



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

Nov 22, 2016 – 03:13 PM EST

PDB ID : 5LZV  
EMDB ID: : EMD-4133  
Title : Structure of the mammalian ribosomal termination complex with accommodated eRF1(AAQ) and ABCE1.  
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.  
Deposited on : 2016-10-02  
Resolution : 3.35 Å(reported)

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

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

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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

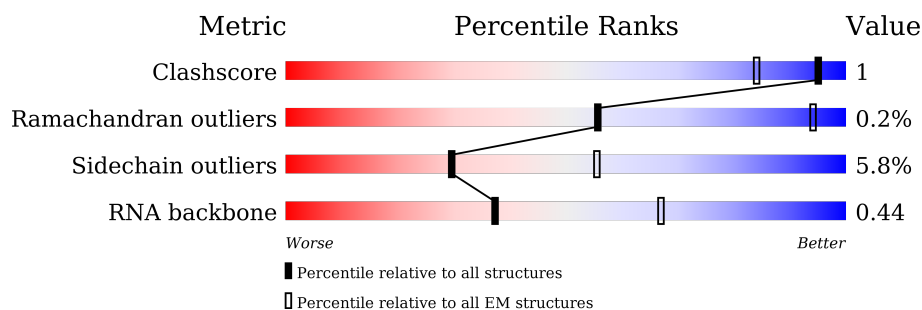
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.35 Å.

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





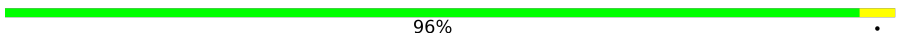














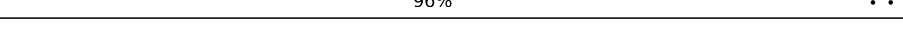
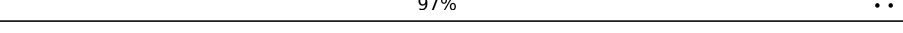




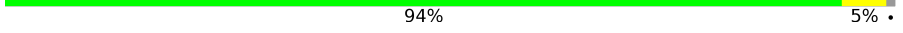
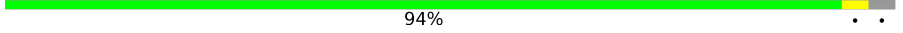
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	A	257	89% 7% .
2	B	403	93% 5% .
3	C	425	82% . 15%
4	D	297	95% ..
5	E	291	70% .. 26%
6	F	247	86% 5% 9%
7	G	319	68% 5% 27%
8	H	192	92% 6% ..



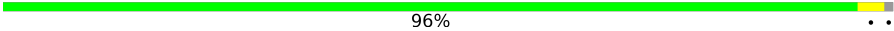
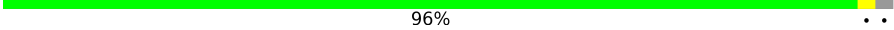


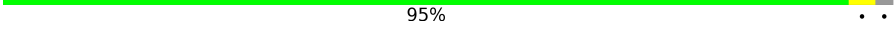
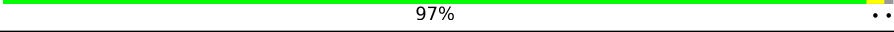



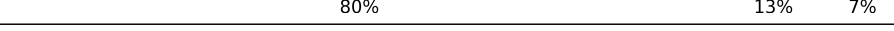







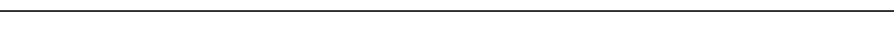

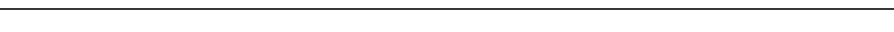
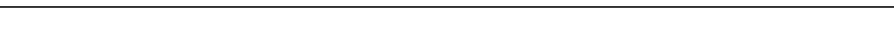


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Mol	Chain	Length	Quality of chain
9	I	214	 92% . .
10	J	178	 90% 6% .
11	L	211	 96% .
12	M	218	 60% . 37%
13	N	204	 95% .
14	O	203	 90% 8% .
15	P	184	 78% 5% 17%
16	Q	188	 95% 5% .
17	R	196	 84% 7% . 8%
18	S	176	 93% 6% .
19	T	160	 91% 8% ..
20	U	128	 77% . 23%
21	V	140	 86% 6% . 6%
22	W	157	 66% . 32%
23	X	156	 72% . 24%
24	Y	145	 88% . . 8%
25	Z	136	 96% . .
26	a	148	 97% . .
27	b	245	 41% . 58%
28	c	115	 83% . 15%
29	d	125	 79% 6% 14%
30	e	135	 89% 6% 5%
31	f	110	 94% 5% .
32	g	117	 94% . .
33	h	123	 96% . .
















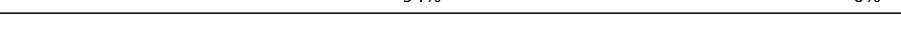





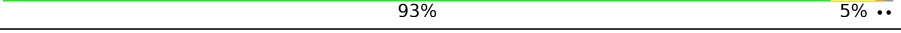

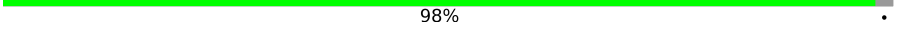

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Mol	Chain	Length	Quality of chain
34	i	105	 94% . .
35	j	97	 84% 5% 11%
36	k	70	 96% . .
37	l	51	 96% . .
38	m	102	 49% . 49%
39	n	25	 92% 8%
40	o	106	 95% . .
41	p	92	 97% . .
42	r	137	 88% . 9%
43	s	318	 58% . 38%
44	t	165	 88% . 7%
45	1	15	 80% 13% 7%
46	2	76	 74% 25% .
47	3	75	 65% 33% .
48	5	3543	 72% 26% .
49	7	120	 88% 13%
50	8	156	 72% 24% . .
51	9	1869	 62% 25% . 9%
52	AA	295	 67% 6% 26%
53	BB	264	 70% 9% . 19%
54	CC	293	 67% 8% . 25%
55	DD	243	 83% 10% . 6%
56	EE	263	 84% 15%
57	FF	204	 78% 10% . 9%
58	GG	249	 86% 8% 5%





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Mol	Chain	Length	Quality of chain
59	HH	194	 85% 10% 5%
60	II	208	 88% 12% .
61	JJ	194	 84% 11% 5%
62	KK	165	 51% 5% . 42%
63	LL	158	 80% 10% 9%
64	MM	132	 67% 15% 5% . 11%
65	NN	151	 88% 10% ..
66	OO	168	 70% 10% . 19%
67	PP	145	 71% 10% . 17%
68	QQ	146	 87% 10% .
69	RR	135	 88% 10% .
70	SS	152	 82% 12% . 5%
71	TT	145	 87% 9% ..
72	UU	119	 78% 6% 16%
73	VV	83	 94% 6%
74	WW	130	 87% 12% .
75	XX	143	 87% 10% ...
76	YY	130	 84% 12% 5%
77	ZZ	125	 54% 6% 40%
78	aa	115	 79% 9% 12%
79	bb	84	 93% 5% ..
80	cc	69	 84% 6% 10%
81	dd	56	 98% .
82	ee	133	 39% . 59%
83	ff	156	 39% . 56%

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Mol	Chain	Length	Quality of chain
84	gg	317	 95% ..
85	hh	15	 53% 47%
86	ii	459	 88% . 9%
87	jj	599	 93% . .

## 2 Entry composition

There are 90 unique types of molecules in this entry. The entry contains 223874 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called uL4.

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

- Molecule 4 is a protein called uL18.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 5 is a protein called eL6.

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

- Molecule 6 is a protein called uL30.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 7 is a protein called eL8.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 8 is a protein called uL6.

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

- Molecule 9 is a protein called uL16.

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

- Molecule 10 is a protein called uL5.



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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called eL15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

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

- Molecule 22 is a protein called eL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

- Molecule 25 is a protein called eL27.

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

- Molecule 26 is a protein called uL15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 27 is a protein called eL29.

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

- Molecule 28 is a protein called eL30.

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

- Molecule 29 is a protein called eL31.

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

- Molecule 30 is a protein called eL32.

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

- Molecule 31 is a protein called eL33.

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

- Molecule 32 is a protein called eL34.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 33 is a protein called uL29.

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

- Molecule 34 is a protein called eL36.

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

- Molecule 35 is a protein called eL37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

- Molecule 39 is a protein called eL41.

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	15	Total	C	N	O	S	0	0
			125	82	20	22	1		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.



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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

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

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

- Molecule 86 is a protein called eRF1(AAQ).

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	419	Total	C	N	O	S	0	0
			3309	2106	562	629	12		

There are 24 discrepancies between the modelled and reference sequences:

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

*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
ii	-2	GLN	-	expression tag	UNP P62495
ii	-1	GLY	-	expression tag	UNP P62495
ii	0	SER	-	expression tag	UNP P62495
ii	183	ALA	GLY	conflict	UNP P62495
ii	184	ALA	GLY	conflict	UNP P62495

- Molecule 87 is a protein called ABCE1.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	577	Total	C	N	O	S	0	0
			4555	2914	780	830	31		

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

Mol	Chain	Residues	Atoms		AltConf
88	P	1	Total	Mg	0
			1	1	
88	g	1	Total	Mg	0
			1	1	
88	j	1	Total	Mg	0
			1	1	
88	Q	1	Total	Mg	0
			1	1	
88	e	1	Total	Mg	0
			1	1	
88	B	1	Total	Mg	0
			1	1	
88	I	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	
88	7	7	Total	Mg	0
			7	7	
88	a	2	Total	Mg	0
			2	2	
88	5	197	Total	Mg	0
			197	197	
88	8	5	Total	Mg	0
			5	5	
88	9	79	Total	Mg	0
			79	79	
88	L	1	Total	Mg	0
			1	1	

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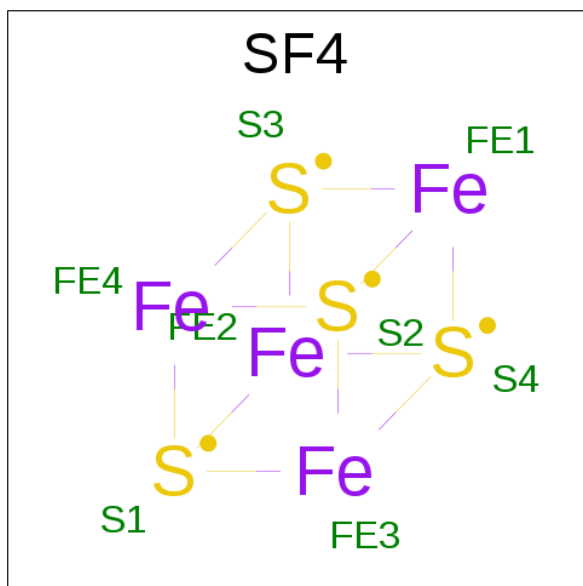
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Mol	Chain	Residues	Atoms		AltConf
88	hh	1	Total	Mg	0
			1	1	

- 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 IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
90	jj	1	Total	Fe	S	0
			16	8	8	
90	jj	1	Total	Fe	S	0
			16	8	8	





MET	GLU	GLY	ALA	GLU	GLY	LYS	LYS	VAL	PRO	ALA	VAL	PRO	GLU	THR	LEU	LYS	LYS	ARG	ARG	ASP	Q38	R46	R65	L88	A89	L124	I134	E151	E187	V196	G197	K198	V227	M246	M247
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------

- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | GLU | GLN | LEU | PRO | THR | CYS | TYR | THR | HIS | HIS | ASP | PHE | THR | TRP | ASP | LYS | VAL | LEU | CYS | TRP | SER | GLN | SER | PRO | GLY | ILE | LEU | ASN | SER | LYS | CYS | LEU | TRP | PRO | PHE | THR | ILE | HIS | LEU | LEU | VAL | GLY | ALA | LEU | PRO | ARG | GLY | ALA | TRP | GLY | GLY |
| MET | SER | SER | TYR | ARG | LEU | TYR | CYS | MET | LYS | GLU | GLU | ARG | HIS | ASN | LEU | VAL | LEU | CYS | LEU | TRP | SER | GLN | SER | PRO | GLY | ILE | LEU | ASN | SER | LYS | CYS | LEU | TRP | PRO | PHE | THR | ILE | HIS | LEU | LEU | VAL | GLY | ALA | LEU | PRO | ARG | GLY | ALA | TRP | GLY | GLY |

- 

- MET  
 G2  
 L36  
 K39  
 L103  
 SER  
 CYS  
 ALA  
 GLY  
 ALA  
 ASP  
 ARG  
 LEU  
 Q112  
 R116  
 E146  
 R153  
 Q163  
 K164  
 K208  
 S214

- MET  
 A1A  
 G1N  
 ASP  
 G1N  
 GLY  
 GLU  
 K8  
 R16  
 G27  
 E28  
 L33  
 R64  
 I68  
 A69  
 V70  
 E81  
 I113  
 L175  
 P176  
 G177  
 LYS

- 
- | Amino Acid | Percentage (%) |
|------------|----------------|
| MET        | 10             |
| A2         | 15             |
| R5         | 10             |
| W18        | 10             |
| T63        | 10             |
| H67        | 10             |
| R74        | 10             |
| R121       | 10             |
| K162       | 10             |
| R186       | 10             |
| K211       | 10             |

- [illegible]

- Molecule 13: eL15

Chain N:  95% .

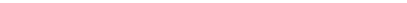


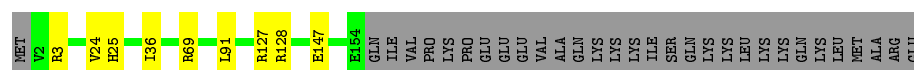
- Molecule 14: uL13

Chain O:  90% 8%



- Molecule 15: uL22

Chain P:  78% 5% 17%



- Molecule 16: eL18

Chain Q:  95% 5%



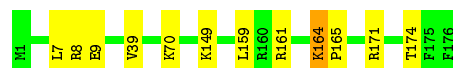
- Molecule 17: eL19

Chain R:  84% 7% 8%



- Molecule 18: eL20

Chain S:  93% 6%

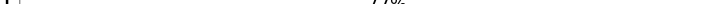


- Molecule 19: eL21

Chain T:  91% 8% ..

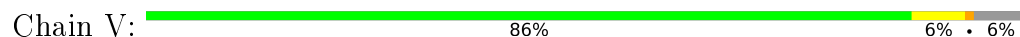


- Molecule 20: eL22

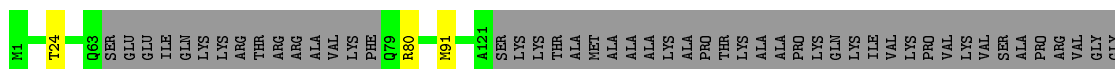
Chain U:  77% 23%



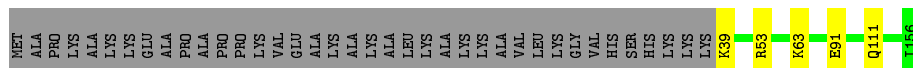
- Molecule 21: uL14



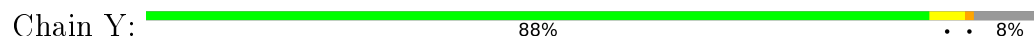
- Molecule 22: eL24



- Molecule 23: uL23



- Molecule 24: uL24



- Molecule 25: eL27

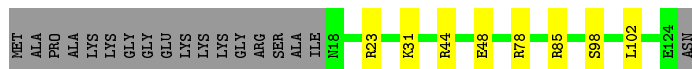
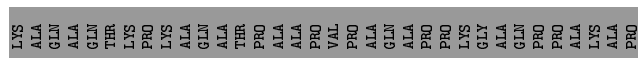


- Molecule 26: uL15



- Molecule 27: eL29









Chain i:  94% . .



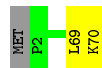
- Molecule 35: eL37

Chain j:  84% 5% 11%



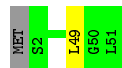
- Molecule 36: eL38

Chain k:  96% . .



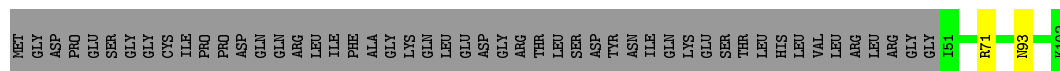
- Molecule 37: eL39

Chain l:  96% . .



- Molecule 38: eL40

Chain m:  49% . 49%



- Molecule 39: eL41

Chain n:  92% 8%



- Molecule 40: eL42

Chain o:  95% . .



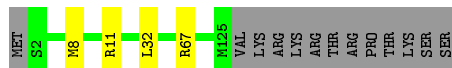
- Molecule 41: eL43

Chain p:  97% . .



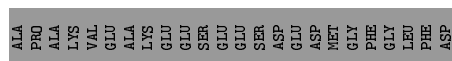
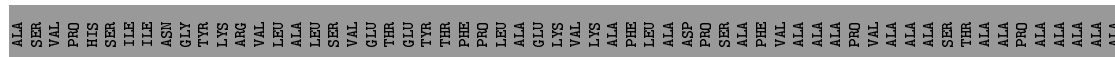
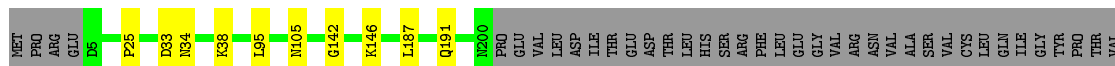
- Molecule 42: eL28

Chain r: 88% 9%



- Molecule 43: uL10

Chain s: 58% 38%



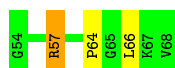
- Molecule 44: uL11

Chain t: 88% 7%



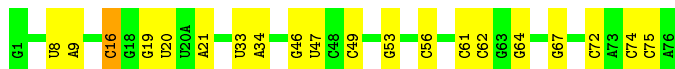
- Molecule 45: Nascent chain

Chain 1: 80% 13% 7%



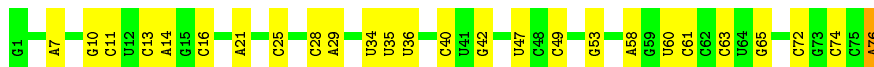
- Molecule 46: P-site tRNA

Chain 2: 74% 25%



- Molecule 47: E-site tRNA

Chain 3: 65% 33%




- Molecule 48: 28S ribosomal RNA

G2479	A2069	G1973	G1819	G1654	C1486	G1377	U1209	A944	G708	G457		C1
G2483	G2331	G1974	U1920	G1655	G1495	C1378	G1210	U945			C143	C6
A2484	A2332	U1974	G1821	C1655	G1495	C1379	G1211	A466	C719	A466	C144	C7
U2485	G2333	G1975	U1822	U1656	G1496	G1380	G1212	A956	G722	U467	C159	U8
	G2348	G1976	G1823	C1661	G1498	U1381	G1214	G956		U468		
		C1977					C1214	G956	G729	C469	A165	A12
C2488	A2088	G1978	C1828	C1676	G1502	A1387	C1215	G959	G730	C480	U13	A12
C2489	G2089	A1979	G1833	U1677	A1503	G1394	G1234	A960	G731	U481	C172	C14
U2490	U2090	U1980	U1834	G1678	G1504		G1235	G961		C481A	C173	A15
C2491	G2091	A1981	G1835	A1679		A1397	C1236	G963	G734	C482		U20
C2493	G2093	A1984	G1836	A1679	U1514	A1398	C1237	G964		C483	G176	U20
C2494	C2094	A1985	A1837	G1691	U1515	A1398	C1238	G965	C738	U484	G177	C24
U2495	A2095	U1986	G1837	G1691	G1516	C1401	C1239	A966	C738A	C485	C178	A25
	A2096	G1987	G1842	G1724	G1517	C1402	C1239	G967	G739	C486	C179	C25
C2499	A2097	C1987		U1725	A1518	G1403	G1272	C968			A336	C30
	G2098	A1990	G1855	U1726		G1403	G1273	C969	G742	C490	U200	
A2502	C2099	A1991		A1523		G1416	A1274			G491	C201	U35
C2503	A2374	U1992	A1867	G1733	A1523	C1417	G1275	G971A	A747	U492	C202	
G2504	A2101	C1993	A1868	G1734	A1525	C1418	C1276		G748	C493	A37	A39
C2505	G2380	G1993	G1869	U1735		G1419	G1276	G973	G749		C205	
G2506	A2103	U1997		A1534		A1420	G1284		U750	C496	C350	A42
	A2395	C1997	C1881	C1740		G1421		C979		C497	U209	
C2509	A2105	G2001		G1741	A1547		G1287		G756	C498	U357	A47
	G2397	A2002	C1893	A1742	A1554	C1429	G1288	C983	G757	C499	C216	G48
A2512	A2107	G2003		A1742					G758	G500	C217	U49
A2513	G2108	U2004	A1997							G504	A362	A218
	A2109	G2005	A1997	G1750		C1291	G1291	C990		G505	A363	A56
G2521	G2110	U2006	G1910	G1753	A1563	A1433	C1292	C1071	U911		C220	G57
	U2111	G2007		A1564		A1434	C1293	C1072	U912		C221	G58
		U2008	G1916	U1754	A1565	G1435	A1294	C1073	U913			A59
G2414	G2259	C2011	A1917	C1755	C1566	C1436	U1295	G1073	U914		U224	A64
U2415	G2260	A2012	U1918	U1756	G1574	C1437	G1075	G1075	A915	C653	G225	A64
G2416	G2261	C2012	G1919	U1757		U1438	G1076	C1076	A917	C654	G226	
A2417	G2262	A2013	C1920	U1578		C1301	C1077	C1077	G918	C657	A227	
		C2014	G1921	G1760		C1441	A1302	A1078		C658		A73
G2421	G2265	U2015	G1922	G1761	G1584	C1442	A1303		C921	C659	U233	
G2422	C2266	C2016	A1923	C1762		U1445	C1304	C1079	C922	A407	G234	U77
G2424	U2267	G2016	A1923	G1763	U1591	C1446	C1304			A408	A235	
U2425	C2268	G2024	C1									

C4957	C4958	C4964	U4965	A4966	A4967	U4976	A4979	U4988	U4989	C4990	U4991	A5014	G5017	U5040	G5041	C5047	C5050	C5051	C5052	U5053	C5054	G5055	A5056	A5061	G5062	U5069																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				</
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• Molecule 49: 5S ribosomal RNA

Chain 7:  88% 13%

G1	G7	A13	U33	U38	A42	U53	A54	G64	G97	A100	U109	G110	G116	G117	U120
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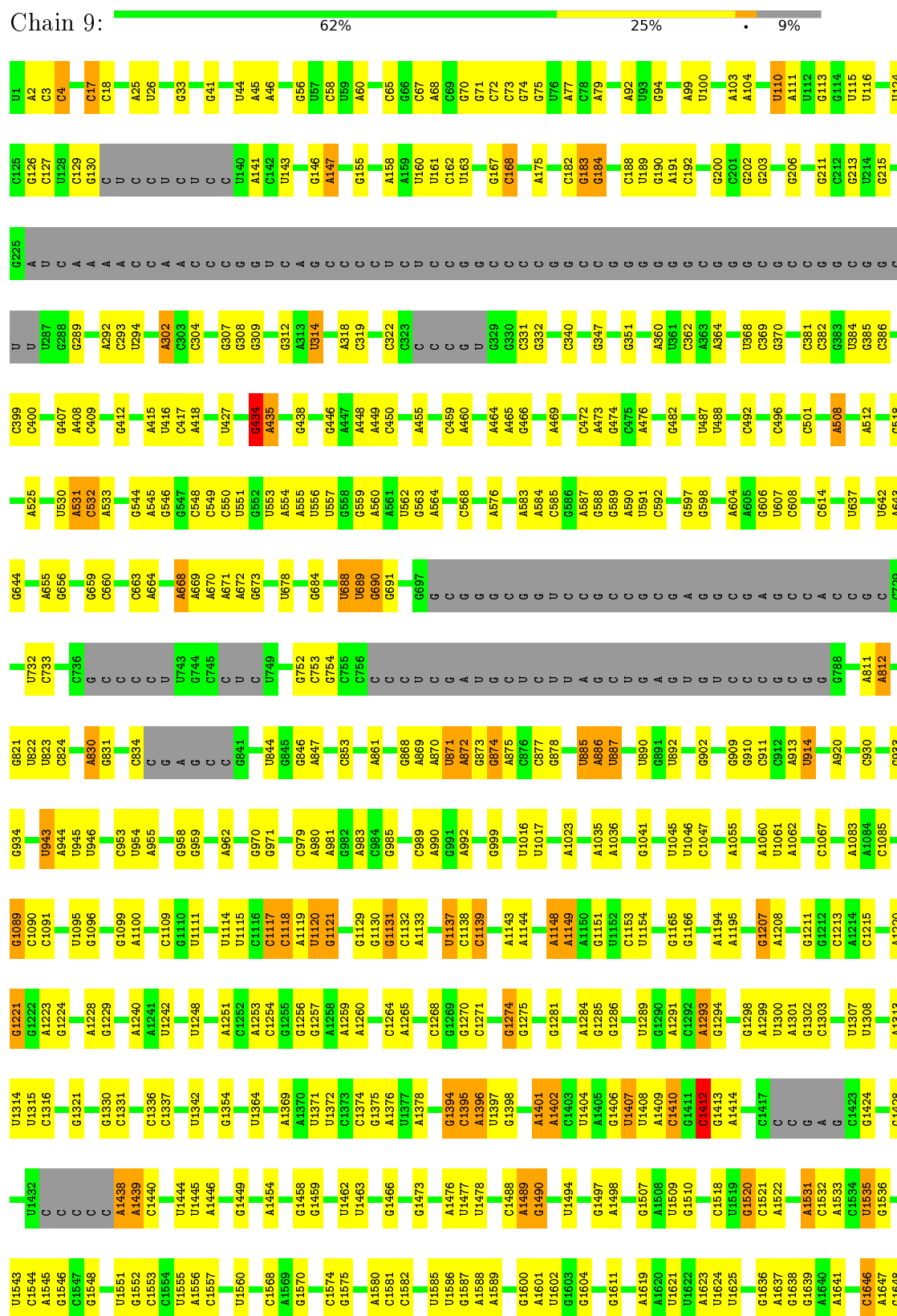
• Molecule 50: 5.8S ribosomal RNA

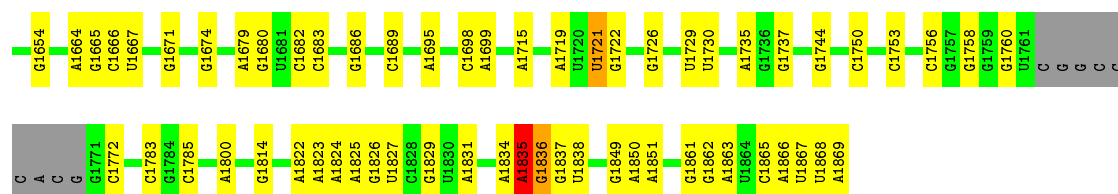
Chain 8:  72% 24%

C1	G2	A3	C32	G33	U34	C35	G49	C50	U51	A52	A59	A62	U63	G75	G79	A	C	A	C	A	U85	U86	G87	G94	A95	C96	A97	A103	A104	C105	G106	C107	A108	C109	U110	U111	G112	C113	G114	G121	G122	U123	U124	C125	C126	U127	A137	G143
G147	C150	C153	U156																																													

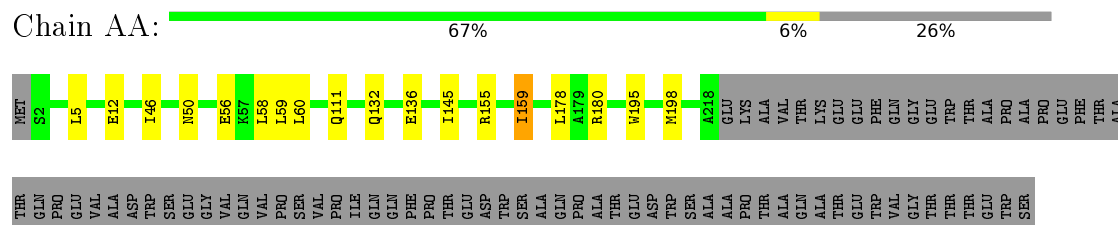


• Molecule 51: 18S ribosomal RNA

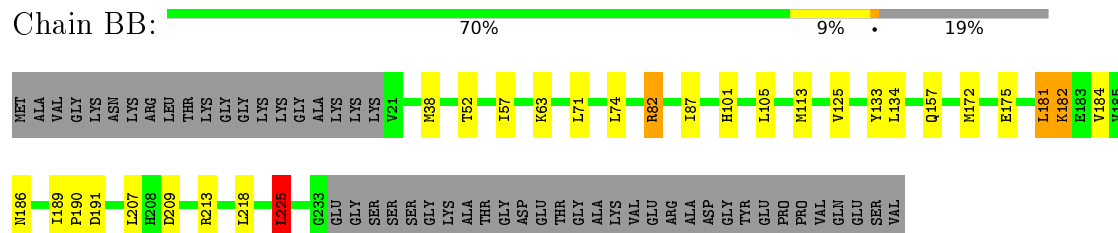




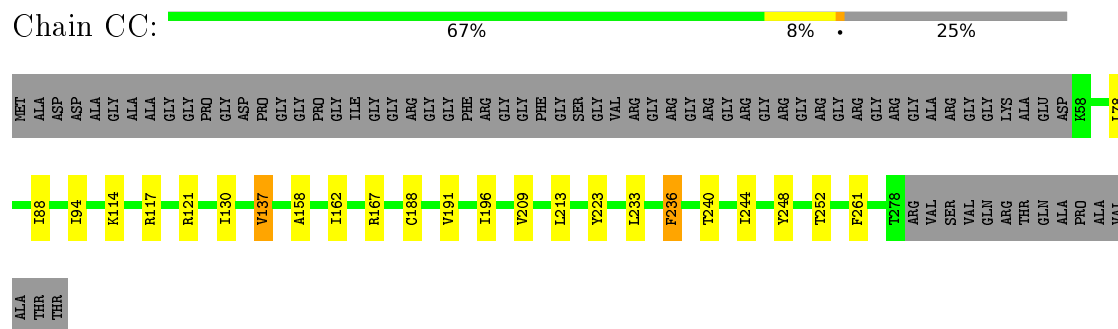
• Molecule 52: uS2



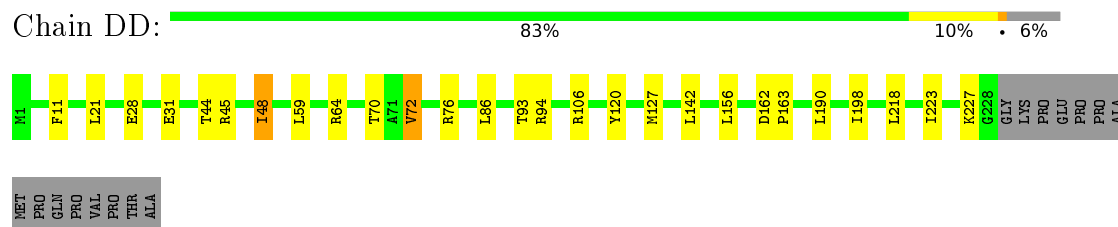
• Molecule 53: eS1



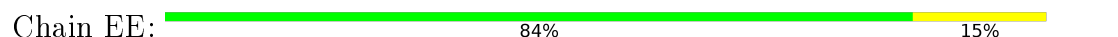
• Molecule 54: uS5

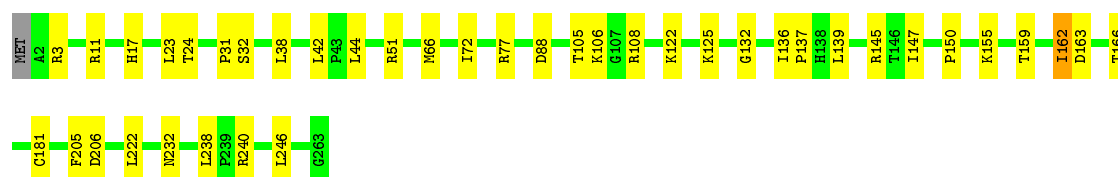


• Molecule 55: uS3



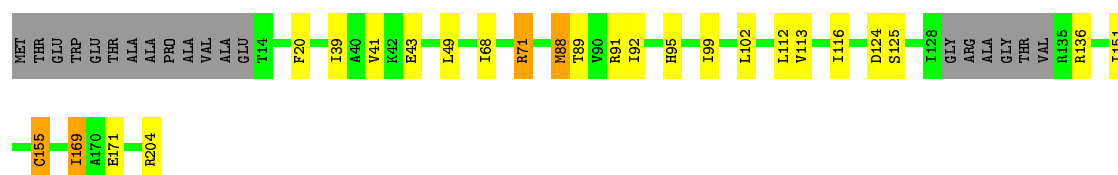
• Molecule 56: eS4





- Molecule 57: uS7

Chain FF: 78% 10% 9%



- Molecule 58: eS6

Chain GG: 86% 8% 5%



- Molecule 59: eS7

Chain HH: 85% 10% 5%



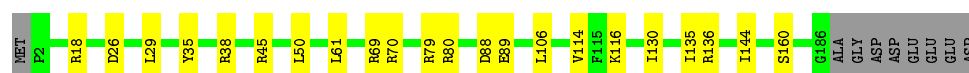
- Molecule 60: eS8

Chain II: 88% 12% 0%



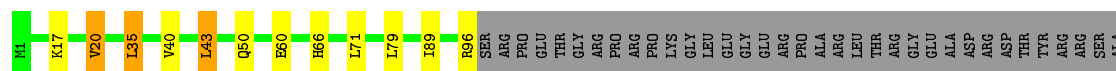
- Molecule 61: uS4

Chain JJ: 84% 11% 5%




- Molecule 62: eS10

Chain KK: 51% 5% 42%



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

• Molecule 63: uS17

Chain LL:  80% 10% 9%

MET  
ALA  
D3  
Y10  
I16  
K20  
V23  
LEU  
LEU  
GLY  
THR  
GLY  
LYS  
GLY  
K32  
T40  
G41  
L42  
E49  
T56  
R69  
T85  
D91  
R101  
K104  
R105  
H106  
Q121  
V126  
L134  
K153  
GLN  
PHE  
GLN  
LYS  
PHE

• Molecule 64: eS12

Chain MM:  67% 15% 5% 11%

MET  
ALA  
GLU  
GLU  
ILE  
ALA  
GLY  
GLY  
VAL  
MET  
ASP  
Y14  
A17  
L18  
Q19  
L22  
L31  
A32  
R33  
R36  
K40  
A41  
L42  
R45  
L49  
N65  
I74  
R83  
R84  
L85  
R89  
G90  
I91  
G92  
R93  
K99  
P100  
R101  
V111  
K112  
D113  
K121  
D122  
V123

I124  
C130  
LYS

• Molecule 65: uS15

Chain NN:  88% 10% ..

MET  
G2  
R3  
R20  
K27  
L54  
R55  
V60  
K78  
L84  
P85  
E86  
L91  
K94  
K107  
D110  
L125  
Y129  
K132  
V150  
ALA

• Molecule 66: uS11

Chain OO:  70% 10% 19%

MET  
LYS  
ALA  
ARG  
LEU  
ALA  
SER  
SER  
GLY  
SER  
GLY  
VAL  
ARG  
ARG  
ARG  
ALA  
ALA  
MET  
MET  
ALA  
PRO  
ARG  
GLY  
LYS  
GLY  
LYS  
GLU  
GLN  
VAL  
ILE  
S16  
Q20  
E25  
F34  
N38  
F41  
K50  
E51  
V56  
S69  
C85  
R98  
A99  
R104  
L119


R128  
D131  
R146  
R150  
L151

• Molecule 67: uS19

Chain PP:  71% 10% 17%


MET  
ALA  
GLU  
VAL  
GLN  
LYS  
LYS  
LYS  
ARG  
THR  
F12  
R13  
K14  
F15  
Y37  
R42  
R43  
R44  
L45  
S46  
R47  
K52  
L56  
T78  
H79  
L80  
M83  
K108  
P109  
R130  
P131  
GLY  
ILE  
GLY  
ALA  
THR  
HIS  
SER  
SER  
ARG  
PHE  
ILE  
PRO  
LEU  
LYS

• Molecule 68: uS9

Chain QQ:  87% 10% .


MET  
PRO  
SER  
LYS  
G5  
R15  
K16  
K17  
T18  
L31  
V34  
M41  
Y49  
K50  
L51  
L52  
E53  
K60  
D67  
I84  
K90  
R140  
R146

• Molecule 69: eS17

Chain RR:  88% 10%




- Molecule 70: uS13

Chain SS:  82% 12% 5%




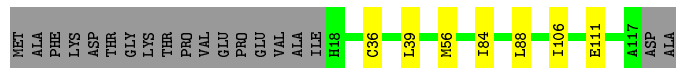
- Molecule 71: eS19

Chain TT:  87% 9%



- Molecule 72: uS10

Chain UU:  78% 6% 16%



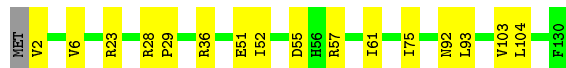
- Molecule 73: eS21

Chain VV:  94% 6%



- Molecule 74: uS8

Chain WW:  87% 12%




- Molecule 75: uS12

Chain XX:  87% 10%



- Molecule 76: eS24

Chain YY:  84% 12% 5%



Chain ff:  39% . 56%

MET GLN ILE PHE VAL LYS THR LEU THR LEU VAL GLN LYS THR ILE THR LEU GLN VAL GLU ASP THR ILE GLU ASN VAL LYS ALA LYS ILE GLN ASP LYS GLU GLY ILE PRO PRO ASP LYS GLN GLN ARG ARG LEU ILE PHE ALA GLY LYS LYS LEU GLU ASP GLY ARG THR LEU SER ASP TYR ASN

ILE GLN LYS SER THR LEU HIS VAL ARG ARG GLY ALA LYS ARG LYS K33 K34 K99 K113 C121 R138 H139 Y140 F150 ASN LYS PRO GLN ASP LYS

- Molecule 84: RACK1

Chain gg:  95% ..


MET T2 W17 Q20 R36 G61 L79 L87 Q119 C207 E273 L289 L306 T314 GLY THR ARG

- Molecule 85: mRNA (UGA stop codon)

Chain hh:  53% 47%

U41 C42 A43 A44 A45 Q46 U49 G52 C55

- Molecule 86: eRF1(AAQ)

Chain ii:  88% . 9%

MET ARG GLY SER HIS HIS HIS HIS MET MET ALA SER GLN ASN LEU TYR PHE GLN SER SER MET ASP ASP S6 N61 I62 K63 S64 R65 R68 N86 E103 R132 Q211 L212 F232 M241 L246 E339 E340 E341 L368 V417

Y424 GLN GLY ASP ASP PHE PHE ASP LEU ASP ASP TYR

- Molecule 87: ABCE1

Chain jj:  93% . .

MET ALA ASP R4 E24 E52 L75 R96 I97 D192 D236 K250 I313 E320 F331 LYS VAL ALA GLU THR ALA ASN GLU GLU VAL LYS LYS R345 L362 E373 R377 R385 F388 R399 GLU GLY GLU V404 Y411 Q468

R506 R510 T526 L597 ASP ASP

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	80571	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: ZN, MG, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.34	0/1936	0.61	0/2596
10	J	0.36	0/1385	0.57	0/1852
11	L	0.36	0/1733	0.62	0/2316
12	M	0.36	0/1158	0.59	0/1547
13	N	0.35	0/1746	0.61	0/2338
14	O	0.36	0/1662	0.59	0/2222
15	P	0.34	0/1268	0.54	0/1700
16	Q	0.35	0/1539	0.64	0/2054
17	R	0.35	0/1524	0.62	0/2013
18	S	0.35	0/1501	0.59	0/2012
19	T	0.34	0/1326	0.55	0/1770
2	B	0.34	0/3240	0.56	0/4339
20	U	0.37	0/823	0.52	0/1104
21	V	0.34	0/993	0.57	0/1332
22	W	0.35	0/873	0.55	0/1158
23	X	0.34	0/984	0.55	0/1323
24	Y	0.34	0/1132	0.56	0/1504
25	Z	0.36	0/1130	0.54	0/1507
26	a	0.32	0/1191	0.56	0/1590
27	b	0.35	0/861	0.57	0/1138
28	c	0.34	0/771	0.50	0/1034
29	d	0.36	0/903	0.61	0/1216
3	C	0.35	0/2937	0.59	0/3946
30	e	0.35	0/1071	0.60	0/1429
31	f	0.35	0/895	0.61	0/1198
32	g	0.35	0/916	0.64	0/1220
33	h	0.34	0/1021	0.56	0/1348
34	i	0.35	0/841	0.56	0/1112
35	j	0.37	0/720	0.67	0/952
36	k	0.33	0/575	0.52	0/761
37	l	0.37	0/459	0.58	0/608
38	m	0.35	0/435	0.57	0/575

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	n	0.35	0/240	0.71	0/305
4	D	0.34	0/2437	0.55	1/3264 (0.0%)
40	o	0.35	0/864	0.58	0/1140
41	p	0.34	0/718	0.54	0/953
42	r	0.36	0/1010	0.62	0/1354
43	s	0.37	0/1530	0.51	0/2064
44	t	0.36	0/1174	0.55	0/1582
45	1	0.42	0/129	0.80	1/173 (0.6%)
46	2	0.25	0/1805	0.67	0/2809
47	3	0.22	0/1777	0.67	0/2763
48	5	0.25	7/84974 (0.0%)	0.68	22/132512 (0.0%)
49	7	0.21	0/2858	0.64	0/4455
5	E	0.34	0/1762	0.57	0/2362
50	8	0.23	0/3581	0.66	0/5577
51	9	0.23	1/40524 (0.0%)	0.70	10/63134 (0.0%)
52	AA	0.35	0/1747	0.60	0/2374
53	BB	0.35	0/1756	0.63	0/2350
54	CC	0.35	0/1753	0.63	0/2369
55	DD	0.36	0/1796	0.64	0/2417
56	EE	0.35	0/2118	0.64	0/2849
57	FF	0.35	0/1492	0.63	0/2005
58	GG	0.35	0/1946	0.68	1/2590 (0.0%)
59	HH	0.36	0/1510	0.59	0/2022
6	F	0.35	0/1911	0.56	1/2549 (0.0%)
60	II	0.35	0/1715	0.64	0/2287
61	JJ	0.35	0/1550	0.70	0/2069
62	KK	0.36	0/834	0.61	0/1125
63	LL	0.34	0/1195	0.64	0/1597
64	MM	0.37	0/918	0.70	1/1233 (0.1%)
65	NN	0.35	0/1226	0.65	0/1649
66	OO	0.35	0/1029	0.76	1/1380 (0.1%)
67	PP	0.36	0/1017	0.68	0/1358
68	QQ	0.34	0/1146	0.62	0/1534
69	RR	0.35	0/1082	0.61	0/1452
7	G	0.36	0/1910	0.58	0/2569
70	SS	0.36	0/1208	0.68	0/1618
71	TT	0.38	0/1115	0.64	1/1493 (0.1%)
72	UU	0.34	0/805	0.63	0/1081
73	VV	0.37	0/643	0.67	0/860
74	WW	0.34	0/1051	0.65	0/1406
75	XX	0.34	0/1116	0.65	0/1490
76	YY	0.36	0/1028	0.65	0/1366
77	ZZ	0.35	0/604	0.63	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  > 2	RMSZ	# Z  > 2
78	aa	0.37	0/828	0.72	0/1109
79	bb	0.34	0/665	0.58	0/891
8	H	0.35	0/1535	0.58	0/2063
80	cc	0.34	0/490	0.68	0/656
81	dd	0.39	0/470	0.62	0/623
82	ee	0.36	0/447	0.68	0/587
83	ff	0.38	0/567	0.61	0/753
84	gg	0.34	0/2493	0.56	0/3394
85	hh	0.28	0/353	0.77	0/547
86	ii	0.36	0/3363	0.58	0/4523
87	jj	0.34	0/4640	0.56	1/6264 (0.0%)
9	I	0.35	0/1702	0.55	0/2272
All	All	0.29	8/239706 (0.0%)	0.65	40/350845 (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
48	5	0	4
56	EE	0	1
75	XX	0	1
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	5	1974	U	C2-N3	20.27	1.51	1.37
51	9	1412	C	O3'-P	-7.90	1.51	1.61
48	5	1974	U	N1-C2	7.38	1.45	1.38
48	5	1986	U	N3-C4	7.08	1.44	1.38
48	5	1986	U	N1-C2	6.78	1.44	1.38
48	5	336	A	C5-C6	6.13	1.46	1.41
48	5	77	U	N3-C4	-5.95	1.33	1.38
48	5	2013	A	N1-C2	5.49	1.39	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	1974	U	C2-N3-C4	-11.71	119.98	127.00
48	5	1986	U	C2-N3-C4	-7.93	122.24	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1394	G	C2'-C3'-O3'	7.89	126.85	109.50
51	9	1835	A	C2'-C3'-O3'	7.67	126.38	109.50
48	5	1979	A	C2'-C3'-O3'	7.12	125.16	109.50
48	5	336	A	N1-C6-N6	-7.09	114.35	118.60
48	5	1174	G	C2'-C3'-O3'	7.02	124.94	109.50
4	D	22	ARG	NE-CZ-NH1	6.35	123.48	120.30
51	9	874	G	C2'-C3'-O3'	6.21	123.63	113.70
51	9	1646	C	C2'-C3'-O3'	6.02	123.33	113.70
48	5	1445	U	C2'-C3'-O3'	5.99	123.28	113.70
48	5	2013	A	C4-N9-C1'	5.95	137.01	126.30
48	5	77	U	C2-N1-C1'	-5.91	110.61	117.70
64	MM	49	LEU	CA-CB-CG	5.88	128.84	115.30
48	5	1291	G	C2'-C3'-O3'	5.84	123.05	113.70
48	5	2013	A	C8-N9-C1'	-5.78	117.30	127.70
48	5	1477	C	C2'-C3'-O3'	5.76	122.91	113.70
48	5	406	C	C2'-C3'-O3'	5.74	122.89	113.70
66	OO	146	ARG	NE-CZ-NH1	5.56	123.08	120.30
48	5	1329	G	C2'-C3'-O3'	5.51	122.51	113.70
58	GG	41	LEU	CA-CB-CG	5.46	127.86	115.30
48	5	4947	U	C2'-C3'-O3'	5.45	122.41	113.70
71	TT	110	LEU	CA-CB-CG	5.42	127.78	115.30
45	1	57	ARG	NE-CZ-NH1	5.37	122.98	120.30
48	5	77	U	C6-N1-C1'	5.37	128.71	121.20
51	9	434	G	C2'-C3'-O3'	5.35	122.27	113.70
6	F	88	LEU	CA-CB-CG	5.30	127.50	115.30
48	5	3888	G	C2'-C3'-O3'	5.28	122.15	113.70
48	5	2474	G	C2'-C3'-O3'	5.24	122.08	113.70
48	5	2046	G	C2'-C3'-O3'	5.22	122.06	113.70
51	9	1438	A	C4-N9-C1'	5.20	135.66	126.30
48	5	1211	G	C2'-C3'-O3'	5.19	122.00	113.70
51	9	887	U	O4'-C1'-N1	5.16	112.33	108.20
51	9	1438	A	C8-N9-C1'	-5.16	118.42	127.70
51	9	110	U	C2'-C3'-O3'	5.15	121.94	113.70
48	5	245	C	C2'-C3'-O3'	5.11	121.88	113.70
87	jj	506	ARG	NE-CZ-NH2	-5.09	117.75	120.30
48	5	2002	A	C6-N1-C2	-5.03	115.58	118.60
51	9	1535	U	N1-C1'-C2'	5.02	120.53	114.00
48	5	1986	U	C2-N1-C1'	5.01	123.71	117.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
48	5	1974	U	Sidechain
48	5	1986	U	Sidechain
48	5	2002	A	Sidechain
48	5	2013	A	Sidechain
56	EE	155	LYS	Peptide
75	XX	61	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	d	888	0	930	0	0
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	999	0	0
33	h	1013	0	1147	0	0
34	i	830	0	916	0	0
35	j	705	0	737	0	0
36	k	569	0	637	0	0
37	l	447	0	480	0	0
38	m	429	0	466	0	0
39	n	239	0	289	0	0
40	o	851	0	920	0	0
41	p	708	0	756	0	0
42	r	994	0	1051	0	0
43	s	1507	0	1564	0	0
44	t	1160	0	1218	0	0
45	1	125	0	117	2	0
46	2	1616	0	824	5	0
47	3	1593	0	811	4	0
48	5	75972	0	38391	124	0
49	7	2558	0	1296	0	0
50	8	3208	0	1629	1	0
51	9	36249	0	18316	150	0
52	AA	1710	0	1708	2	0
53	BB	1729	0	1803	12	0
54	CC	1716	0	1806	10	0
55	DD	1768	0	1866	8	0
56	EE	2076	0	2177	15	0
57	FF	1471	0	1522	12	0
58	GG	1923	0	2089	6	0
59	HH	1488	0	1582	5	0
60	II	1686	0	1772	9	0
61	JJ	1525	0	1640	7	0
62	KK	810	0	836	5	0
63	LL	1175	0	1249	5	0
64	MM	908	0	939	19	0
65	NN	1202	0	1289	3	0
66	OO	1016	0	1039	2	0
67	PP	997	0	1045	5	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	3	0
70	SS	1190	0	1249	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	TT	1097	0	1132	4	0
72	UU	795	0	862	2	0
73	VV	636	0	637	3	0
74	WW	1034	0	1080	6	0
75	XX	1098	0	1167	7	0
76	YY	1011	0	1083	2	0
77	ZZ	598	0	656	5	0
78	aa	814	0	864	0	0
79	bb	651	0	672	0	0
80	cc	488	0	514	0	0
81	dd	459	0	451	0	0
82	ee	443	0	492	0	0
83	ff	555	0	566	0	0
84	gg	2436	0	2393	0	0
85	hh	317	0	161	0	0
86	ii	3309	0	3350	0	0
87	jj	4555	0	4691	0	0
88	5	197	0	0	0	0
88	7	7	0	0	0	0
88	8	5	0	0	0	0
88	9	79	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	L	1	0	0	0	0
88	P	1	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	a	2	0	0	0	0
88	e	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
88	j	1	0	0	0	0
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	16	0	0	0	0
All	All	223874	0	168777	436	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 1.

All (436) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3914:U:O4	48:5:4378:A:N1	1.58	1.34
48:5:1986:U:C2	48:5:2006:U:O4	1.82	1.32
51:9:1137:U:O4	51:9:1148:A:N1	1.70	1.24
48:5:1986:U:O2	48:5:2006:U:C4	1.91	1.23
48:5:1986:U:O2	48:5:2006:U:O4	1.57	1.20
48:5:2367:A:N1	48:5:2788:U:O4	1.73	1.19
51:9:1137:U:C4	51:9:1148:A:N1	2.12	1.17
48:5:1986:U:O4	48:5:2014:C:N4	1.83	1.11
48:5:2367:A:N6	48:5:2788:U:H3	1.51	1.08
51:9:1407:U:H2'	51:9:1408:U:C6	1.91	1.06
48:5:1986:U:H2'	48:5:2007:G:O6	1.56	1.02
48:5:77:U:O4	48:5:336:A:N1	1.99	0.96
51:9:1137:U:O4	51:9:1148:A:C2	2.20	0.94
48:5:3914:U:H3	48:5:4378:A:N6	1.66	0.92
51:9:872:A:N1	51:9:914:U:O4	2.05	0.89
51:9:885:U:O2'	51:9:886:A:O5'	1.89	0.88
48:5:2367:A:H61	48:5:2788:U:H3	0.87	0.85
48:5:1986:U:O2	48:5:2006:U:C5	2.31	0.84
51:9:1407:U:O2'	51:9:1408:U:O4'	1.96	0.84
51:9:1137:U:O4	51:9:1148:A:C6	2.32	0.82
48:5:2367:A:N6	48:5:2788:U:N3	2.17	0.82
51:9:688:U:O2'	51:9:689:U:OP2	1.99	0.81
48:5:3914:U:C4	48:5:4378:A:N1	2.48	0.80
48:5:3914:U:O4	48:5:4378:A:C2	2.35	0.80
48:5:2013:A:C2	48:5:2014:C:C2	2.70	0.79
48:5:3914:U:N3	48:5:4378:A:N6	2.27	0.79
53:BB:182:LYS:O	53:BB:186:ASN:ND2	2.15	0.78
51:9:872:A:N1	51:9:914:U:C4	2.52	0.78
48:5:1974:U:N3	48:5:2002:A:C6	2.52	0.78
51:9:530:U:H5''	51:9:530:U:H6	1.49	0.77
51:9:1137:U:C4	51:9:1148:A:C6	2.74	0.76
64:MM:101:ARG:HA	64:MM:101:ARG:CZ	2.16	0.75
51:9:885:U:HO2'	51:9:886:A:P	2.11	0.73
48:5:3766:A:N1	51:9:1827:U:O2'	2.19	0.73
56:EE:122:LYS:HG2	56:EE:162:ILE:HD11	1.73	0.71
48:5:2005:G:N2	48:5:2014:C:O2	2.17	0.71
51:9:1095:U:O4	51:9:1149:A:N1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:2367:A:N1	48:5:2788:U:C4	2.60	0.69
51:9:530:U:H5''	51:9:530:U:C6	2.27	0.69
51:9:203:G:OP2	60:II:147:LYS:NZ	2.22	0.68
48:5:1986:U:C2'	48:5:2007:G:O6	2.39	0.68
51:9:1401:A:C2	51:9:1402:A:C6	2.83	0.68
56:EE:139:LEU:HD12	56:EE:150:PRO:HB3	1.76	0.67
56:EE:122:LYS:CG	56:EE:162:ILE:HD11	2.24	0.67
51:9:1137:U:N3	51:9:1148:A:N6	2.43	0.67
48:5:1974:U:N3	48:5:2002:A:N6	2.44	0.65
48:5:2007:G:C2	48:5:2013:A:N6	2.65	0.65
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.96	0.64
57:FF:68:ILE:HD12	57:FF:112:LEU:HD22	1.80	0.64
48:5:1978:C:H3'	48:5:1979:A:H5''	1.79	0.63
48:5:2013:A:C2	48:5:2014:C:N1	2.66	0.63
51:9:1438:A:H2'	51:9:1439:A:C8	2.33	0.63
48:5:4744:A:N1	48:5:4956:A:N1	2.46	0.63
48:5:4213:A:N1	48:5:4218:U:O4	2.32	0.63
48:5:1974:U:O2	48:5:2002:A:N7	2.32	0.63
53:BB:189:ILE:HG22	53:BB:190:PRO:HD3	1.81	0.63
51:9:872:A:C6	51:9:914:U:O4	2.52	0.62
48:5:4723:A:H2'	48:5:4724:A:C8	2.34	0.62
51:9:1407:U:O2	51:9:1408:U:C2	2.53	0.62
64:MM:22:LEU:HD11	64:MM:89:VAL:HA	1.80	0.61
48:5:2409:U:C4	48:5:2783:A:N1	2.68	0.61
48:5:1986:U:N3	48:5:2013:A:N6	2.48	0.61
48:5:1986:U:C4	48:5:2013:A:N6	2.69	0.61
51:9:872:A:C6	51:9:914:U:C4	2.90	0.59
51:9:1412:C:H5''	51:9:1412:C:H6	1.66	0.59
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.32	0.59
48:5:1986:U:C4	48:5:2014:C:N4	2.70	0.59
48:5:3712:A:C2	51:9:970:G:C6	2.92	0.58
48:5:3629:A:C1'	51:9:1721:U:O2	2.51	0.58
48:5:3629:A:H4'	51:9:1721:U:O2	2.04	0.58
65:NN:125:LEU:HD22	65:NN:129:TYR:CE2	2.39	0.58
51:9:980:A:H2'	51:9:981:A:C8	2.39	0.58
67:PP:56:LEU:HD13	67:PP:78:THR:HG21	1.86	0.58
48:5:4699:U:N3	48:5:4701:A:N6	2.51	0.57
51:9:1546:G:H5'	68:QQ:18:THR:HG21	1.85	0.57
51:9:183:G:O2'	51:9:184:G:O5'	2.21	0.57
77:ZZ:79:ILE:HB	77:ZZ:83:LEU:HD12	1.86	0.57
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:3629:A:C4'	51:9:1721:U:O2	2.52	0.57
48:5:1986:U:H2'	48:5:2007:G:C6	2.37	0.57
51:9:1149:A:N3	51:9:1149:A:H2'	2.20	0.57
51:9:1117:C:O2'	51:9:1118:C:O4'	2.23	0.57
22:W:80:ARG:NH2	58:GG:129:VAL:O	2.38	0.57
12:M:97:ALA:HB2	14:O:203:VAL:HB	1.86	0.57
64:MM:17:ALA:C	64:MM:124:ILE:HD11	2.25	0.56
51:9:1444:U:P	68:QQ:15:ARG:HH22	2.28	0.56
46:2:74:C:OP2	48:5:4548:A:H2'	2.04	0.56
46:2:16:C:O4'	46:2:16:C:O2	2.24	0.56
51:9:945:U:H2'	51:9:946:U:C6	2.40	0.56
48:5:2007:G:O2'	48:5:2012:A:N6	2.39	0.56
48:5:3712:A:C2	51:9:970:G:C5	2.94	0.56
48:5:77:U:N3	48:5:336:A:N6	2.44	0.56
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	1.88	0.56
48:5:1974:U:C4	48:5:2002:A:N6	2.73	0.56
48:5:3810:C:O4'	48:5:3810:C:O2	2.23	0.56
61:JJ:136:ARG:HD3	61:JJ:160:SER:HA	1.87	0.56
51:9:830:A:N1	51:9:844:U:O4	2.40	0.55
48:5:245:C:O4'	48:5:245:C:O2	2.24	0.55
48:5:1483:C:O2	48:5:1483:C:O4'	2.23	0.55
48:5:2505:C:O4'	48:5:2505:C:O2	2.24	0.55
48:5:4699:U:C4	48:5:4701:A:N6	2.75	0.55
48:5:1974:U:N3	48:5:2002:A:C5	2.73	0.55
51:9:501:C:O2	51:9:501:C:H2'	2.06	0.55
64:MM:33:ARG:NH2	64:MM:91:LEU:HD21	2.22	0.55
61:JJ:35:TYR:CD2	61:JJ:106:LEU:HD23	2.42	0.55
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.89	0.54
51:9:1139:C:O4'	51:9:1139:C:O2	2.25	0.54
51:9:853:C:O2	51:9:853:C:O4'	2.26	0.54
64:MM:22:LEU:HD21	64:MM:89:VAL:HG23	1.89	0.54
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.90	0.54
48:5:4887:C:H6	48:5:4887:C:C5'	2.21	0.54
51:9:94:G:HO2'	51:9:508:A:HO2'	1.52	0.54
56:EE:139:LEU:HD12	56:EE:150:PRO:CB	2.38	0.54
60:II:190:LEU:HD12	60:II:194:GLU:HB3	1.89	0.54
53:BB:82:ARG:NH1	53:BB:189:ILE:O	2.40	0.53
57:FF:92:ILE:HD13	57:FF:169:ILE:HG21	1.90	0.53
48:5:2627:C:O4'	48:5:2627:C:O2	2.25	0.53
51:9:92:A:O4'	56:EE:3:ARG:NH1	2.42	0.53
48:5:4723:A:C2	48:5:4724:A:C6	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1130:G:N3	51:9:1130:G:H2'	2.24	0.53
51:9:1315:U:O2	51:9:1315:U:O4'	2.27	0.53
75:XX:51:VAL:HG13	75:XX:70:VAL:CG1	2.39	0.53
51:9:1444:U:H2'	51:9:1445:U:C6	2.43	0.53
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.42	0.53
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.39	0.53
57:FF:99:ILE:HG23	77:ZZ:67:LEU:HD21	1.90	0.53
48:5:4989:U:O4'	48:5:4989:U:O2	2.28	0.52
51:9:17:C:O2'	51:9:1194:A:N1	2.40	0.52
74:WW:6:VAL:HG13	74:WW:29:PRO:HB2	1.90	0.52
77:ZZ:50:PHE:CE2	77:ZZ:83:LEU:HD11	2.44	0.52
48:5:498:C:O2	48:5:498:C:O4'	2.27	0.52
56:EE:137:PRO:HB2	56:EE:150:PRO:HD2	1.90	0.52
51:9:501:C:O2	51:9:501:C:C2'	2.57	0.52
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.91	0.52
5:E:159:ARG:NH1	48:5:4940:C:OP1	2.42	0.52
64:MM:101:ARG:HA	64:MM:101:ARG:NE	2.25	0.52
54:CC:261:PHE:HB2	73:VV:52:THR:HG21	1.91	0.52
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.91	0.52
51:9:531:A:H3'	51:9:532:C:H5"	1.90	0.52
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.92	0.52
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.52
51:9:1364:U:O4'	51:9:1364:U:O2	2.28	0.52
51:9:94:G:O2'	51:9:508:A:O2'	2.24	0.52
51:9:1137:U:H3	51:9:1148:A:N6	2.07	0.51
51:9:4:C:O2'	61:JJ:18:ARG:NH1	2.43	0.51
75:XX:84:PHE:HB2	75:XX:118:VAL:HG11	1.90	0.51
48:5:1168:G:C2	48:5:1194:G:O6	2.63	0.51
48:5:224:U:O4'	48:5:224:U:O2	2.28	0.51
18:S:164:LYS:HB3	18:S:165:PRO:HD3	1.93	0.51
50:8:125:C:O2	50:8:125:C:O4'	2.28	0.51
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.92	0.50
21:V:99:GLU:HB3	22:W:24:THR:HG23	1.92	0.50
48:5:2763:U:O2	48:5:2763:U:O4'	2.29	0.50
76:YY:25:ILE:HD11	76:YY:44:LEU:HD21	1.93	0.50
64:MM:49:LEU:HB3	64:MM:111:VAL:CG2	2.42	0.50
51:9:17:C:H2'	51:9:18:C:C6	2.47	0.50
45:1:66:LEU:HD12	48:5:3908:A:C2	2.46	0.50
48:5:2013:A:N3	48:5:2014:C:C6	2.80	0.50
17:R:163:ARG:NH1	51:9:871:U:C4	2.79	0.50
51:9:1109:C:H42	69:RR:126:MET:HB3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1237:C:O2	48:5:1237:C:O4'	2.29	0.50
47:3:76:A:C2	48:5:4370:G:C6	2.99	0.49
48:5:1974:U:C2	48:5:2002:A:N7	2.80	0.49
48:5:2409:U:O4	48:5:2783:A:N1	2.46	0.49
51:9:1835:A:HO2'	51:9:1836:G:P	2.36	0.49
51:9:823:U:O2	51:9:823:U:O4'	2.30	0.49
51:9:1118:C:H2'	51:9:1119:A:C8	2.47	0.49
51:9:872:A:N6	51:9:914:U:C4	2.81	0.49
51:9:1130:G:HO2'	51:9:1131:G:C5'	2.26	0.49
62:KK:35:LEU:HD13	62:KK:40:VAL:HG21	1.95	0.49
69:RR:98:VAL:HG21	69:RR:117:LEU:HD22	1.94	0.48
48:5:1986:U:C2	48:5:2006:U:C4	2.72	0.48
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.43	0.48
48:5:1174:G:C2'	48:5:1175:A:O5'	2.61	0.48
51:9:399:C:O2	63:LL:106:HIS:ND1	2.46	0.48
67:PP:15:PHE:CE1	67:PP:109:PRO:HB3	2.48	0.48
48:5:1175:A:C2	48:5:1187:G:N7	2.82	0.48
51:9:943:U:H2'	51:9:944:A:O4'	2.13	0.48
54:CC:130:ILE:HG22	54:CC:158:ALA:HB1	1.95	0.48
51:9:302:A:H1'	60:II:73:THR:HG23	1.95	0.48
51:9:1438:A:C2	51:9:1439:A:C6	3.02	0.48
2:B:252:ALA:HB1	48:5:4524:G:N3	2.28	0.48
60:II:36:THR:HG21	60:II:179:PRO:HB2	1.94	0.48
51:9:1395:C:H2'	51:9:1396:A:N3	2.29	0.48
51:9:302:A:H1'	60:II:73:THR:CG2	2.43	0.48
51:9:872:A:N6	51:9:914:U:C5	2.82	0.48
57:FF:88:MET:HE1	57:FF:92:ILE:HD11	1.95	0.48
61:JJ:114:VAL:HG21	61:JJ:135:ILE:CD1	2.44	0.48
74:WW:52:ILE:HG22	74:WW:61:ILE:HG12	1.96	0.48
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.44	0.47
51:9:690:G:O5'	51:9:690:G:H8	1.97	0.47
51:9:979:C:C4	51:9:980:A:N7	2.82	0.47
59:HH:27:LEU:HD13	59:HH:45:ILE:HD13	1.95	0.47
66:OO:98:ARG:NH1	66:OO:99:ALA:O	2.47	0.47
10:J:64:ARG:HD3	46:2:56:C:O4'	2.13	0.47
17:R:176:ARG:NH1	51:9:909:G:OP1	2.46	0.47
63:LL:101:ARG:HB2	75:XX:10:ALA:HB2	1.96	0.47
48:5:4579:U:H2'	48:5:4580:U:C6	2.48	0.47
48:5:4724:A:C6	48:5:4725:C:C4	3.03	0.47
51:9:1129:G:C6	51:9:1130:G:O6	2.67	0.47
51:9:1551:U:O2	51:9:1551:U:O4'	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:MM:90:GLY:HA2	64:MM:93:LYS:HG3	1.94	0.47
48:5:1381:U:O4'	48:5:1381:U:O2	2.29	0.47
51:9:1520:G:N3	51:9:1520:G:H2'	2.30	0.47
54:CC:137:VAL:HG21	54:CC:244:ILE:HD12	1.97	0.47
8:H:105:ILE:CD1	8:H:136:VAL:HG23	2.45	0.47
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.45	0.47
57:FF:71:ARG:HG2	57:FF:151:ILE:HD13	1.96	0.47
45:1:57:ARG:NH2	48:5:3862:A:O2'	2.47	0.47
14:O:72:HIS:N	48:5:4586:G:OP1	2.44	0.47
51:9:1834:A:C2	51:9:1836:G:C4	3.03	0.47
57:FF:151:ILE:O	57:FF:155:CYS:HB2	2.15	0.47
48:5:2007:G:N3	48:5:2013:A:N6	2.62	0.47
48:5:4699:U:N3	48:5:4701:A:C6	2.83	0.47
51:9:944:A:C5	51:9:945:U:C5	3.03	0.47
10:J:27:GLY:HA2	10:J:68:ILE:HG23	1.95	0.47
63:LL:104:LYS:O	75:XX:11:ARG:NH2	2.48	0.47
74:WW:75:ILE:HD11	74:WW:93:LEU:HD11	1.97	0.47
48:5:3712:A:N1	51:9:970:G:C6	2.83	0.47
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.48	0.47
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.97	0.47
14:O:12:ARG:O	18:S:171:ARG:NH2	2.48	0.47
10:J:33:LEU:HD21	10:J:70:VAL:HB	1.96	0.47
48:5:1194:G:C2	48:5:1195:G:H1'	2.51	0.46
12:M:112:VAL:HG11	14:O:201:LEU:HD11	1.96	0.46
51:9:1143:A:C2	51:9:1144:A:C2	3.03	0.46
48:5:1301:C:O2	48:5:1301:C:O4'	2.33	0.46
5:E:95:VAL:CG2	5:E:112:LEU:HD21	2.45	0.46
68:QQ:49:TYR:O	68:QQ:53:GLU:N	2.48	0.46
48:5:4942:C:H4'	48:5:4943:A:OP1	2.16	0.46
51:9:1095:U:O2	51:9:1151:G:N2	2.49	0.46
51:9:183:G:N3	51:9:183:G:O2'	2.48	0.46
48:5:1563:A:O2'	48:5:1564:A:O4'	2.34	0.46
48:5:77:U:C4	48:5:336:A:N1	2.80	0.46
51:9:1624:U:O2	51:9:1624:U:O4'	2.32	0.46
51:9:1303:C:O2	51:9:1303:C:O4'	2.31	0.46
68:QQ:51:LEU:HD22	68:QQ:84:ILE:HD11	1.98	0.46
68:QQ:34:VAL:HG21	68:QQ:84:ILE:HD12	1.97	0.46
2:B:324:GLY:HA2	48:5:5051:C:H4'	1.96	0.46
51:9:1336:C:H2'	51:9:1337:C:O4'	2.16	0.46
64:MM:19:GLN:NE2	64:MM:19:GLN:HA	2.30	0.46
64:MM:36:ARG:CZ	64:MM:40:LYS:HZ1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:164:LYS:HB3	18:S:165:PRO:CD	2.46	0.46
60:II:60:LEU:HD23	60:II:185:ALA:HB2	1.98	0.46
51:9:1489:A:H4'	51:9:1490:G:OP2	2.16	0.46
1:A:207:VAL:HG12	48:5:3919:C:H5''	1.98	0.46
51:9:146:G:O2'	51:9:147:A:O5'	2.29	0.45
51:9:1834:A:N3	51:9:1834:A:H2'	2.31	0.45
51:9:1568:C:OP1	71:TT:96:SER:OG	2.32	0.45
53:BB:189:ILE:HB	53:BB:190:PRO:CD	2.47	0.45
59:HH:170:VAL:HG13	59:HH:187:PHE:HB2	1.99	0.45
64:MM:121:LYS:HA	64:MM:124:ILE:HD12	1.99	0.45
75:XX:81:ILE:CG2	75:XX:120:PHE:CD1	3.00	0.45
46:2:53:G:C2	46:2:62:C:C2	3.05	0.45
48:5:4758:U:O2	48:5:4758:U:O4'	2.34	0.45
48:5:77:U:O4	48:5:336:A:C2	2.69	0.45
51:9:1401:A:C2	51:9:1402:A:N1	2.85	0.45
58:GG:162:LEU:HD11	58:GG:172:LYS:HB2	1.98	0.45
60:II:194:GLU:HA	63:LL:10:TYR:CE2	2.52	0.45
54:CC:94:ILE:HG13	54:CC:162:ILE:HD11	1.98	0.45
64:MM:36:ARG:NH1	64:MM:40:LYS:HZ1	2.14	0.45
17:R:173:ARG:NH2	51:9:910:G:OP2	2.50	0.45
51:9:1531:A:H2'	51:9:1532:C:C6	2.51	0.45
51:9:953:C:H2'	51:9:954:U:O4'	2.16	0.45
51:9:1407:U:H2'	51:9:1408:U:H6	1.66	0.45
57:FF:102:LEU:HD22	77:ZZ:110:THR:HG21	1.98	0.45
47:3:76:A:C6	48:5:4370:G:C5	3.05	0.45
55:DD:72:VAL:HG23	62:KK:20:VAL:HG21	1.99	0.45
24:Y:55:VAL:HG13	24:Y:104:VAL:HG13	1.99	0.45
17:R:71:ARG:NH1	48:5:3605:C:OP2	2.50	0.45
51:9:183:G:N3	51:9:183:G:C2'	2.79	0.45
48:5:1990:A:H3'	48:5:1991:A:H5''	1.99	0.44
51:9:434:G:H2'	51:9:435:A:C8	2.52	0.44
19:T:80:VAL:HG21	48:5:4305:G:C6	2.52	0.44
59:HH:30:LEU:HD22	59:HH:82:GLU:HG2	1.99	0.44
48:5:2007:G:H5''	48:5:2007:G:H8	1.82	0.44
48:5:2007:G:N2	48:5:2013:A:H62	2.15	0.44
53:BB:134:LEU:CD2	53:BB:218:LEU:HD12	2.47	0.44
48:5:921:C:O2'	48:5:922:C:C5'	2.65	0.44
56:EE:11:ARG:HH22	56:EE:24:THR:HG1	1.61	0.44
66:OO:34:PHE:HB3	66:OO:41:PHE:HB2	2.00	0.44
75:XX:81:ILE:HG21	75:XX:120:PHE:CD1	2.52	0.44
48:5:1974:U:O2	48:5:2002:A:C8	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1518:C:O5'	51:9:1518:C:O2	2.35	0.44
51:9:831:G:N2	51:9:844:U:O2	2.50	0.44
48:5:4119:C:O4'	48:5:4119:C:O2	2.35	0.44
48:5:921:C:O2'	48:5:922:C:H5'	2.18	0.44
51:9:1207:G:C6	51:9:1837:G:C6	3.06	0.44
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	2.00	0.44
48:5:1973:G:C2	48:5:2002:A:N6	2.86	0.43
48:5:2367:A:C2	48:5:2788:U:O4	2.59	0.43
54:CC:191:VAL:HG11	54:CC:236:PHE:HA	2.00	0.43
51:9:314:U:H2'	51:9:314:U:O2	2.18	0.43
46:2:33:U:OP2	68:QQ:146:ARG:NH2	2.52	0.43
48:5:3876:A:HO2'	48:5:3877:A:P	2.42	0.43
48:5:4887:C:H6	48:5:4887:C:H5''	1.81	0.43
64:MM:19:GLN:HE21	64:MM:19:GLN:HA	1.83	0.43
48:5:1173:G:C6	48:5:1174:G:C6	3.07	0.43
51:9:1274:G:N7	62:KK:43:LEU:HD13	2.33	0.43
51:9:407:G:H3'	51:9:408:A:C5'	2.47	0.43
53:BB:189:ILE:CB	53:BB:190:PRO:CD	2.96	0.43
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.81	0.43
62:KK:40:VAL:HG23	62:KK:40:VAL:O	2.18	0.43
64:MM:19:GLN:CA	64:MM:19:GLN:HE21	2.32	0.43
64:MM:42:LEU:HG	64:MM:74:ILE:HD13	2.00	0.43
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.48	0.43
51:9:427:U:O4'	51:9:427:U:O2	2.34	0.43
48:5:496:G:C4	48:5:659:G:N2	2.87	0.43
51:9:1035:A:H2'	51:9:1036:A:O4'	2.17	0.43
51:9:92:A:C6	51:9:446:G:C6	3.06	0.43
56:EE:132:GLY:N	56:EE:136:ILE:O	2.51	0.43
57:FF:41:VAL:HG11	57:FF:113:VAL:HG21	2.00	0.43
53:BB:52:THR:HG23	53:BB:57:ILE:HA	2.00	0.43
18:S:161:ARG:HG3	18:S:161:ARG:O	2.19	0.43
48:5:1773:U:C5	48:5:1774:C:C5	3.07	0.43
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.54	0.43
51:9:1089:G:C6	51:9:1090:C:C4	3.07	0.43
51:9:584:A:C6	51:9:585:C:C4	3.07	0.43
51:9:846:G:OP2	56:EE:108:ARG:NH1	2.51	0.43
51:9:910:G:C2	51:9:911:C:C2	3.07	0.43
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	2.00	0.43
64:MM:18:LEU:N	64:MM:124:ILE:HD11	2.34	0.43
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.53	0.43
48:5:2094:C:O2	48:5:2094:C:O4'	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.99	0.43
62:KK:71:LEU:HD21	62:KK:79:LEU:HD12	2.01	0.43
48:5:4942:C:H3'	48:5:4942:C:O2	2.19	0.42
51:9:1395:C:H2'	51:9:1396:A:O4'	2.19	0.42
51:9:488:U:O2	51:9:488:U:O4'	2.34	0.42
51:9:872:A:C2	51:9:914:U:O4	2.70	0.42
11:L:18:TRP:CE3	13:N:198:LEU:HD12	2.54	0.42
14:O:23:VAL:HG13	14:O:33:VAL:HG11	2.00	0.42
56:EE:125:LYS:HA	56:EE:159:THR:HG22	2.01	0.42
60:II:194:GLU:HG2	63:LL:10:TYR:CD1	2.54	0.42
48:5:1773:U:C4	48:5:1774:C:C4	3.08	0.42
48:5:4423:U:O4'	48:5:4423:U:O2	2.38	0.42
51:9:1220:A:N6	51:9:1221:G:C6	2.88	0.42
56:EE:163:ASP:HB3	56:EE:166:THR:HG22	2.01	0.42
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.48	0.42
51:9:1120:U:H2'	51:9:1121:G:H8	1.85	0.42
51:9:1666:C:H2'	51:9:1667:U:O4'	2.19	0.42
53:BB:87:ILE:HG23	53:BB:101:HIS:CG	2.54	0.42
7:G:317:LYS:HD2	53:BB:225:LEU:HB3	2.02	0.42
13:N:89:VAL:HG13	48:5:3928:A:H5'	2.01	0.42
5:E:165:VAL:HG11	5:E:178:VAL:HG13	2.00	0.42
21:V:26:ILE:HG22	21:V:101:ASN:HB3	2.00	0.42
51:9:1293:A:N6	51:9:1294:G:C6	2.88	0.42
64:MM:22:LEU:C	64:MM:22:LEU:HD13	2.40	0.42
67:PP:37:TYR:OH	67:PP:45:LEU:HD11	2.20	0.42
51:9:1046:U:H2'	51:9:1047:C:O4'	2.20	0.42
51:9:1445:U:O4	51:9:1446:A:N6	2.53	0.42
51:9:1834:A:N3	51:9:1834:A:C2'	2.82	0.42
51:9:962:A:N1	51:9:1055:A:O2'	2.53	0.42
55:DD:21:LEU:CD2	55:DD:48:ILE:HD11	2.50	0.42
6:F:89:ALA:HB2	6:F:124:LEU:HD21	2.01	0.42
57:FF:116:ILE:HD12	57:FF:151:ILE:HG13	2.02	0.42
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	2.01	0.42
14:O:84:VAL:HG11	14:O:102:LEU:HD22	2.01	0.42
51:9:1488:C:O2'	51:9:1490:G:OP2	2.36	0.42
51:9:168:C:OP1	58:GG:131:ARG:NH2	2.53	0.42
51:9:944:A:C2	51:9:983:A:C2	3.07	0.42
53:BB:189:ILE:HB	53:BB:190:PRO:HD2	2.02	0.42
59:HH:51:ILE:HD11	59:HH:176:VAL:HG22	2.02	0.42
47:3:10:G:N2	47:3:11:C:C2	2.88	0.42
51:9:1535:U:O2	51:9:1535:U:H2'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1619:A:OP2	67:PP:47:ARG:NH1	2.49	0.42
53:BB:189:ILE:CG2	53:BB:190:PRO:HD3	2.49	0.42
3:C:150:LEU:HB3	3:C:151:PRO:HD3	2.01	0.42
56:EE:147:ILE:HD11	56:EE:162:ILE:CG2	2.50	0.42
57:FF:125:SER:OG	57:FF:136:ARG:NH2	2.53	0.42
55:DD:11:PHE:CE2	72:UU:84:ILE:HD11	2.55	0.42
55:DD:11:PHE:CZ	72:UU:84:ILE:HD11	2.55	0.42
48:5:1563:A:N7	51:9:678:U:O4'	2.54	0.41
48:5:1973:G:N1	48:5:2002:A:N6	2.69	0.41
7:G:98:ILE:HG21	48:5:4125:C:H4'	2.03	0.41
51:9:1438:A:C2	51:9:1439:A:C2	3.08	0.41
51:9:1719:A:N6	51:9:1814:G:O2'	2.53	0.41
52:AA:180:ARG:HG2	52:AA:195:TRP:CE3	2.55	0.41
51:9:1228:A:H2'	51:9:1229:G:C8	2.55	0.41
51:9:190:G:H5''	60:II:145:ILE:CD1	2.49	0.41
3:C:232:VAL:HG12	3:C:263:LEU:CD1	2.50	0.41
56:EE:105:THR:HG23	56:EE:106:LYS:HD2	2.01	0.41
48:5:1174:G:H2'	48:5:1175:A:O5'	2.21	0.41
48:5:1818:G:O2'	48:5:1819:G:OP1	2.31	0.41
51:9:1374:C:H2'	51:9:1375:G:O4'	2.19	0.41
51:9:1412:C:H6	51:9:1412:C:C5'	2.33	0.41
1:A:11:GLY:O	48:5:3675:G:N2	2.51	0.41
48:5:4305:G:N3	48:5:4305:G:C2'	2.84	0.41
51:9:1520:G:N3	51:9:1520:G:C2'	2.83	0.41
51:9:688:U:HO2'	51:9:689:U:P	2.32	0.41
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.56	0.41
2:B:77:THR:HG21	2:B:337:VAL:HG22	2.03	0.41
58:GG:121:ILE:HG13	58:GG:122:PRO:HD2	2.02	0.41
51:9:1409:A:H5'	51:9:1410:C:OP2	2.20	0.41
51:9:830:A:H2'	51:9:831:G:O4'	2.19	0.41
52:AA:145:ILE:HG12	52:AA:159:ILE:CG2	2.51	0.41
65:NN:54:LEU:HB3	65:NN:60:VAL:HG13	2.02	0.41
51:9:1045:U:H2'	51:9:1046:U:O4'	2.21	0.41
51:9:1518:C:O2	51:9:1518:C:O4'	2.38	0.41
48:5:3629:A:H1'	51:9:1721:U:O2	2.19	0.41
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	2.03	0.41
16:Q:78:LYS:HG2	16:Q:137:VAL:HG23	2.03	0.41
51:9:1674:G:N7	68:QQ:17:LYS:NZ	2.60	0.41
51:9:455:A:O2'	51:9:1735:A:N3	2.40	0.41
55:DD:48:ILE:HG23	55:DD:86:LEU:HD12	2.03	0.41
56:EE:31:PRO:HG2	56:EE:38:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:88:LEU:HD22	6:F:89:ALA:N	2.36	0.41
7:G:215:ASP:HB3	7:G:216:PRO:HD3	2.02	0.41
71:TT:39:LEU:HD11	71:TT:52:TRP:CZ3	2.55	0.41
48:5:4895:C:O2	48:5:4895:C:C2'	2.69	0.40
64:MM:33:ARG:HH22	64:MM:89:VAL:HG21	1.86	0.40
48:5:2013:A:C2	48:5:2014:C:C6	3.09	0.40
51:9:668:A:N1	51:9:1143:A:C5	2.89	0.40
51:9:958:G:H2'	51:9:959:G:O4'	2.22	0.40
53:BB:133:TYR:CE2	53:BB:181:LEU:HD12	2.56	0.40
57:FF:99:ILE:HD13	57:FF:171:GLU:HA	2.03	0.40
57:FF:39:ILE:HG23	57:FF:68:ILE:HG21	2.02	0.40
12:M:112:VAL:CG1	14:O:201:LEU:HD11	2.51	0.40
54:CC:261:PHE:CB	73:VV:52:THR:HG21	2.50	0.40
74:WW:28:ARG:CB	74:WW:29:PRO:HD3	2.51	0.40
48:5:1563:A:C8	51:9:678:U:C4'	3.04	0.40
51:9:415:A:H2'	51:9:416:U:O4'	2.21	0.40
17:R:163:ARG:NH1	51:9:871:U:C5	2.90	0.40
1:A:234:LYS:HG2	1:A:238:ILE:HD12	2.03	0.40
4:D:41:LYS:NZ	19:T:30:TYR:O	2.39	0.40
48:5:3723:A:C2	48:5:3724:A:C6	3.09	0.40
51:9:412:G:O2'	51:9:812:A:N6	2.54	0.40
64:MM:99:LYS:HD3	64:MM:100:PRO:HD2	2.03	0.40
71:TT:18:LEU:HB3	71:TT:58:ALA:HB1	2.02	0.40
74:WW:55:ASP:O	74:WW:57:ARG:N	2.55	0.40
48:5:747:A:H4'	48:5:748:G:OP1	2.22	0.40
51:9:1439:A:C6	51:9:1440:C:C4	3.10	0.40
67:PP:52:LYS:HE3	67:PP:80:LEU:HD21	2.03	0.40
70:SS:3:LEU:HB3	77:ZZ:50:PHE:CD2	2.56	0.40
70:SS:15:VAL:HG22	70:SS:68:ILE:HD11	2.04	0.40
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	2.03	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%)	21 (8%)	1 (0%)	39	78
2	B	392/403 (97%)	365 (93%)	26 (7%)	1 (0%)	46	82
3	C	360/425 (85%)	339 (94%)	21 (6%)	0	100	100
4	D	291/297 (98%)	277 (95%)	14 (5%)	0	100	100
5	E	208/291 (72%)	193 (93%)	15 (7%)	0	100	100
6	F	223/247 (90%)	213 (96%)	9 (4%)	1 (0%)	39	78
7	G	229/319 (72%)	220 (96%)	9 (4%)	0	100	100
8	H	188/192 (98%)	177 (94%)	11 (6%)	0	100	100
9	I	201/214 (94%)	184 (92%)	17 (8%)	0	100	100
10	J	168/178 (94%)	160 (95%)	8 (5%)	0	100	100
11	L	208/211 (99%)	201 (97%)	7 (3%)	0	100	100
12	M	136/218 (62%)	128 (94%)	8 (6%)	0	100	100
13	N	201/204 (98%)	189 (94%)	12 (6%)	0	100	100
14	O	197/203 (97%)	184 (93%)	13 (7%)	0	100	100
15	P	151/184 (82%)	141 (93%)	10 (7%)	0	100	100
16	Q	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
17	R	178/196 (91%)	173 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	164 (94%)	10 (6%)	0	100	100
19	T	157/160 (98%)	150 (96%)	7 (4%)	0	100	100
20	U	97/128 (76%)	86 (89%)	11 (11%)	0	100	100
21	V	129/140 (92%)	115 (89%)	14 (11%)	0	100	100
22	W	102/157 (65%)	97 (95%)	5 (5%)	0	100	100
23	X	116/156 (74%)	107 (92%)	9 (8%)	0	100	100
24	Y	132/145 (91%)	123 (93%)	9 (7%)	0	100	100
25	Z	133/136 (98%)	127 (96%)	4 (3%)	2 (2%)	13	51
26	a	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
27	b	100/245 (41%)	93 (93%)	5 (5%)	2 (2%)	9	45
28	c	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
29	d	105/125 (84%)	95 (90%)	10 (10%)	0	100	100
30	e	126/135 (93%)	118 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	f	107/110 (97%)	101 (94%)	4 (4%)	2 (2%)	10	46
32	g	112/117 (96%)	106 (95%)	6 (5%)	0	100	100
33	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	i	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
35	j	84/97 (87%)	78 (93%)	5 (6%)	1 (1%)	16	56
36	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
38	m	50/102 (49%)	47 (94%)	3 (6%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	99 (97%)	3 (3%)	0	100	100
41	p	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
42	r	122/137 (89%)	114 (93%)	7 (6%)	1 (1%)	24	65
43	s	194/318 (61%)	176 (91%)	16 (8%)	2 (1%)	19	60
44	t	151/165 (92%)	136 (90%)	13 (9%)	2 (1%)	15	54
45	1	13/15 (87%)	8 (62%)	4 (31%)	1 (8%)	1	10
52	AA	215/295 (73%)	201 (94%)	13 (6%)	1 (0%)	34	74
53	BB	211/264 (80%)	201 (95%)	9 (4%)	1 (0%)	34	74
54	CC	219/293 (75%)	209 (95%)	10 (5%)	0	100	100
55	DD	226/243 (93%)	214 (95%)	9 (4%)	3 (1%)	15	54
56	EE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
57	FF	181/204 (89%)	171 (94%)	10 (6%)	0	100	100
58	GG	235/249 (94%)	221 (94%)	14 (6%)	0	100	100
59	HH	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
60	II	204/208 (98%)	195 (96%)	8 (4%)	1 (0%)	34	74
61	JJ	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
62	KK	94/165 (57%)	88 (94%)	6 (6%)	0	100	100
63	LL	139/158 (88%)	127 (91%)	12 (9%)	0	100	100
64	MM	115/132 (87%)	104 (90%)	11 (10%)	0	100	100
65	NN	147/151 (97%)	140 (95%)	7 (5%)	0	100	100
66	OO	134/168 (80%)	122 (91%)	11 (8%)	1 (1%)	26	68
67	PP	118/145 (81%)	108 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	QQ	140/146 (96%)	131 (94%)	9 (6%)	0	100	100
69	RR	130/135 (96%)	120 (92%)	10 (8%)	0	100	100
70	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
71	TT	139/145 (96%)	132 (95%)	7 (5%)	0	100	100
72	UU	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
73	VV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
74	WW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
75	XX	139/143 (97%)	130 (94%)	6 (4%)	3 (2%)	8	43
76	YY	122/130 (94%)	113 (93%)	9 (7%)	0	100	100
77	ZZ	73/125 (58%)	68 (93%)	5 (7%)	0	100	100
78	aa	99/115 (86%)	93 (94%)	6 (6%)	0	100	100
79	bb	81/84 (96%)	71 (88%)	9 (11%)	1 (1%)	16	56
80	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
81	dd	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
82	ee	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
83	ff	66/156 (42%)	61 (92%)	5 (8%)	0	100	100
84	gg	311/317 (98%)	290 (93%)	20 (6%)	1 (0%)	46	82
86	ii	417/459 (91%)	404 (97%)	12 (3%)	1 (0%)	52	86
87	jj	571/599 (95%)	538 (94%)	32 (6%)	1 (0%)	52	86
All	All	12520/14448 (87%)	11763 (94%)	727 (6%)	30 (0%)	56	86

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
75	XX	62	PRO
86	ii	182	ARG
43	s	142	GLY
44	t	125	LEU
52	AA	159	ILE
66	OO	20	GLN
75	XX	61	GLN
1	A	234	LYS
25	Z	91	LEU
27	b	102	PRO
53	BB	225	LEU

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Mol	Chain	Res	Type
55	DD	48	ILE
75	XX	86	PRO
2	B	17	LEU
31	f	106	TYR
44	t	54	LYS
25	Z	90	PRO
27	b	29	TYR
43	s	25	PRO
55	DD	44	THR
79	bb	81	ARG
87	jj	24	GLU
42	r	11	ARG
55	DD	93	THR
84	gg	61	GLY
45	l	64	PRO
6	F	196	VAL
35	j	38	GLY
31	f	107	PRO
60	II	3	ILE

### 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%)	178 (94%)	12 (6%)	22	61
2	B	342/348 (98%)	326 (95%)	16 (5%)	32	71
3	C	302/347 (87%)	290 (96%)	12 (4%)	38	74
4	D	247/250 (99%)	239 (97%)	8 (3%)	46	80
5	E	190/251 (76%)	181 (95%)	9 (5%)	32	71
6	F	196/215 (91%)	187 (95%)	9 (5%)	33	71
7	G	200/272 (74%)	189 (94%)	11 (6%)	27	65
8	H	169/171 (99%)	157 (93%)	12 (7%)	18	56
9	I	175/181 (97%)	167 (95%)	8 (5%)	33	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	143/149 (96%)	138 (96%)	5 (4%)	43	77
11	L	175/176 (99%)	168 (96%)	7 (4%)	38	74
12	M	117/161 (73%)	111 (95%)	6 (5%)	29	67
13	N	171/172 (99%)	162 (95%)	9 (5%)	28	66
14	O	171/173 (99%)	163 (95%)	8 (5%)	32	71
15	P	134/163 (82%)	125 (93%)	9 (7%)	20	59
16	Q	164/165 (99%)	157 (96%)	7 (4%)	35	73
17	R	159/175 (91%)	148 (93%)	11 (7%)	19	58
18	S	157/157 (100%)	149 (95%)	8 (5%)	29	67
19	T	139/140 (99%)	127 (91%)	12 (9%)	13	46
20	U	89/114 (78%)	88 (99%)	1 (1%)	80	91
21	V	101/107 (94%)	93 (92%)	8 (8%)	15	50
22	W	86/126 (68%)	85 (99%)	1 (1%)	78	90
23	X	106/134 (79%)	101 (95%)	5 (5%)	32	71
24	Y	124/135 (92%)	118 (95%)	6 (5%)	31	70
25	Z	117/118 (99%)	115 (98%)	2 (2%)	68	87
26	a	119/120 (99%)	116 (98%)	3 (2%)	55	83
27	b	84/184 (46%)	82 (98%)	2 (2%)	57	84
28	c	84/98 (86%)	82 (98%)	2 (2%)	57	84
29	d	98/110 (89%)	90 (92%)	8 (8%)	14	48
30	e	114/121 (94%)	106 (93%)	8 (7%)	19	57
31	f	88/89 (99%)	84 (96%)	4 (4%)	34	72
32	g	98/100 (98%)	94 (96%)	4 (4%)	37	74
33	h	109/110 (99%)	105 (96%)	4 (4%)	41	76
34	i	86/89 (97%)	83 (96%)	3 (4%)	43	77
35	j	73/80 (91%)	69 (94%)	4 (6%)	27	65
36	k	64/65 (98%)	62 (97%)	2 (3%)	47	80
37	l	47/48 (98%)	46 (98%)	1 (2%)	61	85
38	m	48/90 (53%)	46 (96%)	2 (4%)	36	73
39	n	24/24 (100%)	22 (92%)	2 (8%)	14	48
40	o	92/94 (98%)	89 (97%)	3 (3%)	45	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	p	74/75 (99%)	72 (97%)	2 (3%)	52	82
42	r	108/121 (89%)	105 (97%)	3 (3%)	51	82
43	s	164/258 (64%)	156 (95%)	8 (5%)	31	69
44	t	126/137 (92%)	121 (96%)	5 (4%)	38	74
45	1	13/13 (100%)	13 (100%)	0	100	100
52	AA	180/245 (74%)	166 (92%)	14 (8%)	16	51
53	BB	194/231 (84%)	175 (90%)	19 (10%)	10	37
54	CC	187/225 (83%)	175 (94%)	12 (6%)	22	60
55	DD	190/202 (94%)	172 (90%)	18 (10%)	11	38
56	EE	224/225 (100%)	206 (92%)	18 (8%)	15	50
57	FF	158/170 (93%)	146 (92%)	12 (8%)	16	53
58	GG	207/218 (95%)	195 (94%)	12 (6%)	25	64
59	HH	165/174 (95%)	154 (93%)	11 (7%)	20	59
60	II	178/180 (99%)	164 (92%)	14 (8%)	15	50
61	JJ	161/168 (96%)	148 (92%)	13 (8%)	15	49
62	KK	87/136 (64%)	78 (90%)	9 (10%)	9	34
63	LL	130/142 (92%)	118 (91%)	12 (9%)	11	40
64	MM	99/108 (92%)	83 (84%)	16 (16%)	3	14
65	NN	130/131 (99%)	118 (91%)	12 (9%)	11	40
66	OO	106/130 (82%)	91 (86%)	15 (14%)	4	19
67	PP	109/130 (84%)	99 (91%)	10 (9%)	11	40
68	QQ	117/121 (97%)	111 (95%)	6 (5%)	29	67
69	RR	119/121 (98%)	111 (93%)	8 (7%)	20	59
70	SS	125/132 (95%)	111 (89%)	14 (11%)	7	30
71	TT	111/115 (96%)	101 (91%)	10 (9%)	12	42
72	UU	92/107 (86%)	86 (94%)	6 (6%)	21	60
73	VV	67/67 (100%)	65 (97%)	2 (3%)	48	80
74	WW	112/113 (99%)	106 (95%)	6 (5%)	27	66
75	XX	113/115 (98%)	107 (95%)	6 (5%)	28	66
76	YY	107/112 (96%)	96 (90%)	11 (10%)	9	34
77	ZZ	66/103 (64%)	63 (96%)	3 (4%)	34	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
78	aa	88/98 (90%)	78 (89%)	10 (11%)	7	29
79	bb	75/76 (99%)	70 (93%)	5 (7%)	20	59
80	cc	55/62 (89%)	51 (93%)	4 (7%)	17	54
81	dd	48/49 (98%)	48 (100%)	0	100	100
82	ee	46/106 (43%)	43 (94%)	3 (6%)	21	60
83	ff	61/140 (44%)	54 (88%)	7 (12%)	7	28
84	gg	272/275 (99%)	262 (96%)	10 (4%)	41	76
86	ii	361/394 (92%)	345 (96%)	16 (4%)	35	72
87	jj	509/526 (97%)	489 (96%)	20 (4%)	39	75
All	All	10926/12272 (89%)	10290 (94%)	636 (6%)	29	64

All (636) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	102	LEU
1	A	109	GLU
1	A	128	ARG
1	A	142	GLU
1	A	163	ARG
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	62	ARG
2	B	66	LYS
2	B	74	GLU
2	B	95	THR
2	B	135	LYS
2	B	248	LEU
2	B	261	ARG
2	B	262	VAL
2	B	294	LYS
2	B	309	LEU
2	B	314	ILE

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Mol	Chain	Res	Type
2	B	333	LEU
2	B	356	LYS
2	B	383	GLU
3	C	20	LYS
3	C	95	MET
3	C	113	ARG
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	175	LYS
3	C	188	ARG
3	C	193	LYS
3	C	281	MET
3	C	307	LYS
3	C	312	ARG
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	202	GLN
4	D	264	LYS
4	D	268	ARG
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	141	ARG
5	E	144	ARG
5	E	169	LYS
5	E	178	VAL
5	E	213	LYS
5	E	291	PHE
6	F	38	GLN
6	F	46	ARG
6	F	65	ARG
6	F	88	LEU
6	F	134	ILE
6	F	151	GLU
6	F	187	GLU
6	F	198	LYS
6	F	246	MET
7	G	126	ARG

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Mol	Chain	Res	Type
7	G	148	LEU
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	242	ARG
7	G	273	GLU
7	G	293	ASN
8	H	1	MET
8	H	20	LEU
8	H	23	ARG
8	H	52	LYS
8	H	54	ARG
8	H	59	LYS
8	H	66	GLU
8	H	105	ILE
8	H	106	GLN
8	H	108	ASN
8	H	128	MET
8	H	173	ARG
9	I	36	LEU
9	I	39	LYS
9	I	116	ARG
9	I	146	GLU
9	I	153	ARG
9	I	163	GLN
9	I	164	LYS
9	I	208	LYS
10	J	16	ARG
10	J	28	GLU
10	J	81	GLU
10	J	113	ILE
10	J	175	LEU
11	L	5	ARG
11	L	63	THR
11	L	67	HIS
11	L	74	ARG
11	L	121	ARG
11	L	162	LYS
11	L	186	ARG

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Mol	Chain	Res	Type
12	M	8	GLU
12	M	32	ASP
12	M	37	LEU
12	M	57	LEU
12	M	96	GLU
12	M	119	ARG
13	N	9	GLU
13	N	26	ARG
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	87	HIS
13	N	89	VAL
13	N	162	ARG
13	N	197	THR
14	O	74	ARG
14	O	82	ARG
14	O	128	ARG
14	O	130	LYS
14	O	145	VAL
14	O	175	MET
14	O	179	LYS
14	O	202	LEU
15	P	3	ARG
15	P	24	VAL
15	P	25	HIS
15	P	36	ILE
15	P	69	ARG
15	P	91	LEU
15	P	127	ARG
15	P	128	ARG
15	P	147	GLU
16	Q	61	LEU
16	Q	75	ARG
16	Q	91	ARG
16	Q	97	LYS
16	Q	115	LYS
16	Q	138	LEU
16	Q	143	ARG
17	R	8	LYS
17	R	36	ASN
17	R	50	ILE

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Mol	Chain	Res	Type
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	113	LYS
17	R	133	LYS
17	R	138	LEU
17	R	176	ARG
17	R	178	GLN
18	S	7	LEU
18	S	8	ARG
18	S	9	GLU
18	S	70	LYS
18	S	149	LYS
18	S	159	LEU
18	S	164	LYS
18	S	174	THR
19	T	5	LYS
19	T	33	ILE
19	T	60	LYS
19	T	80	VAL
19	T	96	ILE
19	T	117	LYS
19	T	118	GLU
19	T	142	ARG
19	T	144	ASN
19	T	146	LYS
19	T	157	GLU
19	T	159	MET
20	U	33	ILE
21	V	15	ARG
21	V	18	LEU
21	V	35	LYS
21	V	60	MET
21	V	91	LYS
21	V	99	GLU
21	V	109	LYS
21	V	123	LYS
22	W	91	MET
23	X	39	LYS
23	X	53	ARG
23	X	63	LYS
23	X	91	GLU

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Mol	Chain	Res	Type
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	50	ARG
24	Y	52	ASP
24	Y	72	GLN
24	Y	104	VAL
25	Z	33	THR
25	Z	112	ARG
26	a	4	ARG
26	a	84	GLU
26	a	132	ARG
27	b	40	LEU
27	b	101	HIS
28	c	37	MET
28	c	78	ASN
29	d	23	ARG
29	d	31	LYS
29	d	44	ARG
29	d	48	GLU
29	d	78	ARG
29	d	85	ARG
29	d	98	SER
29	d	102	LEU
30	e	21	ILE
30	e	22	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	91	CYS
30	e	106	LYS
30	e	128	ARG
31	f	16	ARG
31	f	23	GLU
31	f	52	LYS
31	f	101	ILE
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	114	GLN
33	h	15	GLU
33	h	28	LEU

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Mol	Chain	Res	Type
33	h	67	GLU
33	h	77	LYS
34	i	77	VAL
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	11	ARG
35	j	20	ARG
35	j	58	THR
36	k	69	LEU
36	k	70	LYS
37	l	49	LEU
38	m	71	ARG
38	m	93	ASN
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	36	GLN
40	o	82	MET
41	p	8	VAL
41	p	84	ARG
42	r	8	MET
42	r	32	LEU
42	r	67	ARG
43	s	33	ASP
43	s	34	ASN
43	s	38	LYS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	98	ILE
44	t	133	LEU
44	t	137	GLN
44	t	144	ASP
52	AA	5	LEU
52	AA	12	GLU
52	AA	46	ILE
52	AA	50	ASN
52	AA	56	GLU

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Mol	Chain	Res	Type
52	AA	58	LEU
52	AA	59	LEU
52	AA	60	LEU
52	AA	111	GLN
52	AA	132	GLN
52	AA	136	GLU
52	AA	155	ARG
52	AA	178	LEU
52	AA	198	MET
53	BB	38	MET
53	BB	63	LYS
53	BB	71	LEU
53	BB	74	LEU
53	BB	82	ARG
53	BB	105	LEU
53	BB	113	MET
53	BB	125	VAL
53	BB	157	GLN
53	BB	172	MET
53	BB	175	GLU
53	BB	181	LEU
53	BB	182	LYS
53	BB	184	VAL
53	BB	191	ASP
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	117	ARG
54	CC	121	ARG
54	CC	137	VAL
54	CC	167	ARG
54	CC	188	CYS
54	CC	213	LEU
54	CC	236	PHE
54	CC	240	THR
54	CC	248	TYR
54	CC	252	THR
55	DD	28	GLU
55	DD	31	GLU

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Mol	Chain	Res	Type
55	DD	45	ARG
55	DD	59	LEU
55	DD	64	ARG
55	DD	72	VAL
55	DD	76	ARG
55	DD	94	ARG
55	DD	106	ARG
55	DD	120	TYR
55	DD	127	MET
55	DD	142	LEU
55	DD	156	LEU
55	DD	190	LEU
55	DD	198	ILE
55	DD	218	LEU
55	DD	223	ILE
55	DD	227	LYS
56	EE	17	HIS
56	EE	23	LEU
56	EE	32	SER
56	EE	42	LEU
56	EE	51	ARG
56	EE	66	MET
56	EE	77	ARG
56	EE	88	ASP
56	EE	145	ARG
56	EE	162	ILE
56	EE	181	CYS
56	EE	205	PHE
56	EE	206	ASP
56	EE	222	LEU
56	EE	232	ASN
56	EE	238	LEU
56	EE	240	ARG
56	EE	246	LEU
57	FF	20	PHE
57	FF	43	GLU
57	FF	49	LEU
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	91	ARG
57	FF	95	HIS

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Mol	Chain	Res	Type
57	FF	124	ASP
57	FF	155	CYS
57	FF	169	ILE
57	FF	204	ARG
58	GG	41	LEU
58	GG	63	MET
58	GG	64	LYS
58	GG	67	VAL
58	GG	116	LYS
58	GG	137	ARG
58	GG	171	THR
58	GG	178	ARG
58	GG	183	ARG
58	GG	190	ARG
58	GG	216	ARG
58	GG	230	LYS
59	HH	8	ILE
59	HH	36	LEU
59	HH	53	VAL
59	HH	76	GLN
59	HH	79	LEU
59	HH	82	GLU
59	HH	100	ILE
59	HH	137	SER
59	HH	145	ARG
59	HH	160	LYS
59	HH	172	THR
60	II	12	ARG
60	II	23	LYS
60	II	26	LYS
60	II	45	THR
60	II	74	ARG
60	II	93	THR
60	II	100	CYS
60	II	107	THR
60	II	121	LEU
60	II	130	THR
60	II	161	LEU
60	II	168	GLN
60	II	178	ARG
60	II	203	LYS
61	JJ	26	ASP

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Mol	Chain	Res	Type
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	61	LEU
61	JJ	69	ARG
61	JJ	70	ARG
61	JJ	79	ARG
61	JJ	80	ARG
61	JJ	88	ASP
61	JJ	89	GLU
61	JJ	116	LYS
62	KK	17	LYS
62	KK	20	VAL
62	KK	35	LEU
62	KK	43	LEU
62	KK	50	GLN
62	KK	60	GLU
62	KK	66	HIS
62	KK	89	ILE
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	40	ILE
63	LL	42	LEU
63	LL	49	GLU
63	LL	56	ILE
63	LL	69	ARG
63	LL	85	THR
63	LL	91	ASP
63	LL	121	GLN
63	LL	126	VAL
63	LL	134	LEU
64	MM	22	LEU
64	MM	31	LEU
64	MM	33	ARG
64	MM	36	ARG
64	MM	40	LYS
64	MM	42	LEU
64	MM	45	ARG
64	MM	49	LEU
64	MM	55	ASN

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Mol	Chain	Res	Type
64	MM	83	LYS
64	MM	85	LEU
64	MM	99	LYS
64	MM	101	ARG
64	MM	112	LYS
64	MM	113	ASP
64	MM	123	VAL
65	NN	3	ARG
65	NN	20	ARG
65	NN	27	LYS
65	NN	55	ARG
65	NN	60	VAL
65	NN	78	LYS
65	NN	84	LEU
65	NN	86	GLU
65	NN	94	LYS
65	NN	107	LYS
65	NN	110	ASP
65	NN	132	LYS
66	OO	25	GLU
66	OO	34	PHE
66	OO	38	ASN
66	OO	50	LYS
66	OO	51	GLU
66	OO	56	VAL
66	OO	69	SER
66	OO	85	CYS
66	OO	104	ARG
66	OO	119	LEU
66	OO	128	ARG
66	OO	131	ASP
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	42	ARG
67	PP	44	ARG
67	PP	46	SER
67	PP	83	MET

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Mol	Chain	Res	Type
67	PP	108	LYS
67	PP	130	ARG
68	QQ	31	LEU
68	QQ	41	MET
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	105	MET
69	RR	121	GLN
69	RR	132	ARG
70	SS	8	LYS
70	SS	14	ARG
70	SS	21	ASP
70	SS	23	ARG
70	SS	36	VAL
70	SS	46	ARG
70	SS	52	LEU
70	SS	59	LEU
70	SS	63	GLU
70	SS	83	PHE
70	SS	86	ARG
70	SS	110	ASP
70	SS	132	ARG
70	SS	144	ARG
71	TT	41	LYS
71	TT	62	ARG
71	TT	90	SER
71	TT	102	ARG
71	TT	108	GLU
71	TT	110	LEU
71	TT	121	ARG
71	TT	124	THR
71	TT	131	LEU
71	TT	142	LYS
72	UU	36	CYS
72	UU	39	LEU

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Mol	Chain	Res	Type
72	UU	56	MET
72	UU	88	LEU
72	UU	106	ILE
72	UU	111	GLU
73	VV	9	VAL
73	VV	12	TYR
74	WW	23	ARG
74	WW	36	ARG
74	WW	51	GLU
74	WW	92	ASN
74	WW	103	VAL
74	WW	104	LEU
75	XX	64	SER
75	XX	67	ARG
75	XX	71	ARG
75	XX	105	PHE
75	XX	107	ARG
75	XX	115	ILE
76	YY	16	ARG
76	YY	17	LEU
76	YY	20	ARG
76	YY	32	LYS
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	115	LYS
77	ZZ	80	ARG
77	ZZ	89	GLN
77	ZZ	92	LEU
78	aa	12	LYS
78	aa	21	ILE
78	aa	34	LYS
78	aa	41	ILE
78	aa	44	ILE
78	aa	55	GLU
78	aa	67	LEU
78	aa	74	CYS
78	aa	95	ARG
78	aa	100	ARG

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Mol	Chain	Res	Type
79	bb	17	ARG
79	bb	42	LYS
79	bb	64	CYS
79	bb	80	ARG
79	bb	81	ARG
80	cc	26	GLN
80	cc	31	ARG
80	cc	40	ARG
80	cc	44	ARG
82	ee	99	LYS
82	ee	110	GLN
82	ee	113	ARG
83	ff	83	LYS
83	ff	94	LYS
83	ff	99	LYS
83	ff	113	LYS
83	ff	121	CYS
83	ff	138	ARG
83	ff	140	TYR
84	gg	17	TRP
84	gg	20	GLN
84	gg	36	ARG
84	gg	79	LEU
84	gg	87	LEU
84	gg	119	GLN
84	gg	207	CYS
84	gg	273	GLU
84	gg	289	LEU
84	gg	306	LEU
86	ii	61	ASN
86	ii	63	LYS
86	ii	65	ARG
86	ii	68	ARG
86	ii	86	ASN
86	ii	103	GLU
86	ii	211	GLN
86	ii	212	LEU
86	ii	232	PHE
86	ii	241	MET
86	ii	246	LEU
86	ii	339	GLU
86	ii	340	GLU

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Mol	Chain	Res	Type
86	ii	341	GLU
86	ii	368	LEU
86	ii	417	VAL
87	jj	52	GLU
87	jj	75	LEU
87	jj	96	ARG
87	jj	97	LEU
87	jj	192	ASP
87	jj	236	ASP
87	jj	250	LYS
87	jj	313	LEU
87	jj	320	GLU
87	jj	345	MET
87	jj	362	LEU
87	jj	373	GLU
87	jj	377	MET
87	jj	385	LYS
87	jj	388	PHE
87	jj	404	VAL
87	jj	411	TYR
87	jj	468	GLN
87	jj	510	HIS
87	jj	526	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
64	MM	19	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	15 (20%)	0
47	3	72/75 (96%)	22 (30%)	2 (2%)
48	5	3515/3543 (99%)	902 (25%)	167 (4%)
49	7	119/120 (99%)	14 (11%)	1 (0%)
50	8	150/156 (96%)	36 (24%)	7 (4%)
51	9	1679/1869 (89%)	419 (24%)	63 (3%)
85	hh	14/15 (93%)	7 (50%)	0
All	All	5623/5854 (96%)	1415 (25%)	240 (4%)



All (1415) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	8	U
46	2	9	A
46	2	16	C
46	2	19	G
46	2	20	U
46	2	21	A
46	2	34	A
46	2	46	G
46	2	47	U
46	2	49	C
46	2	61	C
46	2	64	G
46	2	67	G
46	2	72	C
46	2	75	C
47	3	7	A
47	3	13	C
47	3	14	A
47	3	21	A
47	3	25	C
47	3	28	C
47	3	29	A
47	3	34	U
47	3	35	U
47	3	36	U
47	3	40	C
47	3	42	G
47	3	47	U
47	3	49	C
47	3	53	G
47	3	58	A
47	3	60	U
47	3	61	C
47	3	63	C
47	3	65	G
47	3	72	C
47	3	76	A
48	5	6	C
48	5	8	U
48	5	12	A
48	5	13	U
48	5	15	A

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Mol	Chain	Res	Type
48	5	25	A
48	5	30	C
48	5	35	U
48	5	39	A
48	5	42	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	73	A
48	5	91	G
48	5	93	G
48	5	108	A
48	5	109	G
48	5	110	C
48	5	118	C
48	5	119	G
48	5	120	A
48	5	121	A
48	5	126	C
48	5	131	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	143	C
48	5	144	G
48	5	159	C
48	5	165	A
48	5	172	C
48	5	173	C
48	5	176	G
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

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Mol	Chain	Res	Type
48	5	217	C
48	5	218	A
48	5	220	C
48	5	221	C
48	5	224	U
48	5	225	G
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	235	A
48	5	246	G
48	5	253	G
48	5	255	C
48	5	263	G
48	5	266	C
48	5	276	C
48	5	279	A
48	5	280	G
48	5	297	U
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	322	C
48	5	328	A
48	5	334	A
48	5	340	C
48	5	347	A
48	5	350	C
48	5	357	U
48	5	361	C
48	5	362	A
48	5	363	A
48	5	379	G
48	5	386	A
48	5	387	G
48	5	407	A
48	5	409	G
48	5	410	A
48	5	412	G

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Mol	Chain	Res	Type
48	5	413	G
48	5	429	A
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	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	481	G
48	5	481(A)	C
48	5	482	G
48	5	483	G
48	5	484	U
48	5	485	C
48	5	486	C
48	5	490	C
48	5	492	U
48	5	493	G
48	5	497	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	510	U
48	5	653	C
48	5	654	C
48	5	657	C
48	5	658	C
48	5	659	G
48	5	660	G
48	5	667	A
48	5	668	C
48	5	669	C
48	5	670	G
48	5	672	C
48	5	683	C

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Mol	Chain	Res	Type
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	702	U
48	5	704	C
48	5	705	G
48	5	708	G
48	5	719	C
48	5	722	G
48	5	729	G
48	5	730	G
48	5	731	G
48	5	734	G
48	5	738	C
48	5	738(A)	C
48	5	739	G
48	5	742	G
48	5	747	A
48	5	748	G
48	5	749	G
48	5	750	U
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	917	A
48	5	918	G
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	929	A
48	5	930	G
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	935	A
48	5	935(A)	G
48	5	936	C

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Mol	Chain	Res	Type
48	5	937	U
48	5	939	G
48	5	941	C
48	5	943	A
48	5	944	A
48	5	945	U
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	963	G
48	5	964	A
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	973	G
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1071	C
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1175	A
48	5	1177	U
48	5	1179	U
48	5	1184	A
48	5	1185	G
48	5	1189	G
48	5	1194	G
48	5	1195	G
48	5	1211	G

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Mol	Chain	Res	Type
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	1284	G
48	5	1287	G
48	5	1288	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	1334	A
48	5	1354	A
48	5	1359	G
48	5	1360	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G
48	5	1378	C
48	5	1379	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A

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Mol	Chain	Res	Type
48	5	1398	A
48	5	1401	C
48	5	1403	G
48	5	1416	G
48	5	1418	C
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1429	C
48	5	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	1456	C
48	5	1457	G
48	5	1458	C
48	5	1459	A
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	1486	C
48	5	1495	G
48	5	1497	A
48	5	1498	G
48	5	1502	G
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1525	A
48	5	1534	A

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Mol	Chain	Res	Type
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1574	G
48	5	1578	U
48	5	1584	G
48	5	1591	U
48	5	1592	G
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	1638	A
48	5	1640	C
48	5	1641	G
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1691	G
48	5	1724	G
48	5	1726	U
48	5	1734	G
48	5	1735	U
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1760	G

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Mol	Chain	Res	Type
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	1799	G
48	5	1800	U
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	1823	G
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1867	A
48	5	1869	G
48	5	1881	C
48	5	1893	C
48	5	1897	A
48	5	1910	G
48	5	1916	G
48	5	1918	U
48	5	1919	G
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1933	G
48	5	1940	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	5	1941	A
48	5	1948	G
48	5	1952	G
48	5	1957	U
48	5	1958	A
48	5	1959	U
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1976	G
48	5	1977	C
48	5	1978	C
48	5	1979	A
48	5	1980	U
48	5	1983	A
48	5	1984	A
48	5	1986	U
48	5	1987	C
48	5	1991	A
48	5	1993	C
48	5	1997	U
48	5	2001	G
48	5	2002	A
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2007	G
48	5	2008	U
48	5	2011	C
48	5	2013	A
48	5	2016	C
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2033	A
48	5	2034	G
48	5	2046	G
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
48	5	2062	C
48	5	2064	G
48	5	2069	A
48	5	2070	U
48	5	2084	U
48	5	2085	G
48	5	2089	G
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G
48	5	2101	A
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2110	G
48	5	2111	U
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	2277	C
48	5	2278	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

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Mol	Chain	Res	Type
48	5	2316	G
48	5	2331	G
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2357	G
48	5	2364	G
48	5	2366	A
48	5	2370	A
48	5	2374	A
48	5	2380	G
48	5	2395	A
48	5	2396	A
48	5	2399	G
48	5	2414	G
48	5	2416	G
48	5	2417	A
48	5	2421	G
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2428	A
48	5	2433	G
48	5	2441	C
48	5	2447	U
48	5	2450	G
48	5	2467	U
48	5	2468	U
48	5	2469	C
48	5	2471	G
48	5	2475	G
48	5	2479	G
48	5	2483	G
48	5	2485	U
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2499	C
48	5	2503	G

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Mol	Chain	Res	Type
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2509	C
48	5	2512	A
48	5	2513	A
48	5	2521	G
48	5	2529	A
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2571	C
48	5	2572	C
48	5	2575	U
48	5	2577	C
48	5	2583	C
48	5	2586	G
48	5	2587	A
48	5	2588	C
48	5	2601	A
48	5	2618	G
48	5	2620	G
48	5	2622	G
48	5	2623	A
48	5	2627	C
48	5	2638	G
48	5	2639	U
48	5	2640	G
48	5	2647	A
48	5	2658	G
48	5	2661	U
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2670	C
48	5	2673	G
48	5	2676	A

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Mol	Chain	Res	Type
48	5	2680	G
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2688	G
48	5	2689	C
48	5	2695	A
48	5	2696	A
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2740	U
48	5	2743	A
48	5	2751	G
48	5	2754	G
48	5	2760	G
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2787	A
48	5	2788	U
48	5	2789	A
48	5	2790	U
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2814	C
48	5	2819	U
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U

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Mol	Chain	Res	Type
48	5	2838	G
48	5	2839	U
48	5	2842	G
48	5	2855	G
48	5	2857	A
48	5	2862	G
48	5	2864	A
48	5	2875	C
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3599	A
48	5	3604	A
48	5	3605	C
48	5	3615	G
48	5	3625	G
48	5	3626	G
48	5	3630	A
48	5	3635	A
48	5	3644	U
48	5	3646	A
48	5	3662	A
48	5	3673	C
48	5	3674	G
48	5	3685	C
48	5	3692	A
48	5	3698	G
48	5	3711	A
48	5	3712	A
48	5	3719	A
48	5	3722	G
48	5	3729	U
48	5	3733	A
48	5	3737	A
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3755	G
48	5	3756	A
48	5	3759	A

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Mol	Chain	Res	Type
48	5	3760	A
48	5	3765	G
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3783	A
48	5	3784	A
48	5	3785	A
48	5	3786	U
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3851	U
48	5	3859	G
48	5	3867	A
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3889	G
48	5	3897	G
48	5	3898	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3908	A
48	5	3915	U
48	5	3916	G
48	5	3927	U
48	5	3939	G
48	5	3943	A
48	5	3946	G

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Mol	Chain	Res	Type
48	5	4067	U
48	5	4069	U
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4150	G
48	5	4162	C
48	5	4163	U
48	5	4166	G
48	5	4171	C
48	5	4183	G
48	5	4184	G
48	5	4190	U
48	5	4191	G
48	5	4203	A
48	5	4212	A
48	5	4218	U
48	5	4222	G
48	5	4225	G
48	5	4229	U
48	5	4232	U
48	5	4233	A
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4267	G
48	5	4268	A

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Mol	Chain	Res	Type
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	4336	A
48	5	4339	A
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4373	G
48	5	4376	A
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4387	C
48	5	4393	G
48	5	4394	A
48	5	4395	U
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4436	U
48	5	4437	U
48	5	4438	U
48	5	4440	G
48	5	4441	A
48	5	4444	C

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Mol	Chain	Res	Type
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	4512	U
48	5	4513	A
48	5	4515	G
48	5	4519	C
48	5	4520	G
48	5	4524	G
48	5	4527	G
48	5	4528	G
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4563	U
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4574	U
48	5	4575	G
48	5	4578	G
48	5	4581	G
48	5	4586	G
48	5	4590	A
48	5	4606	G
48	5	4618	G
48	5	4627	U
48	5	4636	U
48	5	4637	G
48	5	4650	G
48	5	4652	G
48	5	4656	A
48	5	4657	U

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Mol	Chain	Res	Type
48	5	4660	G
48	5	4661	G
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4678	G
48	5	4687	A
48	5	4694	G
48	5	4699	U
48	5	4700	A
48	5	4701	A
48	5	4709	U
48	5	4712	C
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	4756	C
48	5	4757	C
48	5	4759	C
48	5	4761	G
48	5	4765	G
48	5	4771	C
48	5	4772	C
48	5	4868	G
48	5	4870	G
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	A
48	5	4877	G
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4887	C

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Mol	Chain	Res	Type
48	5	4891	G
48	5	4895	C
48	5	4897	G
48	5	4904	G
48	5	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G
48	5	4918	C
48	5	4919	G
48	5	4921	C
48	5	4922	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	4936	G
48	5	4937	C
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
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	4979	A
48	5	4988	U

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Mol	Chain	Res	Type
48	5	4989	U
48	5	4990	C
48	5	4991	U
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	5052	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5061	A
48	5	5062	G
49	7	7	G
49	7	13	A
49	7	33	U
49	7	38	U
49	7	42	A
49	7	53	U
49	7	54	A
49	7	64	G
49	7	97	G
49	7	100	A
49	7	110	G
49	7	116	G
49	7	117	G
49	7	120	U
50	8	2	G
50	8	3	A
50	8	32	C
50	8	34	U
50	8	35	C
50	8	49	G
50	8	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

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Mol	Chain	Res	Type
50	8	87	G
50	8	94	G
50	8	95	A
50	8	97	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	147	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	41	G
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	60	A
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G

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Mol	Chain	Res	Type
51	9	73	C
51	9	74	G
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	129	C
51	9	130	G
51	9	141	A
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	175	A
51	9	182	C
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	191	A
51	9	192	C
51	9	200	G
51	9	202	G
51	9	206	G
51	9	211	G
51	9	213	G

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Mol	Chain	Res	Type
51	9	215	G
51	9	289	G
51	9	292	A
51	9	293	C
51	9	294	U
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	314	U
51	9	318	A
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	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	381	C
51	9	382	C
51	9	384	U
51	9	385	G
51	9	386	C
51	9	400	C
51	9	409	C
51	9	417	C
51	9	418	A
51	9	435	A
51	9	438	G
51	9	448	A
51	9	449	A
51	9	450	C
51	9	459	C
51	9	460	A
51	9	464	A

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Mol	Chain	Res	Type
51	9	465	A
51	9	466	G
51	9	469	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	508	A
51	9	512	A
51	9	518	G
51	9	525	A
51	9	531	A
51	9	532	C
51	9	533	A
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	560	A
51	9	562	U
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G
51	9	589	G
51	9	590	A
51	9	591	U

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Mol	Chain	Res	Type
51	9	592	C
51	9	597	G
51	9	598	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	614	C
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	659	G
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	673	G
51	9	684	G
51	9	688	U
51	9	689	U
51	9	690	G
51	9	691	G
51	9	732	U
51	9	733	C
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

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Mol	Chain	Res	Type
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	886	A
51	9	887	U
51	9	890	U
51	9	892	U
51	9	902	G
51	9	913	A
51	9	914	U
51	9	920	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	955	A
51	9	971	G
51	9	985	G
51	9	989	C
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	1060	A
51	9	1061	U
51	9	1062	A
51	9	1067	C
51	9	1083	A
51	9	1085	C
51	9	1089	G
51	9	1096	G
51	9	1099	G
51	9	1100	A
51	9	1111	U

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Mol	Chain	Res	Type
51	9	1114	U
51	9	1115	U
51	9	1117	C
51	9	1118	C
51	9	1120	U
51	9	1121	G
51	9	1131	G
51	9	1132	C
51	9	1133	A
51	9	1138	C
51	9	1139	C
51	9	1148	A
51	9	1149	A
51	9	1153	C
51	9	1154	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1213	C
51	9	1215	C
51	9	1221	G
51	9	1223	A
51	9	1224	G
51	9	1240	A
51	9	1242	U
51	9	1248	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G
51	9	1259	A
51	9	1260	A
51	9	1265	A
51	9	1268	C
51	9	1270	G
51	9	1271	C
51	9	1274	G
51	9	1275	G

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Mol	Chain	Res	Type
51	9	1281	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
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	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1321	G
51	9	1330	G
51	9	1331	C
51	9	1342	U
51	9	1354	G
51	9	1369	A
51	9	1371	U
51	9	1372	U
51	9	1376	A
51	9	1378	A
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1398	G
51	9	1401	A
51	9	1402	A
51	9	1404	U
51	9	1406	G
51	9	1407	U
51	9	1410	C
51	9	1412	C
51	9	1413	G
51	9	1414	A
51	9	1424	G
51	9	1428	G

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Mol	Chain	Res	Type
51	9	1439	A
51	9	1449	G
51	9	1454	A
51	9	1458	G
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1466	G
51	9	1473	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1490	G
51	9	1494	U
51	9	1497	G
51	9	1498	A
51	9	1507	G
51	9	1509	U
51	9	1510	G
51	9	1521	C
51	9	1522	A
51	9	1531	A
51	9	1533	A
51	9	1536	G
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1582	C
51	9	1585	U
51	9	1586	U
51	9	1587	G

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Mol	Chain	Res	Type
51	9	1588	A
51	9	1589	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1621	U
51	9	1623	A
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1639	G
51	9	1641	A
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1729	U
51	9	1730	U
51	9	1737	G
51	9	1750	C
51	9	1753	C
51	9	1756	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C

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Mol	Chain	Res	Type
51	9	1800	A
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	1850	A
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
85	hh	49	U
85	hh	52	G
85	hh	55	C

All (240) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
47	3	7	A
47	3	74	C
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	125	C
48	5	134	G
48	5	143	C

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Mol	Chain	Res	Type
48	5	217	C
48	5	226	G
48	5	234	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	G
48	5	361	C
48	5	385	A
48	5	387	G
48	5	406	C
48	5	408	A
48	5	409	G
48	5	417	G
48	5	449	C
48	5	466	A
48	5	480	C
48	5	481(A)	C
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	669	C
48	5	696	C
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	748	G
48	5	749	G
48	5	915	A
48	5	916	C
48	5	924	C
48	5	930	G
48	5	933	G
48	5	935(A)	G
48	5	936	C
48	5	956	A
48	5	959	G
48	5	963	G
48	5	965	G

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Mol	Chain	Res	Type
48	5	966	A
48	5	971(A)	G
48	5	1071	C
48	5	1072	C
48	5	1174	G
48	5	1209	U
48	5	1211	G
48	5	1214	C
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1294	A
48	5	1295	U
48	5	1329	G
48	5	1358	G
48	5	1359	G
48	5	1370	G
48	5	1376	C
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	1484	G
48	5	1485	C
48	5	1633	G
48	5	1733	G
48	5	1734	G
48	5	1740	C
48	5	1804	A
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1919	G
48	5	1921	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	2398	U
48	5	2425	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2474	G
48	5	2490	U
48	5	2502	A
48	5	2529	A
48	5	2546	G
48	5	2587	A
48	5	2661	U
48	5	2695	A
48	5	2696	A
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
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G

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Mol	Chain	Res	Type
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4116	C
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4162	C
48	5	4170	A
48	5	4232	U
48	5	4254	G
48	5	4266	G
48	5	4348	A
48	5	4378	A
48	5	4448	G
48	5	4449	A
48	5	4463	U
48	5	4527	G
48	5	4572	U
48	5	4573	G
48	5	4656	A
48	5	4699	U
48	5	4719	G
48	5	4871	C
48	5	4872	G
48	5	4876	A
48	5	4884	G
48	5	4894	A
48	5	4925	U
48	5	4936	G
48	5	4942	C
48	5	4947	U
48	5	4949	G
48	5	4965	U
49	7	109	U
50	8	2	G
50	8	51	U
50	8	85	U
50	8	86	U
50	8	94	G
50	8	110	U
50	8	124	U

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Mol	Chain	Res	Type
51	9	2	A
51	9	72	C
51	9	103	A
51	9	110	U
51	9	126	G
51	9	160	U
51	9	182	C
51	9	293	C
51	9	314	U
51	9	369	C
51	9	434	G
51	9	448	A
51	9	465	A
51	9	473	A
51	9	531	A
51	9	532	C
51	9	553	U
51	9	555	A
51	9	559	G
51	9	563	G
51	9	591	U
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U
51	9	690	G
51	9	752	G
51	9	821	G
51	9	861	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	872	A
51	9	874	G
51	9	885	U
51	9	1016	U
51	9	1114	U
51	9	1115	U
51	9	1120	U
51	9	1137	U
51	9	1165	G
51	9	1253	A

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Mol	Chain	Res	Type
51	9	1264	C
51	9	1284	A
51	9	1286	G
51	9	1313	A
51	9	1330	G
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1489	A
51	9	1520	G
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1664	A
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1835	A
51	9	1867	U
51	9	1868	U

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 310 ligands modelled in this entry, 308 are monoatomic - leaving 2 for Mogul analysis.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
90	SF4	jj	600	87	0,12,12	0.00	-	0,24,24	0.00	-
90	SF4	jj	601	87	0,12,12	0.00	-	0,24,24	0.00	-

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	SF4	jj	600	87	-	0/0/48/48	0/6/5/5
90	SF4	jj	601	87	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

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	29
51	9	7
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	41.35
1	5	1252:C	O3'	1271:G	P	35.93

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1219:G	O3'	1233:G	P	23.06
1	5	3948:C	O3'	4065:G	P	19.73
1	5	1406(C):G	O3'	1411:C	P	18.70
1	5	990:C	O3'	1064:G	P	18.45
1	5	523:C	O3'	638:G	P	18.03
1	5	4138:C	O3'	4146:G	P	17.86
1	5	4101:C	O3'	4107:G	P	17.54
1	5	4777:C	O3'	4859:C	P	16.83
1	5	760:G	O3'	904:C	P	15.36
1	5	5022:U	O3'	5028:G	P	14.91
1	5	1696:C	O3'	1720:C	P	14.34
1	5	182:G	O3'	189:G	P	14.28
1	5	1364:U	O3'	1368:A	P	14.23
1	5	2901:G	O3'	3597:G	P	13.50
1	5	512:U	O3'	515:C	P	10.15
1	5	4729:A	O3'	4735:G	P	10.00
1	5	1180:C	O3'	1183:C	P	8.82
1	5	500:G	O3'	504:G	P	6.45
1	3	19:G	O3'	20:U	P	5.79
1	5	1100:U	O3'	1168:G	P	5.75
1	5	1239:C	O3'	1244:G	P	5.52
1	9	322:C	O3'	323:C	P	5.16
1	5	4740:G	O3'	4743:G	P	4.87
1	3	16:C	O3'	18:U	P	4.78
1	9	309:G	O3'	310:C	P	4.71
1	9	304:C	O3'	305:U	P	4.64
1	9	798:G	O3'	799:U	P	4.41
1	2	16:C	O3'	18:G	P	4.19
1	5	170:C	O3'	171:U	P	3.86
1	5	751:G	O3'	752:G	P	3.52
1	5	5020:G	O3'	5021:C	P	3.42
1	9	902:G	O3'	903:A	P	3.39
1	5	1438:U	O3'	1440:U	P	3.37
1	5	4899:G	O3'	4902:C	P	3.36
1	5	267:G	O3'	268:G	P	3.34
1	9	903:A	O3'	904:A	P	3.33
1	9	1295:A	O3'	1296:U	P	3.29