

wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 03:24 pm GMT

PDB ID	:	5MRE
EMDB ID	:	EMD-3552
Title	:	Structure of the yeast mitochondrial ribosome - Class B
Authors	:	Desai, N.; Brown, A.; Amunts, A.; Ramakrishnan, V.
Deposited on	:	2016-12-22
Resolution	:	3.75 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 3.75 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. 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 $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain	
1	А	3296	60% 19% ·	18%
2	В	393	74% 7% •	18%
3	С	249	86%	13% •
4	D	252	88%	10% •
5	Е	274	90%	9%
6	F	196	91%	9%
7	G	74	95%	5%



Mol	Chain	Length	Quality of chain	
8	Η	160	90%	10%
9	Ι	138	84%	8% 8%
10	J	220	90%	10%
11	K	195	88%	12% •
12	L	237	88%	8% •
13	М	151	91%	9% •
14	Ν	118	95%	•••
15	О	225	93%	7%
16	Р	207	94%	6%
17	Q	296	88%	7% •
18	R	337	91%	7% •
19	S	216	80% 6	% 14%
20	Т	225	85%	11% •
21	U	82	89%	11%
22	V	177	• 50% • 47%	
23	W	112	95%	5%
24	Х	64	84%	16%
25	Y	46	91%	9%
26	Ζ	62	94%	6%
27	0	38	89%	11%
28	1	348	94%	6%
29	2	113	88%	11% •
30	3	130	94%	6%
31	4	138	91%	9%
32	5	324	90%	10%



Mol	Chain	Length	Quality of chain	
33	6	281	75% 8%	17%
34	7	106	87%	13%
35	8	264	71% 5%	25%
36	9	215	86%	7% 6%
37	a	177	97%	•
38	b	155	97%	•
39	с	119	98%	·
40	d	215	94%	• •
41	AA	344	54% 5% 41%	
42	BB	266	83%	15% ·
43	CC	398	72% 12%	• 15%
44	DD	486	51% 7% · 41%	
45	EE	293	86%	12% ••
46	\mathbf{FF}	125	83%	17%
47	GG	161	93%	7%
48	HH	154	79%	18% ••
49	II	244	82%	10% 7%
50	JJ	186	• 82%	14% ••
51	KK	148	77%	19% •
52	LL	124	81%	17% •
53	MM	120	76%	22% •
54	NN	115	• 84%	12% •
55	00	253	82%	11% • 6%
56	PP	119	90%	7% ••
57	QQ	237	75% 119	6 14%



Mol	Chain	Length	Quality of chain	
58	RR	99	84%	8% 8%
59	SS	80	79%	20% •
60	TT	92	88%	12%
61	UU	233	87%	12% ·
62	VV	233	93%	6% ·
63	WW	401	83%	16%
64	XX	96	93%	5% •
65	YY	273	86%	12% ••
66	ZZ	91	76%	19% • •
67	11	34	88%	12%
68	22	99	96%	•
69	33	255	84%	11% • •
70	44	321	79%	6% 16%
71	55	339	17% • 83%	
72	66	319	88%	8% •
73	77	165	92%	8% •
74	88	457	87%	11% ••
75	aa	1649	63%	27% · 9%
76	bb	76	42% 5	7% •
77	сс	94	100%	
78	dd	151	• 100%	



2 Entry composition (i)

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

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

• Molecule 1 is a RNA chain called 21S ribosomal RNA.

Mol	Chain	Residues			AltConf	Trace			
1	А	2709	Total 57598	C 25914	N 10252	O 18729	Р 2703	0	0

• Molecule 2 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	321	Total 2527	$\begin{array}{c} \mathrm{C} \\ 1575 \end{array}$	N 507	0 436	S 9	0	0

• Molecule 3 is a protein called uL3m.

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

• Molecule 4 is a protein called uL4m.

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

• Molecule 5 is a protein called uL5m.

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

• Molecule 6 is a protein called uL6m.

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



• Molecule 7 is a protein called bL9m.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
7	G	74	Total 617	C 393	N 110	0 113	S 1	0	0

• Molecule 8 is a protein called uL13m.

Mol	Chain	Residues		At	oms	AltConf	Trace		
8	Н	160	Total 1275	C 807	N 240	0 224	${S \atop 4}$	0	0

• Molecule 9 is a protein called uL14m.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
9	Ι	127	Total 956	C 595	N 180	0 170	S 11	0	0

• Molecule 10 is a protein called uL15m.

Mol	Chain	Residues		At	oms			AltConf	Trace
10	J	220	Total 1746	C 1119	N 326	O 298	${ m S} { m 3}$	0	0

• Molecule 11 is a protein called uL16m.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
11	K	195	Total 1573	C 1001	N 297	0 270	$\frac{S}{5}$	0	0

• Molecule 12 is a protein called bL17m.

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

• Molecule 13 is a protein called bL19m.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	М	151	Total 1206	C 766	N 220	0 217	${ m S} { m 3}$	0	0

• Molecule 14 is a protein called bL21m.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	Ν	118	Total 948	C 598	N 177	0 171	${ m S} { m 2}$	0	0

• Molecule 15 is a protein called uL22m.

Mol	Chain	Residues		Ate		AltConf	Trace		
15	0	225	Total 1826	C 1169	N 332	O 320	${ m S}{ m 5}$	0	0

• Molecule 16 is a protein called uL23m.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
16	Р	207	Total 1729	C 1104	N 310	O 309	S 6	0	0

• Molecule 17 is a protein called uL24m.

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

• Molecule 18 is a protein called bL27m.

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

• Molecule 19 is a protein called bL28m.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	S	185	Total 1543	C 994	N 281	O 265	${ m S} { m 3}$	0	0

• Molecule 20 is a protein called uL29m.

Mol	Chain	Residues		At	AltConf	Trace			
20	Т	216	Total 1792	C 1139	N 324	O 325	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 21 is a protein called uL30m.



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

• Molecule 22 is a protein called bL31m.

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

• Molecule 23 is a protein called bL32m.

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

• Molecule 24 is a protein called bL33m.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
24	Х	64	Total 512	C 330	N 96	O 86	0	0

• Molecule 25 is a protein called bL34m.

Mol	Chain	Residues		Aton	ns	AltConf	Trace	
25	Y	46	Total 385	С 245	N 82	O 58	0	0

• Molecule 26 is a protein called bL35m.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
26	Ζ	62	Total 508	C 322	N 111	0 74	S 1	0	0

• Molecule 27 is a protein called bL36m.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
27	0	38	Total	С	N	0	S	0	0
	_		324	205	66	50	3	_	-

• Molecule 28 is a protein called mL38.



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

• Molecule 29 is a protein called mL40.

Mol	Chain	Residues		At	oms			AltConf	Trace
29	2	113	Total 944	${ m C} 597$	N 174	0 168	${ m S}{ m 5}$	0	0

• Molecule 30 is a protein called mL41.

Mol	Chain	Residues		At	oms			AltConf	Trace
30	3	130	Total 1046	C 671	N 189	0 183	${ m S} { m 3}$	0	0

• Molecule 31 is a protein called mL43.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	4	138	Total 1117	C 700	N 219	O 193	${ m S}{ m 5}$	0	0

• Molecule 32 is a protein called mL44.

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

• Molecule 33 is a protein called mL46.

Mol	Chain	Residues		At	oms			AltConf	Trace
33	6	234	Total 1932	C 1250	N 327	O 353	${ m S} { m 2}$	0	0

• Molecule 34 is a protein called mL49.

Mol	Chain	Residues		At	oms			AltConf	Trace
34	7	106	Total 858	C 553	N 151	0 152	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 35 is a protein called mL50.



Mol	Chain	Residues		At	AltConf	Trace			
35	8	199	Total 1629	C 1032	N 278	0 315	$\frac{S}{4}$	0	0

• Molecule 36 is a protein called mL57.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
36	9	202	Total 1587	C 1014	N 279	O 289	${f S}{5}$	0	0

• Molecule 37 is a protein called mL58.

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

• Molecule 38 is a protein called mL59.

Mol	Chain	Residues		At	oms			AltConf	Trace
38	b	155	Total 1299	C 850	N 225	0 221	${ m S} { m 3}$	0	0

• Molecule 39 is a protein called mL60.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	с	119	Total 1004	C 645	N 191	O 164	$\frac{S}{4}$	0	0

• Molecule 40 is a protein called mL67.

Mol	Chain	Residues		At	oms			AltConf	Trace
40	d	206	Total 1746	C 1117	N 318	0 304	${f S}7$	0	0

• Molecule 41 is a protein called bS1m.

Mol	Chain	Residues		At	oms			AltConf	Trace
41	AA	203	Total 1610	C 1032	N 285	0 288	${S \atop 5}$	0	0

• Molecule 42 is a protein called uS2m.



Mol	Chain	Residues		At	AltConf	Trace			
42	BB	266	Total 2085	C 1313	N 366	O 404	${ m S} { m 2}$	0	0

• Molecule 43 is a protein called uS3m.

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

• Molecule 44 is a protein called uS4m.

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

• Molecule 45 is a protein called uS5m.

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

• Molecule 46 is a protein called bS6m.

Mol	Chain	Residues		At	oms	AltConf	Trace		
46	\mathbf{FF}	125	Total 1002	C 639	N 182	O 177	${S \over 4}$	0	0

• Molecule 47 is a protein called uS7m.

Mol	Chain	Residues		At	oms	AltConf	Trace		
47	GG	161	Total 1282	C 811	N 238	0 228	${ m S}{ m 5}$	0	0

• Molecule 48 is a protein called uS8m.

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

• Molecule 49 is a protein called uS9m.



Mol	Chain	Residues		Ate	AltConf	Trace			
49	II	226	Total 1820	C 1167	N 332	O 316	${f S}{5}$	0	0

• Molecule 50 is a protein called uS10m.

Mol	Chain	Residues		At	oms	AltConf	Trace		
50	JJ	186	Total 1508	C 964	N 259	0 281	$\frac{S}{4}$	0	0

• Molecule 51 is a protein called uS11m.

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

• Molecule 52 is a protein called uS12m.

Mol	Chain	Residues		At	oms	AltConf	Trace		
52	LL	124	Total 948	C 585	N 194	0 165	${S \atop 4}$	0	0

• Molecule 53 is a protein called uS13m.

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

• Molecule 54 is a protein called uS14m.

Mol	Chain	Residues		At	oms	AltConf	Trace		
54	NN	115	Total 953	C 612	N 182	0 154	${ m S}{ m 5}$	0	0

• Molecule 55 is a protein called uS15m.

Mol	Chain	Residues		Ate	AltConf	Trace			
55	00	238	Total 1962	C 1227	N 371	O 356	S 8	0	0

• Molecule 56 is a protein called bS16m.



Mol	Chain	Residues		At	AltConf	Trace			
56	PP	116	Total 919	$\begin{array}{c} \mathrm{C} \\ 586 \end{array}$	N 172	0 159	${ m S} { m 2}$	0	0

• Molecule 57 is a protein called uS17m.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
57	QQ	204	Total 1683	C 1055	N 315	O 308	${ m S}{ m 5}$	0	0

• Molecule 58 is a protein called bS18m.

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

• Molecule 59 is a protein called uS19m.

Mol	Chain	Residues		At	oms	AltConf	Trace		
59	SS	80	Total 636	C 408	N 115	0 111	${ m S} { m 2}$	0	0

• Molecule 60 is a protein called bS21m.

Mol	Chain	Residues		At	oms	AltConf	Trace		
60	TT	92	Total 760	C 475	N 150	0 130	${ m S}{ m 5}$	0	0

• Molecule 61 is a protein called mS23.

Mol	Chain	Residues		At	AltConf	Trace			
61	UU	233	Total 1907	C 1211	N 331	O 358	${f S}7$	0	0

• Molecule 62 is a protein called mS26.

Mol	Chain	Residues		At	AltConf	Trace			
62	VV	233	Total 1872	C 1189	N 338	0 342	${ m S} { m 3}$	0	0

• Molecule 63 is a protein called mS29.



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

• Molecule 64 is a protein called mS33.

Mol	Chain	Residues		At	oms			AltConf	Trace
64	XX	96	Total 774	C 496	N 140	0 135	${f S}\ 3$	0	0

• Molecule 65 is a protein called mS35.

Mol	Chain	Residues		Ate		AltConf	Trace		
65	YY	269	Total 2258	C 1429	N 404	0 421	$\frac{S}{4}$	0	0

• Molecule 66 is a protein called mS37.

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

• Molecule 67 is a protein called mS38.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
67	11	34	Total 303	C 183	N 75	0 43	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 68 is a protein called mS41.

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

• Molecule 69 is a protein called mS42.

Mol	Chain	Residues		At	oms			AltConf	Trace
69	33	244	Total 1953	C 1261	N 328	O 359	${f S}{5}$	0	0

• Molecule 70 is a protein called mS43.



Mol	Chain	Residues		At	oms			AltConf	Trace
70	44	270	Total 2169	C 1380	N 370	O 412	${f S}{7}$	0	0

• Molecule 71 is a protein called mS44.

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

• Molecule 72 is a protein called mS45.

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

• Molecule 73 is a protein called mS46.

Mol	Chain	Residues		At	oms	AltConf	Trace		
73	77	165	Total 1330	C 854	N 214	O 259	${ m S} { m 3}$	0	0

• Molecule 74 is a protein called mS47.

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

• Molecule 75 is a RNA chain called 15S ribosomal RNA.

Mol	Chain	Residues		1	AltConf	Trace			
75	aa	1501	Total 31883	C 14338	N 5633	O 10411	Р 1501	0	0

• Molecule 76 is a RNA chain called tRNA.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
76	bb	76	Total 1615	C 723	N 289	O 528	Р 75	0	0

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



Mol	Chain	Residues		Aton	ns	AltConf	Trace	
77	сс	94	Total 470	C 282	N 94	O 94	0	0

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

Mol	Chain	Residues	Atoms			AltConf	Trace	
78	dd	151	Total	С	Ν	0	0	0
		-	755	453	151	151	_	_

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

Mol	Chain	Residues	Atoms	AltConf
79	А	183	Total Mg 183 183	0
79	BB	1	Total Mg 1 1	0
79	LL	1	Total Mg 1 1	0
79	MM	1	Total Mg 1 1	0
79	QQ	1	Total Mg 1 1	0
79	WW	1	Total Mg 1 1	0
79	aa	111	Total Mg 111 111	0

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

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

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

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

• Molecule 82 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\rm C_{10}H_{15}N_5O_{11}P_2).$





Mol	Chain	Residues	Atoms				AltConf	
00	11/11/	1	Total	С	Ν	Ο	Р	0
82	VV VV	1	28	10	5	11	2	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 21S ribosomal RNA









• Molecule 6: uL6m

Chain F:	91%	9%
817 124 124 138 148 148 148 148 148 148 148 148 148 14	1111 1115 1116 1116 1122 1122 1122 1122	
• Molecule 7: bL9m		
Chain G:	95%	5%
810 112 112 112 165 166 166 180 183		
• Molecule 8: uL13m		
Chain H:	90%	10%
82 R14 V19 127 137 137 127 146 V46 V46 T60 T60 T68 R83 R83 R83 R83	C102 1123 1123 1140 1140 1158 0161	
\bullet Molecule 9: uL14m		
Chain I:	84%	8% 8%
M1 12 12 12 12 12 14 14 14 14 14 14 14 14 14 14 14 14 14	R62 172 172 199 119 119 119 1138 1138	
• Molecule 10: uL15m		
Chain J:	90%	10%
V58 160 150 150 177 177 177 177 185 185 177 185 185 185 185 185 185 199 1111 11111 11111 111111 1111111111	V125 L130 F141 P156 K162 K162 K209 R241 R241 R241 R246 R246 R246 R246 R246	E273 K277
• Molecule 11: uL16m		
Chain K:	88%	12% •
K38 E40 E40 E40 E40 E40 B94 B94 B94 C114 C110 C114 C1113 C1114 C11	1115 K130 M139 E150 E158 E158 E158 A168 E158 F192 F192 F192 F192 F192 F192 F192 F192	K227 222 8232
\bullet Molecule 12: bL17m		
Chain L:	88%	8% •
12 87 88 842 152 166 166 166 166 166 114 114 114 114	M145 M145 M145 M145 M148 M178 M178 M178 M178 M178 M178 M178 M17	THK LYS PRO S230 R237 P238

 \bullet Molecule 13: bL19m



Chain M:	91%	9% •
Y16 V28 Y29 P30 V76 F90	194 1102 1110 1111 1114 1114 1114 1121 1121	
• Molecule 1	l4: bL21m	
Chain N:	95%	•••
T44 D45 T46 L76 V105 P108	1100 11123 1116 1118 1100	
• Molecule 1	15: uL22m	
Chain O:	93%	7%
885 8103 1107 8111 1112 1112	K117 D135 L140 V163 1203 L265 L228 L228 L228 L228 L228 L228 L228 R276 N276	
• Molecule 1	l6: uL23m	
Chain P:	94%	6%
D65 192 1108 F113 D117	1161 1169 1169 1227 1227 1227 1265 1265 1265	
• Molecule 1	17: uL24m	
Chain Q:	88% 7%	·
82 R14 E51 I83 F86	N119 191 191 191 191 113 113 113	1243 1246 1246 1257 1269
E297		
• Molecule 1	18: bL27m	
Chain R:	91% 7	% •
835 167 163 177 185	R94 197 197 197 197 117 117 1172 1173 1173 1173 1173 1173	GLY LYS LYS SER 1345 L371
• Molecule 1	l9: bL28m	
Chain S:	80% 6% 14%	5
K67 K67 V79 K95	V101 V101 1132 ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	V231



 \bullet Molecule 20: uL29m

Chain T:	85%	11% •
A15 T17 T17 T17 D32 D32 P32 F48 F48 F48 F55 T57 T57 T57 F86	H89 L98 Q117 L122 L122 L122 L122 L122 L127 L144 T144 T144 T144 T145 M149 W150 W150 U151	L170 D192 PRD ASP ASP ASP ASP C203 C213 C213 C213 C213 C213 C213 C213 C21
ASN 1220 R239		
• Molecule 21: uL30m		
Chain U:	89%	11%
V6 V6 11 119 119 122 V23 V23 V23		
• Molecule 22: bL31m		
Chain V:	50% ·	47%
MET LEU LEU LEU SER TLE PHE ALA ALA ALA SER SER SER TVB SER TVB	T20 S61 S61 ASP ASP ASP ASP ASP ASS ASP ASS ASS ASS	S110 VAL VAL SER THR THR FRA SER SER SER CLU CLU CLUS CLUS CLUS CLUS CLUS CLUS C
GLU LYS GLU ASP VAL SER GLU LYS MET ASP TYS ASP TYS LEU V LEU V	LEU ASP ASP ASP ASP ASP CLN GLN CLN CLN CLN CLN CLN CLN CLN CLN CLN C	
• Molecule 23: bL32m		
Chain W:	95%	5%
472 C104 M118 M118 L148 L148 L153 L153 L153 D188		
• Molecule 24: bL33m		
Chain X:	84%	16%
86 111 111 113 113 125 125 135 135 135 135 135 135 135 135 135 13	R67	
\bullet Molecule 25: bL34m		
Chain Y:	91%	9%
K60 R73 G88 R13 H106 H105		
• Molecule 26: bL35m		
Chain Z:	94%	6%

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• Molecule 27: bL36m

Chain 0:	89%	11%
F56 V62 D68 C93		
\bullet Molecule 28: mL38		
Chain 1:	94%	6%
H20 L32 L32 L32 L32 L32 L32 L13 L106 L106 E109 P113	117 1165 1165 1165 1167 1171 1171 1171 1	L315 R367
• Molecule 29: mL40		
Chain 2:	88%	11% •
334 440 841 841 841 843 146 847 847 847 848 847 848 847 848 847 848 847 848 847 848 847 848 847 848 848	R100 L104 R124 M127 R146	
\bullet Molecule 30: mL41		
Chain 3:	94%	6%
L17 K54 161 161 165 178 K78 K78 K91 K91 K91		
• Molecule 31: mL43		
Chain 4:	91%	9%
V2 11 11 11 11 12 72 12 72 12 72 12 72 127 127	R139 R139 R133 R133	
\bullet Molecule 32: mL44		
Chain 5:	90%	10%
687 170 187 187 187 190 190 1110 1111 1110 1111	A138 N142 N167 N188 S192 S192 Q204 N203 Q204 N203 Q204 N203 Q204 N205 C21 C22 C27 C27 C27 C27 C27 C27 C27 C27 C27	K248 V260 W268 A259 V270 V270 V270 V270 V279 V279 V279 V279 V279 V220
V324 R329 H339 V340 V390		
• Molecule 33: mL46		



Chain 6:	75%	8%	17%
MET LYS LYS ASUL ASU MET LEU LEU LEU THR THR THR THR THR THR THR THR THR THR	V27 K47 Y51 F56 B60 M60 W61 T62 T62 T62 T62 T62 T62 T62 T62 T62 T62	K111 L116 SER ASP ASP SER	THR VAL ALA ALA PHE SER ASN ASN ASN GLN GLN GLN GLN
SER LYS ASP ASP ASP ASP A136 A196 A196 A196 A196 A196 A196 A196 A19	VAL VAL ALX SER ASP ASP ASP ASP 1257 1257 1257 1257 1277 1277 1277 1277		
• Molecule 34: mL49			
Chain 7:	87%		13%
441 147 156 156 196 196 1103 1103 1111 1111 1111 1111	1128 V135 K144 F146		
• Molecule 35: mL50			
Chain 8:	/1%	5% 2	25%
MET SER SER LEU LEU LEU LEU HIS PRO PRO PRO PRO CYS PRO PRO CYS FILEU TRP CYS FILEU CYS FILEU CYS FILEU CYS FILEU CYS SER CYS CYS CYS SER CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	LTS CTA ALA ALA ALA ALA ALA ALA ALA ALA ALA A	PRO VAL LYS ASP LYS LYS GLN	LEU LLE LLF LLF ASP ASP GLU GLU ASN GLU
ALA SER SER SER GLN GLN SER SER ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	L194 L194 L258 L258		
\bullet Molecule 36: mL57			
Chain 9:	86%		7% 6%
V29 P36 P36 P36 P36 P36 P36 P36 P36 P36 P36	SELY SELA ALA ALA CUU CVS SELU CVS CVS CVS CVS CVS CUU CUU CUU CUU CUU CUU CUU CUU CUU CU	E210 K211 A212 L221 D222 K223	V230 K243
\bullet Molecule 37: mL58			
Chain a:	97%		•
K19 K25 710 710 8105 8105 8105 8126 8126 8133 8133			
\bullet Molecule 38: mL59			
Chain b:	97%		•
13 132 132 119 119 119 119 119 119 119 119			
\bullet Molecule 39: mL60			
Chain c:	98%		





 \bullet Molecule 40: mL67

Chain d:		94%		
M1 L66 R67 R68 R68 R68 R104 THR THR	ALM ALM CUV LYS CUV LYS CLN CUV ALC PRAL A158 A158 A158 A158 A158 A158 A158 A158			
• Molecule 41:	bS1m			
Chain AA:	54%	5%	41%	
MET 12 143 144 145 145 154	L63 170 171 176 176 176 183 183 183 183	TY US TY US TILE SER ARG CLU CLU ARD ALA ALA ALA LLY LLY	SER LEU PHE LIYS CLYS CLYS CLY MET ALA ALA ALA ALA ALA ALA	LYS LYS ARG LEU
LYS LYS LYS THR THR ALA ALA ILE ILE ARG SER SER SER	ASP ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	LYS LEU ASN SER SER ASN LYS CLU CLU TYR TYR VAL	PHE LEU LEU LYS LYS LYS CLU CLU K195 F196 F196 F206	VAL VAL LYS
GLU ASN ASN ASN ASN LYS LYS LZ44 F26	L297 L298 L298 PR0 PR0 C29 C20 C20 C20 C20 C20 C20 C20 C20 C20 C20	ARG ARG TTYR TTYR TTYR TTYR FRO FRO ARG ARG ARG	ARG PRO SER VAL SER CALY CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	GLY ASN
• Molecule 42:	uS2m			
Chain BB:		83%	15% •	
P128 L132 L146 K159 K159	100 1183 1183 1183 1183 1183 1183 1183 1	H215 H216 1219 L226 L249 K256 K256 K256 K256 K256	1286 1276 1275 1275 1276 1276 1276 1278 1278 1278 1278 1278 1278 1278 1278	N324
N328 R329 E333 E333 R339 R339 T342	13 67 13 75 13 75 13 75 13 75 13 75 13 75 13 75 13 75 13 75			
• Molecule 43:	uS3m			
Chain CC:	7:	2%	12% • 15%	
MET MET LYS LYS LEU LEU LEU ASN MET LEU LEU	A CANADA	TARN LEU ASP ASP ASP AST ASP AST PRO PRO PRO PRO PRO PRO PRO ANA	ILE PRO PRO PRO PRO ISO ISO ISO ISO ISO ISO ISO ISO ISO IS	L119 L119 N129
11 40 H1 44 L1 49 L1 49 M158 ASP ASP	ASN ASN ASN ASN ASN ASN 1166 1179 1179 1181 1181 1181	N1260 N1390 V212 V213 V214 V214 V214 V215 V221 S221 V223 V223 V223 V223 V223	N263 N263 N263 N263 N263 N280 ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	ASN TYR ASN ASN
ASN N295 N295 N304 N304 N306 N306 N306 N306 N306 N306	1310 1311 1311 1311 1319 1319 1320 1324 1329 1329 1329 1329 1330 1331	T344 L358 W359 W359 N374 M379 M382 M382	1391	
• Molecule 44:	uS4m			
Chain DD:	51%	7% •	41%	





• Molecule 49: uS9m



Chain II:	82%	10%	7%	
R35 P39 F61 A 7 A 7	ASN ASN ALV GLU GLN GLN GLN GLN CLS CLS CLS CLS CLS CLS CLS CLS CLS CLS	T164 1176	L183 T215	E225 M228
K248 R254 R257 P264 W275	R277 R278			
• Molecule 50	0: uS10m			
Chain JJ:	82%	14%		
11 7 11 7 11 7 11 9 19 19 19 19 12 9 13 2 13 2	Y38 A43 D51 D51 D51 D51 D50 D50 D50 066 Y67 T70 T70 T71 T71 T73 T73 T73 T73 T73 T73 T73 T73 T73 T73	V120 L121 L124	1125 M133	N174 D175 D176
L200 E201				
• Molecule 5	1: uS11m			
Chain KK:	77%	19%		·
K70 L78 S92 N99 HHE HIS	L15 L16 L16 L16 L16 L124 L124 L124 L124 L124 L124 L128 L124 L128 L128 L128 L128 L128 L161 L161 L161 L161 L161 L161 L161 L16	K186 V192	K193 K194 I198	T202 R210
R216 L217				
• Molecule 52	2: uS12m			
Chain LL:	81%	17	%	•
A29 T30 K35 K35 K44 K44 K44 K46	847 847 V66 V67 L68 K71 K72 K72 R82 R82 R82 R82 R82 V108 L119 V120 V120 V121 V124 K148 K148 K148 K148			
• Molecule 53	3: uS13m			
Chain MM:	76%	229	%	•
V2 I5 L6 F10 A19 V25	L39 L39 L39 L39 L39 L58 L58 L58 L58 L58 L58 L58 L58 L57 L57 L57 L57 L57 L57 L57 L57 L57 L57	R120 G121		
• Molecule 54	4: uS14m			
Chain NN:	84%	1	2% •	-
M1 L12 L22 L22 E35 L37	F43 R46 M69 K70 F86 F86 F86 F86 F89 F89 F89 F89 F89 F89 F89 F89 F89 F89			
• Molecule 5	5: uS15m			



Chain OO:	82%	11% • 6%	
834 141 168 168 168 168 168	A81 195 A112 A112 A112 A112 A124 A124 A124 A128 A128 A128 A128 A128 A173 A181 A181 A181 A182 A173 A182 A173 A181 A182 A173 A182 A173 A182 A176 A176 A176 A176 A176 A176 A176 A176	1192 1205 1206 1206 1206	L219 1227
1231 1232 1233 1234 1234 1234 1234 1234	R275 R280 R283 F286		
• Molecule 5	56: bS16m		
Chain PP:	90%	7% • •	I
T2 R3 N22 V39	L40 V86 K92 K92 K100 K100 K1100 K1100 L120		
• Molecule 5	57: uS17m		
Chain QQ:	75% 11%	14%	I
MET A2 V20 V22 V22 E25	133 134 137 137 137 137 134 144 144 144 144 145 145 176 176 176 178 178 178 178 178 178 178 178 178 178	L135 SER SER SER GLY T140 T140	LIT' R150 TYR
GLY ILE GLN ASP PHE SER GLN E159	L172 1186 1186 C200 C200 C200 C200 C200 C200 C200 C20		
• Molecule 5	58: bS18m		
Chain RR:	84%	8% 8%	
K40 141 L49 D68 Q72 ALA	ASN LYS ASN ASN ASN ASN ASN ASN ASN 1104 1104 1123 1135 1135 1135		
• Molecule 5	59: uS19m		
Chain SS:	79%	20% •	
89 113 114 115 115 116 116 117 117	N2 4 03 0 03 0 15 3 0 15 3 0 15 3 0 15 3 0 15 3 0 15 3 0 15 3 0 15 3 15 4 15 3 15 4 15 3 15 6 5 15 6 5 16 6 16 8 16 8 16 8 16 8		
• Molecule 6	50: bS21m		
Chain TT:	88%	12%	
A86 R99 F117 M124 K144	R153 R156 R156 R156 R156 R156 R156 P171		
• Molecule 6	51: mS23		
Chain UU:	87%	12% •	

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 \bullet Molecule 62: mS26





Chain 11:	88%	12%	
D78 M88 L93 R97 R105			
• Molecule 68	8: mS41		
Chain 22:	96%	•	
130 V38 148 52 E114 E114	M1 28		
• Molecule 69): mS42		
Chain 33:	84% 1	1% ••	
18 121 128 W38 Y44	149 149 167 167 167 167 167 167 198 198 198 198 198 198 198 198	F177 P178 Q181	N186 1204
L210 V214 W217 V237 Y243	1260 822 61 822 62		
• Molecule 70): mS43		
Chain 44:	79% 6%	16%	I
MET LEU LEU ARG PHE THR GLY ALA ALA ALA ILE	ARG ARG TYR TYR ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	ARG ASN ASP MET PRO ASN	ARG D190 N203
P207 R230 ALA LYS GLU ALA GLY ASN	LEU GLU ASP ASP ASP AL E264 E264 E264 CVS CVS E294 CVS CVS CVS CVS CVS CVS CVS CVS CVS CVS		
• Molecule 71	: mS44		
Chain 55:	17% • 83%		I
MET CLY THR THR THR VAL VAL ASN GLU	PRO PRO LEU LEU LEU LEU LEU LEU ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	ARG ASP PRO LYS THR ARG	GLU PRO LEU GLN
PRO ARG PRO PRO VAL LYS PRO LEU SER LYS	TILE ASN ASN ASN ASN ASN ASN ASN SER SER SER FILE FILE FILE FILE FILE FILE FILE FILE	MET VAL GLY LEU LEU TYR	GLY ILE GLU HIS
LYS PHE LEU LYS ALA GLN ASN PRO SER YAL	PHE PHE 1115 PHE PHE PHE PHE ASN PHE PHE ASN PHE PHE ASN PHE PHE ASN PHE PHE ASN PHE PHE ASN PHE PHE ASN PHE PHE PHE PHE PHE PHE PHE PHE PHE PHE	LEU ASN ARG LYS ASN ASN	THR GLY LEU ALA
ASN TLE LEU VAL ALA ALA THR LEU GLY GLN GLN	ILE CLY CLY PHE PHC CLU CLU CLU CLU CLU CLU CLU PHC CLU CLU PHC CLU PHC CLU PHC CLU PHC CLU PHC CLU PHC CLU PHC CLU PHC CLU PHC CLU CLY PHC CLU CLY PHC CLU CLY PHC CLU CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	LEU ILE ALA ARG THR LEU	LEU ASP ILE ASP
GLN HIS ASN ASN ALA GLN CLU CLU CLU CLU CLU	PLE PLE TTRE ARG ALN ALSN ALSN ALSN ALSN ALSN ALSN ALL ALN ALL ALL ALL ALL ALL ALL ALL AL	LYS	

 \bullet Molecule 72: mS45



Chain 66:	88%	8% •	
F27 Y37 T81 Y87 I88	P80 P80 P90 P90 P136 P136 P136 L149 P136 L149 P136 L149 P136 L153 P136 L153 P136 L153 P136 L153 P136 L153 P136 L153 P126 L153 P126 L153 P126 L17 P127 L24 P255 L256 P257 L24 P257 L257 P267 L257 P257 L257 P257 L247 P257 L256 P257 L257 P267 L257 P267 L256 P267 L247 P267 L247 P267 L247 P267 L247 P267 L247 P267 L247 P27	THR ASN LYS LYS Y307 F309 F309	G318
R333 1345			
• Molecule	73: mS46		
Chain 77:	92%	8% •	
8197 L202 E212 P215	C247 47 T256 1256 1256 1256 1265 1256 1265 1265 1265 1270 1265 1270 1265 1270 1265 1270 1265 1270 1270 1270 <tr< td=""><td></td><td></td></tr<>		
• Molecule	74: mS47		
Chain 88:	87%	11% ••	
A36 T46 A47 R48 R48 T82	I118 I131 1131 1131 1138 1138 1145 1145 1145 1145 1145 1145 1155 1145 1155	R237 1297 L304 1320 L325	-
S328 L336 L336 L338 V339 L355	A369 M363 M363 M363 M363 M363 L368 L368 L368 L368 M369 M423 M423 M423 M449 M449 M449 M449 M449 M449 M449 M44		
• Molecule	75: 15S ribosomal RNA		
Chain aa:	63% 27%	• 9%	
9 D A A A A A A	u u U 14 414 414 414 414 435 435 446 446 446 446 455 455 455 455 455 45	U99 100 101 102 102 102 103 104 108	A109
A116 A119 A120 U121 U123	U124 4126 4126 4126 4126 4137 4133 4137 4133 4147 4145 4145 4145 4145 4145 4145 4145	A182 U A185 A197 A198	U208
A209 U210 U A A214 U215 A216	U219 U219 U223 U223 U224 U224 U224 A235 A235 A235 A235 A235 A235 A235 A255 A25	A294 A298 U299 A304 A312	-
C318 U334 A335 U336 A337 A337 U347	A348 U349 A351 G352 G352 C356 G371 C376 C376 C376 A339 A414 C376 C380 C376 C376 C376 C376 C376 C376 C376 C376	PCCAPCCC	U
A A A D A D D A	А С С С С С С С С С С С С С С С С С С С	U495 A496 A497 A498 A502 A503 A503	A509
U510 U526 G527 U531 U532	A 537 A 538 A 540 A 540 A 540 A 542 A 550 A 555 A 5555 A 5555 A 5555 A 5555 A 5555 A 5555 A 5555 A 5555 A	A C C A C C A C C	n



U A A A A A A A A A A A A A A A A A A A
UT14 UT14 A715 A726 UT29 A732 A732 A732 A732 A733 A753 A753 A753 A753 A753 A753 A761 UT75 A769 A764 A764 A764 A763 A764 A763 A764 A764 A764 A764 A764 A764 A764 A764
A880 A881 C882 C882 C882 C882 A881 A881 A881 A892 A912 A913 A915 A915 A916 A916 A916 A916 A933 A933 A923 A916 A916 A933 A936 A933 A936 A936 A936 A936 A93
C1035 A1035 A1035 A1042 A1042 A1043 A1043 A1048 A1048 A1057 A1057 A1056 A1056 A1056 A1056 A1058 A1058 A1058 A1058 A1079 A1079 A1078 A1088 U10888 U10888 U1088 U1088 U1088 U1088 U1088 U1088 U1088 U1088 U1088 U108
A1152 A1152 A1154 C1154 C1155 A1177 U1176 U1177 A1177 A1177 A1178 U1188 U1188 U1188 U1188 U1188 U1188 U1198 U1198 U1198 A1233 A1233 A1233 A1228 A1228 A1228 A1228 A1228 A1228 A1228 A1228 A1228 A1228 A1228 A1228 A1228 A1270 A1277 A1278 A1270 A1277 A1278 A1277 A1278 A1277 A1278 A1277 A1278 A12888 A1288 A1288 A1288 A1288 A12888 A12888 A12888 A12888 A12888 A12888 A12888 A12888 A128888 A128888 A12888 A128888 A128888 A128888 A12888888 A128888 A128888888 A128888888888
A1376 A1376 A1281 A1281 A1281 A1281 A1281 A1281 A1291 A1291 A1291 A1291 A1291 A1291 A1291 A1291 A1291 A1291 A1291 A1291 A1291 A1291 A137 A137 A137 A137 A137 A137 A137 A13
U A 1367 U U U 1368 01372 01372 01372 1372 01372 1388 01372 01388 01388 01388 01388 01388 01388 01414 01414 01414 01414 01445 01433 01445 0145 01
U1474 U1474 C1487 C1487 C1487 A1496 A1500 A1510 A1510 U1500 A1510 A1510 U1511 U1512 U1512 U1523 U1538 U1538 U1538 U1558 U1558 U1558 U1558 U1558 U1558 U1558 U1558 U1558 U1598 U1599 U1599 U1599 U1599 U1599 U1599 U1599 U1599 </td
AI 611 C1 612 C1 612 C1 622 C1 623 D1 625 AI 628 AI 628 AI 628 AI 632 D1 641 C1 644 D1 640 D1 646 D1 649 AI 639 D1 640 D1 640 D1 648 D1 649 D1 649 D1 649 D1 649
• Molecule 76: tRNA
Chain bb: 42% 57% .
G1 G1 1 1
Y V
\bullet Molecule 77: unknown protein sequence 1
Chain cc: 100%
There are no outlier residues recorded for this chain.
\bullet Molecule 78: unknown protein sequence 2
Chain dd: 100%







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55448	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	23.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II $(4k \ge 4k)$	Depositor
Maximum map value	0.590	Depositor
Minimum map value	-0.375	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.00586	Depositor
Map size (Å)	442.2, 442.2, 442.2	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mal	Chain	Bond lengths		Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.23	0/64517	0.70	14/100359~(0.0%)	
2	В	0.34	0/2573	0.69	1/3456~(0.0%)	
3	С	0.32	0/1975	0.61	0/2657	
4	D	0.35	0/2031	0.66	0/2751	
5	Е	0.33	0/2244	0.57	0/3033	
6	F	0.33	0/1551	0.57	0/2093	
7	G	0.33	0/628	0.57	0/844	
8	Н	0.34	0/1302	0.62	0/1749	
9	Ι	0.32	0/962	0.65	0/1285	
10	J	0.33	0/1783	0.63	0/2384	
11	K	0.34	0/1606	0.65	0/2148	
12	L	0.33	0/1845	0.62	0/2489	
13	М	0.34	0/1224	0.67	0/1651	
14	Ν	0.32	0/961	0.65	0/1295	
15	0	0.32	0/1859	0.62	0/2495	
16	Р	0.33	0/1773	0.60	0/2390	
17	Q	0.34	0/2323	0.57	0/3135	
18	R	0.33	0/2783	0.63	0/3723	
19	S	0.34	0/1576	0.60	0/2104	
20	Т	0.34	0/1837	0.59	0/2486	
21	U	0.34	0/648	0.61	0/870	
22	V	0.35	0/741	0.61	0/995	
23	W	0.31	0/955	0.59	0/1273	
24	Х	0.33	0/520	0.66	0/696	
25	Y	0.35	0/392	0.72	0/515	
26	Ζ	0.34	0/522	0.67	0/695	
27	0	0.33	0/329	0.58	0/432	
28	1	0.34	0/2949	0.58	0/3998	
29	2	0.33	0/963	0.61	0/1295	
30	3	0.34	0/1072	0.60	0/1442	
31	4	0.34	$0/1\overline{138}$	0.69	0/1526	
32	5	0.32	0/2604	0.59	0/3526	



Mal	Chain	Bond	lengths	Bond angles		
NIOI	Ullaili	RMSZ	# Z > 5	RMSZ	# Z > 5	
33	6	0.35	0/1978	0.59	0/2664	
34	7	0.35	0/873	0.61	0/1170	
35	8	0.33	0/1659	0.56	0/2230	
36	9	0.35	0/1616	0.56	0/2177	
37	a	0.34	0/1471	0.64	0/1976	
38	b	0.33	0/1333	0.57	0/1783	
39	с	0.33	0/1028	0.61	0/1372	
40	d	0.33	0/1791	0.61	0/2415	
41	AA	0.33	0/1645	0.60	0/2218	
42	BB	0.35	0/2128	0.67	0/2892	
43	CC	0.34	0/2864	0.58	0/3853	
44	DD	0.35	0/2434	0.63	0/3281	
45	EE	0.33	0/2360	0.59	0/3180	
46	FF	0.39	0/1014	0.64	0/1358	
47	GG	0.34	0/1305	0.61	0/1763	
48	HH	0.33	0/1232	0.70	1/1660~(0.1%)	
49	II	0.34	0/1855	0.62	0/2492	
50	JJ	0.34	0/1544	0.68	2/2091~(0.1%)	
51	KK	0.36	0/1136	0.62	0/1515	
52	LL	0.34	0/963	0.68	0/1292	
53	MM	0.34	0/957	0.64	0/1277	
54	NN	0.35	0/972	0.64	0/1300	
55	00	0.34	0/1985	0.65	0/2647	
56	PP	0.34	0/934	0.64	0/1260	
57	QQ	0.32	0/1694	0.64	0/2252	
58	RR	0.37	0/749	0.66	0/998	
59	SS	0.36	0/652	0.69	0/882	
60	TT	0.37	0/771	0.63	0/1019	
61	UU	0.33	0/1950	0.62	0/2636	
62	VV	0.32	0/1900	0.60	0/2540	
63	WW	0.34	0/3282	0.59	1/4438~(0.0%)	
64	XX	0.35	0/786	0.63	0/1046	
65	YY	0.35	0/2313	0.61	0/3119	
66	ZZ	0.32	0/702	0.58	0/945	
67	11	0.34	0/303	0.84	0/386	
68	22	0.34	0/852	0.56	0/1142	
69	33	0.35	0/2002	0.57	0/2721	
70	44	0.34	0/2214	0.57	0/2990	
71	55	0.35	0/521	0.57	0/701	
72	66	0.34	0/2547	0.58	0/3438	
73	77	0.35	0/1358	0.55	0/1839	
74	88	0.35	0/3646	0.57	0/4935	
75	aa	0.26	0/35686	0.75	33/55477~(0.1%)	



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
76	bb	0.45	0/1805	0.90	5/2811~(0.2%)
All	All	0.30	0/212996	0.67	57/307971~(0.0%)

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
75	aa	1455	G	P-O3'-C3'	-11.24	106.21	119.70
75	aa	44	U	O4'-C1'-N1	10.73	116.78	108.20
75	aa	1119	G	C4'-C3'-O3'	-10.10	88.19	109.40
75	aa	1119	G	C2'-C3'-O3'	9.55	130.51	109.50
75	aa	44	U	C2'-C3'-O3'	-9.27	89.11	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	А	57598	0	28892	216	0
2	В	2527	0	2649	54	0
3	С	1932	0	1969	20	0
4	D	1991	0	2032	5	0
5	Ε	2187	0	2203	16	0
6	F	1524	0	1587	4	0
7	G	617	0	626	1	0
8	Н	1275	0	1310	12	0
9	Ι	956	0	1037	4	0
10	J	1746	0	1840	5	0
11	Κ	1573	0	1629	5	0
12	L	1817	0	1878	9	0
13	М	1206	0	1283	7	0
14	N	948	0	1006	3	0
15	0	1826	0	1933	3	0
16	Р	1729	0	1724	8	0



Conti	Continuea from previous page								
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes			
17	Q	2272	0	2334	6	0			
18	R	2738	0	2811	6	0			
19	S	1543	0	1621	14	0			
20	Т	1792	0	1782	11	0			
21	U	639	0	699	4	0			
22	V	729	0	711	1	0			
23	W	937	0	975	4	0			
24	Х	512	0	563	3	0			
25	Y	385	0	423	3	0			
26	Z	508	0	539	0	0			
27	0	324	0	344	3	0			
28	1	2875	0	2881	11	0			
29	2	944	0	969	9	0			
30	3	1046	0	1071	6	0			
31	4	1117	0	1142	7	0			
32	5	2552	0	2600	18	0			
33	6	1932	0	1950	11	0			
34	7	858	0	908	6	0			
35	8	1629	0	1633	2	0			
36	9	1587	0	1628	7	0			
37	a	1440	0	1473	0	0			
38	b	1299	0	1367	0	0			
39	с	1004	0	1065	0	0			
40	d	1746	0	1743	0	0			
41	AA	1610	0	1639	6	0			
42	BB	2085	0	2094	18	0			
43	CC	2821	0	2829	17	0			
44	DD	2369	0	2436	12	0			
45	EE	2306	0	2324	17	0			
46	FF	1002	0	1086	47	0			
47	GG	1282	0	1338	2	0			
48	HH	1213	0	1277	12	0			
49	II	1820	0	1906	11	0			
50	JJ	1508	0	1505	88	0			
51	KK	1121	0	1171	11	0			
52	LL	948	0	1002	14	0			
53	MM	942	0	1001	17	0			
54	NN	953	0	1007	9	0			
55	00	1962	0	2036	21	0			
56	PP	919	0	982	4	0			
57	QQ	1683	0	1769	16	0			
58	RR	738	0	771	2	0			



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	SS	636	0	654	19	0
60	TT	760	0	791	3	0
61	UU	1907	0	1898	18	0
62	VV	1872	0	1978	8	0
63	WW	3216	0	3315	45	0
64	XX	774	0	821	4	0
65	YY	2258	0	2229	49	0
66	ZZ	687	0	719	15	0
67	11	303	0	357	2	0
68	22	833	0	839	1	0
69	33	1953	0	1913	15	0
70	44	2169	0	2155	6	0
71	55	508	0	524	1	0
72	66	2488	0	2520	9	0
73	77	1330	0	1350	6	0
74	88	3573	0	3576	22	0
75	aa	31883	0	16005	0	0
76	bb	1615	0	821	0	0
77	сс	470	0	102	0	0
78	dd	755	0	167	0	0
79	А	183	0	0	0	0
79	BB	1	0	0	0	0
79	LL	1	0	0	0	0
79	MM	1	0	0	0	0
79	QQ	1	0	0	0	0
79	WW	1	0	0	0	0
79	aa	111	0	0	0	0
80	В	1	0	0	0	0
81	0	1	0	0	0	0
81	W	1	0	0	0	0
82	WW	28	0	12	1	0
All	All	201462	0	157749	837	0

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

The worst 5 of 837 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)
50:JJ:71:ILE:CG1	50:JJ:116:THR:HG21	1.17	1.64
50:JJ:71:ILE:CD1	50:JJ:116:THR:HG21	1.32	1.60



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:JJ:71:ILE:HG12	50:JJ:116:THR:CG2	1.35	1.55
63:WW:243:LYS:NZ	63:WW:246:VAL:HG22	1.25	1.44
50:JJ:68:TYR:CE2	65:YY:163:PRO:HG3	1.55	1.42

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	Perce	entiles
2	В	317/393~(81%)	302~(95%)	15 (5%)	0	100	100
3	C	247/249~(99%)	234~(95%)	11 (4%)	2 (1%)	19	56
4	D	250/252~(99%)	237~(95%)	9 (4%)	4 (2%)	9	44
5	Е	272/274~(99%)	256~(94%)	15 (6%)	1 (0%)	34	69
6	F	194/196~(99%)	183 (94%)	10 (5%)	1 (0%)	29	65
7	G	72/74~(97%)	70~(97%)	2 (3%)	0	100	100
8	Н	158/160~(99%)	152 (96%)	6 (4%)	0	100	100
9	Ι	123/138~(89%)	114 (93%)	9 (7%)	0	100	100
10	J	218/220~(99%)	202~(93%)	15 (7%)	1 (0%)	29	65
11	K	193/195~(99%)	184 (95%)	9 (5%)	0	100	100
12	L	225/237~(95%)	217~(96%)	8 (4%)	0	100	100
13	М	149/151~(99%)	139~(93%)	10 (7%)	0	100	100
14	N	116/118~(98%)	105 (90%)	10 (9%)	1 (1%)	17	54
15	Ο	223/225~(99%)	211 (95%)	12 (5%)	0	100	100
16	Р	205/207~(99%)	196 (96%)	9 (4%)	0	100	100
17	Q	280/296~(95%)	268 (96%)	12 (4%)	0	100	100
18	R	327/337~(97%)	314 (96%)	12 (4%)	1 (0%)	41	74



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
19	S	181/216~(84%)	171 (94%)	10 (6%)	0	100	100
20	Т	210/225~(93%)	199 (95%)	11 (5%)	0	100	100
21	U	80/82~(98%)	78 (98%)	2 (2%)	0	100	100
22	V	87/177~(49%)	83 (95%)	4 (5%)	0	100	100
23	W	110/112~(98%)	105 (96%)	5 (4%)	0	100	100
24	Х	62/64~(97%)	59 (95%)	3 (5%)	0	100	100
25	Y	44/46~(96%)	41 (93%)	3 (7%)	0	100	100
26	Z	60/62~(97%)	56 (93%)	4 (7%)	0	100	100
27	0	36/38~(95%)	33 (92%)	3 (8%)	0	100	100
28	1	346/348~(99%)	330 (95%)	16 (5%)	0	100	100
29	2	111/113~(98%)	106 (96%)	5 (4%)	0	100	100
30	3	128/130~(98%)	122 (95%)	6 (5%)	0	100	100
31	4	136/138~(99%)	130 (96%)	6 (4%)	0	100	100
32	5	322/324~(99%)	306 (95%)	16 (5%)	0	100	100
33	6	228/281~(81%)	221 (97%)	7 (3%)	0	100	100
34	7	104/106~(98%)	97 (93%)	7 (7%)	0	100	100
35	8	195/264~(74%)	192 (98%)	3 (2%)	0	100	100
36	9	198/215~(92%)	186 (94%)	12 (6%)	0	100	100
37	a	175/177~(99%)	163 (93%)	12 (7%)	0	100	100
38	b	153/155~(99%)	146 (95%)	7 (5%)	0	100	100
39	с	117/119~(98%)	112 (96%)	4 (3%)	1 (1%)	17	54
40	d	202/215~(94%)	189 (94%)	13 (6%)	0	100	100
41	AA	197/344~(57%)	190 (96%)	7 (4%)	0	100	100
42	BB	264/266~(99%)	247 (94%)	15 (6%)	2 (1%)	19	56
43	CC	331/398~(83%)	302 (91%)	27 (8%)	2 (1%)	25	61
44	DD	281/486~(58%)	265 (94%)	15 (5%)	1 (0%)	34	69
45	EE	284/293~(97%)	262 (92%)	20 (7%)	2 (1%)	22	59
46	FF	123/125~(98%)	113 (92%)	10 (8%)	0	100	100
47	GG	159/161~(99%)	148 (93%)	10 (6%)	1 (1%)	25	61
48	HH	152/154~(99%)	145 (95%)	7 (5%)	0	100	100
49	II	220/244~(90%)	206 (94%)	12 (6%)	2 (1%)	17	54



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
50	JJ	184/186~(99%)	164 (89%)	14 (8%)	6 (3%)	4	32
51	KK	138/148~(93%)	126 (91%)	11 (8%)	1 (1%)	22	59
52	LL	122/124~(98%)	110 (90%)	11 (9%)	1 (1%)	19	56
53	MM	118/120~(98%)	109 (92%)	8 (7%)	1 (1%)	19	56
54	NN	113/115~(98%)	109 (96%)	4 (4%)	0	100	100
55	00	234/253~(92%)	227~(97%)	7 (3%)	0	100	100
56	PP	112/119~(94%)	105 (94%)	7 (6%)	0	100	100
57	QQ	194/237~(82%)	184 (95%)	9 (5%)	1 (0%)	29	65
58	RR	87/99~(88%)	81 (93%)	6 (7%)	0	100	100
59	SS	78/80~(98%)	71 (91%)	6 (8%)	1 (1%)	12	48
60	TT	90/92~(98%)	86 (96%)	4 (4%)	0	100	100
61	UU	231/233~(99%)	223 (96%)	8 (4%)	0	100	100
62	VV	231/233~(99%)	221 (96%)	10 (4%)	0	100	100
63	WW	399/401~(100%)	368 (92%)	29 (7%)	2 (0%)	29	65
64	XX	91/96~(95%)	88 (97%)	3 (3%)	0	100	100
65	YY	265/273~(97%)	244 (92%)	18 (7%)	3 (1%)	14	51
66	ZZ	83/91~(91%)	74 (89%)	9 (11%)	0	100	100
67	11	32/34~(94%)	31 (97%)	1 (3%)	0	100	100
68	22	97/99~(98%)	89 (92%)	7 (7%)	1 (1%)	15	52
69	33	240/255~(94%)	226 (94%)	13 (5%)	1 (0%)	34	69
70	44	264/321 (82%)	251 (95%)	10 (4%)	3 (1%)	14	51
71	55	55/339~(16%)	53 (96%)	2 (4%)	0	100	100
72	66	301/319~(94%)	291 (97%)	10 (3%)	0	100	100
73	77	$\overline{163/165}\ (99\%)$	146 (90%)	16 (10%)	1 (1%)	25	61
74	88	448/457~(98%)	414 (92%)	31 (7%)	3 (1%)	22	59
All	All	13235/14689~(90%)	12478 (94%)	710 (5%)	47 (0%)	38	69

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	DD	423	THR
4	D	52	LEU
4	D	195	VAL



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Mol	Chain	Res	Type
14	Ν	109	ILE
42	BB	303	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	entiles
2	В	272/337~(81%)	256~(94%)	16~(6%)	19	51
3	\mathbf{C}	210/210~(100%)	197~(94%)	13~(6%)	18	50
4	D	218/218~(100%)	197~(90%)	21 (10%)	8	34
5	Ε	242/242~(100%)	230~(95%)	12~(5%)	24	55
6	F	172/172~(100%)	164 (95%)	8 (5%)	26	56
7	G	68/68~(100%)	66~(97%)	2(3%)	42	67
8	Н	138/138~(100%)	131~(95%)	7(5%)	24	55
9	Ι	108/117~(92%)	104 (96%)	4 (4%)	34	62
10	J	181/181~(100%)	165 (91%)	16 (9%)	10	38
11	Κ	167/167~(100%)	151 (90%)	16 (10%)	8	34
12	L	203/211~(96%)	194 (96%)	9(4%)	28	58
13	М	136/136~(100%)	130~(96%)	6 (4%)	28	58
14	Ν	107/107~(100%)	105~(98%)	2(2%)	57	76
15	Ο	200/200~(100%)	189 (94%)	11 (6%)	21	54
16	Р	185/185~(100%)	181 (98%)	4 (2%)	52	73
17	Q	256/267~(96%)	242 (94%)	14 (6%)	21	54
18	R	303/308~(98%)	292~(96%)	11 (4%)	35	63
19	S	167/191~(87%)	161 (96%)	6 (4%)	35	63
20	Т	204/213~(96%)	197~(97%)	7(3%)	37	64
21	U	73/73~(100%)	71 (97%)	2(3%)	44	69
22	V	74/161~(46%)	71~(96%)	3~(4%)	30	59
23	W	$10\overline{4/104}~(100\%)$	101 (97%)	3 (3%)	42	67



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
24	Х	56/56~(100%)	52~(93%)	4 (7%)	14	46
25	Y	40/40~(100%)	39~(98%)	1 (2%)	47	70
26	Ζ	50/50~(100%)	46 (92%)	4 (8%)	12	42
27	0	36/36~(100%)	35~(97%)	1 (3%)	43	68
28	1	323/323~(100%)	312 (97%)	11 (3%)	37	64
29	2	106/106~(100%)	100 (94%)	6 (6%)	20	53
30	3	112/112~(100%)	110 (98%)	2 (2%)	59	78
31	4	121/121~(100%)	118 (98%)	3 (2%)	47	70
32	5	284/284~(100%)	278 (98%)	6 (2%)	53	74
33	6	213/252~(84%)	205 (96%)	8 (4%)	33	61
34	7	95/95~(100%)	91 (96%)	4 (4%)	30	59
35	8	182/240~(76%)	173 (95%)	9 (5%)	25	55
36	9	176/186~(95%)	168 (96%)	8 (4%)	27	57
37	a	158/158~(100%)	152 (96%)	6 (4%)	33	61
38	b	144/144~(100%)	139 (96%)	5 (4%)	36	63
39	с	110/110~(100%)	109 (99%)	1 (1%)	78	88
40	d	191/199~(96%)	187 (98%)	4 (2%)	53	74
41	АА	177/309~(57%)	168 (95%)	9 (5%)	24	55
42	BB	233/233~(100%)	206 (88%)	27 (12%)	5	27
43	CC	328/385~(85%)	297 (90%)	31 (10%)	8	35
44	DD	256/437~(59%)	229 (90%)	27 (10%)	7	30
45	EE	249/252~(99%)	237~(95%)	12 (5%)	25	56
46	FF	114/114~(100%)	105 (92%)	9 (8%)	12	43
47	GG	138/138~(100%)	132 (96%)	6 (4%)	29	58
48	HH	141/141~(100%)	125 (89%)	16 (11%)	6	28
49	II	196/215~(91%)	186 (95%)	10 (5%)	24	55
50	JJ	167/167~(100%)	151 (90%)	16 (10%)	8	34
51	KK	122/127~(96%)	108 (88%)	14 (12%)	5	28
52	LL	103/103~(100%)	92 (89%)	11 (11%)	6	30
53	MM	100/100~(100%)	92 (92%)	8 (8%)	12	42
54	NN	103/103~(100%)	92 (89%)	11 (11%)	6	30



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
55	00	208/220~(94%)	199 (96%)	9 (4%)	29	58
56	PP	101/104~(97%)	96 (95%)	5 (5%)	24	55
57	QQ	187/218~(86%)	178 (95%)	9 (5%)	25	56
58	RR	80/87~(92%)	74 (92%)	6 (8%)	13	44
59	SS	69/69~(100%)	63 (91%)	6 (9%)	10	39
60	TT	81/81 (100%)	73~(90%)	8 (10%)	8	33
61	UU	208/208~(100%)	198 (95%)	10 (5%)	25	56
62	VV	208/210~(99%)	199 (96%)	9 (4%)	29	58
63	WW	368/368~(100%)	328 (89%)	40 (11%)	6	29
64	XX	84/84 (100%)	79 (94%)	5 (6%)	19	51
65	YY	248/250~(99%)	231 (93%)	17 (7%)	15	47
66	ZZ	78/82~(95%)	71 (91%)	7 (9%)	9	37
67	11	32/32~(100%)	31 (97%)	1 (3%)	40	65
68	22	90/90~(100%)	89~(99%)	1 (1%)	73	85
69	33	216/231~(94%)	204 (94%)	12 (6%)	21	53
70	44	238/281~(85%)	229 (96%)	9 (4%)	33	61
71	55	53/303~(18%)	51 (96%)	2 (4%)	33	61
72	66	277/289~(96%)	269~(97%)	8 (3%)	42	67
73	77	158/158 (100%)	152 (96%)	6 (4%)	33	61
74	88	401/404 (99%)	377 (94%)	24 (6%)	19	51
All	All	11997/13111 (92%)	11320 (94%)	677 (6%)	25	53

5 of 677 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
52	LL	148	LYS
63	WW	325	MET
54	NN	37	LEU
52	LL	144	LYS
60	TT	144	LYS

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



Mol	Chain	Res	Type
19	\mathbf{S}	226	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	2677/3296~(81%)	608~(22%)	107 (3%)
75	aa	1473/1649~(89%)	444 (30%)	0
76	bb	75/76~(98%)	42~(56%)	0
All	All	4225/5021 (84%)	1094~(25%)	107 (2%)

5 of 1094 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	А	26	А
1	А	27	А
1	А	28	U
1	А	30	U
1	А	35	U

5 of 107 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	А	1706	G
1	А	2329	А
1	А	3154	U
1	А	1708	А
1	А	2304	А

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 303 ligands modelled in this entry, 302 are monoatomic - leaving 1 for Mogul analysis.



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

Mol Type Chain	hain Res		Ros	Bos	Tink	Bo	ond leng	ths	B	ond ang	les
	Mol Type Chain Res	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
82	GDP	WW	501	79	24,30,30	0.98	1 (4%)	30,47,47	1.33	4 (13%)	

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
82	GDP	WW	501	79	-	5/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
82	WW	501	GDP	C6-N1	-2.22	1.34	1.37

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
82	WW	501	GDP	PA-O3A-PB	-3.71	120.09	132.83
82	WW	501	GDP	C3'-C2'-C1'	2.58	104.87	100.98
82	WW	501	GDP	C5-C6-N1	2.47	118.32	113.95
82	WW	501	GDP	C8-N7-C5	2.44	107.64	102.99

All (4) bond angle outliers are listed below:

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	WW	501	GDP	C5'-O5'-PA-O2A
82	WW	501	GDP	C3'-C4'-C5'-O5'
82	WW	501	GDP	O4'-C4'-C5'-O5'
82	WW	501	GDP	C5'-O5'-PA-O3A
82	WW	501	GDP	C5'-O5'-PA-O1A



There are no ring outliers.

1 monomer is involved in 1 short contact:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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

The worst 5 of 25 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	dd	115:UNK	С	151:UNK	Ν	40.49
1	dd	220:UNK	С	265:UNK	Ν	35.53
1	dd	170:UNK	С	202:UNK	Ν	27.02
1	сс	59:UNK	С	76:UNK	Ν	22.66
1	сс	93:UNK	С	105:UNK	Ν	20.48



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3552. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



The images above show the map projected in three orthogonal directions.



6.2 Central slices (i)

6.2.1 Primary map



X Index: 165





Z Index: 165

6.2.2 Raw map



X Index: 165

Y Index: 165

Z Index: 165

The images above show central slices of the map in three orthogonal directions.



6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 196





Z Index: 163

6.3.2 Raw map



X Index: 196

Y Index: 159

Z Index: 154

The images above show the largest variance slices of the map in three orthogonal directions.



6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00586. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 4197 nm^3 ; this corresponds to an approximate mass of 3791 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.267 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.267 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{B}_{\text{osolution ostimato}}(\hat{\mathbf{A}})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.51	7.42	4.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.51 differs from the reported value 3.75 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3552 and PDB model 5MRE. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.00586 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)

This section was not generated.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00586).



9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00586) and Q-score for the entire model and for each chain.

Chain Atom inclusion		
All	0.9671	
0	0.9808	
1	0.9665	
11	0.9228	
2	0.9674	
22	0.9645	
3	0.9646	
33	0.9600	
4	0.9593	
44	0.9530	
5	0.9589	
55	0.9415	
6	0.9483	
66	0.9576	
7	0.9597	
77	0.9170	
8	0.9532	
88	0.9395	
9	0.9669	
А	0.9856	
AA	0.9499	
В	0.9525	
BB	0.9593	
С	0.9625	
CC	0.9328	
D	0.9584	
DD	0.9538	
E	0.9619	
EE	0.9362	
F	0.9647	
FF	0.9070	
G	0.9521	
GG	0.9234	
Н	0.9624	
HH	0.9497	





Chain	Atom inclusion
Ι	0.9477
II	0.9543
J	0.9654
JJ	0.9227
K	0.9621
KK	0.9347
L	0.9606
LL	0.9576
М	0.9564
MM	0.9457
Ν	0.9620
NN	0.9374
0	0.9641
00	0.9270
Р	0.9608
PP	0.9551
Q	0.9587
QQ	0.9373
R	0.9598
RR	0.9480
S	0.9567
SS	0.9452
Т	0.9601
TT	0.9266
U	0.9553
UU	0.9517
V	0.9545
VV	0.9430
W	0.9573
WW	0.9439
Х	0.9376
XX	0.9484
Y	0.9377
YY	0.9367
Z	0.9508
ZZ	0.9194
a	0.9743
aa	0.9880
b	0.9616
bb	0.9077
с	0.9641
сс	0.9468



Chain	Atom inclusion
d	0.9628
dd	0.9854

