



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

Jan 23, 2017 – 05:00 PM EST

PDB ID : 3JCT  
EMDB ID: : EMD-6615  
Title : Cryo-em structure of eukaryotic pre-60S ribosomal subunits  
Authors : Wu, S.; Kumcuoglu, B.; Yan, K.G.; Brown, H.; Zhang, Y.X.; Tan, D.; Gamalinda, M.; Yuan, Y.; Li, Z.F.; Jakovljevic, J.; Ma, C.Y.; Lei, J.L.; Dong, M.Q.; Woolford Jr., J.L.; Gao, N.  
Deposited on : 2016-03-09  
Resolution : 3.08 Å(reported)  
Based on PDB ID : 4V88

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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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

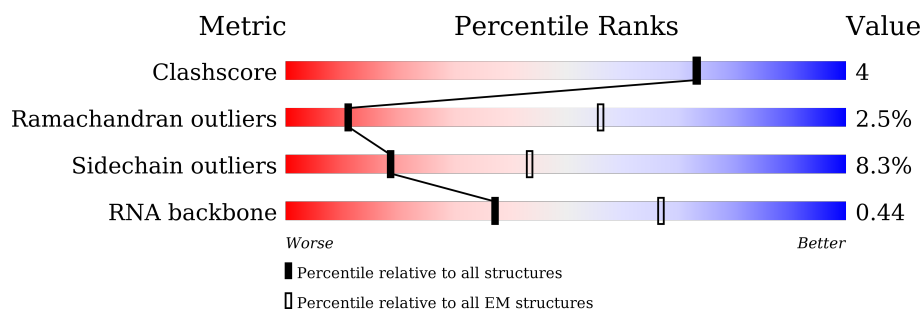
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.08 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.









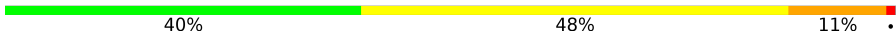




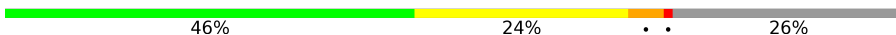




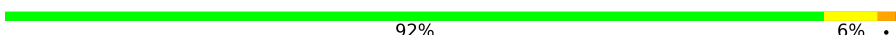








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	254	
2	B	387	
3	C	362	
4	D	297	
5	E	176	
6	F	244	
7	G	256	
8	H	191	









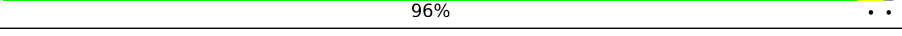

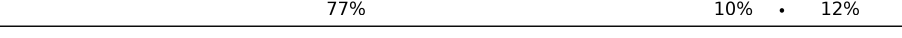
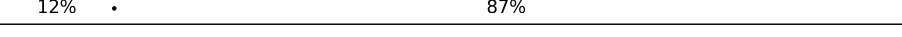

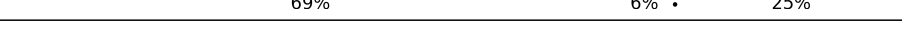


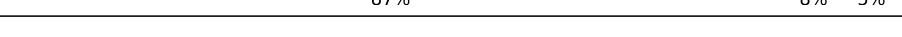

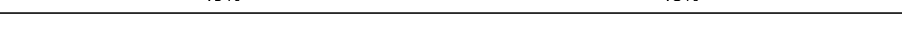






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Mol	Chain	Length	Quality of chain
9	I	166	
10	J	174	
11	K	376	
12	L	199	
13	M	138	
14	N	204	
15	O	199	
16	P	184	
17	Q	186	
18	R	189	
19	S	172	
20	T	160	
21	U	121	
22	V	137	
23	W	236	
24	X	142	
25	Y	127	
26	Z	136	
27	a	149	
28	b	647	
29	c	105	
30	d	113	
31	e	130	
32	f	107	
33	g	121	

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Mol	Chain	Length	Quality of chain
34	h	120	
35	i	100	
36	j	88	
37	k	78	
38	l	51	
39	m	486	
40	n	605	
41	o	220	
42	p	92	
43	q	455	
44	r	261	
45	s	520	
46	t	322	
47	u	199	
48	v	344	
49	w	203	
50	x	515	
51	y	245	
52	z	106	
53	1	3396	
54	2	158	
55	3	121	
56	4	593	
57	5	120	
58	6	232	

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 156562 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	213	Total	C	N	O	S	0	0
			1634	1023	326	284	1		

- Molecule 2 is a protein called 60S ribosomal protein L3.

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

- Molecule 3 is a protein called 60S ribosomal protein L4-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	276	Total	C	N	O	S	0	0
			2211	1397	391	421	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 6 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 7 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 8 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 9 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	131	Total	C	N	O	S	0	0
			1059	662	195	198	4		

- Molecule 10 is a protein called 60S ribosomal protein L11-A.

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

- Molecule 11 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	256	Total	C	N	O	S	0	0
			2064	1332	342	387	3		

- Molecule 12 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	187	Total	C	N	O	0	0
			1499	934	307	258		

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 14 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 15 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L17-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	134	Total	C	N	O	S	0	0
			1035	659	196	179	1		

- Molecule 18 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	156	Total	C	N	O	S	0	0
			1258	781	265	212			

- Molecule 19 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 20 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	119	Total	C	N	O	S	0	0
			943	595	180	165	3		

- Molecule 21 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	106	Total	C	N	O	0	0
			844	545	138	161		

- Molecule 22 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 23 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	234	Total	C	N	O	S	0	0
			1885	1194	323	362	6		

- Molecule 24 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	141	Total	C	N	O	S	0	0
			1100	705	196	197	2		

- Molecule 25 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 27 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	93	Total	C	N	O	S	0	0
			735	479	130	125	1		

- Molecule 28 is a protein called Nucleolar GTP-binding protein 1.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	642	Total	C	N	O	S	0	0
			5185	3251	938	970	26		

- Molecule 29 is a protein called 60S ribosomal protein L30.

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

- Molecule 30 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 31 is a protein called 60S ribosomal protein L32.

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

- Molecule 32 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 33 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 34 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L38.

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

- Molecule 38 is a protein called 60S ribosomal protein L39.

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

- Molecule 39 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	469	Total	C	N	O	S	0	0
			3774	2381	685	699	9		

- Molecule 40 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	371	Total	C	N	O	S	0	0
			3030	1963	523	534	10		

- Molecule 41 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 42 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 43 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	183	Total	C	N	O	S	0	0
			1514	957	268	288	1		

- Molecule 44 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 45 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	69	Total	C	N	O	S	0	0
			573	359	113	98	3		

- Molecule 46 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	t	287	Total	C	N	O	S	0	0
			2306	1459	427	417	3		

- Molecule 47 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 48 is a protein called Ribosome biogenesis protein RPF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	287	Total	C	N	O	S	0	0
			2318	1482	408	412	16		

- Molecule 49 is a protein called Regulator of ribosome biosynthesis.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	w	182	Total	C	N	O	S	0	0
			1448	911	261	271	5		

- Molecule 50 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	x	488	Total	C	N	O	S	0	0
			3807	2398	677	711	21		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

- Molecule 52 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	z	55	Total	C	N	O		
			444	273	88	83	0	0

- Molecule 53 is a RNA chain called RDN25-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	3058	Total	C	N	O	P	0	0
			65427	29223	11807	21339	3058		

- Molecule 54 is a RNA chain called RDN58-1 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 55 is a RNA chain called RDN5-2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 56 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	516	Total	C	N	O	S	0	0
			3999	2530	688	766	15		

- Molecule 57 is a protein called rRNA-processing protein CGR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	73	Total	C	N	O	S	0	0
			645	395	133	114	3		

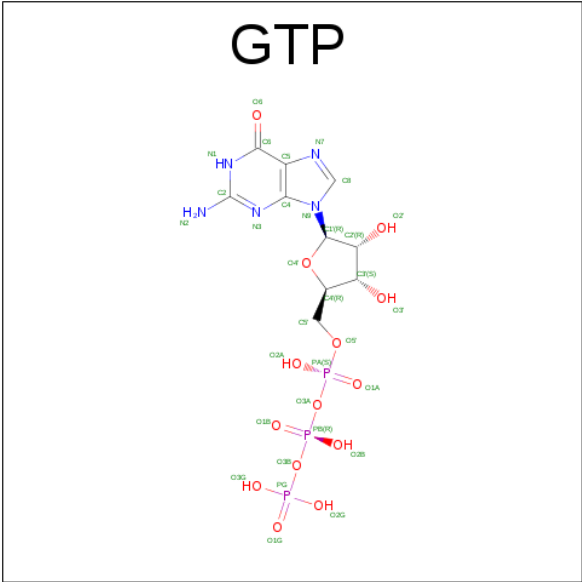
- Molecule 58 is a RNA chain called ITS2-1 miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	65	Total	C	N	O	P	0	0
			1370	614	228	463	65		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	p	1	Total	Zn	0
			1	1	
59	j	1	Total	Zn	0
			1	1	
59	I	1	Total	Zn	0
			1	1	
59	u	1	Total	Zn	0
			1	1	

- Molecule 60 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
60	b	1	Total	C	N	O	P	0
			32	10	5	14	3	
60	m	1	Total	C	N	O	P	0
			32	10	5	14	3	

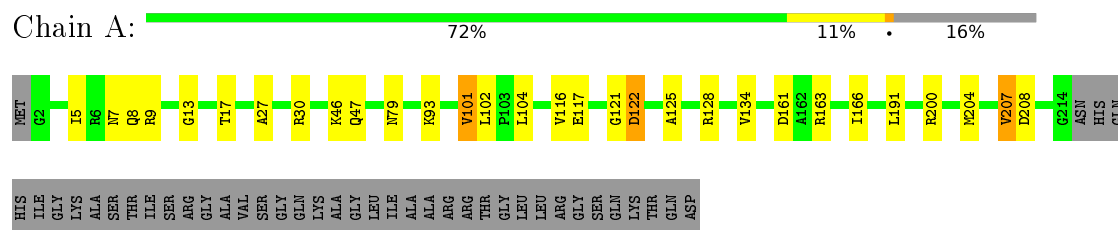
- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
61	b	1	Total	Mg	0
			1	1	
61	m	1	Total	Mg	0
			1	1	

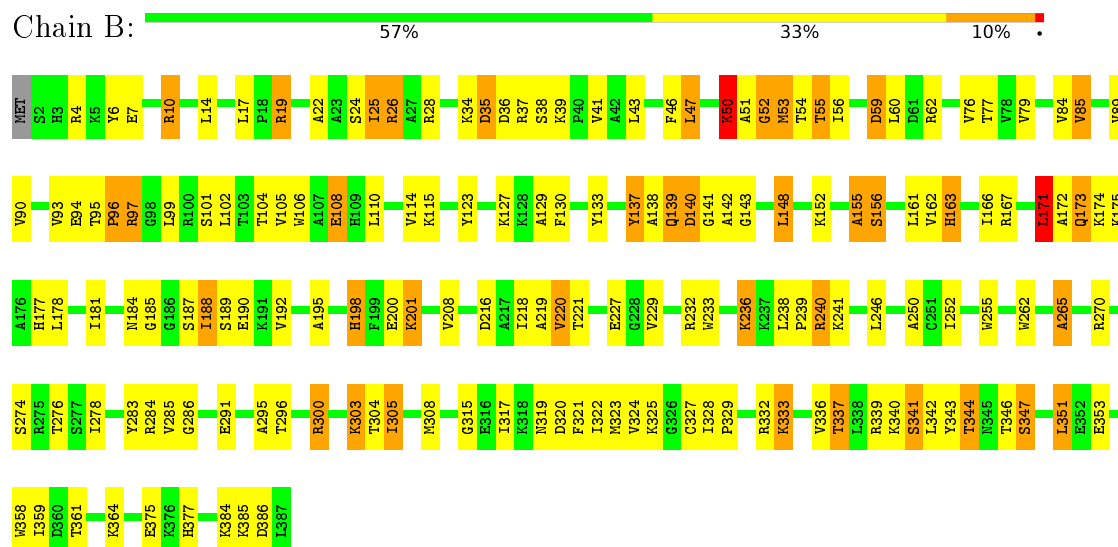
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

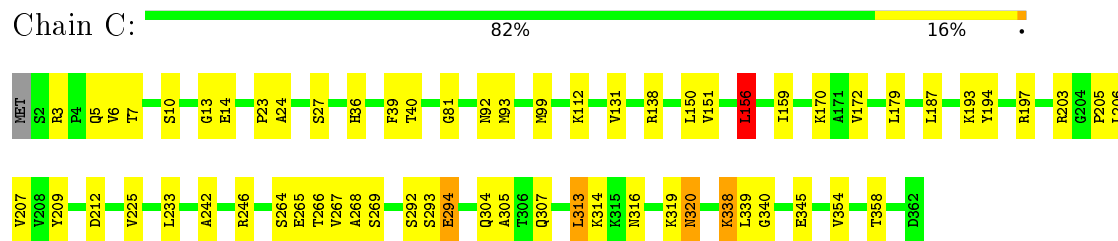
- Molecule 1: 60S ribosomal protein L2-A



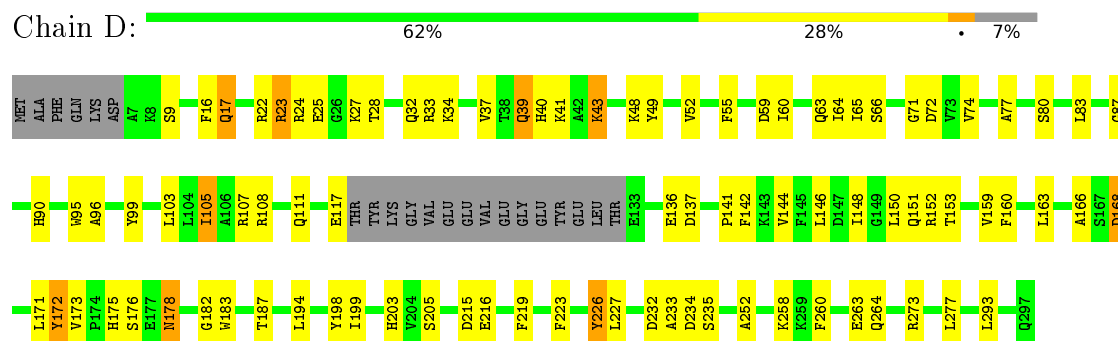
- Molecule 2: 60S ribosomal protein L3



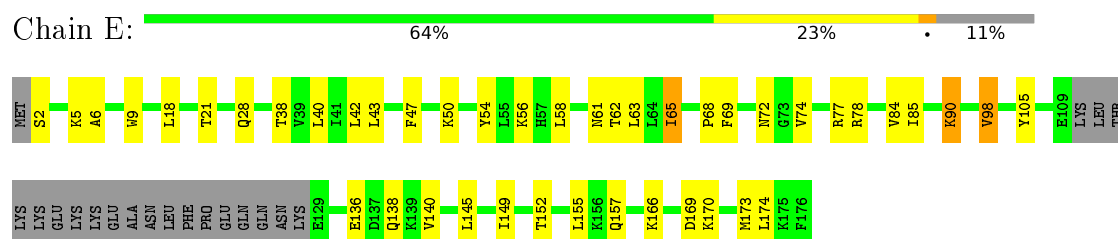
- Molecule 3: 60S ribosomal protein L4-A



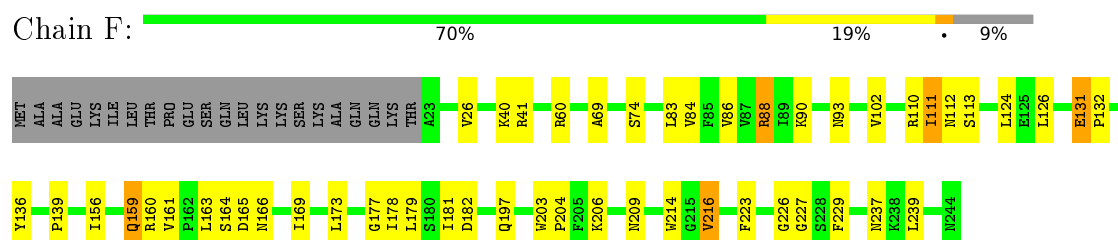
- Molecule 4: 60S ribosomal protein L5



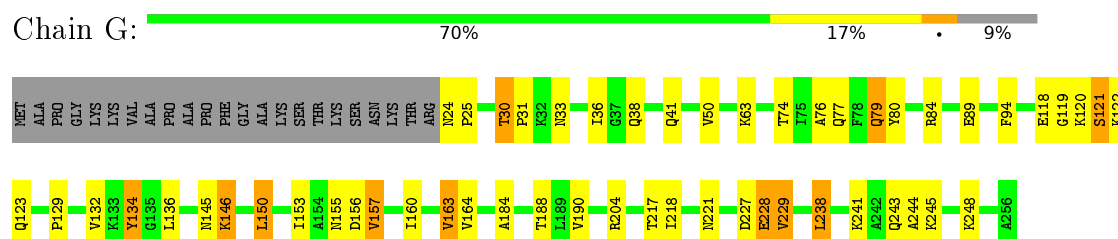
• Molecule 5: 60S ribosomal protein L6-A



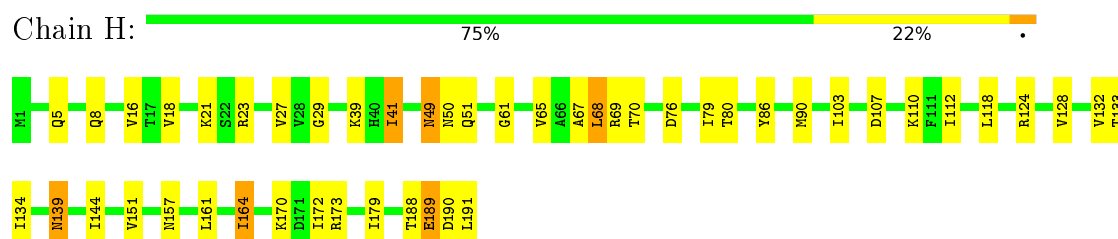
• Molecule 6: 60S ribosomal protein L7-A



• Molecule 7: 60S ribosomal protein L8-A

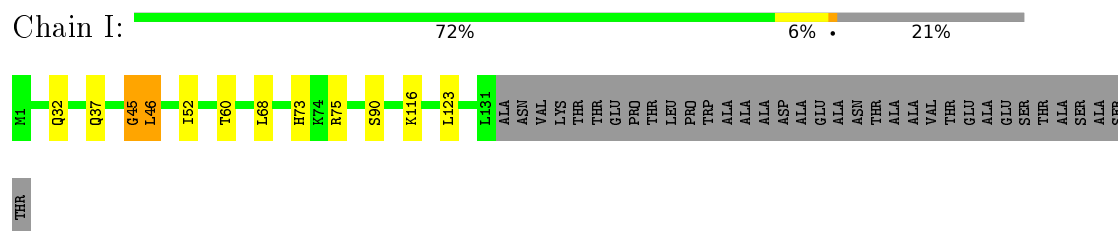


• Molecule 8: 60S ribosomal protein L9-A

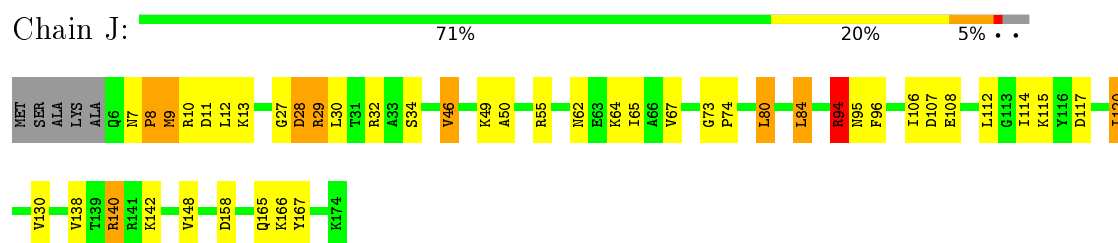




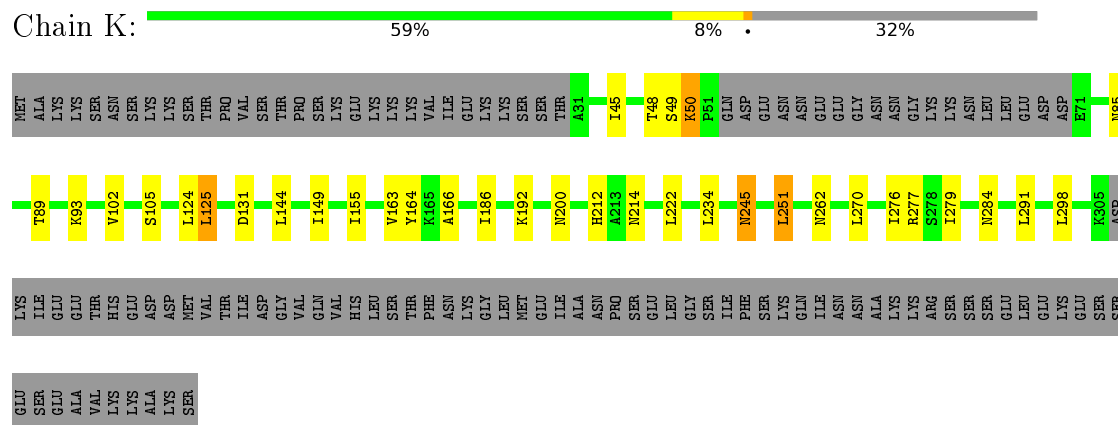
- Molecule 9: Bud site selection protein 20



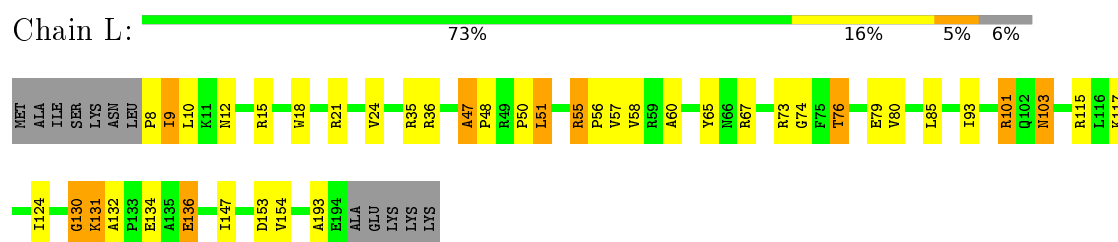
- Molecule 10: 60S ribosomal protein L11-A



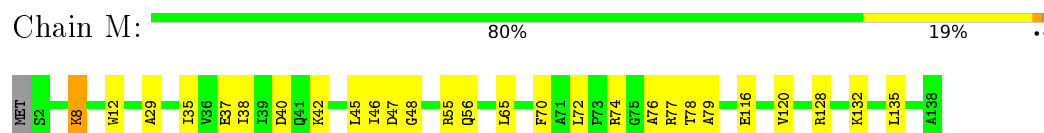
- Molecule 11: Proteasome-interacting protein CIC1



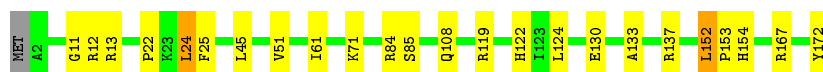
- Molecule 12: 60S ribosomal protein L13-A



- Molecule 13: 60S ribosomal protein L14-A

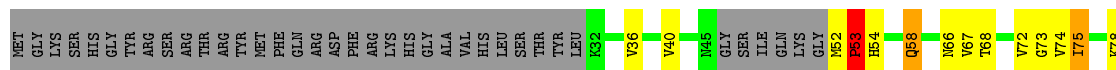


- Chain S:  85% 13% .



- Molecule 20: 60S ribosomal protein L21-A

Chain T: 46% 24% 26%



- Molecule 21: 60S ribosomal protein L22-A

Chain U: 82% 6% 12%



- Molecule 22: 60S ribosomal protein L23-A

Chain V: 88% 10% 2%



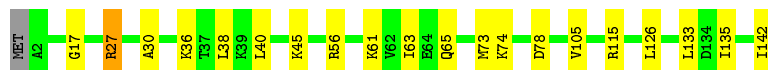
- Molecule 23: Ribosome assembly factor MRT4

Chain W: 87% 11% 2%



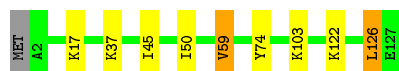
- Molecule 24: 60S ribosomal protein L25

Chain X: 85% 13% 2%



- Molecule 25: 60S ribosomal protein L26-A

Chain Y: 92% 6% 2%



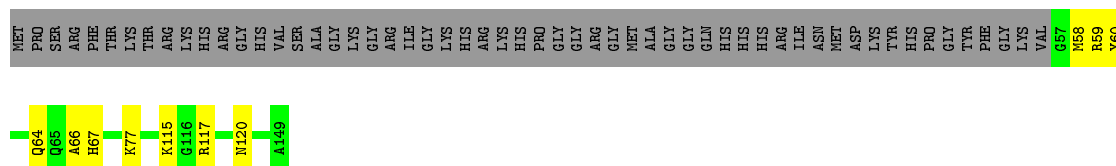
- Molecule 26: 60S ribosomal protein L27-A

Chain Z: 85% 14% 1%



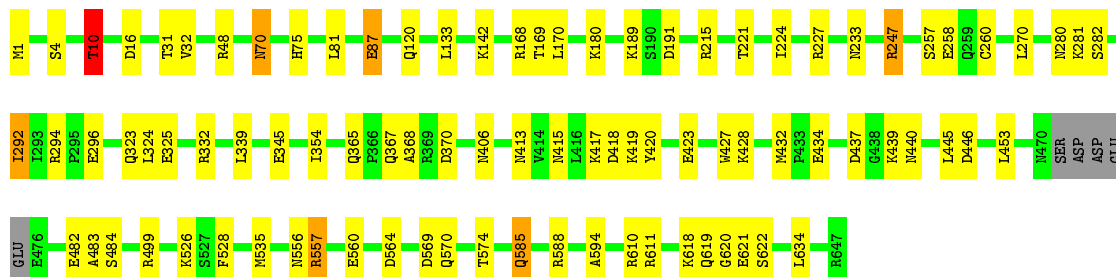
- Molecule 27: 60S ribosomal protein L28

Chain a: 56% 7% 38%



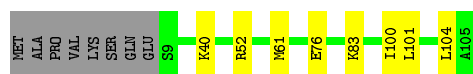
- Molecule 28: Nucleolar GTP-binding protein 1

Chain b: 85% 13% ..



- Molecule 29: 60S ribosomal protein L30

Chain c: 85% 8% 8%



- Molecule 30: 60S ribosomal protein L31-A

Chain d: 83% 11% 5%



- Molecule 31: 60S ribosomal protein L32

Chain e: 92% 6% .



- Molecule 32: 60S ribosomal protein L33-A

Chain f: 93% 5% ..



- Molecule 33: 60S ribosomal protein L34-A

Chain g: 87% 6% 7%



- Molecule 34: 60S ribosomal protein L35-A

Chain h: 88% 11% ..



- Molecule 35: 60S ribosomal protein L36-A

Chain i: 90% 8% ..



- Molecule 36: 60S ribosomal protein L37-A

Chain j: 91% 8% .



- Molecule 37: 60S ribosomal protein L38

Chain k: 92% 6% .



- Molecule 38: 60S ribosomal protein L39

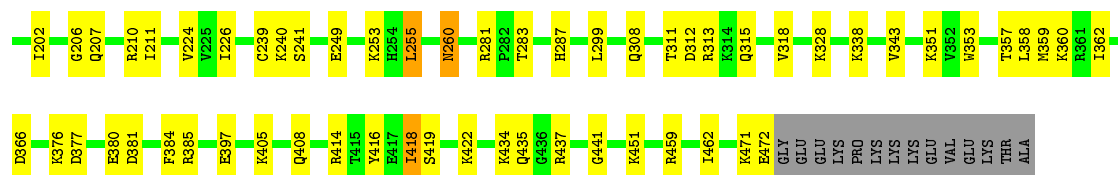
Chain l: 82% 16% .



- Molecule 39: Nucleolar GTP-binding protein 2

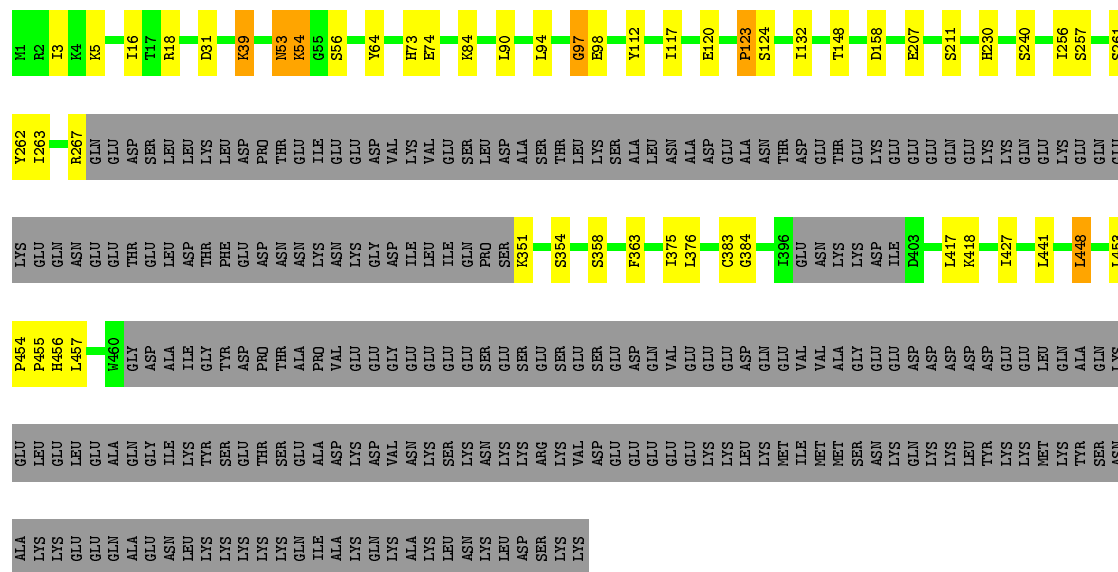
Chain m: 78% 17% ..





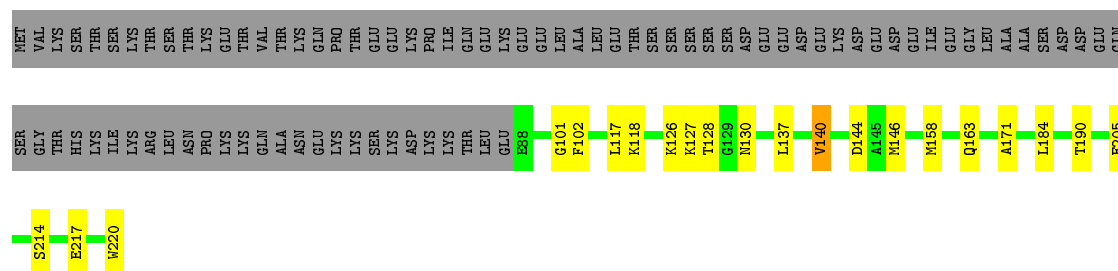
• Molecule 40: Pescadillo homolog

Chain n: 53% 8% 39%



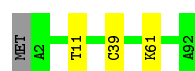
• Molecule 41: Ribosome biogenesis protein 15

Chain o: 51% 9% 40%



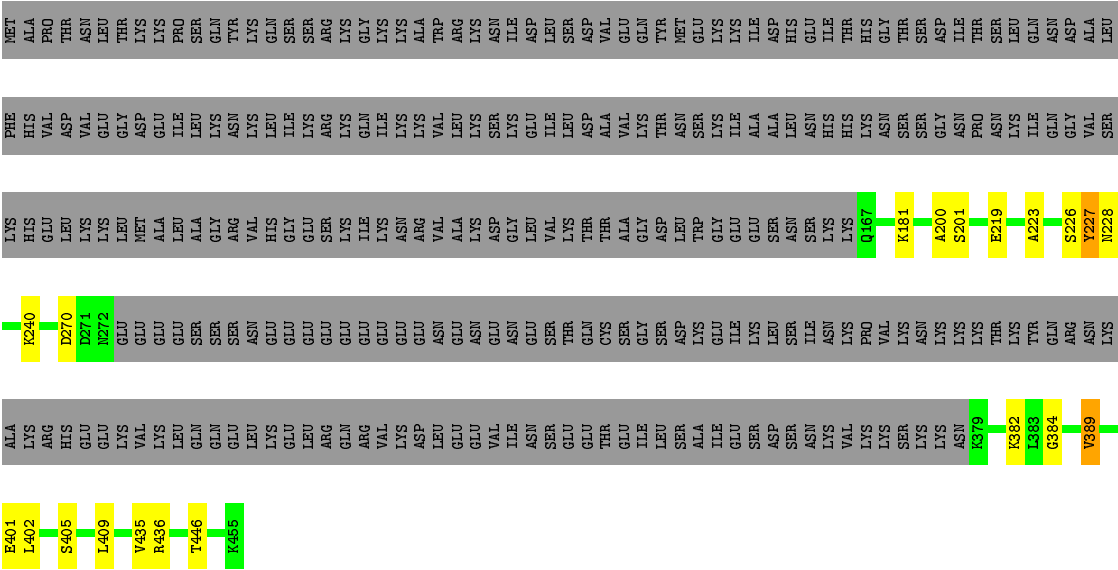
• Molecule 42: 60S ribosomal protein L43-A

Chain p: 96%

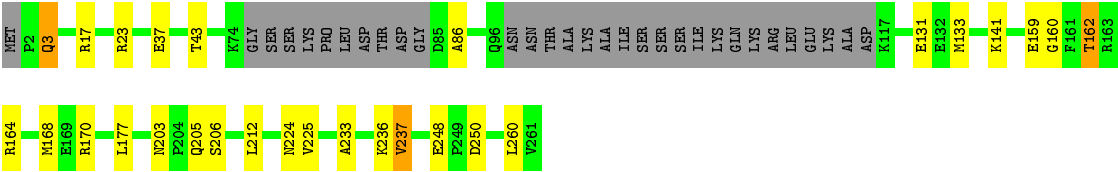


• Molecule 43: Ribosome biogenesis protein NOP53

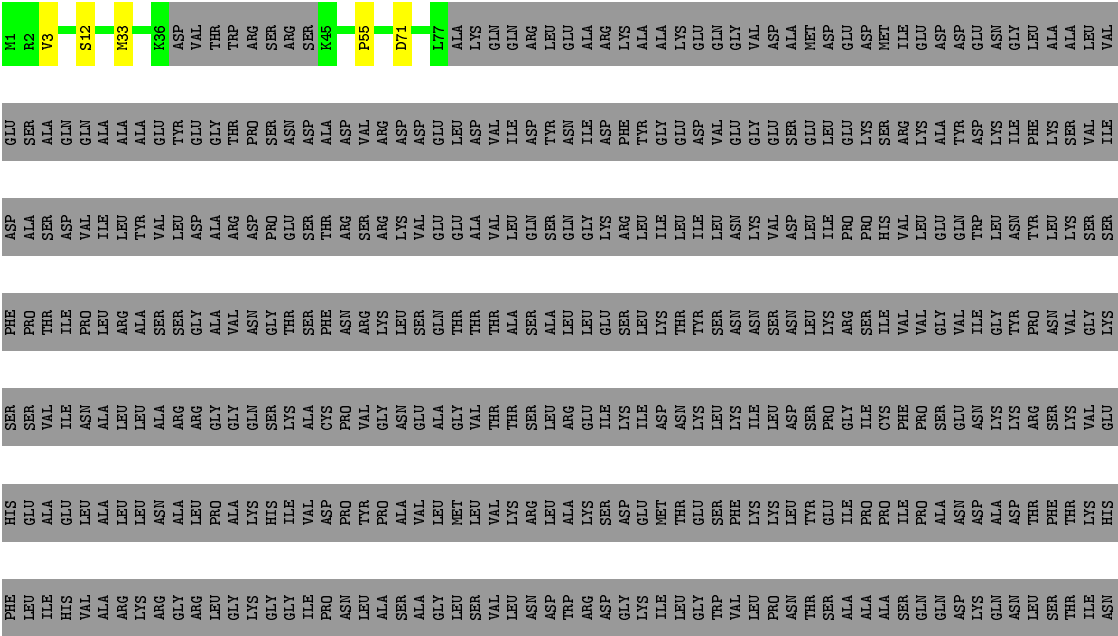
Chain q: 36% 60%



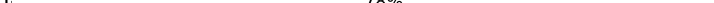
• Molecule 44: Ribosome biogenesis protein NSA2

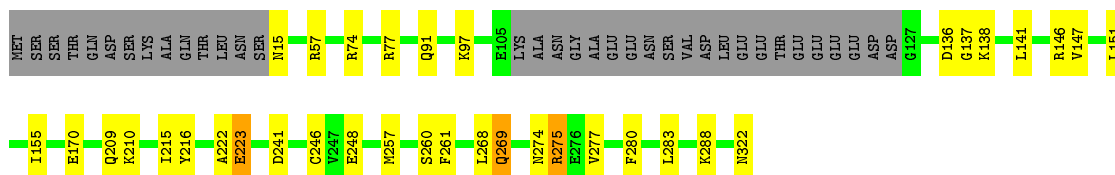


• Molecule 45: Nuclear GTP-binding protein NUG1



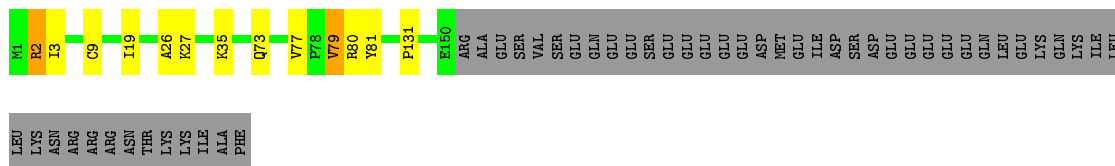
- Molecule 46: Ribosome biogenesis protein RLP7

Chain t:  78% 10% 11%

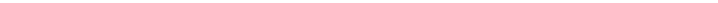


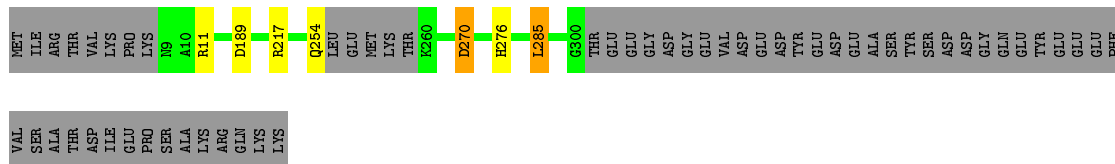
- Molecule 47: Ribosome biogenesis protein RLP24

Chain u:  69% 6% • 25%



- Molecule 48: Ribosome biogenesis protein RPF2

Chain v:  81% .. 17%



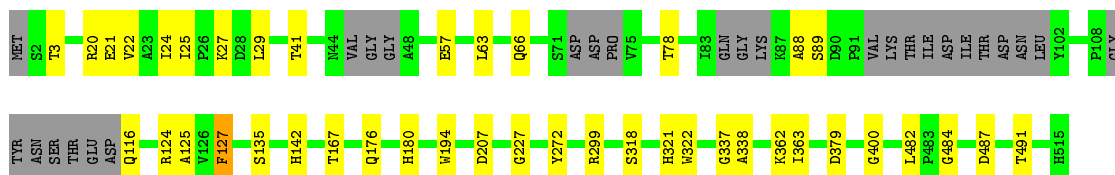
- Molecule 49: Regulator of ribosome biosynthesis

Chain w:  81% 7% • 10%



- Molecule 50: Ribosome assembly protein 4

Chain x:  87% 8% 5%



- Molecule 51: Eukaryotic translation initiation factor 6

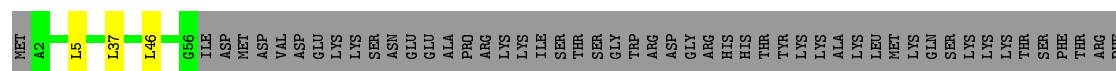


Chain y:  92% 8%



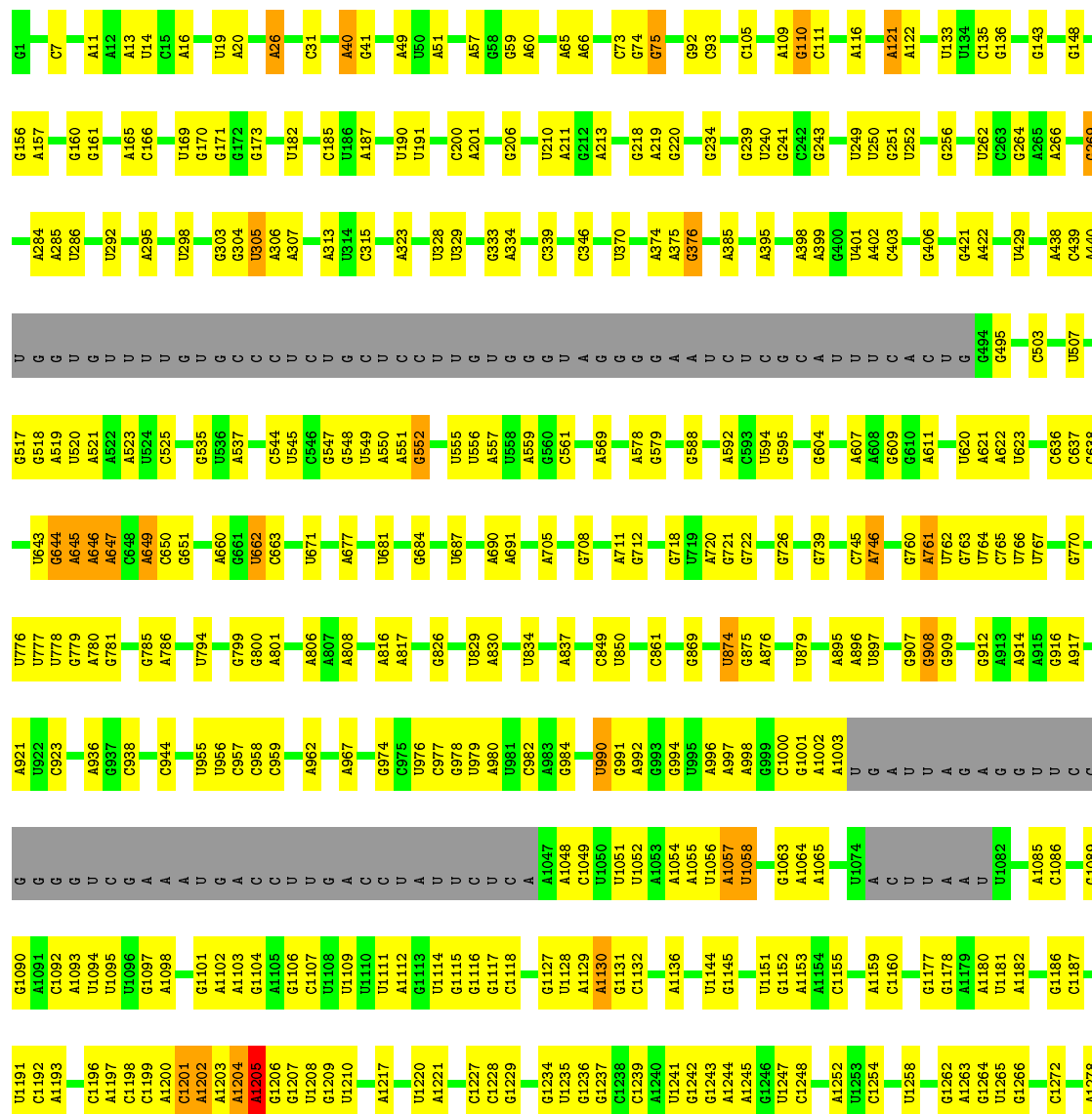
• Molecule 52: UPF0642 protein YBL028C

Chain z:  49% 48%

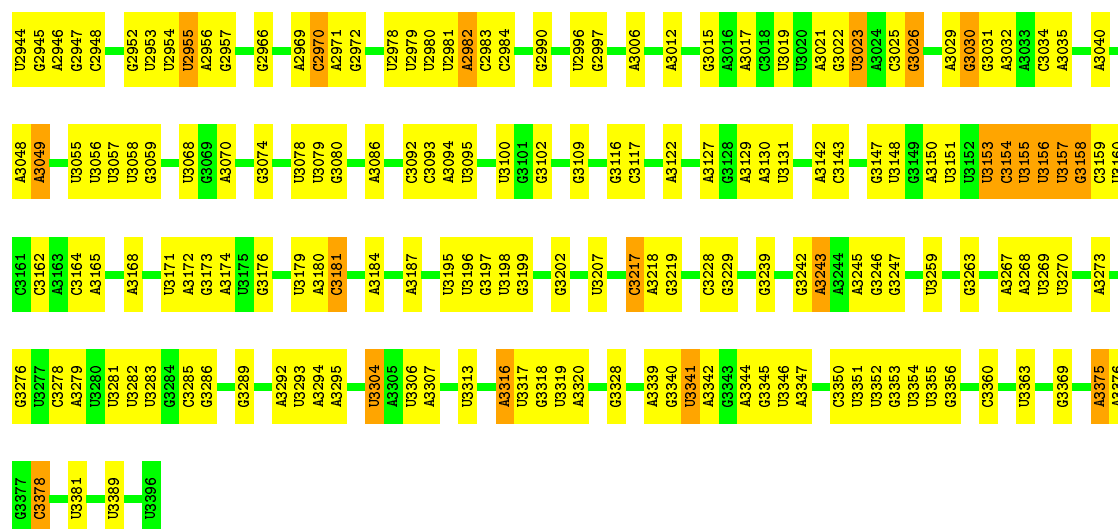


• Molecule 53: RDN25-1 rRNA

Chain 1:  59% 27% 10%

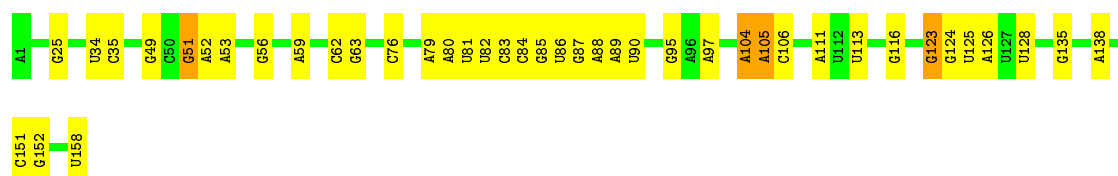


U2846	C2764	U2688	C2583	A2502	C2437	C	C2245	U2137	G	C1866	G1718	A1566	C1420	C1279
A2847	C2765	A2689	C2586	G2503	C2444	A	G2246	U2140	G	A1867	U1721	U1567	G1421	C1280
G2848	U2766	G2690	G2586	U2504	A2445	U	C2247	U2141	A	U1568	U1725	U1568	G1434	G1281
C2857	U2767	A2691	G2586	U2505		A	C2248	A2142	G	U1569	C1725	U1570	U1435	G1282
U2858	A2768	C2693	A2593	C2506	A	A2313	G2249	A2143	G	A1571		U1571	C1436	C1283
U2859	G2770	G2694	C2594	U2507	G	G2316	G2250	A2144	U	U1572		U1572	C1437	A1286
U2860	U2771	A2695	A2595	U2508	A	A2317	A2252	A2145	C	U1573	A1741	C1573	G1443	A1287
U2861	C2772	G2696	U2596	U2509	G	U2318	A2255	C2146	A	C1574		C1574	G1443	C1296
U2862	C2773	A2697	U2597	C2510	G	G2319	A2256	G2150	G	A1575	U1746	A1575	G1447	
U2863	C2774	G2698	C2598	C2512	G	U2318	G2257	G2151	G	G1576		G1576	G1447	U1299
A2864		G2699	U2599	U2513	U	A2332	U2258	A2158	U	G1577		U1577	G1450	
U2865	G2777	U2701	C2600	U2514	G	C2333	A2259		G	A1580		A1580		A1302
U2866	G2778	U2702	A2601	A2515	U	U2334	A2260		G	C1581		C1581	A1460	A1303
C2867	A2779	A2703	G2602		A	G2335	U2261	C2163	U	A1582		A1582	A1304	A1304
U2868		A2704	G2607		A	U2336	A2262	A2164	G	A1583		A1583	A1467	
G2870	A2785	G2705	G2607	G2522	A	C2337	A2263	G2169	U	U1587		U1587	U1471	G1307
G2871	G2786	U2706	G2607	A2524	U	C2338	U2264	U2170	A	U1588		U1588		A1308
G2872	G2787	C2707	G2614	G2525	A	G2370	U2268		G	U1589		U1589	A1481	G1313
U2873	U2788	U2712	G2615	C2526	A	A2371	U2269	G2177	A	A1593		A1593	U1322	U1322
G2874	U2789	U2713	C	G2528	G	A	A2270	U2184	C	G1765		U1765	A1482	
U2875	G2790	G2714	U	A2529	U	A	A2271	G2185	C	G1766		A1593	G1483	
G2876	A2791	A2715	G	G2530	G	G	A2272		U	G1770		U1606	U1484	
G2877	G2792	U2716	G2619	C2531	G	G2376	G2272	U2190	U	G1775		U1607	G1485	U1329
G2878	G2794	U2717	G2620	U2532	G		G2273	U2191	C			C1608	G1487	A1330
C2879	U2795	U2718	C2621	G2534	A	G2385	U2274	C2192	G	G			A1490	A1332
	G2796	U2719	G2622		G	A2275	G2276	U2193	U	G				
A2887	C2797	G2720	G2623		C	U2388	C2277	U2194	U	G1794		A1621	C1502	U1348
U2888	G2798	A2721	G2624	U2538	U	G	C2278	C2195	G	U1795		U1622	A1503	G1349
C2889	A2799	U2722	C2625	C2539	U	G2389	A2279	C2196	C	G1796				A1360
U2890	G2800	U2723	A2626	U2540	C			C2197	U			U1629	U1351	
U2891	A2801	U2724		A2541	G	A2397	A2280	A2198	A	U1797		U1630	C1508	U1352
	A2802	U2725	G2645	U2542	G	A2398			C	A1810		C1631	U1523	U1353
G2898	A2803	C2726	U2650	U2543	C	A2399		G2201	A			A1632	A1524	G1354
C2899	A2804	G2727	G2651	U2544	G	G2400		U2205	A	A1813		C1639	U1525	A1355
G2900		G2728	G2652	C2545	C	A2401		G2206	U	A1814		G1640	U1526	U1356
A2902		U2729	U2653		C	A2402		A2207	U	U1815		A1642	C1527	G1357
	G2810	U2730	C2654	C2546	G			U2208	A	A1817		A1643		G1362
	G2814	U2731	U2655	A2547	U	C2405		G2210	C	U1820		C1644	C1532	G1367
G2918	G2815	G2732	U2656	C2548	G			U2211	U	U1821		U1645	U1533	
	G2816		A2657	G2549	A	U2410			A	C1822				G1380
U2921	U2817	A2740	G2658		A	G2412		U2226	C			C1657	G1536	A1381
G2922	U2818	A2747	G2659	U2552	A	A2413		C2227	C	U1837		G1658		G1382
U2923	A2819	U2748		A2554	U	G2414		A2228	C	G1838			A1539	G1383
U2924	C2820	G2749	G2663	G2555	A				U	A1839		G1662	U1549	A1386
C2925	U2822				C	G2415		A2229	U	U1840			U1549	G1387
A2926	U2823	U2752	A2667	A2561	C	U2418			G					
C2927	G2824	G2753			A	A2419		C2235	U	A1841		C1671	U1554	
C2928	C2825	G2754	A2674	C2568	C	U2427		G2236	U	A1842			U1555	A1399
C2929	U2826	C2755	G2677	A2569	U	U2428		C2237	G				C1556	G1400
	C2836	U2756		U2570	A	G2429		G2238	U	A1683			A1557	
U2935		U2757	A2680	C2571	C	U2430		G2239	U	C1846				
A2936	G2840	U2758	U2681	G2572	C	C2431		G2240	A	U1701			G1404	
	G2841	U2759	U2681	C2573	U	A2432		U2241	C	U1703			G1560	
U2940	G2842	C2760	C2685	G2574	U	A2433		A2242	A				G1561	
		G2761	A2686	G2575	U	G2435		A2243	C	U1716			C1562	G1414
C		A2762			A			A2131	G	A1858				
G2943	G2845	U2763	G2687	U2578	G	U2436		A2244	G	A1859				A1419



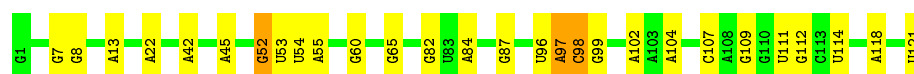
• Molecule 54: RDN58-1 rRNA

Chain 2: 73% 24%



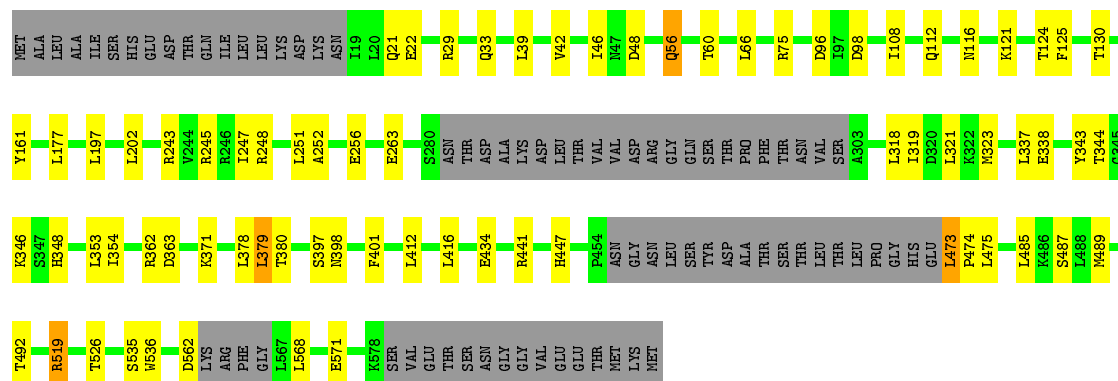
• Molecule 55: RDN5-2 rRNA

Chain 3: 77% 21%



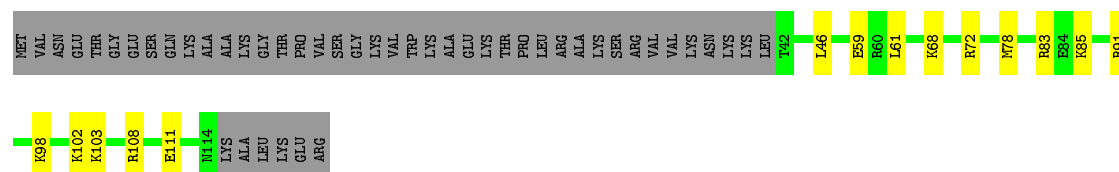
• Molecule 56: Probable metalloprotease ARX1

Chain 4: 75% 12% 13%



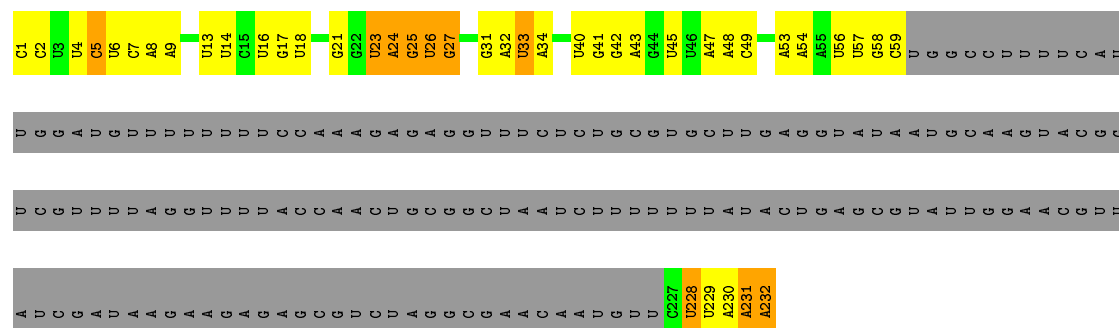
• Molecule 57: rRNA-processing protein CGR1

Chain 5:  49% 12% 39%



- Molecule 58: ITS2-1 miscRNA

Chain 6:  10% 14% • 72%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	191848	Depositor
Resolution determination method	Not provided	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	Gatan k2 summit	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 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	0.37	0/1666	0.66	0/2241
10	J	0.42	0/1374	0.68	0/1842
11	K	0.38	0/2098	0.49	0/2830
12	L	0.38	0/1524	0.71	1/2046 (0.0%)
13	M	0.33	0/1074	0.58	0/1446
14	N	0.38	0/1757	0.70	0/2354
15	O	0.34	0/1585	0.44	0/2128
16	P	0.35	0/1465	0.63	0/1968
17	Q	0.35	0/1050	0.57	0/1419
18	R	0.34	0/1275	0.60	0/1702
19	S	0.35	0/1473	0.57	0/1980
2	B	0.41	0/3152	0.71	1/4239 (0.0%)
20	T	0.37	0/957	0.63	0/1285
21	U	0.36	0/861	0.49	0/1167
22	V	0.34	0/1018	0.55	0/1369
23	W	0.37	0/1918	0.53	0/2586
24	X	0.34	0/1116	0.54	0/1503
25	Y	0.33	0/1004	0.56	1/1341 (0.1%)
26	Z	0.35	0/1118	0.54	0/1497
27	a	0.36	0/751	0.57	0/1013
28	b	0.38	0/5270	0.59	0/7080
29	c	0.35	0/751	0.52	0/1008
3	C	0.37	0/2801	0.62	0/3792
30	d	0.32	0/887	0.53	0/1191
31	e	0.34	0/1041	0.58	0/1394
32	f	0.35	0/868	0.60	0/1168
33	g	0.34	0/891	0.61	0/1191
34	h	0.34	0/978	0.57	0/1301
35	i	0.37	0/778	0.58	0/1034
36	j	0.39	0/696	0.69	1/923 (0.1%)
37	k	0.36	0/618	0.53	0/826
38	l	0.36	0/443	0.69	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  > 2	RMSZ	# Z  > 2
39	m	0.40	1/3848 (0.0%)	0.59	0/5181
4	D	0.39	0/2257	0.63	0/3043
40	n	0.39	0/3101	0.56	0/4187
41	o	0.38	0/1129	0.54	0/1502
42	p	0.35	0/701	0.60	0/934
43	q	0.38	0/1539	0.54	0/2059
44	r	0.38	0/1892	0.62	0/2528
45	s	0.35	0/577	0.53	0/752
46	t	0.40	1/2333 (0.0%)	0.54	0/3128
47	u	0.38	0/1287	0.62	0/1711
48	v	0.35	0/2361	0.47	0/3153
49	w	0.35	0/1471	0.52	0/1980
5	E	0.36	0/1260	0.61	0/1694
50	x	0.35	0/3897	0.50	0/5282
51	y	0.35	0/1872	0.57	1/2548 (0.0%)
52	z	0.39	0/445	0.63	0/585
53	1	0.23	0/73234	0.70	12/114167 (0.0%)
54	2	0.23	0/3746	0.69	1/5832 (0.0%)
55	3	0.20	0/2883	0.65	1/4491 (0.0%)
56	4	0.37	0/4069	0.52	0/5520
57	5	0.39	0/649	0.59	0/848
58	6	0.26	0/1527	0.77	0/2371
6	F	0.37	0/1821	0.60	0/2451
7	G	0.37	0/1849	0.60	0/2495
8	H	0.35	0/1539	0.61	0/2073
9	I	0.37	0/1075	0.52	0/1443
All	All	0.31	2/166620 (0.0%)	0.65	19/241410 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	3
11	K	0	3
13	M	0	1
18	R	0	1
19	S	0	6
2	B	0	10
20	T	0	2
21	U	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
22	V	0	2
23	W	0	3
24	X	0	2
26	Z	0	2
28	b	0	18
3	C	0	1
30	d	0	3
31	e	0	1
32	f	0	1
33	g	0	1
34	h	0	2
36	j	0	1
37	k	0	2
38	l	0	1
39	m	0	16
4	D	0	3
40	n	0	18
41	o	0	4
43	q	0	8
44	r	0	6
46	t	0	7
47	u	0	3
49	w	0	9
50	x	0	8
51	y	0	3
56	4	0	11
6	F	0	1
7	G	0	4
9	I	0	1
All	All	0	169

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	m	182	GLY	C-O	7.46	1.35	1.23
46	t	322	ASN	C-O	6.18	1.35	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1	1307	G	C2'-C3'-O3'	7.51	126.02	109.50
53	1	649	A	C2'-C3'-O3'	7.47	125.94	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	1	2900	A	C2'-C3'-O3'	7.35	125.67	109.50
53	1	3030	G	C2'-C3'-O3'	6.33	123.82	113.70
53	1	3341	U	C2'-C3'-O3'	6.30	123.78	113.70
53	1	1816	A	C2'-C3'-O3'	6.17	123.57	113.70
53	1	305	U	C2'-C3'-O3'	5.60	122.67	113.70
54	2	123	G	C2'-C3'-O3'	5.54	122.57	113.70
2	B	139	GLN	C-N-CA	-5.54	107.86	121.70
53	1	990	U	C2'-C3'-O3'	5.52	122.53	113.70
36	j	45	ARG	NE-CZ-NH1	5.40	123.00	120.30
53	1	3316	A	C2'-C3'-O3'	5.34	122.24	113.70
53	1	1302	A	C2'-C3'-O3'	5.32	122.21	113.70
55	3	52	G	C2'-C3'-O3'	5.25	122.09	113.70
51	y	90	ASP	CB-CG-OD2	5.20	122.98	118.30
53	1	1205	A	C2'-C3'-O3'	5.17	121.97	113.70
53	1	761	A	C2'-C3'-O3'	5.16	121.95	113.70
12	L	101	ARG	NE-CZ-NH1	5.16	122.88	120.30
25	Y	126	LEU	CA-CB-CG	5.14	127.11	115.30

There are no chirality outliers.

All (169) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	4	116	ASN	Peptide
56	4	252	ALA	Peptide
56	4	348	HIS	Peptide
56	4	362	ARG	Peptide
56	4	371	LYS	Peptide
56	4	379	LEU	Peptide
56	4	397	SER	Peptide
56	4	473	LEU	Peptide
56	4	526	THR	Peptide
56	4	535	SER	Peptide
56	4	56	GLN	Peptide
2	B	156	SER	Peptide
2	B	220	VAL	Peptide
2	B	315	GLY	Peptide
2	B	340	LYS	Peptide
2	B	346	THR	Peptide
2	B	347	SER	Peptide
2	B	384	LYS	Peptide
2	B	50	LYS	Peptide
2	B	52	GLY	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	B	59	ASP	Peptide
3	C	81	GLY	Peptide
4	D	137	ASP	Peptide
4	D	172	TYR	Peptide
4	D	71	GLY	Peptide
6	F	214	TRP	Peptide
7	G	24	ASN	Peptide
7	G	30	THR	Peptide
7	G	76	ALA	Peptide
7	G	79	GLN	Peptide
9	I	45	GLY	Peptide
10	J	73	GLY	Peptide
10	J	8	PRO	Peptide
10	J	9	MET	Peptide
11	K	164	TYR	Peptide
11	K	212	HIS	Peptide
11	K	214	ASN	Peptide
13	M	8	LYS	Peptide
18	R	131	ALA	Peptide
19	S	11	GLY	Peptide
19	S	133	ALA	Peptide
19	S	152	LEU	Peptide
19	S	153	PRO	Peptide
19	S	22	PRO	Peptide
19	S	84	ARG	Peptide
20	T	52	MET	Peptide
20	T	53	PRO	Peptide
21	U	49	ASN	Peptide
22	V	88	ARG	Peptide
22	V	89	ASP	Peptide
23	W	100	THR	Peptide
23	W	135	PHE	Peptide
23	W	176	LYS	Peptide
24	X	17	GLY	Peptide
24	X	65	GLN	Peptide
26	Z	31	GLU	Peptide
26	Z	8	GLY	Peptide
28	b	10	THR	Peptide
28	b	221	THR	Peptide
28	b	247	ARG	Peptide
28	b	280	ASN	Peptide
28	b	292	ILE	Peptide

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Mol	Chain	Res	Type	Group
28	b	32	VAL	Peptide
28	b	370	ASP	Peptide
28	b	406	ASN	Peptide
28	b	419	LYS	Peptide
28	b	427	TRP	Peptide
28	b	437	ASP	Peptide
28	b	446	ASP	Peptide
28	b	483	ALA	Peptide
28	b	557	ARG	Peptide
28	b	594	ALA	Peptide
28	b	619	GLN	Peptide
28	b	620	GLY	Peptide
28	b	70	ASN	Peptide
30	d	87	ASN	Peptide
30	d	95	PRO	Peptide
30	d	97	LEU	Peptide
31	e	121	ASN	Peptide
32	f	91	ALA	Peptide
33	g	71	THR	Peptide
34	h	38	ARG	Peptide
34	h	91	ALA	Peptide
36	j	39	TYR	Peptide
37	k	18	ALA	Peptide
37	k	33	LYS	Peptide
38	l	2	ALA	Peptide
39	m	144	LYS	Peptide
39	m	151	ARG	Peptide
39	m	206	GLY	Peptide
39	m	240	LYS	Peptide
39	m	253	LYS	Peptide
39	m	260	ASN	Peptide
39	m	312	ASP	Peptide
39	m	357	THR	Peptide
39	m	376	LYS	Peptide
39	m	384	PHE	Peptide
39	m	416	TYR	Peptide
39	m	419	SER	Peptide
39	m	43	THR	Peptide
39	m	441	GLY	Peptide
39	m	52	LYS	Peptide
39	m	99	THR	Peptide
40	n	123	PRO	Peptide

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Mol	Chain	Res	Type	Group
40	n	124	SER	Peptide
40	n	148	THR	Peptide
40	n	207	GLU	Peptide
40	n	211	SER	Peptide
40	n	240	SER	Peptide
40	n	261	SER	Peptide
40	n	3	ILE	Peptide
40	n	358	SER	Peptide
40	n	383	CYS	Peptide
40	n	39	LYS	Peptide
40	n	418	LYS	Peptide
40	n	453	LEU	Peptide
40	n	454	PRO	Peptide
40	n	53	ASN	Peptide
40	n	54	LYS	Peptide
40	n	56	SER	Peptide
40	n	97	GLY	Peptide
41	o	101	GLY	Peptide
41	o	126	LYS	Peptide
41	o	127	LYS	Peptide
41	o	214	SER	Peptide
43	q	200	ALA	Peptide
43	q	223	ALA	Peptide
43	q	226	SER	Peptide
43	q	382	LYS	Peptide
43	q	384	GLY	Peptide
43	q	389	VAL	Peptide
43	q	401	GLU	Peptide
43	q	409	LEU	Peptide
44	r	141	LYS	Peptide
44	r	159	GLU	Peptide
44	r	160	GLY	Peptide
44	r	233	ALA	Peptide
44	r	260	LEU	Peptide
44	r	43	THR	Peptide
46	t	137	GLY	Peptide
46	t	146	ARG	Peptide
46	t	209	GLN	Peptide
46	t	222	ALA	Peptide
46	t	274	ASN	Peptide
46	t	277	VAL	Peptide
46	t	280	PHE	Peptide

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Mol	Chain	Res	Type	Group
47	u	2	ARG	Peptide
47	u	77	VAL	Peptide
47	u	79	VAL	Peptide
49	w	112	THR	Peptide
49	w	122	GLY	Peptide
49	w	125	PRO	Peptide
49	w	137	ALA	Peptide
49	w	143	PRO	Peptide
49	w	144	LYS	Peptide
49	w	157	GLN	Peptide
49	w	79	GLY	Peptide
49	w	86	VAL	Peptide
50	x	124	ARG	Peptide
50	x	127	PHE	Peptide
50	x	135	SER	Peptide
50	x	167	THR	Peptide
50	x	24	ILE	Peptide
50	x	27	LYS	Peptide
50	x	29	LEU	Peptide
50	x	318	SER	Peptide
51	y	145	ASN	Peptide
51	y	226	ASP	Peptide
51	y	28	VAL	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1634	0	1685	17	0
2	B	3081	0	3165	86	0
3	C	2749	0	2863	30	0
4	D	2211	0	2175	66	0
5	E	1239	0	1326	22	0
6	F	1784	0	1862	23	0
7	G	1817	0	1908	29	0
8	H	1518	0	1587	25	0
9	I	1059	0	1090	4	0
10	J	1353	0	1383	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	2064	0	2156	16	0
12	L	1499	0	1558	20	0
13	M	1059	0	1154	22	0
14	N	1720	0	1779	9	0
15	O	1555	0	1659	165	0
16	P	1442	0	1485	10	0
17	Q	1035	0	1115	4	0
18	R	1258	0	1341	9	0
19	S	1437	0	1475	6	0
20	T	943	0	994	31	0
21	U	844	0	855	1	0
22	V	1003	0	1048	12	0
23	W	1885	0	1921	3	0
24	X	1100	0	1187	5	0
25	Y	993	0	1081	2	0
26	Z	1092	0	1155	12	0
27	a	735	0	776	0	0
28	b	5185	0	5251	0	0
29	c	743	0	797	0	0
30	d	873	0	914	0	0
31	e	1020	0	1090	0	0
32	f	850	0	880	0	0
33	g	881	0	945	0	0
34	h	969	0	1078	0	0
35	i	771	0	849	0	0
36	j	681	0	683	0	0
37	k	612	0	682	0	0
38	l	436	0	475	0	0
39	m	3774	0	3835	0	0
40	n	3030	0	3107	0	0
41	o	1107	0	1159	0	0
42	p	694	0	734	0	0
43	q	1514	0	1570	0	0
44	r	1860	0	1965	0	0
45	s	573	0	644	0	0
46	t	2306	0	2454	0	0
47	u	1265	0	1314	0	0
48	v	2318	0	2398	0	0
49	w	1448	0	1510	0	0
50	x	3807	0	3790	0	0
51	y	1849	0	1835	0	0
52	z	444	0	478	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	1	65427	0	32875	328	0
54	2	3353	0	1695	4	0
55	3	2579	0	1303	12	0
56	4	3999	0	4088	7	0
57	5	645	0	688	0	0
58	6	1370	0	692	20	0
59	I	1	0	0	0	0
59	j	1	0	0	0	0
59	p	1	0	0	0	0
59	u	1	0	0	0	0
60	b	32	0	12	0	0
60	m	32	0	12	0	0
61	b	1	0	0	0	0
61	m	1	0	0	0	0
All	All	156562	0	123585	939	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (939) 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)
53:1:2428:U:C5	53:1:2602:G:N1	1.70	1.54
53:1:2428:U:H5	53:1:2602:G:N1	0.92	1.40
53:1:2255:A:N7	53:1:2261:G:N2	1.70	1.35
53:1:3153:U:O4	53:1:3293:U:N3	1.59	1.35
18:R:62:ARG:NH1	53:1:3068:U:OP2	1.61	1.32
53:1:2528:G:C2	53:1:2529:A:N3	2.02	1.27
53:1:3153:U:C6	53:1:3158:G:C6	2.23	1.27
15:O:121:PRO:HA	15:O:124:LEU:CD2	1.63	1.26
15:O:52:LEU:O	15:O:56:ASP:OD1	1.53	1.24
4:D:151:GLN:NE2	55:3:45:A:OP1	1.72	1.20
53:1:2760:C:H5	53:1:2800:G:N2	1.38	1.19
53:1:3153:U:C6	53:1:3158:G:O6	1.95	1.18
53:1:2428:U:H5	53:1:2602:G:C6	1.63	1.17
15:O:147:TRP:CZ3	15:O:150:GLU:HB2	1.83	1.14
53:1:2760:C:C5	53:1:2800:G:N2	2.14	1.14
2:B:90:VAL:HG22	2:B:104:THR:HG22	1.19	1.13
53:1:2528:G:N1	53:1:2529:A:C2	2.17	1.12
15:O:121:PRO:HA	15:O:124:LEU:HD22	1.25	1.12
53:1:2763:U:O2'	53:1:2764:C:OP1	1.67	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:47:ASP:OD2	13:M:78:THR:HG23	1.48	1.11
53:1:3153:U:C6	53:1:3158:G:N1	2.18	1.09
15:O:48:PHE:CE2	15:O:52:LEU:HD21	1.87	1.09
53:1:2531:C:N4	53:1:2547:A:N6	2.00	1.09
53:1:2428:U:C5	53:1:2602:G:C6	2.38	1.09
15:O:48:PHE:CE2	15:O:52:LEU:CD2	2.36	1.08
2:B:94:GLU:HG3	2:B:99:LEU:CD2	1.83	1.08
15:O:48:PHE:HE2	15:O:52:LEU:HD21	1.10	1.08
53:1:3153:U:H6	53:1:3158:G:C6	1.61	1.07
15:O:106:GLU:OE1	15:O:106:GLU:N	1.88	1.06
53:1:2531:C:H42	53:1:2547:A:N6	1.54	1.06
53:1:3153:U:H6	53:1:3158:G:O6	1.32	1.05
53:1:2761:G:O2'	53:1:2762:A:P	2.13	1.04
53:1:2762:A:O2'	53:1:2794:G:C6	2.11	1.03
53:1:2428:U:O4	53:1:2602:G:O6	1.77	1.03
53:1:2760:C:H2'	53:1:2761:G:C8	1.92	1.02
53:1:2546:C:H3'	53:1:2547:A:H5''	1.42	1.01
53:1:2428:U:H5	53:1:2602:G:C2	1.78	1.01
53:1:2428:U:C5	53:1:2602:G:C2	2.49	1.00
2:B:94:GLU:HG3	2:B:99:LEU:HD22	1.41	0.99
15:O:48:PHE:HE2	15:O:52:LEU:CD2	1.72	0.99
2:B:94:GLU:CG	2:B:99:LEU:CD2	2.39	0.99
53:1:3157:U:H1'	53:1:3158:G:N7	1.78	0.99
2:B:90:VAL:CG2	2:B:104:THR:HG22	1.92	0.98
53:1:2761:G:O2'	53:1:2762:A:OP1	1.83	0.97
53:1:2528:G:C2	53:1:2529:A:C4	2.54	0.96
4:D:152:ARG:HD2	53:1:2663:G:OP1	1.65	0.95
53:1:2428:U:HO2'	53:1:2429:G:H8	0.96	0.95
53:1:2526:C:H2'	53:1:2527:G:H5'	1.47	0.94
53:1:2531:C:N4	53:1:2547:A:H62	1.62	0.94
2:B:94:GLU:HG2	2:B:99:LEU:HD21	1.50	0.93
15:O:8:VAL:HG22	15:O:34:VAL:CG1	1.99	0.93
53:1:2531:C:H42	53:1:2547:A:H61	1.15	0.93
2:B:89:VAL:HG21	2:B:195:ALA:CB	1.99	0.92
53:1:3153:U:C5	53:1:3158:G:O6	2.23	0.92
16:P:138:LYS:NZ	16:P:140:GLU:OE2	2.03	0.92
15:O:121:PRO:HA	15:O:124:LEU:HD23	1.52	0.91
2:B:89:VAL:HG21	2:B:195:ALA:HB1	1.49	0.91
6:F:112:ASN:ND2	6:F:209:ASN:OD1	2.03	0.91
53:1:1229:G:C6	53:1:1281:G:C6	2.59	0.90
53:1:2546:C:O2	53:1:2548:C:N3	2.04	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:GLN:O	2:B:141:GLY:N	2.05	0.90
4:D:150:LEU:HD21	53:1:2703:A:H2	1.33	0.89
53:1:2547:A:O3'	53:1:2548:C:H3'	1.73	0.88
53:1:2761:G:O2'	53:1:2762:A:O5'	1.89	0.88
2:B:56:ILE:HD11	2:B:359:ILE:HG23	1.55	0.88
15:O:148:LYS:H	15:O:148:LYS:HD3	1.38	0.88
15:O:96:LYS:O	15:O:100:GLU:HG3	1.73	0.88
15:O:53:LYS:C	15:O:56:ASP:OD1	2.13	0.87
53:1:3153:U:C4	53:1:3293:U:N3	2.34	0.87
15:O:181:ALA:O	15:O:184:THR:HG22	1.74	0.87
7:G:119:GLY:O	7:G:120:LYS:HG3	1.76	0.86
53:1:2597:U:O2'	53:1:2598:G:H5'	1.76	0.86
53:1:2546:C:O3'	53:1:2548:C:OP1	1.93	0.86
58:6:26:U:O2'	58:6:27:G:H8	1.57	0.86
15:O:121:PRO:CA	15:O:124:LEU:HD22	2.04	0.86
15:O:48:PHE:CE2	15:O:52:LEU:HD22	2.09	0.86
53:1:2526:C:C2'	53:1:2527:G:H5'	2.05	0.85
2:B:94:GLU:CG	2:B:99:LEU:HD21	2.06	0.85
4:D:166:ALA:HB1	4:D:171:LEU:HD12	1.58	0.84
15:O:8:VAL:HG22	15:O:34:VAL:HG11	1.58	0.84
15:O:73:PHE:HB3	15:O:78:ARG:HG2	1.58	0.84
11:K:93:LYS:HB2	58:6:24:A:C2	2.13	0.84
15:O:147:TRP:HZ3	15:O:150:GLU:HB2	1.36	0.84
53:1:2429:G:O6	53:1:2601:A:C6	2.30	0.83
53:1:2238:G:O2'	53:1:2239:G:P	2.35	0.83
15:O:41:LEU:CD2	15:O:80:PHE:HD2	1.91	0.83
53:1:2759:U:C5	53:1:2760:C:C4	2.67	0.83
55:3:82:G:O6	55:3:98:C:C5	2.31	0.82
55:3:97:A:O2'	55:3:98:C:H5'	1.78	0.82
2:B:89:VAL:CG2	2:B:195:ALA:HB1	2.08	0.82
15:O:148:LYS:H	15:O:148:LYS:CD	1.91	0.82
58:6:26:U:O2'	58:6:27:G:C8	2.32	0.82
4:D:52:VAL:HG21	4:D:65:ILE:HD12	1.62	0.82
15:O:77:SER:HB2	15:O:104:VAL:HG12	1.60	0.81
53:1:2528:G:N2	53:1:2529:A:N3	2.29	0.81
15:O:84:LEU:O	15:O:84:LEU:HD23	1.81	0.81
55:3:82:G:O6	55:3:98:C:N4	2.13	0.80
7:G:120:LYS:O	7:G:121:SER:OG	1.99	0.80
6:F:110:ARG:O	6:F:113:SER:OG	1.99	0.80
53:1:2528:G:H1'	53:1:2529:A:O4'	1.81	0.80
4:D:152:ARG:CD	53:1:2663:G:OP1	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:40:LEU:HD13	5:E:84:VAL:HG11	1.64	0.80
15:O:53:LYS:O	15:O:56:ASP:OD1	1.99	0.80
4:D:150:LEU:CD2	53:1:2703:A:H2	1.95	0.79
7:G:244:ALA:HB1	53:1:2528:G:H5'	1.63	0.79
15:O:121:PRO:O	15:O:123:ALA:N	2.14	0.79
53:1:2763:U:HO2'	53:1:2764:C:P	2.06	0.79
15:O:77:SER:HB2	15:O:104:VAL:CG1	2.13	0.79
11:K:276:ILE:HD12	11:K:279:ILE:HD11	1.65	0.78
4:D:153:THR:HG23	4:D:160:PHE:CZ	2.18	0.78
53:1:1282:G:O2'	53:1:1283:C:O5'	2.02	0.77
53:1:2528:G:C2	53:1:2529:A:C2	2.65	0.77
4:D:150:LEU:HD21	53:1:2703:A:C2	2.19	0.77
53:1:2528:G:C4	53:1:2529:A:C4	2.73	0.77
14:N:122:ASN:OD1	14:N:123:GLN:N	2.17	0.77
15:O:26:GLN:HA	15:O:26:GLN:OE1	1.85	0.77
18:R:60:LYS:O	18:R:64:ARG:HG3	1.84	0.77
53:1:2761:G:HO2'	53:1:2762:A:P	2.02	0.76
26:Z:81:LEU:HD23	26:Z:82:PRO:HD2	1.68	0.76
53:1:2528:G:N3	53:1:2529:A:C4	2.54	0.76
53:1:2429:G:C6	53:1:2601:A:C2	2.74	0.76
2:B:104:THR:HG23	53:1:3147:G:O2'	1.85	0.76
15:O:57:PHE:HA	15:O:60:LYS:HZ3	1.51	0.76
53:1:2759:U:H5	53:1:2760:C:C6	2.05	0.75
4:D:152:ARG:NH1	53:1:2663:G:H4'	2.01	0.75
53:1:1229:G:O6	53:1:1281:G:O6	2.05	0.75
58:6:26:U:O2'	58:6:27:G:O5'	2.04	0.75
15:O:48:PHE:CD2	15:O:52:LEU:HD22	2.22	0.75
13:M:35:ILE:HA	13:M:46:ILE:HG22	1.68	0.74
15:O:77:SER:HB3	15:O:106:GLU:OE1	1.87	0.74
53:1:2238:G:O2'	53:1:2239:G:O5'	2.06	0.74
1:A:79:ASN:ND2	1:A:166:ILE:O	2.21	0.74
15:O:121:PRO:C	15:O:123:ALA:H	1.89	0.74
53:1:2427:U:N3	53:1:2428:U:O4	2.20	0.74
4:D:150:LEU:CD2	53:1:2703:A:C2	2.70	0.74
53:1:3157:U:H1'	53:1:3158:G:C8	2.22	0.74
53:1:3153:U:O4	53:1:3293:U:C2	2.40	0.73
22:V:45:ARG:HH11	22:V:46:LEU:H	1.36	0.73
53:1:2429:G:C6	53:1:2601:A:N1	2.56	0.73
53:1:2598:G:O2'	53:1:2599:U:C5'	2.35	0.73
15:O:52:LEU:O	15:O:56:ASP:CG	2.26	0.73
15:O:107:GLY:O	15:O:109:PRO:HD3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:45:ARG:HG2	22:V:48:ARG:NH1	2.03	0.73
53:1:2759:U:H5	53:1:2760:C:C5	2.06	0.72
20:T:152:ALA:HB1	20:T:153:PRO:CD	2.19	0.72
53:1:3156:U:O2'	53:1:3157:U:O5'	2.06	0.72
2:B:90:VAL:HG23	2:B:161:LEU:HD11	1.70	0.72
15:O:170:LYS:CB	15:O:170:LYS:NZ	2.52	0.72
4:D:153:THR:HG23	4:D:160:PHE:HZ	1.53	0.71
53:1:3156:U:H1'	53:1:3157:U:OP1	1.89	0.71
15:O:181:ALA:O	15:O:184:THR:CG2	2.38	0.71
53:1:2763:U:O2'	53:1:2764:C:P	2.46	0.71
2:B:94:GLU:HG2	2:B:99:LEU:CD2	2.12	0.71
15:O:106:GLU:H	15:O:106:GLU:CD	1.92	0.71
15:O:108:ILE:CG2	15:O:113:ASP:HA	2.21	0.71
6:F:223:PHE:HA	6:F:227:GLY:O	1.90	0.71
15:O:19:LEU:HD23	15:O:80:PHE:HE2	1.56	0.71
53:1:2429:G:C5	53:1:2601:A:C2	2.79	0.70
53:1:2427:U:N3	53:1:2428:U:C4	2.59	0.70
15:O:23:VAL:HG11	15:O:84:LEU:HD11	1.74	0.70
15:O:98:ALA:HA	15:O:101:ARG:HH11	1.55	0.70
15:O:186:ALA:O	15:O:187:GLU:HB3	1.92	0.70
15:O:73:PHE:CB	15:O:78:ARG:HG2	2.21	0.70
15:O:157:GLU:OE1	15:O:160:ARG:NH1	2.24	0.70
53:1:2428:U:C4	53:1:2602:G:C6	2.80	0.69
11:K:124:LEU:HD21	11:K:155:ILE:HD13	1.74	0.69
4:D:205:SER:HB2	4:D:233:ALA:HB1	1.73	0.69
53:1:1281:G:O2'	53:1:1282:G:O5'	2.10	0.69
4:D:107:ARG:NE	4:D:107:ARG:HA	2.07	0.69
53:1:3153:U:C5	53:1:3158:G:C6	2.77	0.69
15:O:41:LEU:HD21	15:O:80:PHE:HD2	1.58	0.69
15:O:108:ILE:HG21	15:O:113:ASP:HA	1.73	0.69
53:1:2528:G:C6	53:1:2529:A:C6	2.81	0.69
15:O:104:VAL:O	15:O:105:PHE:CD1	2.46	0.69
15:O:170:LYS:HZ2	15:O:170:LYS:HB2	1.58	0.69
53:1:3153:U:C5	53:1:3158:G:N1	2.59	0.68
53:1:2546:C:O2	53:1:2548:C:C2	2.45	0.68
15:O:41:LEU:HD21	15:O:80:PHE:CD2	2.29	0.68
20:T:152:ALA:O	20:T:154:VAL:N	2.26	0.68
53:1:2511:A:O2'	53:1:2512:C:O4'	2.07	0.67
15:O:25:LYS:O	15:O:25:LYS:HD3	1.94	0.67
8:H:86:TYR:CE2	8:H:151:VAL:HG22	2.29	0.67
53:1:1282:G:O2'	53:1:1283:C:C5'	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:6:26:U:O2'	58:6:27:G:O4'	2.13	0.67
53:1:2511:A:H2'	53:1:2512:C:C6	2.29	0.67
55:3:96:U:O4	55:3:97:A:N6	2.28	0.67
15:O:23:VAL:CG1	15:O:84:LEU:HD11	2.24	0.67
53:1:2759:U:C5	53:1:2760:C:C5	2.83	0.67
53:1:2238:G:HO2'	53:1:2239:G:P	2.16	0.66
53:1:2510:U:O2'	53:1:2511:A:O5'	2.13	0.66
13:M:128:ARG:HD3	13:M:132:LYS:HZ1	1.59	0.66
55:3:82:G:C6	55:3:98:C:H5	2.13	0.66
15:O:121:PRO:CA	15:O:124:LEU:CD2	2.57	0.66
11:K:93:LYS:HB2	58:6:24:A:H2	1.57	0.66
6:F:111:ILE:O	6:F:112:ASN:HB2	1.95	0.66
15:O:170:LYS:NZ	15:O:170:LYS:HB3	2.09	0.66
13:M:128:ARG:HD3	13:M:132:LYS:NZ	2.10	0.66
6:F:173:LEU:O	6:F:177:GLY:O	2.13	0.66
53:1:1229:G:C6	53:1:1281:G:O6	2.49	0.66
53:1:2428:U:C4	53:1:2602:G:O6	2.48	0.66
53:1:3153:U:O4	53:1:3293:U:C4	2.44	0.66
10:J:27:GLY:O	10:J:28:ASP:C	2.33	0.66
53:1:2243:A:OP1	53:1:2243:A:H8	1.79	0.65
53:1:2657:A:O2'	53:1:2658:G:O4'	2.12	0.65
15:O:170:LYS:CB	15:O:170:LYS:HZ2	2.08	0.65
4:D:152:ARG:HD3	53:1:2663:G:H5'	1.78	0.65
53:1:2761:G:OP2	53:1:2761:G:H8	1.80	0.65
55:3:82:G:O6	55:3:98:C:C4	2.49	0.65
7:G:134:TYR:CG	7:G:190:VAL:HG21	2.31	0.65
16:P:36:ILE:HD11	16:P:95:LEU:HD11	1.78	0.65
2:B:43:LEU:HG	2:B:181:ILE:HG21	1.78	0.65
26:Z:81:LEU:HD23	26:Z:82:PRO:CD	2.26	0.65
4:D:52:VAL:N	4:D:63:GLN:O	2.30	0.65
53:1:2758:A:H2'	53:1:2759:U:O2	1.96	0.65
53:1:2760:C:C6	53:1:2800:G:N2	2.64	0.65
20:T:91:LEU:HD13	20:T:96:ILE:HD11	1.77	0.65
7:G:134:TYR:HB3	7:G:190:VAL:HG21	1.79	0.65
53:1:2511:A:H2'	53:1:2512:C:H6	1.61	0.65
53:1:2596:U:C5	53:1:2597:U:C5	2.85	0.65
26:Z:24:VAL:HG11	26:Z:87:LEU:HD23	1.78	0.65
5:E:68:PRO:HG3	5:E:145:LEU:HD23	1.77	0.64
15:O:46:GLU:O	15:O:47:PHE:C	2.34	0.64
4:D:107:ARG:HE	4:D:107:ARG:HA	1.63	0.64
11:K:93:LYS:HE2	58:6:24:A:C2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:2428:U:C6	53:1:2602:G:C2	2.85	0.64
8:H:49:ASN:O	8:H:51:GLN:N	2.31	0.64
53:1:2596:U:C4	53:1:2597:U:C4	2.85	0.64
53:1:2527:G:O2'	53:1:2528:G:H5'	1.98	0.64
15:O:8:VAL:HG12	15:O:117:ARG:HB3	1.80	0.63
53:1:2528:G:C6	53:1:2529:A:C2	2.86	0.63
2:B:219:ALA:C	2:B:221:THR:HG23	2.18	0.63
2:B:90:VAL:HG22	2:B:104:THR:CG2	2.12	0.63
15:O:88:VAL:HG12	15:O:89:SER:N	2.12	0.63
53:1:2528:G:C5	53:1:2529:A:C5	2.87	0.63
3:C:338:LYS:O	3:C:340:GLY:N	2.31	0.63
8:H:41:ILE:HD11	8:H:67:ALA:HB1	1.81	0.63
16:P:126:ARG:HA	16:P:140:GLU:HG2	1.81	0.63
4:D:151:GLN:OE1	4:D:152:ARG:N	2.31	0.63
15:O:130:LYS:HG3	15:O:131:PRO:HD2	1.81	0.63
53:1:2546:C:C2'	53:1:2548:C:OP1	2.47	0.63
53:1:2759:U:C4	53:1:2760:C:C4	2.86	0.62
7:G:119:GLY:O	7:G:120:LYS:CG	2.44	0.62
53:1:2929:C:H2'	53:1:2929:C:O2	1.98	0.62
4:D:144:VAL:O	4:D:173:VAL:HG22	1.99	0.62
20:T:152:ALA:HB1	20:T:153:PRO:HD2	1.82	0.62
2:B:24:SER:O	2:B:26:ARG:N	2.32	0.62
20:T:74:VAL:HG21	20:T:91:LEU:HD12	1.81	0.62
2:B:328:ILE:HG21	2:B:336:VAL:HG11	1.80	0.62
1:A:5:ILE:HG22	1:A:208:ASP:O	2.00	0.62
15:O:108:ILE:HG22	15:O:113:ASP:HB3	1.82	0.62
53:1:2759:U:C5	53:1:2760:C:C2	2.86	0.62
55:3:82:G:C6	55:3:98:C:C5	2.87	0.62
15:O:3:VAL:HG13	15:O:4:GLU:HG3	1.82	0.62
53:1:2546:C:C3'	53:1:2548:C:OP1	2.48	0.62
20:T:100:LYS:O	20:T:102:ARG:N	2.33	0.62
53:1:2429:G:C6	53:1:2601:A:C6	2.88	0.61
2:B:227:GLU:HG2	2:B:270:ARG:HE	1.65	0.61
53:1:2546:C:H3'	53:1:2547:A:C5'	2.24	0.61
53:1:2531:C:H41	53:1:2547:A:H62	1.44	0.61
15:O:53:LYS:CA	15:O:56:ASP:OD1	2.48	0.61
15:O:15:LEU:HA	15:O:42:ASN:O	2.00	0.61
15:O:15:LEU:O	15:O:16:VAL:C	2.38	0.61
2:B:219:ALA:HB2	2:B:336:VAL:HG12	1.83	0.61
2:B:139:GLN:C	2:B:141:GLY:H	2.03	0.61
10:J:27:GLY:O	10:J:30:LEU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:1280:C:H2'	53:1:1281:G:H5'	1.84	0.60
15:O:171:LYS:O	15:O:175:THR:HG23	2.00	0.60
15:O:27:LEU:HD13	15:O:98:ALA:O	2.01	0.60
5:E:47:PHE:CD2	5:E:74:VAL:HG22	2.37	0.60
2:B:139:GLN:O	2:B:140:ASP:C	2.37	0.60
53:1:3154:C:O2'	53:1:3155:U:OP2	2.20	0.60
7:G:119:GLY:C	7:G:120:LYS:HG3	2.22	0.60
2:B:285:VAL:HG22	2:B:322:ILE:HD13	1.84	0.60
53:1:2393:G:O2'	53:1:2982:A:N6	2.35	0.59
53:1:2762:A:O2'	53:1:2794:G:O6	2.20	0.59
53:1:2929:C:C2'	53:1:2929:C:O2	2.49	0.59
15:O:195:ALA:O	15:O:198:GLY:N	2.34	0.59
12:L:50:PRO:O	12:L:51:LEU:HB2	2.02	0.59
15:O:104:VAL:O	15:O:105:PHE:CG	2.56	0.59
4:D:64:ILE:HD11	4:D:105:ILE:HG13	1.83	0.59
15:O:147:TRP:CZ3	15:O:150:GLU:CB	2.74	0.59
2:B:218:ILE:HD11	2:B:337:THR:HB	1.83	0.59
53:1:2759:U:H2'	53:1:2760:C:H5'	1.85	0.59
16:P:36:ILE:CD1	16:P:95:LEU:HD11	2.32	0.59
4:D:150:LEU:HD22	53:1:2703:A:C2	2.38	0.59
23:W:188:VAL:HG11	23:W:202:ILE:HG21	1.85	0.59
15:O:121:PRO:C	15:O:123:ALA:N	2.56	0.58
53:1:2528:G:N3	53:1:2529:A:N9	2.51	0.58
53:1:2758:A:O2'	53:1:2759:U:OP1	2.21	0.58
53:1:2528:G:C4	53:1:2529:A:N9	2.72	0.58
13:M:55:ARG:NH2	13:M:76:ALA:O	2.25	0.58
15:O:19:LEU:O	15:O:23:VAL:HG23	2.03	0.58
2:B:104:THR:OG1	53:1:3148:U:H4'	2.02	0.58
20:T:132:PRO:O	20:T:134:GLN:NE2	2.37	0.58
15:O:187:GLU:OE1	15:O:187:GLU:HA	2.03	0.58
13:M:128:ARG:O	13:M:132:LYS:HG2	2.04	0.58
13:M:47:ASP:OD2	13:M:78:THR:CG2	2.39	0.58
20:T:105:PHE:O	20:T:109:VAL:HG23	2.03	0.58
53:1:2759:U:C5	53:1:2760:C:N3	2.71	0.57
2:B:173:GLN:O	2:B:175:LYS:N	2.37	0.57
53:1:2432:A:C6	53:1:2598:G:O6	2.57	0.57
53:1:2598:G:O2'	53:1:2599:U:H5'	2.03	0.57
53:1:2528:G:N3	53:1:2529:A:C1'	2.68	0.57
53:1:2764:C:H4'	53:1:2765:C:OP2	2.03	0.57
6:F:88:ARG:NH1	6:F:90:LYS:O	2.38	0.57
16:P:127:ARG:O	16:P:139:TYR:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:45:ARG:HG2	22:V:48:ARG:HH12	1.69	0.57
53:1:1481:A:O2'	53:1:1858:A:H1'	2.04	0.57
53:1:2794:G:C2	53:1:2795:U:O4	2.58	0.57
10:J:27:GLY:O	10:J:29:ARG:N	2.37	0.57
53:1:2528:G:C6	53:1:2529:A:N1	2.72	0.57
53:1:2793:G:HO2'	53:1:2794:G:P	2.27	0.57
53:1:2857:C:O2'	53:1:2858:U:O5'	2.21	0.57
2:B:60:LEU:HD21	2:B:62:ARG:CZ	2.35	0.57
4:D:49:TYR:CD1	4:D:142:PHE:CZ	2.93	0.57
4:D:166:ALA:CB	4:D:171:LEU:HD12	2.33	0.56
22:V:46:LEU:O	22:V:47:ASN:HB2	2.04	0.56
53:1:2759:U:C2'	53:1:2760:C:H5'	2.36	0.56
15:O:22:VAL:HG23	15:O:23:VAL:N	2.20	0.56
15:O:67:THR:O	15:O:71:PHE:CE1	2.58	0.56
53:1:1281:G:C2	53:1:1282:G:C5	2.94	0.56
3:C:292:SER:OG	3:C:293:SER:N	2.37	0.56
13:M:37:GLU:OE2	13:M:74:ARG:NE	2.37	0.56
15:O:41:LEU:CD2	15:O:80:PHE:CD2	2.80	0.56
18:R:62:ARG:NH2	53:1:3070:A:OP1	2.37	0.56
53:1:3154:C:HO2'	53:1:3155:U:P	2.28	0.56
53:1:2763:U:C2'	53:1:2764:C:OP1	2.53	0.56
53:1:3153:U:O4	53:1:3292:A:N6	2.39	0.56
6:F:163:LEU:O	6:F:165:ASP:N	2.38	0.56
7:G:122:LYS:O	7:G:123:GLN:HB2	2.05	0.56
53:1:2598:G:O2'	53:1:2599:U:O4'	2.21	0.56
53:1:1281:G:O2'	53:1:1282:G:H8	1.89	0.56
15:O:22:VAL:CG1	15:O:122:GLN:OE1	2.54	0.56
13:M:72:LEU:HD21	13:M:76:ALA:HB3	1.87	0.56
15:O:73:PHE:CG	15:O:78:ARG:HG2	2.41	0.56
4:D:152:ARG:CZ	53:1:2663:G:H4'	2.36	0.56
3:C:156:LEU:HD23	3:C:159:ILE:HD12	1.88	0.56
15:O:187:GLU:OE1	15:O:187:GLU:CA	2.54	0.56
12:L:79:GLU:HG3	12:L:103:ASN:HD21	1.71	0.56
18:R:102:LEU:HD22	18:R:138:LEU:HD12	1.88	0.55
53:1:2598:G:O2'	53:1:2599:U:O5'	2.24	0.55
4:D:178:ASN:HA	4:D:183:TRP:CD2	2.41	0.55
7:G:118:GLU:OE2	7:G:118:GLU:N	2.39	0.55
53:1:2760:C:H5	53:1:2800:G:H22	0.65	0.55
53:1:2793:G:H3'	53:1:2794:G:H5''	1.89	0.55
55:3:82:G:O6	55:3:98:C:H5	1.82	0.55
53:1:1228:C:C2	53:1:1282:G:N1	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:2437:G:C4	53:1:2511:A:C2	2.95	0.55
53:1:2546:C:O2	53:1:2548:C:O2	2.24	0.55
2:B:286:GLY:HA3	2:B:321:PHE:CE2	2.42	0.55
15:O:43:ILE:HD11	15:O:138:LEU:HD13	1.87	0.55
53:1:2237:C:C5	53:1:2238:G:N7	2.74	0.55
26:Z:2:ALA:N	53:1:2891:U:HO2'	150.13	0.55
2:B:104:THR:OG1	53:1:3148:U:C4'	2.54	0.55
8:H:161:LEU:CD2	8:H:179:ILE:HD12	2.36	0.55
15:O:80:PHE:HE1	15:O:84:LEU:HD12	1.72	0.55
19:S:24:LEU:HG	20:T:146:ASN:HD21	1.72	0.55
15:O:184:THR:HG23	15:O:185:ALA:N	2.22	0.55
15:O:22:VAL:HG12	15:O:122:GLN:OE1	2.07	0.55
53:1:3153:U:O4	53:1:3292:A:C6	2.60	0.55
4:D:219:PHE:CE2	4:D:227:LEU:HD21	2.42	0.55
12:L:47:ALA:HB3	12:L:48:PRO:HD3	1.88	0.55
53:1:2528:G:N3	53:1:2529:A:H1'	2.22	0.55
53:1:2761:G:C2'	53:1:2762:A:OP1	2.55	0.55
4:D:32:GLN:CD	4:D:148:ILE:HD12	2.27	0.54
26:Z:81:LEU:HD23	26:Z:82:PRO:N	2.22	0.54
15:O:142:SER:HA	15:O:145:VAL:HG22	1.89	0.54
15:O:170:LYS:HZ3	15:O:170:LYS:HB3	1.73	0.54
20:T:53:PRO:HB2	20:T:54:HIS:HA	1.88	0.54
53:1:3217:C:C2'	53:1:3217:C:O2	2.54	0.54
14:N:110:ALA:HB1	14:N:113:LEU:CD2	2.38	0.54
15:O:56:ASP:O	15:O:59:ARG:HG2	2.07	0.54
2:B:105:VAL:HG21	2:B:148:LEU:HD13	1.89	0.54
6:F:69:ALA:HB1	6:F:74:SER:O	2.08	0.54
15:O:55:HIS:O	15:O:58:LEU:N	2.41	0.54
53:1:2758:A:HO2'	53:1:2759:U:P	2.31	0.54
53:1:2793:G:C3'	53:1:2794:G:C5'	2.86	0.54
56:4:343:TYR:N	56:4:354:ILE:HD11	2.23	0.54
15:O:187:GLU:OE1	15:O:187:GLU:O	2.26	0.54
53:1:2428:U:C6	53:1:2602:G:N2	2.76	0.53
53:1:3153:U:HO2'	53:1:3154:C:H6	1.56	0.53
2:B:163:HIS:HB2	2:B:177:HIS:O	2.07	0.53
53:1:1228:C:N3	53:1:1282:G:C6	2.77	0.53
53:1:646:A:H4'	53:1:647:A:O4'	2.08	0.53
3:C:193:LYS:HZ2	3:C:193:LYS:HB3	1.73	0.53
23:W:135:PHE:CE1	23:W:208:ILE:HD13	2.43	0.53
53:1:2793:G:O2'	53:1:2794:G:OP1	2.23	0.53
53:1:3156:U:O2'	53:1:3157:U:P	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:LEU:HD13	2:B:47:LEU:N	2.24	0.53
13:M:37:GLU:OE2	13:M:74:ARG:CZ	2.57	0.53
53:1:1229:G:N1	53:1:1281:G:C6	2.76	0.53
53:1:2428:U:O2'	53:1:2429:G:O5'	2.26	0.53
53:1:2758:A:H8	53:1:2758:A:H5'	1.73	0.53
2:B:221:THR:HG21	2:B:329:PRO:HB2	1.90	0.53
4:D:77:ALA:O	4:D:108:ARG:NH1	2.41	0.53
7:G:156:ASP:O	7:G:157:VAL:HG23	2.08	0.53
4:D:99:TYR:CZ	4:D:168:ASP:OD2	2.62	0.53
3:C:36:HIS:O	3:C:40:THR:HG23	2.09	0.53
8:H:16:VAL:HG12	8:H:29:GLY:HA3	1.91	0.53
53:1:1280:C:C2'	53:1:1281:G:H5'	2.38	0.53
53:1:2238:G:N2	53:1:2239:G:C4	2.77	0.53
15:O:108:ILE:HG22	15:O:108:ILE:O	2.09	0.52
53:1:2548:C:H2'	53:1:2548:C:O2	2.07	0.52
53:1:2955:U:O2	53:1:2955:U:O4'	2.27	0.52
26:Z:13:VAL:HG22	26:Z:80:LEU:CD2	2.38	0.52
53:1:2527:G:O2'	53:1:2528:G:OP2	2.25	0.52
53:1:2836:C:O2	53:1:2836:C:O4'	2.25	0.52
7:G:150:LEU:HD21	7:G:218:ILE:HD13	1.91	0.52
8:H:189:GLU:HA	8:H:190:ASP:C	2.30	0.52
10:J:50:ALA:HB2	10:J:65:ILE:HD12	1.90	0.52
15:O:16:VAL:CG2	15:O:43:ILE:HG12	2.40	0.52
53:1:1556:C:O2	53:1:1556:C:O4'	2.24	0.52
53:1:745:C:H2'	53:1:746:A:H5'	1.90	0.52
2:B:303:LYS:CD	2:B:361:THR:HG21	2.40	0.52
3:C:39:PHE:CD2	3:C:242:ALA:HB2	2.44	0.52
14:N:4:TYR:CE2	14:N:5:LYS:HB2	2.45	0.52
15:O:195:ALA:O	15:O:196:ALA:C	2.47	0.52
21:U:14:THR:HG23	21:U:66:VAL:HG22	1.92	0.52
53:1:2793:G:H3'	53:1:2794:G:C5'	2.40	0.52
3:C:193:LYS:HZ2	3:C:193:LYS:CB	2.23	0.52
1:A:128:ARG:NH1	53:1:2177:G:OP2	2.38	0.52
53:1:2510:U:HO2'	53:1:2511:A:P	2.31	0.52
53:1:3181:C:O2	53:1:3181:C:O4'	2.27	0.52
17:Q:86:THR:HG22	17:Q:105:ARG:HB2	1.92	0.52
53:1:2531:C:H41	53:1:2547:A:N6	1.98	0.51
3:C:193:LYS:NZ	3:C:193:LYS:CB	2.73	0.51
15:O:8:VAL:CG1	15:O:117:ARG:HB3	2.40	0.51
15:O:148:LYS:N	15:O:148:LYS:CD	2.61	0.51
53:1:2236:G:O2'	53:1:2237:C:H5'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:2429:G:O6	53:1:2601:A:N1	2.41	0.51
53:1:2654:C:O2	53:1:2654:C:C2'	2.58	0.51
5:E:166:LYS:O	5:E:169:ASP:HB2	2.10	0.51
7:G:74:THR:O	7:G:77:GLN:NE2	2.42	0.51
15:O:22:VAL:CG2	15:O:23:VAL:N	2.73	0.51
13:M:40:ASP:OD1	13:M:42:LYS:N	2.41	0.51
13:M:70:PHE:CZ	13:M:72:LEU:HD12	2.46	0.51
2:B:55:THR:HG23	53:1:3049:A:N3	2.25	0.51
15:O:155:LYS:O	15:O:155:LYS:HG2	2.11	0.51
53:1:2724:U:C2'	53:1:2724:U:O2	2.58	0.51
53:1:26:A:N3	53:1:328:U:O2'	2.43	0.51
55:3:82:G:N1	55:3:98:C:C5	2.79	0.51
15:O:57:PHE:HA	15:O:60:LYS:NZ	2.24	0.51
56:4:247:ILE:HD11	56:4:318:LEU:HB2	1.93	0.51
58:6:26:U:O2'	58:6:27:G:P	2.69	0.51
2:B:76:VAL:HB	2:B:324:VAL:O	2.11	0.51
15:O:62:THR:OG1	15:O:69:GLY:HA2	2.11	0.51
2:B:238:LEU:HD21	2:B:250:ALA:HB2	1.93	0.51
26:Z:46:ILE:HD11	26:Z:49:TYR:CE2	2.45	0.51
53:1:1228:C:N3	53:1:1282:G:O6	2.44	0.51
53:1:1282:G:O2'	53:1:1283:C:O4'	2.28	0.51
53:1:3025:C:H2'	53:1:3026:G:H5'	1.93	0.51
12:L:130:GLY:O	12:L:132:ALA:N	2.44	0.51
15:O:34:VAL:HG13	15:O:34:VAL:O	2.10	0.51
16:P:138:LYS:HD2	16:P:140:GLU:OE1	2.12	0.50
53:1:1204:A:H2'	53:1:1205:A:O4'	2.11	0.50
53:1:1281:G:C2	53:1:1282:G:N7	2.80	0.50
53:1:2759:U:O4	53:1:2760:C:N4	2.44	0.50
53:1:2969:A:O2'	53:1:2970:C:O4'	2.29	0.50
3:C:3:ARG:NH1	3:C:27:SER:OG	2.44	0.50
12:L:47:ALA:CB	12:L:48:PRO:HD3	2.41	0.50
53:1:1724:U:H1'	53:1:1725:C:C6	2.46	0.50
58:6:33:U:C2'	58:6:33:U:O2	2.58	0.50
5:E:157:GLN:OE1	5:E:157:GLN:N	2.44	0.50
19:S:124:LEU:HD22	20:T:153:PRO:HB3	1.92	0.50
3:C:205:PRO:HD2	3:C:225:VAL:HG22	1.94	0.50
16:P:138:LYS:O	16:P:138:LYS:HG3	2.10	0.50
19:S:45:LEU:HB3	19:S:51:VAL:HG21	1.94	0.50
53:1:2825:C:O2	53:1:2825:C:O4'	2.30	0.50
2:B:95:THR:HG22	53:1:3243:A:H4'	1.94	0.50
5:E:2:SER:N	53:1:1387:G:HO2'	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:95:TRP:CE3	4:D:198:TYR:HB3	2.47	0.50
4:D:90:HIS:HB3	4:D:226:TYR:CZ	2.47	0.50
6:F:197:GLN:OE1	6:F:197:GLN:N	2.45	0.50
2:B:344:THR:HG23	26:Z:26:VAL:HG21	165.12	0.50
53:1:2862:U:O2	53:1:2862:U:O4'	2.29	0.50
55:3:84:A:C6	55:3:97:A:N1	2.79	0.50
2:B:110:LEU:HD13	2:B:130:PHE:CD2	2.47	0.50
5:E:54:TYR:HE1	5:E:63:LEU:HD22	1.76	0.50
19:S:25:PHE:CD2	20:T:151:LEU:HD13	2.47	0.50
20:T:154:VAL:N	20:T:155:PRO:HA	2.27	0.50
22:V:45:ARG:CG	22:V:48:ARG:NH1	2.73	0.50
53:1:2597:U:HO2'	53:1:2598:G:H5'	1.76	0.50
53:1:2108:C:H1'	53:1:3344:A:C8	2.46	0.50
8:H:188:THR:HA	8:H:189:GLU:HG2	1.94	0.50
15:O:128:ARG:O	15:O:129:LEU:O	2.30	0.50
15:O:48:PHE:O	15:O:49:ARG:C	2.48	0.50
53:1:2887:A:N3	53:1:2887:A:H5'	2.27	0.49
58:6:23:U:O2'	58:6:24:A:OP1	2.21	0.49
2:B:110:LEU:HB3	2:B:114:VAL:HG21	1.94	0.49
15:O:133:ARG:CZ	15:O:133:ARG:HB3	2.40	0.49
53:1:644:G:O2'	53:1:645:A:O5'	2.28	0.49
2:B:139:GLN:C	2:B:141:GLY:N	2.60	0.49
3:C:354:VAL:O	3:C:358:THR:HG23	2.11	0.49
7:G:134:TYR:CB	7:G:190:VAL:HG21	2.41	0.49
7:G:238:LEU:HD13	7:G:243:GLN:HE21	1.76	0.49
22:V:45:ARG:HD2	22:V:46:LEU:H	1.77	0.49
2:B:19:ARG:NH2	2:B:232:ARG:O	2.46	0.49
14:N:4:TYR:CG	14:N:5:LYS:N	2.80	0.49
20:T:119:ALA:HB1	20:T:124:VAL:HG11	1.93	0.49
58:6:231:A:O2'	58:6:232:A:N3	2.36	0.49
2:B:14:LEU:HD22	2:B:262:TRP:CZ3	2.48	0.49
2:B:50:LYS:HA	2:B:79:VAL:HA	1.94	0.49
12:L:36:ARG:NH2	53:1:687:U:OP2	2.45	0.49
53:1:551:A:O2'	53:1:552:G:O5'	2.30	0.49
15:O:36:VAL:HG21	15:O:108:ILE:HG12	1.95	0.49
53:1:2596:U:C4	53:1:2597:U:C5	3.01	0.49
53:1:2731:U:O2	53:1:2731:U:C2'	2.61	0.49
5:E:69:PHE:HB3	5:E:138:GLN:HE21	1.77	0.49
4:D:55:PHE:CE1	4:D:159:VAL:HG22	2.48	0.49
5:E:69:PHE:CB	5:E:138:GLN:HE21	2.25	0.49
53:1:40:A:H2'	53:1:40:A:N3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:79:ALA:HB2	53:1:525:C:H5''	1.95	0.49
15:O:142:SER:HA	15:O:145:VAL:CG2	2.42	0.49
4:D:111:GLN:NE2	4:D:252:ALA:HB2	2.28	0.49
1:A:93:LYS:NZ	53:1:2548:C:C5'	2.76	0.48
53:1:2794:G:N3	53:1:2795:U:O4	2.46	0.48
7:G:50:VAL:HG11	24:X:27:ARG:HG3	1.95	0.48
11:K:124:LEU:CD2	11:K:155:ILE:HD13	2.42	0.48
12:L:93:ILE:HG22	12:L:93:ILE:O	2.13	0.48
20:T:67:VAL:HA	20:T:72:VAL:HG12	1.94	0.48
1:A:101:VAL:C	1:A:102:LEU:HD12	2.34	0.48
2:B:35:ASP:OD1	2:B:184:ASN:O	2.30	0.48
15:O:73:PHE:HB3	15:O:78:ARG:CG	2.37	0.48
53:1:2241:U:O2'	53:1:2244:A:N6	2.45	0.48
15:O:47:PHE:O	15:O:48:PHE:C	2.51	0.48
6:F:159:GLN:O	53:1:1362:G:H4'	2.14	0.48
53:1:2548:C:P	53:1:2548:C:H3'	2.54	0.48
58:6:228:U:C2'	58:6:228:U:O2	2.61	0.48
3:C:10:SER:OG	3:C:13:GLY:O	2.28	0.48
4:D:64:ILE:HD12	4:D:64:ILE:N	2.28	0.48
53:1:2722:U:O2	53:1:2722:U:O4'	2.30	0.48
53:1:1299:U:O2	53:1:1299:U:O4'	2.31	0.48
53:1:2511:A:O2'	53:1:2512:C:C5'	2.61	0.48
5:E:149:ILE:HG23	5:E:155:LEU:HD12	1.96	0.48
14:N:188:ARG:NH2	53:1:31:C:OP2	2.44	0.48
53:1:2428:U:C4	53:1:2602:G:N1	2.62	0.48
2:B:236:LYS:NZ	22:V:47:ASN:HD22	2.11	0.48
2:B:56:ILE:HD13	2:B:76:VAL:CG2	2.44	0.48
3:C:292:SER:OG	3:C:294:GLU:OE1	2.31	0.48
7:G:160:ILE:O	7:G:164:VAL:HG13	2.14	0.48
53:1:2819:A:H4'	53:1:2820:A:OP2	2.13	0.48
12:L:80:VAL:HG12	12:L:85:LEU:O	2.14	0.48
22:V:47:ASN:O	53:1:2338:C:H4'	2.14	0.48
53:1:1281:G:N2	53:1:1282:G:C5	2.82	0.48
2:B:303:LYS:HD3	2:B:361:THR:HG21	1.95	0.48
15:O:108:ILE:CG2	15:O:113:ASP:CA	2.92	0.48
15:O:64:PHE:CE2	15:O:68:ARG:HD3	2.49	0.48
1:A:93:LYS:HZ3	53:1:2548:C:H5''	1.79	0.47
53:1:3023:U:O2	53:1:3023:U:O4'	2.29	0.47
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.46	0.47
7:G:227:ASP:OD1	7:G:228:GLU:N	2.47	0.47
15:O:21:SER:O	15:O:22:VAL:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:41:LEU:HD22	15:O:80:PHE:HD2	1.74	0.47
56:4:66:LEU:HD12	56:4:108:ILE:HD11	1.97	0.47
7:G:153:ILE:HG23	7:G:163:VAL:HG11	1.95	0.47
15:O:192:LYS:O	15:O:195:ALA:HB3	2.14	0.47
3:C:264:SER:OG	3:C:267:VAL:HG22	2.13	0.47
8:H:18:VAL:HG12	8:H:27:VAL:HG22	1.96	0.47
12:L:9:ILE:HD13	12:L:9:ILE:N	2.29	0.47
15:O:84:LEU:HD23	15:O:84:LEU:C	2.35	0.47
17:Q:57:ILE:HD12	53:1:671:U:OP2	2.14	0.47
18:R:115:ILE:HD11	18:R:119:LEU:HG	1.96	0.47
20:T:119:ALA:O	20:T:122:GLN:O	2.32	0.47
11:K:245:ASN:HD22	11:K:245:ASN:C	2.18	0.47
15:O:88:VAL:CG1	15:O:89:SER:N	2.76	0.47
53:1:2759:U:C3'	53:1:2760:C:H5'	2.45	0.47
4:D:103:LEU:HD13	4:D:168:ASP:HB2	1.97	0.47
8:H:16:VAL:HG21	8:H:79:ILE:HG23	1.96	0.47
53:1:2760:C:O2'	53:1:2761:G:O4'	2.23	0.47
53:1:2793:G:C3'	53:1:2794:G:H5''	2.44	0.47
53:1:2793:G:N3	53:1:2793:G:H2'	2.28	0.47
53:1:2901:G:H5''	53:1:2901:G:C8	2.50	0.47
11:K:93:LYS:HE2	58:6:24:A:N3	2.30	0.47
2:B:52:GLY:O	2:B:53:MET:HB2	2.15	0.47
2:B:283:TYR:OH	2:B:325:LYS:HD2	2.15	0.47
8:H:61:GLY:O	8:H:65:VAL:HG23	2.15	0.47
11:K:277:ARG:CZ	11:K:298:LEU:HD21	2.45	0.47
15:O:77:SER:CB	15:O:104:VAL:HG12	2.37	0.47
15:O:133:ARG:HH11	15:O:133:ARG:HA	1.79	0.47
15:O:193:GLN:O	15:O:196:ALA:HB3	2.15	0.47
7:G:217:THR:O	7:G:221:ASN:ND2	2.46	0.46
8:H:86:TYR:CZ	8:H:151:VAL:HG22	2.50	0.46
13:M:77:ARG:HG2	13:M:77:ARG:HH11	1.80	0.46
53:1:2792:A:H2'	53:1:2793:G:O4'	2.14	0.46
53:1:3158:G:HO2'	53:1:3159:C:C5'	2.27	0.46
15:O:129:LEU:HD12	15:O:129:LEU:HA	1.75	0.46
4:D:182:GLY:HA3	4:D:194:LEU:HD22	1.98	0.46
8:H:124:ARG:HG2	8:H:164:ILE:HD12	1.97	0.46
15:O:31:GLN:HE21	15:O:31:GLN:HA	1.80	0.46
16:P:138:LYS:HD2	16:P:140:GLU:CD	2.35	0.46
22:V:37:ILE:HD11	22:V:73:VAL:HG21	1.96	0.46
1:A:9:ARG:NH1	53:1:912:G:OP2	2.49	0.46
3:C:150:LEU:HD23	3:C:151:VAL:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:GLN:HE21	4:D:17:GLN:H	1.63	0.46
8:H:139:ASN:HD22	8:H:139:ASN:C	2.19	0.46
53:1:2137:U:OP2	53:1:2142:A:N6	2.46	0.46
53:1:3156:U:HO2'	53:1:3157:U:P	2.38	0.46
2:B:220:VAL:N	2:B:221:THR:HG23	2.30	0.46
7:G:134:TYR:CD1	7:G:190:VAL:HG21	2.50	0.46
13:M:77:ARG:HG2	13:M:77:ARG:NH1	2.31	0.46
15:O:148:LYS:HD3	15:O:148:LYS:N	2.17	0.46
53:1:3157:U:H4'	53:1:3158:G:O5'	2.16	0.46
2:B:218:ILE:HG23	2:B:276:THR:HG23	1.97	0.46
15:O:168:TYR:CE2	15:O:172:ARG:HD3	2.51	0.46
4:D:65:ILE:HG22	4:D:66:SER:O	2.16	0.46
53:1:2528:G:C6	53:1:2529:A:C5	3.04	0.46
1:A:93:LYS:HZ3	53:1:2548:C:C5'	2.29	0.46
6:F:102:VAL:HG13	6:F:126:LEU:HD22	1.97	0.46
15:O:194:LEU:O	15:O:195:ALA:C	2.54	0.46
4:D:39:GLN:O	53:1:2749:G:O5'	2.33	0.46
2:B:93:VAL:HG22	2:B:155:ALA:H	1.80	0.46
12:L:153:ASP:OD1	12:L:154:VAL:N	2.48	0.46
53:1:2793:G:H2'	53:1:2794:G:H5''	1.97	0.46
1:A:27:ALA:O	1:A:128:ARG:NH2	2.49	0.46
5:E:136:GLU:O	5:E:140:VAL:HG23	2.16	0.46
15:O:190:VAL:HG13	15:O:191:ALA:N	2.31	0.46
26:Z:13:VAL:HG22	26:Z:80:LEU:HD21	1.98	0.46
1:A:117:GLU:OE1	1:A:163:ARG:NE	2.50	0.45
10:J:80:LEU:HD22	10:J:84:LEU:HD12	1.98	0.45
8:H:18:VAL:CG1	8:H:27:VAL:HG22	2.47	0.45
53:1:2190:U:H2'	53:1:2191:U:H5'	1.99	0.45
53:1:2332:A:H2'	53:1:2333:C:O4'	2.16	0.45
2:B:59:ASP:N	2:B:59:ASP:OD1	2.49	0.45
2:B:79:VAL:HG13	2:B:322:ILE:HB	1.99	0.45
15:O:73:PHE:CD1	15:O:78:ARG:HG2	2.52	0.45
53:1:2528:G:C4	53:1:2529:A:C5	3.05	0.45
53:1:2758:A:C4	53:1:2759:U:O2	2.70	0.45
8:H:76:ASP:O	8:H:80:THR:HG23	2.17	0.45
53:1:3217:C:H2'	53:1:3217:C:O2	2.17	0.45
53:1:374:A:HO2'	53:1:376:G:H8	1.64	0.45
7:G:136:LEU:HD23	7:G:136:LEU:C	2.37	0.45
8:H:67:ALA:O	8:H:70:THR:HG22	2.17	0.45
53:1:2236:G:H2'	53:1:2237:C:C6	2.52	0.45
53:1:2428:U:O2	53:1:2428:U:H2'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ILE:HG12	2:B:321:PHE:CE2	2.52	0.45
12:L:73:ARG:NH1	53:1:110:G:OP2	2.50	0.45
13:M:47:ASP:OD1	13:M:48:GLY:N	2.49	0.45
15:O:54:TYR:O	15:O:55:HIS:C	2.53	0.45
26:Z:81:LEU:C	26:Z:81:LEU:CD2	2.86	0.45
3:C:197:ARG:NH1	53:1:1381:A:OP1	2.50	0.45
53:1:908:G:N1	53:1:2414:G:OP1	2.50	0.45
8:H:128:VAL:HG13	8:H:132:VAL:HG13	1.98	0.45
8:H:133:THR:C	8:H:134:ILE:HD12	2.37	0.45
53:1:1130:A:H2'	53:1:1131:G:O4'	2.17	0.45
16:P:67:ILE:HD11	53:1:1447:G:H3'	1.98	0.45
2:B:233:TRP:CG	2:B:265:ALA:HB1	2.52	0.45
4:D:198:TYR:CD2	4:D:203:HIS:CE1	3.05	0.45
4:D:205:SER:CB	4:D:233:ALA:HB1	2.46	0.45
8:H:8:GLN:HG2	8:H:68:LEU:HD11	1.97	0.45
14:N:110:ALA:HB1	14:N:113:LEU:HD22	1.98	0.45
15:O:40:GLU:OE2	15:O:40:GLU:HA	2.17	0.45
17:Q:36:LEU:HB3	17:Q:45:ASN:HD22	1.82	0.45
53:1:1307:G:C2	53:1:1308:A:C2	3.05	0.44
53:1:2527:G:O2'	53:1:2528:G:C8	2.70	0.44
53:1:2546:C:H2'	53:1:2548:C:OP1	2.14	0.44
4:D:23:ARG:O	4:D:25:GLU:O	2.34	0.44
4:D:99:TYR:CE2	4:D:199:ILE:HG23	2.53	0.44
5:E:54:TYR:CE1	5:E:63:LEU:HD22	2.52	0.44
53:1:2427:U:C2	53:1:2428:U:C4	3.05	0.44
53:1:2598:G:H2'	53:1:2599:U:C6	2.52	0.44
11:K:192:LYS:HE3	58:6:25:G:O5'	2.17	0.44
58:6:5:C:O4'	58:6:5:C:O2	2.35	0.44
2:B:47:LEU:HB3	2:B:337:THR:HG23	1.99	0.44
3:C:304:GLN:O	3:C:305:ALA:HB3	2.17	0.44
4:D:146:LEU:HB2	4:D:173:VAL:HG21	1.98	0.44
5:E:58:LEU:HD12	5:E:62:THR:OG1	2.17	0.44
5:E:65:ILE:HD11	5:E:77:ARG:HB3	1.98	0.44
14:N:119:TYR:OH	14:N:131:GLU:OE1	2.27	0.44
53:1:2255:A:C8	53:1:2261:G:N2	2.48	0.44
53:1:2528:G:C5	53:1:2529:A:C4	3.05	0.44
53:1:2432:A:C2	53:1:2598:G:C6	3.05	0.44
2:B:106:TRP:HB2	2:B:133:TYR:CE2	2.51	0.44
2:B:208:VAL:O	2:B:208:VAL:HG12	2.18	0.44
3:C:193:LYS:HB2	3:C:193:LYS:NZ	2.32	0.44
17:Q:71:LEU:HD22	17:Q:99:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:66:ASN:O	20:T:73:GLY:N	2.50	0.44
53:1:2900:A:O2'	53:1:2901:G:OP1	2.33	0.44
9:I:45:GLY:O	9:I:46:LEU:HD22	2.17	0.44
15:O:108:ILE:HG22	15:O:113:ASP:CB	2.46	0.44
15:O:55:HIS:O	15:O:58:LEU:CB	2.66	0.44
53:1:2900:A:C2'	53:1:2901:G:OP1	2.66	0.44
53:1:3153:U:O2'	53:1:3154:C:C6	2.70	0.44
2:B:141:GLY:O	2:B:143:GLY:N	2.51	0.44
4:D:59:ASP:OD1	4:D:80:SER:OG	2.35	0.44
13:M:65:LEU:HG	19:S:152:LEU:HD11	1.98	0.44
15:O:97:ALA:O	15:O:101:ARG:NH1	2.50	0.44
26:Z:23:VAL:HG12	26:Z:45:GLY:HA3	2.00	0.44
53:1:3158:G:O2'	53:1:3159:C:C5'	2.66	0.44
56:4:319:ILE:HG22	56:4:321:LEU:HD23	1.99	0.44
2:B:152:LYS:HG2	2:B:192:VAL:HG11	1.99	0.44
4:D:83:LEU:O	4:D:87:GLY:N	2.51	0.44
15:O:77:SER:HB2	15:O:104:VAL:HG11	1.98	0.44
53:1:2432:A:N1	53:1:2598:G:C6	2.86	0.44
53:1:2793:G:H2'	53:1:2794:G:C5'	2.47	0.44
2:B:41:VAL:HA	2:B:185:GLY:HA3	2.00	0.44
4:D:153:THR:HG23	4:D:160:PHE:CE2	2.51	0.44
15:O:148:LYS:O	15:O:149:TYR:CD1	2.71	0.44
15:O:26:GLN:CB	15:O:33:ILE:HD11	2.47	0.44
53:1:2405:C:N3	53:1:2817:A:N6	2.66	0.44
2:B:218:ILE:HG22	2:B:276:THR:HA	1.99	0.44
5:E:56:LYS:HB2	5:E:98:VAL:HG11	2.00	0.44
14:N:27:VAL:HB	14:N:122:ASN:ND2	2.33	0.44
15:O:45:GLY:O	15:O:135:TYR:C	2.56	0.44
58:6:26:U:C2'	58:6:27:G:C8	3.01	0.44
6:F:88:ARG:HG2	6:F:111:ILE:HA	1.99	0.44
20:T:154:VAL:HB	20:T:155:PRO:C	2.37	0.44
20:T:58:GLN:HA	20:T:58:GLN:NE2	2.33	0.44
2:B:216:ASP:CB	2:B:278:ILE:HA	2.48	0.43
3:C:206:LEU:HD23	3:C:207:VAL:N	2.33	0.43
15:O:104:VAL:HG12	15:O:105:PHE:N	2.33	0.43
24:X:105:VAL:CG1	24:X:126:LEU:HD22	2.48	0.43
53:1:2759:U:O4	53:1:2760:C:C4	2.70	0.43
53:1:2793:G:O6	53:1:2794:G:C5	2.71	0.43
3:C:313:LEU:HD22	3:C:314:LYS:N	2.33	0.43
7:G:155:ASN:OD1	7:G:156:ASP:N	2.51	0.43
12:L:60:ALA:HB3	12:L:65:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:185:ALA:O	15:O:186:ALA:O	2.36	0.43
23:W:64:LYS:HE3	23:W:66:ILE:HD11	1.99	0.43
53:1:2398:A:H2'	53:1:2399:A:O4'	2.17	0.43
53:1:2528:G:C4	53:1:2529:A:C8	3.06	0.43
13:M:77:ARG:HG3	53:1:561:C:OP1	2.19	0.43
58:6:33:U:O2	58:6:33:U:H2'	2.19	0.43
4:D:22:ARG:O	4:D:25:GLU:HB2	2.18	0.43
6:F:156:ILE:HD12	6:F:161:VAL:HB	2.01	0.43
10:J:49:LYS:HB3	10:J:62:ASN:HA	1.99	0.43
13:M:116:GLU:O	13:M:120:VAL:HG23	2.17	0.43
15:O:23:VAL:O	15:O:24:ALA:C	2.57	0.43
15:O:56:ASP:OD1	15:O:56:ASP:N	2.51	0.43
53:1:2399:A:H2'	53:1:2400:G:O4'	2.18	0.43
1:A:117:GLU:OE2	1:A:121:GLY:N	2.52	0.43
4:D:27:LYS:O	4:D:150:LEU:HD12	2.19	0.43
6:F:83:LEU:HD12	6:F:139:PRO:CG	2.48	0.43
15:O:16:VAL:HG21	15:O:43:ILE:HG12	2.00	0.43
18:R:10:LEU:HA	18:R:10:LEU:HD12	1.85	0.43
53:1:651:G:O2'	53:1:1435:A:OP1	2.37	0.43
2:B:138:ALA:C	2:B:139:GLN:HG3	2.39	0.43
6:F:160:ARG:NH2	6:F:206:LYS:HD3	2.32	0.43
15:O:115:LYS:N	15:O:115:LYS:HD2	2.33	0.43
22:V:136:VAL:HG12	22:V:137:VAL:HG23	1.99	0.43
53:1:2432:A:C6	53:1:2598:G:C6	3.06	0.43
6:F:203:TRP:CD1	6:F:204:PRO:HD2	2.53	0.43
15:O:139:GLY:O	15:O:150:GLU:OE2	2.37	0.43
53:1:1057:A:H4'	53:1:1058:U:OP1	2.19	0.43
53:1:3153:U:O2'	53:1:3154:C:H6	2.01	0.43
1:A:7:ASN:OD1	1:A:8:GLN:N	2.51	0.43
2:B:84:VAL:HG13	2:B:162:VAL:HB	1.99	0.43
6:F:139:PRO:HA	6:F:237:ASN:OD1	2.19	0.43
7:G:145:ASN:N	7:G:146:LYS:HA	2.34	0.43
10:J:46:VAL:O	10:J:67:VAL:HA	2.19	0.43
12:L:76:THR:HG23	12:L:101:ARG:NH1	2.34	0.43
15:O:19:LEU:HD23	15:O:80:PHE:CE2	2.45	0.43
20:T:89:LEU:HD23	20:T:90:ASN:N	2.33	0.43
2:B:171:LEU:HD23	2:B:172:ALA:N	2.34	0.43
5:E:42:LEU:HD23	5:E:42:LEU:N	2.34	0.43
6:F:165:ASP:OD1	6:F:166:ASN:N	2.52	0.43
8:H:23:ARG:NH2	8:H:39:LYS:O	2.52	0.43
10:J:94:ARG:O	10:J:96:PHE:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:102:VAL:HG21	11:K:234:LEU:HD13	2.01	0.43
11:K:144:LEU:HD22	11:K:149:ILE:HD11	2.01	0.43
15:O:50:ASN:ND2	15:O:136:THR:HB	2.33	0.43
15:O:160:ARG:O	15:O:161:LYS:C	2.56	0.43
22:V:45:ARG:HH11	22:V:46:LEU:N	2.11	0.43
24:X:105:VAL:HG11	24:X:126:LEU:HD22	2.00	0.43
53:1:2522:G:N3	53:1:2522:G:H2'	2.34	0.43
2:B:240:ARG:NH2	53:1:874:U:OP1	2.52	0.43
15:O:195:ALA:O	15:O:198:GLY:HA2	2.19	0.43
53:1:1187:C:O5'	53:1:1187:C:O2	2.37	0.43
53:1:2528:G:O2'	53:1:2529:A:H8	2.01	0.43
4:D:152:ARG:HD3	53:1:2663:G:OP1	2.14	0.43
1:A:122:ASP:OD2	1:A:125:ALA:HB2	2.19	0.43
2:B:188:ILE:HD12	2:B:189:SER:H	1.84	0.43
8:H:103:ILE:HD11	8:H:134:ILE:HG22	2.01	0.43
20:T:152:ALA:CB	20:T:153:PRO:CD	2.92	0.43
8:H:188:THR:HA	8:H:189:GLU:CB	2.49	0.42
9:I:46:LEU:N	9:I:46:LEU:HD13	2.34	0.42
22:V:81:GLN:O	22:V:82:ALA:HB3	2.19	0.42
53:1:1716:U:HO2'	53:1:1717:U:P	2.42	0.42
4:D:173:VAL:O	4:D:175:HIS:ND1	2.43	0.42
6:F:131:GLU:N	6:F:132:PRO:CD	2.82	0.42
56:4:447:HIS:CE1	56:4:492:THR:HG22	2.54	0.42
3:C:23:PRO:O	3:C:24:ALA:HB3	2.20	0.42
5:E:50:LYS:NZ	5:E:72:ASN:O	2.48	0.42
18:R:128:LYS:NZ	53:1:1721:U:O4	2.52	0.42
53:1:2547:A:O5'	53:1:2548:C:P	2.78	0.42
53:1:2793:G:H2'	53:1:2794:G:O5'	2.18	0.42
53:1:2969:A:O2'	53:1:2970:C:O5'	2.38	0.42
2:B:60:LEU:HD21	2:B:62:ARG:NH1	2.34	0.42
3:C:265:GLU:CD	3:C:266:THR:HG23	2.39	0.42
12:L:57:VAL:HG22	12:L:147:ILE:HD12	2.01	0.42
15:O:128:ARG:O	15:O:129:LEU:C	2.57	0.42
15:O:45:GLY:O	15:O:135:TYR:HA	2.19	0.42
15:O:89:SER:O	15:O:92:THR:OG1	2.37	0.42
20:T:75:ILE:C	20:T:75:ILE:HD13	2.40	0.42
53:1:2921:U:O2	53:1:2921:U:O4'	2.36	0.42
2:B:4:ARG:NH1	2:B:6:TYR:O	2.53	0.42
3:C:209:TYR:CE2	3:C:212:ASP:HB2	2.55	0.42
2:B:85:VAL:HG13	2:B:163:HIS:CD2	2.55	0.42
4:D:146:LEU:CD2	4:D:163:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:58:VAL:HG13	53:1:75:G:H5'	2.01	0.42
7:G:50:VAL:HG12	24:X:30:ALA:HA	2.00	0.42
53:1:1302:A:O2'	53:1:1303:A:O5'	2.24	0.42
54:2:158:U:O2	54:2:158:U:O4'	2.35	0.42
2:B:22:ALA:HB3	2:B:220:VAL:HG11	2.01	0.42
15:O:177:LYS:HB3	15:O:177:LYS:HE2	1.72	0.42
15:O:78:ARG:O	15:O:81:TYR:HB3	2.19	0.42
20:T:58:GLN:HA	20:T:58:GLN:HE21	1.84	0.42
53:1:3306:U:O2	53:1:3306:U:O4'	2.38	0.42
53:1:662:U:H2'	53:1:663:C:C6	2.54	0.42
12:L:18:TRP:NE1	53:1:799:G:O2'	2.44	0.42
4:D:34:LYS:O	4:D:37:VAL:HB	2.20	0.42
15:O:150:GLU:O	15:O:150:GLU:CG	2.66	0.42
15:O:192:LYS:HG2	15:O:192:LYS:H	1.73	0.42
53:1:1561:G:O2'	53:1:1562:C:OP2	2.32	0.42
4:D:232:ASP:OD1	4:D:232:ASP:N	2.52	0.42
4:D:40:HIS:CG	4:D:43:LYS:HD2	2.54	0.42
15:O:104:VAL:C	15:O:105:PHE:CG	2.93	0.42
1:A:191:LEU:HD11	53:1:1795:U:P	2.60	0.42
56:4:42:VAL:HG12	56:4:46:ILE:HD12	2.01	0.42
2:B:54:THR:OG1	2:B:55:THR:N	2.52	0.42
3:C:316:ASN:HD22	3:C:319:LYS:HE3	1.84	0.42
4:D:64:ILE:HG12	4:D:105:ILE:HD11	2.01	0.42
15:O:8:VAL:HA	15:O:34:VAL:HG13	2.02	0.42
53:1:1329:U:O2'	53:1:1330:A:OP1	2.30	0.41
53:1:1481:A:O2'	53:1:1858:A:N3	2.40	0.41
53:1:3158:G:O2'	53:1:3159:C:O5'	2.37	0.41
55:3:98:C:O2	55:3:98:C:H2'	2.19	0.41
2:B:47:LEU:HD12	2:B:337:THR:HG23	2.02	0.41
4:D:40:HIS:HB3	4:D:41:LYS:HA	2.01	0.41
20:T:151:LEU:O	20:T:152:ALA:HB3	2.20	0.41
1:A:13:GLY:O	1:A:17:THR:HG23	2.19	0.41
4:D:59:ASP:OD1	4:D:60:ILE:N	2.53	0.41
5:E:170:LYS:O	5:E:174:LEU:HG	2.20	0.41
8:H:18:VAL:HG12	8:H:27:VAL:HG13	2.02	0.41
10:J:32:ARG:NH1	10:J:120:ILE:O	2.53	0.41
7:G:129:PRO:HB3	53:1:121:A:C2	2.55	0.41
2:B:96:PRO:HB3	15:O:153:VAL:HG22	2.02	0.41
4:D:223:PHE:O	4:D:227:LEU:HD13	2.21	0.41
5:E:38:THR:HA	5:E:90:LYS:HE2	2.00	0.41
7:G:80:TYR:CD2	7:G:229:VAL:CG2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:132:LYS:O	13:M:135:LEU:O	2.39	0.41
15:O:67:THR:C	15:O:69:GLY:H	2.23	0.41
53:1:2625:C:O2	53:1:2656:A:H1'	2.20	0.41
58:6:25:G:O2'	58:6:26:U:P	2.78	0.41
2:B:46:PHE:CE1	2:B:84:VAL:HG23	2.55	0.41
3:C:316:ASN:HD22	3:C:319:LYS:CE	2.34	0.41
3:C:92:ASN:N	3:C:92:ASN:OD1	2.54	0.41
4:D:219:PHE:CD2	4:D:227:LEU:HD21	2.56	0.41
5:E:5:LYS:O	5:E:6:ALA:HB3	2.21	0.41
8:H:90:MET:HB2	8:H:144:ILE:HG23	2.01	0.41
20:T:119:ALA:HB1	20:T:124:VAL:HG21	2.02	0.41
20:T:66:ASN:HB3	20:T:73:GLY:HA3	2.01	0.41
53:1:1201:C:O2'	53:1:1202:A:N3	2.39	0.41
53:1:2761:G:H1	53:1:2798:C:N4	2.19	0.41
3:C:138:ARG:NH2	53:1:1383:G:O3'	2.53	0.41
13:M:128:ARG:CD	13:M:132:LYS:NZ	2.79	0.41
15:O:45:GLY:O	15:O:135:TYR:CA	2.68	0.41
15:O:46:GLU:O	15:O:46:GLU:HG3	2.20	0.41
53:1:19:U:H2'	53:1:20:A:C8	2.55	0.41
53:1:2509:U:O2'	53:1:2510:U:H5'	2.21	0.41
5:E:28:GLN:OE1	5:E:61:ASN:HB3	2.21	0.41
11:K:125:LEU:HD21	11:K:222:LEU:HD11	2.02	0.41
11:K:45:ILE:HA	11:K:48:THR:HG22	2.01	0.41
26:Z:2:ALA:N	53:1:3015:G:OP2	148.11	0.41
3:C:319:LYS:O	3:C:320:ASN:CB	2.69	0.41
6:F:216:VAL:HG11	6:F:226:GLY:O	2.21	0.41
7:G:184:ALA:O	7:G:188:THR:HG23	2.20	0.41
7:G:33:ASN:HB3	7:G:38:GLN:NE2	2.34	0.41
9:I:68:LEU:HD23	9:I:73:HIS:CD2	2.56	0.41
12:L:56:PRO:HG3	12:L:74:GLY:C	2.41	0.41
20:T:94:GLU:H	20:T:94:GLU:CD	2.24	0.41
53:1:2759:U:C5	53:1:2760:C:C6	2.97	0.41
1:A:116:VAL:HG11	1:A:134:VAL:HG21	2.03	0.41
2:B:286:GLY:O	2:B:320:ASP:HA	2.20	0.41
4:D:33:ARG:O	4:D:37:VAL:HG23	2.20	0.41
7:G:94:PHE:CD2	7:G:132:VAL:HG11	2.56	0.41
53:1:1281:G:O2'	53:1:1282:G:C5'	2.69	0.41
53:1:2730:G:C2'	53:1:2730:G:N3	2.84	0.41
53:1:3154:C:O2'	53:1:3155:U:P	2.79	0.41
54:2:104:A:OP2	54:2:105:A:H2'	2.20	0.41
6:F:83:LEU:HD13	6:F:84:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:112:ILE:HD11	8:H:134:ILE:HG12	2.03	0.41
15:O:78:ARG:O	15:O:79:ILE:C	2.58	0.41
15:O:80:PHE:C	15:O:80:PHE:CD1	2.94	0.41
15:O:82:LYS:O	15:O:83:ALA:C	2.59	0.41
53:1:2714:G:C2'	53:1:2714:G:N3	2.84	0.41
53:1:3019:U:O2	53:1:3019:U:O5'	2.39	0.41
2:B:104:THR:HG1	53:1:3148:U:C4'	2.34	0.41
3:C:150:LEU:HD11	3:C:172:VAL:CG1	2.50	0.41
4:D:96:ALA:HB2	4:D:198:TYR:O	2.21	0.41
12:L:55:ARG:O	12:L:115:ARG:NE	2.53	0.41
12:L:8:PRO:HB2	12:L:9:ILE:HD13	2.03	0.41
13:M:45:LEU:HD12	13:M:56:GLN:O	2.21	0.41
15:O:116:LYS:HG3	15:O:117:ARG:N	2.35	0.41
18:R:60:LYS:NZ	53:1:1671:C:OP1	2.53	0.41
53:1:2528:G:N1	53:1:2529:A:C4	2.83	0.41
53:1:3375:A:O2'	53:1:3378:C:OP2	2.35	0.41
24:X:56:ARG:NH2	54:2:135:G:OP2	2.53	0.41
2:B:166:ILE:HD11	2:B:171:LEU:HD22	2.03	0.41
3:C:6:VAL:HG12	3:C:7:THR:N	2.36	0.41
6:F:86:VAL:HG22	6:F:136:TYR:CB	2.50	0.41
11:K:124:LEU:HD23	11:K:125:LEU:N	2.36	0.41
15:O:22:VAL:HG21	15:O:120:VAL:HG11	2.02	0.41
15:O:194:LEU:O	15:O:198:GLY:N	2.46	0.41
15:O:8:VAL:HA	15:O:34:VAL:CG1	2.50	0.41
20:T:154:VAL:N	20:T:155:PRO:CA	2.84	0.41
20:T:78:LYS:O	20:T:85:LEU:N	2.47	0.41
20:T:40:VAL:HG12	20:T:98:HIS:HA	2.03	0.41
2:B:198:HIS:O	2:B:201:LYS:HB2	2.20	0.40
15:O:65:ASN:HD22	15:O:68:ARG:HD2	1.85	0.40
15:O:74:ARG:O	15:O:142:SER:OG	2.26	0.40
1:A:200:ARG:NH1	53:1:2146:C:OP1	2.53	0.40
53:1:2529:A:C6	53:1:2530:G:C6	3.09	0.40
53:1:2758:A:C2'	53:1:2759:U:O5'	2.70	0.40
53:1:303:G:C2	53:1:313:A:C2	3.09	0.40
56:4:124:THR:HG23	56:4:125:PHE:CD2	2.56	0.40
4:D:215:ASP:OD1	4:D:216:GLU:N	2.53	0.40
4:D:65:ILE:HG12	4:D:74:VAL:HG22	2.02	0.40
14:N:120:TRP:CE3	53:1:269:G:H5'	2.56	0.40
15:O:75:ALA:HB3	15:O:78:ARG:HB2	2.03	0.40
53:1:1281:G:O2'	53:1:1282:G:P	2.78	0.40
53:1:2548:C:O2	53:1:2548:C:C2'	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:2758:A:O2'	53:1:2759:U:P	2.79	0.40
6:F:169:ILE:HD13	6:F:181:ILE:HA	2.02	0.40
9:I:52:ILE:HD13	9:I:123:LEU:HD21	2.03	0.40
11:K:200:ASN:OD1	58:6:25:G:N2	2.55	0.40
16:P:22:LEU:HD21	53:1:2150:G:H4'	91.65	0.40
2:B:171:LEU:HD21	53:1:3304:U:O4	2.22	0.40
4:D:234:ASP:OD1	4:D:235:SER:N	2.55	0.40
5:E:43:LEU:HD21	5:E:85:ILE:HD12	2.03	0.40
15:O:181:ALA:C	15:O:184:THR:HG22	2.37	0.40
15:O:195:ALA:O	15:O:198:GLY:CA	2.70	0.40
18:R:23:TRP:CH2	18:R:25:ASP:HB3	2.56	0.40
25:Y:59:VAL:HG12	25:Y:103:LYS:O	2.21	0.40
25:Y:45:ILE:HD11	25:Y:122:LYS:HD3	2.03	0.40
19:S:108:GLN:NE2	53:1:1322:U:O2	2.54	0.40
53:1:2547:A:P	53:1:2548:C:OP1	2.79	0.40
58:6:26:U:HO2'	58:6:27:G:C1'	2.34	0.40
12:L:21:ARG:NH2	54:2:51:G:OP2	60.59	0.40
20:T:151:LEU:HG	20:T:152:ALA:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	211/254 (83%)	205 (97%)	5 (2%)	1 (0%)	34 72
2	B	384/387 (99%)	281 (73%)	67 (17%)	36 (9%)	1 4
3	C	359/362 (99%)	330 (92%)	21 (6%)	8 (2%)	8 36
4	D	272/297 (92%)	246 (90%)	21 (8%)	5 (2%)	11 42
5	E	152/176 (86%)	145 (95%)	6 (4%)	1 (1%)	26 65
6	F	220/244 (90%)	207 (94%)	8 (4%)	5 (2%)	8 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	231/256 (90%)	213 (92%)	12 (5%)	6 (3%)	7	32
8	H	189/191 (99%)	181 (96%)	6 (3%)	2 (1%)	17	55
9	I	129/166 (78%)	110 (85%)	18 (14%)	1 (1%)	24	63
10	J	167/174 (96%)	137 (82%)	15 (9%)	15 (9%)	1	5
11	K	252/376 (67%)	226 (90%)	20 (8%)	6 (2%)	7	33
12	L	185/199 (93%)	170 (92%)	8 (4%)	7 (4%)	4	23
13	M	135/138 (98%)	128 (95%)	6 (4%)	1 (1%)	26	65
14	N	201/204 (98%)	190 (94%)	9 (4%)	2 (1%)	19	58
15	O	195/199 (98%)	150 (77%)	35 (18%)	10 (5%)	2	15
16	P	181/184 (98%)	169 (93%)	9 (5%)	3 (2%)	11	43
17	Q	132/186 (71%)	126 (96%)	6 (4%)	0	100	100
18	R	154/189 (82%)	149 (97%)	4 (3%)	1 (1%)	30	68
19	S	169/172 (98%)	156 (92%)	9 (5%)	4 (2%)	7	33
20	T	115/160 (72%)	102 (89%)	6 (5%)	7 (6%)	2	11
21	U	104/121 (86%)	94 (90%)	8 (8%)	2 (2%)	10	40
22	V	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
23	W	232/236 (98%)	214 (92%)	17 (7%)	1 (0%)	39	75
24	X	139/142 (98%)	130 (94%)	9 (6%)	0	100	100
25	Y	124/127 (98%)	114 (92%)	10 (8%)	0	100	100
26	Z	133/136 (98%)	123 (92%)	9 (7%)	1 (1%)	24	63
27	a	91/149 (61%)	80 (88%)	9 (10%)	2 (2%)	8	36
28	b	638/647 (99%)	561 (88%)	59 (9%)	18 (3%)	6	30
29	c	95/105 (90%)	93 (98%)	1 (1%)	1 (1%)	17	55
30	d	105/113 (93%)	99 (94%)	4 (4%)	2 (2%)	10	40
31	e	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
32	f	104/107 (97%)	99 (95%)	4 (4%)	1 (1%)	19	58
33	g	110/121 (91%)	107 (97%)	2 (2%)	1 (1%)	21	61
34	h	117/120 (98%)	109 (93%)	6 (5%)	2 (2%)	11	43
35	i	97/100 (97%)	87 (90%)	7 (7%)	3 (3%)	5	28
36	j	85/88 (97%)	75 (88%)	9 (11%)	1 (1%)	16	53
37	k	75/78 (96%)	72 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
39	m	465/486 (96%)	399 (86%)	53 (11%)	13 (3%)	6	30
40	n	365/605 (60%)	321 (88%)	27 (7%)	17 (5%)	3	17
41	o	131/220 (60%)	116 (88%)	12 (9%)	3 (2%)	8	35
42	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	17	55
43	q	179/455 (39%)	155 (87%)	18 (10%)	6 (3%)	5	25
44	r	224/261 (86%)	194 (87%)	23 (10%)	7 (3%)	5	28
45	s	65/520 (12%)	59 (91%)	3 (5%)	3 (5%)	3	18
46	t	283/322 (88%)	249 (88%)	24 (8%)	10 (4%)	4	25
47	u	148/199 (74%)	134 (90%)	9 (6%)	5 (3%)	5	25
48	v	283/344 (82%)	269 (95%)	11 (4%)	3 (1%)	17	55
49	w	178/203 (88%)	152 (85%)	21 (12%)	5 (3%)	6	30
50	x	476/515 (92%)	433 (91%)	29 (6%)	14 (3%)	6	29
51	y	242/245 (99%)	222 (92%)	16 (7%)	4 (2%)	11	43
52	z	53/106 (50%)	51 (96%)	2 (4%)	0	100	100
56	4	508/593 (86%)	469 (92%)	31 (6%)	8 (2%)	12	44
57	5	71/120 (59%)	70 (99%)	1 (1%)	0	100	100
All	All	10349/12508 (83%)	9344 (90%)	750 (7%)	255 (2%)	11	33

All (255) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	25	ILE
2	B	34	LYS
2	B	38	SER
2	B	140	ASP
2	B	142	ALA
2	B	229	VAL
2	B	300	ARG
3	C	131	VAL
3	C	268	ALA
3	C	338	LYS
5	E	98	VAL
6	F	216	VAL
7	G	31	PRO
7	G	157	VAL

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Mol	Chain	Res	Type
10	J	9	MET
10	J	28	ASP
10	J	74	PRO
10	J	94	ARG
10	J	165	GLN
12	L	47	ALA
12	L	131	LYS
12	L	136	GLU
12	L	193	ALA
15	O	16	VAL
15	O	122	GLN
15	O	186	ALA
16	P	160	ALA
19	S	85	SER
20	T	53	PRO
20	T	101	CYS
20	T	152	ALA
20	T	153	PRO
28	b	75	HIS
28	b	428	LYS
28	b	484	SER
28	b	621	GLU
29	c	100	ILE
39	m	83	VAL
39	m	100	GLN
39	m	207	GLN
39	m	418	ILE
40	n	98	GLU
41	o	128	THR
41	o	140	VAL
43	q	389	VAL
44	r	17	ARG
44	r	206	SER
46	t	147	VAL
46	t	223	GLU
46	t	261	PHE
47	u	81	TYR
50	x	22	VAL
50	x	207	ASP
51	y	146	ILE
51	y	147	LEU
56	4	344	THR

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Mol	Chain	Res	Type
2	B	51	ALA
2	B	53	MET
2	B	171	LEU
2	B	174	LYS
2	B	187	SER
2	B	265	ALA
2	B	351	LEU
3	C	156	LEU
3	C	269	SER
3	C	339	LEU
4	D	24	ARG
6	F	26	VAL
6	F	159	GLN
8	H	50	ASN
11	K	89	THR
12	L	51	LEU
15	O	47	PHE
15	O	129	LEU
19	S	154	HIS
20	T	36	VAL
20	T	58	GLN
27	a	66	ALA
27	a	77	LYS
28	b	260	CYS
28	b	622	SER
32	f	60	ARG
33	g	46	ASP
35	i	3	VAL
35	i	28	TYR
39	m	125	GLU
39	m	137	TYR
39	m	377	ASP
40	n	97	GLY
40	n	455	PRO
40	n	456	HIS
41	o	171	ALA
43	q	201	SER
43	q	227	TYR
44	r	162	THR
44	r	237	VAL
46	t	136	ASP
47	u	26	ALA

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Mol	Chain	Res	Type
49	w	144	LYS
56	4	98	ASP
56	4	401	PHE
56	4	519	ARG
2	B	26	ARG
2	B	35	ASP
2	B	36	ASP
2	B	97	ARG
2	B	108	GLU
2	B	127	LYS
2	B	200	GLU
2	B	239	PRO
2	B	342	LEU
3	C	233	LEU
3	C	320	ASN
4	D	72	ASP
6	F	164	SER
10	J	11	ASP
10	J	114	ILE
10	J	167	TYR
13	M	29	ALA
14	N	145	ASP
15	O	21	SER
18	R	53	LYS
26	Z	59	ALA
28	b	10	THR
28	b	368	ALA
28	b	417	LYS
28	b	418	ASP
28	b	528	PHE
34	h	75	TYR
34	h	97	ALA
39	m	111	ASN
39	m	120	GLU
40	n	73	HIS
40	n	257	SER
40	n	376	LEU
40	n	457	LEU
43	q	435	VAL
44	r	3	GLN
46	t	151	LEU
46	t	260	SER

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Mol	Chain	Res	Type
46	t	275	ARG
50	x	88	ALA
50	x	89	SER
50	x	125	ALA
51	y	8	GLU
51	y	229	PRO
56	4	474	PRO
2	B	155	ALA
2	B	188	ILE
2	B	295	ALA
2	B	333	LYS
2	B	341	SER
2	B	347	SER
2	B	358	TRP
4	D	260	PHE
7	G	121	SER
8	H	110	LYS
10	J	8	PRO
10	J	95	ASN
10	J	108	GLU
10	J	117	ASP
10	J	140	ARG
11	K	50	LYS
11	K	166	ALA
11	K	251	LEU
15	O	196	ALA
16	P	156	ALA
16	P	158	ALA
19	S	24	LEU
28	b	574	THR
39	m	241	SER
39	m	283	THR
39	m	360	LYS
40	n	54	LYS
40	n	64	TYR
40	n	123	PRO
40	n	262	TYR
43	q	181	LYS
44	r	170	ARG
45	s	55	PRO
46	t	138	LYS
48	v	276	HIS

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Mol	Chain	Res	Type
49	w	142	VAL
50	x	21	GLU
50	x	25	ILE
50	x	41	THR
50	x	180	HIS
50	x	338	ALA
56	4	256	GLU
56	4	380	THR
2	B	10	ARG
2	B	129	ALA
2	B	137	TYR
2	B	343	TYR
4	D	258	LYS
10	J	55	ARG
10	J	64	LYS
11	K	49	SER
11	K	284	ASN
12	L	76	THR
14	N	94	TYR
15	O	48	PHE
21	U	11	ILE
21	U	110	VAL
28	b	87	GLU
28	b	247	ARG
28	b	585	GLN
35	i	27	SER
36	j	85	LYS
40	n	74	GLU
44	r	86	ALA
45	s	3	VAL
45	s	12	SER
46	t	57	ARG
47	u	3	ILE
48	v	270	ASP
48	v	285	LEU
50	x	337	GLY
56	4	363	ASP
2	B	317	ILE
4	D	141	PRO
6	F	178	ILE
28	b	4	SER
28	b	282	SER

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Mol	Chain	Res	Type
30	d	7	VAL
39	m	255	LEU
40	n	5	LYS
40	n	441	LEU
42	p	61	LYS
43	q	405	SER
46	t	269	GLN
49	w	77	VAL
50	x	484	GLY
40	n	448	LEU
47	u	131	PRO
49	w	123	ILE
49	w	143	PRO
50	x	400	GLY
7	G	36	ILE
15	O	79	ILE
15	O	88	VAL
23	W	171	ILE
40	n	384	GLY
7	G	30	THR
9	I	37	GLN
12	L	130	GLY
19	S	167	ARG
47	u	79	VAL
2	B	96	PRO
28	b	227	ARG
50	x	227	GLY
1	A	207	VAL
7	G	25	PRO
30	d	87	ASN
20	T	155	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	166/196 (85%)	157 (95%)	9 (5%)	27 64
2	B	322/323 (100%)	261 (81%)	61 (19%)	2 8
3	C	288/289 (100%)	272 (94%)	16 (6%)	26 63
4	D	227/245 (93%)	206 (91%)	21 (9%)	11 39
5	E	134/153 (88%)	125 (93%)	9 (7%)	20 56
6	F	186/205 (91%)	174 (94%)	12 (6%)	21 57
7	G	191/208 (92%)	175 (92%)	16 (8%)	14 46
8	H	171/171 (100%)	155 (91%)	16 (9%)	11 39
9	I	117/141 (83%)	111 (95%)	6 (5%)	29 66
10	J	147/150 (98%)	125 (85%)	22 (15%)	3 15
11	K	236/346 (68%)	224 (95%)	12 (5%)	29 66
12	L	149/159 (94%)	135 (91%)	14 (9%)	11 39
13	M	108/109 (99%)	105 (97%)	3 (3%)	51 82
14	N	175/176 (99%)	164 (94%)	11 (6%)	22 58
15	O	160/162 (99%)	145 (91%)	15 (9%)	11 39
16	P	145/146 (99%)	135 (93%)	10 (7%)	19 55
17	Q	110/151 (73%)	104 (94%)	6 (6%)	27 63
18	R	129/154 (84%)	119 (92%)	10 (8%)	16 50
19	S	155/156 (99%)	146 (94%)	9 (6%)	25 61
20	T	102/137 (74%)	89 (87%)	13 (13%)	5 22
21	U	93/107 (87%)	91 (98%)	2 (2%)	60 86
22	V	104/105 (99%)	98 (94%)	6 (6%)	25 61
23	W	211/213 (99%)	192 (91%)	19 (9%)	12 41
24	X	117/118 (99%)	103 (88%)	14 (12%)	6 24
25	Y	109/110 (99%)	103 (94%)	6 (6%)	27 63
26	Z	115/116 (99%)	109 (95%)	6 (5%)	29 65
27	a	76/119 (64%)	68 (90%)	8 (10%)	8 32
28	b	568/573 (99%)	506 (89%)	62 (11%)	8 31
29	c	81/88 (92%)	74 (91%)	7 (9%)	13 45
30	d	94/97 (97%)	85 (90%)	9 (10%)	10 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	e	109/111 (98%)	102 (94%)	7 (6%)	22	57
32	f	90/91 (99%)	85 (94%)	5 (6%)	26	63
33	g	95/103 (92%)	90 (95%)	5 (5%)	28	64
34	h	104/105 (99%)	93 (89%)	11 (11%)	8	32
35	i	81/82 (99%)	74 (91%)	7 (9%)	13	45
36	j	70/71 (99%)	66 (94%)	4 (6%)	25	62
37	k	68/69 (99%)	65 (96%)	3 (4%)	35	71
38	l	45/46 (98%)	38 (84%)	7 (16%)	3	14
39	m	413/428 (96%)	349 (84%)	64 (16%)	3	14
40	n	334/548 (61%)	310 (93%)	24 (7%)	18	53
41	o	118/199 (59%)	103 (87%)	15 (13%)	5	22
42	p	71/72 (99%)	69 (97%)	2 (3%)	51	82
43	q	171/420 (41%)	163 (95%)	8 (5%)	32	69
44	r	203/229 (89%)	185 (91%)	18 (9%)	12	42
45	s	62/445 (14%)	60 (97%)	2 (3%)	46	80
46	t	256/287 (89%)	235 (92%)	21 (8%)	14	47
47	u	133/180 (74%)	126 (95%)	7 (5%)	28	64
48	v	258/309 (84%)	252 (98%)	6 (2%)	58	84
49	w	161/179 (90%)	154 (96%)	7 (4%)	35	73
50	x	428/451 (95%)	407 (95%)	21 (5%)	31	68
51	y	210/211 (100%)	199 (95%)	11 (5%)	29	65
52	z	48/95 (50%)	45 (94%)	3 (6%)	22	58
56	4	453/520 (87%)	409 (90%)	44 (10%)	10	36
57	5	67/106 (63%)	53 (79%)	14 (21%)	1	6
All	All	9034/10780 (84%)	8288 (92%)	746 (8%)	19	47

All (746) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	46	LYS
1	A	47	GLN
1	A	101	VAL
1	A	104	LEU

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Mol	Chain	Res	Type
1	A	122	ASP
1	A	161	ASP
1	A	204	MET
1	A	207	VAL
2	B	7	GLU
2	B	10	ARG
2	B	17	LEU
2	B	19	ARG
2	B	25	ILE
2	B	28	ARG
2	B	37	ARG
2	B	39	LYS
2	B	47	LEU
2	B	50	LYS
2	B	55	THR
2	B	77	THR
2	B	85	VAL
2	B	97	ARG
2	B	101	SER
2	B	102	LEU
2	B	108	GLU
2	B	115	LYS
2	B	123	TYR
2	B	137	TYR
2	B	148	LEU
2	B	156	SER
2	B	163	HIS
2	B	167	ARG
2	B	171	LEU
2	B	173	GLN
2	B	178	LEU
2	B	190	GLU
2	B	198	HIS
2	B	201	LYS
2	B	236	LYS
2	B	240	ARG
2	B	241	LYS
2	B	246	LEU
2	B	252	ILE
2	B	255	TRP
2	B	274	SER
2	B	284	ARG

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Mol	Chain	Res	Type
2	B	291	GLU
2	B	296	THR
2	B	300	ARG
2	B	303	LYS
2	B	304	THR
2	B	305	ILE
2	B	308	MET
2	B	319	ASN
2	B	323	MET
2	B	327	CYS
2	B	332	ARG
2	B	333	LYS
2	B	337	THR
2	B	339	ARG
2	B	341	SER
2	B	344	THR
2	B	351	LEU
2	B	353	GLU
2	B	364	LYS
2	B	375	GLU
2	B	377	HIS
2	B	385	LYS
2	B	386	ASP
3	C	5	GLN
3	C	14	GLU
3	C	93	MET
3	C	99	MET
3	C	112	LYS
3	C	156	LEU
3	C	170	LYS
3	C	179	LEU
3	C	187	LEU
3	C	194	TYR
3	C	203	ARG
3	C	246	ARG
3	C	294	GLU
3	C	307	GLN
3	C	313	LEU
3	C	345	GLU
4	D	9	SER
4	D	16	PHE
4	D	17	GLN

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Mol	Chain	Res	Type
4	D	23	ARG
4	D	39	GLN
4	D	43	LYS
4	D	48	LYS
4	D	105	ILE
4	D	117	GLU
4	D	136	GLU
4	D	168	ASP
4	D	172	TYR
4	D	176	SER
4	D	178	ASN
4	D	187	THR
4	D	226	TYR
4	D	263	GLU
4	D	264	GLN
4	D	273	ARG
4	D	277	LEU
4	D	293	LEU
5	E	9	TRP
5	E	18	LEU
5	E	21	THR
5	E	65	ILE
5	E	78	ARG
5	E	90	LYS
5	E	105	TYR
5	E	152	THR
5	E	173	MET
6	F	40	LYS
6	F	41	ARG
6	F	60	ARG
6	F	88	ARG
6	F	93	ASN
6	F	111	ILE
6	F	124	LEU
6	F	131	GLU
6	F	179	LEU
6	F	182	ASP
6	F	229	PHE
6	F	239	LEU
7	G	41	GLN
7	G	63	LYS
7	G	79	GLN

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Mol	Chain	Res	Type
7	G	84	ARG
7	G	89	GLU
7	G	134	TYR
7	G	146	LYS
7	G	150	LEU
7	G	163	VAL
7	G	204	ARG
7	G	228	GLU
7	G	229	VAL
7	G	238	LEU
7	G	241	LYS
7	G	245	LYS
7	G	248	LYS
8	H	5	GLN
8	H	21	LYS
8	H	41	ILE
8	H	49	ASN
8	H	68	LEU
8	H	69	ARG
8	H	107	ASP
8	H	118	LEU
8	H	139	ASN
8	H	157	ASN
8	H	164	ILE
8	H	170	LYS
8	H	172	ILE
8	H	173	ARG
8	H	189	GLU
8	H	191	LEU
9	I	32	GLN
9	I	46	LEU
9	I	60	THR
9	I	75	ARG
9	I	90	SER
9	I	116	LYS
10	J	7	ASN
10	J	10	ARG
10	J	12	LEU
10	J	13	LYS
10	J	29	ARG
10	J	34	SER
10	J	46	VAL

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Mol	Chain	Res	Type
10	J	80	LEU
10	J	84	LEU
10	J	94	ARG
10	J	106	ILE
10	J	107	ASP
10	J	112	LEU
10	J	115	LYS
10	J	120	ILE
10	J	130	VAL
10	J	138	VAL
10	J	140	ARG
10	J	142	LYS
10	J	148	VAL
10	J	158	ASP
10	J	166	LYS
11	K	50	LYS
11	K	85	ASN
11	K	105	SER
11	K	125	LEU
11	K	131	ASP
11	K	163	VAL
11	K	186	ILE
11	K	245	ASN
11	K	251	LEU
11	K	262	ASN
11	K	270	LEU
11	K	291	LEU
12	L	9	ILE
12	L	10	LEU
12	L	12	ASN
12	L	15	ARG
12	L	24	VAL
12	L	35	ARG
12	L	55	ARG
12	L	67	ARG
12	L	103	ASN
12	L	117	LYS
12	L	124	ILE
12	L	131	LYS
12	L	134	GLU
12	L	136	GLU
13	M	8	LYS

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Mol	Chain	Res	Type
13	M	12	TRP
13	M	38	ILE
14	N	10	LEU
14	N	38	ARG
14	N	62	TYR
14	N	83	LYS
14	N	87	GLN
14	N	105	ARG
14	N	113	LEU
14	N	133	ILE
14	N	151	ILE
14	N	183	THR
14	N	201	ARG
15	O	25	LYS
15	O	31	GLN
15	O	52	LEU
15	O	56	ASP
15	O	78	ARG
15	O	106	GLU
15	O	116	LYS
15	O	117	ARG
15	O	124	LEU
15	O	129	LEU
15	O	134	LYS
15	O	142	SER
15	O	148	LYS
15	O	151	ASP
15	O	187	GLU
16	P	49	GLU
16	P	55	GLN
16	P	69	ARG
16	P	96	GLN
16	P	120	ASN
16	P	125	GLN
16	P	139	TYR
16	P	168	LEU
16	P	173	ARG
16	P	180	LYS
17	Q	20	LYS
17	Q	41	ASP
17	Q	49	LEU
17	Q	138	LEU

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Mol	Chain	Res	Type
17	Q	147	ARG
17	Q	148	GLU
18	R	8	LYS
18	R	43	LYS
18	R	74	ARG
18	R	99	LEU
18	R	103	ARG
18	R	104	ARG
18	R	105	LEU
18	R	130	ASN
18	R	138	LEU
18	R	150	GLN
19	S	12	ARG
19	S	13	ARG
19	S	61	ILE
19	S	71	LYS
19	S	119	ARG
19	S	122	HIS
19	S	130	GLU
19	S	137	ARG
19	S	172	TYR
20	T	68	THR
20	T	75	ILE
20	T	79	MET
20	T	92	ARG
20	T	102	ARG
20	T	118	GLU
20	T	127	GLN
20	T	128	LEU
20	T	131	GLN
20	T	136	ARG
20	T	139	ARG
20	T	151	LEU
20	T	156	TYR
21	U	52	ASN
21	U	70	LYS
22	V	11	PHE
22	V	33	ASN
22	V	48	ARG
22	V	72	LYS
22	V	74	MET
22	V	88	ARG

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Mol	Chain	Res	Type
23	W	3	ARG
23	W	5	LYS
23	W	6	ARG
23	W	42	VAL
23	W	45	LEU
23	W	46	ASP
23	W	48	VAL
23	W	49	ARG
23	W	55	GLU
23	W	57	ARG
23	W	60	TRP
23	W	113	LYS
23	W	123	ASP
23	W	133	LEU
23	W	165	MET
23	W	170	GLU
23	W	174	LYS
23	W	187	LEU
23	W	216	LYS
24	X	27	ARG
24	X	36	LYS
24	X	38	LEU
24	X	40	LEU
24	X	45	LYS
24	X	61	LYS
24	X	63	ILE
24	X	73	MET
24	X	74	LYS
24	X	78	ASP
24	X	115	ARG
24	X	133	LEU
24	X	135	ILE
24	X	142	ILE
25	Y	17	LYS
25	Y	37	LYS
25	Y	50	ILE
25	Y	59	VAL
25	Y	74	TYR
25	Y	126	LEU
26	Z	3	LYS
26	Z	15	ARG
26	Z	17	ARG

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Mol	Chain	Res	Type
26	Z	64	LYS
26	Z	81	LEU
26	Z	99	GLU
27	a	58	MET
27	a	59	ARG
27	a	60	TYR
27	a	64	GLN
27	a	67	HIS
27	a	115	LYS
27	a	117	ARG
27	a	120	ASN
28	b	1	MET
28	b	10	THR
28	b	16	ASP
28	b	31	THR
28	b	48	ARG
28	b	70	ASN
28	b	81	LEU
28	b	87	GLU
28	b	120	GLN
28	b	133	LEU
28	b	142	LYS
28	b	168	ARG
28	b	169	THR
28	b	170	LEU
28	b	180	LYS
28	b	189	LYS
28	b	191	ASP
28	b	215	ARG
28	b	224	ILE
28	b	233	ASN
28	b	257	SER
28	b	258	GLU
28	b	270	LEU
28	b	281	LYS
28	b	292	ILE
28	b	294	ARG
28	b	296	GLU
28	b	323	GLN
28	b	324	LEU
28	b	325	GLU
28	b	332	ARG

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Mol	Chain	Res	Type
28	b	339	LEU
28	b	345	GLU
28	b	354	ILE
28	b	365	GLN
28	b	367	GLN
28	b	413	ASN
28	b	415	ASN
28	b	420	TYR
28	b	423	GLU
28	b	432	MET
28	b	434	GLU
28	b	439	LYS
28	b	440	ASN
28	b	445	LEU
28	b	453	LEU
28	b	482	GLU
28	b	499	ARG
28	b	526	LYS
28	b	535	MET
28	b	556	ASN
28	b	557	ARG
28	b	560	GLU
28	b	564	ASP
28	b	569	ASP
28	b	570	GLN
28	b	585	GLN
28	b	588	ARG
28	b	610	ARG
28	b	611	ARG
28	b	618	LYS
28	b	634	LEU
29	c	40	LYS
29	c	52	ARG
29	c	61	MET
29	c	76	GLU
29	c	83	LYS
29	c	101	LEU
29	c	104	LEU
30	d	6	ASP
30	d	26	LYS
30	d	31	ARG
30	d	50	ARG

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Mol	Chain	Res	Type
30	d	55	LEU
30	d	61	LYS
30	d	86	LYS
30	d	102	LYS
30	d	111	GLU
31	e	19	ARG
31	e	21	HIS
31	e	33	ARG
31	e	82	LEU
31	e	87	MET
31	e	103	LYS
31	e	126	LEU
32	f	10	LYS
32	f	19	SER
32	f	48	ARG
32	f	60	ARG
32	f	70	LYS
33	g	29	ILE
33	g	44	CYS
33	g	47	CYS
33	g	58	ARG
33	g	80	ARG
34	h	20	GLN
34	h	21	LEU
34	h	27	GLU
34	h	28	LEU
34	h	38	ARG
34	h	48	ARG
34	h	49	LYS
34	h	71	LYS
34	h	85	THR
34	h	89	ARG
34	h	119	LYS
35	i	28	TYR
35	i	45	ARG
35	i	51	SER
35	i	57	LEU
35	i	58	ILE
35	i	60	LEU
35	i	68	ARG
36	j	15	SER
36	j	25	ARG

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Mol	Chain	Res	Type
36	j	67	LEU
36	j	75	LYS
37	k	31	LEU
37	k	67	GLN
37	k	77	ARG
38	l	4	GLN
38	l	6	SER
38	l	21	ARG
38	l	23	LEU
38	l	29	LEU
38	l	47	THR
38	l	48	LYS
39	m	22	LEU
39	m	30	TYR
39	m	32	ASP
39	m	34	LYS
39	m	35	ARG
39	m	41	MET
39	m	62	GLN
39	m	83	VAL
39	m	98	GLU
39	m	100	GLN
39	m	106	VAL
39	m	125	GLU
39	m	130	ARG
39	m	132	LEU
39	m	133	ASP
39	m	148	LYS
39	m	152	LEU
39	m	166	GLU
39	m	172	GLU
39	m	174	LYS
39	m	191	GLU
39	m	202	ILE
39	m	210	ARG
39	m	211	ILE
39	m	224	VAL
39	m	226	ILE
39	m	239	CYS
39	m	249	GLU
39	m	255	LEU
39	m	260	ASN

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Mol	Chain	Res	Type
39	m	281	ARG
39	m	287	HIS
39	m	299	LEU
39	m	308	GLN
39	m	311	THR
39	m	313	ARG
39	m	315	GLN
39	m	318	VAL
39	m	328	LYS
39	m	338	LYS
39	m	343	VAL
39	m	351	LYS
39	m	353	TRP
39	m	358	LEU
39	m	359	MET
39	m	362	ILE
39	m	366	ASP
39	m	380	GLU
39	m	381	ASP
39	m	385	ARG
39	m	397	GLU
39	m	405	LYS
39	m	408	GLN
39	m	414	ARG
39	m	418	ILE
39	m	422	LYS
39	m	434	LYS
39	m	435	GLN
39	m	437	ARG
39	m	451	LYS
39	m	459	ARG
39	m	462	ILE
39	m	471	LYS
39	m	472	GLU
40	n	16	ILE
40	n	18	ARG
40	n	31	ASP
40	n	39	LYS
40	n	53	ASN
40	n	84	LYS
40	n	90	LEU
40	n	94	LEU

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Mol	Chain	Res	Type
40	n	112	TYR
40	n	117	ILE
40	n	120	GLU
40	n	132	ILE
40	n	158	ASP
40	n	230	HIS
40	n	256	ILE
40	n	263	ILE
40	n	267	ARG
40	n	351	LYS
40	n	354	SER
40	n	363	PHE
40	n	375	ILE
40	n	417	LEU
40	n	427	ILE
40	n	448	LEU
41	o	102	PHE
41	o	117	LEU
41	o	118	LYS
41	o	130	ASN
41	o	137	LEU
41	o	140	VAL
41	o	144	ASP
41	o	146	MET
41	o	158	MET
41	o	163	GLN
41	o	184	LEU
41	o	190	THR
41	o	205	GLU
41	o	217	GLU
41	o	220	TRP
42	p	11	THR
42	p	39	CYS
43	q	219	GLU
43	q	227	TYR
43	q	228	ASN
43	q	240	LYS
43	q	270	ASP
43	q	402	LEU
43	q	436	ARG
43	q	446	THR
44	r	3	GLN

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Mol	Chain	Res	Type
44	r	23	ARG
44	r	37	GLU
44	r	131	GLU
44	r	133	MET
44	r	162	THR
44	r	164	ARG
44	r	168	MET
44	r	177	LEU
44	r	203	ASN
44	r	205	GLN
44	r	212	LEU
44	r	224	ASN
44	r	225	VAL
44	r	236	LYS
44	r	237	VAL
44	r	248	GLU
44	r	250	ASP
45	s	33	MET
45	s	71	ASP
46	t	15	ASN
46	t	74	ARG
46	t	77	ARG
46	t	91	GLN
46	t	97	LYS
46	t	141	LEU
46	t	155	ILE
46	t	170	GLU
46	t	210	LYS
46	t	215	ILE
46	t	216	TYR
46	t	223	GLU
46	t	241	ASP
46	t	246	CYS
46	t	248	GLU
46	t	257	MET
46	t	268	LEU
46	t	269	GLN
46	t	275	ARG
46	t	283	LEU
46	t	288	LYS
47	u	2	ARG
47	u	9	CYS

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Mol	Chain	Res	Type
47	u	19	ILE
47	u	27	LYS
47	u	35	LYS
47	u	73	GLN
47	u	80	ARG
48	v	11	ARG
48	v	189	ASP
48	v	217	ARG
48	v	254	GLN
48	v	270	ASP
48	v	285	LEU
49	w	70	MET
49	w	88	THR
49	w	126	LYS
49	w	153	LYS
49	w	156	ASP
49	w	157	GLN
49	w	197	ARG
50	x	3	THR
50	x	20	ARG
50	x	57	GLU
50	x	63	LEU
50	x	66	GLN
50	x	78	THR
50	x	116	GLN
50	x	127	PHE
50	x	142	HIS
50	x	176	GLN
50	x	194	TRP
50	x	272	TYR
50	x	299	ARG
50	x	321	HIS
50	x	322	TRP
50	x	362	LYS
50	x	363	ILE
50	x	379	ASP
50	x	482	LEU
50	x	487	ASP
50	x	491	THR
51	y	57	ARG
51	y	74	THR
51	y	79	GLN

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Mol	Chain	Res	Type
51	y	85	ARG
51	y	101	LEU
51	y	109	CYS
51	y	139	ARG
51	y	150	SER
51	y	197	MET
51	y	209	ASP
51	y	232	ILE
52	z	5	LEU
52	z	37	LEU
52	z	46	LEU
56	4	21	GLN
56	4	22	GLU
56	4	29	ARG
56	4	33	GLN
56	4	39	LEU
56	4	48	ASP
56	4	56	GLN
56	4	60	THR
56	4	75	ARG
56	4	96	ASP
56	4	112	GLN
56	4	121	LYS
56	4	130	THR
56	4	161	TYR
56	4	177	LEU
56	4	197	LEU
56	4	202	LEU
56	4	243	ARG
56	4	245	ARG
56	4	248	ARG
56	4	251	LEU
56	4	263	GLU
56	4	323	MET
56	4	337	LEU
56	4	338	GLU
56	4	346	LYS
56	4	353	LEU
56	4	378	LEU
56	4	379	LEU
56	4	398	ASN
56	4	412	LEU

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Mol	Chain	Res	Type
56	4	416	LEU
56	4	434	GLU
56	4	441	ARG
56	4	473	LEU
56	4	475	LEU
56	4	485	LEU
56	4	487	SER
56	4	489	MET
56	4	519	ARG
56	4	536	TRP
56	4	562	ASP
56	4	568	LEU
56	4	571	GLU
57	5	46	LEU
57	5	59	GLU
57	5	61	LEU
57	5	68	LYS
57	5	72	ARG
57	5	78	MET
57	5	83	ARG
57	5	85	LYS
57	5	91	ARG
57	5	98	LYS
57	5	102	LYS
57	5	103	LYS
57	5	108	ARG
57	5	111	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	97	ASN
1	A	209	HIS
2	B	139	GLN
2	B	319	ASN
3	C	48	GLN
3	C	114	ASN
3	C	221	ASN
3	C	260	GLN
3	C	304	GLN
3	C	307	GLN

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Mol	Chain	Res	Type
4	D	17	GLN
4	D	39	GLN
5	E	57	HIS
5	E	167	ASN
6	F	37	ASN
6	F	244	ASN
7	G	33	ASN
7	G	38	GLN
7	G	41	GLN
7	G	85	ASN
7	G	95	ASN
7	G	145	ASN
7	G	243	GLN
8	H	49	ASN
8	H	125	ASN
8	H	139	ASN
9	I	97	ASN
12	L	103	ASN
12	L	114	GLN
14	N	182	ASN
15	O	31	GLN
15	O	50	ASN
15	O	65	ASN
16	P	28	ASN
16	P	133	HIS
19	S	8	GLN
19	S	63	GLN
20	T	58	GLN
21	U	87	ASN
22	V	33	ASN
22	V	47	ASN
22	V	98	ASN
23	W	74	GLN
23	W	91	GLN
23	W	167	ASN
23	W	205	GLN
23	W	223	ASN
26	Z	57	HIS
27	a	64	GLN
27	a	67	HIS
28	b	26	GLN
28	b	323	GLN

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Mol	Chain	Res	Type
28	b	333	ASN
28	b	367	GLN
28	b	406	ASN
28	b	500	GLN
28	b	546	GLN
28	b	579	ASN
30	d	57	GLN
30	d	87	ASN
31	e	104	ASN
33	g	3	GLN
33	g	33	GLN
34	h	34	GLN
34	h	62	GLN
38	l	4	GLN
38	l	20	ASN
39	m	146	GLN
39	m	455	ASN
40	n	208	ASN
40	n	428	GLN
41	o	130	ASN
41	o	199	ASN
44	r	4	ASN
44	r	10	HIS
44	r	14	HIS
44	r	203	ASN
44	r	224	ASN
46	t	44	GLN
47	u	37	HIS
47	u	42	GLN
50	x	154	HIS
50	x	176	GLN
50	x	208	ASN
50	x	406	ASN
51	y	6	GLN
51	y	11	ASN
51	y	33	ASN
51	y	106	ASN
51	y	145	ASN
56	4	21	GLN
56	4	33	GLN
56	4	51	HIS
56	4	118	ASN

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Mol	Chain	Res	Type
56	4	447	HIS
56	4	577	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	1	3048/3396 (89%)	923 (30%)	216 (7%)
54	2	157/158 (99%)	38 (24%)	5 (3%)
55	3	120/121 (99%)	22 (18%)	4 (3%)
58	6	64/232 (27%)	41 (64%)	10 (15%)
All	All	3389/3907 (86%)	1024 (30%)	235 (6%)

All (1024) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	1	7	C
53	1	11	A
53	1	13	A
53	1	14	U
53	1	16	A
53	1	26	A
53	1	40	A
53	1	41	G
53	1	49	A
53	1	51	A
53	1	57	A
53	1	59	G
53	1	60	A
53	1	65	A
53	1	66	A
53	1	74	G
53	1	75	G
53	1	92	G
53	1	93	C
53	1	105	C
53	1	109	A
53	1	110	G
53	1	111	C
53	1	116	A
53	1	121	A
53	1	122	A

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Mol	Chain	Res	Type
53	1	133	U
53	1	135	C
53	1	136	G
53	1	143	G
53	1	148	G
53	1	156	G
53	1	157	A
53	1	161	G
53	1	165	A
53	1	166	C
53	1	170	G
53	1	171	G
53	1	173	G
53	1	182	U
53	1	185	C
53	1	187	A
53	1	190	U
53	1	191	U
53	1	200	C
53	1	201	A
53	1	206	G
53	1	210	U
53	1	211	A
53	1	213	A
53	1	218	G
53	1	219	A
53	1	220	G
53	1	234	G
53	1	240	U
53	1	241	G
53	1	243	G
53	1	249	U
53	1	250	U
53	1	251	G
53	1	252	U
53	1	256	G
53	1	262	U
53	1	264	G
53	1	266	A
53	1	269	G
53	1	284	A
53	1	285	A

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Mol	Chain	Res	Type
53	1	286	U
53	1	292	U
53	1	295	A
53	1	298	U
53	1	304	G
53	1	305	U
53	1	306	A
53	1	307	A
53	1	315	C
53	1	323	A
53	1	329	U
53	1	333	G
53	1	334	A
53	1	339	C
53	1	346	C
53	1	370	U
53	1	375	A
53	1	376	G
53	1	385	A
53	1	395	A
53	1	398	A
53	1	399	A
53	1	401	U
53	1	402	A
53	1	403	C
53	1	421	G
53	1	422	A
53	1	429	U
53	1	438	A
53	1	439	C
53	1	440	A
53	1	495	G
53	1	503	C
53	1	507	U
53	1	517	G
53	1	518	G
53	1	519	A
53	1	520	U
53	1	521	A
53	1	523	A
53	1	535	G
53	1	537	A

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Mol	Chain	Res	Type
53	1	544	C
53	1	545	U
53	1	547	G
53	1	548	G
53	1	549	U
53	1	550	A
53	1	552	G
53	1	555	U
53	1	556	U
53	1	557	A
53	1	559	A
53	1	569	A
53	1	578	A
53	1	579	G
53	1	592	A
53	1	594	U
53	1	595	G
53	1	604	G
53	1	607	A
53	1	609	G
53	1	611	A
53	1	620	U
53	1	621	A
53	1	622	A
53	1	623	U
53	1	636	C
53	1	637	C
53	1	638	C
53	1	643	U
53	1	644	G
53	1	645	A
53	1	646	A
53	1	647	A
53	1	650	C
53	1	660	A
53	1	662	U
53	1	677	A
53	1	681	U
53	1	684	G
53	1	690	A
53	1	691	A
53	1	705	A

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Mol	Chain	Res	Type
53	1	708	G
53	1	711	A
53	1	712	G
53	1	721	G
53	1	722	G
53	1	726	G
53	1	739	G
53	1	746	A
53	1	762	U
53	1	763	G
53	1	764	U
53	1	765	C
53	1	766	U
53	1	767	U
53	1	776	U
53	1	777	U
53	1	778	U
53	1	779	G
53	1	780	A
53	1	781	G
53	1	785	G
53	1	786	A
53	1	794	U
53	1	800	G
53	1	801	A
53	1	806	A
53	1	808	A
53	1	817	A
53	1	826	G
53	1	829	U
53	1	830	A
53	1	834	U
53	1	837	A
53	1	849	C
53	1	850	U
53	1	861	C
53	1	869	G
53	1	874	U
53	1	875	G
53	1	876	A
53	1	879	U
53	1	895	A

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Mol	Chain	Res	Type
53	1	896	A
53	1	897	U
53	1	907	G
53	1	908	G
53	1	909	G
53	1	914	A
53	1	916	G
53	1	917	A
53	1	921	A
53	1	923	C
53	1	936	A
53	1	938	C
53	1	944	C
53	1	955	U
53	1	956	U
53	1	957	C
53	1	958	C
53	1	959	C
53	1	962	A
53	1	967	A
53	1	974	G
53	1	976	U
53	1	977	C
53	1	978	G
53	1	979	U
53	1	980	A
53	1	982	C
53	1	984	G
53	1	991	G
53	1	992	A
53	1	994	G
53	1	996	A
53	1	997	A
53	1	998	A
53	1	1000	C
53	1	1001	G
53	1	1002	A
53	1	1003	A
53	1	1048	A
53	1	1049	C
53	1	1051	U
53	1	1052	U

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Mol	Chain	Res	Type
53	1	1054	A
53	1	1055	A
53	1	1056	U
53	1	1057	A
53	1	1058	U
53	1	1063	G
53	1	1064	A
53	1	1065	A
53	1	1085	A
53	1	1086	C
53	1	1089	G
53	1	1090	G
53	1	1092	C
53	1	1093	A
53	1	1094	U
53	1	1095	U
53	1	1098	A
53	1	1101	G
53	1	1103	A
53	1	1104	G
53	1	1106	G
53	1	1107	C
53	1	1109	U
53	1	1111	U
53	1	1112	A
53	1	1114	U
53	1	1115	G
53	1	1116	G
53	1	1117	G
53	1	1118	C
53	1	1127	G
53	1	1129	A
53	1	1130	A
53	1	1132	C
53	1	1136	A
53	1	1145	G
53	1	1151	U
53	1	1153	A
53	1	1155	C
53	1	1160	C
53	1	1177	G
53	1	1178	G

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Mol	Chain	Res	Type
53	1	1180	A
53	1	1181	U
53	1	1182	A
53	1	1186	G
53	1	1191	U
53	1	1192	C
53	1	1193	A
53	1	1196	C
53	1	1197	A
53	1	1198	C
53	1	1199	C
53	1	1200	A
53	1	1201	C
53	1	1202	A
53	1	1203	A
53	1	1204	A
53	1	1206	G
53	1	1207	G
53	1	1208	U
53	1	1209	G
53	1	1210	U
53	1	1217	A
53	1	1220	U
53	1	1221	A
53	1	1227	C
53	1	1234	G
53	1	1235	U
53	1	1236	G
53	1	1237	G
53	1	1239	C
53	1	1241	U
53	1	1242	G
53	1	1243	G
53	1	1244	A
53	1	1245	A
53	1	1247	U
53	1	1248	C
53	1	1252	A
53	1	1254	C
53	1	1258	U
53	1	1262	G
53	1	1263	A

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Mol	Chain	Res	Type
53	1	1264	G
53	1	1265	U
53	1	1266	G
53	1	1272	C
53	1	1278	A
53	1	1279	C
53	1	1281	G
53	1	1282	G
53	1	1283	C
53	1	1286	A
53	1	1287	A
53	1	1296	C
53	1	1299	U
53	1	1302	A
53	1	1303	A
53	1	1304	A
53	1	1307	G
53	1	1308	A
53	1	1313	G
53	1	1330	A
53	1	1331	U
53	1	1332	A
53	1	1348	U
53	1	1349	G
53	1	1351	U
53	1	1352	A
53	1	1353	U
53	1	1354	G
53	1	1356	U
53	1	1357	G
53	1	1367	G
53	1	1380	G
53	1	1383	G
53	1	1386	A
53	1	1399	A
53	1	1400	G
53	1	1404	G
53	1	1414	G
53	1	1419	A
53	1	1421	G
53	1	1434	G
53	1	1437	C

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Mol	Chain	Res	Type
53	1	1443	G
53	1	1450	G
53	1	1460	A
53	1	1471	U
53	1	1481	A
53	1	1483	G
53	1	1485	G
53	1	1487	G
53	1	1490	A
53	1	1503	A
53	1	1508	C
53	1	1523	U
53	1	1527	C
53	1	1531	C
53	1	1533	U
53	1	1536	G
53	1	1539	A
53	1	1549	U
53	1	1555	U
53	1	1556	C
53	1	1557	A
53	1	1560	G
53	1	1561	G
53	1	1562	C
53	1	1566	A
53	1	1567	U
53	1	1568	U
53	1	1569	U
53	1	1570	U
53	1	1571	A
53	1	1573	G
53	1	1575	A
53	1	1577	G
53	1	1580	A
53	1	1581	C
53	1	1582	C
53	1	1583	A
53	1	1587	A
53	1	1589	A
53	1	1593	A
53	1	1607	U
53	1	1608	C

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Mol	Chain	Res	Type
53	1	1620	U
53	1	1622	U
53	1	1629	U
53	1	1631	C
53	1	1632	A
53	1	1639	C
53	1	1641	U
53	1	1642	A
53	1	1643	A
53	1	1645	U
53	1	1657	C
53	1	1658	G
53	1	1662	G
53	1	1683	A
53	1	1701	C
53	1	1703	U
53	1	1716	U
53	1	1717	U
53	1	1718	G
53	1	1724	U
53	1	1725	C
53	1	1741	A
53	1	1746	U
53	1	1750	A
53	1	1751	G
53	1	1759	C
53	1	1760	A
53	1	1762	C
53	1	1763	U
53	1	1765	U
53	1	1766	G
53	1	1770	G
53	1	1775	G
53	1	1780	G
53	1	1794	G
53	1	1797	A
53	1	1810	A
53	1	1813	A
53	1	1814	A
53	1	1815	U
53	1	1816	A
53	1	1817	G

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Mol	Chain	Res	Type
53	1	1820	U
53	1	1821	U
53	1	1822	C
53	1	1837	U
53	1	1839	A
53	1	1841	A
53	1	1842	A
53	1	1849	C
53	1	1850	A
53	1	1858	A
53	1	1859	A
53	1	1866	C
53	1	1867	A
53	1	1871	U
53	1	1880	U
53	1	1886	A
53	1	1893	A
53	1	1906	G
53	1	1926	C
53	1	1937	U
53	1	1951	C
53	1	1952	G
53	1	1953	G
53	1	2094	C
53	1	2099	A
53	1	2100	A
53	1	2101	C
53	1	2102	U
53	1	2112	U
53	1	2121	G
53	1	2122	G
53	1	2126	A
53	1	2131	A
53	1	2140	U
53	1	2144	A
53	1	2145	A
53	1	2158	A
53	1	2163	C
53	1	2164	A
53	1	2169	G
53	1	2170	U
53	1	2184	U

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Mol	Chain	Res	Type
53	1	2185	G
53	1	2191	U
53	1	2193	U
53	1	2194	G
53	1	2195	C
53	1	2196	C
53	1	2198	A
53	1	2201	G
53	1	2205	U
53	1	2207	A
53	1	2208	A
53	1	2209	U
53	1	2210	G
53	1	2211	U
53	1	2226	U
53	1	2227	C
53	1	2228	A
53	1	2229	A
53	1	2235	C
53	1	2236	G
53	1	2238	G
53	1	2239	G
53	1	2242	A
53	1	2243	A
53	1	2244	A
53	1	2245	C
53	1	2246	G
53	1	2247	G
53	1	2248	C
53	1	2249	G
53	1	2250	G
53	1	2252	A
53	1	2255	A
53	1	2256	A
53	1	2257	C
53	1	2259	A
53	1	2263	C
53	1	2264	U
53	1	2268	U
53	1	2269	U
53	1	2270	A
53	1	2271	A

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Mol	Chain	Res	Type
53	1	2272	G
53	1	2273	G
53	1	2274	U
53	1	2276	G
53	1	2277	C
53	1	2278	C
53	1	2279	A
53	1	2280	A
53	1	2316	G
53	1	2317	A
53	1	2318	U
53	1	2334	U
53	1	2335	G
53	1	2336	U
53	1	2370	G
53	1	2371	G
53	1	2385	G
53	1	2388	U
53	1	2393	G
53	1	2397	A
53	1	2398	A
53	1	2401	A
53	1	2402	A
53	1	2410	U
53	1	2411	U
53	1	2412	G
53	1	2414	G
53	1	2418	G
53	1	2419	A
53	1	2428	U
53	1	2429	G
53	1	2430	A
53	1	2435	G
53	1	2437	G
53	1	2444	C
53	1	2445	A
53	1	2502	A
53	1	2503	G
53	1	2504	U
53	1	2505	U
53	1	2506	U
53	1	2508	U

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Mol	Chain	Res	Type
53	1	2510	U
53	1	2511	A
53	1	2514	U
53	1	2515	A
53	1	2522	G
53	1	2523	A
53	1	2526	C
53	1	2527	G
53	1	2528	G
53	1	2529	A
53	1	2530	G
53	1	2531	C
53	1	2532	U
53	1	2533	G
53	1	2534	G
53	1	2538	U
53	1	2539	C
53	1	2540	A
53	1	2541	U
53	1	2542	U
53	1	2543	U
53	1	2544	U
53	1	2545	C
53	1	2546	C
53	1	2547	A
53	1	2548	C
53	1	2549	G
53	1	2552	C
53	1	2554	A
53	1	2555	G
53	1	2561	A
53	1	2569	A
53	1	2570	U
53	1	2571	U
53	1	2572	C
53	1	2573	G
53	1	2575	G
53	1	2578	U
53	1	2583	C
53	1	2586	G
53	1	2593	A
53	1	2594	C

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Mol	Chain	Res	Type
53	1	2598	G
53	1	2602	G
53	1	2606	G
53	1	2607	G
53	1	2614	G
53	1	2615	G
53	1	2620	G
53	1	2621	G
53	1	2623	G
53	1	2625	C
53	1	2626	A
53	1	2645	G
53	1	2650	U
53	1	2651	G
53	1	2652	U
53	1	2653	C
53	1	2654	C
53	1	2655	U
53	1	2656	A
53	1	2657	A
53	1	2659	G
53	1	2663	G
53	1	2667	A
53	1	2674	A
53	1	2677	G
53	1	2681	U
53	1	2685	C
53	1	2686	A
53	1	2688	U
53	1	2690	G
53	1	2691	A
53	1	2692	A
53	1	2693	C
53	1	2694	A
53	1	2696	A
53	1	2697	A
53	1	2698	G
53	1	2700	G
53	1	2701	U
53	1	2702	A
53	1	2703	A
53	1	2704	A

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Mol	Chain	Res	Type
53	1	2707	C
53	1	2712	U
53	1	2713	U
53	1	2714	G
53	1	2715	A
53	1	2716	U
53	1	2717	U
53	1	2718	U
53	1	2719	U
53	1	2720	G
53	1	2721	A
53	1	2724	U
53	1	2725	U
53	1	2726	C
53	1	2727	A
53	1	2728	G
53	1	2729	U
53	1	2730	G
53	1	2731	U
53	1	2732	G
53	1	2740	A
53	1	2747	A
53	1	2749	G
53	1	2752	U
53	1	2754	G
53	1	2756	C
53	1	2758	A
53	1	2759	U
53	1	2760	C
53	1	2761	G
53	1	2762	A
53	1	2763	U
53	1	2764	C
53	1	2765	C
53	1	2766	U
53	1	2767	U
53	1	2768	U
53	1	2769	A
53	1	2770	G
53	1	2771	U
53	1	2772	C
53	1	2773	C

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Mol	Chain	Res	Type
53	1	2774	C
53	1	2777	G
53	1	2778	G
53	1	2779	A
53	1	2785	A
53	1	2786	G
53	1	2787	G
53	1	2788	C
53	1	2790	A
53	1	2791	G
53	1	2793	G
53	1	2794	G
53	1	2795	U
53	1	2796	G
53	1	2797	C
53	1	2798	C
53	1	2799	A
53	1	2801	A
53	1	2802	A
53	1	2803	A
53	1	2804	A
53	1	2810	C
53	1	2814	G
53	1	2816	G
53	1	2817	A
53	1	2818	U
53	1	2819	A
53	1	2820	A
53	1	2821	C
53	1	2822	U
53	1	2824	G
53	1	2825	C
53	1	2826	U
53	1	2840	C
53	1	2842	U
53	1	2845	A
53	1	2847	A
53	1	2848	G
53	1	2857	C
53	1	2858	U
53	1	2859	U
53	1	2861	U

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Mol	Chain	Res	Type
53	1	2863	G
53	1	2864	A
53	1	2865	U
53	1	2866	U
53	1	2867	C
53	1	2868	U
53	1	2869	U
53	1	2870	C
53	1	2871	G
53	1	2872	A
53	1	2873	U
53	1	2874	G
53	1	2875	U
53	1	2876	C
53	1	2877	G
53	1	2878	G
53	1	2879	C
53	1	2887	A
53	1	2889	C
53	1	2891	U
53	1	2898	G
53	1	2899	C
53	1	2901	G
53	1	2902	A
53	1	2918	G
53	1	2923	U
53	1	2924	U
53	1	2925	C
53	1	2926	A
53	1	2927	C
53	1	2928	C
53	1	2930	A
53	1	2935	U
53	1	2936	A
53	1	2944	U
53	1	2945	G
53	1	2946	A
53	1	2947	G
53	1	2948	C
53	1	2952	G
53	1	2953	U
53	1	2954	U

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Mol	Chain	Res	Type
53	1	2955	U
53	1	2956	A
53	1	2957	G
53	1	2966	G
53	1	2970	C
53	1	2971	A
53	1	2972	G
53	1	2978	U
53	1	2979	U
53	1	2980	U
53	1	2981	U
53	1	2982	A
53	1	2983	C
53	1	2984	C
53	1	2990	G
53	1	2996	U
53	1	2997	G
53	1	3006	A
53	1	3012	A
53	1	3017	A
53	1	3021	A
53	1	3022	G
53	1	3023	U
53	1	3026	G
53	1	3029	A
53	1	3030	G
53	1	3031	G
53	1	3032	A
53	1	3034	C
53	1	3035	A
53	1	3040	A
53	1	3049	A
53	1	3056	U
53	1	3057	U
53	1	3058	U
53	1	3059	G
53	1	3074	G
53	1	3078	U
53	1	3079	U
53	1	3080	G
53	1	3086	A
53	1	3092	C

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Mol	Chain	Res	Type
53	1	3093	C
53	1	3094	A
53	1	3095	U
53	1	3100	U
53	1	3102	G
53	1	3109	G
53	1	3116	G
53	1	3117	C
53	1	3122	A
53	1	3127	A
53	1	3129	A
53	1	3130	A
53	1	3131	U
53	1	3142	A
53	1	3143	C
53	1	3150	A
53	1	3151	U
53	1	3153	U
53	1	3154	C
53	1	3155	U
53	1	3156	U
53	1	3157	U
53	1	3158	G
53	1	3160	U
53	1	3162	C
53	1	3164	C
53	1	3165	A
53	1	3168	A
53	1	3172	A
53	1	3173	G
53	1	3174	A
53	1	3176	G
53	1	3179	U
53	1	3180	A
53	1	3181	C
53	1	3184	A
53	1	3187	A
53	1	3196	U
53	1	3197	G
53	1	3198	U
53	1	3199	G
53	1	3202	G

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Mol	Chain	Res	Type
53	1	3207	U
53	1	3217	C
53	1	3218	A
53	1	3219	G
53	1	3229	G
53	1	3239	G
53	1	3242	G
53	1	3243	A
53	1	3245	A
53	1	3246	G
53	1	3247	G
53	1	3259	U
53	1	3263	G
53	1	3268	A
53	1	3270	U
53	1	3273	A
53	1	3276	G
53	1	3278	C
53	1	3279	A
53	1	3281	U
53	1	3282	U
53	1	3283	U
53	1	3285	C
53	1	3286	G
53	1	3289	G
53	1	3294	A
53	1	3295	A
53	1	3304	U
53	1	3307	A
53	1	3313	U
53	1	3316	A
53	1	3317	U
53	1	3318	G
53	1	3319	U
53	1	3320	A
53	1	3328	G
53	1	3339	A
53	1	3341	U
53	1	3342	A
53	1	3345	G
53	1	3346	U
53	1	3347	A

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Mol	Chain	Res	Type
53	1	3350	C
53	1	3351	U
53	1	3352	U
53	1	3353	G
53	1	3354	U
53	1	3355	U
53	1	3356	G
53	1	3360	C
53	1	3363	U
53	1	3369	G
53	1	3375	A
53	1	3376	A
53	1	3378	C
53	1	3381	U
53	1	3389	U
54	2	25	G
54	2	34	U
54	2	35	C
54	2	49	G
54	2	51	G
54	2	52	A
54	2	53	A
54	2	56	G
54	2	59	A
54	2	62	C
54	2	63	G
54	2	76	C
54	2	79	A
54	2	80	A
54	2	81	U
54	2	82	U
54	2	84	C
54	2	85	G
54	2	86	U
54	2	87	G
54	2	88	A
54	2	89	A
54	2	90	U
54	2	95	G
54	2	97	A
54	2	104	A
54	2	105	A

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Mol	Chain	Res	Type
54	2	106	C
54	2	111	A
54	2	113	U
54	2	116	G
54	2	124	G
54	2	125	U
54	2	126	A
54	2	128	U
54	2	138	A
54	2	151	C
54	2	152	G
55	3	7	G
55	3	8	G
55	3	13	A
55	3	22	A
55	3	42	A
55	3	53	U
55	3	54	U
55	3	55	A
55	3	60	G
55	3	65	G
55	3	87	G
55	3	97	A
55	3	98	C
55	3	99	G
55	3	102	A
55	3	104	A
55	3	107	C
55	3	109	G
55	3	112	G
55	3	114	U
55	3	118	A
55	3	121	U
58	6	2	C
58	6	4	U
58	6	5	C
58	6	6	U
58	6	7	C
58	6	8	A
58	6	9	A
58	6	13	U
58	6	14	U

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Mol	Chain	Res	Type
58	6	16	U
58	6	17	G
58	6	18	U
58	6	21	G
58	6	23	U
58	6	24	A
58	6	25	G
58	6	26	U
58	6	27	G
58	6	31	G
58	6	32	A
58	6	33	U
58	6	34	A
58	6	40	U
58	6	41	G
58	6	42	G
58	6	43	A
58	6	45	U
58	6	47	A
58	6	48	A
58	6	49	C
58	6	53	A
58	6	54	A
58	6	56	U
58	6	57	U
58	6	58	G
58	6	59	C
58	6	228	U
58	6	229	U
58	6	230	A
58	6	231	A
58	6	232	A

All (235) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	1	13	A
53	1	40	A
53	1	73	C
53	1	133	U
53	1	148	G
53	1	160	G

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Mol	Chain	Res	Type
53	1	169	U
53	1	210	U
53	1	239	G
53	1	284	A
53	1	285	A
53	1	304	G
53	1	305	U
53	1	402	A
53	1	406	G
53	1	439	C
53	1	518	G
53	1	588	G
53	1	594	U
53	1	607	A
53	1	637	C
53	1	645	A
53	1	649	A
53	1	718	G
53	1	720	A
53	1	760	G
53	1	761	A
53	1	765	C
53	1	766	U
53	1	770	G
53	1	800	G
53	1	806	A
53	1	816	A
53	1	849	C
53	1	896	A
53	1	916	G
53	1	990	U
53	1	994	G
53	1	998	A
53	1	1056	U
53	1	1057	A
53	1	1064	A
53	1	1097	G
53	1	1102	A
53	1	1103	A
53	1	1111	U
53	1	1128	U
53	1	1144	U

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Mol	Chain	Res	Type
53	1	1152	G
53	1	1159	A
53	1	1191	U
53	1	1192	C
53	1	1201	C
53	1	1203	A
53	1	1205	A
53	1	1241	U
53	1	1244	A
53	1	1281	G
53	1	1282	G
53	1	1286	A
53	1	1302	A
53	1	1307	G
53	1	1329	U
53	1	1355	A
53	1	1467	A
53	1	1482	A
53	1	1484	U
53	1	1502	C
53	1	1525	G
53	1	1554	U
53	1	1556	C
53	1	1560	G
53	1	1567	U
53	1	1568	U
53	1	1569	U
53	1	1570	U
53	1	1573	G
53	1	1574	C
53	1	1580	A
53	1	1581	C
53	1	1582	C
53	1	1606	U
53	1	1607	U
53	1	1630	U
53	1	1641	U
53	1	1643	A
53	1	1657	C
53	1	1716	U
53	1	1814	A
53	1	1816	A

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Mol	Chain	Res	Type
53	1	1820	U
53	1	1841	A
53	1	1846	C
53	1	1858	A
53	1	2101	C
53	1	2113	A
53	1	2144	A
53	1	2209	U
53	1	2235	C
53	1	2238	G
53	1	2243	A
53	1	2244	A
53	1	2255	A
53	1	2256	A
53	1	2261	G
53	1	2263	C
53	1	2268	U
53	1	2269	U
53	1	2271	A
53	1	2272	G
53	1	2275	A
53	1	2277	C
53	1	2316	G
53	1	2317	A
53	1	2410	U
53	1	2411	U
53	1	2428	U
53	1	2429	G
53	1	2444	C
53	1	2510	U
53	1	2511	A
53	1	2513	U
53	1	2522	G
53	1	2525	G
53	1	2527	G
53	1	2528	G
53	1	2537	U
53	1	2541	U
53	1	2547	A
53	1	2548	C
53	1	2554	A
53	1	2568	C

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Mol	Chain	Res	Type
53	1	2570	U
53	1	2572	C
53	1	2593	A
53	1	2598	G
53	1	2624	G
53	1	2625	C
53	1	2650	U
53	1	2651	G
53	1	2652	U
53	1	2654	C
53	1	2655	U
53	1	2658	G
53	1	2680	A
53	1	2688	U
53	1	2691	A
53	1	2692	A
53	1	2695	A
53	1	2716	U
53	1	2719	U
53	1	2725	U
53	1	2726	C
53	1	2727	A
53	1	2728	G
53	1	2729	U
53	1	2753	G
53	1	2758	A
53	1	2761	G
53	1	2763	U
53	1	2770	G
53	1	2793	G
53	1	2795	U
53	1	2796	G
53	1	2797	C
53	1	2798	C
53	1	2802	A
53	1	2817	A
53	1	2818	U
53	1	2819	A
53	1	2825	C
53	1	2857	C
53	1	2858	U
53	1	2865	U

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Mol	Chain	Res	Type
53	1	2866	U
53	1	2868	U
53	1	2869	U
53	1	2870	C
53	1	2875	U
53	1	2900	A
53	1	2946	A
53	1	2954	U
53	1	2970	C
53	1	2983	C
53	1	3030	G
53	1	3048	A
53	1	3055	U
53	1	3056	U
53	1	3057	U
53	1	3078	U
53	1	3093	C
53	1	3116	G
53	1	3153	U
53	1	3154	C
53	1	3155	U
53	1	3156	U
53	1	3157	U
53	1	3158	G
53	1	3171	U
53	1	3195	U
53	1	3207	U
53	1	3218	A
53	1	3228	C
53	1	3242	G
53	1	3267	A
53	1	3269	U
53	1	3278	C
53	1	3279	A
53	1	3316	A
53	1	3340	G
53	1	3341	U
53	1	3350	C
53	1	3351	U
53	1	3353	G
53	1	3375	A
53	1	3389	U

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Mol	Chain	Res	Type
54	2	80	A
54	2	81	U
54	2	83	C
54	2	88	A
54	2	123	G
55	3	52	G
55	3	97	A
55	3	98	C
55	3	111	U
58	6	1	C
58	6	5	C
58	6	16	U
58	6	23	U
58	6	24	A
58	6	25	G
58	6	26	U
58	6	57	U
58	6	228	U
58	6	231	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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	GTP	b	701	61	26,34,34	1.15	2 (7%)	29,54,54	1.83	6 (20%)
60	GTP	m	501	61	26,34,34	1.05	2 (7%)	29,54,54	1.64	4 (13%)

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
60	GTP	b	701	61	-	0/18/38/38	0/3/3/3
60	GTP	m	501	61	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	m	501	GTP	C5-C4	2.82	1.46	1.40
60	b	701	GTP	C5-C4	3.04	1.47	1.40
60	m	501	GTP	C6-C5	3.18	1.47	1.41
60	b	701	GTP	C6-C5	3.86	1.49	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	b	701	GTP	C6-C5-C4	-3.71	116.62	120.86
60	b	701	GTP	C5-C6-N1	-3.66	118.73	123.52
60	m	501	GTP	C5-C6-N1	-3.54	118.89	123.52
60	b	701	GTP	N3-C2-N1	-3.50	122.79	127.56
60	m	501	GTP	N3-C2-N1	-3.27	123.10	127.56
60	m	501	GTP	C6-C5-C4	-3.05	117.37	120.86
60	b	701	GTP	C1'-N9-C4	-2.75	123.74	126.81
60	b	701	GTP	O4'-C1'-N9	2.74	113.27	108.11
60	m	501	GTP	C6-N1-C2	4.66	121.34	115.88
60	b	701	GTP	C6-N1-C2	5.03	121.78	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.