03	0.40
57:FF:20:PHE:C	57:FF:20:PHE:CD1	2.93	0.40
51:9:1284:A:C6	64:MM:91:LEU:HD22	2.45	0.40
70:SS:10:GLN:HA	70:SS:10:GLN:HE21	1.86	0.40
74:WW:7:LEU:O	74:WW:11:LEU:HG	2.22	0.40
48:5:2081:C:H2'	48:5:2082:G:O4'	2.20	0.40
48:5:4124:G:O2'	48:5:4125:C:OP1	2.32	0.40
13:N:91:GLN:NE2	48:5:4178:A:OP2	2.54	0.40
53:BB:107:ARG:NH1	66:OO:133:THR:O	2.54	0.40
5:E:184:LEU:O	48:5:4883:C:N4	2.55	0.40
63:LL:4:ILE:CD1	63:LL:56:ILE:HD11	2.49	0.40
12:M:112:VAL:CG1	14:O:201:LEU:HD11	2.50	0.40
16:Q:67:ILE:HD12	16:Q:96:PRO:HD2	2.03	0.40
21:V:82:ILE:HD12	21:V:104:VAL:HG13	2.02	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	220 (89%)	24 (10%)	2 (1%)	22	65
2	B	392/403 (97%)	355 (91%)	35 (9%)	2 (0%)	32	73
3	C	360/425 (85%)	332 (92%)	23 (6%)	5 (1%)	13	52
4	D	291/297 (98%)	278 (96%)	10 (3%)	3 (1%)	18	60
5	E	208/291 (72%)	189 (91%)	19 (9%)	0	100	100
6	F	223/247 (90%)	204 (92%)	16 (7%)	3 (1%)	14	54
7	G	229/319 (72%)	216 (94%)	11 (5%)	2 (1%)	20	63
8	H	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
9	I	201/214 (94%)	177 (88%)	23 (11%)	1 (0%)	32	73
10	J	168/178 (94%)	157 (94%)	9 (5%)	2 (1%)	15	56
11	L	208/211 (99%)	193 (93%)	14 (7%)	1 (0%)	32	73
12	M	136/218 (62%)	125 (92%)	11 (8%)	0	100	100
13	N	201/204 (98%)	181 (90%)	19 (10%)	1 (0%)	32	73
14	O	197/203 (97%)	183 (93%)	13 (7%)	1 (0%)	32	73
15	P	151/184 (82%)	140 (93%)	9 (6%)	2 (1%)	14	54
16	Q	185/188 (98%)	168 (91%)	16 (9%)	1 (0%)	32	73
17	R	178/196 (91%)	171 (96%)	6 (3%)	1 (1%)	28	70
18	S	174/176 (99%)	159 (91%)	12 (7%)	3 (2%)	11	48
19	T	157/160 (98%)	142 (90%)	15 (10%)	0	100	100
20	U	97/128 (76%)	86 (89%)	9 (9%)	2 (2%)	8	44
21	V	129/140 (92%)	113 (88%)	16 (12%)	0	100	100
22	W	102/157 (65%)	93 (91%)	8 (8%)	1 (1%)	18	60
23	X	116/156 (74%)	109 (94%)	6 (5%)	1 (1%)	20	63
24	Y	132/145 (91%)	126 (96%)	5 (4%)	1 (1%)	22	65
25	Z	133/136 (98%)	123 (92%)	8 (6%)	2 (2%)	12	51

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	a	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
27	b	100/245 (41%)	93 (93%)	6 (6%)	1 (1%)	18	60
28	c	96/115 (84%)	89 (93%)	7 (7%)	0	100	100
29	d	105/125 (84%)	94 (90%)	10 (10%)	1 (1%)	18	60
30	e	126/135 (93%)	121 (96%)	5 (4%)	0	100	100
31	f	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	9	45
32	g	112/117 (96%)	103 (92%)	8 (7%)	1 (1%)	20	63
33	h	120/123 (98%)	116 (97%)	3 (2%)	1 (1%)	22	65
34	i	100/105 (95%)	92 (92%)	8 (8%)	0	100	100
35	j	84/97 (87%)	74 (88%)	9 (11%)	1 (1%)	15	56
36	k	67/70 (96%)	63 (94%)	3 (4%)	1 (2%)	12	51
37	l	48/51 (94%)	41 (85%)	7 (15%)	0	100	100
38	m	50/102 (49%)	46 (92%)	4 (8%)	0	100	100
39	n	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
40	o	102/106 (96%)	92 (90%)	9 (9%)	1 (1%)	18	60
41	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	17	58
42	r	122/137 (89%)	104 (85%)	14 (12%)	4 (3%)	4	34
43	s	194/318 (61%)	174 (90%)	18 (9%)	2 (1%)	18	60
44	t	151/165 (92%)	134 (89%)	15 (10%)	2 (1%)	14	54
45	1	5/7 (71%)	2 (40%)	3 (60%)	0	100	100
52	AA	215/295 (73%)	195 (91%)	19 (9%)	1 (0%)	32	73
53	BB	211/264 (80%)	199 (94%)	12 (6%)	0	100	100
54	CC	219/293 (75%)	202 (92%)	16 (7%)	1 (0%)	32	73
55	DD	226/243 (93%)	206 (91%)	18 (8%)	2 (1%)	20	63
56	EE	260/263 (99%)	242 (93%)	18 (7%)	0	100	100
57	FF	181/204 (89%)	168 (93%)	10 (6%)	3 (2%)	11	48
58	GG	235/249 (94%)	217 (92%)	17 (7%)	1 (0%)	38	77
59	HH	181/194 (93%)	168 (93%)	13 (7%)	0	100	100
60	II	204/208 (98%)	191 (94%)	11 (5%)	2 (1%)	18	60
61	JJ	183/194 (94%)	175 (96%)	8 (4%)	0	100	100
62	KK	94/165 (57%)	85 (90%)	6 (6%)	3 (3%)	5	34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	LL	139/158 (88%)	124 (89%)	14 (10%)	1 (1%)	25	67
64	MM	115/132 (87%)	99 (86%)	16 (14%)	0	100	100
65	NN	147/151 (97%)	134 (91%)	13 (9%)	0	100	100
66	OO	134/168 (80%)	120 (90%)	13 (10%)	1 (1%)	25	67
67	PP	118/145 (81%)	103 (87%)	14 (12%)	1 (1%)	22	65
68	QQ	140/146 (96%)	132 (94%)	8 (6%)	0	100	100
69	RR	130/135 (96%)	115 (88%)	14 (11%)	1 (1%)	22	65
70	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
71	TT	139/145 (96%)	131 (94%)	7 (5%)	1 (1%)	25	67
72	UU	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
73	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
74	WW	127/130 (98%)	116 (91%)	9 (7%)	2 (2%)	11	49
75	XX	139/143 (97%)	124 (89%)	12 (9%)	3 (2%)	8	43
76	YY	122/130 (94%)	116 (95%)	6 (5%)	0	100	100
77	ZZ	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
78	aa	99/115 (86%)	88 (89%)	9 (9%)	2 (2%)	9	45
79	bb	81/84 (96%)	73 (90%)	7 (9%)	1 (1%)	15	56
80	cc	60/69 (87%)	55 (92%)	3 (5%)	2 (3%)	4	34
81	dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
82	ee	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
83	ff	66/156 (42%)	60 (91%)	5 (8%)	1 (2%)	12	51
84	gg	311/317 (98%)	284 (91%)	24 (8%)	3 (1%)	18	60
86	ii	370/403 (92%)	343 (93%)	26 (7%)	1 (0%)	44	81
87	jj	423/710 (60%)	381 (90%)	38 (9%)	4 (1%)	20	63
All	All	12317/14495 (85%)	11302 (92%)	923 (8%)	92 (1%)	30	67

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	236	GLU
18	S	155	PRO
31	f	107	PRO
75	XX	62	PRO
87	jj	605	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	217	GLN
11	L	63	THR
13	N	89	VAL
14	O	200	GLY
20	U	24	ASP
20	U	62	SER
22	W	27	LYS
29	d	58	GLY
33	h	89	ARG
42	r	11	ARG
42	r	68	SER
43	s	142	GLY
44	t	125	LEU
66	OO	20	GLN
75	XX	61	GLN
75	XX	86	PRO
84	gg	224	GLY
87	jj	269	VAL
1	A	14	SER
3	C	275	SER
6	F	99	GLY
7	G	105	THR
10	J	141	ILE
15	P	25	HIS
18	S	166	ARG
31	f	106	TYR
35	j	59	THR
42	r	33	LYS
52	AA	159	ILE
78	aa	47	ALA
80	cc	22	GLY
87	jj	596	LYS
2	B	17	LEU
4	D	44	TYR
16	Q	14	ARG
17	R	3	MET
25	Z	90	PRO
25	Z	91	LEU
55	DD	93	THR
57	FF	21	GLY
57	FF	63	LYS
60	II	123	ARG

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
62	KK	64	TRP
67	PP	82	ASP
74	WW	78	ARG
78	aa	26	CYS
86	ii	12	ASN
3	C	254	GLU
4	D	119	TYR
6	F	125	ASN
24	Y	78	TYR
36	k	20	ALA
40	o	96	ASP
43	s	25	PRO
44	t	54	LYS
57	FF	43	GLU
62	KK	30	PRO
63	LL	66	VAL
71	TT	109	GLY
80	cc	18	LEU
83	ff	128	ALA
7	G	216	PRO
18	S	165	PRO
27	b	102	PRO
41	p	51	ALA
69	RR	119	VAL
74	WW	29	PRO
79	bb	51	GLN
87	jj	618	SER
10	J	68	ILE
58	GG	135	PRO
3	C	90	GLY
3	C	99	GLY
4	D	125	VAL
15	P	114	ILE
23	X	119	ILE
32	g	48	VAL
55	DD	48	ILE
62	KK	40	VAL
2	B	98	GLY
3	C	247	GLY
9	I	135	ILE
54	CC	171	GLY
84	gg	13	GLY

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
42	r	29	PRO
60	II	3	ILE
84	gg	243	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	176 (93%)	14 (7%)	16	51
2	B	342/348 (98%)	312 (91%)	30 (9%)	12	43
3	C	302/347 (87%)	278 (92%)	24 (8%)	14	48
4	D	247/250 (99%)	236 (96%)	11 (4%)	32	68
5	E	190/251 (76%)	179 (94%)	11 (6%)	23	60
6	F	196/215 (91%)	177 (90%)	19 (10%)	9	37
7	G	200/272 (74%)	186 (93%)	14 (7%)	18	54
8	H	169/171 (99%)	155 (92%)	14 (8%)	13	45
9	I	175/181 (97%)	161 (92%)	14 (8%)	14	48
10	J	143/149 (96%)	134 (94%)	9 (6%)	21	58
11	L	175/176 (99%)	165 (94%)	10 (6%)	24	61
12	M	117/161 (73%)	109 (93%)	8 (7%)	18	55
13	N	171/172 (99%)	161 (94%)	10 (6%)	23	60
14	O	171/173 (99%)	156 (91%)	15 (9%)	12	43
15	P	134/163 (82%)	124 (92%)	10 (8%)	16	51
16	Q	164/165 (99%)	149 (91%)	15 (9%)	11	41
17	R	159/175 (91%)	143 (90%)	16 (10%)	9	36
18	S	157/157 (100%)	145 (92%)	12 (8%)	15	50
19	T	139/140 (99%)	126 (91%)	13 (9%)	10	39
20	U	89/114 (78%)	87 (98%)	2 (2%)	57	83
21	V	101/107 (94%)	90 (89%)	11 (11%)	7	32

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	W	86/126 (68%)	85 (99%)	1 (1%)	75	90
23	X	106/134 (79%)	101 (95%)	5 (5%)	30	67
24	Y	124/135 (92%)	116 (94%)	8 (6%)	20	57
25	Z	117/118 (99%)	112 (96%)	5 (4%)	33	69
26	a	119/120 (99%)	115 (97%)	4 (3%)	42	75
27	b	84/184 (46%)	80 (95%)	4 (5%)	30	66
28	c	84/98 (86%)	77 (92%)	7 (8%)	13	45
29	d	98/110 (89%)	85 (87%)	13 (13%)	4	24
30	e	114/121 (94%)	106 (93%)	8 (7%)	18	54
31	f	88/89 (99%)	81 (92%)	7 (8%)	14	48
32	g	98/100 (98%)	92 (94%)	6 (6%)	22	59
33	h	109/110 (99%)	104 (95%)	5 (5%)	31	67
34	i	86/89 (97%)	82 (95%)	4 (5%)	30	67
35	j	73/80 (91%)	68 (93%)	5 (7%)	18	55
36	k	64/65 (98%)	61 (95%)	3 (5%)	30	67
37	l	47/48 (98%)	45 (96%)	2 (4%)	33	69
38	m	48/90 (53%)	44 (92%)	4 (8%)	13	45
39	n	24/24 (100%)	22 (92%)	2 (8%)	13	45
40	o	92/94 (98%)	89 (97%)	3 (3%)	43	75
41	p	74/75 (99%)	69 (93%)	5 (7%)	18	55
42	r	108/121 (89%)	97 (90%)	11 (10%)	8	35
43	s	164/258 (64%)	158 (96%)	6 (4%)	39	73
44	t	126/137 (92%)	122 (97%)	4 (3%)	44	76
45	1	6/6 (100%)	6 (100%)	0	100	100
52	AA	180/245 (74%)	161 (89%)	19 (11%)	8	33
53	BB	194/231 (84%)	176 (91%)	18 (9%)	10	40
54	CC	187/225 (83%)	170 (91%)	17 (9%)	11	41
55	DD	190/202 (94%)	173 (91%)	17 (9%)	11	42
56	EE	224/225 (100%)	204 (91%)	20 (9%)	11	42
57	FF	158/170 (93%)	147 (93%)	11 (7%)	18	54
58	GG	207/218 (95%)	185 (89%)	22 (11%)	8	33

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	HH	165/174 (95%)	152 (92%)	13 (8%)	14	48
60	II	178/180 (99%)	167 (94%)	11 (6%)	21	59
61	JJ	161/168 (96%)	142 (88%)	19 (12%)	6	28
62	KK	87/136 (64%)	81 (93%)	6 (7%)	18	55
63	LL	130/142 (92%)	114 (88%)	16 (12%)	5	26
64	MM	99/108 (92%)	86 (87%)	13 (13%)	5	24
65	NN	130/131 (99%)	114 (88%)	16 (12%)	5	26
66	OO	106/130 (82%)	97 (92%)	9 (8%)	12	44
67	PP	109/130 (84%)	97 (89%)	12 (11%)	7	32
68	QQ	117/121 (97%)	110 (94%)	7 (6%)	22	59
69	RR	119/121 (98%)	109 (92%)	10 (8%)	13	45
70	SS	125/132 (95%)	107 (86%)	18 (14%)	4	20
71	TT	111/115 (96%)	102 (92%)	9 (8%)	14	47
72	UU	92/107 (86%)	83 (90%)	9 (10%)	9	37
73	VV	67/67 (100%)	63 (94%)	4 (6%)	22	59
74	WW	112/113 (99%)	103 (92%)	9 (8%)	14	48
75	XX	113/115 (98%)	105 (93%)	8 (7%)	17	54
76	YY	107/112 (96%)	92 (86%)	15 (14%)	4	21
77	ZZ	66/103 (64%)	59 (89%)	7 (11%)	8	33
78	aa	88/98 (90%)	75 (85%)	13 (15%)	3	19
79	bb	75/76 (99%)	66 (88%)	9 (12%)	6	27
80	cc	55/62 (89%)	47 (86%)	8 (14%)	4	20
81	dd	48/49 (98%)	44 (92%)	4 (8%)	13	45
82	ee	46/106 (43%)	39 (85%)	7 (15%)	3	18
83	ff	61/140 (44%)	58 (95%)	3 (5%)	29	65
84	gg	272/275 (99%)	257 (94%)	15 (6%)	25	62
86	ii	326/353 (92%)	310 (95%)	16 (5%)	29	65
87	jj	358/608 (59%)	331 (92%)	27 (8%)	16	51
All	All	10733/12306 (87%)	9892 (92%)	841 (8%)	19	48

All (841) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	5	ILE
1	A	64	ARG
1	A	102	LEU
1	A	125	LYS
1	A	128	ARG
1	A	163	ARG
1	A	165	VAL
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	227	ARG
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	74	GLU
2	B	97	ARG
2	B	103	LYS
2	B	135	LYS
2	B	146	LEU
2	B	214	ASP
2	B	228	TYR
2	B	231	VAL
2	B	234	ARG
2	B	244	THR
2	B	248	LEU
2	B	261	ARG
2	B	262	VAL
2	B	264	PHE
2	B	279	GLU
2	B	294	LYS
2	B	298	LEU
2	B	309	LEU
2	B	314	ILE
2	B	333	LEU
2	B	351	LEU
2	B	352	LEU
2	B	356	LYS
2	B	357	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	B	383	GLU
3	C	20	LYS
3	C	29	LYS
3	C	84	THR
3	C	95	MET
3	C	113	ARG
3	C	122	TYR
3	C	143	ARG
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	173	LYS
3	C	175	LYS
3	C	188	ARG
3	C	193	LYS
3	C	208	CYS
3	C	213	GLU
3	C	219	LYS
3	C	232	VAL
3	C	246	VAL
3	C	281	MET
3	C	284	MET
3	C	307	LYS
3	C	312	ARG
3	C	333	LYS
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	208	MET
4	D	264	LYS
4	D	268	ARG
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	141	ARG
5	E	143	LEU
5	E	144	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	E	169	LYS
5	E	178	VAL
5	E	213	LYS
5	E	289	LEU
5	E	291	PHE
6	F	30	LYS
6	F	46	ARG
6	F	65	ARG
6	F	73	MET
6	F	88	LEU
6	F	95	ARG
6	F	100	VAL
6	F	115	GLN
6	F	120	THR
6	F	123	LYS
6	F	128	SER
6	F	134	ILE
6	F	151	GLU
6	F	186	MET
6	F	187	GLU
6	F	198	LYS
6	F	211	LYS
6	F	231	ASP
6	F	245	ARG
7	G	105	THR
7	G	126	ARG
7	G	154	LYS
7	G	163	LYS
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	207	LEU
7	G	220	VAL
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	242	ARG
7	G	293	ASN
8	H	1	MET
8	H	23	ARG
8	H	52	LYS
8	H	54	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
8	H	57	VAL
8	H	59	LYS
8	H	66	GLU
8	H	74	CYS
8	H	105	ILE
8	H	108	ASN
8	H	128	MET
8	H	149	ASN
8	H	173	ARG
8	H	177	ASP
9	I	36	LEU
9	I	39	LYS
9	I	76	MET
9	I	116	ARG
9	I	123	GLN
9	I	142	LEU
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	168	SER
9	I	195	CYS
9	I	200	ILE
9	I	207	ASP
9	I	208	LYS
10	J	16	ARG
10	J	28	GLU
10	J	33	LEU
10	J	72	CYS
10	J	81	GLU
10	J	113	ILE
10	J	136	ARG
10	J	167	GLN
10	J	175	LEU
11	L	10	LEU
11	L	35	ARG
11	L	63	THR
11	L	67	HIS
11	L	74	ARG
11	L	106	SER
11	L	129	ARG
11	L	162	LYS
11	L	186	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
11	L	195	ARG
12	M	2	VAL
12	M	37	LEU
12	M	54	CYS
12	M	57	LEU
12	M	89	THR
12	M	96	GLU
12	M	105	THR
12	M	119	ARG
13	N	9	GLU
13	N	26	ARG
13	N	32	GLN
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	87	HIS
13	N	89	VAL
13	N	162	ARG
13	N	182	HIS
14	O	18	ARG
14	O	37	ARG
14	O	49	ARG
14	O	61	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	188	LYS
14	O	202	LEU
15	P	21	ASN
15	P	24	VAL
15	P	25	HIS
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	127	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	5	ILE
16	Q	13	VAL
16	Q	31	LEU
16	Q	61	LEU
16	Q	63	LEU
16	Q	75	ARG
16	Q	91	ARG
16	Q	95	VAL
16	Q	97	LYS
16	Q	101	CYS
16	Q	115	LYS
16	Q	138	LEU
16	Q	143	ARG
16	Q	168	ARG
17	R	8	LYS
17	R	15	LEU
17	R	36	ASN
17	R	40	GLN
17	R	50	ILE
17	R	52	ARG
17	R	63	CYS
17	R	89	MET
17	R	99	MET
17	R	106	LEU
17	R	113	LYS
17	R	130	ASN
17	R	133	LYS
17	R	138	LEU
17	R	176	ARG
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	17	LEU
18	S	24	THR
18	S	43	ARG
18	S	70	LYS
18	S	83	ARG
18	S	102	THR
18	S	120	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	17	ARG
19	T	33	ILE
19	T	52	MET
19	T	60	LYS
19	T	63	ARG
19	T	96	ILE
19	T	117	LYS
19	T	142	ARG
19	T	144	ASN
19	T	146	LYS
19	T	157	GLU
19	T	159	MET
20	U	33	ILE
20	U	80	LYS
21	V	15	ARG
21	V	18	LEU
21	V	35	LYS
21	V	45	ILE
21	V	59	ASP
21	V	60	MET
21	V	71	GLU
21	V	82	ILE
21	V	91	LYS
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	59	LYS
23	X	63	LYS
24	Y	2	LYS
24	Y	8	THR
24	Y	28	LYS
24	Y	50	ARG
24	Y	72	GLN
24	Y	74	TYR
24	Y	104	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
24	Y	112	ASP
25	Z	5	MET
25	Z	65	ARG
25	Z	83	THR
25	Z	84	ARG
25	Z	112	ARG
26	a	4	ARG
26	a	84	GLU
26	a	122	VAL
26	a	132	ARG
27	b	22	LYS
27	b	40	LEU
27	b	41	ARG
27	b	101	HIS
28	c	37	MET
28	c	50	ASN
28	c	78	ASN
28	c	81	LEU
28	c	83	THR
28	c	90	ARG
28	c	92	CYS
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	44	ARG
29	d	48	GLU
29	d	56	GLU
29	d	78	ARG
29	d	79	ASN
29	d	83	ARG
29	d	85	ARG
29	d	90	ARG
29	d	98	SER
29	d	117	LEU
30	e	21	ILE
30	e	22	ARG
30	e	48	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	106	LYS
30	e	128	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
31	f	16	ARG
31	f	23	GLU
31	f	28	LEU
31	f	33	VAL
31	f	52	LYS
31	f	90	SER
31	f	101	ILE
32	g	22	LEU
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	90	ARG
32	g	114	GLN
33	h	16	GLU
33	h	28	LEU
33	h	67	GLU
33	h	77	LYS
33	h	89	ARG
34	i	34	THR
34	i	48	CYS
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	11	ARG
35	j	20	ARG
35	j	58	THR
35	j	79	ARG
36	k	37	ARG
36	k	69	LEU
36	k	70	LYS
37	l	33	ASN
37	l	49	LEU
38	m	71	ARG
38	m	72	LYS
38	m	92	THR
38	m	93	ASN
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	61	LYS
40	o	82	MET
41	p	8	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
41	p	30	GLU
41	p	47	MET
41	p	62	LYS
41	p	70	THR
42	r	8	MET
42	r	14	SER
42	r	18	ILE
42	r	20	ARG
42	r	26	SER
42	r	32	LEU
42	r	35	ARG
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	144	ASP
52	AA	9	GLN
52	AA	12	GLU
52	AA	25	LEU
52	AA	44	ASP
52	AA	46	ILE
52	AA	50	ASN
52	AA	56	GLU
52	AA	58	LEU
52	AA	60	LEU
52	AA	85	ARG
52	AA	111	GLN
52	AA	122	LEU
52	AA	132	GLN
52	AA	136	GLU
52	AA	142	LEU
52	AA	155	ARG
52	AA	169	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
52	AA	170	SER
52	AA	178	LEU
53	BB	29	ASP
53	BB	38	MET
53	BB	50	THR
53	BB	71	LEU
53	BB	82	ARG
53	BB	96	CYS
53	BB	105	LEU
53	BB	125	VAL
53	BB	126	ASP
53	BB	139	CYS
53	BB	157	GLN
53	BB	175	GLU
53	BB	180	ASP
53	BB	181	LEU
53	BB	207	LEU
53	BB	209	ASP
53	BB	213	ARG
53	BB	225	LEU
54	CC	78	LEU
54	CC	114	LYS
54	CC	115	GLN
54	CC	117	ARG
54	CC	120	GLN
54	CC	121	ARG
54	CC	137	VAL
54	CC	167	ARG
54	CC	188	CYS
54	CC	192	LEU
54	CC	227	ARG
54	CC	235	ASN
54	CC	236	PHE
54	CC	244	ILE
54	CC	251	LEU
54	CC	255	LEU
54	CC	271	ASP
55	DD	28	GLU
55	DD	31	GLU
55	DD	45	ARG
55	DD	64	ARG
55	DD	65	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
55	DD	76	ARG
55	DD	127	MET
55	DD	134	CYS
55	DD	142	LEU
55	DD	146	ARG
55	DD	160	SER
55	DD	168	VAL
55	DD	190	LEU
55	DD	206	ASP
55	DD	215	ASP
55	DD	218	LEU
55	DD	227	LYS
56	EE	17	HIS
56	EE	30	ARG
56	EE	41	CYS
56	EE	42	LEU
56	EE	51	ARG
56	EE	59	ASP
56	EE	66	MET
56	EE	77	ARG
56	EE	108	ARG
56	EE	115	THR
56	EE	145	ARG
56	EE	165	GLU
56	EE	171	ASP
56	EE	181	CYS
56	EE	205	PHE
56	EE	222	LEU
56	EE	232	ASN
56	EE	245	ARG
56	EE	246	LEU
56	EE	247	THR
57	FF	20	PHE
57	FF	36	GLN
57	FF	63	LYS
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	95	HIS
57	FF	122	ARG
57	FF	125	SER
57	FF	146	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
57	FF	204	ARG
58	GG	41	LEU
58	GG	59	GLN
58	GG	63	MET
58	GG	64	LYS
58	GG	67	VAL
58	GG	70	HIS
58	GG	72	ARG
58	GG	76	LEU
58	GG	92	ARG
58	GG	95	LYS
58	GG	103	ASP
58	GG	107	SER
58	GG	150	GLU
58	GG	159	ARG
58	GG	171	THR
58	GG	178	ARG
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	216	ARG
58	GG	230	LYS
58	GG	237	LEU
59	HH	8	ILE
59	HH	36	LEU
59	HH	40	LEU
59	HH	46	THR
59	HH	76	GLN
59	HH	82	GLU
59	HH	100	ILE
59	HH	105	THR
59	HH	119	SER
59	HH	132	ASP
59	HH	145	ARG
59	HH	153	LEU
59	HH	158	LEU
60	II	6	ASP
60	II	10	LYS
60	II	22	HIS
60	II	23	LYS
60	II	47	ARG
60	II	49	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
60	II	92	ARG
60	II	121	LEU
60	II	130	THR
60	II	168	GLN
60	II	175	ILE
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	70	ARG
61	JJ	79	ARG
61	JJ	80	ARG
61	JJ	86	VAL
61	JJ	89	GLU
61	JJ	95	ASP
61	JJ	103	GLU
61	JJ	109	ARG
61	JJ	110	LEU
61	JJ	116	LYS
61	JJ	128	VAL
61	JJ	131	ARG
61	JJ	133	ARG
62	KK	1	MET
62	KK	35	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	89	ILE
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	39	ASN
63	LL	40	ILE
63	LL	42	LEU
63	LL	54	THR
63	LL	56	ILE
63	LL	60	CYS
63	LL	69	ARG
63	LL	85	THR
63	LL	108	ASN
63	LL	110	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
63	LL	121	GLN
63	LL	126	VAL
63	LL	132	ARG
63	LL	134	LEU
64	MM	31	LEU
64	MM	33	ARG
64	MM	40	LYS
64	MM	43	ASP
64	MM	45	ARG
64	MM	49	LEU
64	MM	55	ASN
64	MM	69	CYS
64	MM	76	LEU
64	MM	83	LYS
64	MM	85	LEU
64	MM	96	ARG
64	MM	101	ARG
65	NN	20	ARG
65	NN	27	LYS
65	NN	36	GLN
65	NN	39	LYS
65	NN	55	ARG
65	NN	60	VAL
65	NN	75	LEU
65	NN	76	LYS
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	94	LYS
65	NN	107	LYS
65	NN	110	ASP
65	NN	125	LEU
65	NN	132	LYS
66	OO	28	PHE
66	OO	34	PHE
66	OO	38	ASN
66	OO	51	GLU
66	OO	56	VAL
66	OO	128	ARG
66	OO	146	ARG
66	OO	150	ARG
66	OO	151	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE
67	PP	37	TYR
67	PP	44	ARG
67	PP	45	LEU
67	PP	76	VAL
67	PP	78	THR
67	PP	83	MET
67	PP	104	GLN
67	PP	108	LYS
67	PP	130	ARG
68	QQ	7	LEU
68	QQ	31	LEU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	67	ASP
68	QQ	89	SER
68	QQ	140	ARG
69	RR	5	ARG
69	RR	31	ASN
69	RR	43	SER
69	RR	44	LYS
69	RR	62	GLN
69	RR	78	ARG
69	RR	98	VAL
69	RR	99	ASP
69	RR	105	MET
69	RR	132	ARG
70	SS	7	GLU
70	SS	8	LYS
70	SS	13	LEU
70	SS	14	ARG
70	SS	21	ASP
70	SS	23	ARG
70	SS	46	ARG
70	SS	49	ASP
70	SS	52	LEU
70	SS	59	LEU
70	SS	60	THR
70	SS	63	GLU
70	SS	75	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
70	SS	81	ASP
70	SS	83	PHE
70	SS	86	ARG
70	SS	115	LYS
70	SS	132	ARG
71	TT	37	VAL
71	TT	55	THR
71	TT	62	ARG
71	TT	90	SER
71	TT	102	ARG
71	TT	110	LEU
71	TT	121	ARG
71	TT	124	THR
71	TT	142	LYS
72	UU	18	HIS
72	UU	25	THR
72	UU	33	GLU
72	UU	56	MET
72	UU	68	THR
72	UU	79	ARG
72	UU	90	ASP
72	UU	106	ILE
72	UU	111	GLU
73	VV	1	MET
73	VV	10	ASP
73	VV	12	TYR
73	VV	68	SER
74	WW	18	GLU
74	WW	23	ARG
74	WW	36	ARG
74	WW	51	GLU
74	WW	52	ILE
74	WW	85	ASP
74	WW	92	ASN
74	WW	97	ARG
74	WW	103	VAL
75	XX	15	SER
75	XX	18	ARG
75	XX	48	LYS
75	XX	61	GLN
75	XX	67	ARG
75	XX	105	PHE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
75	XX	115	ILE
75	XX	127	ASN
76	YY	9	THR
76	YY	16	ARG
76	YY	17	LEU
76	YY	20	ARG
76	YY	40	ILE
76	YY	46	LYS
76	YY	47	MET
76	YY	53	ASP
76	YY	61	ARG
76	YY	63	HIS
76	YY	74	MET
76	YY	80	ASP
76	YY	88	LYS
76	YY	101	LYS
76	YY	115	LYS
77	ZZ	54	THR
77	ZZ	59	CYS
77	ZZ	74	SER
77	ZZ	80	ARG
77	ZZ	89	GLN
77	ZZ	92	LEU
77	ZZ	106	GLN
78	aa	18	VAL
78	aa	19	GLN
78	aa	21	ILE
78	aa	23	CYS
78	aa	34	LYS
78	aa	41	ILE
78	aa	42	ARG
78	aa	44	ILE
78	aa	55	GLU
78	aa	81	SER
78	aa	86	ASN
78	aa	96	THR
78	aa	100	ARG
79	bb	11	SER
79	bb	17	ARG
79	bb	34	ASP
79	bb	37	CYS
79	bb	42	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
79	bb	64	CYS
79	bb	77	CYS
79	bb	80	ARG
79	bb	81	ARG
80	cc	18	LEU
80	cc	20	ARG
80	cc	31	ARG
80	cc	36	ASP
80	cc	40	ARG
80	cc	44	ARG
80	cc	51	ARG
80	cc	68	LEU
81	dd	9	SER
81	dd	11	PRO
81	dd	27	ARG
81	dd	49	ASP
82	ee	85	VAL
82	ee	99	LYS
82	ee	107	ARG
82	ee	108	ARG
82	ee	109	MET
82	ee	113	ARG
82	ee	121	THR
83	ff	99	LYS
83	ff	138	ARG
83	ff	140	TYR
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	38	LYS
84	gg	47	ARG
84	gg	113	PHE
84	gg	149	GLU
84	gg	191	HIS
84	gg	198	VAL
84	gg	207	CYS
84	gg	273	GLU
84	gg	287	THR
84	gg	289	LEU
84	gg	298	LEU
84	gg	306	LEU
86	ii	40	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
86	ii	68	CYS
86	ii	81	LEU
86	ii	90	GLU
86	ii	107	ASN
86	ii	149	ILE
86	ii	156	MET
86	ii	170	LYS
86	ii	198	HIS
86	ii	243	VAL
86	ii	258	CYS
86	ii	297	LYS
86	ii	311	LEU
86	ii	313	ILE
86	ii	319	ARG
86	ii	349	LEU
87	jj	269	VAL
87	jj	276	LEU
87	jj	297	GLN
87	jj	298	GLU
87	jj	304	LYS
87	jj	313	LEU
87	jj	330	MET
87	jj	361	GLN
87	jj	369	VAL
87	jj	385	GLN
87	jj	389	HIS
87	jj	408	MET
87	jj	425	LEU
87	jj	434	PHE
87	jj	436	GLU
87	jj	482	ARG
87	jj	489	ARG
87	jj	499	GLN
87	jj	505	ILE
87	jj	548	ASP
87	jj	557	MET
87	jj	585	ILE
87	jj	613	ILE
87	jj	640	ASN
87	jj	653	LEU
87	jj	664	ARG
87	jj	668	ARG



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
2	B	167	GLN
2	B	204	GLN
5	E	45	HIS
5	E	194	GLN
6	F	57	HIS
6	F	79	ASN
6	F	247	ASN
7	G	134	ASN
7	G	138	GLN
8	H	15	ASN
9	I	144	ASN
9	I	147	HIS
10	J	112	HIS
14	O	65	ASN
15	P	56	GLN
17	R	130	ASN
18	S	163	HIS
19	T	131	GLN
22	W	48	GLN
23	X	93	ASN
29	d	30	HIS
32	g	14	ASN
34	i	20	ASN
38	m	91	HIS
42	r	70	GLN
42	r	103	HIS
43	s	34	ASN
52	AA	29	ASN
54	CC	115	GLN
54	CC	235	ASN
55	DD	145	GLN
56	EE	67	GLN
56	EE	98	ASN
56	EE	260	GLN
57	FF	118	ASN
58	GG	13	GLN
58	GG	186	GLN
59	HH	114	GLN
60	II	88	ASN
61	JJ	154	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
63	LL	39	ASN
66	OO	79	GLN
68	QQ	35	ASN
68	QQ	142	GLN
69	RR	31	ASN
70	SS	10	GLN
70	SS	125	HIS
74	WW	92	ASN
75	XX	77	ASN
79	bb	26	GLN
79	bb	49	HIS
81	dd	3	HIS
81	dd	10	HIS
83	ff	93	HIS
86	ii	109	GLN
86	ii	216	GLN
87	jj	385	GLN
87	jj	389	HIS
87	jj	605	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	15 (20%)	0
47	3	72/75 (96%)	21 (29%)	1 (1%)
48	5	3506/3543 (98%)	881 (25%)	182 (5%)
49	7	119/120 (99%)	13 (10%)	1 (0%)
50	8	149/156 (95%)	38 (25%)	6 (4%)
51	9	1680/1869 (89%)	435 (25%)	85 (5%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5607/5847 (95%)	1407 (25%)	275 (4%)

All (1407) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	9	A
46	2	13	U
46	2	14	A
46	2	16	C
46	2	19	G
46	2	21	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
46	2	42	A
46	2	43	A
46	2	46	G
46	2	47	U
46	2	49	C
46	2	58	A
46	2	61	C
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
47	3	72	C
47	3	76	A
48	5	12	A
48	5	13	U
48	5	15	A
48	5	17	A
48	5	25	A
48	5	30	C
48	5	36	U
48	5	39	A
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	72	C
48	5	73	A
48	5	75	G
48	5	84	A
48	5	91	G
48	5	93	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	116	G
48	5	118	C
48	5	119	G
48	5	120	A
48	5	122	U
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	159	C
48	5	160	G
48	5	172	C
48	5	173	C
48	5	177	G
48	5	179	G
48	5	200	U
48	5	201	C
48	5	202	C
48	5	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	224	U
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	236	G
48	5	245	C
48	5	246	G
48	5	253	G
48	5	262	G
48	5	265	C
48	5	266	C
48	5	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	321	U
48	5	322	C
48	5	334	A
48	5	340	C
48	5	347	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	363	A
48	5	365	U
48	5	386	A
48	5	387	G
48	5	399	G
48	5	401	G
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	482	G
48	5	483	G
48	5	484	U
48	5	485	C
48	5	486	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	647	G
48	5	649	A
48	5	654	C
48	5	658	C
48	5	666	G
48	5	667	A
48	5	668	C
48	5	672	C
48	5	683	C
48	5	684	G
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	704	C
48	5	705	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	729	G
48	5	730	G
48	5	731	G
48	5	739	G
48	5	742	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	917	A
48	5	918	G
48	5	922(A)	G
48	5	922(B)	C
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	929	A
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	936	C
48	5	938	C
48	5	939	G
48	5	941	C
48	5	943	A
48	5	944	A
48	5	945	U
48	5	955	G
48	5	956	A
48	5	959	G
48	5	960	A
48	5	961	G
48	5	962	C
48	5	965	G
48	5	966	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	967	C
48	5	968	C
48	5	969	C
48	5	972	C
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1177	U
48	5	1179	U
48	5	1195	G
48	5	1209	U
48	5	1210	C
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1280	C
48	5	1284	G
48	5	1287	G
48	5	1288	G
48	5	1291	G
48	5	1292	C
48	5	1293	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	1329	G
48	5	1330	A
48	5	1337	A
48	5	1353	G
48	5	1354	A
48	5	1359	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1411(B)	C
48	5	1411(C)	C
48	5	1412	G
48	5	1416	G
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1422	G
48	5	1429	C
48	5	1432	G
48	5	1433	A
48	5	1435	G
48	5	1436	C
48	5	1437	C
48	5	1438	U
48	5	1441	C
48	5	1442	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	1478	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1503	A
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1524	A
48	5	1525	A
48	5	1534	A
48	5	1535	C
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1568	C
48	5	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1640	C
48	5	1641	G
48	5	1649	U
48	5	1652	U
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1691	G
48	5	1694	C
48	5	1724	G
48	5	1729	A
48	5	1733	G
48	5	1734	G
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1761	G
48	5	1763	C
48	5	1764	G
48	5	1768	C
48	5	1770	A
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1781	U
48	5	1785	C
48	5	1787	A
48	5	1799	G
48	5	1803	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	1804	A
48	5	1805	A
48	5	1819	G
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1869	G
48	5	1882	U
48	5	1890	G
48	5	1893	C
48	5	1897	A
48	5	1910	G
48	5	1918	U
48	5	1919	G
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1938	C
48	5	1948	G
48	5	1951	G
48	5	1952	G
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1966	C
48	5	1967	A
48	5	1976	G
48	5	1977	C
48	5	1978	C
48	5	1980	U
48	5	1982	G
48	5	1983	A
48	5	1984	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	1986	U
48	5	1987	C
48	5	1991	A
48	5	1992	U
48	5	1993	C
48	5	1997	U
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2011	C
48	5	2017	A
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2044	U
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2069	A
48	5	2072	C
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	2274	C
48	5	2275	G
48	5	2279	A
48	5	2280	G
48	5	2289	C
48	5	2294	G
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2325	C
48	5	2332	A
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2360	A
48	5	2364	G
48	5	2366	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	2421	G
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2433	G
48	5	2441	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	2447	U
48	5	2450	G
48	5	2469	C
48	5	2471	G
48	5	2475	G
48	5	2479	G
48	5	2483	G
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2511	A
48	5	2513	A
48	5	2514	G
48	5	2521	G
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2549	G
48	5	2553	A
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2575	U
48	5	2583	C
48	5	2587	A
48	5	2601	A
48	5	2611	A
48	5	2620	G
48	5	2627	C
48	5	2638	G
48	5	2647	A
48	5	2660	A
48	5	2662	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	2663	G
48	5	2669	C
48	5	2670	C
48	5	2676	A
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2695	A
48	5	2696	A
48	5	2704	C
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2735	G
48	5	2740	U
48	5	2743	A
48	5	2744	A
48	5	2754	G
48	5	2760	G
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2787	A
48	5	2788	U
48	5	2790	U
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2826	U
48	5	2827	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	2844	A
48	5	2855	G
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3604	A
48	5	3605	C
48	5	3606	U
48	5	3615	G
48	5	3618	C
48	5	3625	G
48	5	3626	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3662	A
48	5	3667	C
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	3740	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3759	A
48	5	3760	A
48	5	3761	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	3765	G
48	5	3766	A
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3784	A
48	5	3785	A
48	5	3786	U
48	5	3798	U
48	5	3799	A
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3813	A
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3824	A
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3843	C
48	5	3859	G
48	5	3867	A
48	5	3874	G
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3888	G
48	5	3889	G
48	5	3892	U
48	5	3897	G
48	5	3898	G
48	5	3901	A
48	5	3905	A
48	5	3906	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	3941	G
48	5	3943	A
48	5	4067	U
48	5	4069	U
48	5	4071	U
48	5	4073	A
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4092	G
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4138	C
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4165	C
48	5	4166	G
48	5	4171	C
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4201	G
48	5	4203	A
48	5	4212	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	4218	U
48	5	4221	C
48	5	4222	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4237	C
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4266	G
48	5	4267	G
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4297	G
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4329	G
48	5	4330	G
48	5	4332	C
48	5	4335	C
48	5	4336	A
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4368	G
48	5	4373	G
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	4387	C
48	5	4391	G
48	5	4393	G
48	5	4394	A
48	5	4395	U
48	5	4396	A
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4440	G
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4464	A
48	5	4472	G
48	5	4474	A
48	5	4475	G
48	5	4476	C
48	5	4488	A
48	5	4495	G
48	5	4500	U
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4524	G
48	5	4531	U
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4561	C
48	5	4567	G
48	5	4570	G
48	5	4572	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	4573	G
48	5	4575	G
48	5	4584	A
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4599	A
48	5	4606	G
48	5	4618	G
48	5	4620	U
48	5	4636	U
48	5	4637	G
48	5	4652	G
48	5	4656	A
48	5	4661	G
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4678	G
48	5	4700	A
48	5	4701	A
48	5	4703	U
48	5	4709	U
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4728	U
48	5	4729	A
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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	4881	U
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	4919	G
48	5	4921	C
48	5	4924	C
48	5	4926	C
48	5	4927	G
48	5	4928	C
48	5	4931	G
48	5	4935	C
48	5	4937	C
48	5	4938	A
48	5	4940	C
48	5	4942	C
48	5	4943	A
48	5	4944	C
48	5	4945	G
48	5	4947	U
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	4981	G
48	5	4985	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4991	U
48	5	4994	G
48	5	4997	G
48	5	4999	G
48	5	5014	A
48	5	5017	G
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5058	A
48	5	5061	A
48	5	5062	G
48	5	5066	U
49	7	7	G
49	7	22	A
49	7	25	G
49	7	33	U
49	7	53	U
49	7	54	A
49	7	64	G
49	7	76	U
49	7	97	G
49	7	100	A
49	7	110	G
49	7	111	C
49	7	120	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
50	8	2	G
50	8	3	A
50	8	21	C
50	8	32	C
50	8	34	U
50	8	35	C
50	8	49	G
50	8	51	U
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	G
50	8	79	G
50	8	86	U
50	8	87	G
50	8	90	C
50	8	94	G
50	8	95	A
50	8	103	A
50	8	104	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	114	G
50	8	121	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	153	C
50	8	156	U
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	60	A
51	9	64	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	128	U
51	9	129	C
51	9	130	G
51	9	141	A
51	9	142	C
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	292	A
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	313	A
51	9	314	U
51	9	317	C
51	9	318	A
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	335	G
51	9	340	C
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	370	G
51	9	372	U
51	9	379	C
51	9	381	C
51	9	382	C
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G
51	9	409	C
51	9	417	C
51	9	418	A
51	9	434	G
51	9	435	A
51	9	438	G
51	9	441	C
51	9	448	A
51	9	449	A
51	9	450	C
51	9	453	C
51	9	459	C
51	9	460	A
51	9	462	C
51	9	463	C
51	9	464	A
51	9	465	A
51	9	466	G
51	9	468	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	501	C
51	9	523	A
51	9	525	A
51	9	531	A
51	9	532	C
51	9	533	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	559	G
51	9	562	U
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	595	U
51	9	597	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	613	G
51	9	614	C
51	9	615	C
51	9	616	A
51	9	617	G
51	9	620	G
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	630	U
51	9	631	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	632	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	646	G
51	9	659	G
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	684	G
51	9	688	U
51	9	689	U
51	9	733	C
51	9	752	G
51	9	753	C
51	9	754	G
51	9	798	G
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	834	C
51	9	844	U
51	9	847	A
51	9	861	A
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	876	C
51	9	877	C
51	9	878	G
51	9	885	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	887	U
51	9	890	U
51	9	892	U
51	9	913	A
51	9	914	U
51	9	919	A
51	9	920	A
51	9	921	G
51	9	922	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	971	G
51	9	981	A
51	9	985	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1002	U
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1055	A
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1067	C
51	9	1078	C
51	9	1083	A
51	9	1085	C
51	9	1100	A
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G
51	9	1131	G
51	9	1138	C
51	9	1139	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	1144	A
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1161	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1196	A
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1215	C
51	9	1221	G
51	9	1224	G
51	9	1227	G
51	9	1230	C
51	9	1240	A
51	9	1242	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1259	A
51	9	1260	A
51	9	1265	A
51	9	1266	C
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1280	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1303	C
51	9	1304	U
51	9	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1330	G
51	9	1331	C
51	9	1341	C
51	9	1342	U
51	9	1348	G
51	9	1369	A
51	9	1371	U
51	9	1372	U
51	9	1376	A
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	1405	A
51	9	1412	C
51	9	1424	G
51	9	1428	G
51	9	1439	A
51	9	1449	G
51	9	1454	A
51	9	1455	A
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1466	G
51	9	1473	G
51	9	1476	A
51	9	1477	U
51	9	1487	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	1490	G
51	9	1494	U
51	9	1498	A
51	9	1509	U
51	9	1510	G
51	9	1519	U
51	9	1521	C
51	9	1522	A
51	9	1523	C
51	9	1531	A
51	9	1533	A
51	9	1536	G
51	9	1539	U
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1585	U
51	9	1587	G
51	9	1588	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1624	U
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1641	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1683	C
51	9	1686	G
51	9	1695	A
51	9	1698	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	1732	G
51	9	1744	G
51	9	1745	A
51	9	1748	G
51	9	1753	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C
51	9	1800	A
51	9	1801	A
51	9	1805	G
51	9	1822	A
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	1849	G
51	9	1851	A
51	9	1852	C
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A
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

All (275) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	74	C
48	5	12	A
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	119	G
48	5	125	C
48	5	134	G
48	5	143	C
48	5	159	C
48	5	217	C
48	5	224	U
48	5	226	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	G
48	5	315	G
48	5	385	A
48	5	387	G
48	5	406	C
48	5	408	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	409	G
48	5	417	G
48	5	449	C
48	5	453	G
48	5	466	A
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	916	C
48	5	922	C
48	5	922(B)	C
48	5	930	G
48	5	933	G
48	5	935(A)	G
48	5	936	C
48	5	955	G
48	5	956	A
48	5	959	G
48	5	966	A
48	5	968	C
48	5	969	C
48	5	971(A)	G
48	5	1072	C
48	5	1209	U
48	5	1211	G
48	5	1214	C
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1295	U
48	5	1329	G
48	5	1358	G
48	5	1370	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	1378	C
48	5	1380	G
48	5	1432	G
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1481	C
48	5	1485	C
48	5	1497	A
48	5	1523	A
48	5	1533	A
48	5	1625	G
48	5	1633	G
48	5	1654	G
48	5	1678	C
48	5	1733	G
48	5	1740	C
48	5	1804	A
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1892	A
48	5	1919	G
48	5	1921	C
48	5	1935	C
48	5	1947	U
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2046	G
48	5	2068	C
48	5	2088	A
48	5	2089	G
48	5	2100	G
48	5	2265	G
48	5	2266	C
48	5	2278	G
48	5	2313	A
48	5	2333	G
48	5	2398	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	A
48	5	2513	A
48	5	2529	A
48	5	2530	U
48	5	2546	G
48	5	2553	A
48	5	2587	A
48	5	2661	U
48	5	2695	A
48	5	2724	G
48	5	2739	C
48	5	2754	G
48	5	2794	C
48	5	2806	A
48	5	2845	A
48	5	2874	U
48	5	3603	G
48	5	3625	G
48	5	3673	C
48	5	3697	U
48	5	3710	G
48	5	3759	A
48	5	3760	A
48	5	3765	G
48	5	3784	A
48	5	3785	A
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	3938	G
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4116	C
48	5	4119	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
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	4291	G
48	5	4378	A
48	5	4379	A
48	5	4395	U
48	5	4404	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4510	A
48	5	4527	G
48	5	4572	U
48	5	4699	U
48	5	4719	G
48	5	4753	U
48	5	4756	C
48	5	4872	G
48	5	4884	G
48	5	4925	U
48	5	4936	G
48	5	4942	C
48	5	4944	C
48	5	4947	U
48	5	4965	U
48	5	5013	C
48	5	5047	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

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	3	C
51	9	72	C
51	9	110	U
51	9	126	G
51	9	128	U
51	9	141	A
51	9	142	C
51	9	160	U
51	9	182	C
51	9	214	U
51	9	293	C
51	9	312	G
51	9	360	A
51	9	363	A
51	9	369	C
51	9	434	G
51	9	465	A
51	9	492	C
51	9	500	A
51	9	532	C
51	9	550	C
51	9	553	U
51	9	555	A
51	9	559	G
51	9	563	G
51	9	587	A
51	9	591	U
51	9	594	A
51	9	606	G
51	9	613	G
51	9	615	C
51	9	620	G
51	9	625	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U
51	9	752	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
51	9	821	G
51	9	869	A
51	9	870	A
51	9	872	A
51	9	874	G
51	9	875	A
51	9	1016	U
51	9	1087	A
51	9	1114	U
51	9	1130	G
51	9	1137	U
51	9	1165	G
51	9	1253	A
51	9	1264	C
51	9	1274	G
51	9	1285	G
51	9	1313	A
51	9	1330	G
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1438	A
51	9	1476	A
51	9	1489	A
51	9	1493	C
51	9	1519	U
51	9	1520	G
51	9	1581	C
51	9	1621	U
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1663	A
51	9	1664	A
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1825	A
51	9	1835	A
51	9	1867	U
51	9	1868	U



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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 273 ligands modelled in this entry, 272 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	25,34,34	2.60	7 (28%)	28,54,54	0.93	1 (3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C4-N9	-10.51	1.33	1.47
90	jj	700	GCP	C8-N9	-3.89	1.35	1.46
90	jj	700	GCP	C5-C6	-2.26	1.48	1.53
90	jj	700	GCP	PB-O2B	2.28	1.61	1.56
90	jj	700	GCP	PB-O3A	2.54	1.61	1.58
90	jj	700	GCP	PG-O2G	2.77	1.61	1.54
90	jj	700	GCP	PG-O3G	2.95	1.61	1.54



All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	PA-O3A-PB	-2.64	123.88	132.39

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	42
51	9	8
47	3	2
46	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.91
1	5	1252:C	O3'	1271:G	P	36.05
1	5	1405:C	O3'	1406:G	P	23.79
1	5	1219:G	O3'	1233:G	P	22.30
1	5	1406:G	O3'	1406(A):G	P	20.51
1	5	3948:C	O3'	4065:G	P	19.69
1	5	990:C	O3'	1064:G	P	18.04
1	5	523:C	O3'	638:G	P	18.03
1	5	4138:C	O3'	4146:G	P	18.02
1	5	4101:C	O3'	4107:G	P	17.30
1	5	4777:C	O3'	4859:C	P	16.29
1	5	5022:U	O3'	5028:G	P	15.23
1	5	760:G	O3'	904:C	P	14.93
1	5	1696:C	O3'	1720:C	P	14.86

*Continued on next page...*



*Continued from previous page...*

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1364:U	O3'	1368:A	P	14.43
1	5	182:G	O3'	189:G	P	14.08
1	5	1406(C):G	O3'	1411:C	P	13.56
1	5	2901:G	O3'	3597:G	P	13.16
1	5	1411:C	O3'	1411(A):G	P	13.03
1	5	921:C	O3'	922:C	P	12.78
1	5	481:G	O3'	481(A):C	P	12.48
1	5	934:C	O3'	935:A	P	10.82
1	5	970:G	O3'	971:U	P	10.67
1	5	737:C	O3'	738:C	P	9.93
1	5	4729:A	O3'	4735:G	P	9.81
1	5	512:U	O3'	515:C	P	9.70
1	5	971:U	O3'	971(A):G	P	9.68
1	5	1180:C	O3'	1183:C	P	9.47
1	5	500:G	O3'	504:G	P	6.88
1	5	1100:U	O3'	1168:G	P	5.94
1	3	19:G	O3'	20:U	P	5.60
1	5	480:C	O3'	481:G	P	5.46
1	3	16:C	O3'	18:U	P	5.24
1	5	4740:G	O3'	4743:G	P	5.13
1	9	322:C	O3'	323:C	P	5.02
1	9	798:G	O3'	799:U	P	4.84
1	5	1239:C	O3'	1244:G	P	4.76
1	2	16:C	O3'	18:G	P	4.39
1	9	304:C	O3'	305:U	P	4.29
1	5	935:A	O3'	935(A):G	P	4.26
1	9	309:G	O3'	310:C	P	4.26
1	5	170:C	O3'	171:U	P	3.83
1	5	738:C	O3'	738(A):C	P	3.67
1	5	1438:U	O3'	1440:U	P	3.47
1	5	4899:G	O3'	4902:C	P	3.40
1	9	902:G	O3'	903:A	P	3.37
1	9	903:A	O3'	904:A	P	3.27
1	9	1295:A	O3'	1296:U	P	3.25
1	5	267:G	O3'	268:G	P	3.08
1	5	5020:G	O3'	5021:C	P	3.05
1	5	751:G	O3'	752:G	P	2.99
1	9	593:C	O3'	594:A	P	2.98
1	5	2031:C	O3'	2032:U	P	2.33