



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 8, 2017 – 12:02 PM EST

PDB ID : 5MRC
EMDB ID: : EMD-3551
Title : Structure of the yeast mitochondrial ribosome - Class A
Authors : Desai, N.; Brown, A.; Amunts, A.; Ramakrishnan, V.
Deposited on : 2016-12-22
Resolution : 3.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

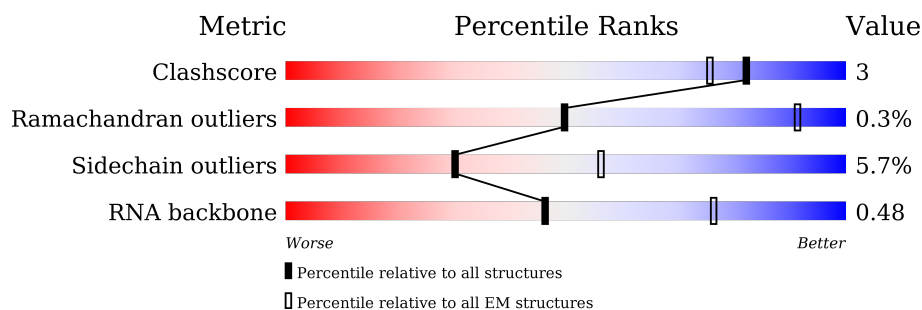
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.25 Å.

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








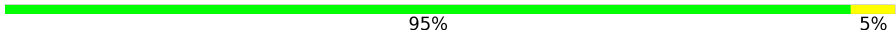
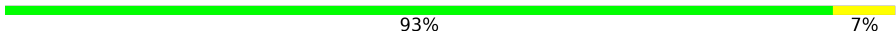
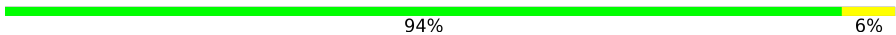






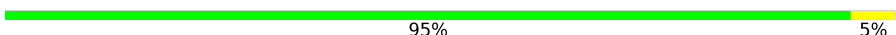


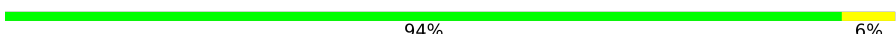

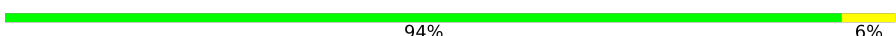

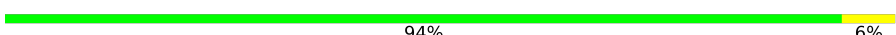



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A	3296	60% 19% 18%
2	B	393	73% 8% 18%
3	C	249	86% 13%
4	D	252	87% 12% .
5	E	274	93% 6% .
6	F	196	91% 9%
7	G	74	95% 5%
8	H	160	91% 9%

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Mol	Chain	Length	Quality of chain
9	I	138	
10	J	220	
11	K	195	
12	L	237	
13	M	151	
14	N	118	
15	O	225	
16	P	207	
17	Q	296	
18	R	337	
19	S	216	
20	T	225	
21	U	82	
22	V	177	
23	W	112	
24	X	64	
25	Y	46	
26	Z	62	
27	0	38	
28	1	348	
29	2	113	
30	3	130	
31	4	138	
32	5	324	
33	6	281	










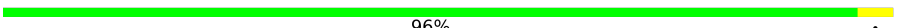







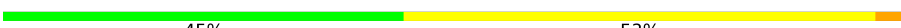
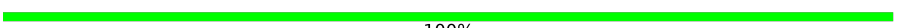
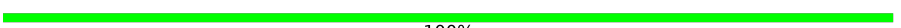
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Mol	Chain	Length	Quality of chain
34	7	106	
35	8	264	
36	9	215	
37	a	177	
38	b	155	
39	c	119	
40	d	215	
41	AA	344	
42	BB	266	
43	CC	398	
44	DD	486	
45	EE	293	
46	FF	125	
47	GG	161	
48	HH	154	
49	II	244	
50	JJ	186	
51	KK	148	
52	LL	124	
53	MM	120	
54	NN	115	
55	OO	253	
56	PP	119	
57	QQ	237	
58	RR	99	

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Mol	Chain	Length	Quality of chain
59	SS	80	 79% 18% .
60	TT	92	 88% 11% .
61	UU	233	 86% 12% .
62	VV	233	 93% 6% .
63	WW	401	 85% 15%
64	XX	96	 92% 6% .
65	YY	273	 85% 13% .
66	ZZ	91	 80% 14% . .
67	11	34	 91% 9%
68	22	99	 96% .
69	33	255	 84% 11% . .
70	44	321	 79% 6% 16%
71	55	339	 17% . 83%
72	66	319	 88% 8% .
73	77	165	 92% 8% .
74	88	457	 87% 11% ..
75	aa	1649	 63% 27% 9%
76	bb	76	 45% 53% .
77	cc	94	 100%
78	dd	151	 100%

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 201462 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 21S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2709	Total	C	N	O	P	0	0
			57598	25914	10252	18729	2703		

- Molecule 2 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	321	Total	C	N	O	S	0	0
			2527	1575	507	436	9		

- Molecule 3 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	249	Total	C	N	O	S	0	0
			1932	1218	360	344	10		

- Molecule 4 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	252	Total	C	N	O	S	0	0
			1991	1264	355	369	3		

- Molecule 5 is a protein called uL5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	274	Total	C	N	O	S	0	0
			2187	1396	391	394	6		

- Molecule 6 is a protein called uL6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	196	Total	C	N	O	S	0	0
			1524	967	273	280	4		

- Molecule 7 is a protein called bL9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	74	Total	C	N	O	S	0	0
			617	393	110	113	1		

- Molecule 8 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	160	Total	C	N	O	S	0	0
			1275	807	240	224	4		

- Molecule 9 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	127	Total	C	N	O	S	0	0
			956	595	180	170	11		

- Molecule 10 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	220	Total	C	N	O	S	0	0
			1746	1119	326	298	3		

- Molecule 11 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	195	Total	C	N	O	S	0	0
			1573	1001	297	270	5		

- Molecule 12 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	229	Total	C	N	O	S	0	0
			1817	1140	333	336	8		

- Molecule 13 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	151	Total	C	N	O	S	0	0
			1206	766	220	217	3		

- Molecule 14 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	118	Total	C	N	O	S	0	0
			948	598	177	171	2		

- Molecule 15 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	225	Total	C	N	O	S	0	0
			1826	1169	332	320	5		

- Molecule 16 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	207	Total	C	N	O	S	0	0
			1729	1104	310	309	6		

- Molecule 17 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	284	Total	C	N	O	S	0	0
			2272	1451	396	417	8		

- Molecule 18 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	331	Total	C	N	O	S	0	0
			2738	1728	497	509	4		

- Molecule 19 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	185	Total	C	N	O	S	0	0
			1543	994	281	265	3		

- Molecule 20 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1792	1139	324	325	4		

- Molecule 21 is a protein called uL30m.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	82	Total	C	N	O	0	0
			639	410	116	113		

- Molecule 22 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	93	Total	C	N	O	S	0	0
			729	456	145	127	1		

- Molecule 23 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	112	Total	C	N	O	S	0	0
			937	587	181	163	6		

- Molecule 24 is a protein called bL33m.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	64	Total	C	N	O	0	0
			512	330	96	86		

- Molecule 25 is a protein called bL34m.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	46	Total	C	N	O	0	0
			385	245	82	58		

- Molecule 26 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	62	Total	C	N	O	S	0	0
			508	322	111	74	1		

- Molecule 27 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	38	Total	C	N	O	S	0	0
			324	205	66	50	3		

- Molecule 28 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	348	Total	C	N	O	S	0	0
			2875	1847	499	523	6		

- Molecule 29 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	113	Total	C	N	O	S	0	0
			944	597	174	168	5		

- Molecule 30 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	130	Total	C	N	O	S	0	0
			1046	671	189	183	3		

- Molecule 31 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	138	Total	C	N	O	S	0	0
			1117	700	219	193	5		

- Molecule 32 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	324	Total	C	N	O	S	0	0
			2552	1630	431	480	11		

- Molecule 33 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	234	Total	C	N	O	S	0	0
			1932	1250	327	353	2		

- Molecule 34 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	7	106	Total	C	N	O	S	0	0
			858	553	151	152	2		

- Molecule 35 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	8	199	Total	C	N	O	S	0	0
			1629	1032	278	315	4		

- Molecule 36 is a protein called mL57.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	9	202	Total	C	N	O	S	0	0
			1587	1014	279	289	5		

- Molecule 37 is a protein called mL58.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	177	Total	C	N	O	S	0	0
			1440	907	267	260	6		

- Molecule 38 is a protein called mL59.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	155	Total	C	N	O	S	0	0
			1299	850	225	221	3		

- Molecule 39 is a protein called mL60.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	119	Total	C	N	O	S	0	0
			1004	645	191	164	4		

- Molecule 40 is a protein called mL67.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	206	Total	C	N	O	S	0	0
			1746	1117	318	304	7		

- Molecule 41 is a protein called bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AA	203	Total	C	N	O	S	0	0
			1610	1032	285	288	5		

- Molecule 42 is a protein called uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BB	266	Total	C	N	O	S	0	0
			2085	1313	366	404	2		

- Molecule 43 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	CC	339	Total	C	N	O	S	0	0
			2821	1772	502	517	30		

- Molecule 44 is a protein called uS4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	DD	287	Total	C	N	O	S	0	0
			2369	1542	420	403	4		

- Molecule 45 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	EE	288	Total	C	N	O	S	0	0
			2306	1473	408	417	8		

- Molecule 46 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	FF	125	Total	C	N	O	S	0	0
			1002	639	182	177	4		

- Molecule 47 is a protein called uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	GG	161	Total	C	N	O	S	0	0
			1282	811	238	228	5		

- Molecule 48 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	HH	154	Total	C	N	O	S	0	0
			1213	767	217	220	9		

- Molecule 49 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	II	226	Total	C	N	O	S	0	0
			1820	1167	332	316	5		

- Molecule 50 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	JJ	186	Total	C	N	O	S	0	0
			1508	964	259	281	4		

- Molecule 51 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	KK	142	Total	C	N	O	S	0	0
			1121	717	195	203	6		

- Molecule 52 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LL	124	Total	C	N	O	S	0	0
			948	585	194	165	4		

- Molecule 53 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	MM	120	Total	C	N	O	S	0	0
			942	596	179	161	6		

- Molecule 54 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	NN	115	Total	C	N	O	S	0	0
			953	612	182	154	5		

- Molecule 55 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	OO	238	Total	C	N	O	S	0	0
			1962	1227	371	356	8		

- Molecule 56 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	PP	116	Total	C	N	O	S	0	0
			919	586	172	159	2		

- Molecule 57 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	QQ	204	Total	C	N	O	S	0	0
			1683	1055	315	308	5		

- Molecule 58 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	RR	91	Total	C	N	O	S	0	0
			738	463	143	128	4		

- Molecule 59 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	SS	80	Total	C	N	O	S	0	0
			636	408	115	111	2		

- Molecule 60 is a protein called bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	TT	92	Total	C	N	O	S	0	0
			760	475	150	130	5		

- Molecule 61 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	UU	233	Total	C	N	O	S	0	0
			1907	1211	331	358	7		

- Molecule 62 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	VV	233	Total	C	N	O	S	0	0
			1872	1189	338	342	3		

- Molecule 63 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	WW	401	Total	C	N	O	S	0	0
			3216	2072	540	596	8		

- Molecule 64 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	XX	96	Total	C	N	O	S	0	0
			774	496	140	135	3		

- Molecule 65 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	YY	269	Total	C	N	O	S	0	0
			2258	1429	404	421	4		

- Molecule 66 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	ZZ	87	Total	C	N	O	S	0	0
			687	435	128	118	6		

- Molecule 67 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	11	34	Total	C	N	O	S	0	0
			303	183	75	43	2		

- Molecule 68 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	22	99	Total	C	N	O	S	0	0
			833	530	156	146	1		

- Molecule 69 is a protein called mS42.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	33	244	Total	C	N	O	S	0	0
			1953	1261	328	359	5		

- Molecule 70 is a protein called mS43.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	44	270	Total	C	N	O	S	0	0
			2169	1380	370	412	7		

- Molecule 71 is a protein called mS44.

Mol	Chain	Residues	Atoms				AltConf	Trace
71	55	59	Total	C	N	O	0	0
			508	338	84	86		

- Molecule 72 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	66	305	Total	C	N	O	S	0	0
			2488	1587	445	450	6		

- Molecule 73 is a protein called mS46.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	77	165	Total	C	N	O	S	0	0
			1330	854	214	259	3		

- Molecule 74 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	88	452	Total	C	N	O	S	0	0
			3573	2272	600	681	20		

- Molecule 75 is a RNA chain called 15S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	aa	1501	Total	C	N	O	P	0	0
			31883	14338	5633	10411	1501		

- Molecule 76 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	bb	76	Total	C	N	O	P	0	0
			1615	723	289	528	75		

- Molecule 77 is a protein called unknown protein sequence 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
77	cc	94	Total	C	N	O	0	0
			470	282	94	94		

- Molecule 78 is a protein called unknown protein sequence 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
78	dd	151	Total	C	N	O	0	0
			755	453	151	151		

- Molecule 79 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
79	BB	1	Total	Mg	0
			1	1	
79	WW	1	Total	Mg	0
			1	1	
79	d	1	Total	Mg	0
			1	1	
79	NN	1	Total	Mg	0
			1	1	
79	MM	1	Total	Mg	0
			1	1	
79	A	181	Total	Mg	0
			181	181	
79	aa	111	Total	Mg	0
			111	111	
79	3	1	Total	Mg	0
			1	1	
79	QQ	1	Total	Mg	0
			1	1	

- Molecule 80 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
80	B	1	Total	Na	0
			1	1	

- Molecule 81 is ZINC ION (three-letter code: ZN) (formula: Zn).

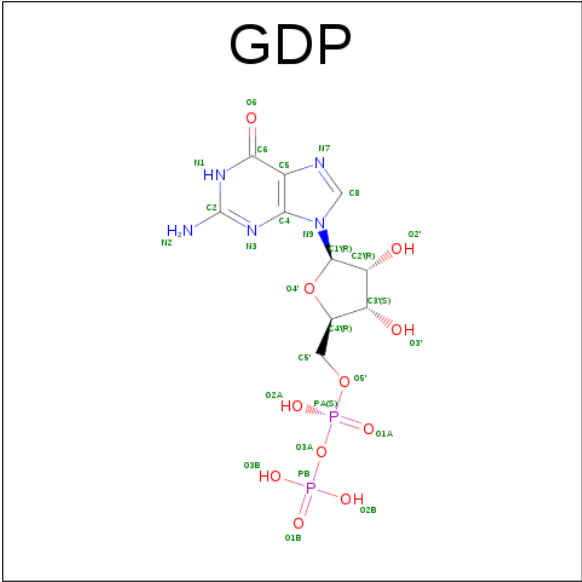
Mol	Chain	Residues	Atoms		AltConf
81	0	1	Total	Zn	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
81	W	1	Total	Zn	0
			1	1	

- Molecule 82 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

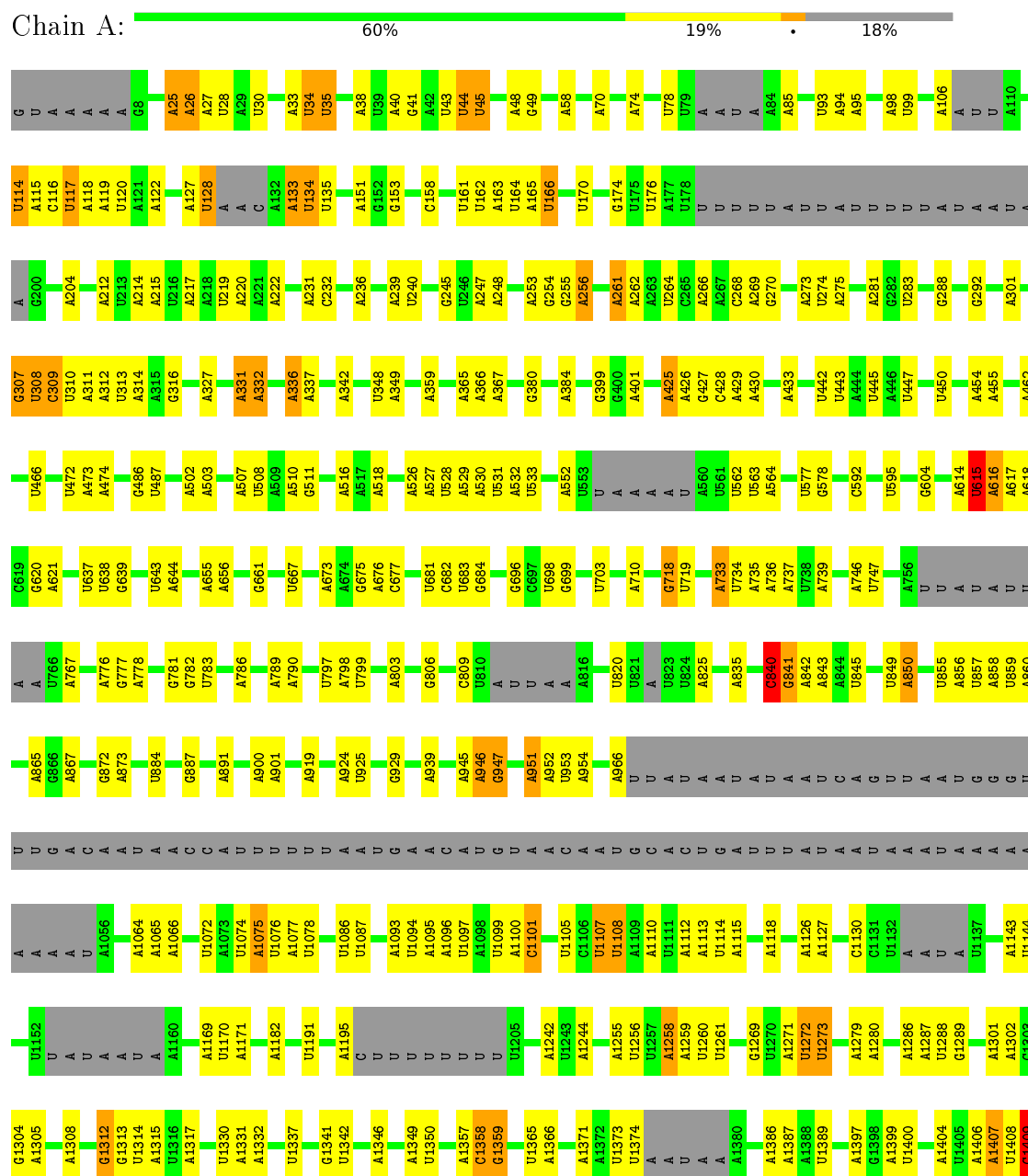


Mol	Chain	Residues	Atoms					AltConf
82	WW	1	Total	C	N	O	P	0
			28	10	5	11	2	

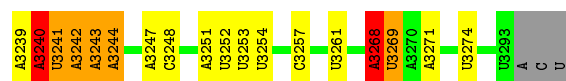
3 Residue-property plots [i](#)

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

• Molecule 1: 21S RNA









- Molecule 2: uL2m

Chain B: 73% 8% 18%



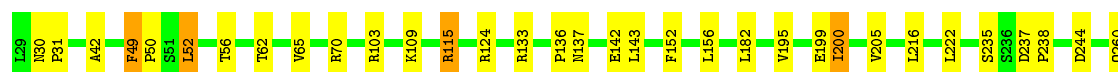
- Molecule 3: uL3m

Chain C:  86% 13%



- Molecule 4: uL4m

Chain D: 87% 12%



- Molecule 5: uL5m

Chain E:  93% 6%



- Molecule 6: uL6m

Chain F: 91% 9%



- Molecule 7: bL9m

Chain G:  95% 5%




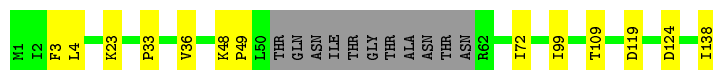
- Molecule 8: uL13m

Chain H:  91% 9%




- Molecule 9: uL14m

Chain I:  83% 9% 8%




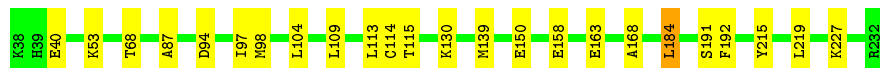
- Molecule 10: uL15m

Chain J:  90% 10%




- Molecule 11: uL16m

Chain K:  88% 12%




- Molecule 12: bL17m

Chain L:  88% 8%



- Molecule 13: bL19m

Chain M:  91% 8%



- Molecule 14: bL21m

Chain N:  95% 5%



- Molecule 15: uL22m

Chain O: 93% 7%



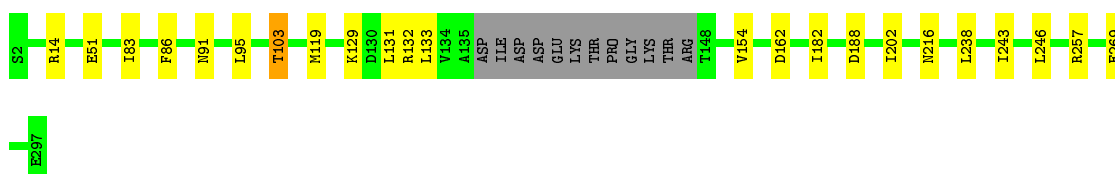
- Molecule 16: uL23m

Chain P: 94% 6%



- Molecule 17: uL24m

Chain Q: 88% 7% .



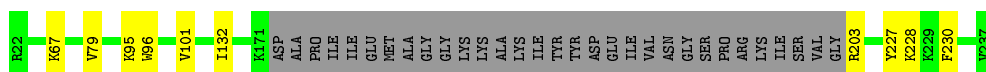
- Molecule 18: bL27m

Chain R: 91% 7% .



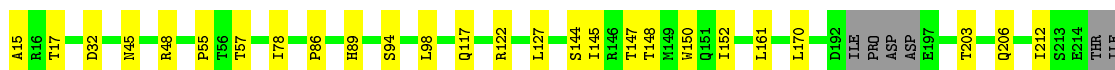
- Molecule 19: bL28m

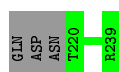
Chain S: 81% 5% 14%



- Molecule 20: uL29m

Chain T: 84% 12% .





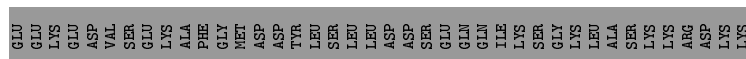
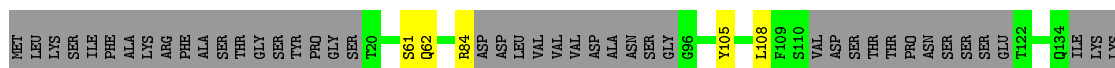
- Molecule 21: uL30m

Chain U: 84% 15%



- Molecule 22: bL31m

Chain V: 50% 47%



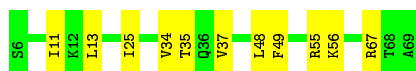
- Molecule 23: bL32m

Chain W: 95% 5%



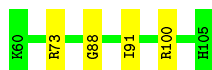
- Molecule 24: bL33m

Chain X: 83% 17%



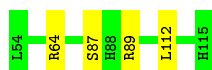
- Molecule 25: bL34m

Chain Y: 91% 9%



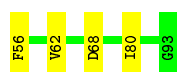
- Molecule 26: bL35m

Chain Z: 94% 6%



- Molecule 27: bL36m

Chain 0: 89% 11%



- Molecule 28: mL38

Chain 1: 94% 6%



- Molecule 29: mL40

Chain 2: 88% 11% .



- Molecule 30: mL41

Chain 3: 94% 6%



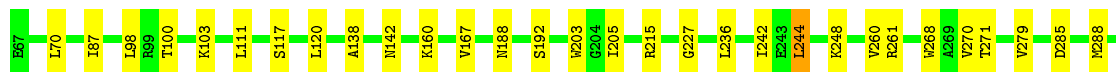
- Molecule 31: mL43

Chain 4: 91% 9%



- Molecule 32: mL44

Chain 5: 89% 11%




- Molecule 33: mL46

Chain 6: 75% 8% 17%



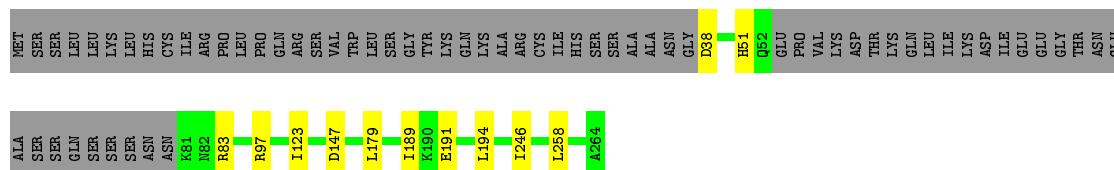
- Molecule 34: mL49

Chain 7:  87% 13%



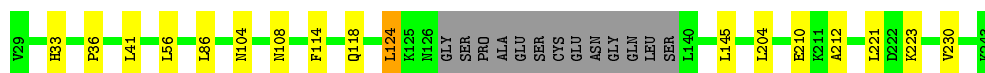
- Molecule 35: mL50

Chain 8:  71% 5% 25%



- Molecule 36: mL57

Chain 9:  86% 7% 6%



- Molecule 37: mL58

Chain a:  96%



- Molecule 38: mL59

Chain b:  97%



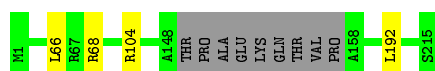
- Molecule 39: mL60

Chain c:  98%



- Molecule 40: mL67

Chain d:  94%



- Molecule 41: bS1m

Device Type	Percentage
Smartphone	54%
Tablet	5%
Feature phone	41%



83% 16% .

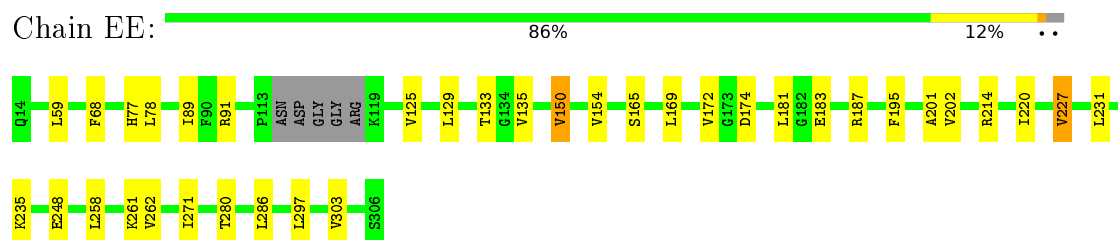


Response	Percentage
Used	71%
Not used	13%
Don't know	15%

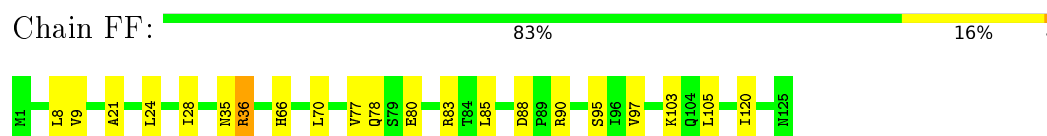


Device Type	Percentage
Smartphone	50%
Tablet	8%
Feature phone	41%

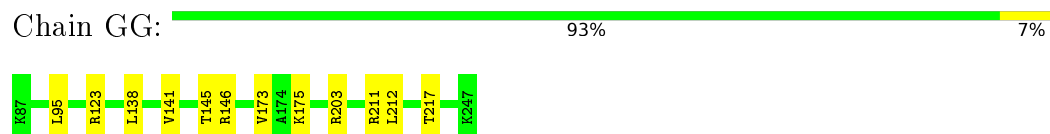
- Molecule 45: uS5m



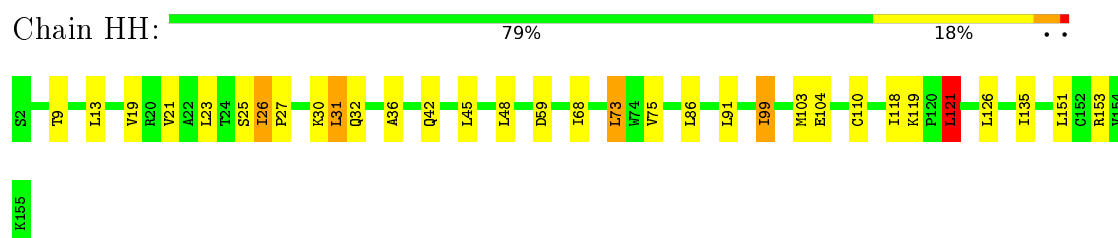
- Molecule 46: bS6m



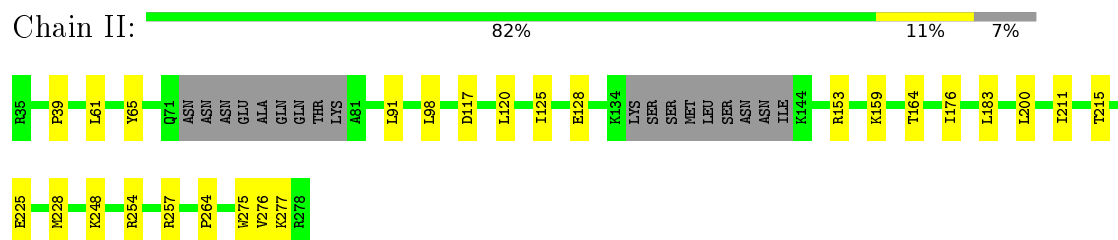
- Molecule 47: uS7m



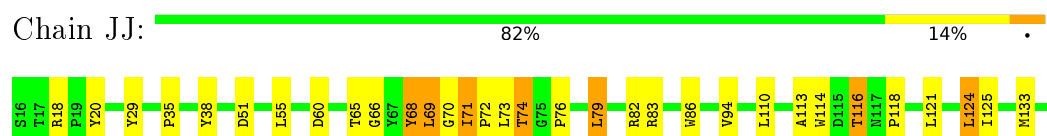
- Molecule 48: uS8m




- Molecule 49: uS9m

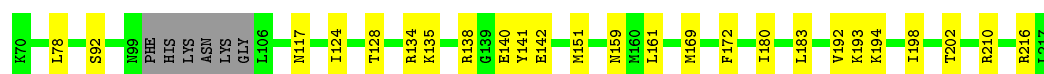


- Molecule 50: uS10m




- Molecule 51: uS11m

Chain KK:  79% 17% .



- Molecule 52: uS12m

Chain LL:  85% 13% .




- Molecule 53: uS13m

Chain MM:  91% 8% .




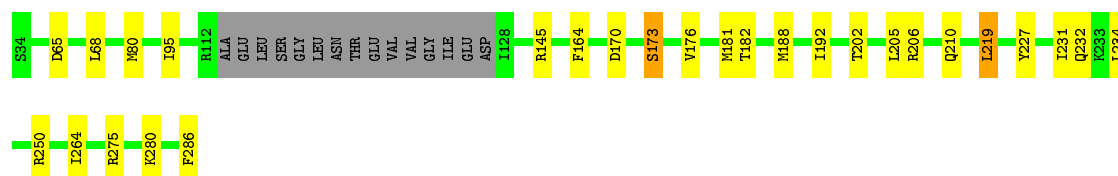
- Molecule 54: uS14m

Chain NN:  85% 11% .



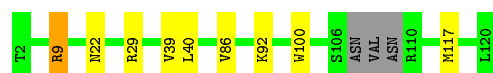
- Molecule 55: uS15m

Chain OO:  83% 10% 6% .




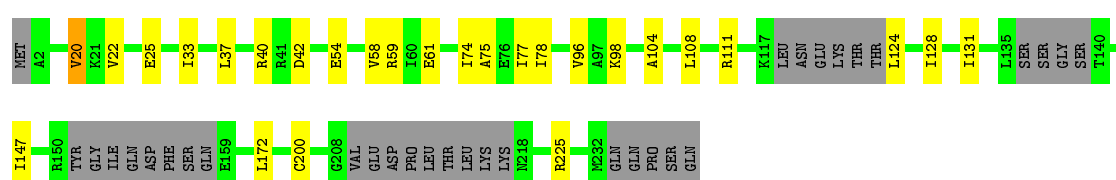
- Molecule 56: bS16m

Chain PP:  90% 7% . .




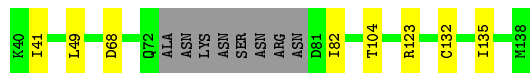
- Molecule 57: uS17m

Chain QQ:  75% 11% 14%




- Molecule 58: bS18m

Chain RR:  84% 8% 8%



- Molecule 59: uS19m

Chain SS:  79% 18% .



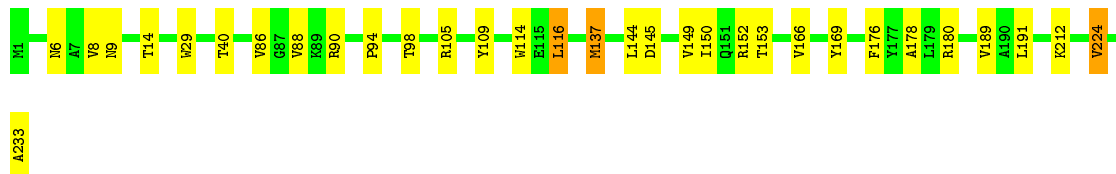
- Molecule 60: bS21m

Chain TT:  88% 11% .



- Molecule 61: mS23

Chain UU:  86% 12% .



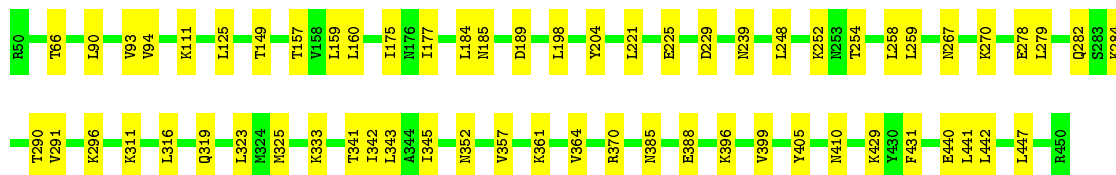
- Molecule 62: mS26

Chain VV:  93% 6% .



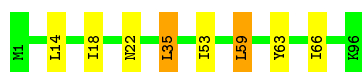
- Molecule 63: mS29

Chain WW:  85% 15%



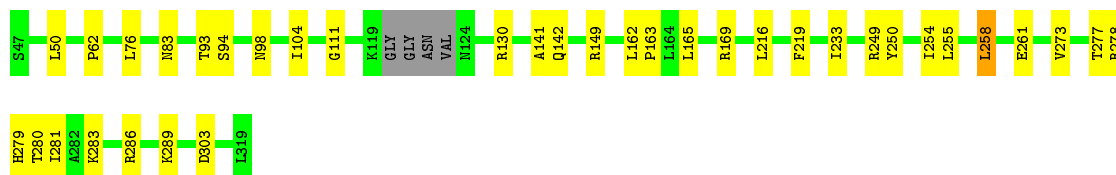
- Molecule 64: mS33

Chain XX:  92% 6% .



• Molecule 65: mS35

Chain YY: 85% 13% .



• Molecule 66: mS37

Chain ZZ: 80% 14% . .



• Molecule 67: mS38

Chain 11: 91% 9%



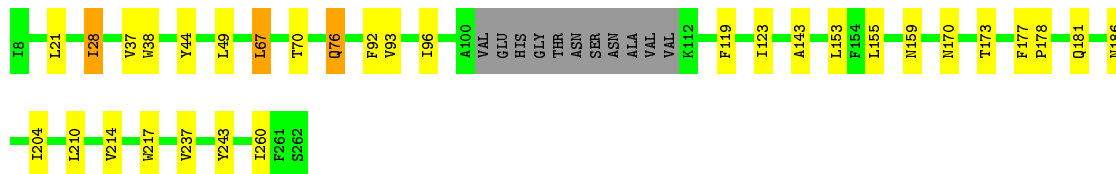
• Molecule 68: mS41

Chain 22: 96% .



• Molecule 69: mS42

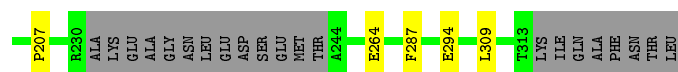
Chain 33: 84% 11% . .



• Molecule 70: mS43

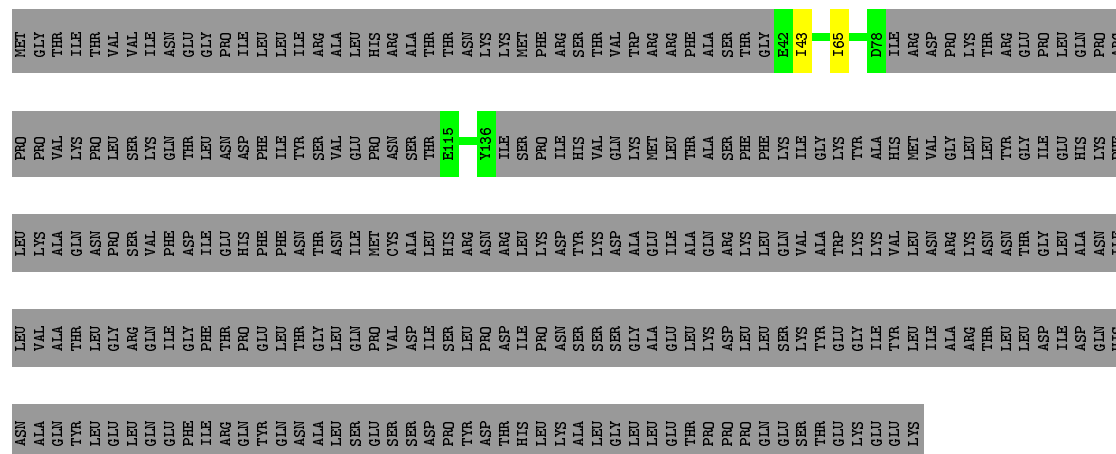
Chain 44: 79% 6% 16%





• Molecule 71: mS44

Chain 55: 17% 83%



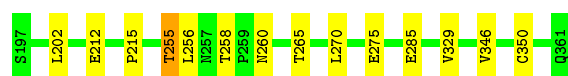
• Molecule 72: mS45

Chain 66: 88% 8%



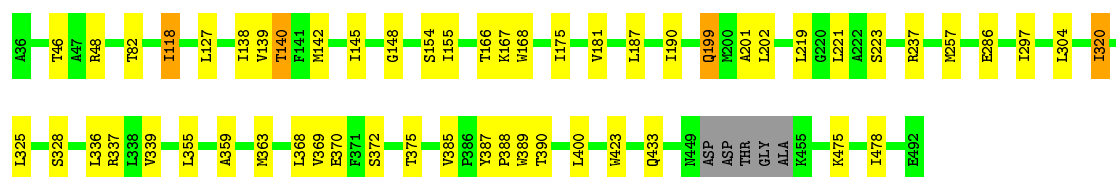
• Molecule 73: mS46

Chain 77: 92% 8%



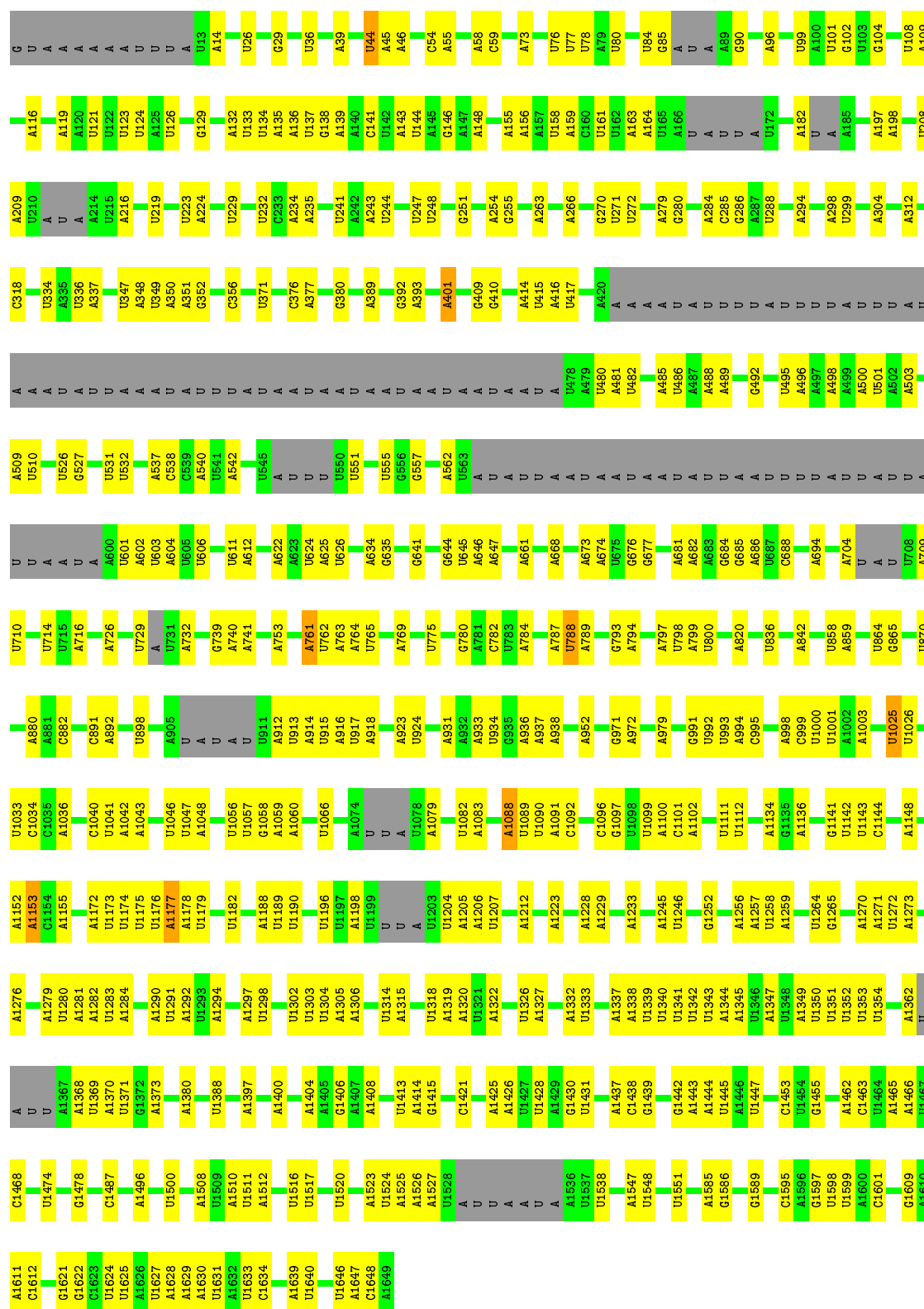
• Molecule 74: mS47

Chain 88: 87% 11%



• Molecule 75: 15S RNA

Chain aa: 63% 27% 9%



• Molecule 76: tRNA

Chain bb: 45% 53%



- Molecule 77: unknown protein sequence 1

Chain cc: 100%

There are no outlier residues recorded for this chain.

- Molecule 78: unknown protein sequence 2

Chain dd: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	141795	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, NA, 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	0.23	0/64517	0.71	19/100359 (0.0%)
10	J	0.33	0/1783	0.64	0/2384
11	K	0.34	0/1606	0.66	0/2148
12	L	0.32	0/1845	0.63	0/2489
13	M	0.35	0/1224	0.67	0/1651
14	N	0.33	0/961	0.66	0/1295
15	O	0.32	0/1859	0.63	0/2495
16	P	0.33	0/1773	0.61	0/2390
17	Q	0.34	0/2323	0.57	0/3135
18	R	0.33	0/2783	0.64	0/3723
19	S	0.34	0/1576	0.61	0/2104
2	B	0.34	0/2573	0.67	0/3456
20	T	0.34	0/1837	0.60	0/2486
21	U	0.41	0/648	0.64	0/870
22	V	0.35	0/741	0.61	0/995
23	W	0.31	0/955	0.59	0/1273
24	X	0.33	0/520	0.66	0/696
25	Y	0.35	0/392	0.72	0/515
26	Z	0.34	0/522	0.68	0/695
27	0	0.33	0/329	0.58	0/432
28	1	0.34	0/2949	0.59	0/3998
29	2	0.33	0/963	0.62	0/1295
3	C	0.32	0/1975	0.62	0/2657
30	3	0.34	0/1072	0.61	0/1442
31	4	0.34	0/1138	0.70	0/1526
32	5	0.32	0/2604	0.59	0/3526
33	6	0.34	0/1978	0.59	0/2664
34	7	0.35	0/873	0.61	0/1170
35	8	0.33	0/1659	0.56	0/2230
36	9	0.34	0/1616	0.57	0/2177
37	a	0.34	0/1471	0.65	0/1976
38	b	0.33	0/1333	0.58	0/1783

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	c	0.33	0/1028	0.61	0/1372
4	D	0.35	0/2031	0.66	0/2751
40	d	0.33	0/1791	0.62	0/2415
41	AA	0.33	0/1645	0.61	0/2218
42	BB	0.36	0/2128	0.67	0/2892
43	CC	0.34	0/2864	0.58	0/3853
44	DD	0.35	0/2434	0.64	0/3281
45	EE	0.33	0/2360	0.60	0/3180
46	FF	0.32	0/1014	0.63	0/1358
47	GG	0.35	0/1305	0.62	0/1763
48	HH	0.33	0/1232	0.71	1/1660 (0.1%)
49	II	0.34	0/1855	0.62	0/2492
5	E	0.32	0/2244	0.56	0/3033
50	JJ	0.33	0/1544	0.66	1/2091 (0.0%)
51	KK	0.36	0/1136	0.63	0/1515
52	LL	0.34	0/963	0.70	0/1292
53	MM	0.33	0/957	0.65	0/1277
54	NN	0.35	0/972	0.64	0/1300
55	OO	0.34	0/1985	0.68	0/2647
56	PP	0.33	0/934	0.64	0/1260
57	QQ	0.32	0/1694	0.65	0/2252
58	RR	0.37	0/749	0.67	0/998
59	SS	0.34	0/652	0.66	1/882 (0.1%)
6	F	0.33	0/1551	0.58	0/2093
60	TT	0.37	0/771	0.64	0/1019
61	UU	0.33	0/1950	0.62	0/2636
62	VV	0.32	0/1900	0.60	0/2540
63	WW	0.34	0/3282	0.58	0/4438
64	XX	0.35	0/786	0.63	0/1046
65	YY	0.35	0/2313	0.62	0/3119
66	ZZ	0.43	0/702	0.71	1/945 (0.1%)
67	11	0.33	0/303	0.81	0/386
68	22	0.34	0/852	0.56	0/1142
69	33	0.35	0/2002	0.58	0/2721
7	G	0.33	0/628	0.58	0/844
70	44	0.34	0/2214	0.58	0/2990
71	55	0.35	0/521	0.57	0/701
72	66	0.34	0/2547	0.59	0/3438
73	77	0.35	0/1358	0.56	0/1839
74	88	0.35	0/3646	0.58	0/4935
75	aa	0.26	0/35686	0.74	24/55477 (0.0%)
76	bb	0.42	0/1805	0.87	2/2811 (0.1%)
8	H	0.34	0/1302	0.63	0/1749

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
9	I	0.32	0/962	0.66	0/1285
All	All	0.30	0/212996	0.67	49/307971 (0.0%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	ZZ	24	ARG	NE-CZ-NH2	11.40	126.00	120.30
76	bb	33	U	N1-C1'-C2'	-8.48	102.67	112.00
1	A	2897	A	C2'-C3'-O3'	8.30	127.76	109.50
1	A	840	C	C2'-C3'-O3'	8.25	127.64	109.50
50	JJ	71	ILE	C-N-CD	-8.03	102.93	120.60
1	A	615	U	C2'-C3'-O3'	7.46	125.90	109.50
75	aa	798	U	C2'-C3'-O3'	7.35	125.68	109.50
75	aa	509	A	C2'-C3'-O3'	7.33	125.63	109.50
75	aa	971	G	C2'-C3'-O3'	7.29	125.53	109.50
75	aa	415	U	C2'-C3'-O3'	7.11	125.14	109.50
1	A	2359	U	C2'-C3'-O3'	6.95	124.82	113.70
75	aa	1430	G	C2'-C3'-O3'	6.93	124.78	113.70
1	A	733	A	C2'-C3'-O3'	6.90	124.74	113.70
1	A	3268	A	C2'-C3'-O3'	6.77	124.53	113.70
75	aa	1082	U	C2'-C3'-O3'	6.69	124.40	113.70
75	aa	1332	A	C2'-C3'-O3'	6.65	124.35	113.70
75	aa	739	G	C2'-C3'-O3'	6.63	124.31	113.70
1	A	3241	U	C1'-C2'-O2'	-6.61	90.76	110.60
75	aa	392	G	C2'-C3'-O3'	6.51	124.12	113.70
1	A	1892	G	C2'-C3'-O3'	6.48	124.07	113.70
75	aa	1152	A	P-O3'-C3'	-6.41	112.01	119.70
59	SS	15	GLY	C-N-CD	-6.20	106.96	120.60
75	aa	1343	U	C2'-C3'-O3'	6.18	123.59	113.70
1	A	1409	C	C2'-C3'-O3'	6.16	123.55	113.70
1	A	44	U	C2'-C3'-O3'	6.14	123.52	113.70
75	aa	1297	A	C2'-C3'-O3'	6.08	123.43	113.70
1	A	3017	U	C2'-C3'-O3'	6.07	123.41	113.70
75	aa	488	A	C2'-C3'-O3'	6.05	123.37	113.70
75	aa	1152	A	C4'-C3'-O3'	5.94	124.87	113.00
75	aa	1088	A	C2'-C3'-O3'	5.89	123.12	113.70
1	A	1312	G	C2'-C3'-O3'	5.83	123.03	113.70
76	bb	63	C	C1'-C2'-O2'	-5.80	93.20	110.60
1	A	946	A	N1-C6-N6	-5.75	115.15	118.60
75	aa	761	A	C2'-C3'-O3'	5.65	122.74	113.70
75	aa	709	A	C2'-C3'-O3'	5.44	122.40	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	HH	121	LEU	CA-CB-CG	5.41	127.75	115.30
75	aa	401	A	N1-C6-N6	-5.39	115.37	118.60
1	A	336	A	C2'-C3'-O3'	5.37	122.29	113.70
75	aa	44	U	C4'-C3'-O3'	5.28	123.55	113.00
75	aa	788	U	N3-C4-O4	-5.14	115.81	119.40
1	A	2941	A	N9-C1'-C2'	5.11	120.65	114.00
1	A	114	U	O4'-C1'-N1	5.11	112.29	108.20
75	aa	1177	A	C2'-C3'-O3'	5.08	121.82	113.70
75	aa	485	A	C2'-C3'-O3'	5.07	121.81	113.70
1	A	3242	A	N9-C1'-C2'	-5.04	106.45	112.00
1	A	1410	U	C2'-C3'-O3'	5.04	121.76	113.70
1	A	3240	A	N9-C1'-C2'	-5.02	106.47	112.00
75	aa	1025	U	C4'-C3'-O3'	5.02	123.04	113.00
75	aa	1153	A	O5'-P-OP1	5.02	116.72	110.70

There are no chirality outliers.

There are no planarity outliers.

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	57598	0	28892	190	0
2	B	2527	0	2649	36	0
3	C	1932	0	1969	21	0
4	D	1991	0	2032	10	0
5	E	2187	0	2203	8	0
6	F	1524	0	1587	4	0
7	G	617	0	626	1	0
8	H	1275	0	1310	6	0
9	I	956	0	1037	5	0
10	J	1746	0	1840	5	0
11	K	1573	0	1629	5	0
12	L	1817	0	1878	10	0
13	M	1206	0	1283	6	0
14	N	948	0	1006	2	0
15	O	1826	0	1933	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	1729	0	1724	8	0
17	Q	2272	0	2334	6	0
18	R	2738	0	2811	6	0
19	S	1543	0	1621	5	0
20	T	1792	0	1782	12	0
21	U	639	0	699	6	0
22	V	729	0	711	12	0
23	W	937	0	975	4	0
24	X	512	0	563	3	0
25	Y	385	0	423	3	0
26	Z	508	0	539	0	0
27	0	324	0	344	3	0
28	1	2875	0	2881	11	0
29	2	944	0	969	9	0
30	3	1046	0	1071	6	0
31	4	1117	0	1142	7	0
32	5	2552	0	2600	19	0
33	6	1932	0	1950	12	0
34	7	858	0	908	6	0
35	8	1629	0	1633	2	0
36	9	1587	0	1628	7	0
37	a	1440	0	1473	0	0
38	b	1299	0	1367	0	0
39	c	1004	0	1065	0	0
40	d	1746	0	1743	0	0
41	AA	1610	0	1639	6	0
42	BB	2085	0	2094	20	0
43	CC	2821	0	2829	20	0
44	DD	2369	0	2436	22	0
45	EE	2306	0	2323	16	0
46	FF	1002	0	1086	27	0
47	GG	1282	0	1339	5	0
48	HH	1213	0	1277	12	0
49	II	1820	0	1906	9	0
50	JJ	1508	0	1505	64	0
51	KK	1121	0	1172	10	0
52	LL	948	0	1005	8	0
53	MM	942	0	1001	3	0
54	NN	953	0	1007	10	0
55	OO	1962	0	2036	18	0
56	PP	919	0	982	4	0
57	QQ	1683	0	1769	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	RR	738	0	771	2	0
59	SS	636	0	654	27	0
60	TT	760	0	791	4	0
61	UU	1907	0	1898	23	0
62	VV	1872	0	1978	7	0
63	WW	3216	0	3315	14	0
64	XX	774	0	821	5	0
65	YY	2258	0	2229	45	0
66	ZZ	687	0	719	11	0
67	11	303	0	357	1	0
68	22	833	0	839	1	0
69	33	1953	0	1913	16	0
70	44	2169	0	2155	6	0
71	55	508	0	524	0	0
72	66	2488	0	2520	10	0
73	77	1330	0	1350	6	0
74	88	3573	0	3576	23	0
75	aa	31883	0	16010	0	0
76	bb	1615	0	821	0	0
77	cc	470	0	102	0	0
78	dd	755	0	167	0	0
79	3	1	0	0	0	0
79	A	181	0	0	0	0
79	BB	1	0	0	0	0
79	MM	1	0	0	0	0
79	NN	1	0	0	0	0
79	QQ	1	0	0	0	0
79	WW	1	0	0	0	0
79	aa	111	0	0	0	0
79	d	1	0	0	0	0
80	B	1	0	0	0	0
81	0	1	0	0	0	0
81	W	1	0	0	0	0
82	WW	28	0	12	1	0
All	All	201462	0	157758	733	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 (733) 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)
22:V:105:TYR:CE2	59:SS:16:PRO:HG3	1.09	1.60
50:JJ:71:ILE:HG12	50:JJ:116:THR:CG2	1.18	1.57
22:V:105:TYR:CE2	59:SS:16:PRO:CG	1.93	1.50
50:JJ:71:ILE:CG1	50:JJ:116:THR:HG21	1.56	1.34
22:V:105:TYR:CD2	59:SS:16:PRO:HD3	1.64	1.31
50:JJ:68:TYR:CE2	65:YY:162:LEU:C	2.03	1.30
1:A:945:A:C2	1:A:1107:U:O2	1.85	1.28
1:A:3243:A:O2'	1:A:3244:A:O5'	1.53	1.27
50:JJ:68:TYR:CD2	65:YY:162:LEU:C	2.09	1.26
1:A:1689:U:O4	1:A:2853:A:N1	1.68	1.26
1:A:1913:A:N1	1:A:2880:U:O4	1.69	1.25
50:JJ:68:TYR:OH	65:YY:163:PRO:HG3	1.09	1.25
50:JJ:68:TYR:OH	65:YY:163:PRO:CG	1.84	1.24
22:V:105:TYR:CD2	59:SS:16:PRO:CG	2.20	1.22
22:V:105:TYR:CD2	59:SS:16:PRO:HG3	1.75	1.22
22:V:105:TYR:CD2	59:SS:16:PRO:CD	2.23	1.22
22:V:105:TYR:CZ	59:SS:16:PRO:HG3	1.76	1.19
1:A:114:U:O4	1:A:118:A:N1	1.76	1.18
59:SS:9:SER:CB	59:SS:14:LYS:HE2	1.73	1.18
50:JJ:68:TYR:CE2	65:YY:163:PRO:N	2.10	1.18
50:JJ:68:TYR:CD2	65:YY:162:LEU:O	1.96	1.18
50:JJ:71:ILE:CG1	50:JJ:116:THR:CG2	2.13	1.17
44:DD:128:GLY:O	44:DD:136:LYS:HE3	1.42	1.15
59:SS:9:SER:HB3	59:SS:14:LYS:CE	1.77	1.12
1:A:127:A:O2'	1:A:128:U:H5'	1.50	1.09
61:UU:233:ALA:HB1	66:ZZ:32:VAL:HG13	1.30	1.09
50:JJ:68:TYR:CE2	65:YY:163:PRO:CD	2.37	1.08
50:JJ:71:ILE:HG12	50:JJ:116:THR:HG23	1.09	1.06
1:A:1097:U:C4	3:C:210:ASP:O	2.08	1.06
3:C:210:ASP:HB3	3:C:211:PRO:HD3	1.37	1.05
61:UU:233:ALA:CB	66:ZZ:32:VAL:HG13	1.87	1.04
1:A:45:U:O4	1:A:2895:A:N1	1.91	1.02
50:JJ:68:TYR:CD2	65:YY:162:LEU:HB3	1.96	1.01
50:JJ:65:THR:O	50:JJ:69:LEU:HD21	1.61	1.00
50:JJ:71:ILE:CD1	50:JJ:116:THR:HG21	1.91	1.00
50:JJ:68:TYR:CE2	65:YY:163:PRO:HD3	1.96	1.00
59:SS:17:ASN:ND2	59:SS:39:ALA:O	1.93	0.99
50:JJ:68:TYR:CE2	65:YY:162:LEU:CB	2.46	0.99
2:B:80:ILE:HD11	46:FF:83:ARG:NH2	1.78	0.98
22:V:105:TYR:CE2	59:SS:16:PRO:CD	2.43	0.98
1:A:3162:U:N3	1:A:3243:A:N6	2.13	0.97
22:V:105:TYR:HD2	59:SS:16:PRO:HD3	0.96	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:A:N6	1:A:134:U:O4	1.99	0.96
2:B:71:VAL:HG11	46:FF:35:ASN:HA	1.44	0.96
50:JJ:65:THR:O	50:JJ:69:LEU:CD2	2.14	0.96
1:A:3162:U:H3	1:A:3243:A:N6	1.63	0.95
1:A:1689:U:H3	1:A:2853:A:H61	1.11	0.95
14:N:94:VAL:O	14:N:109:ILE:HG13	1.66	0.95
1:A:3162:U:H3	1:A:3243:A:H61	1.07	0.95
50:JJ:68:TYR:CZ	65:YY:163:PRO:HG3	2.00	0.94
74:88:328:SER:HB3	74:88:389:TRP:CH2	2.02	0.94
50:JJ:71:ILE:HG12	50:JJ:116:THR:HG21	0.94	0.93
74:88:328:SER:HB3	74:88:389:TRP:CZ2	2.03	0.92
1:A:45:U:H3	1:A:2895:A:H61	1.12	0.92
1:A:1913:A:N6	1:A:2880:U:N3	2.19	0.90
59:SS:13:TRP:O	59:SS:14:LYS:HB3	1.71	0.90
2:B:71:VAL:HG11	46:FF:35:ASN:CA	2.01	0.90
50:JJ:68:TYR:CZ	65:YY:163:PRO:CD	2.55	0.89
1:A:1097:U:O4	3:C:210:ASP:O	1.89	0.89
2:B:71:VAL:HG11	46:FF:35:ASN:CB	2.02	0.88
50:JJ:68:TYR:CD2	65:YY:162:LEU:CB	2.55	0.88
50:JJ:69:LEU:HD23	50:JJ:69:LEU:H	1.38	0.88
1:A:947:G:C6	1:A:1107:U:C5	2.61	0.88
50:JJ:68:TYR:CE2	65:YY:162:LEU:HB2	2.10	0.87
50:JJ:68:TYR:HE2	65:YY:163:PRO:HD3	1.36	0.86
1:A:166:U:C4	1:A:212:A:N1	2.43	0.86
51:KK:142:GLU:N	51:KK:142:GLU:OE1	2.08	0.86
44:DD:136:LYS:HE2	44:DD:138:LYS:HE2	1.54	0.86
1:A:945:A:C2	1:A:1107:U:C2	2.64	0.85
48:HH:99:ILE:HD11	48:HH:118:ILE:HD11	1.58	0.85
55:OO:170:ASP:OD2	55:OO:173:SER:HB2	1.77	0.84
50:JJ:68:TYR:CZ	65:YY:163:PRO:CG	2.59	0.84
44:DD:128:GLY:HA3	44:DD:136:LYS:CE	2.09	0.83
50:JJ:68:TYR:OH	65:YY:163:PRO:CD	2.26	0.83
50:JJ:68:TYR:HE2	65:YY:162:LEU:HB2	1.42	0.82
61:UU:233:ALA:CB	66:ZZ:32:VAL:CG1	2.57	0.82
50:JJ:66:GLY:HA3	50:JJ:73:LEU:HD12	1.62	0.82
28:1:109:GLU:HB3	28:1:138:VAL:HG21	1.60	0.82
16:P:255:LEU:HD13	35:8:246:ILE:HD11	1.59	0.82
1:A:945:A:N3	1:A:1107:U:O2	2.12	0.81
59:SS:9:SER:HB3	59:SS:14:LYS:HE2	0.89	0.81
44:DD:128:GLY:C	44:DD:136:LYS:HE3	2.00	0.80
50:JJ:68:TYR:HD2	65:YY:162:LEU:HB3	1.43	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3162:U:H2'	1:A:3163:U:C6	2.17	0.79
2:B:97:LYS:HZ3	55:OO:275:ARG:HH22	1.29	0.79
1:A:1913:A:N1	1:A:2880:U:C4	2.50	0.78
50:JJ:68:TYR:CE2	65:YY:162:LEU:CA	2.67	0.78
1:A:3162:U:O2	1:A:3243:A:N1	2.17	0.78
50:JJ:68:TYR:HH	65:YY:163:PRO:HG3	0.94	0.78
50:JJ:71:ILE:CG1	50:JJ:116:THR:HG23	1.98	0.77
1:A:45:U:H3	1:A:2895:A:N6	1.83	0.77
1:A:127:A:H2	1:A:134:U:O2	1.63	0.77
1:A:98:A:O2'	4:D:136:PRO:HB3	1.84	0.76
66:ZZ:78:ILE:HD13	66:ZZ:78:ILE:O	1.84	0.76
1:A:127:A:C2	1:A:134:U:O2	2.32	0.76
50:JJ:69:LEU:HD23	50:JJ:69:LEU:N	2.00	0.76
2:B:71:VAL:CG1	46:FF:35:ASN:HA	2.15	0.76
1:A:2941:A:H2'	1:A:2942:A:C8	2.21	0.75
1:A:1689:U:H3	1:A:2853:A:N6	1.84	0.75
1:A:127:A:O2'	1:A:128:U:C5'	2.33	0.74
59:SS:17:ASN:O	59:SS:18:ILE:HD12	1.87	0.74
1:A:114:U:N3	1:A:118:A:N6	2.36	0.73
1:A:366:A:C6	1:A:367:A:N6	2.57	0.72
2:B:68:THR:O	55:OO:145:ARG:NH2	2.22	0.72
59:SS:16:PRO:O	59:SS:18:ILE:HD13	1.88	0.72
1:A:1689:U:O4	1:A:2853:A:C2	2.43	0.72
42:BB:278:GLY:HA2	42:BB:334:GLU:OE2	1.90	0.72
50:JJ:68:TYR:HE2	65:YY:163:PRO:CD	1.92	0.72
50:JJ:68:TYR:CD2	65:YY:162:LEU:CA	2.73	0.72
44:DD:136:LYS:HE2	44:DD:138:LYS:CE	2.19	0.71
69:33:92:PHE:CZ	69:33:96:ILE:HD11	2.26	0.71
3:C:210:ASP:CB	3:C:211:PRO:HD3	2.18	0.71
44:DD:128:GLY:CA	44:DD:136:LYS:CE	2.68	0.71
46:FF:9:VAL:HG21	46:FF:21:ALA:HB2	1.72	0.71
44:DD:128:GLY:HA3	44:DD:136:LYS:HE2	1.72	0.70
1:A:127:A:N6	1:A:134:U:C4	2.60	0.70
1:A:3271:A:HO2'	13:M:16:TYR:N	1.89	0.70
1:A:114:U:H3	1:A:118:A:N6	1.90	0.70
50:JJ:68:TYR:CZ	65:YY:163:PRO:HD3	2.25	0.70
55:OO:227:TYR:CE1	55:OO:231:ILE:HD11	2.27	0.69
44:DD:128:GLY:CA	44:DD:136:LYS:HE3	2.22	0.69
61:UU:233:ALA:HB1	66:ZZ:32:VAL:CG1	2.15	0.69
1:A:2792:G:HO2'	27:0:56:PHE:N	1.89	0.69
1:A:3243:A:O2'	1:A:3244:A:P	2.49	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:A:C2'	1:A:128:U:H5'	2.22	0.69
42:BB:278:GLY:CA	42:BB:334:GLU:OE2	2.40	0.69
50:JJ:68:TYR:CZ	65:YY:163:PRO:N	2.61	0.69
43:CC:190:ASN:N	43:CC:190:ASN:HD22	1.91	0.68
44:DD:136:LYS:CE	44:DD:138:LYS:HE2	2.24	0.68
1:A:273:A:H2'	1:A:274:U:H5'	1.76	0.68
1:A:1493:U:O2'	1:A:1494:A:O4'	2.11	0.68
2:B:73:LEU:HD23	46:FF:77:VAL:HG13	1.76	0.68
59:SS:17:ASN:O	59:SS:41:THR:OG1	2.10	0.68
2:B:71:VAL:HG11	46:FF:35:ASN:HB3	1.74	0.67
1:A:166:U:O4	1:A:212:A:N1	2.27	0.67
44:DD:125:ILE:HD11	44:DD:140:PRO:HA	1.76	0.67
50:JJ:68:TYR:HE2	65:YY:162:LEU:CB	1.93	0.66
28:1:73:ILE:CD1	33:6:51:TYR:HB2	2.25	0.66
1:A:273:A:C2'	1:A:274:U:H5'	2.25	0.66
1:A:127:A:H2'	1:A:128:U:O4'	1.96	0.66
1:A:2839:A:N7	3:C:209:GLN:NE2	2.42	0.66
55:OO:227:TYR:CZ	55:OO:231:ILE:HD11	2.31	0.66
18:R:198:LEU:HD21	18:R:254:LEU:HD22	1.76	0.66
1:A:3162:U:C2	1:A:3243:A:N1	2.64	0.66
1:A:946:A:N3	1:A:946:A:H3'	2.11	0.66
50:JJ:65:THR:O	50:JJ:69:LEU:HD23	1.94	0.65
7:G:37:VAL:HG21	7:G:65:ILE:HD11	1.76	0.65
52:LL:35:LYS:HB2	57:QQ:33:ILE:HD12	1.77	0.65
28:1:106:ILE:HA	28:1:138:VAL:HG22	1.77	0.65
1:A:3160:U:H5''	12:L:52:THR:HG21	1.79	0.65
69:33:178:PRO:HG3	69:33:204:ILE:HD11	1.79	0.64
22:V:105:TYR:HE2	59:SS:16:PRO:CG	1.99	0.64
1:A:1689:U:C4	1:A:2853:A:N1	2.62	0.64
50:JJ:68:TYR:OH	65:YY:163:PRO:HD3	1.97	0.64
32:5:138:ALA:HB2	32:5:244:LEU:HD12	1.80	0.64
1:A:274:U:H2'	1:A:275:A:H8	1.62	0.63
1:A:274:U:O2'	1:A:275:A:C5'	2.46	0.63
50:JJ:68:TYR:O	65:YY:169:ARG:NH1	2.31	0.63
31:4:18:ALA:HB2	32:5:285:ASP:HB3	1.81	0.63
1:A:128:U:H3	1:A:133:A:H61	1.47	0.63
46:FF:28:ILE:HD12	46:FF:85:LEU:HD21	1.81	0.63
56:PP:39:VAL:HG11	72:66:318:GLY:HA3	1.81	0.62
44:DD:125:ILE:HG22	44:DD:130:VAL:HB	1.81	0.62
55:OO:170:ASP:OD2	55:OO:173:SER:CB	2.47	0.62
50:JJ:70:GLY:O	50:JJ:72:PRO:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:U:C4	1:A:118:A:N1	2.64	0.62
1:A:273:A:C5	1:A:274:U:C5	2.87	0.62
1:A:425:A:N3	1:A:425:A:H2'	2.14	0.62
45:EE:129:LEU:HD13	45:EE:202:VAL:HG11	1.82	0.62
50:JJ:79:LEU:HD21	50:JJ:110:LEU:HB2	1.80	0.62
66:ZZ:28:ASN:O	66:ZZ:32:VAL:HG23	2.00	0.62
1:A:273:A:C6	1:A:274:U:C5	2.88	0.62
2:B:73:LEU:HD12	46:FF:80:GLU:HG2	1.82	0.62
1:A:1696:A:OP2	2:B:334:ARG:NH1	2.33	0.61
45:EE:220:ILE:HD11	45:EE:231:LEU:HD12	1.81	0.61
1:A:3162:U:C4	1:A:3243:A:N6	2.61	0.61
44:DD:128:GLY:CA	44:DD:136:LYS:HE2	2.30	0.61
1:A:615:U:O2'	1:A:616:A:OP1	2.09	0.61
54:NN:107:LEU:HD12	54:NN:110:VAL:HG21	1.82	0.61
1:A:3239:A:H8	1:A:3240:A:C8	2.18	0.61
16:P:181:PHE:HB3	20:T:127:LEU:HD11	1.82	0.61
1:A:1913:A:N6	1:A:2880:U:H3	1.95	0.60
1:A:945:A:N1	1:A:1107:U:O2	2.32	0.60
22:V:108:LEU:CD1	59:SS:15:GLY:O	2.50	0.60
74:88:370:GLU:OE1	74:88:390:THR:HG22	2.02	0.60
42:BB:278:GLY:N	42:BB:334:GLU:OE2	2.34	0.60
63:WW:111:LYS:HD2	63:WW:157:THR:HG21	1.84	0.60
42:BB:210:ILE:HD11	61:UU:94:PRO:CB	2.31	0.60
42:BB:210:ILE:HD11	61:UU:94:PRO:HB2	1.83	0.59
2:B:73:LEU:CD1	46:FF:80:GLU:HG2	2.33	0.59
74:88:328:SER:CB	74:88:389:TRP:CH2	2.82	0.59
1:A:114:U:H3	1:A:118:A:H61	1.41	0.59
50:JJ:66:GLY:HA3	50:JJ:73:LEU:CD1	2.31	0.59
19:S:227:TYR:O	19:S:230:PHE:N	2.35	0.59
59:SS:9:SER:CB	59:SS:14:LYS:HG2	2.32	0.59
49:II:276:VAL:HG23	49:II:276:VAL:O	2.00	0.59
1:A:127:A:H2'	1:A:128:U:H6	1.67	0.59
1:A:307:G:O2'	1:A:308:U:O5'	2.21	0.59
63:WW:157:THR:OG1	82:WW:501:GDP:O2A	2.20	0.59
65:YY:250:TYR:CZ	65:YY:254:ILE:HD11	2.38	0.59
3:C:210:ASP:HB3	3:C:211:PRO:CD	2.21	0.59
1:A:947:G:C5	1:A:1107:U:C5	2.91	0.59
43:CC:213:ILE:HD11	43:CC:223:TYR:CD2	2.38	0.58
48:HH:110:CYS:HA	48:HH:121:LEU:HD12	1.85	0.58
66:ZZ:10:LEU:HD13	66:ZZ:13:LEU:HD11	1.84	0.58
1:A:841:G:OP1	5:E:110:ASN:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ILE:CD1	57:QQ:108:LEU:CD2	2.82	0.57
8:H:102:GLY:HA2	8:H:128:VAL:HG11	1.86	0.57
50:JJ:73:LEU:HD23	50:JJ:113:ALA:HA	1.86	0.57
62:VV:107:LEU:HD22	62:VV:111:PHE:CE2	2.40	0.57
3:C:207:GLN:HB2	3:C:211:PRO:HG2	1.85	0.57
63:WW:177:ILE:HB	63:WW:291:VAL:HG12	1.85	0.57
45:EE:262:VAL:HG11	45:EE:271:ILE:HD11	1.87	0.57
2:B:97:LYS:HZ3	55:OO:275:ARG:NH2	2.01	0.56
1:A:1107:U:H3'	1:A:1108:U:H5'	1.87	0.56
50:JJ:68:TYR:HD2	65:YY:162:LEU:CB	2.10	0.56
1:A:3160:U:C5'	12:L:52:THR:HG21	2.36	0.56
16:P:92:ILE:HG23	20:T:122:ARG:HA	1.88	0.56
59:SS:17:ASN:C	59:SS:18:ILE:HD12	2.26	0.56
45:EE:172:VAL:HG12	45:EE:201:ALA:HB1	1.88	0.56
69:33:67:LEU:HD13	69:33:173:THR:HG21	1.88	0.55
50:JJ:68:TYR:HE2	65:YY:162:LEU:CA	2.13	0.55
1:A:2673:A:C5	10:J:125:VAL:HG21	2.41	0.55
1:A:2941:A:C2	1:A:2942:A:C2	2.95	0.55
47:GG:175:LYS:HD3	51:KK:141:TYR:CD1	2.42	0.55
2:B:73:LEU:CD1	46:FF:80:GLU:CG	2.84	0.55
2:B:66:ASN:HB3	57:QQ:111:ARG:HH21	1.72	0.55
59:SS:9:SER:HB2	59:SS:14:LYS:HG2	1.87	0.55
8:H:139:ASN:HB3	32:5:329:ARG:O	2.07	0.55
2:B:63:ILE:HD13	57:QQ:108:LEU:CD2	2.36	0.55
1:A:114:U:O4	1:A:118:A:C2	2.58	0.55
50:JJ:71:ILE:HD11	50:JJ:116:THR:HG21	1.85	0.55
2:B:71:VAL:HG12	46:FF:35:ASN:OD1	2.07	0.55
18:R:205:LEU:HD11	18:R:211:ILE:HG22	1.89	0.55
61:UU:105:ARG:HG3	61:UU:150:ILE:HD13	1.90	0.55
69:33:38:TRP:CE3	69:33:93:VAL:HG21	2.42	0.54
74:88:370:GLU:CD	74:88:390:THR:HG22	2.27	0.54
2:B:63:ILE:HD13	57:QQ:108:LEU:HD21	1.88	0.54
73:77:329:VAL:HG21	73:77:350:CYS:HB3	1.87	0.54
30:3:61:ILE:HG23	30:3:77:VAL:HG22	1.89	0.54
1:A:127:A:H2'	1:A:128:U:C6	2.42	0.54
4:D:133:ARG:HH21	4:D:137:ASN:HD22	1.54	0.54
48:HH:99:ILE:CD1	48:HH:118:ILE:HD11	2.35	0.54
1:A:99:U:H5'	4:D:136:PRO:HG3	1.88	0.54
49:II:65:TYR:CD2	49:II:125:ILE:HD11	2.42	0.54
63:WW:357:VAL:HG13	63:WW:364:VAL:HG22	1.88	0.54
3:C:209:GLN:O	3:C:209:GLN:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:WW:175:ILE:HD11	63:WW:279:LEU:HD13	1.89	0.54
6:F:73:LEU:CD2	6:F:103:VAL:HG11	2.38	0.54
54:NN:107:LEU:N	54:NN:107:LEU:HD23	2.23	0.54
33:6:217:ILE:HD12	33:6:277:LEU:HG	1.90	0.54
51:KK:128:THR:HG23	51:KK:138:ARG:HB2	1.90	0.54
1:A:45:U:C4	1:A:2895:A:N1	2.75	0.53
1:A:947:G:C6	1:A:1107:U:C6	2.96	0.53
1:A:2608:C:H2'	1:A:2609:G:O4'	2.09	0.53
52:LL:99:GLY:O	52:LL:127:ARG:NH2	2.42	0.53
1:A:274:U:O2'	1:A:275:A:H5'	2.09	0.53
10:J:77:LEU:HD23	10:J:85:LEU:HD13	1.90	0.53
52:LL:74:ASN:ND2	52:LL:74:ASN:O	2.41	0.53
54:NN:12:LEU:HD22	54:NN:22:LEU:HD21	1.90	0.53
2:B:71:VAL:CG1	46:FF:35:ASN:OD1	2.56	0.53
17:Q:83:ILE:HG22	17:Q:95:LEU:HD22	1.91	0.53
50:JJ:125:ILE:HG21	73:77:215:PRO:HG3	1.88	0.53
18:R:286:LEU:HD12	18:R:324:TYR:CG	2.44	0.53
20:T:57:THR:HG21	23:W:148:LEU:HD12	1.91	0.53
32:5:167:VAL:HG13	32:5:288:MET:HE1	1.91	0.53
1:A:1272:U:O2'	1:A:1273:U:OP2	2.27	0.53
1:A:1913:A:C6	1:A:2880:U:N3	2.77	0.53
61:UU:137:MET:HE1	61:UU:176:PHE:HB2	1.91	0.52
27:0:62:VAL:HG12	27:0:80:ILE:HD12	1.92	0.52
1:A:1708:A:O2'	1:A:1709:G:OP1	2.25	0.52
1:A:2324:U:C6	33:6:99:ILE:HD11	2.44	0.52
42:BB:218:HIS:HB2	42:BB:348:THR:HG21	1.90	0.52
43:CC:224:ILE:HG22	43:CC:391:ILE:HD13	1.90	0.52
1:A:3243:A:O2'	1:A:3244:A:O4'	2.28	0.52
1:A:26:A:N6	36:9:41:LEU:HD11	2.25	0.52
1:A:1869:A:O2'	1:A:1872:G:N3	2.38	0.52
1:A:127:A:C6	1:A:134:U:O4	2.62	0.52
1:A:486:G:OP2	10:J:79:ARG:NH2	2.43	0.52
43:CC:329:ILE:HD11	43:CC:331:PHE:CZ	2.45	0.52
45:EE:154:VAL:O	45:EE:165:SER:N	2.41	0.52
72:66:88:ILE:HG22	72:66:90:PRO:HD3	1.92	0.51
74:88:175:ILE:CG2	74:88:375:THR:HG22	2.40	0.51
55:OO:192:ILE:HD11	55:OO:202:THR:HA	1.92	0.51
61:UU:233:ALA:HB3	66:ZZ:32:VAL:HG13	1.89	0.51
74:88:202:LEU:HD21	74:88:339:VAL:HG11	1.92	0.51
1:A:166:U:O4	1:A:212:A:C6	2.64	0.51
11:K:97:ILE:HG21	11:K:109:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:12:LEU:HD11	21:U:23:VAL:HG11	1.91	0.51
1:A:158:C:O2'	30:3:54:LYS:O	2.20	0.51
74:88:387:TYR:CG	74:88:388:PRO:HD2	2.45	0.51
48:HH:31:LEU:HD23	48:HH:135:ILE:HD11	1.92	0.51
17:Q:133:LEU:HD12	17:Q:154:VAL:HG21	1.92	0.51
42:BB:339:ARG:HE	61:UU:14:THR:HG22	1.75	0.51
28:1:73:ILE:HD13	33:6:51:TYR:HB2	1.91	0.51
2:B:241:LEU:HD12	2:B:241:LEU:N	2.26	0.51
59:SS:9:SER:CA	59:SS:14:LYS:HE2	2.39	0.51
59:SS:53:ILE:HD12	59:SS:62:ILE:HD12	1.92	0.51
20:T:147:THR:HA	20:T:150:TRP:CD1	2.46	0.51
74:88:387:TYR:CD1	74:88:388:PRO:HD2	2.45	0.51
9:I:48:LYS:HG3	9:I:49:PRO:HD2	1.92	0.51
69:33:119:PHE:CE2	69:33:123:ILE:HD11	2.46	0.51
69:33:119:PHE:CZ	69:33:123:ILE:HD11	2.46	0.51
50:JJ:69:LEU:HD11	50:JJ:124:LEU:HB2	1.92	0.51
57:QQ:20:VAL:HG11	57:QQ:74:ILE:HD11	1.92	0.51
1:A:273:A:C6	1:A:274:U:C4	2.99	0.51
1:A:3162:U:N3	1:A:3243:A:C6	2.79	0.51
43:CC:332:LYS:HG3	43:CC:344:THR:HG22	1.92	0.51
44:DD:423:THR:HB	44:DD:424:PRO:CD	2.41	0.51
46:FF:80:GLU:OE2	46:FF:83:ARG:NH2	2.40	0.51
55:OO:206:ARG:O	55:OO:210:GLN:HG2	2.11	0.51
55:OO:192:ILE:HD12	55:OO:205:LEU:HD22	1.92	0.50
5:E:154:LEU:HB3	29:2:42:VAL:HG21	1.94	0.50
46:FF:9:VAL:HG21	46:FF:21:ALA:CB	2.40	0.50
44:DD:125:ILE:HD11	44:DD:140:PRO:CA	2.42	0.50
1:A:1493:U:H2'	1:A:1494:A:C8	2.47	0.50
1:A:3161:U:C4	1:A:3162:U:C5	3.00	0.50
50:JJ:73:LEU:HD23	50:JJ:113:ALA:CA	2.41	0.50
61:UU:14:THR:HG21	61:UU:29:TRP:CZ2	2.47	0.50
1:A:840:C:H2'	1:A:841:G:H5''	1.93	0.50
50:JJ:68:TYR:CZ	65:YY:163:PRO:CA	2.94	0.50
51:KK:172:PHE:CE2	51:KK:202:THR:HG21	2.47	0.50
54:NN:91:PHE:O	54:NN:93:LEU:N	2.44	0.50
1:A:945:A:C4	1:A:1107:U:O2	2.64	0.50
55:OO:182:THR:HG21	55:OO:234:LEU:HD12	1.92	0.50
50:JJ:68:TYR:CG	65:YY:162:LEU:O	2.60	0.50
36:9:114:PHE:CD2	36:9:204:LEU:HD21	2.47	0.50
44:DD:136:LYS:CE	44:DD:138:LYS:CE	2.88	0.50
54:NN:107:LEU:CD1	54:NN:110:VAL:HG21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:KK:140:GLU:OE2	51:KK:140:GLU:HA	2.11	0.50
51:KK:141:TYR:C	51:KK:141:TYR:CD1	2.86	0.50
69:33:237:VAL:HG21	70:44:44:ARG:HG2	1.94	0.49
19:S:132:ILE:N	19:S:132:ILE:HD12	2.27	0.49
63:WW:290:THR:HG22	63:WW:342:ILE:HB	1.94	0.49
33:6:62:THR:HG22	33:6:106:ARG:HD2	1.94	0.49
36:9:221:LEU:HA	36:9:230:VAL:HG23	1.94	0.49
1:A:1889:A:H2'	1:A:1890:C:O4'	2.12	0.49
3:C:61:LEU:HB2	3:C:90:VAL:HG11	1.93	0.49
47:GG:175:LYS:CD	51:KK:141:TYR:CD1	2.89	0.49
31:4:60:GLN:HB3	32:5:100:THR:HG21	1.92	0.49
69:33:237:VAL:HG21	70:44:44:ARG:CG	2.43	0.49
1:A:127:A:HO2'	1:A:128:U:C4'	2.25	0.49
1:A:1913:A:C6	1:A:2880:U:C4	3.01	0.49
1:A:1913:A:C2	1:A:2880:U:O4	2.56	0.49
2:B:73:LEU:HB2	46:FF:35:ASN:ND2	2.27	0.49
16:P:92:ILE:HB	16:P:108:ILE:HB	1.92	0.49
1:A:1913:A:N6	1:A:2880:U:C4	2.74	0.49
1:A:443:U:O4	31:4:24:ARG:NH2	2.46	0.49
42:BB:315:VAL:HG11	49:II:39:PRO:HD3	1.93	0.49
63:WW:291:VAL:CG2	63:WW:343:LEU:HD22	2.43	0.49
65:YY:62:PRO:HA	65:YY:93:THR:HG22	1.94	0.49
74:88:304:LEU:HD21	74:88:320:ILE:HD11	1.95	0.49
1:A:947:G:C6	1:A:1107:U:H5	2.23	0.49
42:BB:180:PRO:HA	42:BB:183:ILE:HD12	1.94	0.49
3:C:210:ASP:CB	3:C:211:PRO:CD	2.88	0.49
61:UU:189:VAL:HB	70:44:162:ALA:HB1	1.94	0.49
1:A:1301:A:H2'	1:A:1302:A:O4'	2.12	0.49
1:A:2590:U:H3'	1:A:2591:A:H5'	1.95	0.49
48:HH:36:ALA:HB1	48:HH:48:LEU:HD13	1.95	0.49
63:WW:149:THR:HG22	63:WW:345:ILE:HD12	1.95	0.49
42:BB:146:LEU:HD21	69:33:217:TRP:CD2	2.47	0.49
70:44:170:TRP:CE2	70:44:207:PRO:HG3	2.47	0.49
3:C:59:CYS:SG	3:C:60:GLY:N	2.86	0.48
48:HH:9:THR:HG21	48:HH:32:GLN:CD	2.33	0.48
42:BB:146:LEU:HD21	69:33:217:TRP:CE2	2.48	0.48
32:5:188:ASN:O	32:5:192:SER:N	2.46	0.48
1:A:737:A:O2'	1:A:739:A:N7	2.46	0.48
52:LL:31:LEU:HG	57:QQ:33:ILE:HD11	1.95	0.48
55:OO:173:SER:HB3	55:OO:176:VAL:HG13	1.95	0.48
24:X:35:THR:HB	24:X:48:LEU:HD11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3241:U:H2'	1:A:3242:A:C8	2.48	0.48
56:PP:100:TRP:CZ3	62:VV:102:LEU:HD12	2.49	0.48
18:R:172:LEU:HD21	18:R:202:ARG:HD3	1.96	0.48
66:ZZ:16:LEU:HB2	66:ZZ:86:TYR:CD1	2.48	0.48
15:O:117:LYS:HB2	32:5:242:ILE:HD11	1.96	0.48
2:B:73:LEU:CD2	46:FF:77:VAL:HG13	2.43	0.48
22:V:108:LEU:HD11	59:SS:15:GLY:O	2.13	0.48
1:A:3137:A:O2'	1:A:3142:A:N1	2.42	0.48
1:A:592:C:H5''	25:Y:91:ILE:HD11	1.95	0.48
61:UU:153:THR:HG22	61:UU:169:TYR:HA	1.95	0.48
54:NN:43:PHE:CE1	64:XX:35:LEU:HD11	2.48	0.48
42:BB:263:ALA:O	42:BB:266:THR:O	2.32	0.48
63:WW:221:LEU:HD21	63:WW:259:LEU:CD2	2.43	0.48
48:HH:119:LYS:O	48:HH:153:ARG:NH2	2.46	0.48
63:WW:111:LYS:HD2	63:WW:157:THR:CG2	2.44	0.48
64:XX:59:LEU:HD23	64:XX:59:LEU:N	2.29	0.48
60:TT:168:ILE:HG21	66:ZZ:89:ILE:HG23	1.95	0.48
28:1:109:GLU:CB	28:1:138:VAL:HG21	2.37	0.48
1:A:1493:U:O2'	1:A:1494:A:O5'	2.31	0.48
2:B:66:ASN:HB3	57:QQ:111:ARG:NH2	2.28	0.48
9:I:72:ILE:HD12	9:I:99:ILE:HG21	1.96	0.48
1:A:3164:A:N1	1:A:3241:U:H5	2.12	0.48
6:F:115:THR:HG23	6:F:116:GLU:HG2	1.96	0.48
13:M:76:VAL:HG21	13:M:94:ILE:HD11	1.96	0.48
1:A:399:G:N7	25:Y:100:ARG:NH1	2.61	0.47
61:UU:149:VAL:O	61:UU:153:THR:HG23	2.13	0.47
73:77:255:THR:HG23	73:77:275:GLU:HB2	1.95	0.47
1:A:33:A:N6	1:A:34:U:C4	2.82	0.47
1:A:1938:A:H2'	1:A:1939:U:O4'	2.15	0.47
3:C:63:THR:HG22	3:C:87:VAL:HG22	1.95	0.47
4:D:133:ARG:HB3	4:D:137:ASN:HD21	1.77	0.47
23:W:118:MET:HE2	23:W:118:MET:HA	1.96	0.47
33:6:27:VAL:HG11	33:6:195:ALA:HB2	1.95	0.47
59:SS:16:PRO:O	59:SS:18:ILE:CD1	2.59	0.47
1:A:1075:A:C6	1:A:1076:U:H1'	2.49	0.47
1:A:2462:A:OP1	5:E:178:ASN:N	2.46	0.47
5:E:161:LEU:HD22	29:2:45:GLN:HB3	1.95	0.47
49:II:176:ILE:HD13	49:II:183:LEU:HG	1.95	0.47
51:KK:198:ILE:HD13	60:TT:117:PHE:CD1	2.50	0.47
21:U:15:VAL:CG1	21:U:19:THR:HB	2.44	0.47
31:4:26:ILE:HG21	31:4:98:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:88:175:ILE:HG23	74:88:375:THR:HG22	1.97	0.47
1:A:3239:A:C8	1:A:3240:A:C8	3.02	0.47
52:LL:74:ASN:C	52:LL:74:ASN:HD22	2.13	0.47
32:5:203:TRP:CZ3	32:5:260:VAL:HG23	2.50	0.47
1:A:3122:U:O2'	1:A:3123:A:OP2	2.28	0.47
44:DD:64:ARG:O	44:DD:68:VAL:HG13	2.15	0.47
63:WW:399:VAL:HG13	63:WW:441:LEU:HD11	1.97	0.47
63:WW:93:VAL:HG21	63:WW:405:TYR:CD1	2.49	0.47
43:CC:171:TYR:CG	65:YY:104:ILE:HD13	2.49	0.47
33:6:255:ALA:HB3	33:6:257:LEU:HD11	1.96	0.47
34:7:96:ILE:HG21	34:7:100:VAL:HG12	1.97	0.47
1:A:261:A:C4	1:A:307:G:N7	2.83	0.47
12:L:148:LEU:HD21	12:L:169:ASN:HB2	1.97	0.47
61:UU:6:ASN:HA	61:UU:9:ASN:OD1	2.14	0.47
33:6:207:ILE:CD1	33:6:236:ILE:HD13	2.44	0.47
72:66:81:THR:HA	72:66:214:ARG:HB3	1.96	0.47
34:7:91:THR:HG23	34:7:135:VAL:HG22	1.97	0.47
74:88:142:MET:O	74:88:166:THR:HG22	2.15	0.47
74:88:48:ARG:HG2	74:88:82:THR:HG22	1.97	0.47
55:OO:164:PHE:HB3	55:OO:176:VAL:HG12	1.97	0.47
1:A:1666:A:C2'	1:A:1667:A:O5'	2.63	0.46
43:CC:278:LEU:HD11	43:CC:304:ASN:HB3	1.96	0.46
2:B:73:LEU:HD22	46:FF:35:ASN:HD22	1.80	0.46
56:PP:22:ASN:OD1	56:PP:39:VAL:HG13	2.15	0.46
54:NN:36:ILE:HD11	73:77:346:VAL:CG2	2.45	0.46
35:8:189:ILE:HG22	35:8:194:LEU:HD23	1.96	0.46
50:JJ:68:TYR:HD2	65:YY:162:LEU:CA	2.25	0.46
3:C:31:ILE:HD13	8:H:140:ILE:CD1	2.45	0.46
4:D:200:ILE:HD11	4:D:205:VAL:CG2	2.45	0.46
50:JJ:69:LEU:CD2	50:JJ:69:LEU:N	2.73	0.46
61:UU:86:VAL:HG12	61:UU:88:VAL:HG23	1.98	0.46
32:5:203:TRP:CH2	32:5:260:VAL:HG23	2.51	0.46
33:6:56:GLU:O	33:6:60:MET:N	2.49	0.46
50:JJ:69:LEU:HD12	50:JJ:71:ILE:CD1	2.46	0.46
17:Q:103:THR:HG22	17:Q:119:MET:HG3	1.96	0.46
19:S:227:TYR:O	19:S:228:LYS:C	2.54	0.46
1:A:1581:U:H2'	1:A:1582:A:H5'	1.96	0.46
45:EE:125:VAL:HG23	45:EE:195:PHE:CE2	2.51	0.46
15:O:163:VAL:HG13	15:O:267:LEU:HB2	1.98	0.46
29:2:40:GLN:O	29:2:44:THR:HG23	2.16	0.46
1:A:275:A:C2	1:A:367:A:C2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
74:88:145:ILE:HG22	74:88:167:LYS:CG	2.46	0.46
1:A:425:A:N3	1:A:425:A:C2'	2.78	0.46
67:11:93:LEU:HD11	67:11:97:ARG:CZ	2.46	0.46
46:FF:8:LEU:HD22	46:FF:66:HIS:ND1	2.30	0.46
8:H:37:ILE:HG23	8:H:42:ARG:HB2	1.97	0.46
41:AA:70:THR:HG21	41:AA:76:THR:HG23	1.97	0.46
43:CC:190:ASN:N	43:CC:190:ASN:ND2	2.62	0.46
48:HH:45:LEU:HD22	48:HH:75:VAL:HG13	1.97	0.46
1:A:2612:A:OP1	1:A:2638:G:N2	2.49	0.45
1:A:2712:G:H2'	1:A:2713:G:O4'	2.16	0.45
1:A:786:A:N3	5:E:107:TYR:OH	2.41	0.45
72:66:149:LEU:HD22	72:66:153:LEU:HD22	1.99	0.45
32:5:87:ILE:HG21	32:5:117:SER:HB3	1.99	0.45
43:CC:144:HIS:CE1	43:CC:149:LEU:HD13	2.51	0.45
49:II:61:LEU:HD11	49:II:128:GLU:HG3	1.97	0.45
69:33:177:PHE:CE2	69:33:214:VAL:HG21	2.52	0.45
17:Q:202:ILE:HD13	30:3:89:GLU:HB3	1.98	0.45
1:A:698:U:H2'	1:A:699:G:O4'	2.16	0.45
9:I:36:VAL:HG21	9:I:119:ASP:HB2	1.99	0.45
72:66:307:TYR:HB3	72:66:309:PHE:CE1	2.51	0.45
1:A:1702:C:H2'	1:A:1703:U:O4'	2.16	0.45
1:A:2437:U:H4'	1:A:2438:A:OP1	2.17	0.45
1:A:3261:U:O4'	1:A:3261:U:O2	2.35	0.45
45:EE:59:LEU:HD11	50:JJ:20:TYR:CE2	2.51	0.45
6:F:122:LEU:HD22	6:F:201:VAL:HG22	1.98	0.45
20:T:55:PRO:HG2	23:W:153:LEU:HD21	1.98	0.45
5:E:154:LEU:HG	29:2:42:VAL:HG11	1.98	0.45
69:33:143:ALA:HB2	69:33:153:LEU:HD22	1.99	0.45
1:A:1708:A:H4'	1:A:1709:G:OP2	2.16	0.45
1:A:3135:U:H4'	1:A:3136:U:OP1	2.16	0.45
57:QQ:61:GLU:HG2	57:QQ:75:ALA:HB2	1.98	0.45
46:FF:95:SER:HB2	58:RR:135:ILE:HD12	1.98	0.45
1:A:1366:A:O4'	1:A:1534:G:N2	2.49	0.45
1:A:3164:A:N1	1:A:3241:U:C5	2.85	0.45
48:HH:9:THR:HG22	48:HH:27:PRO:HD2	1.99	0.45
20:T:144:SER:O	20:T:148:THR:HG23	2.16	0.45
28:1:117:TYR:HB2	29:2:67:ILE:HD13	1.99	0.45
32:5:268:TRP:HA	32:5:279:VAL:HG22	1.99	0.45
74:88:328:SER:CB	74:88:389:TRP:CZ2	2.89	0.45
28:1:73:ILE:HG12	33:6:47:LYS:HB3	1.99	0.45
1:A:1561:G:H3'	1:A:1561:G:N3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:U:O2'	1:A:275:A:O5'	2.34	0.45
1:A:2361:A:C6	28:1:202:VAL:HG13	2.52	0.45
32:5:98:LEU:HG	32:5:227:GLY:HA2	1.99	0.45
1:A:1581:U:C3'	1:A:1582:A:H5'	2.47	0.45
1:A:2911:U:H2'	1:A:2912:C:O4'	2.17	0.45
3:C:43:ASN:O	3:C:52:ARG:NH2	2.46	0.45
43:CC:224:ILE:HG22	43:CC:391:ILE:CD1	2.47	0.45
28:1:113:PRO:HG3	29:2:71:THR:HG21	1.99	0.44
1:A:127:A:C2'	1:A:128:U:O4'	2.65	0.44
1:A:3241:U:H2'	1:A:3242:A:H8	1.83	0.44
47:GG:203:ARG:HB2	47:GG:211:ARG:HG2	2.00	0.44
43:CC:321:TYR:O	65:YY:141:ALA:HB2	2.17	0.44
64:XX:66:ILE:N	64:XX:66:ILE:HD12	2.32	0.44
25:Y:88:GLY:HA2	25:Y:91:ILE:HD12	1.99	0.44
50:JJ:72:PRO:HB2	50:JJ:114:TRP:HB2	1.98	0.44
13:M:90:PHE:CE1	13:M:121:ILE:HD12	2.53	0.44
14:N:76:LEU:HD11	14:N:153:LEU:HD11	1.99	0.44
57:QQ:131:ILE:HD11	57:QQ:147:ILE:HG21	2.00	0.44
5:E:266:ILE:HG21	5:E:280:LEU:HD21	2.00	0.44
6:F:30:VAL:HG11	6:F:111:ILE:HD13	2.00	0.44
20:T:86:PRO:HG2	20:T:89:HIS:CG	2.53	0.44
1:A:1493:U:O2'	1:A:1494:A:P	2.76	0.44
74:88:140:THR:HG21	74:88:154:SER:HA	2.00	0.44
2:B:80:ILE:CD1	46:FF:83:ARG:NH2	2.66	0.44
9:I:3:PHE:CZ	9:I:33:PRO:HB3	2.52	0.44
20:T:206:GLN:HB3	20:T:212:ILE:HG23	2.00	0.44
36:9:124:LEU:CD1	36:9:145:LEU:HD11	2.48	0.44
1:A:117:U:O4'	1:A:117:U:O2	2.35	0.44
41:AA:97:ILE:HD12	41:AA:206:LEU:HD21	2.00	0.44
3:C:93:ILE:HD11	3:C:109:GLY:HA3	1.98	0.44
55:OO:188:MET:HG2	55:OO:205:LEU:HB2	1.99	0.44
55:OO:250:ARG:HG2	55:OO:264:ILE:HD11	2.00	0.44
61:UU:105:ARG:CG	61:UU:150:ILE:HD13	2.47	0.44
1:A:366:A:N1	1:A:367:A:N1	2.66	0.43
53:MM:113:LYS:HB3	53:MM:114:LEU:HD13	2.00	0.43
18:R:63:ILE:HG21	18:R:107:ILE:HG21	2.00	0.43
32:5:142:ASN:O	32:5:215:ARG:NH2	2.50	0.43
74:88:145:ILE:HG22	74:88:167:LYS:HG3	2.00	0.43
36:9:204:LEU:HD22	36:9:212:ALA:CB	2.48	0.43
1:A:2913:U:N3	1:A:2941:A:C2	2.83	0.43
42:BB:183:ILE:HD11	42:BB:375:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:GLU:OE2	46:FF:36:ARG:NH1	2.51	0.43
47:GG:175:LYS:HE2	51:KK:141:TYR:HB3	0.87	0.43
48:HH:13:LEU:HD23	48:HH:86:LEU:HD21	2.00	0.43
17:Q:133:LEU:HD13	17:Q:182:ILE:HG21	1.99	0.43
69:33:44:TYR:HB2	70:44:287:PHE:CE2	2.53	0.43
42:BB:183:ILE:HD11	42:BB:375:VAL:CG2	2.48	0.43
44:DD:109:LEU:HD11	44:DD:152:VAL:HG22	2.01	0.43
16:P:181:PHE:HB2	20:T:78:ILE:HD11	2.00	0.43
46:FF:105:LEU:HD12	62:VV:198:GLU:HB3	2.01	0.43
28:1:249:LEU:HB3	28:1:252:ILE:HD11	2.00	0.43
1:A:849:U:H2'	1:A:850:A:C8	2.52	0.43
11:K:215:TYR:CE2	11:K:219:LEU:HD11	2.53	0.43
41:AA:206:LEU:HB3	61:UU:114:TRP:CG	2.54	0.43
68:22:48:ILE:HD11	68:22:52:CYS:SG	2.59	0.43
1:A:74:A:O2'	4:D:238:PRO:O	2.36	0.43
52:LL:68:LEU:HB3	52:LL:118:LEU:HD22	2.00	0.43
57:QQ:58:VAL:HG12	57:QQ:77:ILE:HD13	2.00	0.43
24:X:13:LEU:HB3	24:X:49:PHE:HB3	2.00	0.43
72:66:37:TYR:CG	72:66:95:GLY:HA3	2.53	0.43
73:77:256:LEU:HG	73:77:270:LEU:HD21	2.00	0.43
1:A:2968:A:O2'	12:L:79:LEU:O	2.34	0.43
52:LL:43:ARG:O	52:LL:43:ARG:HG2	2.19	0.43
1:A:3268:A:H2'	1:A:3269:U:C6	2.54	0.43
1:A:466:U:OP2	10:J:87:LYS:NZ	2.50	0.43
43:CC:190:ASN:H	43:CC:190:ASN:HD22	1.64	0.43
55:OO:188:MET:HB3	55:OO:205:LEU:HD13	2.01	0.43
57:QQ:59:ARG:NH2	62:VV:48:GLY:O	2.52	0.43
57:QQ:225:ARG:HB3	62:VV:171:GLU:CD	2.39	0.43
1:A:1725:G:OP1	2:B:176:ARG:NH2	2.48	0.43
1:A:254:G:N2	1:A:256:A:N3	2.64	0.43
1:A:3122:U:O4'	1:A:3122:U:O2	2.35	0.43
1:A:34:U:HO2'	1:A:35:U:P	2.41	0.43
3:C:115:LEU:HD11	13:M:28:VAL:HG21	2.01	0.43
12:L:237:ARG:NH1	13:M:30:PRO:O	2.51	0.43
32:5:111:LEU:HA	32:5:270:VAL:HG11	2.01	0.43
74:88:187:LEU:HB3	74:88:201:ALA:HB1	2.01	0.43
41:AA:196:PHE:CZ	61:UU:166:VAL:HG22	2.54	0.43
20:T:117:GLN:HG3	20:T:145:ILE:HG21	2.00	0.43
32:5:307:LEU:HD21	32:5:340:VAL:HG11	1.99	0.43
2:B:210:ARG:NH2	2:B:261:GLY:O	2.52	0.43
45:EE:227:VAL:HG21	45:EE:271:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:6:VAL:HG23	21:U:28:LEU:HD21	2.01	0.43
50:JJ:68:TYR:HD2	65:YY:162:LEU:O	1.85	0.43
1:A:1258:A:H2'	1:A:1259:A:O4'	2.19	0.42
1:A:3242:A:O2'	1:A:3243:A:H5'	2.19	0.42
1:A:366:A:N6	1:A:367:A:N6	2.67	0.42
45:EE:150:VAL:HG13	45:EE:169:LEU:HB3	2.01	0.42
48:HH:26:ILE:HG22	48:HH:73:LEU:HB3	2.00	0.42
51:KK:183:LEU:HD23	51:KK:192:VAL:HG22	2.01	0.42
55:OO:219:LEU:HD13	55:OO:227:TYR:HA	2.01	0.42
56:PP:9:ARG:HA	56:PP:86:VAL:HG21	2.00	0.42
1:A:247:A:H2'	1:A:248:A:O4'	2.19	0.42
42:BB:206:THR:HG21	42:BB:348:THR:HA	1.99	0.42
11:K:184:LEU:HD13	11:K:192:PHE:HB3	2.01	0.42
9:I:138:ILE:HD11	13:M:114:ILE:HD12	2.01	0.42
57:QQ:78:ILE:HD11	62:VV:44:VAL:HG22	2.01	0.42
72:66:179:ILE:N	72:66:180:PRO:HD2	2.34	0.42
54:NN:36:ILE:HD11	73:77:346:VAL:HG22	2.01	0.42
3:C:58:ARG:NH1	3:C:159:PHE:O	2.53	0.42
44:DD:402:ILE:CD1	44:DD:411:VAL:HG12	2.49	0.42
12:L:107:ARG:HG3	12:L:125:GLU:HG2	2.00	0.42
12:L:7:ARG:HB2	12:L:42:GLU:HG3	2.01	0.42
54:NN:94:CYS:SG	54:NN:95:ARG:N	2.92	0.42
61:UU:8:VAL:HB	61:UU:40:THR:HG22	2.01	0.42
1:A:45:U:C5	1:A:2894:A:C5	3.08	0.42
42:BB:214:TYR:HB3	42:BB:219:ILE:HD12	2.01	0.42
1:A:639:G:C8	15:O:249:ALA:HB1	2.54	0.42
16:P:169:ILE:HD12	23:W:148:LEU:HD11	2.01	0.42
17:Q:238:LEU:HD13	17:Q:243:ILE:HD11	2.01	0.42
32:5:324:VAL:HG21	32:5:339:HIS:CG	2.53	0.42
43:CC:278:LEU:HD11	43:CC:304:ASN:CB	2.50	0.42
49:II:176:ILE:HD11	63:WW:431:PHE:CG	2.55	0.42
27:0:62:VAL:HG12	27:0:80:ILE:CD1	2.50	0.42
16:P:117:ASP:OD2	30:3:78:ARG:NH1	2.53	0.42
74:88:372:SER:O	74:88:375:THR:OG1	2.33	0.42
1:A:1358:C:C6	1:A:1359:G:C8	3.08	0.42
1:A:1913:A:N6	1:A:1914:A:C2	2.88	0.42
2:B:241:LEU:HD13	2:B:246:ILE:HD11	2.01	0.42
2:B:73:LEU:HD23	46:FF:77:VAL:HA	2.01	0.42
43:CC:87:LEU:HD22	43:CC:91:ASN:HB2	2.00	0.42
11:K:97:ILE:HG13	11:K:168:ALA:HB2	2.01	0.42
61:UU:109:TYR:CD1	61:UU:116:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:A:HI'	1:A:1409:C:O4'	2.19	0.42
4:D:70:ARG:NH1	34:7:124:GLN:O	2.53	0.42
12:L:179:GLU:HG3	12:L:214:LEU:HD12	2.01	0.42
52:LL:74:ASN:C	52:LL:74:ASN:ND2	2.73	0.42
31:4:57:PRO:HB2	32:5:103:LYS:HG3	2.02	0.42
50:JJ:69:LEU:CD1	50:JJ:124:LEU:HB2	2.50	0.42
53:MM:25:TYR:OH	53:MM:120:ARG:NH1	2.44	0.42
19:S:132:ILE:N	19:S:132:ILE:CD1	2.83	0.42
62:VV:21:ILE:HB	62:VV:114:GLU:HG3	2.02	0.42
65:YY:219:PHE:CD2	65:YY:258:LEU:HD22	2.55	0.42
69:33:28:ILE:HD11	69:33:96:ILE:HG23	2.01	0.42
1:A:2597:G:O2'	1:A:2602:A:N1	2.47	0.42
1:A:25:A:O2'	1:A:26:A:O5'	2.32	0.42
44:DD:423:THR:CB	44:DD:424:PRO:CD	2.97	0.42
24:X:11:ILE:HD11	24:X:25:ILE:HD11	2.01	0.42
5:E:161:LEU:HD22	29:2:45:GLN:CB	2.50	0.41
1:A:1413:A:H5'	30:3:65:THR:HG23	2.01	0.41
72:66:87:TYR:CG	72:66:136:PRO:HA	2.55	0.41
34:7:121:VAL:HB	34:7:128:ILE:HG22	2.01	0.41
1:A:308:U:C2'	1:A:309:C:O5'	2.68	0.41
41:AA:75:THR:HG22	60:TT:177:TYR:OH	2.19	0.41
42:BB:203:ARG:O	42:BB:206:THR:HG22	2.19	0.41
45:EE:68:PHE:O	65:YY:149:ARG:NH1	2.53	0.41
3:C:32:ALA:HA	8:H:158:ILE:HD11	2.02	0.41
50:JJ:68:TYR:CE2	65:YY:163:PRO:CA	2.99	0.41
11:K:87:ALA:HA	11:K:115:THR:HG21	2.01	0.41
54:NN:91:PHE:CD2	54:NN:107:LEU:HD13	2.54	0.41
59:SS:21:LEU:HD11	59:SS:35:THR:HG22	2.02	0.41
21:U:31:ARG:HD2	21:U:31:ARG:HH21	1.71	0.41
74:88:155:ILE:HD11	74:88:190:ILE:HD11	2.02	0.41
1:A:2948:C:OP2	3:C:173:LYS:HE3	2.20	0.41
45:EE:133:THR:HG23	45:EE:135:VAL:HG23	2.02	0.41
49:II:159:LYS:HG2	49:II:164:THR:HG22	2.02	0.41
55:OO:232:GLN:HB3	57:QQ:96:VAL:HG21	2.02	0.41
61:UU:178:ALA:HB2	70:44:123:ASN:HB2	2.01	0.41
64:XX:18:ILE:HD11	65:YY:261:GLU:HB2	2.02	0.41
28:1:252:ILE:HG21	28:1:261:ILE:HD12	2.01	0.41
50:JJ:35:PRO:O	50:JJ:72:PRO:HG3	2.19	0.41
32:5:120:LEU:CD2	32:5:205:ILE:HG23	2.49	0.41
45:EE:77:HIS:ND1	45:EE:78:LEU:O	2.53	0.41
31:4:27:THR:HB	31:4:73:ARG:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1993:U:O2'	19:S:101:VAL:HG21	2.21	0.41
2:B:63:ILE:HD11	57:QQ:104:ALA:HB1	2.03	0.41
48:HH:19:VAL:HG23	48:HH:21:VAL:HG13	2.03	0.41
1:A:2673:A:C6	10:J:125:VAL:HG21	2.55	0.41
18:R:77:VAL:HG13	18:R:85:ILE:HG23	2.02	0.41
58:RR:41:ILE:HD11	61:UU:224:VAL:HG22	2.02	0.41
1:A:2426:A:H1'	29:2:46:LEU:HD21	2.01	0.41
34:7:66:TYR:CE1	34:7:103:LEU:HD13	2.55	0.41
74:88:118:ILE:HD11	74:88:359:ALA:HB2	2.02	0.41
2:B:143:HIS:CE1	2:B:332:THR:HG22	2.55	0.41
57:QQ:124:LEU:HD23	57:QQ:128:ILE:HD13	2.01	0.41
65:YY:277:THR:O	65:YY:281:ILE:HG23	2.21	0.41
1:A:1412:U:H1'	30:3:65:THR:HG21	2.03	0.41
1:A:1913:A:N6	1:A:2880:U:C2	2.88	0.41
1:A:3112:A:H2'	1:A:3113:U:O4'	2.20	0.41
1:A:331:A:O2'	1:A:332:A:P	2.79	0.41
43:CC:119:LEU:HD13	43:CC:140:THR:HG21	2.02	0.41
43:CC:212:TYR:HB2	43:CC:215:LEU:HD13	2.03	0.41
4:D:49:PHE:HB3	4:D:50:PRO:HD3	2.03	0.41
44:DD:53:ARG:HD3	44:DD:481:TYR:OH	2.20	0.41
45:EE:286:LEU:HD22	45:EE:297:LEU:HD22	2.03	0.41
2:B:73:LEU:HD11	46:FF:80:GLU:CG	2.51	0.41
49:II:200:LEU:HD11	49:II:211:ILE:HD12	2.02	0.41
1:A:951:A:OP1	1:A:1101:C:O2'	2.38	0.41
47:GG:141:VAL:HG22	47:GG:217:THR:HG23	2.02	0.41
53:MM:10:PHE:CE1	53:MM:19:ALA:HB1	2.56	0.41
63:WW:177:ILE:HG23	63:WW:204:TYR:OH	2.21	0.41
65:YY:279:HIS:CD2	65:YY:280:THR:HG23	2.56	0.41
1:A:1261:U:C5'	31:4:71:LEU:HD21	2.50	0.41
74:88:168:TRP:CD2	74:88:221:LEU:HD13	2.56	0.41
1:A:718:G:H2'	1:A:1968:U:C2	2.56	0.41
3:C:210:ASP:N	3:C:211:PRO:CD	2.81	0.41
21:U:19:THR:HA	21:U:22:ILE:HD12	2.03	0.41
69:33:70:THR:HG23	69:33:76:GLN:HG3	2.03	0.41
29:2:48:VAL:HG21	33:6:67:PHE:CG	2.55	0.41
1:A:1341:G:N2	1:A:1562:A:O2'	2.54	0.41
16:P:227:ILE:HG22	16:P:232:LYS:HB2	2.02	0.41
1:A:366:A:C6	1:A:367:A:C6	3.09	0.41
41:AA:51:LYS:HZ3	42:BB:197:GLN:HA	1.86	0.41
43:CC:192:CYS:SG	43:CC:193:ASN:N	2.94	0.41
4:D:42:ALA:HB2	34:7:56:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:9:33:HIS:NE2	36:9:36:PRO:O	2.54	0.40
45:EE:303:VAL:HG12	72:66:255:PRO:HA	2.01	0.40
3:C:27:VAL:HG21	8:H:158:ILE:HD13	2.03	0.40
49:II:275:TRP:CZ3	49:II:277:LYS:HB2	2.56	0.40
12:L:148:LEU:HD21	12:L:169:ASN:CB	2.51	0.40
43:CC:171:TYR:CG	65:YY:104:ILE:CD1	3.05	0.40
1:A:3243:A:O2'	1:A:3244:A:H8	2.04	0.40
43:CC:302:ILE:HD11	50:JJ:29:TYR:CE2	2.56	0.40
43:CC:306:TYR:HB2	45:EE:59:LEU:HB2	2.02	0.40
20:T:98:LEU:HD22	20:T:152:ILE:HG12	2.02	0.40
60:TT:165:LEU:HD22	66:ZZ:10:LEU:HD12	2.04	0.40
32:5:160:LYS:HA	32:5:261:ARG:HD3	2.04	0.40
74:88:199:GLN:HG3	74:88:286:GLU:HA	2.04	0.40
36:9:145:LEU:N	36:9:145:LEU:HD12	2.36	0.40
1:A:1582:A:H2'	1:A:1583:G:O4'	2.22	0.40
1:A:2711:G:OP1	4:D:115:ARG:NH2	2.55	0.40
2:B:104:ARG:O	2:B:107:ARG:NH2	2.52	0.40
1:A:510:A:H2'	1:A:511:G:O4'	2.22	0.40
2:B:80:ILE:HD11	46:FF:83:ARG:HH22	1.74	0.40
42:BB:275:TRP:CZ2	42:BB:279:THR:OG1	2.74	0.40
44:DD:106:ASP:OD1	44:DD:122:ARG:N	2.55	0.40
50:JJ:71:ILE:HA	50:JJ:72:PRO:HD2	1.79	0.40
21:U:26:LEU:HD21	21:U:47:LEU:CD2	2.52	0.40
45:EE:286:LEU:HD11	72:66:244:PHE:CE1	2.57	0.40
33:6:62:THR:HG22	33:6:106:ARG:CD	2.50	0.40
1:A:1107:U:H3'	1:A:1108:U:C5'	2.51	0.40
1:A:1424:U:O4'	1:A:1533:G:H1'	2.21	0.40
1:A:1901:U:OP1	12:L:8:LYS:NZ	2.54	0.40
1:A:231:A:H2'	1:A:232:C:C6	2.56	0.40
1:A:366:A:C2	1:A:367:A:N1	2.90	0.40
1:A:946:A:N3	1:A:946:A:C3'	2.81	0.40
42:BB:146:LEU:HD11	69:33:217:TRP:CD1	2.57	0.40
44:DD:49:LYS:HD2	44:DD:480:TYR:CE1	2.56	0.40
1:A:1583:G:HO2'	20:T:15:ALA:N	2.20	0.40
64:XX:59:LEU:HD21	64:XX:63:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	317/393 (81%)	303 (96%)	14 (4%)	0	100	100
3	C	247/249 (99%)	233 (94%)	13 (5%)	1 (0%)	39	78
4	D	250/252 (99%)	236 (94%)	10 (4%)	4 (2%)	12	52
5	E	272/274 (99%)	254 (93%)	16 (6%)	2 (1%)	26	70
6	F	194/196 (99%)	183 (94%)	10 (5%)	1 (0%)	34	75
7	G	72/74 (97%)	70 (97%)	2 (3%)	0	100	100
8	H	158/160 (99%)	152 (96%)	6 (4%)	0	100	100
9	I	123/138 (89%)	114 (93%)	9 (7%)	0	100	100
10	J	218/220 (99%)	202 (93%)	15 (7%)	1 (0%)	34	75
11	K	193/195 (99%)	184 (95%)	9 (5%)	0	100	100
12	L	225/237 (95%)	217 (96%)	8 (4%)	0	100	100
13	M	149/151 (99%)	139 (93%)	10 (7%)	0	100	100
14	N	116/118 (98%)	106 (91%)	10 (9%)	0	100	100
15	O	223/225 (99%)	211 (95%)	12 (5%)	0	100	100
16	P	205/207 (99%)	196 (96%)	9 (4%)	0	100	100
17	Q	280/296 (95%)	268 (96%)	12 (4%)	0	100	100
18	R	327/337 (97%)	314 (96%)	12 (4%)	1 (0%)	46	83
19	S	181/216 (84%)	171 (94%)	10 (6%)	0	100	100
20	T	210/225 (93%)	199 (95%)	11 (5%)	0	100	100
21	U	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
22	V	87/177 (49%)	83 (95%)	4 (5%)	0	100	100
23	W	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
24	X	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
25	Y	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
26	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	0	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
28	1	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
29	2	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
30	3	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
31	4	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
32	5	322/324 (99%)	306 (95%)	16 (5%)	0	100	100
33	6	228/281 (81%)	221 (97%)	7 (3%)	0	100	100
34	7	104/106 (98%)	97 (93%)	7 (7%)	0	100	100
35	8	195/264 (74%)	192 (98%)	3 (2%)	0	100	100
36	9	198/215 (92%)	186 (94%)	12 (6%)	0	100	100
37	a	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
38	b	153/155 (99%)	146 (95%)	7 (5%)	0	100	100
39	c	117/119 (98%)	112 (96%)	4 (3%)	1 (1%)	21	64
40	d	202/215 (94%)	189 (94%)	13 (6%)	0	100	100
41	AA	197/344 (57%)	190 (96%)	7 (4%)	0	100	100
42	BB	264/266 (99%)	247 (94%)	15 (6%)	2 (1%)	24	66
43	CC	331/398 (83%)	302 (91%)	27 (8%)	2 (1%)	30	72
44	DD	281/486 (58%)	265 (94%)	15 (5%)	1 (0%)	39	78
45	EE	284/293 (97%)	262 (92%)	20 (7%)	2 (1%)	26	70
46	FF	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
47	GG	159/161 (99%)	149 (94%)	9 (6%)	1 (1%)	30	72
48	HH	152/154 (99%)	144 (95%)	8 (5%)	0	100	100
49	II	220/244 (90%)	205 (93%)	13 (6%)	2 (1%)	21	64
50	JJ	184/186 (99%)	166 (90%)	13 (7%)	5 (3%)	6	37
51	KK	138/148 (93%)	126 (91%)	11 (8%)	1 (1%)	26	70
52	LL	122/124 (98%)	110 (90%)	12 (10%)	0	100	100
53	MM	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
54	NN	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
55	OO	234/253 (92%)	226 (97%)	8 (3%)	0	100	100
56	PP	112/119 (94%)	105 (94%)	7 (6%)	0	100	100
57	QQ	194/237 (82%)	184 (95%)	9 (5%)	1 (0%)	34	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	RR	87/99 (88%)	81 (93%)	6 (7%)	0	100	100
59	SS	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	15	56
60	TT	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
61	UU	231/233 (99%)	223 (96%)	8 (4%)	0	100	100
62	VV	231/233 (99%)	220 (95%)	11 (5%)	0	100	100
63	WW	399/401 (100%)	368 (92%)	28 (7%)	3 (1%)	24	66
64	XX	91/96 (95%)	88 (97%)	3 (3%)	0	100	100
65	YY	265/273 (97%)	244 (92%)	18 (7%)	3 (1%)	17	60
66	ZZ	83/91 (91%)	73 (88%)	10 (12%)	0	100	100
67	11	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
68	22	97/99 (98%)	89 (92%)	7 (7%)	1 (1%)	19	62
69	33	240/255 (94%)	225 (94%)	14 (6%)	1 (0%)	39	78
70	44	264/321 (82%)	251 (95%)	10 (4%)	3 (1%)	17	60
71	55	55/339 (16%)	53 (96%)	2 (4%)	0	100	100
72	66	301/319 (94%)	291 (97%)	10 (3%)	0	100	100
73	77	163/165 (99%)	146 (90%)	16 (10%)	1 (1%)	30	72
74	88	448/457 (98%)	414 (92%)	31 (7%)	3 (1%)	26	70
All	All	13235/14689 (90%)	12473 (94%)	718 (5%)	44 (0%)	50	83

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	DD	423	THR
4	D	52	LEU
4	D	195	VAL
42	BB	303	GLU
45	EE	89	ILE
59	SS	30	GLY
63	WW	385	ASN
65	YY	98	ASN
68	22	114	GLU
70	44	62	LYS
70	44	128	ASN
70	44	203	ASN
42	BB	197	GLN
49	II	257	ARG

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Mol	Chain	Res	Type
50	JJ	94	VAL
50	JJ	199	HIS
73	77	212	GLU
5	E	218	ARG
50	JJ	74	THR
51	KK	135	LYS
57	QQ	54	GLU
63	WW	239	ASN
63	WW	410	ASN
65	YY	94	SER
65	YY	111	GLY
74	88	385	VAL
3	C	197	ILE
4	D	49	PHE
5	E	42	PRO
10	J	115	LYS
39	c	124	ILE
43	CC	324	LEU
49	II	264	PRO
69	33	170	ASN
18	R	185	LYS
45	EE	214	ARG
74	88	148	GLY
6	F	196	GLY
4	D	31	PRO
47	GG	173	VAL
50	JJ	76	PRO
43	CC	66	GLY
50	JJ	118	PRO
74	88	181	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	272/337 (81%)	255 (94%)	17 (6%)	22 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	210/210 (100%)	197 (94%)	13 (6%)	23	62
4	D	218/218 (100%)	196 (90%)	22 (10%)	9	36
5	E	242/242 (100%)	230 (95%)	12 (5%)	30	70
6	F	172/172 (100%)	164 (95%)	8 (5%)	32	71
7	G	68/68 (100%)	66 (97%)	2 (3%)	50	81
8	H	138/138 (100%)	131 (95%)	7 (5%)	29	69
9	I	108/117 (92%)	104 (96%)	4 (4%)	41	77
10	J	181/181 (100%)	166 (92%)	15 (8%)	14	48
11	K	167/167 (100%)	151 (90%)	16 (10%)	10	38
12	L	203/211 (96%)	194 (96%)	9 (4%)	35	73
13	M	136/136 (100%)	130 (96%)	6 (4%)	35	73
14	N	107/107 (100%)	105 (98%)	2 (2%)	65	87
15	O	200/200 (100%)	189 (94%)	11 (6%)	27	67
16	P	185/185 (100%)	181 (98%)	4 (2%)	60	86
17	Q	256/267 (96%)	242 (94%)	14 (6%)	27	67
18	R	303/308 (98%)	291 (96%)	12 (4%)	38	76
19	S	167/191 (87%)	162 (97%)	5 (3%)	48	81
20	T	204/213 (96%)	196 (96%)	8 (4%)	39	76
21	U	73/73 (100%)	69 (94%)	4 (6%)	27	67
22	V	74/161 (46%)	71 (96%)	3 (4%)	37	75
23	W	104/104 (100%)	101 (97%)	3 (3%)	50	81
24	X	56/56 (100%)	51 (91%)	5 (9%)	12	43
25	Y	40/40 (100%)	39 (98%)	1 (2%)	55	84
26	Z	50/50 (100%)	46 (92%)	4 (8%)	15	50
27	0	36/36 (100%)	35 (97%)	1 (3%)	51	82
28	1	323/323 (100%)	312 (97%)	11 (3%)	44	79
29	2	106/106 (100%)	100 (94%)	6 (6%)	25	66
30	3	112/112 (100%)	110 (98%)	2 (2%)	66	88
31	4	121/121 (100%)	118 (98%)	3 (2%)	55	84
32	5	284/284 (100%)	278 (98%)	6 (2%)	61	86
33	6	213/252 (84%)	205 (96%)	8 (4%)	40	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	7	95/95 (100%)	91 (96%)	4 (4%)	36	74
35	8	182/240 (76%)	173 (95%)	9 (5%)	31	70
36	9	176/186 (95%)	168 (96%)	8 (4%)	34	73
37	a	158/158 (100%)	151 (96%)	7 (4%)	35	73
38	b	144/144 (100%)	139 (96%)	5 (4%)	43	78
39	c	110/110 (100%)	109 (99%)	1 (1%)	84	94
40	d	191/199 (96%)	187 (98%)	4 (2%)	61	86
41	AA	177/309 (57%)	168 (95%)	9 (5%)	29	69
42	BB	233/233 (100%)	205 (88%)	28 (12%)	6	28
43	CC	328/385 (85%)	296 (90%)	32 (10%)	10	38
44	DD	256/437 (59%)	229 (90%)	27 (10%)	8	34
45	EE	249/252 (99%)	237 (95%)	12 (5%)	31	71
46	FF	114/114 (100%)	105 (92%)	9 (8%)	15	51
47	GG	138/138 (100%)	132 (96%)	6 (4%)	35	73
48	HH	141/141 (100%)	125 (89%)	16 (11%)	7	31
49	II	196/215 (91%)	186 (95%)	10 (5%)	29	69
50	JJ	167/167 (100%)	151 (90%)	16 (10%)	10	38
51	KK	122/127 (96%)	108 (88%)	14 (12%)	7	30
52	LL	103/103 (100%)	89 (86%)	14 (14%)	5	22
53	MM	100/100 (100%)	94 (94%)	6 (6%)	24	64
54	NN	103/103 (100%)	92 (89%)	11 (11%)	8	33
55	OO	208/220 (94%)	199 (96%)	9 (4%)	35	73
56	PP	101/104 (97%)	96 (95%)	5 (5%)	30	70
57	QQ	187/218 (86%)	178 (95%)	9 (5%)	31	71
58	RR	80/87 (92%)	74 (92%)	6 (8%)	17	53
59	SS	69/69 (100%)	64 (93%)	5 (7%)	18	55
60	TT	81/81 (100%)	73 (90%)	8 (10%)	10	37
61	UU	208/208 (100%)	197 (95%)	11 (5%)	28	68
62	VV	208/210 (99%)	199 (96%)	9 (4%)	35	73
63	WW	368/368 (100%)	330 (90%)	38 (10%)	9	35
64	XX	84/84 (100%)	79 (94%)	5 (6%)	24	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
65	YY	248/250 (99%)	231 (93%)	17 (7%)	19	58
66	ZZ	78/82 (95%)	72 (92%)	6 (8%)	16	52
67	11	32/32 (100%)	31 (97%)	1 (3%)	47	80
68	22	90/90 (100%)	89 (99%)	1 (1%)	80	92
69	33	216/231 (94%)	203 (94%)	13 (6%)	24	64
70	44	238/281 (85%)	229 (96%)	9 (4%)	40	76
71	55	53/303 (18%)	51 (96%)	2 (4%)	40	76
72	66	277/289 (96%)	269 (97%)	8 (3%)	50	81
73	77	158/158 (100%)	152 (96%)	6 (4%)	40	76
74	88	401/404 (99%)	376 (94%)	25 (6%)	23	62
All	All	11997/13111 (92%)	11312 (94%)	685 (6%)	30	66

All (685) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	93	MET
2	B	127	ARG
2	B	134	ASN
2	B	194	ILE
2	B	239	ASN
2	B	240	CYS
2	B	241	LEU
2	B	250	THR
2	B	267	ARG
2	B	287	VAL
2	B	294	HIS
2	B	312	ASP
2	B	316	ARG
2	B	324	SER
2	B	338	MET
2	B	356	LYS
2	B	376	ASN
3	C	23	ARG
3	C	61	LEU
3	C	86	GLU
3	C	97	THR
3	C	106	CYS
3	C	164	GLN

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Mol	Chain	Res	Type
3	C	169	ARG
3	C	175	LYS
3	C	218	ARG
3	C	234	VAL
3	C	248	VAL
3	C	258	SER
3	C	263	GLN
4	D	30	ASN
4	D	52	LEU
4	D	56	THR
4	D	62	THR
4	D	65	VAL
4	D	103	ARG
4	D	109	LYS
4	D	115	ARG
4	D	124	ARG
4	D	142	GLU
4	D	143	LEU
4	D	152	PHE
4	D	156	LEU
4	D	182	LEU
4	D	199	GLU
4	D	200	ILE
4	D	216	LEU
4	D	222	LEU
4	D	235	SER
4	D	237	ASP
4	D	244	ASP
4	D	260	GLN
5	E	32	LEU
5	E	38	SER
5	E	82	LEU
5	E	83	LEU
5	E	117	ARG
5	E	138	GLU
5	E	154	LEU
5	E	165	GLN
5	E	189	HIS
5	E	200	LYS
5	E	218	ARG
5	E	231	PHE
6	F	24	LEU

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Mol	Chain	Res	Type
6	F	48	THR
6	F	78	ASP
6	F	80	LYS
6	F	86	VAL
6	F	97	ARG
6	F	104	ARG
6	F	130	ARG
7	G	12	LEU
7	G	80	LEU
8	H	14	ARG
8	H	19	VAL
8	H	46	VAL
8	H	60	THR
8	H	83	ARG
8	H	99	LYS
8	H	123	LEU
9	I	4	LEU
9	I	23	LYS
9	I	109	THR
9	I	124	ASP
10	J	99	ARG
10	J	101	LYS
10	J	111	THR
10	J	119	LYS
10	J	130	LEU
10	J	141	PHE
10	J	156	ASP
10	J	162	LYS
10	J	193	SER
10	J	209	LYS
10	J	227	GLN
10	J	241	ARG
10	J	246	ARG
10	J	265	ASP
10	J	273	GLU
11	K	40	GLU
11	K	53	LYS
11	K	68	THR
11	K	94	ASP
11	K	98	MET
11	K	104	LEU
11	K	113	LEU

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Mol	Chain	Res	Type
11	K	114	CYS
11	K	130	LYS
11	K	139	MET
11	K	150	GLU
11	K	158	GLU
11	K	163	GLU
11	K	184	LEU
11	K	191	SER
11	K	227	LYS
12	L	8	LYS
12	L	62	ASN
12	L	68	GLU
12	L	69	LEU
12	L	114	ARG
12	L	138	VAL
12	L	145	MET
12	L	177	LYS
12	L	194	LEU
13	M	28	VAL
13	M	102	LEU
13	M	109	LEU
13	M	110	LEU
13	M	111	ARG
13	M	161	LEU
14	N	46	THR
14	N	105	VAL
15	O	103	GLN
15	O	107	LEU
15	O	110	GLN
15	O	112	LEU
15	O	135	ASP
15	O	140	LEU
15	O	203	ILE
15	O	212	GLN
15	O	228	LEU
15	O	265	CYS
15	O	276	ARG
16	P	113	PHE
16	P	161	THR
16	P	197	ARG
16	P	231	LEU
17	Q	14	ARG

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Mol	Chain	Res	Type
17	Q	51	GLU
17	Q	86	PHE
17	Q	91	ASN
17	Q	103	THR
17	Q	129	LYS
17	Q	131	LEU
17	Q	132	ARG
17	Q	162	ASP
17	Q	188	ASP
17	Q	216	ASN
17	Q	246	LEU
17	Q	257	ARG
17	Q	269	GLU
18	R	57	VAL
18	R	94	ARG
18	R	97	LEU
18	R	117	LEU
18	R	159	LEU
18	R	173	GLN
18	R	178	LYS
18	R	181	ARG
18	R	276	GLN
18	R	279	LYS
18	R	293	GLU
18	R	304	LEU
19	S	67	LYS
19	S	79	VAL
19	S	95	LYS
19	S	96	TRP
19	S	203	ARG
20	T	17	THR
20	T	32	ASP
20	T	45	ASN
20	T	48	ARG
20	T	94	SER
20	T	161	LEU
20	T	170	LEU
20	T	203	THR
21	U	8	LEU
21	U	24	LYS
21	U	31	ARG
21	U	60	GLU

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Mol	Chain	Res	Type
22	V	61	SER
22	V	62	GLN
22	V	84	ARG
23	W	104	CYS
23	W	142	GLU
23	W	167	LYS
24	X	34	VAL
24	X	37	VAL
24	X	55	ARG
24	X	56	LYS
24	X	67	ARG
25	Y	73	ARG
26	Z	64	ARG
26	Z	87	SER
26	Z	89	ARG
26	Z	112	LEU
27	0	68	ASP
28	1	32	LEU
28	1	45	GLN
28	1	58	ARG
28	1	102	ASP
28	1	165	ILE
28	1	167	ASP
28	1	171	THR
28	1	173	VAL
28	1	243	THR
28	1	246	CYS
28	1	315	LEU
29	2	46	LEU
29	2	64	GLU
29	2	100	ARG
29	2	104	LEU
29	2	124	ARG
29	2	127	MET
30	3	25	ARG
30	3	91	LYS
31	4	11	ILE
31	4	100	LEU
31	4	102	LYS
32	5	70	LEU
32	5	236	LEU
32	5	244	LEU

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Mol	Chain	Res	Type
32	5	248	LYS
32	5	271	THR
32	5	320	VAL
33	6	111	LYS
33	6	159	GLU
33	6	160	ARG
33	6	161	GLN
33	6	198	GLU
33	6	213	SER
33	6	266	VAL
33	6	277	LEU
34	7	47	LEU
34	7	84	ASN
34	7	111	LEU
34	7	144	LYS
35	8	38	ASP
35	8	51	HIS
35	8	83	ARG
35	8	97	ARG
35	8	123	ILE
35	8	147	ASP
35	8	179	LEU
35	8	191	GLU
35	8	258	LEU
36	9	56	LEU
36	9	86	LEU
36	9	104	ASN
36	9	108	ASN
36	9	118	GLN
36	9	124	LEU
36	9	210	GLU
36	9	223	LYS
37	a	25	LYS
37	a	45	LEU
37	a	70	THR
37	a	105	SER
37	a	126	ARG
37	a	166	ARG
37	a	173	ARG
38	b	32	THR
38	b	88	LEU
38	b	119	LEU

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Mol	Chain	Res	Type
38	b	130	ASP
38	b	152	GLN
39	c	121	LYS
40	d	66	LEU
40	d	68	ARG
40	d	104	ARG
40	d	192	LEU
41	AA	43	LEU
41	AA	45	ARG
41	AA	54	ILE
41	AA	63	LEU
41	AA	71	LEU
41	AA	83	THR
41	AA	89	ARG
41	AA	256	PHE
41	AA	297	LEU
42	BB	132	LEU
42	BB	159	LYS
42	BB	164	ILE
42	BB	199	THR
42	BB	204	SER
42	BB	206	THR
42	BB	210	ILE
42	BB	217	ILE
42	BB	226	LEU
42	BB	249	LEU
42	BB	256	LYS
42	BB	257	ARG
42	BB	260	GLU
42	BB	274	ARG
42	BB	276	ILE
42	BB	280	LEU
42	BB	304	ARG
42	BB	310	GLU
42	BB	314	GLN
42	BB	324	ASN
42	BB	328	ASN
42	BB	329	ARG
42	BB	333	LEU
42	BB	342	THR
42	BB	348	THR
42	BB	367	ARG

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Mol	Chain	Res	Type
42	BB	372	LEU
42	BB	382	ARG
43	CC	80	ILE
43	CC	84	LEU
43	CC	88	ASN
43	CC	102	LYS
43	CC	118	LEU
43	CC	129	ASN
43	CC	158	ASN
43	CC	166	ASN
43	CC	179	LEU
43	CC	180	MET
43	CC	181	ASN
43	CC	184	ASN
43	CC	188	ASN
43	CC	190	ASN
43	CC	220	PHE
43	CC	222	LYS
43	CC	244	LEU
43	CC	248	MET
43	CC	263	ASN
43	CC	278	LEU
43	CC	308	ASN
43	CC	310	THR
43	CC	312	ASP
43	CC	319	LEU
43	CC	324	LEU
43	CC	329	ILE
43	CC	358	LEU
43	CC	360	SER
43	CC	374	ASN
43	CC	379	ASN
43	CC	382	ASN
43	CC	390	ASN
44	DD	9	LYS
44	DD	13	ARG
44	DD	30	LYS
44	DD	34	VAL
44	DD	41	LEU
44	DD	51	GLU
44	DD	52	THR
44	DD	58	GLU

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Mol	Chain	Res	Type
44	DD	61	THR
44	DD	64	ARG
44	DD	68	VAL
44	DD	104	ARG
44	DD	119	ARG
44	DD	127	HIS
44	DD	132	VAL
44	DD	138	LYS
44	DD	144	LEU
44	DD	155	ASP
44	DD	175	ASP
44	DD	394	ASP
44	DD	401	LEU
44	DD	431	LEU
44	DD	432	SER
44	DD	436	ILE
44	DD	453	LEU
44	DD	455	ASP
44	DD	484	ASN
45	EE	91	ARG
45	EE	150	VAL
45	EE	174	ASP
45	EE	181	LEU
45	EE	183	GLU
45	EE	187	ARG
45	EE	227	VAL
45	EE	235	LYS
45	EE	248	GLU
45	EE	258	LEU
45	EE	261	LYS
45	EE	280	THR
46	FF	24	LEU
46	FF	36	ARG
46	FF	70	LEU
46	FF	78	GLN
46	FF	88	ASP
46	FF	90	ARG
46	FF	97	VAL
46	FF	103	LYS
46	FF	120	ILE
47	GG	95	LEU
47	GG	123	ARG

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Mol	Chain	Res	Type
47	GG	138	LEU
47	GG	145	THR
47	GG	146	ARG
47	GG	212	LEU
48	HH	23	LEU
48	HH	25	SER
48	HH	26	ILE
48	HH	30	LYS
48	HH	31	LEU
48	HH	42	GLN
48	HH	59	ASP
48	HH	68	ILE
48	HH	73	LEU
48	HH	91	LEU
48	HH	99	ILE
48	HH	103	MET
48	HH	104	GLU
48	HH	121	LEU
48	HH	126	LEU
48	HH	151	LEU
49	II	91	LEU
49	II	98	LEU
49	II	117	ASP
49	II	120	LEU
49	II	153	ARG
49	II	215	THR
49	II	225	GLU
49	II	228	MET
49	II	248	LYS
49	II	254	ARG
50	JJ	18	ARG
50	JJ	38	TYR
50	JJ	51	ASP
50	JJ	55	LEU
50	JJ	60	ASP
50	JJ	68	TYR
50	JJ	69	LEU
50	JJ	74	THR
50	JJ	79	LEU
50	JJ	82	ARG
50	JJ	83	ARG
50	JJ	86	TRP

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Mol	Chain	Res	Type
50	JJ	116	THR
50	JJ	121	LEU
50	JJ	124	LEU
50	JJ	133	MET
51	KK	78	LEU
51	KK	92	SER
51	KK	117	ASN
51	KK	124	ILE
51	KK	134	ARG
51	KK	151	MET
51	KK	159	ASN
51	KK	161	LEU
51	KK	169	MET
51	KK	180	ILE
51	KK	193	LYS
51	KK	194	LYS
51	KK	210	ARG
51	KK	216	ARG
52	LL	43	ARG
52	LL	44	LYS
52	LL	66	MET
52	LL	67	VAL
52	LL	74	ASN
52	LL	82	ARG
52	LL	91	VAL
52	LL	108	VAL
52	LL	121	VAL
52	LL	126	ILE
52	LL	127	ARG
52	LL	132	LEU
52	LL	144	LYS
52	LL	148	LYS
53	MM	5	ILE
53	MM	6	LEU
53	MM	91	MET
53	MM	97	LEU
53	MM	114	LEU
53	MM	118	ASP
54	NN	1	MET
54	NN	22	LEU
54	NN	35	GLU
54	NN	36	ILE

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Mol	Chain	Res	Type
54	NN	37	LEU
54	NN	69	MET
54	NN	70	ARG
54	NN	72	THR
54	NN	86	PHE
54	NN	91	PHE
54	NN	94	CYS
55	OO	65	ASP
55	OO	68	LEU
55	OO	80	MET
55	OO	95	ILE
55	OO	173	SER
55	OO	181	MET
55	OO	219	LEU
55	OO	280	LYS
55	OO	286	PHE
56	PP	9	ARG
56	PP	29	ARG
56	PP	40	LEU
56	PP	92	LYS
56	PP	117	MET
57	QQ	20	VAL
57	QQ	22	VAL
57	QQ	25	GLU
57	QQ	37	LEU
57	QQ	40	ARG
57	QQ	42	ASP
57	QQ	98	LYS
57	QQ	172	LEU
57	QQ	200	CYS
58	RR	49	LEU
58	RR	68	ASP
58	RR	82	ILE
58	RR	104	THR
58	RR	123	ARG
58	RR	132	CYS
59	SS	9	SER
59	SS	24	ARG
59	SS	35	THR
59	SS	81	LYS
59	SS	82	ARG
60	TT	99	ARG

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Mol	Chain	Res	Type
60	TT	124	MET
60	TT	144	LYS
60	TT	153	ARG
60	TT	155	ARG
60	TT	156	LYS
60	TT	165	LEU
60	TT	171	ASP
61	UU	90	ARG
61	UU	98	THR
61	UU	116	LEU
61	UU	137	MET
61	UU	144	LEU
61	UU	145	ASP
61	UU	152	ARG
61	UU	180	ARG
61	UU	191	LEU
61	UU	212	LYS
61	UU	224	VAL
62	VV	31	ASP
62	VV	74	LEU
62	VV	102	LEU
62	VV	107	LEU
62	VV	141	GLU
62	VV	172	GLU
62	VV	186	LEU
62	VV	199	LEU
62	VV	216	LEU
63	WW	66	THR
63	WW	90	LEU
63	WW	94	VAL
63	WW	125	LEU
63	WW	159	LEU
63	WW	160	LEU
63	WW	184	LEU
63	WW	185	ASN
63	WW	189	ASP
63	WW	198	LEU
63	WW	225	GLU
63	WW	229	ASP
63	WW	248	LEU
63	WW	252	LYS
63	WW	254	THR

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Mol	Chain	Res	Type
63	WW	258	LEU
63	WW	267	ASN
63	WW	270	LYS
63	WW	278	GLU
63	WW	282	GLN
63	WW	284	LYS
63	WW	296	LYS
63	WW	311	LYS
63	WW	316	LEU
63	WW	319	GLN
63	WW	323	LEU
63	WW	325	MET
63	WW	333	LYS
63	WW	341	THR
63	WW	352	ASN
63	WW	361	LYS
63	WW	370	ARG
63	WW	388	GLU
63	WW	396	LYS
63	WW	429	LYS
63	WW	440	GLU
63	WW	442	LEU
63	WW	447	LEU
64	XX	14	LEU
64	XX	22	ASN
64	XX	35	LEU
64	XX	53	ILE
64	XX	59	LEU
65	YY	50	LEU
65	YY	76	LEU
65	YY	83	ASN
65	YY	130	ARG
65	YY	142	GLN
65	YY	165	LEU
65	YY	216	LEU
65	YY	233	ILE
65	YY	249	ARG
65	YY	255	LEU
65	YY	258	LEU
65	YY	273	VAL
65	YY	278	ARG
65	YY	283	LYS

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Mol	Chain	Res	Type
65	YY	286	ARG
65	YY	289	LYS
65	YY	303	ASP
66	ZZ	15	ARG
66	ZZ	38	LEU
66	ZZ	48	SER
66	ZZ	58	LEU
66	ZZ	78	ILE
66	ZZ	88	ARG
67	11	88	MET
68	22	38	VAL
69	33	21	LEU
69	33	28	ILE
69	33	37	VAL
69	33	49	LEU
69	33	67	LEU
69	33	76	GLN
69	33	155	LEU
69	33	159	ASN
69	33	181	GLN
69	33	186	ASN
69	33	210	LEU
69	33	243	TYR
69	33	260	ILE
70	44	22	LEU
70	44	98	GLN
70	44	131	LEU
70	44	149	LEU
70	44	155	LEU
70	44	174	ARG
70	44	264	GLU
70	44	294	GLU
70	44	309	LEU
71	55	43	ILE
71	55	65	ILE
72	66	132	ARG
72	66	152	GLN
72	66	181	ARG
72	66	229	ASN
72	66	247	ILE
72	66	257	ASP
72	66	271	LEU

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Mol	Chain	Res	Type
72	66	333	ARG
73	77	202	LEU
73	77	255	THR
73	77	258	THR
73	77	260	ASN
73	77	265	THR
73	77	285	GLU
74	88	46	THR
74	88	118	ILE
74	88	127	LEU
74	88	138	ILE
74	88	139	VAL
74	88	140	THR
74	88	199	GLN
74	88	219	LEU
74	88	223	SER
74	88	237	ARG
74	88	257	MET
74	88	297	ILE
74	88	320	ILE
74	88	325	LEU
74	88	336	LEU
74	88	337	ARG
74	88	355	LEU
74	88	363	MET
74	88	368	LEU
74	88	369	VAL
74	88	400	LEU
74	88	423	TRP
74	88	433	GLN
74	88	475	LYS
74	88	478	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2677/3296 (81%)	605 (22%)	104 (3%)
75	aa	1473/1649 (89%)	442 (30%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
76	bb	75/76 (98%)	42 (56%)	0
All	All	4225/5021 (84%)	1089 (25%)	104 (2%)

All (1089) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	26	A
1	A	27	A
1	A	28	U
1	A	30	U
1	A	35	U
1	A	38	A
1	A	40	A
1	A	41	G
1	A	43	U
1	A	45	U
1	A	48	A
1	A	49	G
1	A	58	A
1	A	70	A
1	A	78	U
1	A	85	A
1	A	93	U
1	A	94	A
1	A	95	A
1	A	106	A
1	A	115	A
1	A	116	C
1	A	117	U
1	A	119	A
1	A	120	U
1	A	122	A
1	A	128	U
1	A	133	A
1	A	134	U
1	A	135	U
1	A	151	A
1	A	153	G
1	A	161	U
1	A	162	U
1	A	163	A
1	A	165	A

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Mol	Chain	Res	Type
1	A	166	U
1	A	170	U
1	A	174	G
1	A	176	U
1	A	204	A
1	A	214	A
1	A	215	A
1	A	217	A
1	A	219	U
1	A	220	A
1	A	222	A
1	A	236	A
1	A	239	A
1	A	240	U
1	A	245	G
1	A	253	A
1	A	255	G
1	A	256	A
1	A	261	A
1	A	262	A
1	A	264	U
1	A	266	A
1	A	269	A
1	A	270	G
1	A	281	A
1	A	283	U
1	A	288	G
1	A	292	G
1	A	301	A
1	A	307	G
1	A	308	U
1	A	309	C
1	A	310	U
1	A	311	A
1	A	312	A
1	A	313	U
1	A	314	A
1	A	316	G
1	A	327	A
1	A	331	A
1	A	332	A
1	A	337	A

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Mol	Chain	Res	Type
1	A	342	A
1	A	348	U
1	A	349	A
1	A	359	A
1	A	365	A
1	A	380	G
1	A	384	A
1	A	401	A
1	A	425	A
1	A	426	A
1	A	427	G
1	A	428	C
1	A	429	A
1	A	430	A
1	A	433	A
1	A	442	U
1	A	445	U
1	A	447	U
1	A	450	U
1	A	454	A
1	A	455	A
1	A	462	A
1	A	472	U
1	A	473	A
1	A	474	A
1	A	487	U
1	A	502	A
1	A	503	A
1	A	508	U
1	A	516	A
1	A	518	A
1	A	526	A
1	A	527	A
1	A	528	U
1	A	529	A
1	A	530	A
1	A	531	U
1	A	533	U
1	A	552	A
1	A	562	U
1	A	563	U
1	A	564	A

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Mol	Chain	Res	Type
1	A	577	U
1	A	578	G
1	A	595	U
1	A	604	G
1	A	614	A
1	A	615	U
1	A	616	A
1	A	617	A
1	A	618	A
1	A	620	G
1	A	621	A
1	A	637	U
1	A	638	U
1	A	644	A
1	A	655	A
1	A	656	A
1	A	661	G
1	A	667	U
1	A	673	A
1	A	675	G
1	A	676	A
1	A	677	C
1	A	681	U
1	A	682	C
1	A	683	U
1	A	684	G
1	A	696	G
1	A	703	U
1	A	710	A
1	A	718	G
1	A	719	U
1	A	733	A
1	A	734	U
1	A	735	A
1	A	736	A
1	A	747	U
1	A	767	A
1	A	776	A
1	A	777	G
1	A	778	A
1	A	782	G
1	A	783	U

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Mol	Chain	Res	Type
1	A	789	A
1	A	790	A
1	A	797	U
1	A	798	A
1	A	799	U
1	A	803	A
1	A	806	G
1	A	809	C
1	A	820	U
1	A	825	A
1	A	835	A
1	A	840	C
1	A	841	G
1	A	842	A
1	A	843	A
1	A	845	U
1	A	850	A
1	A	855	U
1	A	856	A
1	A	857	U
1	A	858	A
1	A	859	U
1	A	860	A
1	A	865	A
1	A	867	A
1	A	872	G
1	A	873	A
1	A	884	U
1	A	887	G
1	A	891	A
1	A	900	A
1	A	901	A
1	A	919	A
1	A	924	A
1	A	925	U
1	A	929	G
1	A	939	A
1	A	947	G
1	A	951	A
1	A	952	A
1	A	953	U
1	A	954	A

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Mol	Chain	Res	Type
1	A	966	A
1	A	1065	A
1	A	1066	A
1	A	1072	U
1	A	1074	U
1	A	1075	A
1	A	1077	A
1	A	1078	U
1	A	1086	U
1	A	1087	U
1	A	1094	U
1	A	1095	A
1	A	1096	A
1	A	1099	U
1	A	1101	C
1	A	1105	U
1	A	1107	U
1	A	1108	U
1	A	1110	A
1	A	1112	A
1	A	1113	A
1	A	1114	U
1	A	1115	A
1	A	1118	A
1	A	1126	A
1	A	1127	A
1	A	1130	C
1	A	1143	A
1	A	1144	U
1	A	1169	A
1	A	1170	U
1	A	1171	A
1	A	1182	A
1	A	1191	U
1	A	1195	A
1	A	1242	A
1	A	1244	A
1	A	1255	A
1	A	1256	U
1	A	1258	A
1	A	1260	U
1	A	1269	G

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Mol	Chain	Res	Type
1	A	1271	A
1	A	1272	U
1	A	1273	U
1	A	1279	A
1	A	1280	A
1	A	1286	A
1	A	1287	A
1	A	1288	U
1	A	1289	G
1	A	1304	G
1	A	1305	A
1	A	1308	A
1	A	1313	G
1	A	1314	U
1	A	1315	A
1	A	1317	A
1	A	1330	U
1	A	1331	A
1	A	1332	A
1	A	1337	U
1	A	1342	U
1	A	1346	A
1	A	1350	U
1	A	1357	A
1	A	1358	C
1	A	1359	G
1	A	1365	U
1	A	1371	A
1	A	1373	U
1	A	1374	U
1	A	1386	A
1	A	1387	A
1	A	1389	U
1	A	1397	A
1	A	1399	A
1	A	1400	U
1	A	1404	A
1	A	1406	A
1	A	1407	A
1	A	1408	U
1	A	1409	C
1	A	1410	U

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Mol	Chain	Res	Type
1	A	1411	A
1	A	1412	U
1	A	1418	U
1	A	1424	U
1	A	1431	U
1	A	1439	A
1	A	1487	A
1	A	1490	A
1	A	1494	A
1	A	1501	A
1	A	1507	U
1	A	1516	U
1	A	1523	A
1	A	1528	G
1	A	1531	C
1	A	1534	G
1	A	1537	A
1	A	1542	U
1	A	1546	G
1	A	1548	A
1	A	1549	U
1	A	1551	C
1	A	1560	A
1	A	1563	C
1	A	1568	U
1	A	1569	C
1	A	1577	U
1	A	1578	A
1	A	1579	A
1	A	1582	A
1	A	1598	A
1	A	1600	U
1	A	1603	G
1	A	1604	A
1	A	1605	U
1	A	1606	A
1	A	1618	G
1	A	1626	G
1	A	1633	U
1	A	1634	A
1	A	1648	U
1	A	1649	C

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Mol	Chain	Res	Type
1	A	1652	U
1	A	1653	A
1	A	1655	A
1	A	1662	U
1	A	1666	A
1	A	1667	A
1	A	1672	G
1	A	1680	A
1	A	1687	A
1	A	1689	U
1	A	1698	C
1	A	1706	G
1	A	1707	C
1	A	1709	G
1	A	1715	A
1	A	1717	A
1	A	1719	G
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1741	C
1	A	1746	C
1	A	1755	A
1	A	1756	U
1	A	1757	A
1	A	1767	A
1	A	1768	A
1	A	1769	U
1	A	1770	U
1	A	1776	A
1	A	1777	C
1	A	1782	A
1	A	1786	A
1	A	1789	U
1	A	1790	A
1	A	1797	G
1	A	1807	A
1	A	1811	U
1	A	1812	U
1	A	1814	U
1	A	1816	A
1	A	1819	A

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Mol	Chain	Res	Type
1	A	1820	G
1	A	1830	G
1	A	1831	U
1	A	1833	G
1	A	1836	A
1	A	1837	A
1	A	1838	A
1	A	1841	C
1	A	1855	U
1	A	1863	C
1	A	1865	C
1	A	1867	U
1	A	1869	A
1	A	1870	A
1	A	1871	U
1	A	1872	G
1	A	1882	U
1	A	1891	U
1	A	1892	G
1	A	1893	U
1	A	1897	C
1	A	1920	A
1	A	1923	C
1	A	1931	A
1	A	1933	A
1	A	1943	C
1	A	1949	G
1	A	1951	A
1	A	1952	A
1	A	1955	C
1	A	1956	G
1	A	1959	A
1	A	1961	G
1	A	1963	C
1	A	1969	G
1	A	1989	U
1	A	1991	G
1	A	1995	G
1	A	2084	G
1	A	2093	A
1	A	2188	A
1	A	2199	U

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Mol	Chain	Res	Type
1	A	2205	G
1	A	2220	U
1	A	2235	A
1	A	2251	A
1	A	2252	C
1	A	2264	G
1	A	2272	U
1	A	2274	A
1	A	2276	G
1	A	2283	C
1	A	2293	A
1	A	2301	C
1	A	2304	A
1	A	2305	A
1	A	2310	U
1	A	2314	U
1	A	2315	A
1	A	2316	A
1	A	2317	A
1	A	2323	A
1	A	2324	U
1	A	2325	A
1	A	2329	A
1	A	2330	A
1	A	2331	U
1	A	2332	U
1	A	2333	A
1	A	2349	A
1	A	2356	A
1	A	2358	A
1	A	2360	U
1	A	2361	A
1	A	2362	U
1	A	2372	U
1	A	2373	U
1	A	2374	A
1	A	2378	A
1	A	2379	U
1	A	2388	G
1	A	2390	U
1	A	2415	A
1	A	2419	U

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Mol	Chain	Res	Type
1	A	2424	U
1	A	2425	A
1	A	2426	A
1	A	2427	U
1	A	2430	A
1	A	2435	A
1	A	2436	A
1	A	2437	U
1	A	2438	A
1	A	2439	U
1	A	2446	U
1	A	2447	A
1	A	2453	G
1	A	2455	A
1	A	2457	G
1	A	2458	G
1	A	2459	A
1	A	2461	A
1	A	2462	A
1	A	2464	A
1	A	2467	A
1	A	2470	A
1	A	2575	A
1	A	2580	A
1	A	2586	U
1	A	2587	U
1	A	2588	A
1	A	2591	A
1	A	2599	A
1	A	2600	U
1	A	2601	A
1	A	2611	U
1	A	2612	A
1	A	2614	U
1	A	2616	G
1	A	2618	A
1	A	2650	G
1	A	2652	C
1	A	2666	A
1	A	2671	U
1	A	2672	G
1	A	2673	A

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Mol	Chain	Res	Type
1	A	2674	U
1	A	2691	A
1	A	2695	A
1	A	2696	A
1	A	2701	A
1	A	2705	A
1	A	2707	G
1	A	2711	G
1	A	2713	G
1	A	2714	A
1	A	2725	A
1	A	2735	A
1	A	2740	A
1	A	2741	G
1	A	2742	A
1	A	2750	A
1	A	2757	U
1	A	2760	G
1	A	2764	C
1	A	2766	U
1	A	2773	C
1	A	2784	U
1	A	2795	U
1	A	2796	G
1	A	2797	U
1	A	2802	G
1	A	2814	U
1	A	2815	U
1	A	2816	G
1	A	2821	U
1	A	2833	A
1	A	2834	A
1	A	2836	G
1	A	2840	C
1	A	2841	G
1	A	2845	G
1	A	2852	U
1	A	2853	A
1	A	2869	A
1	A	2870	G
1	A	2876	U
1	A	2877	U

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Mol	Chain	Res	Type
1	A	2880	U
1	A	2881	A
1	A	2894	A
1	A	2896	U
1	A	2897	A
1	A	2898	U
1	A	2901	U
1	A	2909	A
1	A	2913	U
1	A	2930	G
1	A	2940	G
1	A	2956	U
1	A	2957	A
1	A	2982	U
1	A	3004	A
1	A	3014	C
1	A	3018	A
1	A	3020	U
1	A	3021	A
1	A	3032	U
1	A	3034	A
1	A	3050	G
1	A	3062	A
1	A	3068	U
1	A	3069	A
1	A	3070	A
1	A	3092	U
1	A	3093	U
1	A	3094	A
1	A	3098	A
1	A	3102	A
1	A	3103	G
1	A	3106	G
1	A	3122	U
1	A	3123	A
1	A	3124	A
1	A	3125	U
1	A	3134	U
1	A	3136	U
1	A	3141	U
1	A	3148	A
1	A	3150	U

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Mol	Chain	Res	Type
1	A	3151	A
1	A	3152	A
1	A	3153	U
1	A	3155	A
1	A	3169	U
1	A	3171	A
1	A	3172	U
1	A	3177	A
1	A	3232	U
1	A	3234	A
1	A	3235	U
1	A	3240	A
1	A	3243	A
1	A	3244	A
1	A	3247	A
1	A	3248	C
1	A	3251	A
1	A	3252	U
1	A	3253	U
1	A	3254	U
1	A	3257	C
1	A	3269	U
1	A	3274	U
75	aa	14	A
75	aa	26	U
75	aa	29	G
75	aa	36	U
75	aa	39	A
75	aa	44	U
75	aa	45	A
75	aa	46	A
75	aa	54	C
75	aa	55	A
75	aa	58	A
75	aa	59	C
75	aa	73	A
75	aa	76	U
75	aa	77	U
75	aa	78	U
75	aa	80	U
75	aa	84	U
75	aa	85	G

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Mol	Chain	Res	Type
75	aa	90	G
75	aa	96	A
75	aa	99	U
75	aa	101	U
75	aa	102	G
75	aa	104	G
75	aa	108	U
75	aa	109	A
75	aa	116	A
75	aa	119	A
75	aa	121	U
75	aa	123	U
75	aa	124	U
75	aa	126	U
75	aa	129	G
75	aa	132	A
75	aa	133	U
75	aa	134	U
75	aa	135	A
75	aa	136	A
75	aa	137	U
75	aa	138	G
75	aa	139	A
75	aa	141	C
75	aa	143	A
75	aa	144	U
75	aa	146	G
75	aa	148	A
75	aa	155	A
75	aa	156	A
75	aa	158	U
75	aa	159	A
75	aa	161	U
75	aa	163	A
75	aa	164	A
75	aa	182	A
75	aa	197	A
75	aa	198	A
75	aa	208	U
75	aa	209	A
75	aa	216	A
75	aa	219	U

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Mol	Chain	Res	Type
75	aa	223	U
75	aa	224	A
75	aa	229	U
75	aa	232	U
75	aa	234	A
75	aa	235	A
75	aa	241	U
75	aa	243	A
75	aa	244	U
75	aa	247	U
75	aa	248	U
75	aa	251	G
75	aa	254	A
75	aa	255	G
75	aa	263	A
75	aa	266	A
75	aa	270	G
75	aa	271	U
75	aa	272	U
75	aa	279	A
75	aa	280	G
75	aa	284	A
75	aa	285	C
75	aa	286	G
75	aa	288	U
75	aa	294	A
75	aa	298	A
75	aa	299	U
75	aa	304	A
75	aa	312	A
75	aa	318	C
75	aa	334	U
75	aa	336	U
75	aa	337	A
75	aa	347	U
75	aa	348	A
75	aa	349	U
75	aa	350	A
75	aa	351	A
75	aa	352	G
75	aa	356	C
75	aa	371	U

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Mol	Chain	Res	Type
75	aa	376	C
75	aa	377	A
75	aa	380	G
75	aa	389	A
75	aa	393	A
75	aa	401	A
75	aa	409	G
75	aa	410	G
75	aa	414	A
75	aa	416	A
75	aa	417	U
75	aa	480	U
75	aa	481	A
75	aa	482	U
75	aa	486	U
75	aa	489	A
75	aa	492	G
75	aa	495	U
75	aa	496	A
75	aa	498	A
75	aa	500	A
75	aa	501	U
75	aa	503	A
75	aa	510	U
75	aa	526	U
75	aa	527	G
75	aa	531	U
75	aa	532	U
75	aa	537	A
75	aa	538	C
75	aa	540	A
75	aa	542	A
75	aa	551	U
75	aa	555	U
75	aa	557	G
75	aa	562	A
75	aa	601	U
75	aa	602	A
75	aa	603	U
75	aa	604	A
75	aa	606	U
75	aa	611	U

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Mol	Chain	Res	Type
75	aa	612	A
75	aa	622	A
75	aa	624	U
75	aa	625	A
75	aa	626	U
75	aa	634	A
75	aa	635	G
75	aa	641	G
75	aa	644	G
75	aa	645	U
75	aa	646	A
75	aa	647	A
75	aa	661	A
75	aa	668	A
75	aa	673	A
75	aa	674	A
75	aa	676	G
75	aa	677	G
75	aa	681	A
75	aa	682	A
75	aa	684	G
75	aa	685	G
75	aa	686	A
75	aa	688	C
75	aa	694	A
75	aa	704	A
75	aa	710	U
75	aa	714	U
75	aa	716	A
75	aa	726	A
75	aa	729	U
75	aa	732	A
75	aa	740	A
75	aa	741	A
75	aa	753	A
75	aa	761	A
75	aa	762	U
75	aa	763	A
75	aa	764	A
75	aa	765	U
75	aa	769	A
75	aa	775	U

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Mol	Chain	Res	Type
75	aa	780	G
75	aa	782	C
75	aa	784	A
75	aa	787	A
75	aa	788	U
75	aa	789	A
75	aa	793	G
75	aa	794	A
75	aa	797	A
75	aa	799	A
75	aa	800	U
75	aa	820	A
75	aa	836	U
75	aa	842	A
75	aa	858	U
75	aa	859	A
75	aa	864	U
75	aa	865	G
75	aa	870	U
75	aa	880	A
75	aa	882	C
75	aa	891	C
75	aa	892	A
75	aa	898	U
75	aa	912	A
75	aa	913	U
75	aa	914	A
75	aa	915	U
75	aa	916	A
75	aa	917	U
75	aa	918	A
75	aa	923	A
75	aa	924	U
75	aa	931	A
75	aa	933	A
75	aa	934	U
75	aa	936	A
75	aa	937	A
75	aa	938	A
75	aa	952	A
75	aa	972	A
75	aa	979	A

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Mol	Chain	Res	Type
75	aa	991	G
75	aa	992	U
75	aa	993	U
75	aa	994	A
75	aa	995	C
75	aa	998	A
75	aa	999	C
75	aa	1000	U
75	aa	1001	U
75	aa	1003	A
75	aa	1025	U
75	aa	1026	U
75	aa	1033	U
75	aa	1034	C
75	aa	1036	A
75	aa	1040	C
75	aa	1041	U
75	aa	1042	A
75	aa	1043	A
75	aa	1046	U
75	aa	1047	U
75	aa	1048	A
75	aa	1056	U
75	aa	1057	U
75	aa	1058	G
75	aa	1059	A
75	aa	1060	A
75	aa	1066	U
75	aa	1079	A
75	aa	1083	A
75	aa	1088	A
75	aa	1089	U
75	aa	1090	U
75	aa	1091	A
75	aa	1092	C
75	aa	1096	C
75	aa	1097	G
75	aa	1099	U
75	aa	1100	A
75	aa	1101	C
75	aa	1102	A
75	aa	1111	U

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Mol	Chain	Res	Type
75	aa	1112	U
75	aa	1134	A
75	aa	1136	A
75	aa	1141	G
75	aa	1142	U
75	aa	1143	U
75	aa	1144	C
75	aa	1148	A
75	aa	1153	A
75	aa	1155	A
75	aa	1172	A
75	aa	1173	U
75	aa	1174	U
75	aa	1175	U
75	aa	1176	U
75	aa	1177	A
75	aa	1178	A
75	aa	1179	U
75	aa	1182	U
75	aa	1188	A
75	aa	1189	U
75	aa	1190	U
75	aa	1196	U
75	aa	1198	A
75	aa	1204	U
75	aa	1205	A
75	aa	1206	A
75	aa	1207	U
75	aa	1212	A
75	aa	1223	A
75	aa	1228	A
75	aa	1229	A
75	aa	1233	A
75	aa	1245	A
75	aa	1246	U
75	aa	1252	G
75	aa	1256	A
75	aa	1257	A
75	aa	1258	U
75	aa	1259	A
75	aa	1264	U
75	aa	1265	G

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Mol	Chain	Res	Type
75	aa	1270	A
75	aa	1271	A
75	aa	1272	U
75	aa	1273	A
75	aa	1276	A
75	aa	1279	A
75	aa	1280	U
75	aa	1281	A
75	aa	1282	A
75	aa	1283	U
75	aa	1284	A
75	aa	1290	A
75	aa	1291	U
75	aa	1292	A
75	aa	1294	A
75	aa	1298	U
75	aa	1302	U
75	aa	1303	U
75	aa	1304	U
75	aa	1305	A
75	aa	1306	A
75	aa	1314	U
75	aa	1315	A
75	aa	1318	U
75	aa	1319	A
75	aa	1320	A
75	aa	1322	A
75	aa	1326	U
75	aa	1327	A
75	aa	1333	U
75	aa	1337	A
75	aa	1338	A
75	aa	1339	U
75	aa	1340	U
75	aa	1341	U
75	aa	1342	U
75	aa	1344	A
75	aa	1345	A
75	aa	1347	A
75	aa	1349	A
75	aa	1350	U
75	aa	1351	U

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Mol	Chain	Res	Type
75	aa	1352	U
75	aa	1353	U
75	aa	1354	U
75	aa	1362	A
75	aa	1368	A
75	aa	1369	U
75	aa	1370	A
75	aa	1371	U
75	aa	1373	A
75	aa	1380	A
75	aa	1388	U
75	aa	1397	A
75	aa	1400	A
75	aa	1404	A
75	aa	1406	G
75	aa	1408	A
75	aa	1413	U
75	aa	1414	A
75	aa	1415	G
75	aa	1421	C
75	aa	1425	A
75	aa	1426	A
75	aa	1428	U
75	aa	1431	U
75	aa	1437	A
75	aa	1438	C
75	aa	1439	G
75	aa	1442	G
75	aa	1443	A
75	aa	1444	A
75	aa	1445	U
75	aa	1447	U
75	aa	1453	C
75	aa	1455	G
75	aa	1462	A
75	aa	1463	C
75	aa	1465	A
75	aa	1466	A
75	aa	1468	C
75	aa	1474	U
75	aa	1478	G
75	aa	1487	C

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Mol	Chain	Res	Type
75	aa	1496	A
75	aa	1500	U
75	aa	1508	A
75	aa	1510	A
75	aa	1511	U
75	aa	1512	A
75	aa	1516	U
75	aa	1517	U
75	aa	1520	U
75	aa	1523	A
75	aa	1524	U
75	aa	1525	A
75	aa	1526	A
75	aa	1527	A
75	aa	1538	U
75	aa	1547	A
75	aa	1548	U
75	aa	1551	U
75	aa	1585	A
75	aa	1586	G
75	aa	1589	G
75	aa	1595	C
75	aa	1597	G
75	aa	1598	U
75	aa	1599	U
75	aa	1601	C
75	aa	1609	G
75	aa	1611	A
75	aa	1612	C
75	aa	1621	G
75	aa	1622	G
75	aa	1624	U
75	aa	1625	U
75	aa	1627	U
75	aa	1628	A
75	aa	1629	A
75	aa	1630	A
75	aa	1631	U
75	aa	1633	U
75	aa	1634	C
75	aa	1639	A
75	aa	1640	U

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Mol	Chain	Res	Type
75	aa	1646	U
75	aa	1647	A
75	aa	1648	C
76	bb	7	G
76	bb	8	U
76	bb	14	A
76	bb	15	G
76	bb	16	U
76	bb	18	G
76	bb	19	G
76	bb	20	U
76	bb	21	A
76	bb	22	G
76	bb	23	A
76	bb	24	G
76	bb	25	C
76	bb	26	A
76	bb	28	A
76	bb	32	C
76	bb	33	U
76	bb	34	C
76	bb	36	U
76	bb	37	A
76	bb	39	U
76	bb	42	U
76	bb	43	G
76	bb	45	G
76	bb	46	G
76	bb	47	U
76	bb	48	C
76	bb	52	G
76	bb	55	U
76	bb	56	C
76	bb	58	A
76	bb	59	A
76	bb	61	C
76	bb	62	C
76	bb	63	C
76	bb	64	G
76	bb	65	U
76	bb	66	C
76	bb	67	G

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Mol	Chain	Res	Type
76	bb	68	U
76	bb	70	G
76	bb	72	C

All (104) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	25	A
1	A	34	U
1	A	44	U
1	A	134	U
1	A	162	U
1	A	164	U
1	A	261	A
1	A	268	C
1	A	311	A
1	A	336	A
1	A	426	A
1	A	429	A
1	A	454	A
1	A	507	A
1	A	529	A
1	A	532	A
1	A	563	U
1	A	614	A
1	A	615	U
1	A	616	A
1	A	617	A
1	A	637	U
1	A	643	U
1	A	655	A
1	A	696	G
1	A	733	A
1	A	746	A
1	A	781	G
1	A	782	G
1	A	840	C
1	A	857	U
1	A	951	A
1	A	1064	A
1	A	1093	A
1	A	1100	A

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Mol	Chain	Res	Type
1	A	1107	U
1	A	1112	A
1	A	1113	A
1	A	1272	U
1	A	1286	A
1	A	1312	G
1	A	1331	A
1	A	1349	A
1	A	1407	A
1	A	1408	U
1	A	1409	C
1	A	1410	U
1	A	1489	U
1	A	1493	U
1	A	1522	A
1	A	1547	U
1	A	1618	G
1	A	1635	G
1	A	1651	A
1	A	1706	G
1	A	1707	C
1	A	1708	A
1	A	1727	A
1	A	1837	A
1	A	1892	G
1	A	2263	U
1	A	2301	C
1	A	2304	A
1	A	2314	U
1	A	2316	A
1	A	2322	U
1	A	2323	A
1	A	2324	U
1	A	2329	A
1	A	2330	A
1	A	2331	U
1	A	2357	U
1	A	2359	U
1	A	2373	U
1	A	2378	A
1	A	2425	A
1	A	2426	A

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Mol	Chain	Res	Type
1	A	2437	U
1	A	2446	U
1	A	2457	G
1	A	2458	G
1	A	2461	A
1	A	2586	U
1	A	2590	U
1	A	2599	A
1	A	2610	A
1	A	2613	A
1	A	2734	A
1	A	2881	A
1	A	2897	A
1	A	2956	U
1	A	3017	U
1	A	3068	U
1	A	3122	U
1	A	3124	A
1	A	3135	U
1	A	3136	U
1	A	3150	U
1	A	3154	U
1	A	3171	A
1	A	3177	A
1	A	3234	A
1	A	3252	U
1	A	3268	A

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 303 ligands modelled in this entry, 302 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$
82	GDP	WW	501	79	24,30,30	1.22	2 (8%)	26,47,47	1.89	6 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	GDP	WW	501	79	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	WW	501	GDP	C5-C4	3.36	1.48	1.40
82	WW	501	GDP	C6-C5	3.75	1.48	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
82	WW	501	GDP	C5-C6-N1	-3.94	118.37	123.52
82	WW	501	GDP	N3-C2-N1	-3.44	122.88	127.56
82	WW	501	GDP	C4'-O4'-C1'	-2.76	106.72	109.64
82	WW	501	GDP	C6-C5-C4	-2.72	117.75	120.86
82	WW	501	GDP	O4'-C1'-N9	3.39	114.51	108.11
82	WW	501	GDP	C6-N1-C2	5.20	121.97	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	WW	501	GDP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
75	aa	13
78	dd	7
77	cc	3
64	XX	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	dd	115:UNK	C	151:UNK	N	40.49
1	dd	220:UNK	C	265:UNK	N	35.53
1	dd	170:UNK	C	202:UNK	N	27.03
1	cc	59:UNK	C	76:UNK	N	22.66
1	cc	93:UNK	C	105:UNK	N	20.49
1	dd	66:UNK	C	71:UNK	N	15.23
1	dd	89:UNK	C	95:UNK	N	14.85
1	cc	37:UNK	C	40:UNK	N	10.31
1	dd	42:UNK	C	45:UNK	N	10.16
1	aa	194:A	O3'	195:U	P	6.91
1	dd	20:UNK	C	23:UNK	N	6.25
1	XX	59:LEU	C	60:LYS	N	6.10
1	XX	58:HIS	C	59:LEU	N	5.25
1	aa	195:U	O3'	196:A	P	3.64
1	aa	518:U	O3'	519:A	P	3.46
1	aa	193:A	O3'	194:A	P	3.40
1	aa	558:A	O3'	559:U	P	3.37
1	aa	260:U	O3'	261:U	P	3.36
1	aa	996:A	O3'	997:G	P	3.35
1	aa	1083:A	O3'	1084:U	P	3.23
1	aa	751:U	O3'	752:A	P	3.20
1	aa	958:C	O3'	959:G	P	3.13
1	aa	1296:A	O3'	1297:A	P	3.10
1	aa	1182:U	O3'	1183:A	P	2.89
1	aa	1268:A	O3'	1269:U	P	2.71