



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 22, 2016 – 03:08 PM EST

PDB ID : 5LZX
EMDB ID: : EMD-4135
Title : Structure of the mammalian rescue complex with Pelota and Hbs1l assembled on a UGA stop codon.
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.67 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

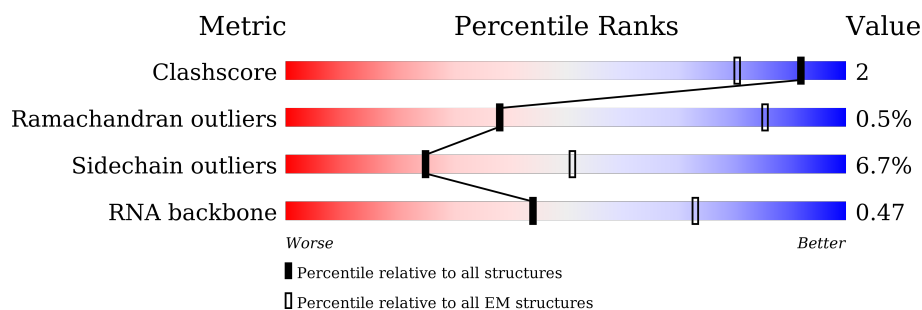
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.67 Å.

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
















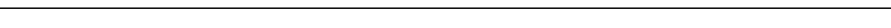




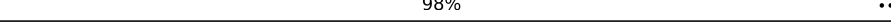




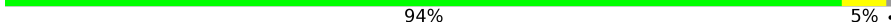

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A	257	82% 14% . .
2	B	403	89% 9% .
3	C	425	76% 8% . 15%
4	D	297	89% 9% .
5	E	291	67% 6% . 26%
6	F	247	80% 11% . 9%
7	G	319	65% 8% 27%
8	H	192	89% 10% .

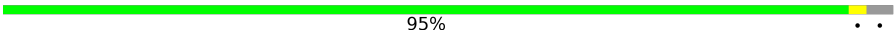

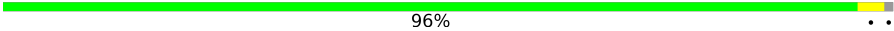
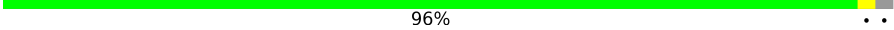



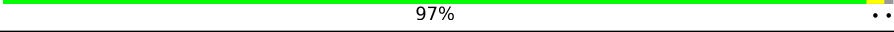



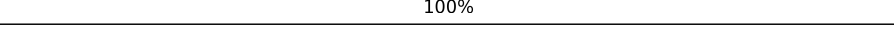







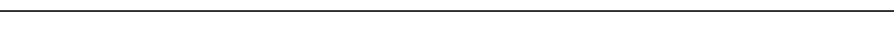

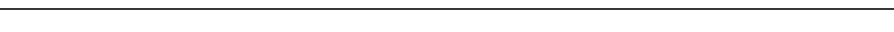
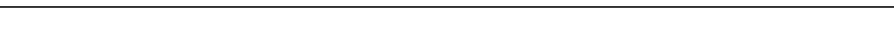


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Mol	Chain	Length	Quality of chain
9	I	214	 88% 7% .
10	J	178	 88% 7% .
11	L	211	 92% 7%
12	M	218	 55% 8% 37%
13	N	204	 89% 10%
14	O	203	 88% 10% .
15	P	184	 78% . . 17%
16	Q	188	 90% 10% .
17	R	196	 82% 9% . 8%
18	S	176	 86% 14%
19	T	160	 91% 9% .
20	U	128	 70% 6% . 23%
21	V	140	 82% 11% . 6%
22	W	157	 62% 6% 32%
23	X	156	 71% . 24%
24	Y	145	 87% 6% 8%
25	Z	136	 90% 10% .
26	a	148	 98% ..
27	b	245	 41% . 58%
28	c	115	 83% . 15%
29	d	125	 77% 9% 14%
30	e	135	 88% 7% 5%
31	f	110	 94% 5% .
32	g	117	 92% 5% .
33	h	123	 95% . .









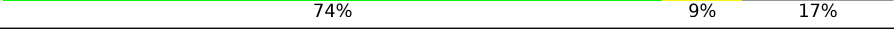

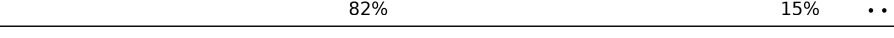
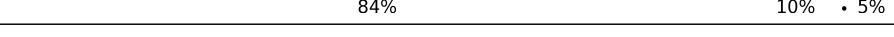

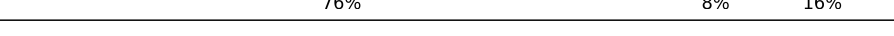
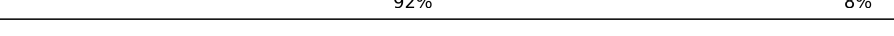

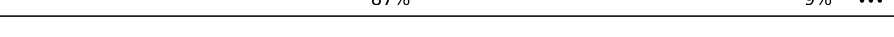

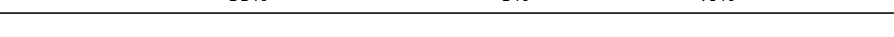






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Mol	Chain	Length	Quality of chain
34	i	105	95% 
35	j	97	84%  5% 11%
36	k	70	96% 
37	l	51	96% 
38	m	102	49%  49%
39	n	25	92% 
40	o	106	92%  6%
41	p	92	97% 
42	r	137	82%  8% 9%
43	s	318	59%  38%
44	t	165	90%  7%
45	1	7	100% 
46	2	76	83%  16%
47	3	75	64%  32%
48	5	3543	70%  26%
49	7	120	85%  14%
50	8	156	72%  24%
51	9	1869	62%  26% 9%
52	AA	295	64%  10% 26%
53	BB	264	71%  8% 19%
54	CC	293	67%  8% 25%
55	DD	243	83%  10% 6%
56	EE	263	87% 
57	FF	204	81%  9% 9%
58	GG	249	85%  10% 5%





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

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Mol	Chain	Length	Quality of chain
84	gg	317	
85	hh	8	
86	ii	403	
87	jj	710	

2 Entry composition

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

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called Ul3.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called uL4.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 6 is a protein called uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called Ribosomal protein L10 (Predicted).

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

- Molecule 10 is a protein called uL5.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called Ribosomal protein L15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called 60S ribosomal protein L27.

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

- Molecule 26 is a protein called uL15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

- Molecule 33 is a protein called uL29.

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

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

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

- Molecule 35 is a protein called Ribosomal protein L37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	1	7	Total	C	N	O	0	0
			49	31	8	10		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called 40S ribosomal protein S3a.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called 40S ribosomal protein S6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

- Molecule 61 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called 40S ribosomal protein S12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called 40S ribosomal protein S27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA (UGA stop codon).

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

- Molecule 86 is a protein called Protein pelota homolog.

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

There are 19 discrepancies between the modelled and reference sequences:

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

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

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

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
jj	-25	MET	-	initiating methionine	UNP Q9Y450
jj	-24	ASP	-	expression tag	UNP Q9Y450

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

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

Mol	Chain	Residues	Atoms	AltConf
88	P	1	Total Mg 1 1	0
88	jj	1	Total Mg 1 1	0
88	V	1	Total Mg 1 1	0
88	7	5	Total Mg 5 5	0
88	a	1	Total Mg 1 1	0
88	5	182	Total Mg 182 182	0
88	8	6	Total Mg 6 6	0

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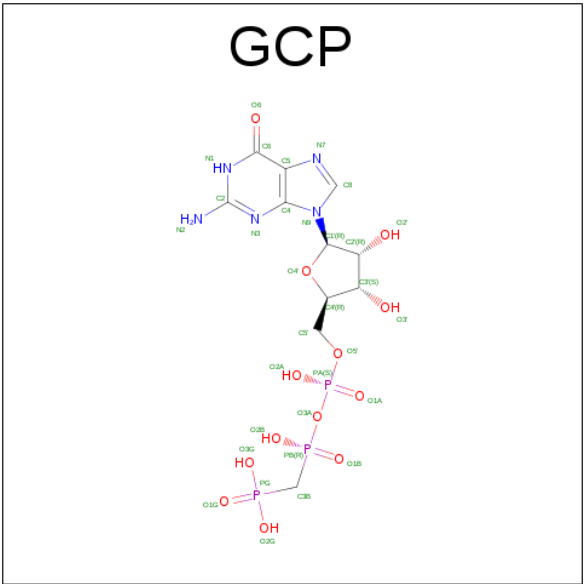
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Mol	Chain	Residues	Atoms		AltConf
88	9	66	Total	Mg	0
			66	66	
88	L	1	Total	Mg	0
			1	1	

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

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

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

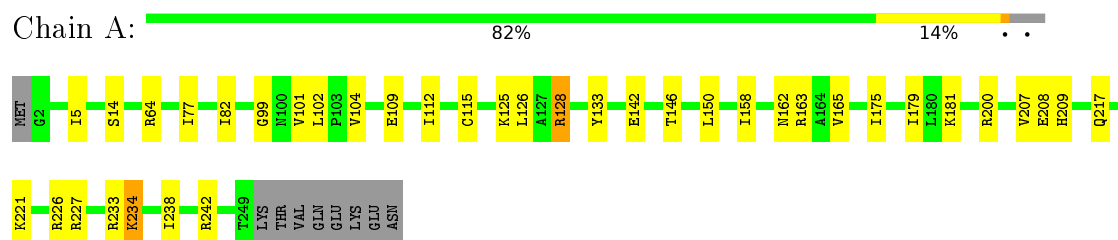


Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

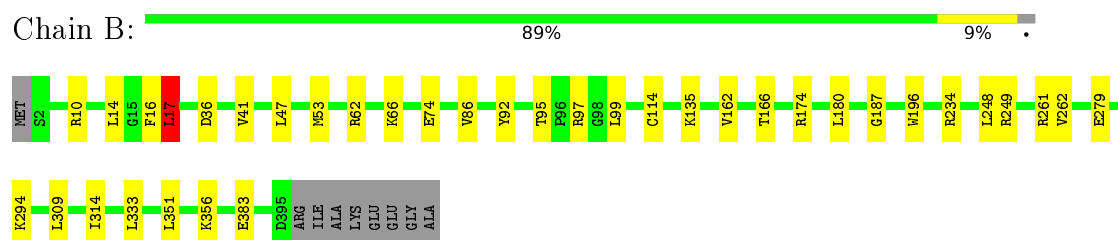
3 Residue-property plots

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

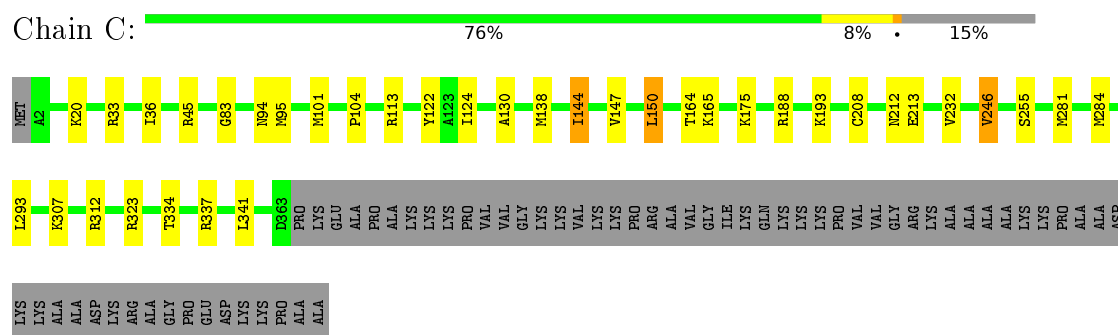
- Molecule 1: uL2



- Molecule 2: U13



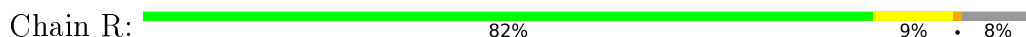
- Molecule 3: uL4



- Molecule 4: 60S ribosomal protein L5

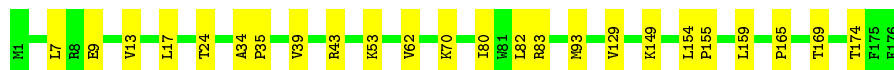
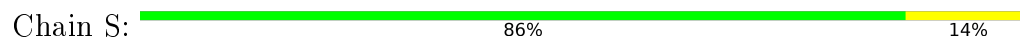


- Molecule 5: 60S ribosomal protein L6

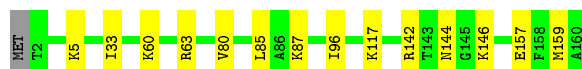




- Molecule 18: eL20



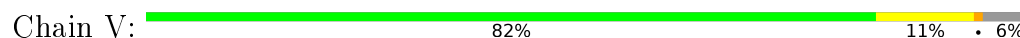
- Molecule 19: eL21



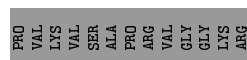
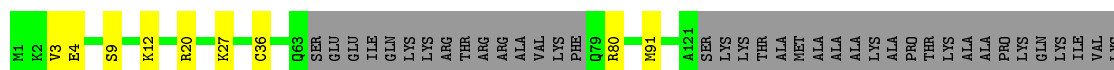
- Molecule 20: eL22



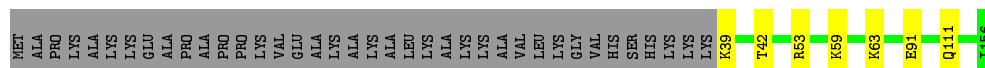
- Molecule 21: uL14



- Molecule 22: eL24



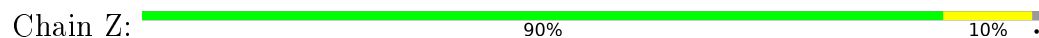
- Molecule 23: uL23



- Molecule 24: uL24



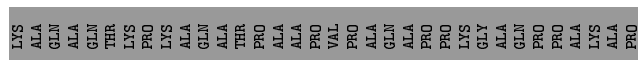
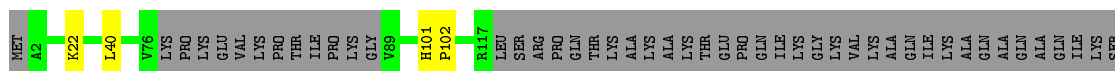
- Molecule 25: 60S ribosomal protein L27



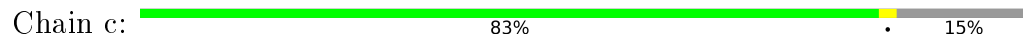
- Molecule 26: uL15



- Molecule 27: eL29



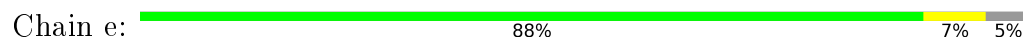
- Molecule 28: eL30



- Molecule 29: eL31



- Molecule 30: eL32



- Molecule 31: eL33

Chain f:  94% 5%



- Molecule 32: eL34

Chain g:  92% 5%



- Molecule 33: uL29

Chain h:  95% . .




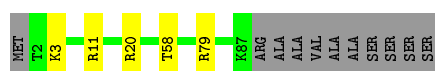
- Molecule 34: 60S ribosomal protein L36

Chain i:  95% . .



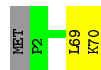
- Molecule 35: Ribosomal protein L37

Chain j:  84% 5% 11%



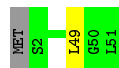
- Molecule 36: eL38

Chain k:  96% . .



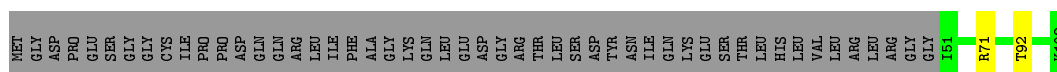
- Molecule 37: eL39

Chain l:  96% . .



- Molecule 38: eL40

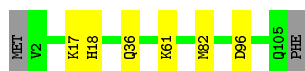
Chain m:  49% . 49%



- Molecule 39: eL41



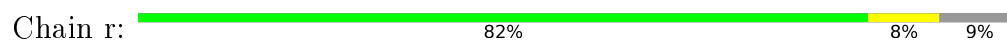
- Molecule 40: eL42



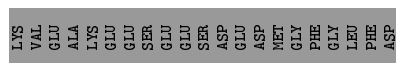
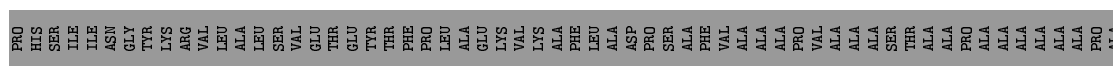
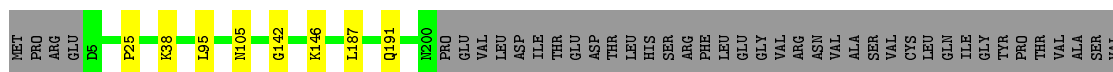
- Molecule 41: eL43



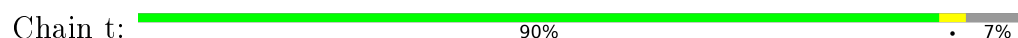
- Molecule 42: eL28



- Molecule 43: uL10

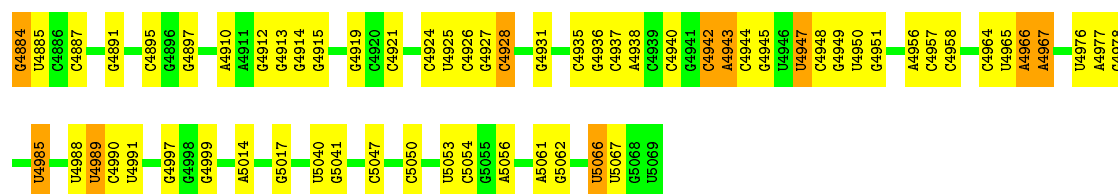


- Molecule 44: uL11



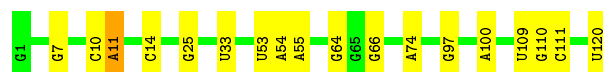
- Molecule 45: Nascent chain



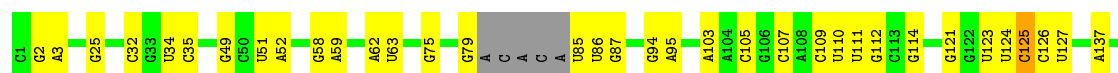
• Molecule 49: 5S ribosomal RNA

Chain 7: 85% 14%



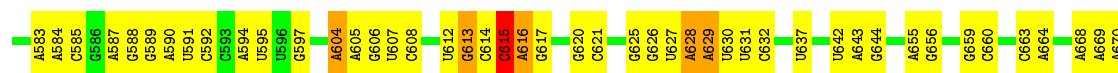
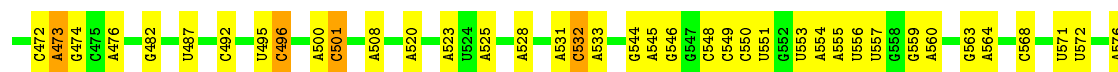
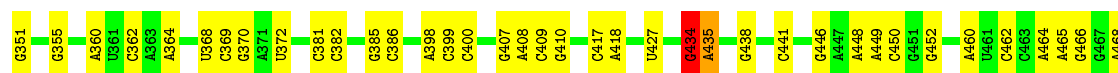
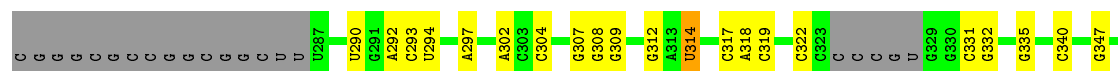
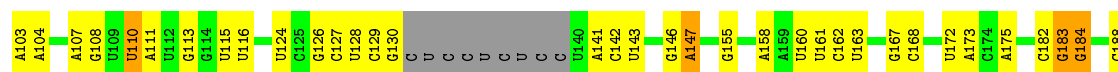
• Molecule 50: 5.8S ribosomal RNA

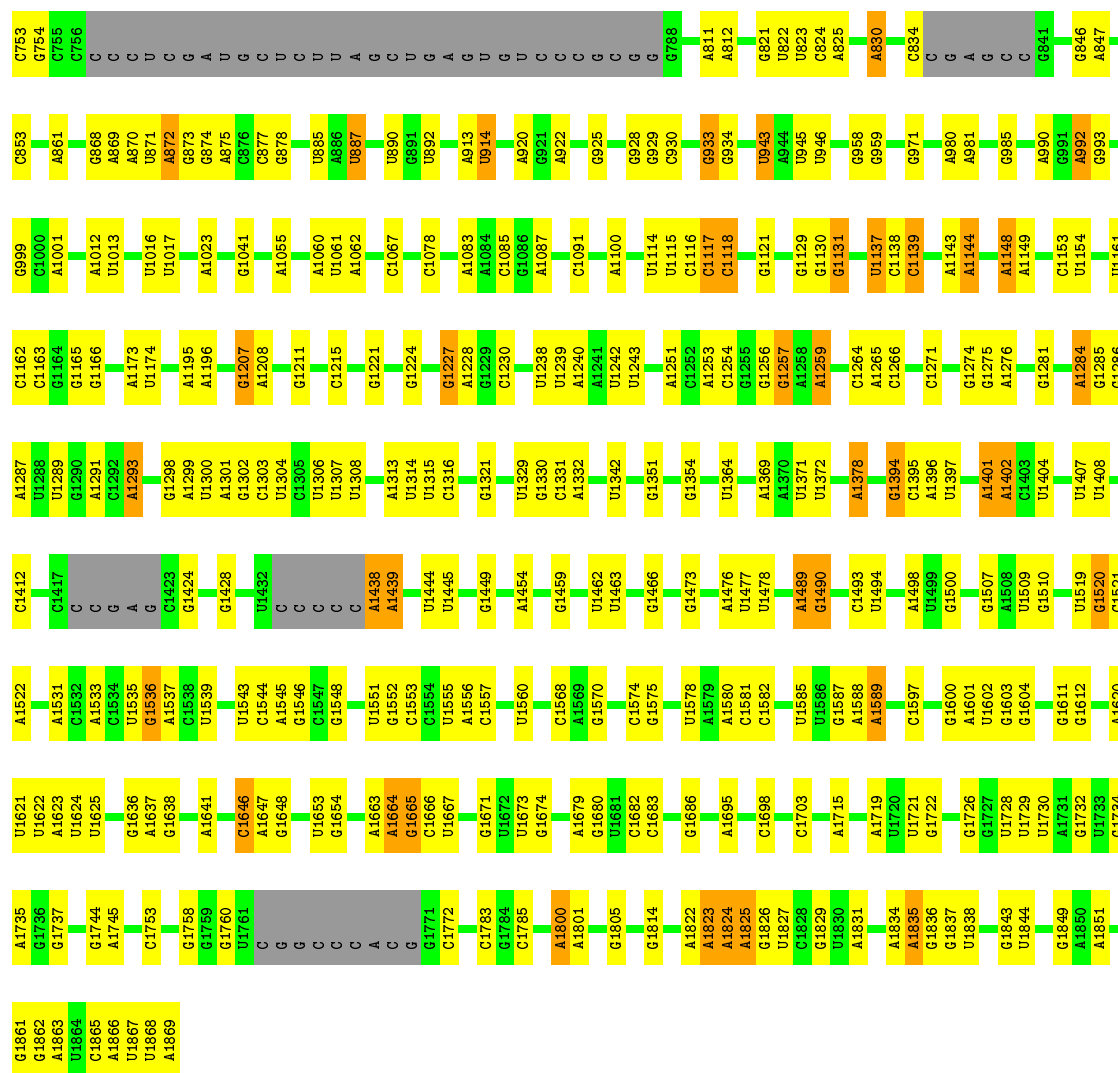
Chain 8: 72% 24%



• Molecule 51: 18S ribosomal RNA

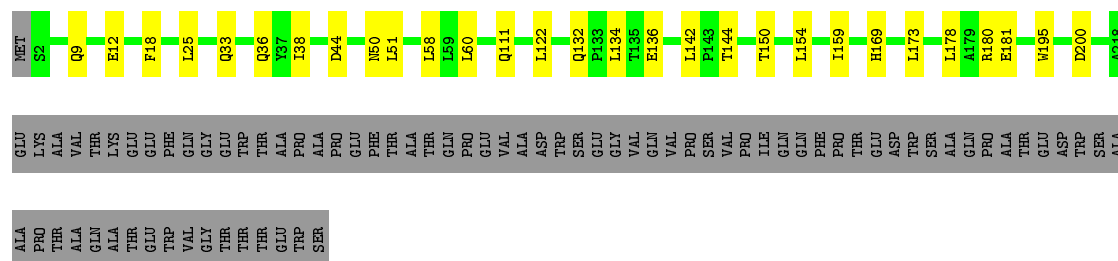
Chain 9: 62% 26% 9%





• Molecule 52: uS2

Chain AA: 64% 10% 26%



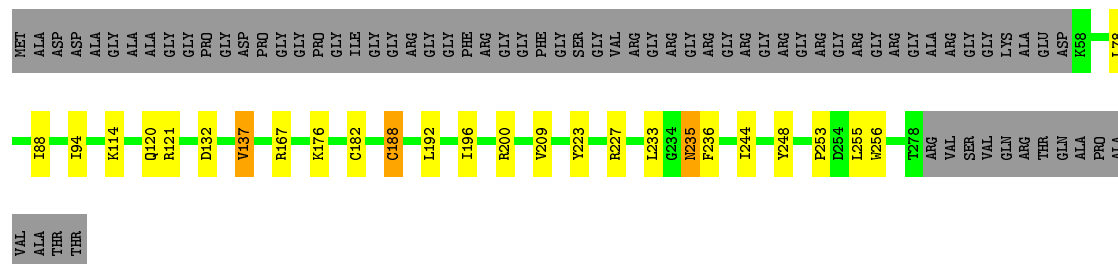
• Molecule 53: 40S ribosomal protein S3a

Chain BB: 71% 8% 19%

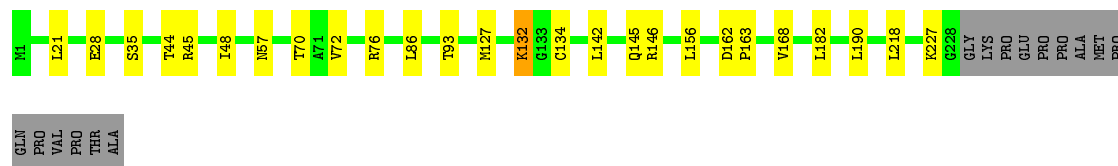
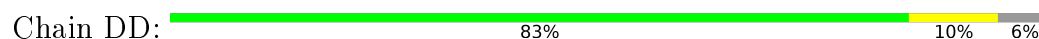




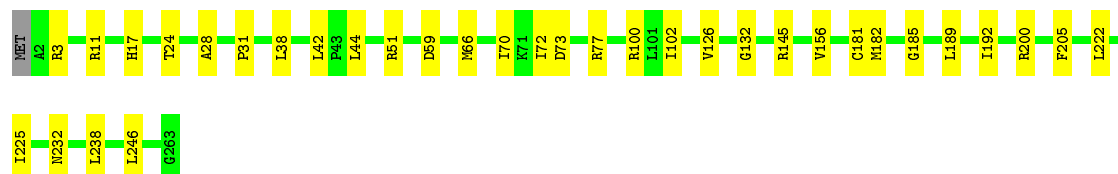
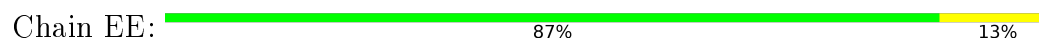
- Molecule 54: uS5



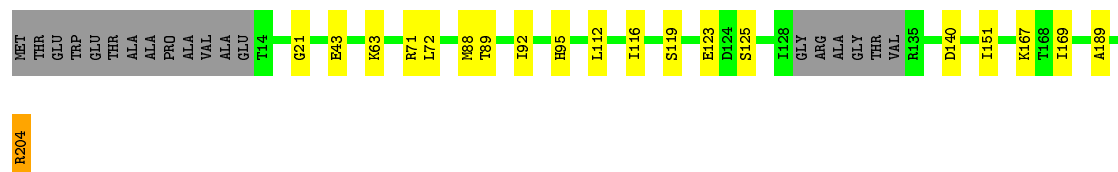
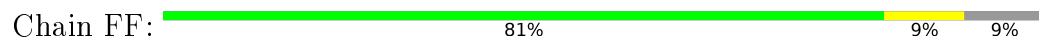
- Molecule 55: uS3



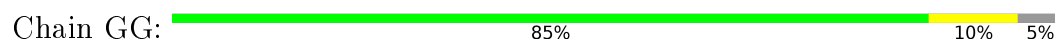
- Molecule 56: eS4



- Molecule 57: uS7




- Molecule 58: 40S ribosomal protein S6



SER
GLN
LYS


- Molecule 59: eS7

Chain HH:  81% 14% 5%

MET PHE SER SER A6 A7 I8 D17 S21 L27 L36 L40 L45 L46 V53 I61 V66 Q76 L79 E82 I95 A96 I100 S108 ARG THR LYS ASN K113 R118 S119 R120 T121 L122 L133 V134 R145 D149 K160

F173 L194

- Molecule 60: eS8

Chain II:  89% 10% .

MET G2 I3 D6 R12 K23 K26 Y27 E28 T36 R49 R82 N99 Y117 L121 K128 L129 T130 A156 Q168 R178 P179 L190 E194 G207 LYS

- Molecule 61: Ribosomal protein S9 (Predicted)

Chain JJ:  86% 9% 5%

MET P2 R18 L29 Y35 R38 R45 L61 R69 R70 R79 R80 E89 N92 L106 K116 I130 I135 I144 F147 G186 ALA GLY ASP ASP GLU GLU ASP

- Molecule 62: eS10

Chain KK:  50% 7% 42%

M1 K6 I11 K17 H32 L35 V40 V45 Q50 E60 R64 I89 R96 SER ARG PRO GLU THR ARG GLY ARG PRO PRO LYS GLY LEU GLU GLY GLU ASP ASP LYS LYS ALA ALA GLY GLY SER THR LYS THR GLU PHE GLN PHE ARG GLY PHE GLY ARG PRO GLN

VAL PRO PRO GLY ALA ASP LYS LYS ALA ALA ALA ALA GLY SER THR LYS THR GLU PHE GLN PHE ARG GLY PHE GLY ARG PRO GLN


- Molecule 63: uS17

Chain LL:  74% 15% 9%

MET ALA D3 T4 I16 K20 V23 LEU LEU GLY THR GLY LYS K32 Y37 K38 N39 I40 I41 L42 T51 I56 P61 V66 R69 M82 T85 I96 I99 H100 R101 H106 S110 L113 Q121 V126 R132 P133 SER L134

V142 L143 K144 K153 GLN PHE GLN PHE

- Molecule 64: 40S ribosomal protein S12

Chain MM:  77% 12% 11%



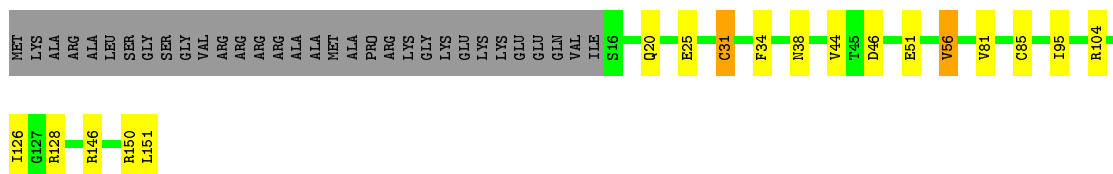
• Molecule 65: uS15

Chain NN: 85% 12% ..



• Molecule 66: uS11

Chain OO: 70% 10% • 19%



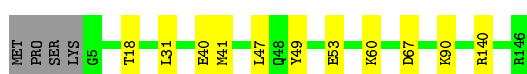
• Molecule 67: uS19

Chain PP: 74% 9% 17%



• Molecule 68: uS9

Chain QQ: 90% 8% •



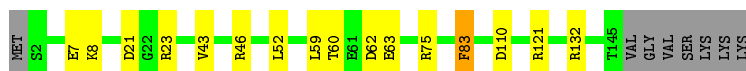
• Molecule 69: eS17

Chain RR: 82% 15% ..



• Molecule 70: uS13

Chain SS: 84% 10% • 5%

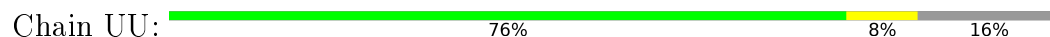


• Molecule 71: eS19

Chain TT: 88% 8% ..



- Molecule 72: uS10



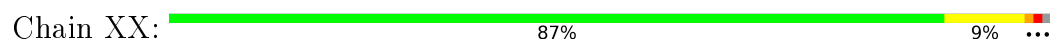
- Molecule 73: eS21



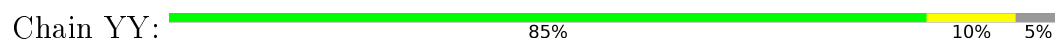
- Molecule 74: uS8



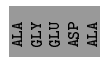
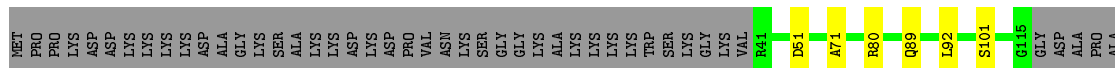
- Molecule 75: uS12



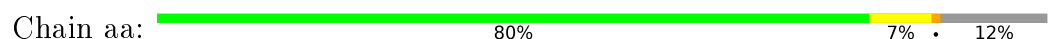
- Molecule 76: eS24



- Molecule 77: eS25



- Molecule 78: eS26





- Molecule 79: 40S ribosomal protein S27

Chain bb: 89% 8% ..



- Molecule 80: eS28

Chain cc: 83% 7% 10%



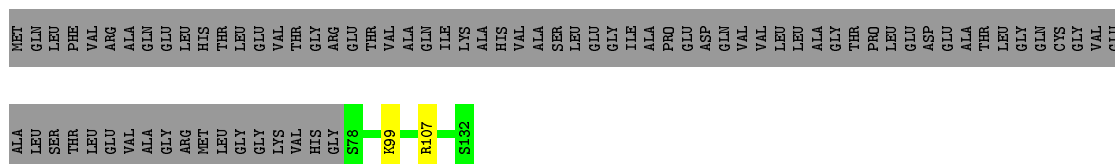
- Molecule 81: uS14

Chain dd: 89% 9% .



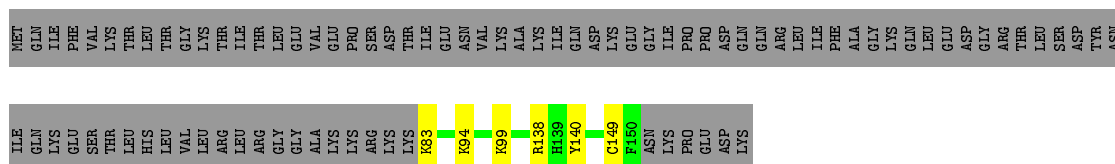
- Molecule 82: eS30

Chain ee: 40% . 59%



- Molecule 83: eS31

Chain ff: 40% . 56%



- Molecule 84: RACK1

Chain gg: 95% . .



- Molecule 85: mRNA (UGA stop codon)

Chain hh:

50%

50%

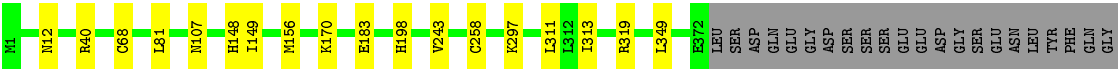


• Molecule 86: Protein pelota homolog

Chain ii:

88%

8%

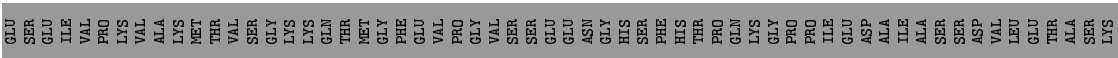
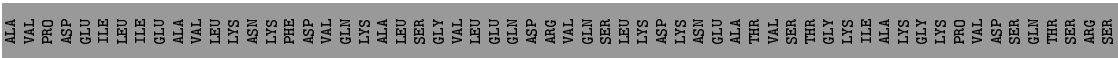
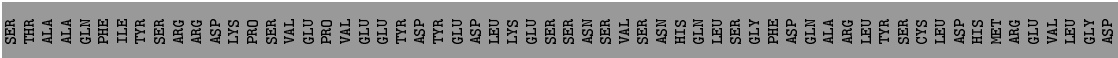


• Molecule 87: HBS1-like protein

Chain jj:

55%

40%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	37432	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	104478	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.35	0/1936	0.70	0/2596
10	J	0.34	0/1385	0.61	0/1852
11	L	0.34	0/1733	0.68	0/2316
12	M	0.36	0/1158	0.68	0/1547
13	N	0.35	0/1746	0.67	0/2338
14	O	0.36	0/1662	0.66	0/2222
15	P	0.36	0/1268	0.64	0/1700
16	Q	0.35	0/1539	0.73	0/2054
17	R	0.34	0/1524	0.66	0/2013
18	S	0.35	0/1501	0.65	0/2012
19	T	0.34	0/1326	0.62	0/1770
2	B	0.36	0/3240	0.65	0/4339
20	U	0.35	0/823	0.56	0/1104
21	V	0.34	0/993	0.63	0/1332
22	W	0.35	0/873	0.57	0/1158
23	X	0.31	0/984	0.60	0/1323
24	Y	0.32	0/1132	0.62	0/1504
25	Z	0.36	0/1130	0.63	0/1507
26	a	0.33	0/1191	0.63	0/1590
27	b	0.33	0/861	0.58	0/1138
28	c	0.31	0/771	0.54	0/1034
29	d	0.35	0/903	0.66	0/1216
3	C	0.34	0/2937	0.67	0/3946
30	e	0.34	0/1071	0.64	0/1429
31	f	0.38	0/895	0.70	0/1198
32	g	0.34	0/916	0.69	0/1220
33	h	0.31	0/1021	0.61	0/1348
34	i	0.34	0/841	0.60	0/1112
35	j	0.35	0/720	0.70	0/952
36	k	0.31	0/575	0.54	0/761
37	l	0.35	0/459	0.63	0/608
38	m	0.31	0/435	0.60	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	n	0.36	0/240	0.67	0/305
4	D	0.34	0/2437	0.62	2/3264 (0.1%)
40	o	0.34	0/864	0.62	0/1140
41	p	0.34	0/718	0.59	0/953
42	r	0.34	0/1010	0.65	0/1354
43	s	0.37	0/1530	0.50	0/2064
44	t	0.36	0/1174	0.53	0/1582
45	1	0.44	0/49	0.61	0/65
46	2	0.21	0/1805	0.66	0/2809
47	3	0.21	0/1777	0.65	0/2763
48	5	0.31	14/84961 (0.0%)	0.76	62/132460 (0.0%)
49	7	0.28	0/2858	0.67	0/4455
5	E	0.33	0/1762	0.62	0/2362
50	8	0.27	0/3581	0.67	0/5577
51	9	0.27	1/40523 (0.0%)	0.70	8/63130 (0.0%)
52	AA	0.35	0/1747	0.61	0/2374
53	BB	0.33	0/1756	0.58	0/2350
54	CC	0.34	0/1753	0.63	0/2369
55	DD	0.35	0/1796	0.62	0/2417
56	EE	0.35	0/2118	0.64	0/2849
57	FF	0.34	0/1492	0.61	0/2005
58	GG	0.35	0/1946	0.66	0/2590
59	HH	0.35	0/1510	0.58	0/2022
6	F	0.36	0/1911	0.65	0/2549
60	II	0.34	0/1715	0.66	0/2287
61	JJ	0.34	0/1550	0.70	0/2069
62	KK	0.35	0/834	0.57	0/1125
63	LL	0.34	0/1195	0.69	0/1597
64	MM	0.36	0/918	0.59	0/1233
65	NN	0.33	0/1226	0.64	0/1649
66	OO	0.34	0/1029	0.72	0/1380
67	PP	0.37	0/1017	0.65	0/1358
68	QQ	0.34	0/1146	0.60	0/1534
69	RR	0.35	0/1082	0.61	0/1452
7	G	0.34	0/1910	0.62	0/2569
70	SS	0.35	0/1208	0.66	0/1618
71	TT	0.37	0/1115	0.63	1/1493 (0.1%)
72	UU	0.33	0/805	0.64	0/1081
73	VV	0.36	0/643	0.65	0/860
74	WW	0.34	0/1051	0.68	0/1406
75	XX	0.34	0/1116	0.65	0/1490
76	YY	0.37	0/1028	0.64	0/1366
77	ZZ	0.35	0/604	0.61	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
78	aa	0.35	0/828	0.73	0/1109
79	bb	0.35	0/665	0.62	0/891
8	H	0.33	0/1535	0.61	0/2063
80	cc	0.33	0/490	0.68	0/656
81	dd	0.38	0/470	0.65	0/623
82	ee	0.35	0/447	0.65	0/587
83	ff	0.37	0/567	0.57	0/753
84	gg	0.33	0/2493	0.55	0/3394
85	hh	0.28	0/188	0.81	0/290
86	ii	0.34	0/2996	0.57	0/4050
87	jj	0.34	0/3352	0.55	0/4523
9	I	0.34	0/1702	0.63	0/2272
All	All	0.32	15/237792 (0.0%)	0.70	73/348210 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
48	5	0	2
75	XX	0	1
78	aa	0	1
All	All	0	5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	935	A	C5-C6	-17.76	1.25	1.41
48	5	922(A)	G	O3'-P	13.89	1.77	1.61
48	5	935	A	C6-N1	-12.33	1.26	1.35
48	5	935	A	C2-N3	10.66	1.43	1.33
48	5	1411(B)	C	O3'-P	9.43	1.72	1.61
48	5	481	G	N1-C2	-9.42	1.30	1.37
48	5	481	G	C5-C6	8.11	1.50	1.42
48	5	935	A	N3-C4	7.71	1.39	1.34
48	5	1411(C)	C	O5'-C5'	7.46	1.56	1.44
48	5	922	C	O3'-P	6.70	1.69	1.61
48	5	481	G	C2-N3	-6.37	1.27	1.32
48	5	1411(C)	C	C5'-C4'	6.12	1.58	1.51
48	5	481	G	C2-N2	-5.86	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	922(A)	G	C3'-O3'	5.82	1.50	1.42
51	9	615	C	O3'-P	5.12	1.67	1.61

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	481	G	N1-C2-N2	-51.75	69.62	116.20
48	5	481	G	C8-N9-C1'	-51.47	60.09	127.00
48	5	935	A	C5-C6-N6	-47.28	85.88	123.70
48	5	935	A	C6-N1-C2	-34.46	97.92	118.60
48	5	935	A	N1-C6-N6	-34.37	97.98	118.60
48	5	481	G	N3-C2-N2	-31.28	98.00	119.90
48	5	935	A	C4-C5-C6	-29.50	102.25	117.00
48	5	481	G	C6-N1-C2	-22.06	111.86	125.10
48	5	481	G	C2-N3-C4	-20.13	101.84	111.90
48	5	481	G	N9-C1'-C2'	14.58	132.96	114.00
48	5	922	C	C2'-C3'-O3'	13.20	138.53	109.50
48	5	935	A	N3-C4-C5	-13.06	117.66	126.80
48	5	935	A	N1-C2-N3	-11.86	123.37	129.30
48	5	481	G	C4-N9-C1'	-10.14	113.32	126.50
48	5	922	C	N1-C1'-C2'	-10.06	100.92	114.00
48	5	922	C	C4'-C3'-C2'	-8.81	93.78	102.60
48	5	922	C	C5'-C4'-O4'	8.80	119.66	109.10
48	5	1411	C	C4'-C3'-O3'	8.55	130.10	113.00
48	5	922	C	O4'-C4'-C3'	-8.35	95.65	104.00
48	5	1411(C)	C	P-O5'-C5'	8.29	134.17	120.90
51	9	1835	A	C2'-C3'-O3'	8.10	127.32	109.50
48	5	922(B)	C	C1'-C2'-O2'	-7.69	87.54	110.60
51	9	1394	G	C2'-C3'-O3'	7.62	126.26	109.50
48	5	481	G	N3-C4-C5	-7.41	124.90	128.60
4	D	22	ARG	NE-CZ-NH1	7.17	123.88	120.30
48	5	922(A)	G	P-O3'-C3'	7.17	128.30	119.70
48	5	3888	G	C2'-C3'-O3'	7.02	124.95	109.50
48	5	922(A)	G	N9-C1'-C2'	6.92	123.00	114.00
48	5	1411	C	C5'-C4'-C3'	6.92	127.07	116.00
48	5	1477	C	C2'-C3'-O3'	6.88	124.70	113.70
48	5	1411(C)	C	C5'-C4'-O4'	6.87	117.34	109.10
51	9	615	C	N1-C1'-C2'	-6.86	104.45	112.00
48	5	481	G	C5-C6-N1	-6.75	108.12	111.50
51	9	434	G	C2'-C3'-O3'	6.73	124.47	113.70
48	5	922	C	O4'-C1'-N1	6.35	113.28	108.20
51	9	1646	C	C2'-C3'-O3'	6.28	123.74	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4947	U	C2'-C3'-O3'	6.24	123.69	113.70
48	5	2046	G	C2'-C3'-O3'	6.16	123.55	113.70
51	9	615	C	C3'-C2'-C1'	6.00	106.30	101.50
48	5	3697	U	C2'-C3'-O3'	6.00	123.30	113.70
48	5	1411	C	O4'-C4'-C3'	-6.00	98.00	104.00
48	5	406	C	C2'-C3'-O3'	5.99	123.28	113.70
48	5	90	G	C2'-C3'-O3'	5.99	123.28	113.70
48	5	1211	G	C2'-C3'-O3'	5.97	123.25	113.70
48	5	275	C	C2'-C3'-O3'	5.96	123.23	113.70
48	5	125	C	C2'-C3'-O3'	5.93	123.19	113.70
51	9	110	U	C2'-C3'-O3'	5.87	123.10	113.70
48	5	1455	G	C2'-C3'-O3'	5.84	123.04	113.70
48	5	47	A	C4'-C3'-O3'	5.71	124.42	113.00
48	5	1563	A	N9-C1'-C2'	-5.63	105.81	112.00
48	5	1818	G	C2'-C3'-O3'	5.62	122.70	113.70
48	5	2695	A	C2'-C3'-O3'	5.58	122.63	113.70
48	5	385	A	C4'-C3'-O3'	5.56	124.13	113.00
48	5	481	G	N3-C4-N9	5.56	129.34	126.00
48	5	1329	G	C2'-C3'-O3'	5.55	122.58	113.70
48	5	922(B)	C	C5'-C4'-O4'	5.41	115.59	109.10
48	5	922(A)	G	C2'-C3'-O3'	5.40	122.33	113.70
48	5	4884	G	C2'-C3'-O3'	5.39	122.33	113.70
48	5	245	C	C2'-C3'-O3'	5.32	122.21	113.70
48	5	922(B)	C	P-O5'-C5'	5.29	129.36	120.90
48	5	1445	U	C2'-C3'-O3'	5.29	122.16	113.70
4	D	22	ARG	CG-CD-NE	5.22	122.76	111.80
48	5	1291	G	C2'-C3'-O3'	5.18	121.99	113.70
48	5	2474	G	C2'-C3'-O3'	5.16	121.96	113.70
48	5	1411	C	O4'-C1'-N1	5.14	112.31	108.20
51	9	532	C	C2'-C3'-O3'	5.12	121.89	113.70
71	TT	110	LEU	CA-CB-CG	5.11	127.06	115.30
48	5	4448	G	C4'-C3'-O3'	5.08	123.16	113.00
48	5	971(A)	G	C4'-C3'-O3'	5.08	123.15	113.00
48	5	930	G	C2'-C3'-O3'	5.07	121.81	113.70
48	5	1411	C	C2'-C3'-O3'	-5.06	98.37	109.50
48	5	1834	U	C2'-C3'-O3'	5.03	121.75	113.70
48	5	1411(B)	C	P-O3'-C3'	5.00	125.70	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	481	G	Sidechain
48	5	935	A	Sidechain
2	B	16	PHE	Peptide
75	XX	61	GLN	Peptide
78	aa	26	CYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	15	0
2	B	3172	0	3310	12	0
3	C	2883	0	3053	13	0
4	D	2391	0	2424	11	0
5	E	1729	0	1887	7	0
6	F	1875	0	1995	10	0
7	G	1879	0	2027	9	0
8	H	1516	0	1597	6	0
9	I	1664	0	1712	3	0
10	J	1362	0	1399	4	0
11	L	1702	0	1820	4	0
12	M	1137	0	1211	9	0
13	N	1701	0	1749	7	0
14	O	1630	0	1778	9	0
15	P	1242	0	1274	2	0
16	Q	1515	0	1634	4	0
17	R	1508	0	1664	7	0
18	S	1462	0	1508	11	0
19	T	1298	0	1366	2	0
20	U	809	0	833	5	0
21	V	979	0	1039	4	0
22	W	860	0	903	4	0
23	X	967	0	1040	1	0
24	Y	1115	0	1205	1	0
25	Z	1107	0	1182	4	0
26	a	1162	0	1209	0	0
27	b	848	0	920	0	0
28	c	761	0	794	0	0
29	d	888	0	930	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	1000	0	0
33	h	1013	0	1147	0	0
34	i	830	0	916	0	0
35	j	705	0	738	0	0
36	k	569	0	637	0	0
37	l	447	0	480	0	0
38	m	429	0	467	0	0
39	n	239	0	289	0	0
40	o	851	0	920	0	0
41	p	708	0	758	0	0
42	r	994	0	1051	0	0
43	s	1507	0	1564	0	0
44	t	1160	0	1218	0	0
45	1	49	0	51	0	0
46	2	1616	0	824	1	0
47	3	1593	0	811	2	0
48	5	75972	0	38400	244	0
49	7	2558	0	1296	4	0
50	8	3208	0	1629	3	0
51	9	36249	0	18317	131	0
52	AA	1710	0	1708	6	0
53	BB	1729	0	1803	9	0
54	CC	1716	0	1806	8	0
55	DD	1768	0	1866	6	0
56	EE	2076	0	2177	12	0
57	FF	1471	0	1522	6	0
58	GG	1923	0	2089	4	0
59	HH	1488	0	1582	7	0
60	II	1686	0	1772	5	0
61	JJ	1525	0	1640	5	0
62	KK	810	0	836	5	0
63	LL	1175	0	1249	8	0
64	MM	908	0	939	2	0
65	NN	1202	0	1289	5	0
66	OO	1016	0	1039	5	0
67	PP	997	0	1045	1	0
68	QQ	1128	0	1195	2	0
69	RR	1068	0	1121	5	0
70	SS	1190	0	1249	2	0
71	TT	1097	0	1132	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	UU	795	0	862	1	0
73	VV	636	0	637	2	0
74	WW	1034	0	1080	6	0
75	XX	1098	0	1167	6	0
76	YY	1011	0	1083	1	0
77	ZZ	598	0	656	1	0
78	aa	814	0	863	0	0
79	bb	651	0	672	0	0
80	cc	488	0	514	0	0
81	dd	459	0	448	0	0
82	ee	443	0	492	0	0
83	ff	555	0	567	0	0
84	gg	2436	0	2393	0	0
85	hh	169	0	86	0	0
86	ii	2947	0	2957	0	0
87	jj	3292	0	3371	0	0
88	5	182	0	0	0	0
88	7	5	0	0	0	0
88	8	6	0	0	0	0
88	9	66	0	0	0	0
88	L	1	0	0	0	0
88	P	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	0	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	0	0
90	jj	32	0	14	0	0
All	All	222005	0	166949	604	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (604) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:C5'	48:5:922(A):G:H3'	1.43	1.44
48:5:3914:U:O4	48:5:4378:A:N1	1.57	1.37
48:5:922:C:H5''	48:5:922(B):C:O5'	1.25	1.32
48:5:922:C:H5'	48:5:922(A):G:C3'	1.57	1.31
51:9:1137:U:O4	51:9:1148:A:N1	1.67	1.27
48:5:922:C:H2'	48:5:922(B):C:C2	1.67	1.26
48:5:922:C:H5''	48:5:922(B):C:P	1.74	1.26
48:5:77:U:O4	48:5:336:A:N1	1.73	1.21
48:5:1524:A:N6	48:5:1652:U:H3	1.36	1.20
48:5:922:C:C5'	48:5:922(B):C:O5'	1.89	1.20
51:9:1137:U:C4	51:9:1148:A:N1	2.10	1.20
48:5:922:C:P	48:5:922(B):C:O5'	2.08	1.12
48:5:922:C:C5'	48:5:922(B):C:P	2.39	1.09
51:9:1293:A:N6	51:9:1306:U:N3	2.03	1.06
48:5:77:U:H3	48:5:336:A:N6	1.54	1.04
48:5:1524:A:N1	48:5:1652:U:O4	1.93	1.01
51:9:613:G:N2	51:9:629:A:OP1	1.92	1.01
51:9:1137:U:O4	51:9:1148:A:C2	2.14	1.00
48:5:1411:C:O4'	48:5:1411(B):C:H2'	1.61	0.99
51:9:628:A:N6	51:9:1500:G:H21	1.61	0.98
48:5:922(B):C:O2'	48:5:923:C:C5'	2.12	0.97
48:5:1411:C:H5'	48:5:1411(B):C:O3'	1.65	0.96
48:5:2409:U:C4	48:5:2783:A:N1	2.36	0.93
48:5:922:C:C2'	48:5:922(B):C:C2	2.52	0.93
48:5:1411:C:H4'	48:5:1411(C):C:O4'	1.68	0.92
51:9:872:A:N1	51:9:914:U:O4	2.05	0.89
48:5:922:C:O3'	48:5:922(B):C:C6	2.29	0.86
51:9:1137:U:O4	51:9:1148:A:C6	2.30	0.85
48:5:922(B):C:O2'	48:5:923:C:H5''	1.76	0.84
48:5:922:C:H5'	48:5:922(A):G:H3'	0.84	0.83
48:5:922(B):C:O2'	48:5:923:C:O5'	1.97	0.82
48:5:1974:U:N3	48:5:2002:A:C6	2.47	0.82
48:5:922:C:C5'	48:5:922(A):G:C3'	2.31	0.82
48:5:2409:U:O4	48:5:2783:A:N1	2.14	0.81
48:5:922:C:O5'	48:5:922(A):G:H3'	1.80	0.80
48:5:3914:U:C4	48:5:4378:A:N1	2.50	0.79
48:5:922(B):C:O2'	48:5:923:C:P	2.41	0.77
51:9:612:U:O2	51:9:629:A:N6	2.17	0.76
51:9:872:A:N1	51:9:914:U:C4	2.53	0.76
48:5:922:C:H2'	48:5:922(B):C:N1	2.01	0.75
48:5:922:C:O5'	48:5:922(B):C:O5'	2.05	0.75
51:9:628:A:H62	51:9:1500:G:H21	1.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:77:U:C4	48:5:336:A:N1	2.54	0.74
48:5:1411:C:C4'	48:5:1411(C):C:O4'	2.36	0.74
48:5:922:C:P	48:5:922(B):C:P	2.86	0.73
48:5:3914:U:O4	48:5:4378:A:C2	2.41	0.73
48:5:922:C:C6	48:5:922(A):G:C5	2.77	0.73
51:9:1293:A:C6	51:9:1306:U:N3	2.57	0.72
51:9:1137:U:C4	51:9:1148:A:C6	2.78	0.72
51:9:1293:A:N6	51:9:1306:U:C2	2.59	0.70
48:5:3914:U:H3	48:5:4378:A:N6	1.88	0.70
48:5:3914:U:N3	48:5:4378:A:N6	2.40	0.69
48:5:922:C:H5'	48:5:922(A):G:C2'	2.22	0.68
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.74	0.68
48:5:922:C:C3'	48:5:922(B):C:O4'	2.42	0.68
48:5:738:C:O2'	48:5:738(A):C:O4'	2.05	0.67
48:5:1411:C:HO2'	48:5:1411(C):C:H6	1.41	0.67
48:5:2395:A:O2'	48:5:2806:A:H1'	1.94	0.67
48:5:922(B):C:HO2'	48:5:923:C:P	2.18	0.66
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.93	0.66
48:5:922:C:H3'	48:5:922:C:C6	2.30	0.66
48:5:922:C:C2'	48:5:922(B):C:N1	2.58	0.66
51:9:1293:A:N6	51:9:1306:U:C4	2.56	0.66
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.77	0.66
51:9:613:G:C2	51:9:629:A:OP1	2.48	0.65
53:BB:139:CYS:SG	53:BB:140:VAL:N	2.70	0.65
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.79	0.65
48:5:747:A:H4'	48:5:748:G:OP1	1.97	0.65
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.78	0.65
48:5:922:C:H2'	48:5:922(B):C:N3	2.11	0.65
48:5:222:C:H2'	48:5:223:G:O4'	1.97	0.64
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.31	0.64
48:5:1974:U:C4	48:5:2002:A:N6	2.67	0.63
48:5:1411:C:O2'	48:5:1411(C):C:C6	2.51	0.63
74:WW:75:ILE:HD11	74:WW:93:LEU:HD11	1.81	0.63
51:9:613:G:N1	51:9:629:A:OP1	2.30	0.62
48:5:922:C:O5'	48:5:922(A):G:P	2.57	0.62
3:C:341:LEU:HD21	5:E:52:LEU:HD21	1.82	0.62
48:5:1411:C:O2'	48:5:1411(C):C:H6	1.83	0.62
51:9:1130:G:N3	51:9:1130:G:H2'	2.14	0.62
3:C:101:MET:SD	3:C:104:PRO:HA	2.40	0.62
51:9:613:G:H22	51:9:629:A:P	2.21	0.61
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.49	0.61
51:9:628:A:N6	51:9:1500:G:N2	2.41	0.61
48:5:922:C:C5'	48:5:922(A):G:O3'	2.49	0.61
51:9:96:C:O2	51:9:473:A:O2'	2.18	0.61
51:9:1407:U:H2'	51:9:1408:U:C6	2.35	0.60
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.83	0.60
51:9:1293:A:N1	51:9:1306:U:O4	2.33	0.60
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	1.84	0.60
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	1.82	0.60
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.82	0.60
48:5:922:C:P	48:5:922(B):C:C5'	2.89	0.60
48:5:1406(B):C:H2'	48:5:1406(C):G:O4'	2.01	0.60
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.34	0.60
48:5:742:G:C2	48:5:922(A):G:C6	2.90	0.60
48:5:3723:A:H2'	48:5:3724:A:C8	2.37	0.60
48:5:4942:C:H4'	48:5:4943:A:OP1	2.02	0.60
48:5:4510:A:O2'	48:5:4511:A:O4'	2.20	0.60
51:9:183:G:O2'	51:9:184:G:O5'	2.20	0.59
51:9:872:A:C6	51:9:914:U:O4	2.55	0.59
48:5:922:C:O5'	48:5:922:C:O3'	2.20	0.59
14:O:72:HIS:N	48:5:4586:G:OP1	2.33	0.59
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.38	0.58
48:5:1370:G:O2'	48:5:1371:A:OP2	2.18	0.58
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.38	0.58
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.69	0.57
51:9:501:C:O2	51:9:501:C:H2'	2.04	0.57
51:9:945:U:H2'	51:9:946:U:C6	2.40	0.57
51:9:29:G:H4'	75:XX:129:SER:HB2	1.86	0.57
48:5:961:G:C6	48:5:962:C:C4	2.93	0.57
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.36	0.57
20:U:87:THR:HG23	20:U:102:VAL:HG21	1.86	0.56
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.87	0.56
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.41	0.56
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.56
46:2:16:C:O4'	46:2:16:C:O2	2.23	0.56
48:5:245:C:O4'	48:5:245:C:O2	2.23	0.56
2:B:249:ARG:NH1	48:5:2837:U:OP1	2.39	0.56
48:5:481:G:O6	48:5:481(A):C:H5''	2.05	0.56
48:5:1524:A:N6	48:5:1652:U:N3	2.18	0.56
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.87	0.56
48:5:77:U:O4	48:5:336:A:C2	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD13	1:A:150:LEU:HD21	1.86	0.56
3:C:334:THR:HG21	6:F:50:TYR:OH	2.06	0.56
11:L:71:ARG:NH2	48:5:74:G:O3'	2.39	0.55
51:9:1401:A:C2	51:9:1402:A:C6	2.94	0.55
48:5:1974:U:N3	48:5:2002:A:N6	2.55	0.55
65:NN:125:LEU:HD22	65:NN:129:TYR:CE2	2.41	0.55
74:WW:3:ARG:HD3	74:WW:6:VAL:HG22	1.88	0.55
48:5:738(A):C:H5''	48:5:739:G:H5''	1.89	0.55
48:5:4723:A:H2'	48:5:4724:A:C8	2.42	0.55
51:9:1824:A:N3	51:9:1824:A:H2'	2.22	0.55
51:9:980:A:H2'	51:9:981:A:C8	2.42	0.55
48:5:2409:U:C4	48:5:2783:A:C2	2.95	0.54
48:5:294:G:O6	48:5:315:G:H1'	2.07	0.54
48:5:3810:C:O4'	48:5:3810:C:O2	2.25	0.54
48:5:922:C:O5'	48:5:922(A):G:C3'	2.49	0.54
51:9:94:G:O2'	51:9:508:A:O2'	2.26	0.54
60:II:27:TYR:CE1	60:II:28:GLU:HG3	2.43	0.54
48:5:922:C:C3'	48:5:922(B):C:C6	2.91	0.54
48:5:1411:C:HO2'	48:5:1411(C):C:C1'	2.20	0.54
48:5:922:C:C3'	48:5:922:C:C6	2.91	0.54
51:9:1589:A:N3	51:9:1653:U:O2'	2.38	0.54
51:9:1438:A:H2'	51:9:1439:A:C8	2.43	0.54
51:9:1012:A:H2'	51:9:1013:U:O4'	2.08	0.54
51:9:872:A:C6	51:9:914:U:C4	2.96	0.54
2:B:14:LEU:HD23	2:B:17:LEU:HD23	1.90	0.54
48:5:2505:C:O4'	48:5:2505:C:O2	2.24	0.54
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.37	0.54
48:5:113:A:H2'	48:5:114:G:O4'	2.08	0.53
48:5:1483:C:O2	48:5:1483:C:O4'	2.24	0.53
15:P:127:ARG:NH2	48:5:2422:C:OP1	2.41	0.53
51:9:1535:U:O2	51:9:1535:U:H2'	2.08	0.53
12:M:119:ARG:NH1	14:O:202:LEU:HD21	2.24	0.53
48:5:935:A:N6	48:5:935(A):G:H3'	2.22	0.53
51:9:1117:C:O2'	51:9:1118:C:O4'	2.26	0.53
51:9:1823:A:H3'	51:9:1824:A:H5'	1.90	0.53
48:5:2088:A:O2'	48:5:2089:G:OP2	2.25	0.53
48:5:2627:C:O4'	48:5:2627:C:O2	2.27	0.53
51:9:1315:U:O2	51:9:1315:U:O4'	2.27	0.53
51:9:434:G:H2'	51:9:435:A:C8	2.44	0.53
51:9:853:C:O2	51:9:853:C:O4'	2.24	0.53
6:F:90:PHE:CD2	6:F:243:ILE:HD11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1524:A:N1	48:5:1652:U:C4	2.74	0.53
52:AA:38:ILE:HD11	52:AA:150:THR:HG22	1.89	0.53
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.49	0.53
5:E:165:VAL:HG12	5:E:178:VAL:HG22	1.91	0.53
51:9:1139:C:O4'	51:9:1139:C:O2	2.23	0.52
51:9:1137:U:N3	51:9:1148:A:N6	2.57	0.52
5:E:286:PRO:HA	5:E:289:LEU:CD2	2.39	0.52
7:G:101:LYS:HB3	23:X:42:THR:HG23	1.90	0.52
48:5:4989:U:O4'	48:5:4989:U:O2	2.27	0.52
59:HH:27:LEU:HD13	59:HH:45:ILE:HD13	1.91	0.52
48:5:922:C:H5'	48:5:922(A):G:O3'	2.08	0.52
51:9:501:C:O2	51:9:501:C:C2'	2.58	0.52
53:BB:66:VAL:HG22	53:BB:87:ILE:HG22	1.90	0.52
48:5:1411:C:H1'	48:5:1411(C):C:C6	2.44	0.52
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.92	0.52
48:5:1961:G:O2'	48:5:2025:A:N6	2.43	0.52
48:5:1411(C):C:H2'	48:5:1412:G:O4'	2.10	0.52
2:B:174:ARG:NH1	48:5:4985:U:O2	2.43	0.52
4:D:16:TYR:O	49:7:11:A:N6	2.42	0.52
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.45	0.52
48:5:224:U:O2	48:5:224:U:O4'	2.27	0.52
48:5:738:C:O3'	48:5:738(A):C:H5'	2.10	0.52
57:FF:92:ILE:HD13	57:FF:169:ILE:HG21	1.92	0.52
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.40	0.52
48:5:922:C:H5''	48:5:922(B):C:OP1	2.09	0.52
58:GG:132:ARG:HB3	58:GG:133:LEU:HD12	1.92	0.52
48:5:2408:U:O4'	48:5:2409:U:C5	2.63	0.51
22:W:9:SER:HG	22:W:36:CYS:HG	1.57	0.51
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.44	0.51
48:5:934:C:O4'	48:5:935(A):G:O4'	2.28	0.51
51:9:925:G:N2	65:NN:48:SER:OG	2.44	0.51
51:9:146:G:O2'	51:9:147:A:O5'	2.22	0.51
48:5:2409:U:O4	48:5:2783:A:C6	2.64	0.51
48:5:4579:U:H2'	48:5:4580:U:C6	2.46	0.51
12:M:94:LYS:NZ	48:5:4872:G:OP2	2.43	0.51
48:5:4305:G:C2'	48:5:4305:G:N3	2.74	0.51
48:5:922:C:O5'	48:5:922(A):G:O5'	2.29	0.51
51:9:1130:G:HO2'	51:9:1131:G:C5'	2.23	0.51
51:9:1364:U:O4'	51:9:1364:U:O2	2.29	0.51
48:5:922(B):C:C4	48:5:923:C:C5	2.99	0.51
3:C:138:MET:HG2	3:C:144:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4871:C:O2	48:5:4871:C:O4'	2.29	0.51
4:D:106:ALA:HB1	4:D:171:LEU:HD13	1.93	0.51
48:5:923:C:C5	48:5:926:G:O4'	2.64	0.51
52:AA:180:ARG:HG2	52:AA:195:TRP:CE3	2.46	0.51
54:CC:253:PRO:HA	54:CC:256:TRP:CD1	2.45	0.51
48:5:1888:A:N6	48:5:3873:G:O2'	2.44	0.50
48:5:4476:C:O2'	48:5:4478:G:OP2	2.28	0.50
51:9:823:U:O2	51:9:823:U:O4'	2.29	0.50
50:8:125:C:O2	50:8:125:C:O4'	2.30	0.50
21:V:82:ILE:HD12	21:V:104:VAL:HG13	1.93	0.50
48:5:2097:A:OP1	48:5:2107:A:N6	2.45	0.50
51:9:1130:G:O2'	51:9:1131:G:O5'	2.30	0.50
48:5:1381:U:O4'	48:5:1381:U:O2	2.29	0.50
4:D:62:CYS:HB3	4:D:105:LEU:HD22	1.93	0.50
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.94	0.50
51:9:1444:U:H2'	51:9:1445:U:C6	2.47	0.50
53:BB:134:LEU:HD23	53:BB:218:LEU:HD12	1.94	0.50
48:5:3766:A:N1	51:9:1827:U:O2'	2.37	0.50
5:E:185:ASN:ND2	5:E:274:LEU:O	2.45	0.49
61:JJ:35:TYR:CD2	61:JJ:106:LEU:HD23	2.46	0.49
48:5:2094:C:O2	48:5:2094:C:O4'	2.30	0.49
51:9:1129:G:C6	51:9:1130:G:O6	2.65	0.49
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.93	0.49
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.44	0.49
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.41	0.49
14:O:160:ARG:NH2	48:5:4760:G:OP1	2.45	0.49
75:XX:51:VAL:HG22	75:XX:70:VAL:HG11	1.95	0.49
51:9:1719:A:N6	51:9:1814:G:O2'	2.44	0.49
54:CC:137:VAL:HG21	54:CC:244:ILE:HD12	1.94	0.49
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.94	0.49
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.94	0.49
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.93	0.49
13:N:68:ARG:HG2	48:5:302:C:OP1	2.12	0.49
48:5:964:A:H2'	48:5:965:G:O4'	2.12	0.49
20:U:23:LEU:HD11	20:U:83:LEU:CD2	2.43	0.49
48:5:1237:C:O2	48:5:1237:C:O4'	2.30	0.49
51:9:107:A:C2	51:9:355:G:C2	3.01	0.49
48:5:922:C:O3'	48:5:922(B):C:O4'	2.31	0.49
51:9:584:A:C6	51:9:585:C:C4	3.01	0.49
8:H:18:ILE:HG22	8:H:27:VAL:HG22	1.94	0.49
10:J:63:ARG:NH2	50:8:58:G:N7	130.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:604:A:C6	51:9:605:A:N1	2.81	0.49
62:KK:35:LEU:HD13	62:KK:40:VAL:HG21	1.94	0.49
17:R:102:LEU:HD22	17:R:138:LEU:HD12	1.95	0.49
51:9:1520:G:N3	51:9:1520:G:H2'	2.28	0.48
2:B:41:VAL:HA	2:B:187:GLY:HA3	1.95	0.48
2:B:47:LEU:HD23	2:B:166:THR:HG23	1.94	0.48
6:F:161:ILE:HD12	6:F:166:ILE:HB	1.94	0.48
2:B:234:ARG:NH2	48:5:4566:U:O2'	2.46	0.48
3:C:130:ALA:HB3	3:C:246:VAL:HG12	1.95	0.48
8:H:41:ILE:HG21	8:H:73:ILE:HD11	1.96	0.48
66:OO:56:VAL:HG12	66:OO:81:VAL:HG23	1.95	0.48
66:OO:44:VAL:HG11	66:OO:85:CYS:SG	2.53	0.48
48:5:1074:G:C2	48:5:1238:A:C2	3.00	0.48
48:5:2763:U:O2	48:5:2763:U:O4'	2.31	0.48
51:9:612:U:H3	51:9:629:A:H62	1.62	0.48
13:N:179:LYS:O	48:5:297:U:O2'	2.30	0.48
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.95	0.48
53:BB:105:LEU:HD23	53:BB:213:ARG:HA	1.95	0.48
60:II:190:LEU:HD12	60:II:194:GLU:HB3	1.96	0.48
17:R:45:ILE:HG12	17:R:50:ILE:HD11	1.95	0.48
73:VV:55:ILE:HD11	73:VV:69:ILE:HG12	1.94	0.48
51:9:520:A:O2'	51:9:825:A:N3	2.40	0.48
48:5:4709:U:C4	48:5:4710:C:C4	3.01	0.48
14:O:193:THR:HG23	14:O:202:LEU:HD23	1.96	0.48
75:XX:41:PHE:CE1	75:XX:47:ALA:HB3	2.48	0.48
51:9:887:U:O2	51:9:887:U:O4'	2.31	0.48
7:G:210:ILE:HG23	7:G:220:VAL:HG11	1.96	0.48
17:R:98:ARG:NH2	48:5:2262:G:OP2	170.71	0.48
7:G:189:LEU:HD21	7:G:257:PHE:CE1	2.49	0.48
63:LL:4:ILE:HD12	63:LL:56:ILE:HD11	1.95	0.48
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.43	0.47
1:A:207:VAL:HG23	1:A:208:GLU:HG3	1.96	0.47
3:C:334:THR:HG22	3:C:337:ARG:HH22	1.79	0.47
74:WW:55:ASP:O	74:WW:57:ARG:N	2.47	0.47
48:5:1411:C:O5'	48:5:1411(C):C:C5'	2.62	0.47
8:H:117:PHE:CZ	8:H:118:LEU:HD23	2.49	0.47
18:S:80:ILE:HG23	18:S:129:VAL:HG22	1.95	0.47
51:9:1568:C:OP1	71:TT:96:SER:OG	2.29	0.47
48:5:1406:G:C8	48:5:1406(C):G:H2'	2.49	0.47
51:9:1551:U:O2	51:9:1551:U:O4'	2.32	0.47
51:9:290:U:O2'	51:9:292:A:N7	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:C5	48:5:922(A):G:C5	3.02	0.47
52:AA:18:PHE:HD2	52:AA:51:LEU:HD22	1.79	0.47
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.45	0.47
48:5:2473:A:C2	48:5:2506:G:C2	3.02	0.47
6:F:88:LEU:HD22	6:F:89:ALA:N	2.29	0.47
48:5:1411:C:O4'	48:5:1411(B):C:C2'	2.49	0.47
48:5:4524:G:OP2	48:5:4524:G:H4'	2.13	0.47
51:9:1130:G:O2'	51:9:1131:G:P	2.72	0.47
51:9:943:U:OP2	53:BB:216:LYS:NZ	2.43	0.47
59:HH:66:VAL:HG22	59:HH:96:ALA:HB1	1.96	0.47
11:L:108:GLU:N	11:L:108:GLU:OE1	2.47	0.47
18:S:13:VAL:HG23	18:S:62:VAL:HB	1.96	0.47
48:5:4977:A:H2'	48:5:4978:G:O4'	2.14	0.47
51:9:1624:U:O4'	51:9:1624:U:O2	2.32	0.47
48:5:2268:A:H4'	48:5:2269:C:H5'	1.96	0.47
48:5:1337:A:C2	48:5:2349:A:C2	3.03	0.47
48:5:481(A):C:O2	48:5:481(A):C:O4'	2.30	0.47
51:9:1597:C:H4'	51:9:1603:G:O6	2.15	0.47
54:CC:176:LYS:O	54:CC:200:ARG:NH1	2.48	0.47
51:9:495:U:H2'	51:9:496:C:O4'	2.15	0.47
52:AA:18:PHE:CD1	52:AA:173:LEU:HD11	2.49	0.47
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.49	0.47
18:S:82:LEU:HB2	18:S:93:MET:HB2	1.96	0.47
10:J:128:LEU:HD11	10:J:130:PHE:CE1	2.50	0.47
48:5:1332:C:H2'	48:5:1333:A:C8	2.50	0.46
48:5:1990:A:H3'	48:5:1991:A:H5''	1.97	0.46
48:5:356:G:O2'	50:8:25:G:N3	2.46	0.46
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.44	0.46
63:LL:113:LEU:HD23	63:LL:142:VAL:HG21	1.97	0.46
9:I:91:LEU:HD12	9:I:135:ILE:HG23	1.96	0.46
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	1.97	0.46
48:5:4260:U:H2'	48:5:4261:C:C6	2.50	0.46
66:OO:31:CYS:HB2	66:OO:44:VAL:HG22	1.98	0.46
68:QQ:49:TYR:O	68:QQ:53:GLU:N	2.48	0.46
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.97	0.46
48:5:1974:U:C4	48:5:2002:A:C6	3.04	0.46
48:5:922:C:C6	48:5:922(A):G:C6	3.03	0.46
51:9:928:G:H2'	51:9:929:G:C8	2.51	0.46
66:OO:44:VAL:HG23	66:OO:81:VAL:HG11	1.98	0.46
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.51	0.46
6:F:119:GLY:O	6:F:120:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:69:ARG:NH2	48:5:4568:A:N3	2.64	0.46
1:A:179:ILE:O	48:5:3653:A:H4'	2.15	0.46
48:5:3723:A:C2	48:5:3724:A:C6	3.03	0.46
51:9:297:A:H4'	56:EE:132:GLY:O	2.16	0.46
63:LL:37:TYR:CE2	63:LL:51:ILE:HG23	2.51	0.46
3:C:323:ARG:NH1	48:5:1281:G:C8	2.84	0.46
48:5:1411:C:H1'	48:5:1411(C):C:N1	2.30	0.46
48:5:4390:A:H2'	48:5:4391:G:O4'	2.15	0.46
48:5:498:C:O4'	48:5:498:C:O2	2.29	0.46
51:9:1143:A:C2	51:9:1144:A:C2	3.03	0.46
12:M:72:TYR:CE1	48:5:738:C:H4'	2.51	0.46
72:UU:50:VAL:HG23	72:UU:91:LEU:HD23	1.97	0.46
48:5:5066:U:H2'	48:5:5067:U:C6	2.50	0.46
51:9:183:G:N3	51:9:183:G:C2'	2.78	0.46
56:EE:11:ARG:HA	56:EE:28:ALA:HB2	1.98	0.46
8:H:118:LEU:HD21	8:H:177:ASP:HB2	1.98	0.46
64:MM:22:LEU:HD11	64:MM:89:VAL:HA	1.98	0.46
6:F:69:ARG:NH1	48:5:1209:U:O2'	2.49	0.46
48:5:2408:U:C1'	48:5:2409:U:C5	2.99	0.46
1:A:227:ARG:NH2	48:5:3659:G:O2'	2.49	0.45
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.45	0.45
48:5:922:C:C3'	48:5:922(B):C:N1	2.79	0.45
13:N:178:HIS:HA	13:N:181:HIS:NE2	2.31	0.45
51:9:92:A:O4'	56:EE:3:ARG:NH1	2.49	0.45
7:G:111:PRO:HD2	7:G:114:ILE:HD12	1.97	0.45
51:9:1238:U:H2'	51:9:1239:U:O4'	2.17	0.45
51:9:1834:A:N3	51:9:1834:A:C2'	2.80	0.45
51:9:872:A:N6	51:9:914:U:C4	2.85	0.45
58:GG:52:ILE:O	58:GG:52:ILE:HG23	2.17	0.45
48:5:3867:A:C6	48:5:3868:G:C6	3.04	0.45
10:J:141:ILE:HD11	49:7:55:A:N3	2.31	0.45
51:9:1823:A:C3'	51:9:1824:A:H5'	2.46	0.45
20:U:33:ILE:HD12	20:U:96:LEU:HD22	1.98	0.45
48:5:2439:G:C6	48:5:2440:U:C4	3.04	0.45
3:C:33:ARG:HD2	3:C:36:ILE:HD12	1.98	0.45
4:D:22:ARG:HH11	4:D:22:ARG:HG3	1.81	0.45
48:5:114:G:N2	48:5:276:C:O2'	2.50	0.45
51:9:1673:U:H2'	51:9:1674:G:O4'	2.17	0.45
2:B:14:LEU:HD23	2:B:17:LEU:CD2	2.46	0.45
3:C:144:ILE:HD11	3:C:150:LEU:HD23	1.99	0.45
25:Z:75:TYR:CD2	25:Z:80:LEU:HD21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1303:C:O2	51:9:1303:C:O4'	2.33	0.45
51:9:1329:U:O2'	51:9:1332:A:OP2	2.27	0.45
51:9:4:C:O2'	61:JJ:18:ARG:NH1	2.50	0.45
53:BB:150:ILE:HD13	69:RR:129:LYS:HB2	1.98	0.45
3:C:212:ASN:HD22	3:C:255:SER:HB2	1.82	0.45
4:D:39:GLN:HG2	4:D:48:LYS:HB2	1.99	0.45
13:N:48:ALA:HB1	13:N:53:TYR:CB	2.46	0.45
13:N:76:PRO:O	13:N:79:ALA:HB3	2.16	0.45
65:NN:91:LEU:CD1	65:NN:125:LEU:HD12	2.47	0.45
48:5:2363:A:C2	48:5:3860:A:C4	3.05	0.45
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.80	0.45
11:L:116:ARG:NH1	11:L:155:MET:O	2.50	0.45
48:5:1751:A:C2	48:5:1780:A:C2	3.05	0.45
48:5:1411:C:C2'	48:5:1411(C):C:O4'	2.65	0.44
57:FF:123:GLU:OE1	57:FF:204:ARG:NH1	2.50	0.44
48:5:4872:G:H4'	48:5:4873:G:H5''	2.00	0.44
51:9:183:G:N3	51:9:183:G:O2'	2.50	0.44
63:LL:82:MET:HB3	63:LL:85:THR:HG23	2.00	0.44
48:5:4583:C:O2'	48:5:4718:G:N2	2.50	0.44
51:9:399:C:O2	63:LL:106:HIS:ND1	2.51	0.44
57:FF:72:LEU:HD22	57:FF:112:LEU:HD11	1.99	0.44
7:G:132:ALA:HB3	13:N:18:VAL:HG22	1.99	0.44
18:S:53:LYS:NZ	49:7:74:A:O2'	2.51	0.44
48:5:3620:G:OP1	48:5:3622:C:N4	2.50	0.44
62:KK:11:ILE:CD1	62:KK:45:VAL:HG22	2.47	0.44
56:EE:192:ILE:HD13	56:EE:238:LEU:HD23	2.00	0.44
48:5:1411(A):G:C6	48:5:1411(B):C:C4	3.05	0.44
48:5:1854:G:N2	48:5:4394:A:O4'	2.51	0.44
48:5:4928:C:O2	48:5:4928:C:O4'	2.35	0.44
12:M:7:VAL:HG21	18:S:154:LEU:HD21	1.99	0.44
57:FF:119:SER:OG	57:FF:189:ALA:HB1	2.17	0.44
8:H:12:ILE:HG22	8:H:81:ILE:HD11	2.00	0.44
5:E:131:HIS:CD2	48:5:1281:G:C5	3.05	0.44
12:M:97:ALA:HB2	14:O:203:VAL:HB	2.00	0.44
48:5:1339:U:H2'	48:5:1340:C:C6	2.53	0.44
48:5:2693:G:C6	48:5:2694:G:N1	2.86	0.44
48:5:3760:A:H2	51:9:1825:A:N3	2.16	0.44
51:9:1489:A:H4'	51:9:1490:G:OP2	2.17	0.44
7:G:96:GLN:O	48:5:4124:G:N2	2.50	0.44
63:LL:99:TYR:O	63:LL:101:ARG:N	2.50	0.44
48:5:1358:G:H4'	48:5:1359:G:OP1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3648:A:C4	48:5:3785:A:C6	3.06	0.43
69:RR:28:PHE:HA	69:RR:55:THR:HG21	1.99	0.43
48:5:1633:G:H5'	48:5:1634:A:OP1	2.19	0.43
48:5:4423:U:O4'	48:5:4423:U:O2	2.36	0.43
51:9:1243:U:O4	51:9:1257:G:N2	2.51	0.43
51:9:314:U:H2'	51:9:314:U:O2	2.18	0.43
51:9:958:G:C6	51:9:959:G:C6	3.06	0.43
51:9:992:A:C2	51:9:993:G:C8	3.06	0.43
10:J:27:GLY:HA2	10:J:68:ILE:HG23	1.99	0.43
48:5:2729:C:H2'	48:5:2730:U:O4'	2.18	0.43
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.51	0.43
69:RR:119:VAL:HG13	69:RR:119:VAL:O	2.18	0.43
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	2.01	0.43
48:5:1411:C:C4	48:5:1411(B):C:C4	3.07	0.43
48:5:978:G:O2'	48:5:979:C:OP2	2.29	0.43
51:9:628:A:H61	51:9:1500:G:H21	1.55	0.43
6:F:161:ILE:HB	6:F:166:ILE:HD12	1.99	0.43
3:C:164:THR:HG21	48:5:223:G:H2'	2.00	0.43
48:5:4758:U:O2	48:5:4758:U:O4'	2.35	0.43
1:A:77:ILE:HD13	1:A:128:ARG:HB2	2.00	0.43
62:KK:11:ILE:HD12	62:KK:45:VAL:HG22	2.00	0.43
22:W:3:VAL:HG21	22:W:12:LYS:CE	2.48	0.43
51:9:92:A:C6	51:9:446:G:C6	3.06	0.43
1:A:181:LYS:HB2	48:5:1577:G:C5	2.54	0.43
22:W:80:ARG:NH2	58:GG:129:VAL:O	2.52	0.43
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.53	0.43
47:3:75:C:H2'	47:3:76:A:H4'	1.99	0.43
48:5:1632:A:N3	48:5:1632:A:H2'	2.33	0.43
48:5:33:A:C6	48:5:34:A:C6	3.06	0.43
48:5:975:C:C5	48:5:976:G:N7	2.87	0.43
52:AA:134:LEU:CD2	52:AA:144:THR:HG21	2.49	0.43
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.99	0.43
66:OO:95:ILE:HD11	66:OO:126:ILE:HD12	2.00	0.43
18:S:80:ILE:HG22	18:S:82:LEU:CD2	2.49	0.43
48:5:369:G:N1	48:5:373:G:C6	2.87	0.43
53:BB:136:ARG:HB2	53:BB:218:LEU:HD11	2.00	0.43
8:H:12:ILE:HG22	8:H:81:ILE:CD1	2.49	0.43
60:II:3:ILE:O	60:II:3:ILE:HG23	2.18	0.43
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	2.01	0.43
48:5:3690:U:H2'	48:5:3691:G:O4'	2.19	0.43
48:5:77:U:H3	48:5:336:A:H61	0.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:922:C:H5'	48:5:922(B):C:P	2.47	0.43
48:5:922(B):C:N3	48:5:923:C:C5	2.87	0.43
51:9:1284:A:C6	64:MM:91:LEU:HD22	2.54	0.43
14:O:116:LYS:HD3	18:S:169:THR:HG21	2.01	0.43
17:R:60:ARG:NH1	17:R:63:CYS:SG	2.91	0.43
24:Y:49:ILE:HD11	24:Y:55:VAL:HG21	2.01	0.43
48:5:1390:G:N2	48:5:1393:G:OP2	2.49	0.43
51:9:1666:C:H2'	51:9:1667:U:O4'	2.19	0.43
60:II:117:TYR:CD1	60:II:156:ALA:HB2	2.54	0.43
12:M:17:PHE:CE1	12:M:54:CYS:HA	2.54	0.43
25:Z:23:ALA:HA	25:Z:45:GLY:HA2	2.01	0.43
51:9:1664:A:H4'	51:9:1665:G:OP1	2.19	0.42
56:EE:126:VAL:HG23	56:EE:156:VAL:O	2.19	0.42
59:HH:133:LEU:HD22	59:HH:173:PHE:CD1	2.54	0.42
14:O:42:ASN:OD1	14:O:42:ASN:N	2.52	0.42
48:5:66:A:O2'	48:5:326:C:O2	2.35	0.42
48:5:750:U:H2'	48:5:751:G:O4'	2.18	0.42
51:9:107:A:C6	51:9:108:G:C6	3.07	0.42
4:D:33:ARG:NH1	4:D:72:ASP:OD2	2.52	0.42
55:DD:48:ILE:HG23	55:DD:86:LEU:HD12	2.01	0.42
17:R:4:LEU:HD11	17:R:29:THR:HG23	2.01	0.42
71:TT:42:HIS:HB2	71:TT:83:GLN:HA	2.01	0.42
48:5:209:U:C4	48:5:233:U:C4	3.08	0.42
48:5:2750:G:H2'	48:5:2751:G:O4'	2.19	0.42
49:7:14:C:C4	49:7:66:G:N2	2.87	0.42
51:9:830:A:OP2	51:9:846:G:N2	2.52	0.42
51:9:933:G:H1'	51:9:1001:A:O4'	2.19	0.42
5:E:167:PHE:CE1	5:E:176:LEU:HD22	2.54	0.42
9:I:191:ILE:HD11	9:I:212:LEU:HD11	2.00	0.42
48:5:1493:G:C6	48:5:1494:U:C2	3.07	0.42
48:5:3656:A:O4'	48:5:3747:A:C2	2.72	0.42
48:5:4305:G:H2'	48:5:4305:G:N3	2.33	0.42
16:Q:186:TYR:CD2	48:5:4307:A:H4'	2.54	0.42
20:U:84:LYS:HA	20:U:87:THR:HG22	2.02	0.42
14:O:18:ARG:NH2	48:5:2057:A:OP1	2.51	0.42
48:5:67:C:OP2	48:5:312:G:N2	2.52	0.42
48:5:916:C:O4'	48:5:916:C:O2	2.37	0.42
51:9:615:C:H2'	51:9:616:A:C8	2.54	0.42
51:9:62:G:H4'	51:9:172:U:C5	2.55	0.42
51:9:625:G:H4'	51:9:629:A:C4	2.55	0.42
48:5:1563:A:O2'	48:5:1564:A:O4'	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:VAL:HG11	48:5:1633:G:C6	2.54	0.42
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.54	0.42
48:5:3724:A:N6	48:5:3725:G:C6	2.87	0.42
48:5:4291:G:N3	48:5:4291:G:H5''	2.35	0.42
48:5:4966:A:C2	48:5:4967:A:C2	3.08	0.42
55:DD:21:LEU:CD2	55:DD:48:ILE:HD11	2.49	0.42
56:EE:185:GLY:N	56:EE:189:LEU:HD13	2.35	0.42
59:HH:118:ARG:O	59:HH:121:THR:HG22	2.19	0.42
48:5:4525:C:H2'	48:5:4526:U:O4'	2.20	0.42
1:A:101:VAL:HB	1:A:165:VAL:HG12	2.02	0.42
21:V:64:THR:HG21	48:5:3799:A:OP1	2.19	0.42
51:9:183:G:O2'	51:9:184:G:O4'	2.36	0.42
60:II:36:THR:HG21	60:II:179:PRO:HB2	2.01	0.42
62:KK:35:LEU:CD1	62:KK:40:VAL:HG21	2.49	0.42
21:V:39:ILE:HG23	21:V:61:VAL:CG2	2.49	0.42
53:BB:212:VAL:O	53:BB:212:VAL:HG23	2.20	0.41
48:5:2031:C:O3'	48:5:2032:U:P	2.78	0.41
48:5:4515:G:C2	48:5:4516:G:C8	3.09	0.41
51:9:1843:G:H2'	51:9:1844:U:O4'	2.20	0.41
51:9:35:C:O2	51:9:520:A:N1	2.53	0.41
56:EE:181:CYS:SG	56:EE:225:ILE:HG23	2.60	0.41
13:N:42:PRO:HD3	13:N:61:ILE:HD12	2.01	0.41
75:XX:105:PHE:CG	75:XX:112:VAL:HG21	2.55	0.41
48:5:1301:C:O2	48:5:1301:C:O4'	2.34	0.41
48:5:976:G:N2	48:5:977:C:C2	2.88	0.41
51:9:1162:C:H2'	51:9:1163:C:O4'	2.20	0.41
2:B:41:VAL:HG21	2:B:196:TRP:CG	2.56	0.41
2:B:36:ASP:OD1	2:B:36:ASP:N	2.53	0.41
4:D:61:ILE:HG23	4:D:79:TYR:CE2	2.55	0.41
9:I:3:ARG:NH2	48:5:4431:U:OP2	2.51	0.41
48:5:922(A):G:OP1	48:5:922(B):C:C5	2.74	0.41
12:M:23:LYS:HE3	48:5:935:A:H3'	2.03	0.41
48:5:961:G:C6	48:5:971(A):G:C4	3.09	0.41
51:9:1137:U:H3	51:9:1148:A:N6	2.18	0.41
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	2.02	0.41
48:5:1411:C:O2'	48:5:1411(C):C:H3'	2.21	0.41
48:5:3876:A:O2'	48:5:3877:A:P	2.79	0.41
48:5:492:U:O2'	48:5:493:G:P	2.78	0.41
51:9:1351:G:O2'	51:9:1378:A:N1	2.36	0.41
51:9:1734:G:O2'	51:9:1800:A:N6	2.52	0.41
2:B:92:TYR:HB3	2:B:99:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EE:31:PRO:HD2	56:EE:38:LEU:CD1	2.50	0.41
7:G:241:ALA:O	7:G:245:ARG:N	2.54	0.41
63:LL:96:ILE:N	63:LL:96:ILE:HD12	2.35	0.41
17:R:11:ALA:HB1	17:R:50:ILE:HD13	2.03	0.41
74:WW:104:LEU:HB3	74:WW:125:ILE:HA	2.01	0.41
25:Z:41:ALA:HB2	25:Z:77:TYR:HE1	1.85	0.41
48:5:1411:C:C1'	48:5:1411(C):C:O4'	2.69	0.41
48:5:922:C:C2'	48:5:922(B):C:C1'	2.98	0.41
1:A:77:ILE:HD12	1:A:115:CYS:SG	2.60	0.41
56:EE:182:MET:CE	56:EE:192:ILE:HD11	2.50	0.41
6:F:113:LEU:HD22	6:F:118:ASN:O	2.20	0.41
7:G:215:ASP:HB3	7:G:216:PRO:HD3	2.01	0.41
69:RR:111:PHE:HB3	69:RR:114:LEU:HD21	2.03	0.41
48:5:1651:G:N1	48:5:1652:U:C4	2.89	0.41
48:5:314:G:O2'	48:5:4355:G:OP1	2.34	0.41
51:9:1520:G:N3	51:9:1520:G:C2'	2.83	0.41
57:FF:116:ILE:HD12	57:FF:151:ILE:HG13	2.01	0.41
59:HH:122:LEU:HD13	59:HH:122:LEU:C	2.41	0.41
16:Q:43:PHE:CD2	16:Q:133:GLY:HA3	2.56	0.41
51:9:1276:A:N6	51:9:1321:G:O2'	2.54	0.41
51:9:15:U:H2'	51:9:16:G:O4'	2.21	0.41
55:DD:132:LYS:HE3	55:DD:156:LEU:HD23	2.01	0.41
20:U:23:LEU:HD11	20:U:83:LEU:HD23	2.03	0.41
48:5:1523:A:N7	48:5:1652:U:C4	2.89	0.41
51:9:427:U:O2	51:9:427:U:O4'	2.38	0.41
52:AA:33:GLN:HB3	52:AA:154:LEU:HD12	2.02	0.41
48:5:119:G:H3'	48:5:120:A:C5'	2.50	0.41
48:5:1804:A:O2'	48:5:1805:A:OP2	2.33	0.41
51:9:1735:A:C4	51:9:1800:A:C2	3.08	0.41
54:CC:188:CYS:SG	54:CC:235:ASN:HA	2.61	0.41
48:5:1411:C:C4	48:5:1411(B):C:C5	3.09	0.41
48:5:2690:C:H2'	48:5:2691:U:O4'	2.21	0.41
48:5:3668:C:C2	48:5:3675:G:C2	3.09	0.41
48:5:922:C:O2'	48:5:922(B):C:C2	2.74	0.41
51:9:1259:A:H3'	51:9:1259:A:N3	2.35	0.41
3:C:144:ILE:HG12	3:C:147:VAL:HG21	2.02	0.41
57:FF:167:LYS:HA	77:ZZ:71:ALA:HB1	2.02	0.41
48:5:3706:C:H2'	48:5:3707:U:O4'	2.21	0.40
48:5:4289:U:H2'	48:5:4290:U:C6	2.56	0.40
48:5:1963:C:N4	48:5:4694:G:O6	2.54	0.40
51:9:1834:A:N3	51:9:1834:A:H2'	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1207:G:C6	51:9:1837:G:C6	3.09	0.40
51:9:398:A:C8	51:9:398:A:H5'	2.56	0.40
48:5:1802:A:O2'	48:5:1837:A:OP1	2.39	0.40
48:5:3765:G:O2'	48:5:3766:A:N7	2.54	0.40
48:5:492:U:HO2'	48:5:493:G:P	2.43	0.40
51:9:1130:G:N3	51:9:1130:G:C2'	2.82	0.40
51:9:12:U:H2'	51:9:13:C:C6	2.57	0.40
51:9:571:U:C5	51:9:572:U:C5	3.09	0.40
53:BB:143:THR:HG22	53:BB:205:TYR:CD1	2.56	0.40
56:EE:100:ARG:HD2	56:EE:102:ILE:HD11	2.02	0.40
51:9:1620:A:O2'	67:PP:40:ARG:NH2	2.54	0.40
51:9:1536:G:H2'	51:9:1537:A:C8	2.56	0.40
56:EE:44:LEU:HD21	56:EE:70:ILE:HG21	2.03	0.40
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	2.03	0.40
18:S:35:PRO:HD2	18:S:39:VAL:HG21	2.02	0.40
48:5:3851:U:H2'	48:5:3852:A:O4'	2.21	0.40
4:D:4:VAL:HG11	48:5:4247:G:C5'	2.51	0.40
48:5:922(B):C:C2	48:5:923:C:C6	3.10	0.40
2:B:86:VAL:HG13	2:B:162:VAL:HG22	2.04	0.40
22:W:4:GLU:OE1	22:W:20:ARG:NH2	2.54	0.40
48:5:1748:U:C2	48:5:1783:C:C2	3.09	0.40
51:9:1173:A:H2'	51:9:1174:U:O4'	2.21	0.40
51:9:1227:G:C2	51:9:1228:A:C8	3.10	0.40
51:9:584:A:N6	51:9:585:C:N4	2.69	0.40
1:A:82:ILE:HD11	1:A:99:GLY:HA3	2.04	0.40
5:E:156:LEU:HD11	5:E:198:ILE:HG13	2.02	0.40
7:G:139:VAL:HG11	7:G:238:LYS:HG3	2.04	0.40
62:KK:32:HIS:CD2	62:KK:45:VAL:HG21	2.57	0.40
18:S:80:ILE:HG22	18:S:82:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	224 (91%)	19 (8%)	3 (1%)	16	63
2	B	392/403 (97%)	367 (94%)	24 (6%)	1 (0%)	46	83
3	C	360/425 (85%)	338 (94%)	20 (6%)	2 (1%)	30	74
4	D	291/297 (98%)	279 (96%)	10 (3%)	2 (1%)	26	72
5	E	208/291 (72%)	190 (91%)	18 (9%)	0	100	100
6	F	223/247 (90%)	210 (94%)	11 (5%)	2 (1%)	21	68
7	G	229/319 (72%)	221 (96%)	8 (4%)	0	100	100
8	H	188/192 (98%)	172 (92%)	16 (8%)	0	100	100
9	I	201/214 (94%)	183 (91%)	17 (8%)	1 (0%)	34	77
10	J	168/178 (94%)	161 (96%)	7 (4%)	0	100	100
11	L	208/211 (99%)	196 (94%)	11 (5%)	1 (0%)	34	77
12	M	136/218 (62%)	123 (90%)	13 (10%)	0	100	100
13	N	201/204 (98%)	186 (92%)	14 (7%)	1 (0%)	34	77
14	O	197/203 (97%)	183 (93%)	14 (7%)	0	100	100
15	P	151/184 (82%)	142 (94%)	8 (5%)	1 (1%)	26	72
16	Q	185/188 (98%)	168 (91%)	15 (8%)	2 (1%)	17	65
17	R	178/196 (91%)	170 (96%)	8 (4%)	0	100	100
18	S	174/176 (99%)	163 (94%)	9 (5%)	2 (1%)	17	65
19	T	157/160 (98%)	142 (90%)	15 (10%)	0	100	100
20	U	97/128 (76%)	86 (89%)	10 (10%)	1 (1%)	19	66
21	V	129/140 (92%)	121 (94%)	8 (6%)	0	100	100
22	W	102/157 (65%)	97 (95%)	4 (4%)	1 (1%)	19	66
23	X	116/156 (74%)	111 (96%)	5 (4%)	0	100	100
24	Y	132/145 (91%)	128 (97%)	4 (3%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	5 (4%)	2 (2%)	13	59
26	a	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
27	b	100/245 (41%)	92 (92%)	7 (7%)	1 (1%)	19	66
28	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
29	d	105/125 (84%)	90 (86%)	14 (13%)	1 (1%)	19	66
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	99 (92%)	6 (6%)	2 (2%)	10	55
32	g	112/117 (96%)	104 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	h	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
34	i	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
35	j	84/97 (87%)	75 (89%)	9 (11%)	0	100	100
36	k	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
37	l	48/51 (94%)	42 (88%)	6 (12%)	0	100	100
38	m	50/102 (49%)	48 (96%)	2 (4%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	96 (94%)	5 (5%)	1 (1%)	19	66
41	p	89/92 (97%)	81 (91%)	7 (8%)	1 (1%)	17	65
42	r	122/137 (89%)	109 (89%)	11 (9%)	2 (2%)	12	58
43	s	194/318 (61%)	175 (90%)	17 (9%)	2 (1%)	19	66
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	15	61
45	l	5/7 (71%)	2 (40%)	3 (60%)	0	100	100
52	AA	215/295 (73%)	198 (92%)	16 (7%)	1 (0%)	34	77
53	BB	211/264 (80%)	201 (95%)	10 (5%)	0	100	100
54	CC	219/293 (75%)	204 (93%)	15 (7%)	0	100	100
55	DD	226/243 (93%)	207 (92%)	17 (8%)	2 (1%)	21	68
56	EE	260/263 (99%)	248 (95%)	11 (4%)	1 (0%)	39	80
57	FF	181/204 (89%)	169 (93%)	10 (6%)	2 (1%)	17	65
58	GG	235/249 (94%)	226 (96%)	8 (3%)	1 (0%)	39	80
59	HH	181/194 (93%)	172 (95%)	9 (5%)	0	100	100
60	II	204/208 (98%)	190 (93%)	13 (6%)	1 (0%)	34	77
61	JJ	183/194 (94%)	176 (96%)	6 (3%)	1 (0%)	34	77
62	KK	94/165 (57%)	87 (93%)	6 (6%)	1 (1%)	17	65
63	LL	139/158 (88%)	127 (91%)	11 (8%)	1 (1%)	26	72
64	MM	115/132 (87%)	100 (87%)	15 (13%)	0	100	100
65	NN	147/151 (97%)	139 (95%)	8 (5%)	0	100	100
66	OO	134/168 (80%)	124 (92%)	9 (7%)	1 (1%)	26	72
67	PP	118/145 (81%)	104 (88%)	14 (12%)	0	100	100
68	QQ	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
69	RR	130/135 (96%)	117 (90%)	12 (9%)	1 (1%)	24	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
70	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
71	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	26	72
72	UU	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
73	VV	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
74	WW	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	24	70
75	XX	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	8	52
76	YY	122/130 (94%)	115 (94%)	7 (6%)	0	100	100
77	ZZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
78	aa	99/115 (86%)	90 (91%)	7 (7%)	2 (2%)	9	54
79	bb	81/84 (96%)	70 (86%)	10 (12%)	1 (1%)	16	63
80	cc	60/69 (87%)	57 (95%)	3 (5%)	0	100	100
81	dd	53/56 (95%)	48 (91%)	4 (8%)	1 (2%)	10	55
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/156 (42%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/317 (98%)	282 (91%)	26 (8%)	3 (1%)	19	66
86	ii	370/403 (92%)	342 (92%)	27 (7%)	1 (0%)	46	83
87	jj	423/710 (60%)	388 (92%)	31 (7%)	4 (1%)	21	68
All	All	12317/14495 (85%)	11449 (93%)	804 (6%)	64 (0%)	38	77

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	S	155	PRO
75	XX	62	PRO
75	XX	86	PRO
1	A	217	GLN
3	C	83	GLY
3	C	94	ASN
6	F	99	GLY
13	N	89	VAL
43	s	142	GLY
44	t	125	LEU
1	A	14	SER
11	L	63	THR
22	W	27	LYS
25	Z	91	LEU

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Mol	Chain	Res	Type
27	b	102	PRO
31	f	107	PRO
42	r	68	SER
62	KK	64	TRP
66	OO	20	GLN
74	WW	56	HIS
78	aa	47	ALA
79	bb	81	ARG
87	jj	605	GLN
87	jj	618	SER
1	A	234	LYS
2	B	17	LEU
4	D	44	TYR
16	Q	14	ARG
25	Z	90	PRO
31	f	106	TYR
52	AA	159	ILE
56	EE	73	ASP
81	dd	7	TYR
86	ii	12	ASN
87	jj	269	VAL
87	jj	596	LYS
20	U	24	ASP
42	r	33	LYS
44	t	54	LYS
55	DD	44	THR
55	DD	93	THR
61	JJ	147	PHE
75	XX	61	GLN
78	aa	26	CYS
15	P	114	ILE
29	d	58	GLY
40	o	96	ASP
43	s	25	PRO
57	FF	43	GLU
63	LL	66	VAL
16	Q	92	VAL
58	GG	135	PRO
9	I	201	PRO
18	S	165	PRO
60	II	3	ILE
84	gg	224	GLY

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Mol	Chain	Res	Type
4	D	125	VAL
69	RR	119	VAL
71	TT	109	GLY
84	gg	61	GLY
6	F	196	VAL
41	p	9	GLY
57	FF	21	GLY
84	gg	13	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	175 (92%)	15 (8%)	15	56
2	B	342/348 (98%)	322 (94%)	20 (6%)	25	67
3	C	302/347 (87%)	282 (93%)	20 (7%)	21	63
4	D	247/250 (99%)	235 (95%)	12 (5%)	31	71
5	E	190/251 (76%)	178 (94%)	12 (6%)	22	65
6	F	196/215 (91%)	182 (93%)	14 (7%)	18	60
7	G	200/272 (74%)	188 (94%)	12 (6%)	24	66
8	H	169/171 (99%)	158 (94%)	11 (6%)	21	64
9	I	175/181 (97%)	165 (94%)	10 (6%)	25	68
10	J	143/149 (96%)	136 (95%)	7 (5%)	31	71
11	L	175/176 (99%)	166 (95%)	9 (5%)	29	71
12	M	117/161 (73%)	110 (94%)	7 (6%)	24	66
13	N	171/172 (99%)	162 (95%)	9 (5%)	28	70
14	O	171/173 (99%)	159 (93%)	12 (7%)	19	61
15	P	134/163 (82%)	125 (93%)	9 (7%)	20	63
16	Q	164/165 (99%)	153 (93%)	11 (7%)	20	63
17	R	159/175 (91%)	148 (93%)	11 (7%)	19	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S	157/157 (100%)	147 (94%)	10 (6%)	22	64
19	T	139/140 (99%)	128 (92%)	11 (8%)	15	56
20	U	89/114 (78%)	87 (98%)	2 (2%)	60	85
21	V	101/107 (94%)	91 (90%)	10 (10%)	10	45
22	W	86/126 (68%)	85 (99%)	1 (1%)	78	91
23	X	106/134 (79%)	100 (94%)	6 (6%)	25	68
24	Y	124/135 (92%)	118 (95%)	6 (5%)	31	72
25	Z	117/118 (99%)	114 (97%)	3 (3%)	54	83
26	a	119/120 (99%)	117 (98%)	2 (2%)	68	89
27	b	84/184 (46%)	81 (96%)	3 (4%)	42	78
28	c	84/98 (86%)	82 (98%)	2 (2%)	57	84
29	d	98/110 (89%)	88 (90%)	10 (10%)	9	44
30	e	114/121 (94%)	105 (92%)	9 (8%)	15	56
31	f	88/89 (99%)	84 (96%)	4 (4%)	34	74
32	g	98/100 (98%)	92 (94%)	6 (6%)	23	66
33	h	109/110 (99%)	104 (95%)	5 (5%)	33	73
34	i	86/89 (97%)	84 (98%)	2 (2%)	58	85
35	j	73/80 (91%)	68 (93%)	5 (7%)	20	62
36	k	64/65 (98%)	62 (97%)	2 (3%)	47	81
37	l	47/48 (98%)	46 (98%)	1 (2%)	61	86
38	m	48/90 (53%)	46 (96%)	2 (4%)	36	75
39	n	24/24 (100%)	22 (92%)	2 (8%)	14	54
40	o	92/94 (98%)	87 (95%)	5 (5%)	27	69
41	p	74/75 (99%)	73 (99%)	1 (1%)	74	90
42	r	108/121 (89%)	99 (92%)	9 (8%)	14	54
43	s	164/258 (64%)	158 (96%)	6 (4%)	41	77
44	t	126/137 (92%)	123 (98%)	3 (2%)	57	84
45	1	6/6 (100%)	6 (100%)	0	100	100
52	AA	180/245 (74%)	163 (91%)	17 (9%)	11	48
53	BB	194/231 (84%)	180 (93%)	14 (7%)	18	59
54	CC	187/225 (83%)	172 (92%)	15 (8%)	15	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	DD	190/202 (94%)	173 (91%)	17 (9%)	12	51
56	EE	224/225 (100%)	211 (94%)	13 (6%)	25	67
57	FF	158/170 (93%)	150 (95%)	8 (5%)	29	71
58	GG	207/218 (95%)	188 (91%)	19 (9%)	11	49
59	HH	165/174 (95%)	150 (91%)	15 (9%)	12	50
60	II	178/180 (99%)	166 (93%)	12 (7%)	20	63
61	JJ	161/168 (96%)	150 (93%)	11 (7%)	20	62
62	KK	87/136 (64%)	79 (91%)	8 (9%)	11	49
63	LL	130/142 (92%)	116 (89%)	14 (11%)	8	41
64	MM	99/108 (92%)	86 (87%)	13 (13%)	5	31
65	NN	130/131 (99%)	114 (88%)	16 (12%)	6	34
66	OO	106/130 (82%)	94 (89%)	12 (11%)	7	39
67	PP	109/130 (84%)	97 (89%)	12 (11%)	8	40
68	QQ	117/121 (97%)	109 (93%)	8 (7%)	20	62
69	RR	119/121 (98%)	106 (89%)	13 (11%)	8	41
70	SS	125/132 (95%)	111 (89%)	14 (11%)	7	39
71	TT	111/115 (96%)	101 (91%)	10 (9%)	12	50
72	UU	92/107 (86%)	84 (91%)	8 (9%)	13	52
73	VV	67/67 (100%)	64 (96%)	3 (4%)	34	74
74	WW	112/113 (99%)	107 (96%)	5 (4%)	34	74
75	XX	113/115 (98%)	106 (94%)	7 (6%)	23	65
76	YY	107/112 (96%)	96 (90%)	11 (10%)	9	43
77	ZZ	66/103 (64%)	61 (92%)	5 (8%)	16	57
78	aa	88/98 (90%)	81 (92%)	7 (8%)	15	55
79	bb	75/76 (99%)	67 (89%)	8 (11%)	8	42
80	cc	55/62 (89%)	50 (91%)	5 (9%)	12	50
81	dd	48/49 (98%)	44 (92%)	4 (8%)	14	54
82	ee	46/106 (43%)	44 (96%)	2 (4%)	35	75
83	ff	61/140 (44%)	55 (90%)	6 (10%)	10	46
84	gg	272/275 (99%)	262 (96%)	10 (4%)	41	77
86	ii	326/353 (92%)	309 (95%)	17 (5%)	29	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
87	jj	358/608 (59%)	330 (92%)	28 (8%)	16	56
All	All	10733/12306 (87%)	10017 (93%)	716 (7%)	25	63

All (716) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	64	ARG
1	A	102	LEU
1	A	109	GLU
1	A	125	LYS
1	A	128	ARG
1	A	142	GLU
1	A	163	ARG
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	226	ARG
1	A	233	ARG
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	53	MET
2	B	62	ARG
2	B	66	LYS
2	B	74	GLU
2	B	95	THR
2	B	97	ARG
2	B	135	LYS
2	B	248	LEU
2	B	261	ARG
2	B	262	VAL
2	B	279	GLU
2	B	294	LYS
2	B	309	LEU
2	B	314	ILE
2	B	333	LEU
2	B	351	LEU
2	B	356	LYS
2	B	383	GLU
3	C	20	LYS

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Mol	Chain	Res	Type
3	C	45	ARG
3	C	95	MET
3	C	113	ARG
3	C	122	TYR
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	188	ARG
3	C	193	LYS
3	C	208	CYS
3	C	213	GLU
3	C	232	VAL
3	C	246	VAL
3	C	281	MET
3	C	284	MET
3	C	307	LYS
3	C	312	ARG
4	D	22	ARG
4	D	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	128	ASP
4	D	234	ASP
4	D	264	LYS
4	D	268	ARG
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	123	ASP
5	E	141	ARG
5	E	143	LEU
5	E	144	ARG
5	E	169	LYS
5	E	178	VAL
5	E	213	LYS
5	E	289	LEU

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Mol	Chain	Res	Type
5	E	291	PHE
6	F	30	LYS
6	F	38	GLN
6	F	46	ARG
6	F	65	ARG
6	F	67	GLU
6	F	88	LEU
6	F	120	THR
6	F	134	ILE
6	F	151	GLU
6	F	186	MET
6	F	187	GLU
6	F	198	LYS
6	F	211	LYS
6	F	245	ARG
7	G	126	ARG
7	G	154	LYS
7	G	163	LYS
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	215	ASP
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	242	ARG
7	G	293	ASN
8	H	1	MET
8	H	20	LEU
8	H	52	LYS
8	H	54	ARG
8	H	59	LYS
8	H	66	GLU
8	H	74	CYS
8	H	105	ILE
8	H	108	ASN
8	H	128	MET
8	H	173	ARG
9	I	13	LYS
9	I	36	LEU
9	I	39	LYS
9	I	116	ARG

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Mol	Chain	Res	Type
9	I	142	LEU
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	195	CYS
9	I	208	LYS
10	J	16	ARG
10	J	28	GLU
10	J	33	LEU
10	J	72	CYS
10	J	81	GLU
10	J	113	ILE
10	J	175	LEU
11	L	10	LEU
11	L	63	THR
11	L	67	HIS
11	L	74	ARG
11	L	121	ARG
11	L	129	ARG
11	L	162	LYS
11	L	186	ARG
11	L	195	ARG
12	M	37	LEU
12	M	42	CYS
12	M	57	LEU
12	M	89	THR
12	M	96	GLU
12	M	105	THR
12	M	119	ARG
13	N	9	GLU
13	N	26	ARG
13	N	32	GLN
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	87	HIS
13	N	162	ARG
13	N	182	HIS
14	O	37	ARG
14	O	49	ARG
14	O	61	ARG
14	O	67	SER

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Mol	Chain	Res	Type
14	O	82	ARG
14	O	106	ASP
14	O	128	ARG
14	O	130	LYS
14	O	140	ARG
14	O	145	VAL
14	O	175	MET
14	O	179	LYS
15	P	24	VAL
15	P	25	HIS
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	5	ILE
16	Q	13	VAL
16	Q	61	LEU
16	Q	63	LEU
16	Q	75	ARG
16	Q	91	ARG
16	Q	97	LYS
16	Q	101	CYS
16	Q	143	ARG
16	Q	188	ASN
17	R	8	LYS
17	R	36	ASN
17	R	50	ILE
17	R	89	MET
17	R	99	MET
17	R	113	LYS
17	R	130	ASN
17	R	133	LYS
17	R	138	LEU
17	R	176	ARG
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	17	LEU

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Mol	Chain	Res	Type
18	S	24	THR
18	S	43	ARG
18	S	70	LYS
18	S	83	ARG
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	33	ILE
19	T	60	LYS
19	T	63	ARG
19	T	96	ILE
19	T	117	LYS
19	T	142	ARG
19	T	144	ASN
19	T	146	LYS
19	T	157	GLU
19	T	159	MET
20	U	33	ILE
20	U	80	LYS
21	V	15	ARG
21	V	18	LEU
21	V	35	LYS
21	V	41	SER
21	V	60	MET
21	V	71	GLU
21	V	82	ILE
21	V	91	LYS
21	V	109	LYS
21	V	123	LYS
22	W	91	MET
23	X	39	LYS
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	91	GLU
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	50	ARG
24	Y	72	GLN
24	Y	74	TYR

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Mol	Chain	Res	Type
24	Y	112	ASP
25	Z	11	VAL
25	Z	33	THR
25	Z	112	ARG
26	a	4	ARG
26	a	132	ARG
27	b	22	LYS
27	b	40	LEU
27	b	101	HIS
28	c	37	MET
28	c	78	ASN
29	d	23	ARG
29	d	26	THR
29	d	31	LYS
29	d	44	ARG
29	d	48	GLU
29	d	78	ARG
29	d	83	ARG
29	d	85	ARG
29	d	90	ARG
29	d	98	SER
30	e	21	ILE
30	e	22	ARG
30	e	48	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	106	LYS
30	e	113	GLU
30	e	128	ARG
31	f	16	ARG
31	f	23	GLU
31	f	52	LYS
31	f	101	ILE
32	g	5	LEU
32	g	15	THR
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	114	GLN
33	h	16	GLU
33	h	28	LEU

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Mol	Chain	Res	Type
33	h	67	GLU
33	h	77	LYS
33	h	89	ARG
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	11	ARG
35	j	20	ARG
35	j	58	THR
35	j	79	ARG
36	k	69	LEU
36	k	70	LYS
37	l	49	LEU
38	m	71	ARG
38	m	92	THR
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	18	HIS
40	o	36	GLN
40	o	61	LYS
40	o	82	MET
41	p	8	VAL
42	r	8	MET
42	r	20	ARG
42	r	32	LEU
42	r	35	ARG
42	r	39	ARG
42	r	67	ARG
42	r	80	THR
42	r	103	HIS
42	r	118	LEU
43	s	38	LYS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	98	ILE
44	t	133	LEU
52	AA	9	GLN

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Mol	Chain	Res	Type
52	AA	12	GLU
52	AA	25	LEU
52	AA	36	GLN
52	AA	44	ASP
52	AA	50	ASN
52	AA	58	LEU
52	AA	60	LEU
52	AA	111	GLN
52	AA	122	LEU
52	AA	132	GLN
52	AA	136	GLU
52	AA	142	LEU
52	AA	169	HIS
52	AA	178	LEU
52	AA	181	GLU
52	AA	200	ASP
53	BB	38	MET
53	BB	71	LEU
53	BB	82	ARG
53	BB	96	CYS
53	BB	105	LEU
53	BB	126	ASP
53	BB	134	LEU
53	BB	157	GLN
53	BB	180	ASP
53	BB	181	LEU
53	BB	207	LEU
53	BB	209	ASP
53	BB	213	ARG
53	BB	225	LEU
54	CC	78	LEU
54	CC	114	LYS
54	CC	120	GLN
54	CC	121	ARG
54	CC	132	ASP
54	CC	137	VAL
54	CC	167	ARG
54	CC	182	CYS
54	CC	188	CYS
54	CC	192	LEU
54	CC	227	ARG
54	CC	235	ASN

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Mol	Chain	Res	Type
54	CC	236	PHE
54	CC	248	TYR
54	CC	255	LEU
55	DD	28	GLU
55	DD	35	SER
55	DD	45	ARG
55	DD	57	ASN
55	DD	72	VAL
55	DD	76	ARG
55	DD	127	MET
55	DD	132	LYS
55	DD	134	CYS
55	DD	142	LEU
55	DD	145	GLN
55	DD	146	ARG
55	DD	168	VAL
55	DD	182	LEU
55	DD	190	LEU
55	DD	218	LEU
55	DD	227	LYS
56	EE	17	HIS
56	EE	24	THR
56	EE	42	LEU
56	EE	51	ARG
56	EE	59	ASP
56	EE	66	MET
56	EE	77	ARG
56	EE	145	ARG
56	EE	200	ARG
56	EE	205	PHE
56	EE	222	LEU
56	EE	232	ASN
56	EE	246	LEU
57	FF	63	LYS
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	95	HIS
57	FF	125	SER
57	FF	140	ASP
57	FF	204	ARG
58	GG	41	LEU

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Mol	Chain	Res	Type
58	GG	48	TYR
58	GG	63	MET
58	GG	64	LYS
58	GG	67	VAL
58	GG	72	ARG
58	GG	95	LYS
58	GG	103	ASP
58	GG	116	LYS
58	GG	137	ARG
58	GG	159	ARG
58	GG	171	THR
58	GG	183	ARG
58	GG	190	ARG
58	GG	191	ARG
58	GG	216	ARG
58	GG	217	MET
58	GG	230	LYS
58	GG	235	SER
59	HH	8	ILE
59	HH	17	ASP
59	HH	21	SER
59	HH	36	LEU
59	HH	40	LEU
59	HH	46	THR
59	HH	53	VAL
59	HH	76	GLN
59	HH	79	LEU
59	HH	82	GLU
59	HH	100	ILE
59	HH	119	SER
59	HH	145	ARG
59	HH	149	ASP
59	HH	160	LYS
60	II	6	ASP
60	II	12	ARG
60	II	23	LYS
60	II	26	LYS
60	II	49	ARG
60	II	92	ARG
60	II	99	ASN
60	II	121	LEU
60	II	128	LYS

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Mol	Chain	Res	Type
60	II	130	THR
60	II	168	GLN
60	II	178	ARG
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	70	ARG
61	JJ	79	ARG
61	JJ	80	ARG
61	JJ	89	GLU
61	JJ	92	MET
61	JJ	116	LYS
62	KK	1	MET
62	KK	6	LYS
62	KK	17	LYS
62	KK	35	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	89	ILE
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	39	ASN
63	LL	40	ILE
63	LL	42	LEU
63	LL	56	ILE
63	LL	69	ARG
63	LL	85	THR
63	LL	110	SER
63	LL	121	GLN
63	LL	126	VAL
63	LL	132	ARG
63	LL	134	LEU
63	LL	144	LYS
64	MM	31	LEU
64	MM	33	ARG
64	MM	40	LYS
64	MM	49	LEU
64	MM	55	ASN
64	MM	76	LEU

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Mol	Chain	Res	Type
64	MM	83	LYS
64	MM	85	LEU
64	MM	96	ARG
64	MM	99	LYS
64	MM	101	ARG
64	MM	112	LYS
64	MM	122	ASP
65	NN	3	ARG
65	NN	20	ARG
65	NN	27	LYS
65	NN	29	THR
65	NN	36	GLN
65	NN	55	ARG
65	NN	60	VAL
65	NN	75	LEU
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	107	LYS
65	NN	110	ASP
65	NN	120	SER
65	NN	125	LEU
65	NN	132	LYS
66	OO	25	GLU
66	OO	31	CYS
66	OO	34	PHE
66	OO	38	ASN
66	OO	46	ASP
66	OO	51	GLU
66	OO	56	VAL
66	OO	104	ARG
66	OO	128	ARG
66	OO	146	ARG
66	OO	150	ARG
66	OO	151	LEU
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE
67	PP	37	TYR
67	PP	44	ARG
67	PP	51	ARG
67	PP	58	LYS

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Mol	Chain	Res	Type
67	PP	76	VAL
67	PP	78	THR
67	PP	83	MET
67	PP	108	LYS
67	PP	130	ARG
68	QQ	31	LEU
68	QQ	40	GLU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	60	LYS
68	QQ	67	ASP
68	QQ	90	LYS
68	QQ	140	ARG
69	RR	5	ARG
69	RR	31	ASN
69	RR	33	ARG
69	RR	44	LYS
69	RR	62	GLN
69	RR	78	ARG
69	RR	82	ASP
69	RR	98	VAL
69	RR	99	ASP
69	RR	105	MET
69	RR	109	LEU
69	RR	120	THR
69	RR	132	ARG
70	SS	7	GLU
70	SS	8	LYS
70	SS	21	ASP
70	SS	23	ARG
70	SS	46	ARG
70	SS	52	LEU
70	SS	59	LEU
70	SS	60	THR
70	SS	62	ASP
70	SS	63	GLU
70	SS	75	ARG
70	SS	83	PHE
70	SS	110	ASP
70	SS	132	ARG
71	TT	41	LYS
71	TT	55	THR

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Mol	Chain	Res	Type
71	TT	62	ARG
71	TT	102	ARG
71	TT	110	LEU
71	TT	121	ARG
71	TT	123	LEU
71	TT	124	THR
71	TT	131	LEU
71	TT	142	LYS
72	UU	18	HIS
72	UU	25	THR
72	UU	56	MET
72	UU	60	THR
72	UU	88	LEU
72	UU	90	ASP
72	UU	106	ILE
72	UU	111	GLU
73	VV	10	ASP
73	VV	12	TYR
73	VV	66	ASP
74	WW	23	ARG
74	WW	51	GLU
74	WW	92	ASN
74	WW	103	VAL
74	WW	104	LEU
75	XX	8	ARG
75	XX	15	SER
75	XX	67	ARG
75	XX	105	PHE
75	XX	115	ILE
75	XX	119	ARG
75	XX	135	LYS
76	YY	9	THR
76	YY	16	ARG
76	YY	17	LEU
76	YY	20	ARG
76	YY	40	ILE
76	YY	47	MET
76	YY	61	ARG
76	YY	74	MET
76	YY	88	LYS
76	YY	101	LYS
76	YY	103	SER

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Mol	Chain	Res	Type
77	ZZ	51	ASP
77	ZZ	80	ARG
77	ZZ	89	GLN
77	ZZ	92	LEU
77	ZZ	101	SER
78	aa	18	VAL
78	aa	19	GLN
78	aa	21	ILE
78	aa	23	CYS
78	aa	41	ILE
78	aa	42	ARG
78	aa	100	ARG
79	bb	17	ARG
79	bb	36	LYS
79	bb	37	CYS
79	bb	42	LYS
79	bb	64	CYS
79	bb	78	SER
79	bb	80	ARG
79	bb	81	ARG
80	cc	31	ARG
80	cc	40	ARG
80	cc	44	ARG
80	cc	51	ARG
80	cc	68	LEU
81	dd	18	SER
81	dd	22	ARG
81	dd	48	LYS
81	dd	49	ASP
82	ee	99	LYS
82	ee	107	ARG
83	ff	83	LYS
83	ff	94	LYS
83	ff	99	LYS
83	ff	138	ARG
83	ff	140	TYR
83	ff	149	CYS
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	38	LYS
84	gg	119	GLN

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Mol	Chain	Res	Type
84	gg	198	VAL
84	gg	207	CYS
84	gg	273	GLU
84	gg	289	LEU
84	gg	306	LEU
86	ii	40	ARG
86	ii	68	CYS
86	ii	81	LEU
86	ii	107	ASN
86	ii	148	HIS
86	ii	149	ILE
86	ii	156	MET
86	ii	170	LYS
86	ii	183	GLU
86	ii	198	HIS
86	ii	243	VAL
86	ii	258	CYS
86	ii	297	LYS
86	ii	311	LEU
86	ii	313	ILE
86	ii	319	ARG
86	ii	349	LEU
87	jj	269	VAL
87	jj	276	LEU
87	jj	297	GLN
87	jj	298	GLU
87	jj	304	LYS
87	jj	313	LEU
87	jj	325	THR
87	jj	330	MET
87	jj	361	GLN
87	jj	369	VAL
87	jj	385	GLN
87	jj	389	HIS
87	jj	408	MET
87	jj	425	LEU
87	jj	434	PHE
87	jj	436	GLU
87	jj	482	ARG
87	jj	489	ARG
87	jj	499	GLN
87	jj	505	ILE

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Mol	Chain	Res	Type
87	jj	524	PRO
87	jj	548	ASP
87	jj	557	MET
87	jj	590	ILE
87	jj	613	ILE
87	jj	640	ASN
87	jj	653	LEU
87	jj	664	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
7	G	135	GLN
12	M	48	GLN
14	O	65	ASN
17	R	130	ASN
22	W	48	GLN
23	X	93	ASN
23	X	105	ASN
28	c	78	ASN
42	r	70	GLN
42	r	103	HIS
42	r	121	GLN
43	s	34	ASN
52	AA	132	GLN
54	CC	235	ASN
56	EE	260	GLN
59	HH	114	GLN
61	JJ	111	GLN
66	OO	20	GLN
67	PP	41	GLN
67	PP	79	HIS
68	QQ	35	ASN
68	QQ	142	GLN
70	SS	10	GLN
70	SS	97	GLN
74	WW	92	ASN
75	XX	77	ASN
79	bb	49	HIS
82	ee	117	ASN
86	ii	109	GLN

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Mol	Chain	Res	Type
87	jj	385	GLN
87	jj	389	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	13 (17%)	0
47	3	72/75 (96%)	27 (37%)	1 (1%)
48	5	3506/3543 (98%)	849 (24%)	165 (4%)
49	7	119/120 (99%)	12 (10%)	2 (1%)
50	8	150/156 (96%)	35 (23%)	7 (4%)
51	9	1680/1869 (89%)	425 (25%)	84 (5%)
85	hh	7/8 (87%)	4 (57%)	0
All	All	5608/5847 (95%)	1365 (24%)	259 (4%)

All (1365) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	8	U
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G
46	2	21	A
46	2	43	A
46	2	46	G
46	2	47	U
46	2	49	C
46	2	61	C
46	2	72	C
46	2	75	C
47	3	7	A
47	3	13	C
47	3	14	A
47	3	16	C
47	3	21	A
47	3	25	C
47	3	28	C
47	3	29	A
47	3	34	U
47	3	35	U

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Mol	Chain	Res	Type
47	3	36	U
47	3	40	C
47	3	42	G
47	3	47	U
47	3	49	C
47	3	51	G
47	3	53	G
47	3	58	A
47	3	60	U
47	3	61	C
47	3	63	C
47	3	65	G
47	3	71	G
47	3	72	C
47	3	74	C
47	3	75	C
47	3	76	A
48	5	12	A
48	5	13	U
48	5	15	A
48	5	25	A
48	5	30	C
48	5	35	U
48	5	39	A
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	72	C
48	5	73	A
48	5	91	G
48	5	93	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	116	G

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Mol	Chain	Res	Type
48	5	118	C
48	5	119	G
48	5	120	A
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	157	U
48	5	159	C
48	5	160	G
48	5	172	C
48	5	173	C
48	5	177	G
48	5	179	G
48	5	200	U
48	5	201	C
48	5	202	C
48	5	205	C
48	5	209	U
48	5	216	C
48	5	217	C
48	5	218	A
48	5	220	C
48	5	221	C
48	5	224	U
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	246	G
48	5	253	G
48	5	262	G
48	5	263	G
48	5	265	C
48	5	266	C
48	5	276	C
48	5	279	A
48	5	280	G
48	5	281	U
48	5	297	U

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Mol	Chain	Res	Type
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	322	C
48	5	334	A
48	5	340	C
48	5	347	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	363	A
48	5	386	A
48	5	387	G
48	5	399	G
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	431	G
48	5	432	U
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	482	G
48	5	483	G
48	5	484	U
48	5	485	C
48	5	486	C
48	5	490	C
48	5	492	U

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Mol	Chain	Res	Type
48	5	493	G
48	5	495	C
48	5	497	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	510	U
48	5	649	A
48	5	654	C
48	5	658	C
48	5	667	A
48	5	668	C
48	5	672	C
48	5	683	C
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	704	C
48	5	705	G
48	5	708	G
48	5	729	G
48	5	730	G
48	5	731	G
48	5	739	G
48	5	742	G
48	5	744	G
48	5	747	A
48	5	748	G
48	5	749	G
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	915	A
48	5	917	A
48	5	918	G
48	5	922(A)	G
48	5	922(B)	C
48	5	923	C
48	5	924	C

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Mol	Chain	Res	Type
48	5	925	C
48	5	926	G
48	5	929	A
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	936	C
48	5	939	G
48	5	941	C
48	5	943	A
48	5	944	A
48	5	945	U
48	5	955	G
48	5	956	A
48	5	957	G
48	5	959	G
48	5	960	A
48	5	961	G
48	5	962	C
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C
48	5	969	C
48	5	972	C
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1070	G
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1177	U
48	5	1179	U
48	5	1184	A
48	5	1185	G

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Mol	Chain	Res	Type
48	5	1195	G
48	5	1211	G
48	5	1212	G
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1280	C
48	5	1284	G
48	5	1287	G
48	5	1288	G
48	5	1291	G
48	5	1292	C
48	5	1293	G
48	5	1295	U
48	5	1296	G
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1328	G
48	5	1330	A
48	5	1337	A
48	5	1353	G
48	5	1354	A
48	5	1359	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1379	C
48	5	1380	G

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Mol	Chain	Res	Type
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1411(B)	C
48	5	1411(C)	C
48	5	1416	G
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1429	C
48	5	1433	A
48	5	1435	G
48	5	1436	C
48	5	1437	C
48	5	1438	U
48	5	1441	C
48	5	1442	C
48	5	1445	U
48	5	1446	C
48	5	1453	G
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1458	C
48	5	1465	G
48	5	1475	G
48	5	1478	C
48	5	1481	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1504	G
48	5	1514	U

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Mol	Chain	Res	Type
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1525	A
48	5	1534	A
48	5	1535	C
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1568	C
48	5	1578	U
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1640	C
48	5	1641	G
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1670	G
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1724	G
48	5	1726	U
48	5	1729	A
48	5	1734	G
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G

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Mol	Chain	Res	Type
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1761	G
48	5	1763	C
48	5	1764	G
48	5	1768	C
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1781	U
48	5	1787	A
48	5	1797	G
48	5	1799	G
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1819	G
48	5	1821	G
48	5	1822	U
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1869	G
48	5	1882	U
48	5	1893	C
48	5	1897	A
48	5	1910	G
48	5	1918	U
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1933	G
48	5	1941	A
48	5	1948	G

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Mol	Chain	Res	Type
48	5	1952	G
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1966	C
48	5	1967	A
48	5	1976	G
48	5	1977	C
48	5	1978	C
48	5	1980	U
48	5	1982	G
48	5	1983	A
48	5	1984	A
48	5	1986	U
48	5	1987	C
48	5	1991	A
48	5	1992	U
48	5	1993	C
48	5	1997	U
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2011	C
48	5	2017	A
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2033	A
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2069	A
48	5	2084	U
48	5	2085	G
48	5	2089	G

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Mol	Chain	Res	Type
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G
48	5	2101	A
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2109	A
48	5	2110	G
48	5	2259	G
48	5	2260	C
48	5	2262	G
48	5	2266	C
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2275	G
48	5	2279	A
48	5	2289	C
48	5	2294	G
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2316	G
48	5	2332	A
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2352	U
48	5	2360	A
48	5	2364	G
48	5	2370	A

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Mol	Chain	Res	Type
48	5	2395	A
48	5	2396	A
48	5	2399	G
48	5	2416	G
48	5	2417	A
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2428	A
48	5	2433	G
48	5	2441	C
48	5	2447	U
48	5	2450	G
48	5	2469	C
48	5	2471	G
48	5	2475	G
48	5	2483	G
48	5	2485	U
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2513	A
48	5	2521	G
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2553	A
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2571	C
48	5	2572	C
48	5	2575	U

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Mol	Chain	Res	Type
48	5	2583	C
48	5	2587	A
48	5	2601	A
48	5	2620	G
48	5	2627	C
48	5	2638	G
48	5	2639	U
48	5	2640	G
48	5	2647	A
48	5	2661	U
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2676	A
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2689	C
48	5	2695	A
48	5	2696	A
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2735	G
48	5	2740	U
48	5	2743	A
48	5	2754	G
48	5	2755	A
48	5	2760	G
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U

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Mol	Chain	Res	Type
48	5	2787	A
48	5	2789	A
48	5	2790	U
48	5	2794	C
48	5	2795	A
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2835	A
48	5	2838	G
48	5	2842	G
48	5	2855	G
48	5	2875	C
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3604	A
48	5	3605	C
48	5	3606	U
48	5	3615	G
48	5	3625	G
48	5	3626	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3662	A
48	5	3671	G
48	5	3673	C
48	5	3674	G
48	5	3692	A
48	5	3696	C
48	5	3698	G
48	5	3711	A
48	5	3712	A

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Mol	Chain	Res	Type
48	5	3722	G
48	5	3729	U
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3759	A
48	5	3760	A
48	5	3761	C
48	5	3763	A
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3780	G
48	5	3784	A
48	5	3785	A
48	5	3786	U
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3813	A
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3859	G
48	5	3867	A
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3889	G
48	5	3892	U
48	5	3897	G
48	5	3898	G
48	5	3901	A

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Mol	Chain	Res	Type
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3915	U
48	5	3916	G
48	5	3927	U
48	5	3939	G
48	5	3943	A
48	5	4067	U
48	5	4069	U
48	5	4071	U
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4092	G
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4158	C
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4165	C
48	5	4166	G
48	5	4171	C
48	5	4177	C
48	5	4183	G
48	5	4184	G
48	5	4191	G
48	5	4201	G
48	5	4203	A
48	5	4212	A

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Mol	Chain	Res	Type
48	5	4213	A
48	5	4218	U
48	5	4219	A
48	5	4225	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4237	C
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4297	G
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4326	G
48	5	4329	G
48	5	4330	G
48	5	4335	C
48	5	4336	A
48	5	4339	A
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4373	G
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C

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Mol	Chain	Res	Type
48	5	4391	G
48	5	4393	G
48	5	4394	A
48	5	4395	U
48	5	4396	A
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4437	U
48	5	4440	G
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4464	A
48	5	4471	U
48	5	4475	G
48	5	4476	C
48	5	4488	A
48	5	4495	G
48	5	4500	U
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4524	G
48	5	4531	U
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4561	C
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G

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Mol	Chain	Res	Type
48	5	4584	A
48	5	4585	U
48	5	4586	G
48	5	4590	A
48	5	4599	A
48	5	4606	G
48	5	4618	G
48	5	4635	A
48	5	4636	U
48	5	4637	G
48	5	4656	A
48	5	4657	U
48	5	4658	G
48	5	4661	G
48	5	4667	C
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4700	A
48	5	4701	A
48	5	4709	U
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4728	U
48	5	4736	C
48	5	4737	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4755	G
48	5	4756	C
48	5	4757	C
48	5	4758	U
48	5	4759	C
48	5	4760	G
48	5	4761	G
48	5	4765	G
48	5	4771	C
48	5	4772	C
48	5	4868	G
48	5	4870	G

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Mol	Chain	Res	Type
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	A
48	5	4877	G
48	5	4881	U
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4887	C
48	5	4891	G
48	5	4895	C
48	5	4897	G
48	5	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G
48	5	4919	G
48	5	4921	C
48	5	4924	C
48	5	4925	U
48	5	4926	C
48	5	4927	G
48	5	4928	C
48	5	4931	G
48	5	4935	C
48	5	4937	C
48	5	4938	A
48	5	4940	C
48	5	4942	C
48	5	4943	A
48	5	4944	C
48	5	4945	G
48	5	4947	U
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A

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Mol	Chain	Res	Type
48	5	4957	C
48	5	4958	C
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4976	U
48	5	4985	U
48	5	4988	U
48	5	4989	U
48	5	4990	C
48	5	4991	U
48	5	4997	G
48	5	4999	G
48	5	5014	A
48	5	5017	G
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5061	A
48	5	5062	G
48	5	5066	U
49	7	7	G
49	7	11	A
49	7	25	G
49	7	33	U
49	7	53	U
49	7	54	A
49	7	64	G
49	7	97	G
49	7	100	A
49	7	110	G
49	7	111	C
49	7	120	U
50	8	2	G
50	8	3	A
50	8	32	C
50	8	34	U

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Mol	Chain	Res	Type
50	8	35	C
50	8	49	G
50	8	51	U
50	8	52	A
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	G
50	8	79	G
50	8	86	U
50	8	87	G
50	8	94	G
50	8	95	A
50	8	103	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	114	G
50	8	121	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
50	8	150	C
50	8	153	C
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	37	C
51	9	44	U
51	9	45	A
51	9	46	A

Continued on next page...

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Mol	Chain	Res	Type
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	128	U
51	9	129	C
51	9	130	G
51	9	141	A
51	9	142	C
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C
51	9	173	A
51	9	175	A

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Mol	Chain	Res	Type
51	9	182	C
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	192	C
51	9	200	G
51	9	202	G
51	9	206	G
51	9	213	G
51	9	215	G
51	9	293	C
51	9	294	U
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	314	U
51	9	317	C
51	9	318	A
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	335	G
51	9	340	C
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	370	G
51	9	372	U
51	9	381	C
51	9	382	C
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G

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Mol	Chain	Res	Type
51	9	408	A
51	9	409	C
51	9	410	G
51	9	417	C
51	9	418	A
51	9	434	G
51	9	435	A
51	9	438	G
51	9	441	C
51	9	448	A
51	9	449	A
51	9	450	C
51	9	452	G
51	9	460	A
51	9	462	C
51	9	464	A
51	9	465	A
51	9	466	G
51	9	468	A
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	501	C
51	9	523	A
51	9	525	A
51	9	528	A
51	9	531	A
51	9	532	C
51	9	533	A
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A

Continued on next page...

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Mol	Chain	Res	Type
51	9	555	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	595	U
51	9	597	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	613	G
51	9	614	C
51	9	615	C
51	9	616	A
51	9	617	G
51	9	620	G
51	9	621	C
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	630	U
51	9	631	U
51	9	632	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	659	G
51	9	660	C

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Mol	Chain	Res	Type
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	684	G
51	9	688	U
51	9	689	U
51	9	732	U
51	9	752	G
51	9	753	C
51	9	754	G
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A
51	9	834	C
51	9	847	A
51	9	861	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	885	U
51	9	887	U
51	9	890	U
51	9	892	U
51	9	913	A
51	9	914	U
51	9	920	A
51	9	922	A
51	9	930	C
51	9	933	G

Continued on next page...

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Mol	Chain	Res	Type
51	9	934	G
51	9	943	U
51	9	971	G
51	9	985	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1055	A
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1067	C
51	9	1078	C
51	9	1083	A
51	9	1085	C
51	9	1100	A
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1121	G
51	9	1131	G
51	9	1138	C
51	9	1139	C
51	9	1144	A
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1161	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1196	A
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1215	C

Continued on next page...

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Mol	Chain	Res	Type
51	9	1221	G
51	9	1224	G
51	9	1227	G
51	9	1230	C
51	9	1240	A
51	9	1242	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1259	A
51	9	1265	A
51	9	1266	C
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1281	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1287	A
51	9	1289	U
51	9	1291	A
51	9	1293	A
51	9	1298	G
51	9	1299	A
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1304	U
51	9	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1330	G
51	9	1331	C
51	9	1342	U
51	9	1354	G
51	9	1369	A
51	9	1371	U

Continued on next page...

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Mol	Chain	Res	Type
51	9	1372	U
51	9	1378	A
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1401	A
51	9	1402	A
51	9	1404	U
51	9	1412	C
51	9	1424	G
51	9	1428	G
51	9	1439	A
51	9	1449	G
51	9	1454	A
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1466	G
51	9	1473	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1489	A
51	9	1490	G
51	9	1493	C
51	9	1494	U
51	9	1498	A
51	9	1507	G
51	9	1509	U
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1531	A
51	9	1533	A
51	9	1536	G
51	9	1539	U
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U

Continued on next page...

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Mol	Chain	Res	Type
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1582	C
51	9	1585	U
51	9	1587	G
51	9	1588	A
51	9	1589	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1612	G
51	9	1621	U
51	9	1622	U
51	9	1623	A
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1641	A
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1695	A
51	9	1698	C
51	9	1703	C
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G

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Mol	Chain	Res	Type
51	9	1728	U
51	9	1729	U
51	9	1730	U
51	9	1732	G
51	9	1737	G
51	9	1744	G
51	9	1745	A
51	9	1753	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C
51	9	1800	A
51	9	1801	A
51	9	1805	G
51	9	1822	A
51	9	1823	A
51	9	1824	A
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1868	U
51	9	1869	A
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G

All (259) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	74	C
48	5	12	A
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	119	G
48	5	125	C
48	5	134	G
48	5	143	C
48	5	159	C
48	5	217	C
48	5	224	U
48	5	226	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	G
48	5	315	G
48	5	385	A
48	5	406	C
48	5	408	A
48	5	409	G
48	5	417	G
48	5	449	C
48	5	466	A
48	5	484	U
48	5	485	C
48	5	492	U
48	5	497	G
48	5	498	C
48	5	504	G
48	5	696	C
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	916	C
48	5	922	C
48	5	922(B)	C
48	5	930	G
48	5	933	G
48	5	935(A)	G
48	5	936	C

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Mol	Chain	Res	Type
48	5	955	G
48	5	956	A
48	5	959	G
48	5	963	G
48	5	966	A
48	5	968	C
48	5	969	C
48	5	971(A)	G
48	5	1072	C
48	5	1211	G
48	5	1214	C
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1295	U
48	5	1329	G
48	5	1358	G
48	5	1359	G
48	5	1370	G
48	5	1378	C
48	5	1380	G
48	5	1420	A
48	5	1432	G
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1481	C
48	5	1485	C
48	5	1534	A
48	5	1563	A
48	5	1633	G
48	5	1654	G
48	5	1678	C
48	5	1733	G
48	5	1740	C
48	5	1804	A
48	5	1818	G
48	5	1833	G
48	5	1834	U

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Mol	Chain	Res	Type
48	5	1835	G
48	5	1892	A
48	5	1921	C
48	5	1935	C
48	5	1947	U
48	5	1979	A
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2046	G
48	5	2068	C
48	5	2088	A
48	5	2089	G
48	5	2100	G
48	5	2265	G
48	5	2266	C
48	5	2278	G
48	5	2313	A
48	5	2396	A
48	5	2398	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	A
48	5	2529	A
48	5	2546	G
48	5	2553	A
48	5	2661	U
48	5	2695	A
48	5	2724	G
48	5	2754	G
48	5	2794	C
48	5	2806	A
48	5	3603	G
48	5	3625	G
48	5	3648	A
48	5	3673	C
48	5	3697	U
48	5	3710	G

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Mol	Chain	Res	Type
48	5	3759	A
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4162	C
48	5	4170	A
48	5	4221	C
48	5	4232	U
48	5	4254	G
48	5	4266	G
48	5	4272	G
48	5	4291	G
48	5	4378	A
48	5	4395	U
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4510	A
48	5	4527	G
48	5	4572	U
48	5	4626	A
48	5	4634	U
48	5	4699	U
48	5	4719	G
48	5	4872	G
48	5	4884	G
48	5	4925	U
48	5	4936	G
48	5	4942	C
48	5	4947	U
48	5	4965	U
48	5	4966	A
49	7	10	C
49	7	109	U
50	8	2	G

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Mol	Chain	Res	Type
50	8	51	U
50	8	85	U
50	8	86	U
50	8	94	G
50	8	110	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	72	C
51	9	110	U
51	9	126	G
51	9	128	U
51	9	142	C
51	9	160	U
51	9	182	C
51	9	293	C
51	9	312	G
51	9	369	C
51	9	434	G
51	9	465	A
51	9	500	A
51	9	532	C
51	9	550	C
51	9	553	U
51	9	555	A
51	9	559	G
51	9	563	G
51	9	591	U
51	9	594	A
51	9	606	G
51	9	607	U
51	9	613	G
51	9	614	C
51	9	620	G
51	9	626	G
51	9	627	U
51	9	628	A
51	9	629	A
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U

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Mol	Chain	Res	Type
51	9	752	G
51	9	821	G
51	9	869	A
51	9	870	A
51	9	872	A
51	9	874	G
51	9	875	A
51	9	1016	U
51	9	1087	A
51	9	1114	U
51	9	1115	U
51	9	1137	U
51	9	1165	G
51	9	1253	A
51	9	1264	C
51	9	1274	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1313	A
51	9	1330	G
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1438	A
51	9	1476	A
51	9	1489	A
51	9	1493	C
51	9	1519	U
51	9	1520	G
51	9	1578	U
51	9	1581	C
51	9	1621	U
51	9	1622	U
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1663	A
51	9	1664	A
51	9	1665	G
51	9	1679	A
51	9	1721	U

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Mol	Chain	Res	Type
51	9	1744	G
51	9	1824	A
51	9	1825	A
51	9	1835	A
51	9	1867	U
51	9	1868	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 273 ligands modelled in this entry, 272 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
90	GCP	jj	700	88	29,34,34	2.51	8 (27%)	31,54,54	1.12	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	GCP	jj	700	88	-	0/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	C4-N9	-10.40	1.33	1.47
90	jj	700	GCP	C8-N9	-3.75	1.35	1.47
90	jj	700	GCP	C5-C6	-2.18	1.49	1.53
90	jj	700	GCP	PB-O2B	2.16	1.61	1.56
90	jj	700	GCP	PG-O2G	2.67	1.61	1.54
90	jj	700	GCP	PG-O3G	2.67	1.61	1.54
90	jj	700	GCP	PB-O3A	2.71	1.61	1.58
90	jj	700	GCP	C1'-N9	3.75	1.49	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C4-C5-N7	2.49	106.55	102.67
90	jj	700	GCP	C8-N9-C4	3.39	108.64	104.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	43
51	9	8
47	3	2
46	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	40.91
1	5	1252:C	O3'	1271:G	P	35.78
1	5	1405:C	O3'	1406:G	P	23.41

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1219:G	O3'	1233:G	P	22.71
1	5	1406:G	O3'	1406(A):G	P	20.12
1	5	3948:C	O3'	4065:G	P	19.81
1	5	4138:C	O3'	4146:G	P	18.04
1	5	990:C	O3'	1064:G	P	18.02
1	5	523:C	O3'	638:G	P	18.01
1	5	4101:C	O3'	4107:G	P	17.41
1	5	4777:C	O3'	4859:C	P	16.47
1	5	1406(C):G	O3'	1411:C	P	15.34
1	5	760:G	O3'	904:C	P	14.93
1	5	5022:U	O3'	5028:G	P	14.86
1	5	1696:C	O3'	1720:C	P	14.79
1	5	1364:U	O3'	1368:A	P	14.36
1	5	182:G	O3'	189:G	P	13.89
1	5	1411:C	O3'	1411(A):G	P	13.71
1	5	2901:G	O3'	3597:G	P	13.37
1	5	921:C	O3'	922:C	P	13.07
1	5	970:G	O3'	971:U	P	10.72
1	5	481:G	O3'	481(A):C	P	10.70
1	5	934:C	O3'	935:A	P	10.36
1	5	512:U	O3'	515:C	P	9.76
1	5	4729:A	O3'	4735:G	P	9.75
1	5	737:C	O3'	738:C	P	9.61
1	5	971:U	O3'	971(A):G	P	9.59
1	5	1180:C	O3'	1183:C	P	9.18
1	5	500:G	O3'	504:G	P	6.68
1	5	1100:U	O3'	1168:G	P	5.83
1	3	19:G	O3'	20:U	P	5.67
1	5	1239:C	O3'	1244:G	P	5.15
1	9	322:C	O3'	323:C	P	5.12
1	5	4740:G	O3'	4743:G	P	5.00
1	3	16:C	O3'	18:U	P	4.98
1	5	480:C	O3'	481:G	P	4.96
1	9	798:G	O3'	799:U	P	4.62
1	9	309:G	O3'	310:C	P	4.59
1	9	304:C	O3'	305:U	P	4.45
1	2	16:C	O3'	18:G	P	4.28
1	5	935:A	O3'	935(A):G	P	4.20
1	5	738:C	O3'	738(A):C	P	3.96
1	5	170:C	O3'	171:U	P	3.88
1	5	1438:U	O3'	1440:U	P	3.39
1	5	4899:G	O3'	4902:C	P	3.38

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	902:G	O3'	903:A	P	3.37
1	9	903:A	O3'	904:A	P	3.33
1	9	1295:A	O3'	1296:U	P	3.27
1	5	267:G	O3'	268:G	P	3.19
1	9	593:C	O3'	594:A	P	3.16
1	5	5020:G	O3'	5021:C	P	3.14
1	5	751:G	O3'	752:G	P	2.96
1	5	2031:C	O3'	2032:U	P	2.78
1	5	922(A):G	O3'	922(B):C	P	1.77