



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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

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

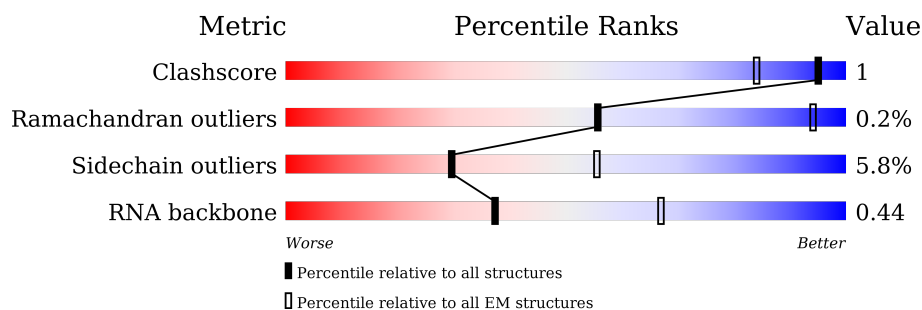
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 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.





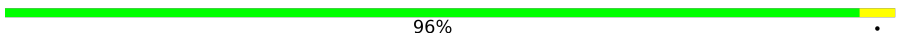














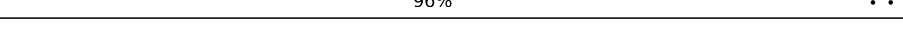
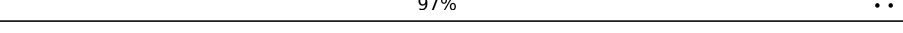




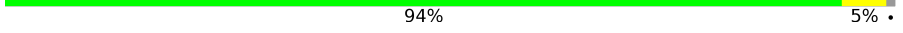
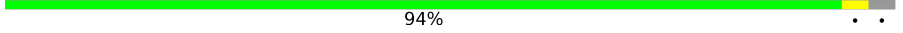
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 ≥ 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	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	
















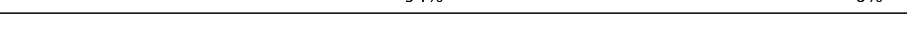







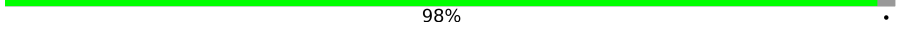

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Mol	Chain	Length	Quality of chain
34	i	105	94%
35	j	97	84%
36	k	70	96%
37	l	51	96%
38	m	102	49%
39	n	25	92%
40	o	106	95%
41	p	92	97%
42	r	137	88%
43	s	318	58%
44	t	165	88%
45	1	15	80%
46	2	76	74%
47	3	75	65%
48	5	3543	72%
49	7	120	88%
50	8	156	72%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

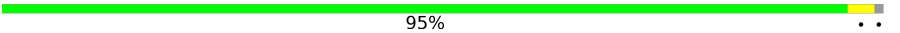



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Mol	Chain	Length	Quality of chain
59	HH	194	 85% 10% 5%
60	II	208	 88% 12% .
61	JJ	194	 84% 11% 5%
62	KK	165	 51% 5% . 42%
63	LL	158	 80% 10% 9%
64	MM	132	 67% 15% 5% . 11%
65	NN	151	 88% 10% ..
66	OO	168	 70% 10% . 19%
67	PP	145	 71% 10% . 17%
68	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

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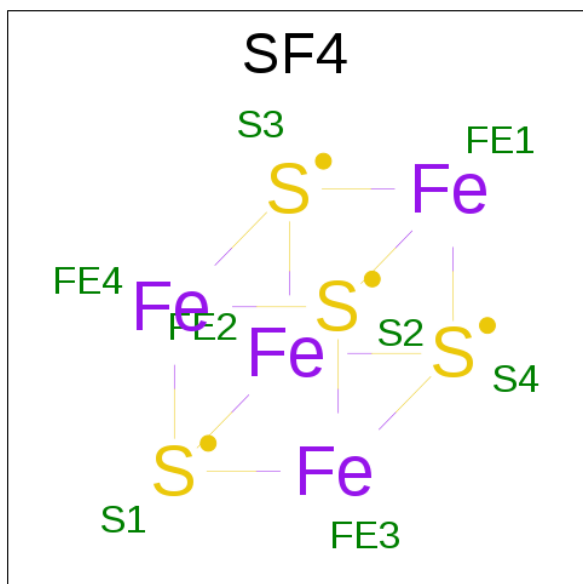
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Mol	Chain	Residues	Atoms		AltConf
88	hh	1	Total	Mg	0
			1	1	

- 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: Fe₄S₄).

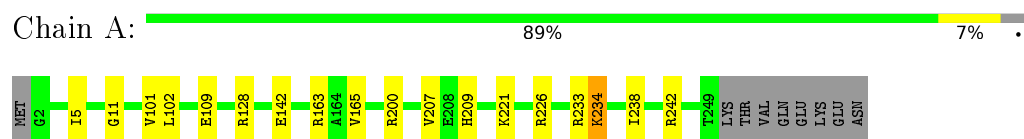


Mol	Chain	Residues	Atoms			AltConf
90	jj	1	Total 16	Fe 8	S 8	0
90	jj	1	Total 16	Fe 8	S 8	0

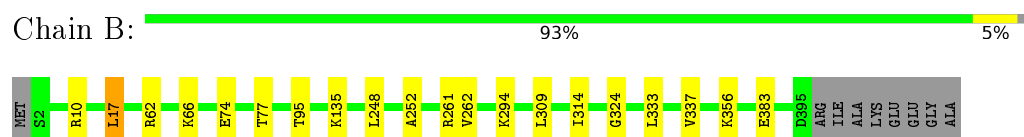
3 Residue-property plots

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

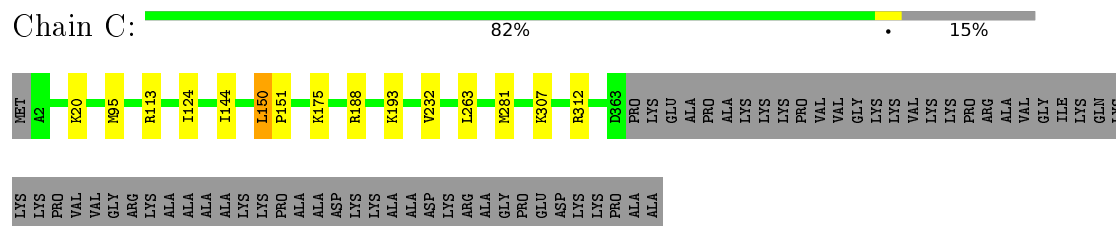
- Molecule 1: uL2



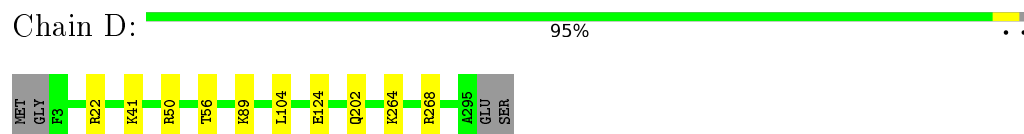
- Molecule 2: uL3



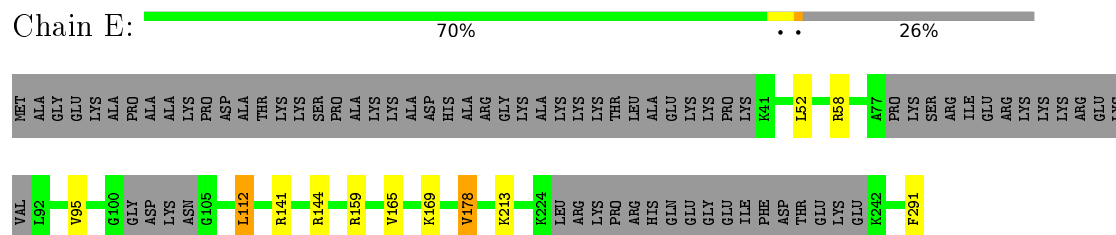
- Molecule 3: uL4



- Molecule 4: uL18



- Molecule 5: eL6



- Molecule 6: uL30

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
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | GLU | GLN | LEU | PRO | THR | CYS | TYR | TRP | HIS | ASP | PHE | THR | TRP | ASP | LYS | V80 | I98 | R126 | L148 | A176 | GLY | LYS | GLY | ASP | VAL | PRO | THR | K184 | K203 | K204 | D215 | P216 | L223 | L226 | M230 | R242 | E273 | N293 | K317 | L318 | G319 | | | | | | | | | | | | |
| MET | SER | SER | TYR | ARG | LEU | GLY | TYR | CYS | MET | LYS | GLU | GLU | ARG | HIS | ASN | LEU | VAL | LEU | CYS | LEU | TRP | SER | GLN | PRO | GLY | ILE | LEU | ASN | SER | LYS | CYS | LEU | TRP | PRO | PHE | THR | ASN | ILE | HIS | LEU | LEU | VAL | GLY | ALA | LEU | PRO | ARG | GLY | 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% .

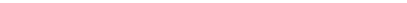


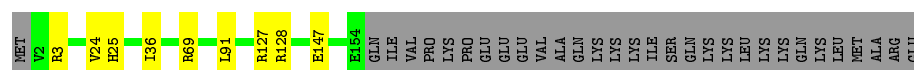
- Molecule 14: uL13

Chain 0: 90% 8%



- Molecule 15: uL22

Chain P:  78% 5% 17%



- Molecule 16: eL18

Chain Q: 95% 5%



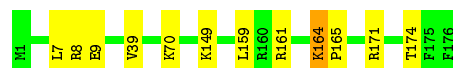
- Molecule 17: eL19

Chain R: 84% 7% 8%

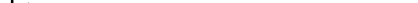


- Molecule 18: eL20

Chain S: 93% 6%

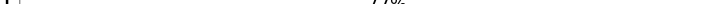


- Molecule 19: eL21

Chain T:  91% 8% ..

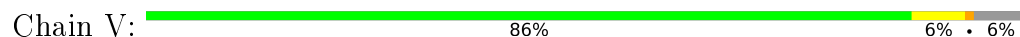


- Molecule 20: eL22

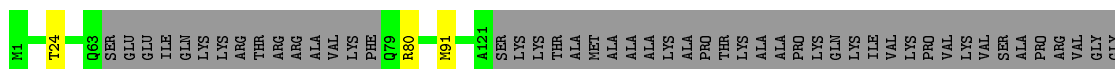
Chain U:  77% 23%



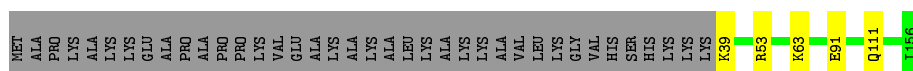
- Molecule 21: uL14



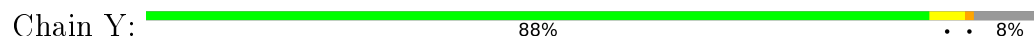
- Molecule 22: eL24



- Molecule 23: uL23



- Molecule 24: uL24



- Molecule 25: eL27

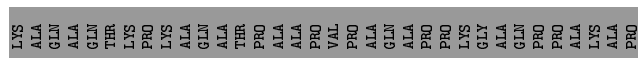


- Molecule 26: uL15



- Molecule 27: eL29





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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | VAL | ALA | ALA | LYS | LYS | THR | LYS | LYS | S10 | M37 | N78 | S107 | MET | PRO | GLU | GLN | THR | GLY | GLU | LYS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|
| MET | ALA | PRO | ALA | LYS | LYS | GLY | GLY | GLU | LYS | LYS | LYS | GLY | ARG | SER | ALA | ILE | M18 | R23 | K31 | R44 | E48 | R78 | R85 | S98 | L102 | E124 | ASN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|-----|

- | |
|------------|
| MET |
| A2 |
| I21
R22 |
| K64 |
| L78 |
| E86 |
| C91 |
| K106 |
| R128 |
| L129 |
| ARG |
| SER |
| GLU |
| GLU |
| ASN |
| GLU |

-

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-

- 


Chain i:  94% . .



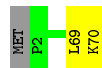
- Molecule 35: eL37

Chain j:  84% 5% 11%



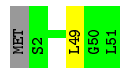
- Molecule 36: eL38

Chain k:  96% . .



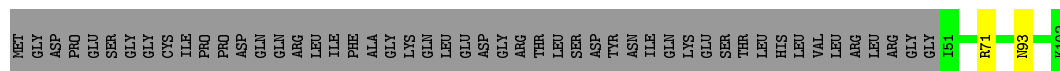
- Molecule 37: eL39

Chain l:  96% . .



- Molecule 38: eL40

Chain m:  49% . 49%



- Molecule 39: eL41

Chain n:  92% 8%



- Molecule 40: eL42

Chain o:  95% . .



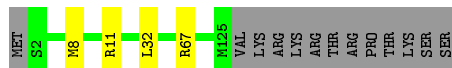
- Molecule 41: eL43

Chain p:  97% . .



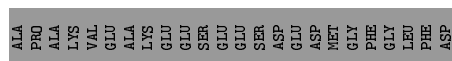
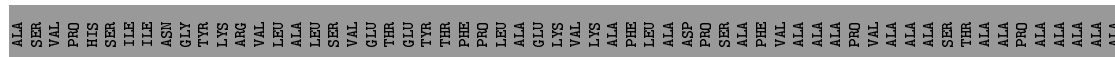
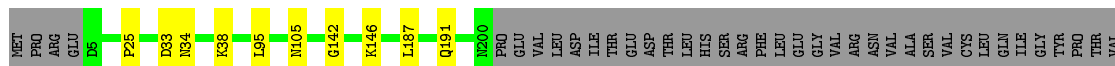
- Molecule 42: eL28

Chain r: 88% 9%



- Molecule 43: uL10

Chain s: 58% 38%



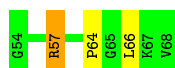
- Molecule 44: uL11

Chain t: 88% 7%



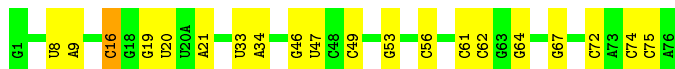
- Molecule 45: Nascent chain

Chain 1: 80% 13% 7%



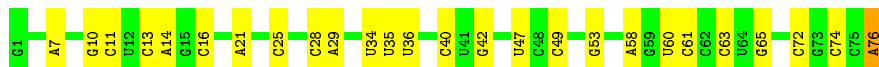
- Molecule 46: P-site tRNA

Chain 2: 74% 25%



- Molecule 47: E-site tRNA

Chain 3: 65% 33%




- Molecule 48: 28S ribosomal RNA

Chain 5:  72% 26%

G1	C143	A306	G457	G708	A944	U1209	G1377	C1486	G1654	G1819	G1973	A2069	G2381	G2479
C6	G144	A309	A466	C719	U945	C1210	C1378	G1495	C1655	U1820	U1974	U2070	A2382	G2483
U8	C159	G310	U467	G722	A956	G1212	C1379	G1496	U1656	U1822	G1975	U2084	G2383	A2484
A12	A165	G315	U468	G729	G958	G1214	U1381	A1497	C1661	G1823	G1976	G2085	G2348	U2485
U13	C172	U316	C460	U730	A960	G1215	A1387	G1502	C1676	C1828	C1978	A2088	C2351	C2488
C14	C173	U322	G481	G731	G961	G1234	G1394	A1503	U1677	U1833	A1979	G2089	C2352	U2490
A15	C176	C328	C481A	G734	G963	G1236	A1397	G1504	C1678	U1835	U1980	U2090	G2357	C2491
U20	G177	A328	G482	G738	A964	C1237	A1398	U1514	A1679	G1836	A1983	G2092	G2364	C2492
A25	G178	A334	U484	C738A	G965	A1238	C1401	U1515	G1691	U1837	G1984	G2093	G2365	G2493
C30	G179	A335	C486	G739	A966	A1239	C1403	U1516	G1724	G1842	U1985	C2094	A2366	U2494
U35	U200	A336	C490	G742	C967	C1272	G1402	A1517	U1725	C1844	U1986	A2095	A2367	U2495
A39	C201	C340	G491	G747	C969	A1274	G1416	A1523	U1726	G1855	A1990	G2096	A2370	C2499
A42	C202	A347	U492	G748	G971A	G1275	C1417	U1524	G1733	U1857	A1991	C2099	A2374	A2502
A47	C205	A350	G496	G749	G973	G1276	C1418	A1525	U1734	A1868	U1992	G2100	G2374	G2503
G48	U209	C350	G497	U750	C979	G1284	G1419	A1534	U1735	U1869	C1993	A2101	G2380	C2504
U49	C216	U357	C498	G756	C983	G1287	A1420	A1547	C1740	C1881	U1997	A2102	G2389	G2506
G49	C217	C361	G500	G757	C988	G1288	C1429	A1554	A1742	C1893	G2001	A2103	A2395	C2509
U56	A218	A362	G509	G758	C990	G1291	G1432	A1563	G1750	A1897	A2002	G2104	A2396	C2512
G57	C220	A363	G505	U911	C1071	G1292	A1433	U1564	G1753	C1899	A2003	A2105	G2397	A2513
G58	C221	G379	U510	U912	A1072	G1293	G1434	A1565	U1754	G1910	G2004	G2106	U2398	G2521
A59	C224	A385	C853	U914	C1073	G1295	C1437	C1566	C1755	G1916	U2005	A2107	G2399	A2529
A64	U224	A386	C854	A915	G1074	G1296	U1438	G1574	U1756	A1917	U2006	A2108	U2409	U2530
A65	G225	G387	C855	A916	C1075	C1301	U1439	U1578	U1757	G1918	C2011	G2259	G2414	U2537
A73	G226	A406	G659	A917	C1076	A1303	U1440	G1584	G1760	G1919	A2012	C2260	G2415	G2546
U77	A227	A408	G660	G918	C1077	C1304	C1441	U1591	G1761	C1920	C2013	G2261	A2417	G2547
G91	A235	A409	G670	G921	C1078	G1304	C1442	G1592	C1762	G1922	C2014	G2262	G2421	U2554
C92	G233	A410	G671	C922	C1079	C1313	U1445	G1596	G1763	A1923	U2015	G2266	A2428	G2555
G93	G234	A417	C872	C923	C1082	C1326	C1446	U1596	C1764	C1931	G2024	A2267	G2433	G2564
A108	G235	A429	C883	C924	G1168	A1327	G1453	U1596	C1768	G1933	A2025	A2268	C2441	A2565
G109	G236	G430	G884	C925	G1173	G1328	G1454	U1602	C1772	A1934	A2026	C2269	G2447	G2566
C110	G237	G431	G885	G926	C1174	G1329	C1455	U1612	C1773	C1935	A2033	G2275	U2457	C2571
C118	G238	G432	U887	G927	C1175	A1330	G1456	G1613	C1774	G1940	G2046	A2277	G2471	U2575
G119	C239	U432	C887	C930	C1176	G1334	C1457	G1624	U1781	U1947	U2047	C2279	G2474	G2576
A120	C240	C446	U887	A935	C1177	A1354	G1458	G1625	A1787	G1948	G2048	C2289	U2467	C2577
A121	C241	C449	C887	G933	C1178	G1358	G1475	A1631	G1799	G1952	G2052	G2294	U2468	C2583
C131	G242	C450	U887	A936	C1179	G1359	C1476	A1632	U1800	U1957	G2055	G2295	C2469	G2586
G134	G243	G451	U887	C934	U1179	G1360	C1477	A1633	U1800	A1958	G2056	G2300	G2470	U2587
G135	G244	A452	U887	C935	C1180	U1364	C1478	A1634	G1803	U1959	C2062	G2301	G2471	C2588
C136	G245	G453	U887	C936	G1189	G1370	C1481	A1638	A1804	A1960	G2063	A2313	G2474	G2601
	G246	G454	U887	C937	C1190	A1371	C1482	U1639	A1805	G1961	G2064	G2314	G2475	
	G247	U454	U887	C938	G1191	C1376	C1483	G1641	G1848	C1963	C2068	G2316		

C4957	C4958	C4964	C4966	C4967	U4976	U4979	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%

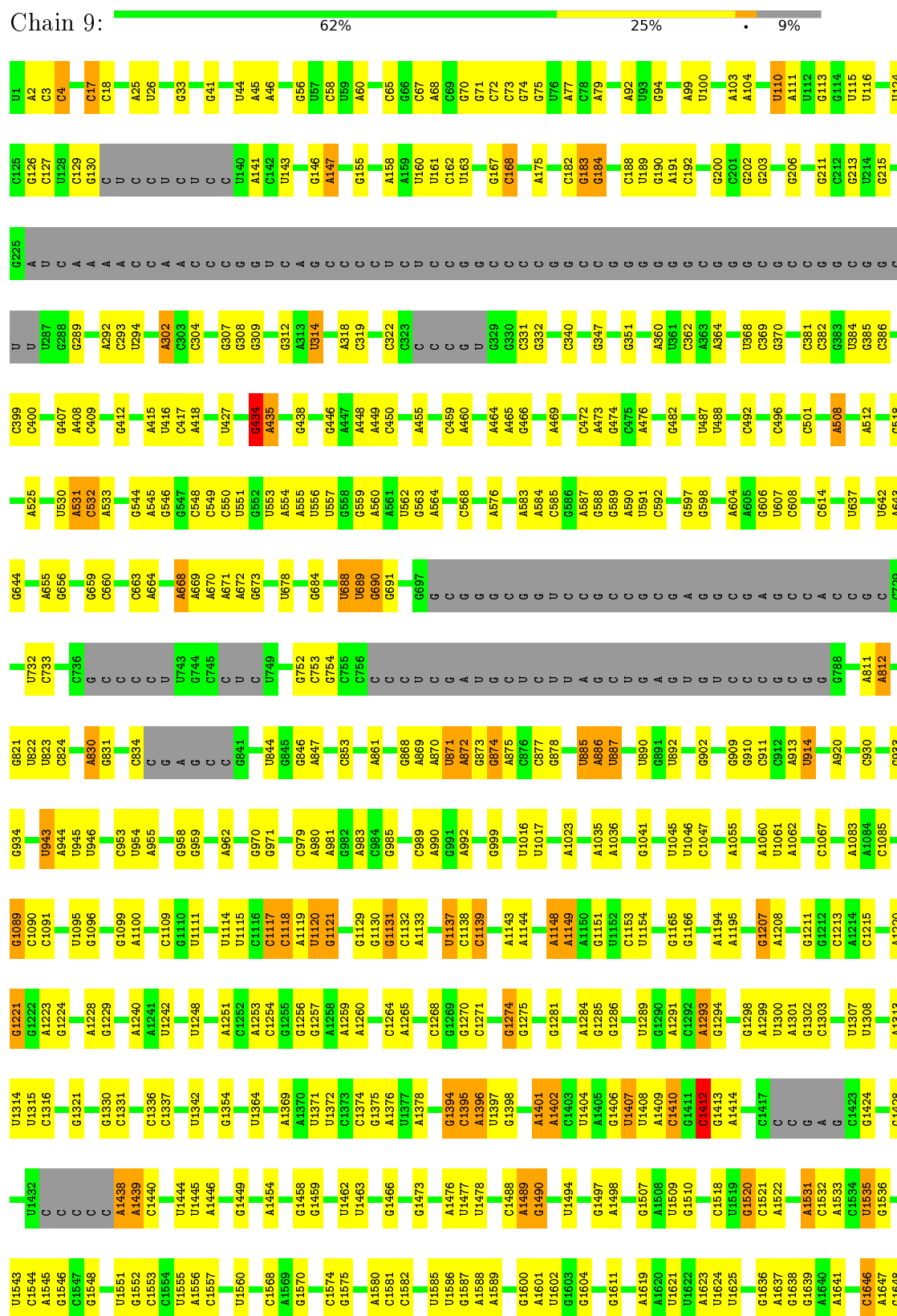
G1	G7	A13	U33	U38	A42	U53	A54	G64	G97	A100	U109	G110	G116	G117	U120
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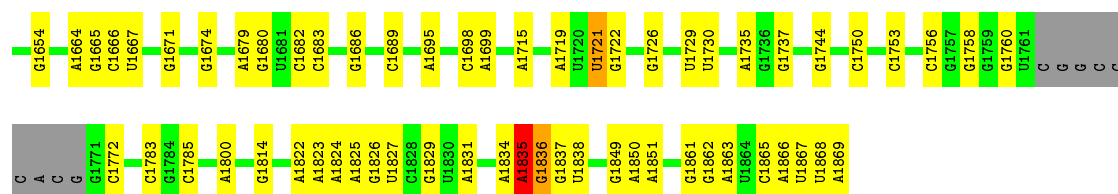
• Molecule 50: 5.8S ribosomal RNA

Chain 8:  72% 24%

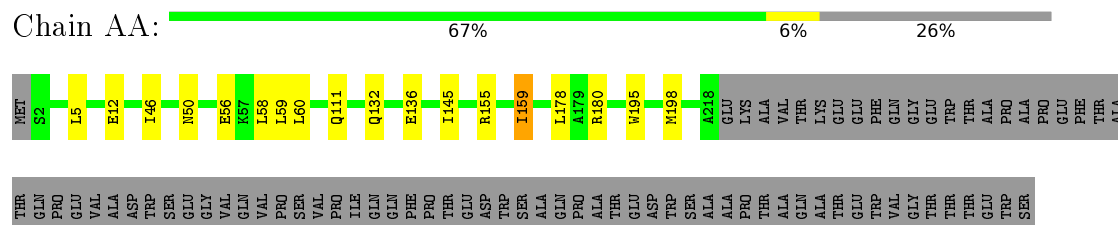
C1	G2	A3	C32	G33	U34	C35	G49	C50	U51	A52	A59	A62	U63	G75	G79	A	C	A	C	A	U85	U86	G87	G94	A95	C96	A97	A103	A104	C105	G106	C107	A108	C109	U110	U111	G112	C113	G114	G121	G122	U123	U124	C125	C126	U127	A137	C142
G147	C150	C153	U156																																													

• Molecule 51: 18S ribosomal RNA

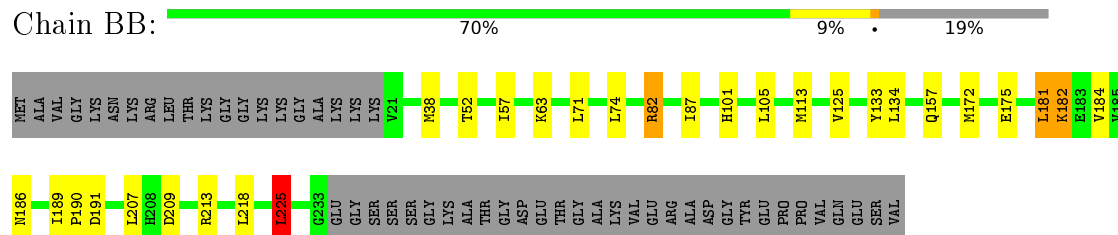




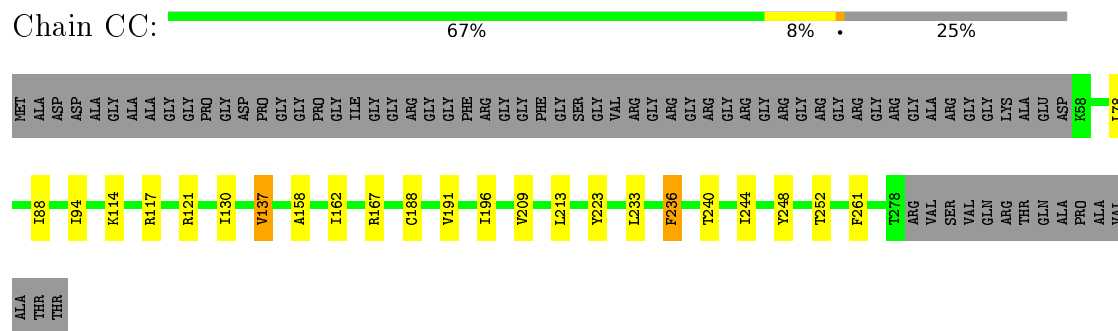
• Molecule 52: uS2



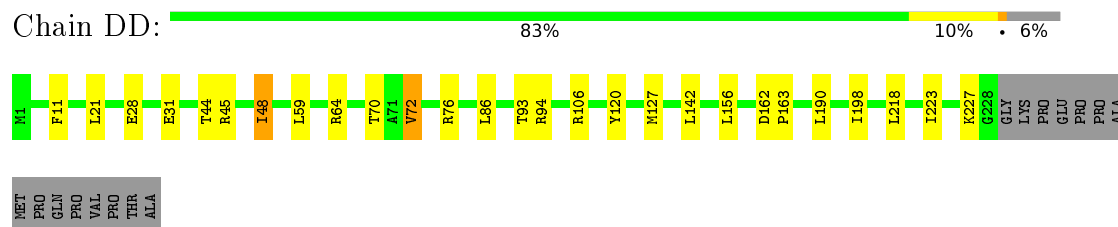
• Molecule 53: eS1



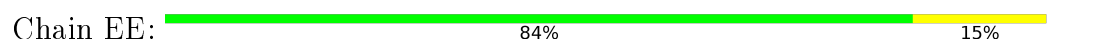
• Molecule 54: uS5

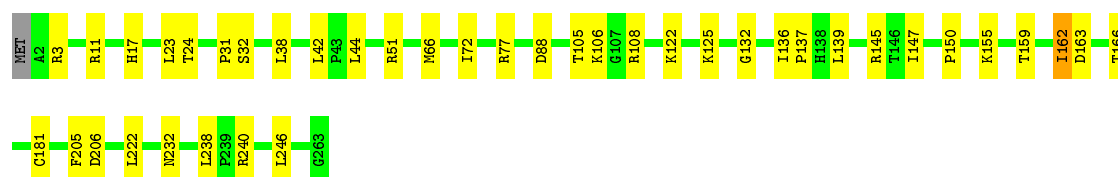


• Molecule 55: uS3



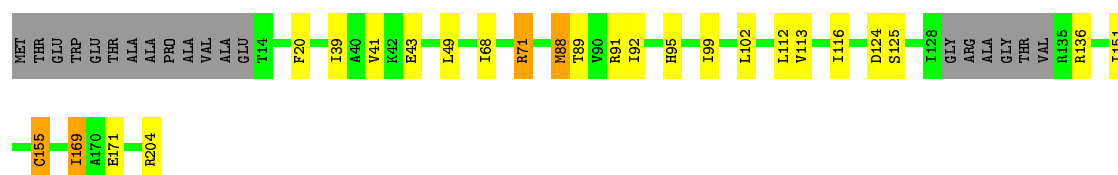
• Molecule 56: eS4





- Molecule 57: uS7

Chain FF: 78% 10% 9%



- Molecule 58: eS6

Chain GG: 86% 8% 5%



- Molecule 59: eS7

Chain HH: 85% 10% 5%



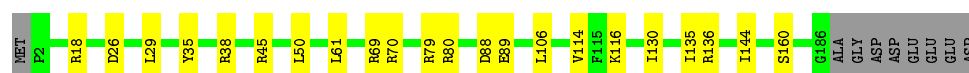
- Molecule 60: eS8

Chain II: 88% 12%



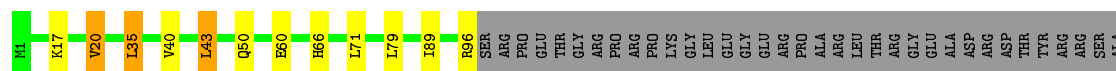
- Molecule 61: uS4

Chain JJ: 84% 11% 5%




- Molecule 62: eS10

Chain KK: 51% 5% 42%



VAL
PRO
PRO
GLY
GLY
ALA
ASP
LYS
LYS
ALA
GLU
GLU
ALA
GLY
GLY
GLY
SER
ALA
ALA
THR
GLY
GLY
PHE
GLN
PHE
ARG
GLY
GLY
PHE
GLY
ARG
GLY
GLY
GLN
PRO
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
I40
G41
L42
E49
I56
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
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
F100
R101
V111
K112
D113
K121
D122
V123

I124
C130
LYS
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
SER
GLY
GLY
VAL
ARG
ARG
ARG
ALA
ALA
MET
MET
ALA
PRO
ARG
GLY
LYS
GLY
LYS
GLY
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
SER
ARG
PHE
ILE
PRO
PRO
LEU
LYS

• Molecule 68: uS9

Chain QQ:  87% 10% .


MET
PRO
SER
LYS
G5
R15
R16
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%



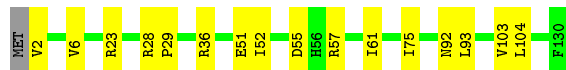
• Molecule 73: eS21

Chain VV:  94% 6%



• Molecule 74: uS8

Chain WW:  87% 12%




• Molecule 75: uS12

Chain XX:  87% 10%



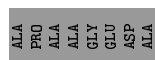
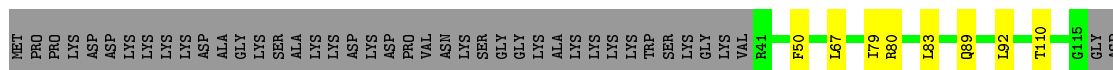
• Molecule 76: eS24

Chain YY:  84% 12% 5%



- Molecule 77: eS25

Chain ZZ: 54% 6% 40%



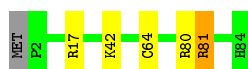
- Molecule 78: eS26

Chain aa: 79% 9% 12%



- Molecule 79: eS27

Chain bb: 93% 5% ..



- Molecule 80: eS28

Chain cc: 84% 6% 10%



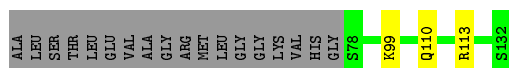
- Molecule 81: uS14

Chain dd: 98% .



- Molecule 82: eS30

Chain ee: 39% . 59%



- Molecule 83: eS31

Chain ff:  39% 56%

MET GLN ILE PHE VAL LYS THR LEU THR THR GLY LYS THR ILE THR LEU GLU VAL GLU PRO SER ASP THR ILE GLU ASN VAL LYS ALA LYS ILE GLN ASP LYS GLU GLY ILE PRO PRO ASP 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 VAL ARG ARG ARG GLY ALA LYS 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 HIS MET MET ALA SER GLU ASN LEU TYR PHE GLN SER SER MET ASP ASP PRO 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 GLU PHE PHE ASP 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 K385 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

The worst 5 of 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

The worst 5 of 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
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

There are no chirality outliers.

5 of 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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	b	848	0	920	0	0
28	c	761	0	794	0	0
29	d	888	0	930	0	0
30	e	1053	0	1147	0	0
31	f	876	0	912	0	0
32	g	906	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	RR	1068	0	1121	3	0
70	SS	1190	0	1249	4	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

5.3.2 Protein sidechains [i](#)

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	l	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 636 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	BB	63	LYS
57	FF	71	ARG
83	ff	121	CYS
53	BB	175	GLU
55	DD	72	VAL

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%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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%)

5 of 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

5 of 240 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
48	5	2398	U
48	5	3904	G
51	9	1286	G
48	5	2467	U
48	5	2696	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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

The worst 5 of 39 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