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PDB ID	:	6NU2
EMDB ID	:	EMD-0514
Title	:	Structural insights into unique features of the human mitochondrial ribosome
		recycling
Authors	:	Sharma, M.R.; Koripella, R.K.; Agrawal, R.K.
Deposited on	:	2019-01-30
Resolution	:	3.90  Å(reported)
Based on initial model	:	3JD5

This is a Full wwPDB EM Validation 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.

EMDB validation analysis MolProbity	:	0.0.1.dev43 4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
$\operatorname{MapQ}$	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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

## 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 3.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
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 >=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 <=5%

Mol	Chain	Length	Quality of chain	
1	А	1472	73%	27%
2	В	56	77%	23%
3	D	236	96%	•
4	Е	304	95%	••
5	F	250	96%	••
6	Н	95	96%	•
7	Ι	168	92%	• 6%
8	J	140	96%	•
9	K	177	95%	5%



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Mol	Chain	Length	Quality of chain	
10	L	115	95%	5%
11	М	287	96%	•
12	Ν	205	99%	·
13	О	152	99%	•
14	Р	138	94%	••
15	Q	219	97%	•
16	R	140	98%	•
17	S	156	97%	•
18	Т	166	98%	•
19	U	111	96%	•
20	V	202	87%	6% 6%
21	W	115	96%	· ·
22	Х	243	94%	6%
23	Y	176	98%	•
24	Z	120	97%	•
25	0	108	96%	•
26	1	52	94%	6%
27	2	46	100%	
28	3	95	98%	•
29	4	36	100%	
30	5	392	92%	••
31	6	354	88%	• 8%
32	7	287	89%	• 7%
33	8	99	97%	·
34	9	123	84%	5% 11%



Conti	inued fron	n previous	page	
Mol	Chain	Length	Quality of chain	
35	a	108	73% •	24%
36	b	148	97%	•
37	с	286	94%	••
38	d	171	92%	•• 5%
39	е	237	88%	• 8%
40	f	146	89%	• 10%
41	g	129	95%	5%
42	h	103	95%	••
43	i	97	94%	6%
44	j	85	98%	
45	k	84	93%	7%
46	1	23	100%	
47	m	45	93%	7%
48	0	94	96%	·
49	р	156	79% •	19%
50	q	128	96%	·
51	r	162	86%	• 10%
52	s	390	93%	• 5%
53	t	28	100%	
54	u	2	100%	
55	z	204	97%	•
56	AA	923	66% 34%	
57	AB	217	99%	
58	AC	132	97%	•
59	AD	343	88%	6% 6%



Conti	nued from	<i>i previous</i>	page	
Mol	Chain	Length	Quality of chain	
60	AE	122	97%	•
61	AF	208	95%	• •
62	AG	326	88%	5% 6%
63	AH	122	94%	6%
64	AI	136	96%	•
65	AJ	108	95%	5%
66	AK	101	92%	8%
67	AL	164	99%	•
68	AM	116	97%	•
69	AN	107	93%	7%
70	AO	185	94%	6%
71	AP	96	98%	
72	AQ	86	97%	•
73	AR	242	94%	6%
74	AS	126	98%	•
75	AT	162	98%	•
76	AU	173	95%	5%
77	AV	365	87%	• 10%
78	AW	97	97%	•
79	AX	348	84%	5% 9%
80	AY	108	95%	5%
81	AZ	87	94%	6%
82	A0	208	93%	
83	A1	272	90%	• 6%
84	A2	116	95%	5%

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Mol	Chain	Length	Quality of chain	
85	A3	69	99%	·
86	A4	474	86%	• 13%



## 2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 294948 atoms, of which 134991 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 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	А	1472	Total 47118	C 14025	H 15857	N 5642	O 10122	Р 1472	0	0

• Molecule 2 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	В	56	Total 1794	C 534	Н 603	N 214	0 387	Р 56	0	0

• Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	236	Total 3738	C 1145	Н 1896	N 373	0 315	S 9	0	0

• Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	300	Total	С	Η	Ν	0	$\mathbf{S}$	0	0
4	Ľ	500	4743	1523	2378	410	422	10	0	0

• Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
5	F	250	Total 4058	C 1294	Н 2045	N 365	0 348	S 6	0	0

• Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues		Α	toms			AltConf	Trace
6	Н	95	Total 1616	C 498	Н 832	N 152	О 134	0	0



• Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues			Atom	ıs			AltConf	Trace
7	Ι	158	Total	C	H 1260	N 225	0	S 10	0	0
			2002	828	1309	233	210	10		

• Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues			Atom	s			AltConf	Trace
8	J	140	Total 2202	C 680	H 1141	N 192	0 187	${S \over 2}$	0	0

• Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
9	K	177	Total 2899	C 934	Н 1448	N 259	O 251	${ m S} 7$	0	0

• Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
10	L	115	Total 1830	C 559	Н 941	N 171	O 154	${ m S}{ m 5}$	0	0

• Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues			Atom	5			AltConf	Trace
11	М	287	Total 4683	C 1472	Н 2378	N 425	O 402	S 6	0	0

• Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
12	Ν	205	Total 3334	C 1056	Н 1680	N 308	O 280	S 10	0	0

• Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
13	Ο	152	Total 2528	C 784	Н 1283	N 239	0 215	S 7	0	0

• Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.



Mol	Chain	Residues			Atom	S			AltConf	Trace
14	Р	133	Total 2162	C 677	Н 1082	N 209	O 189	${ m S}{ m 5}$	0	0

• Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
15	Q	219	Total 3681	C 1168	Н 1859	N 322	O 323	S 9	0	0

• Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
16	R	140	Total 2367	С 732	Н 1214	N 231	O 186	${S \over 4}$	0	0

• Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
17	S	156	Total	С	Н	Ν	Ο	$\mathbf{S}$	0	0
11	D	100	2573	806	1322	222	219	4	0	0

• Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
18	Т	166	Total 2778	C 875	Н 1410	N 254	0 232	S 7	0	0

• Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
19	U	111	Total 1857	C 591	Н 935	N 176	0 153	${S \over 2}$	0	0

• Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
20	V	189	Total 3109	C 987	Н 1558	N 278	0 278	S 8	0	0

• Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.



Mol	Chain	Residues			Atom	ns			AltConf	Trace
21	W	115	Total 1816	C 571	Н 922	N 169	0 151	${ m S} { m 3}$	0	0

• Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
22	X	243	Total 4089	C 1317	Н 2054	N 351	O 362	${ m S}{ m 5}$	0	0

• Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues			Atom	s			AltConf	Trace
23	Y	176	Total 3078	C 970	Н 1561	N 291	O 252	${S \atop 4}$	0	0

• Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
24	Ζ	120	Total 2008	C 626	Н 1030	N 183	O 166	${ m S} { m 3}$	0	0

• Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
25	0	108	Total 1782	C 545	Н 902	N 172	0 157	S 6	0	0

• Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues		A	Atom	s			AltConf	Trace
26	1	52	Total 908	C 278	Н 475	N 83	O 70	${ m S} { m 2}$	0	0

• Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues		ŀ	Atom	s			AltConf	Trace
27	2	46	Total 782	C 233	Н 406	N 83	O 59	S 1	0	0

• Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.



Mol	Chain	Residues			Atom	ns			AltConf	Trace
28	3	95	Total 1714	C 539	Н 883	N 162	0 127	${ m S} { m 3}$	0	0

• Molecule 29 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues		ŀ	Atoms							
29	4	36	Total 666	C 203	Н 344	N 70	O 46	${ m S} { m 3}$	0	0		

• Molecule 30 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues			Atom	s			AltConf	Trace
30	5	376	Total 6123	C 1987	Н 3059	N 529	O 538	S 10	0	0

• Molecule 31 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
31	6	325	Total 5087	C 1692	Н 2451	N 465	0 470	S 9	0	0

• Molecule 32 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues			Atom	s			AltConf	Trace
32	7	266	Total 4331	C 1383	Н 2173	N 371	O 388	S 16	0	0

• Molecule 33 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
33	8	99	Total 1680	C 535	Н 844	N 144	0 155	${ m S} { m 2}$	0	0

• Molecule 34 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
34	9	109	Total 1751	C 565	Н 878	N 152	0 154	${S \over 2}$	0	0

• Molecule 35 is a protein called 39S ribosomal protein L42, mitochondrial.



Mol	Chain	Residues			Atom	ns			AltConf	Trace
35	a	82	Total 1344	C 434	Н 658	N 124	0 123	${ m S}{ m 5}$	0	0

• Molecule 36 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
36	b	148	Total 2358	C 733	Н 1180	N 229	0 213	${ m S} { m 3}$	0	0

• Molecule 37 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
37	с	275	Total 4437	C 1415	Н 2220	N 383	O 410	S 9	0	0

• Molecule 38 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
20	d	169	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0
30	u	102	2690	870	1343	234	235	8	0	0

• Molecule 39 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
39	е	217	Total 3529	C 1124	H 1767	N 310	0 323	${ m S}{ m 5}$	0	0

• Molecule 40 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
40	f	131	Total 2083	C 663	Н 1044	N 169	O 203	${S \atop 4}$	0	0

• Molecule 41 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
41	g	129	Total 2123	C 690	Н 1056	N 185	O 190	${ m S} { m 2}$	0	0

• Molecule 42 is a protein called 39S ribosomal protein L50, mitochondrial.



Mol	Chain	Residues			Aton	ns			AltConf	Trace
42	h	100	Total 1633	С 524	Н 806	N 146	0 155	${ m S} { m 2}$	0	0

• Molecule 43 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
43	i	97	Total 1684	C 532	Н 857	N 165	O 126	$\frac{S}{4}$	0	0

• Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
44	j	85	Total 1357	C 423	Н 673	N 133	O 126	${ m S} { m 2}$	0	0

• Molecule 45 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
45	k	84	Total 1311	C 407	Н 656	N 122	0 121	${ m S}{ m 5}$	0	0

• Molecule 46 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
46	1	23	Total 448	C 137	Н 227	N 52	O 32	0	0

• Molecule 47 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues		A	Atom	s			AltConf	Trace
47	m	45	Total 759	C 232	Н 387	N 76	O 62	${ m S} { m 2}$	0	0

• Molecule 48 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
48	О	94	Total 1601	C 501	Н 804	N 165	0 128	${ m S} { m 3}$	0	0

• Molecule 49 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.



Mol	Chain	Residues			Atom	IS			AltConf	Trace
49	р	127	Total 2141	C 661	Н 1083	N 201	O 192	${ m S}$ $4$	0	0

• Molecule 50 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
50	q	128	Total 2125	C 671	H 1049	N 208	O 192	${ m S}{ m 5}$	0	0

• Molecule 51 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
51	r	146	Total 2423	С 764	Н 1220	N 232	O 199	S 8	0	0

• Molecule 52 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
52	s	370	Total 6058	C 1946	Н 3022	N 542	0 534	S 14	0	0

• Molecule 53 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues		At	$\mathbf{oms}$			AltConf	Trace
53	t	28	Total 170	C 84	Н 30	N 28	O 28	0	0

• Molecule 54 is a RNA chain called E-site tRNA.

Mol	Chain	Residues		A	Aton	ıs			AltConf	Trace
54	u	2	Total 65	C 19	Н 23	N 8	O 13	Р 2	0	0

• Molecule 55 is a protein called Ribosome-recycling factor, mitochondrial.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
55	Z	204	Total 3240	C 974	Н 1665	N 285	O 308	S 8	0	0

• Molecule 56 is a RNA chain called 12S rRNA.



Mol	Chain	Residues			Ato	$\mathbf{ms}$			AltConf	Trace
56	AA	923	Total 29552	C 8790	Н 9946	N 3535	O 6358	Р 923	0	0

• Molecule 57 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
57	AB	217	Total	С	Η	Ν	0	S	0	0
			3533	1131	1765	321	306	10		

• Molecule 58 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
58	AC	132	Total 2170	C 699	Н 1088	N 195	0 184	${S \over 4}$	0	0

• Molecule 59 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
59	AD	322	Total	С	Н	Ν	0	S	0	0
	112	022	5153	1611	2596	476	457	13		0

• Molecule 60 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
60	AE	122	Total 1973	C 614	Н 1001	N 177	0 177	S 4	0	0

• Molecule 61 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues			Atom	s			AltConf	Trace
61	AF	201	Total 3385	C 1069	H 1717	N 305	O 283	S 11	0	0

• Molecule 62 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
62	AG	305	Total 5019	C 1599	Н 2503	N 448	0 455	S 14	0	0

• Molecule 63 is a protein called 28S ribosomal protein S10, mitochondrial.



Mol	Chain	Residues			Atom	S			AltConf	Trace
63	AH	122	Total 2023	C 643	Н 1024	N 168	O 185	${ m S} { m 3}$	0	0

• Molecule 64 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues			AltConf	Trace				
64	AI	136	Total 2063	C 637	H 1052	N 192	0 178	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 65 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
65	AJ	108	Total 1725	C 521	Н 887	N 169	0 142	S 6	0	0

• Molecule 66 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
66	AK	101	Total 1746	C 537	Н 885	N 179	O 140	${f S}{5}$	0	0

• Molecule 67 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
67	AL	164	Total 2855	C 883	Н 1473	N 257	O 235	S 7	0	0

• Molecule 68 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
68	AM	116	Total 1870	C 582	Н 950	N 182	O 150	S 6	0	0

• Molecule 69 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
69	AN	107	Total 1754	C 549	Н 908	N 153	0 141	${ m S} { m 3}$	0	0

• Molecule 70 is a protein called 28S ribosomal protein S18b, mitochondrial.



Mol	Chain	Residues			Atom	IS			AltConf	Trace
70		185	Total	С	Η	Ν	Ο	$\mathbf{S}$	0	0
10	ло	100	3016	970	1488	285	267	6	0	0

• Molecule 71 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
71	AP	96	Total 1578	C 498	Н 804	N 133	0 135	S 8	0	0

• Molecule 72 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
72	AQ	86	Total 1481	C 455	Н 746	N 147	0 124	S 9	0	0

• Molecule 73 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
73	AR	242	Total	C	H	N	0	S	0	0
			4039	1285	2031	343	372	8		

• Molecule 74 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues			Atom	S			AltConf	Trace
74	AS	126	Total 2079	C 673	Н 1037	N 183	0 185	S 1	0	0

• Molecule 75 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
75	AT	162	Total 2674	C 850	Н 1344	N 231	O 238	S 11	0	0

• Molecule 76 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
76	AU	173	Total 2932	C 900	H 1471	N 294	O 263	${S \over 4}$	0	0

• Molecule 77 is a protein called 28S ribosomal protein S27, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace	
77	AV	328	Total 5392	C 1737	Н 2690	N 452	O 502	S 11	0	0

• Molecule 78 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace		
78	AW	97	Total 1551	C 486	Н 785	N 137	O 139	$\frac{S}{4}$	0	0

• Molecule 79 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace		
79	AX	316	Total 5051	C 1625	Н 2520	N 440	O 455	S 11	0	0

• Molecule 80 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace		
80	AY	108	Total 1773	C 593	Н 859	N 150	O 169	${ m S} { m 2}$	0	0

• Molecule 81 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues		Atoms				AltConf	Trace	
81	AZ	87	Total 1487	C 473	Н 747	N 133	0 130	$\frac{S}{4}$	0	0

• Molecule 82 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
82	A0	201	Total 3369	C 1065	Н 1685	N 322	O 292	${ m S}{ m 5}$	0	0

• Molecule 83 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues		Atoms					AltConf	Trace
83	A1	256	Total 4173	C 1321	Н 2097	N 350	O 395	S 10	0	0

• Molecule 84 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.



Mol	Chain	Residues			Aton	ns			AltConf	Trace
84	A2	116	Total 1887	C 574	Н 962	N 181	O 162	S 8	0	0

• Molecule 85 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
85	A3	69	Total 1292	C 393	Н 682	N 130	O 86	S 1	0	0

• Molecule 86 is a protein called Pentatric opeptide repeat domain-containing protein 3, mito-chondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
86	A4	414	Total 5103	C 1805	Н 2265	N 490	O 529	S 14	0	0

• Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
87	А	97	Total Mg 97 97	0
87	М	1	Total Mg 1 1	0
87	g	1	Total Mg 1 1	0
87	АА	28	TotalMg2828	0

• Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
88	0	1	Total Zn 1 1	0
88	4	1	Total Zn 1 1	0
88	r	1	Total Zn 1 1	0
88	AB	1	Total Zn 1 1	0
88	AO	1	Total Zn 1 1	0
88	AP	1	Total Zn 1 1	0



Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
88	AT	1	Total Zn 1 1	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. 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.

Chain A:	73%	27%
G1671         C1672           U1673         U1673           U1674         U1679           U1679         U1679           C1685         C1685           C1685         C1685           C1685         C1685           C1685         C1685           U1679         C1685           U1700         U1700	A1705 A1708 A1708 A1713 C1714 C1714 C1715 C1715 C1715 A1724 A1731 C1732 A1731 C1732	C1748 C1749 G1750 A1751 A1773 C173 C173 C173 C173 A1775 A1775 A1795 A1795 A1795 A1795 A1795
A1805 U1806 U1806 U1808 U1809 A1810 A1810 A1810 C1813 C1813 C1813 C1813 C1813 C1823 U1824 U1824 U1824 A1825 A1835 A1835 A1835 A1835 A1835 A1835 A1835	A1844 A1844 U1848 C1849 A1853 A1855 A1859 A1859 A1859 A1870 A1870 A1871 U1872 A1871 A1872 A1872 A1872 A1872 A1872 A1872	41886 41887 61890 61890 41893 61901 61901 61902 61918 61918 61918 61918 61939 61939
C1944 G1958 A1972 G1973 A1974 A1974 A1974 A1995 A1955 A1995	2015 U2021 U2021 U2022 A2031 A2039 U2041 U2041 U2063 U2063 U2063 A2060 C2061 A2065	A2074 C2079 U2080 U2081 U2083 U2083 U2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2083 C2084 C2084 C2079 C2084 C2084 C2084 C2084 C2085 C2084 C2085
A2131 A2135 A2135 A2135 G2143 G2143 G2143 A2160 A2166 A2166 A2178 A2178	A2175 A2180 A2181 A2181 C2183 C2183 C2183 A2195 A2195 A2195 A2195 A2195 C2206 C2206 C2215	C2217 C2218 A2230 A2235 C2235 A2235 A2245 A2245 A2245 A2245 A2245 A2245 A2245 A2245
A2260 C2265 C2265 C2265 C2265 C2265 A2280 A2293 A2295 U2295 U2295 U2295 U2295 U2295 U2295 U2295 A2293 A2293 A2293 A2293 A2293 A2293 A2293 A2293 A2293 A2295 A2293 A2295 A2293 A2295 A2205 A205 A	2314 2314 72315 72314 72315 72345 72345 72345 72355 725577 725577 725577 725577 72557777777 725577777777	A2369 A2371 U2371 U2372 A2373 A2373 A2373 A2373 A2385 C2389 A2386 C2389 A2396 A2396 A2395
A2398 U2404 C2405 C2415 C2415 C2415 C2415 C2415 C2415 C2415 C2415 C2415 C2433 C2445 C2443 C2445 A2445 A2445 A2445 A2445	C2453 C2454 U2455 C2454 A2458 A2458 C2471 A2470 C2471 A2473 A2472 A2472 A2473 C2493 U2499 U2499 U2510	22511 A2512 C2520 C2520 C2523 C2523 A2524 A2532 A2530 C2535 A2530 C2535 C2536 C2530 C2546 C2546 C2546
A2556 C2556 A22556 U2559 A2564 A2564 C2533 C2533 C2533 C2533 C2533 C2533 C2533 C2533 C2533 C2533 C2535 C2535 C2535 C2535 C2535 C2535 C25555 C2555 C2555 C2555 C2555 C2555 C2555 C2555 C2555 C255	A2604 C2606 U2606 U2614 U2618 U2618 U2628 U2628 U2628 U2628 U2630 U2630 U2630 U2630 U2630 U2630 U2630 U2630	02634 02635 02645 02645 02656 02656 02656 02653 02653 02653 02653 02653 02653 02653 02653 02695 02695 02695
62702 C2708 C2708 A2711 A2713 A2713 C2718 C2713 A2720 C2719 C2713 A2720 C2713 C2713 C2713 C2713 A2720 C2714 A2710 C2773 C2773 C2773 C2774 A2711 C2773 C2774 C2773 C2774 C2773 C2774 C2773 C2774 C2773 C2773 C2774 C2773 C2774 C2773 C2773 C2774 C2773 C2774 C2773 C2774 C2773 C2774 C2773 C2773 C2774 C2773 C2774 C2773 C2774 C2774 C2774 C2773 C2774 C2773 C2774 C2773 C2774 C2773 C2774 C2774 C2774 C2775 C2774 C2775 C2774 C2775 C2	U2744 U2754 A2755 A2755 C2756 C2756 C2756 C2756 C2756 C2759 C2759 C2759 C2759 C2759 C2759 C2759 C2759 C2759 C2756 C2810 C2813 C2756 C27577 C2757 C2757 C2757 C2757 C2757 C2757 C2757 C2757 C2757 C2757	A2837 A2836 C2839 C2847 C2847 A2848 A2848 A2848 C2855 A2859 C2855 A2859 C2855 A2859 C2855
C2881 A2904 A2910 A2913 A2913 A2913 C2916 G2916 G2916 G2916 C2916 C2920 A2918 C2920 C2928 C2928 C2928 C2928 C2928	U2956 C2955 U2955 A2955 A2956 A2966 A2965 C2963 U2977 U2979 U2977 C2985 C2985 C2985 C2985	42900 12991 72992 43000 43003 73005 73005 73005 73015 73015 73015 73016 73016 73016 73018 73018 73018 73018 73018 73018 73018 73018 73018 73018 73018 73017 730000000000
U3042 43053 43055 43055 63056 03066 13066 03066 03068 13065 03068 A3068 A3069 03072 03073 03073 03073 03073 03073 03073 03073 03073 03073 03073 03073 03073 03073 03073 03063 03063 03063 03065 03005 03065 03065 03065 03065 03065 03065 03065 03065 03065 03065 03065 03065 03065 03065 03065 0306 0306	0305 0305 0305 03055 03055 03100 03100 03100 03105 03114 03113 03125 03123 03123 03123 03123	A3133 C3134 A3135 C3152 U3153 C3157 A3156 A3176 A3176 A3177 A3177 A3177

• Molecule 1: 16S rRNA





#### **G18** A29 A29 A31 P31 P31 P31 C50 C50 C50 C50 K157

• Molecule 9: 39S ribosomal protein L13, mitochondrial



Chain Q:

97%





• Molecule 16: 39S ribosomal protein L20, mitochondrial

Chain R:



• Molecule 17: 39S ribosomal protein L21, mitochondrial

Chain S: 97%



• Molecule 18: 39S ribosomal protein L22, mitochondrial

Chain T:

98%

98%

#### 147 R69 Q79 0133 Y158 L212

• Molecule 19: 39S ribosomal protein L23, mitochondrial

Chain U: 96% ·



• Molecule 20: 39S ribosomal protein L24, mitochondrial

Chain V: 87% 6% 6%

• Molecule 21: 39S ribosomal protein L27, mitochondrial

Chain W:

96%

94%



• Molecule 22: 39S ribosomal protein L28, mitochondrial

Chain X:



6%

6%

#### P2 E18 R23 R36 R44 R44 R44 R36 R36 R36 R36 R35 R216 R216 R216 R216 R220 R221 S24

• Molecule 23: 39S ribosomal protein L47, mitochondrial

Chain Y:

663 A83 R162 Q183 R198 R198 R198 R238

• Molecule 24: 39S ribosomal protein L30, mitochondrial

Chain Z: 97%



• Molecule 25: 39S ribosomal protein L32, mitochondrial

Chain 0:

96%

98%

### A79 R84 L116 E163 R179 R179

• Molecule 26: 39S ribosomal protein L33, mitochondrial

Chain 1: 94%

## K1 4 R3 4 R3 8 K6 0 L6 5

• Molecule 27: 39S ribosomal protein L34, mitochondrial

Chain 2:

100%

There are no outlier residues recorded for this chain.

• Molecule 28: 39S ribosomal protein L35, mitochondrial

Chain 3:

98%



 $\bullet$  Molecule 29: 39S ribosomal protein L36, mitochondrial

Chain 4:

100%

There are no outlier residues recorded for this chain.

• Molecule 30: 39S ribosomal protein L37, mitochondrial



Chain 5:	92%	• •
Y31 L70 L70 ASP PR0 ASS PR0 ASS ASS ASS ASS ASS ASS ASS ASS ASS AS	L294 L294 K297 A297 D348 D348 D348 D348 C38 C38 C38 C38 C38 C38 C38 C38 C38 C3	ARG VAL VAL V398 V398 V398 V398 V398 V398 V398 V398
• Molecule 31: 39S ribosomal protein	n L38, mitochondrial	
Chain 6:	88%	• 8%
R27 R27 R5 C79 C79 C79 C79 C79 C79 C79 C79 C79 C79	E118 GLU E120 E120 E120 E120 E123 E209 GLU C109 C109 GLU C133 SER	1225 1277 1277 1277 1277 1277 127 127 127 12
A314 1334 H351 H359 C378 1379 1379		
• Molecule 32: 39S ribosomal protein	n L39, mitochondrial	
Chain 7:	89%	• 7%
S36 K121 K121 K121 F158 F158 F158 F158 F158 C1U T2N K15 K15 K15 K15 K15 K15 K15 K15 K15 K15	D213 N256 P270 P270 P270 P281 P285 P281 P285 P281 P281 P281 P281 P281 P281 P281 P281	8221 R321 K322
• Molecule 33: 39S ribosomal protein	n L40, mitochondrial	
Chain 8:	97%	·
183 196 196 191 191		
• Molecule 34: 39S ribosomal protein	n L41, mitochondrial	
Chain 9: 84	4% 59	% 11%
A15 815 836 838 838 838 838 838 838 846 838 846 846 846 846 846 846 846 846 846 84	G118 R133 R137	
• Molecule 35: 39S ribosomal protein	n L42, mitochondrial	
Chain a: 73%	• 2	24%
T35 N44 N44 N44 N44 ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	VAL GLU HIS LEU EIO4 R122 R122 R122	
• Molecule 36: 39S ribosomal protein	n L43, mitochondrial	
Chain b:	97%	<del>.</del>
12 115 15 15 15 15 115 16 14 14 14		
	PROTEIN DATA BANK	

• Molecule 37: 39S ribosomal protein L44, mitochondrial

Chain c:	94%	•••
V31 R52 P64 P64 P64 P64 P107 P107 P107 P112 P128 P128 P128 P128 P128 P128 P128	ASN 6162 E183 8206 9313 <b>7316</b> <b>7316</b>	
• Molecule 38: 39S rib	osomal protein L45, mitochondrial	
Chain d:	92%	•• 5%
A117 E190 E190 C199 SER MET MET ASN C1N C1N C1N C1N N207 R227	L231 L252 THR ASN P255 L287	
• Molecule 39: 39S rib	osomal protein L46, mitochondrial	
Chain e:	88%	• 8%
843 R55 D104 D104 CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	A135 A135 R151 K152 V171 P174 P174 P174 P174 A1A A1A A1A A1A A1A A1A A1A A1A A13 A1A A1A	1279
• Molecule 40: 39S ribe	osomal protein L48, mitochondrial	
Chain f:	89%	• 10%
Y48           66           GLU           CLYS           LYS           LYS           LYS           LYS           LYS           LYS           QLU           QLY           QLY	GLN SER LYE H144 P193	
• Molecule 41: 39S ribe	osomal protein L49, mitochondrial	
Chain g:	95%	5%
F38 155 750 869 8121 1143 1144 1145 1166		
• Molecule 42: 39S rib	osomal protein L50, mitochondrial	
Chain h:	95%	
R56 F78 GLY SER SER SER L82 N137 N147 Y158		
• Molecule 43: 39S rib	osomal protein L51, mitochondrial	
Chain i:	94%	6%
132 R35 F66 R101 R101 R107 R113 F127 F127 R128		
• Molecule 44: 39S rib	osomal protein L52, mitochondrial	

IN DATA BANK

Chain j:	98% .	
G24 G25 A34 A108 A108		
• Molecule 45	: 39S ribosomal protein L53, mitochondrial	
Chain k:	93% 7%	
V13 339 N46 D58	C 863 A 664 A 664	
• Molecule 46	: 39S ribosomal protein L54, mitochondrial	
Chain l:	100%	
There are no	outlier residues recorded for this chain.	
• Molecule 47	: 39S ribosomal protein L55, mitochondrial	
Chain m:	93% 7%	I
D34 R42 E70 P71 P71		
• Molecule 48	: Ribosomal protein 63, mitochondrial	
Chain o:	96% .	
R9 R15 G61 K81 S102		
• Molecule 49	: Peptidyl-tRNA hydrolase ICT1, mitochondrial	
Chain p:	79% · 19%	1
E38 V61 PRO ASN GLY ALA CLY GLN GLN ALA	ASP ASP SER SER SER SER SER SER SER SER SER SER	
• Molecule 50	: Growth arrest and DNA damage-inducible proteins-interact	ing protein 1
Chain q:	96%	
<b>725</b> 828 942 152 152 878		
• Molecule 51	: 39S ribosomal protein S18a, mitochondrial	
Chain r:	86% • 10%	

L D W I D E

wiw





• Molecule 61: 28S ribosomal protein S7, mitochondrial

Chain AF:



. .

95%



• Molecule 62: 28S ribosomal protein S9, mitochondrial

Chain AG:	88%	5% 6%
E71 R106 L111 L111 L111 R106 R176 G154 R176 G154 R176 R176 R176 C154 LEU	PEU PEU THR THR THR THR THR ASP ASP ASP ASP ASP C233 C233 C233 C233 C233 C233 C233 C23	q261 R276 R276 C289 C289 G291 Q301 Q301 R310 R310 R310 R310 R389
1398 1398 1398 1398 1398		
• Molecule 63: 28S ribo	somal protein S10, mitochondrial	
Chain AH:	94%	6%
P61 E92 K113 K127 H147 H147 M170 Q179 Q179		
• Molecule 64: 28S ribo	somal protein S11, mitochondrial	
Chain AI:	96%	· ·
K59 F60 A108 1144 1145 R189 R189 L194		
• Molecule 65: 28S ribo	somal protein S12, mitochondrial	
Chain AJ:	95%	5%
431 K43 G54 K129 Y130 Y130 K137 K137 K138		
• Molecule 66: 28S ribo	somal protein S14, mitochondrial	
Chain AK:	92%	8%
H28 Y29 V30 V30 S82 S95 S95 S95 S95 S95 S95 S95 S95 S95 S95	112/ W128	
• Molecule 67: 28S ribo	somal protein S15, mitochondrial	
Chain AL:	99%	
D 66 K145 L194 A 239		
• Molecule 68: 28S ribo	somal protein S16, mitochondrial	



Chain AM:	97%	•
K10 G G 62 E 63 E 63 T 126 T 126		
• Molecule 69: 28S riboson	nal protein S17, mitochondrial	
Chain AN:	93%	7%
R5 L65 K73 K73 K78 K78 C100 C100 C100 C100 C100 C100 C100 C10		
• Molecule 70: 28S riboson	nal protein S18b, mitochondrial	
Chain AO:	94%	6%
K62 D53 C34 C34 R96 R196 R196 R136 K143 C128 K143 L163 L163 R173	021 1238	
• Molecule 71: 28S riboson	nal protein S18c, mitochondrial	
Chain AP:	98%	·
N47 M54 E142 E142		
• Molecule 72: 28S riboson	nal protein S21, mitochondrial	
Chain AQ:	97%	·
A2 R10 C87		
• Molecule 73: 28S riboson	nal protein S22, mitochondrial	
Chain AR:	94%	6%
K67 195 K199 K127 K127 K127 L144 E144 L153 T154 K155 K155	R256 (257 7267 1291 1292 11308	
• Molecule 74: 28S riboson	nal protein S23, mitochondrial	
Chain AS:	98%	
A2 R42 G54 A127 A127		
• Molecule 75: 28S riboson	nal protein S25, mitochondrial	



Chain AT:	98%	•
P2 M66 R137 V163 V163		
• Molecule 76: 28	S ribosomal protein S26, mitochondrial	
Chain AU:	95%	5%
R27 R30 H31 D32 D33 D33 P33 P33 P33 P33 P33 P33 P33 P50 P50	R155 E171 R199	
• Molecule 77: 28	S ribosomal protein S27, mitochondrial	
Chain AV:	87% •	10%
D36 E41 A42 V119 R241 A243 V243 P253 C254	V266 8369 8369 8369 840 841 111. 111. 111. 111. 111. 111. 111.	LYS TLE GLU SER CLU CLU LEU LEU SER
1355 1371 1380 1400		
• Molecule 78: 28	S ribosomal protein S28, mitochondrial	
Chain AW:	97%	•
V77 D97 G117 D146 Q173		
• Molecule 79: 28	S ribosomal protein S29, mitochondrial	
Chain AX:	84% 6%	9%
151 159 160 160 172 160 160 160 160 116	P120 1331 1332 1333 1332 133 13 1 13 13 13 13 13 13 13 13 13 13 13 13	LYS TYR VAL TRP ASN LYS ASS GLU SER
THR GLU LYS GLY GLY G220 C220 C270 C270 C270 C270 C270 C270 C	W301 P342 P386 P386 P386 L398	
• Molecule 80: 28	S ribosomal protein S31, mitochondrial	
Chain AY:	95%	5%
2276 A319 C325 C325 C325 C325 C325 C325 C325 C325		
• Molecule 81: 28	S ribosomal protein S33, mitochondrial	
Chain AZ:	94%	6%
	PROTEIN DATA BANK	



• Molecule 82: 28S ribosomal protein S34, mitochondrial



• Molecule 83: 28S ribosomal protein S35, mitochondrial



• Molecule 84: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1

Chain A2:	95%	5%
A2 R337 R337 R337 R337 R337 R337 R337 R33		
• Molecule 85: Aurora kina	se A-interacting protein	

# Chain A3: 99%

• Molecule 86: Pentatricopeptide repeat domain-containing protein 3, mitochondrial





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67116	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	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: 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	
WIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.14	0/34967	0.71	4/54407~(0.0%)
2	В	0.13	0/1328	0.69	0/2056
3	D	0.23	0/1879	0.40	0/2527
4	Е	0.23	0/2433	0.39	0/3299
5	F	0.23	0/2071	0.37	0/2817
6	Н	0.22	0/798	0.40	0/1073
7	Ι	0.23	0/1308	0.37	0/1761
8	J	0.23	0/1077	0.38	0/1452
9	Κ	0.23	0/1495	0.36	0/2029
10	L	0.22	0/904	0.40	0/1218
11	М	0.24	0/2359	0.38	0/3185
12	Ν	0.23	0/1697	0.38	0/2281
13	0	0.22	0/1269	0.36	0/1708
14	Р	0.23	0/1103	0.38	0/1491
15	Q	0.23	0/1863	0.38	0/2509
16	R	0.23	0/1174	0.35	0/1572
17	S	0.23	0/1276	0.40	0/1729
18	Т	0.23	0/1402	0.36	0/1886
19	U	0.24	0/946	0.39	0/1283
20	V	0.22	0/1590	0.39	0/2151
21	W	0.23	0/916	0.39	0/1233
22	Х	0.23	0/2090	0.35	0/2825
23	Y	0.23	0/1552	0.34	0/2079
24	Ζ	0.22	0/1003	0.38	0/1354
25	0	0.23	0/895	0.39	0/1201
26	1	0.23	0/438	0.41	0/583
27	2	0.23	0/382	0.40	0/507
28	3	0.23	0/852	0.38	0/1136
29	4	0.21	0/329	0.40	0/435
30	5	0.23	0/3154	0.39	0/4295
31	6	0.23	0/2722	0.37	0/3709
32	7	0.23	0/2207	0.36	0/2978


Mal	Chain	Bond	lengths	B	ond angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
33	8	0.23	0/855	0.36	0/1152
34	9	0.24	0/896	0.37	0/1205
35	a	0.22	0/709	0.37	0/963
36	b	0.23	0/1202	0.39	0/1626
37	с	0.24	0/2264	0.35	0/3059
38	d	0.22	0/1385	0.38	0/1877
39	е	0.23	0/1797	0.37	0/2422
40	f	0.23	0/1055	0.39	0/1427
41	g	0.24	0/1102	0.38	0/1503
42	h	0.23	0/847	0.35	0/1150
43	i	0.23	0/849	0.35	0/1135
44	j	0.23	0/698	0.33	0/940
45	k	0.22	0/665	0.38	0/897
46	1	0.20	0/226	0.29	0/299
47	m	0.22	0/379	0.40	0/510
48	0	0.22	0/818	0.35	0/1097
49	р	0.22	0/1071	0.37	0/1433
50	q	0.23	0/1107	0.33	0/1498
51	r	0.22	0/1238	0.36	0/1676
52	S	0.23	0/3114	0.38	0/4225
54	u	0.06	0/46	0.62	0/69
55	Z	0.23	0/1584	0.37	0/2126
56	AA	0.15	0/21926	0.74	7/34121~(0.0%)
57	AB	0.24	0/1811	0.37	0/2451
58	AC	0.23	0/1112	0.37	0/1505
59	AD	0.23	0/2607	0.38	0/3498
60	AE	0.23	0/989	0.39	0/1335
61	AF	0.23	0/1708	0.36	0/2291
62	AG	0.23	0/2570	0.37	0/3443
63	AH	0.22	0/1019	0.38	0/1379
64	AI	0.23	0/1031	0.40	0/1390
65	AJ	0.23	0/854	0.41	0/1148
66	AK	0.21	0/879	0.36	0/1182
67	AL	0.23	0/1406	0.34	0/1878
68	AM	0.23	0/941	0.37	0/1265
69	AN	0.23	0/864	0.40	0/1169
70	AO	0.23	0/1580	0.38	0/2150
71	AP	0.23	0/791	0.38	0/1062
72	AQ	0.22	0/747	0.37	0/995
73	AR	0.23	0/2050	0.36	0/2770
74	AS	$0.2\overline{3}$	$0/10\overline{69}$	$0.3\overline{5}$	$0/144\overline{1}$
75	AT	0.24	0/1361	0.38	0/1829
76	AU	0.23	$0/1\overline{482}$	0.34	$0/1\overline{987}$



Mol Chain		Bond lengths		Bond angles	
IVIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
77	AV	0.23	0/2758	0.34	0/3724
78	AW	0.23	0/778	0.40	0/1048
79	AX	0.23	0/2596	0.37	0/3519
80	AY	0.23	0/943	0.32	0/1274
81	AZ	0.23	0/757	0.36	0/1011
82	A0	0.22	0/1727	0.38	0/2338
83	A1	0.23	0/2121	0.37	0/2873
84	A2	0.23	0/939	0.37	0/1256
85	A3	0.22	0/621	0.35	0/820
86	A4	0.23	0/2137	0.31	0/2872
All	All	0.20	0/167560	0.53	11/238082~(0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(°)	$Ideal(^{o})$
1	А	3206	С	C2-N1-C1'	6.09	125.50	118.80
1	А	1890	С	N3-C2-O2	-6.02	117.68	121.90
56	AA	984	С	N3-C2-O2	-5.93	117.75	121.90
56	AA	765	C	C2-N1-C1'	5.86	125.24	118.80
1	А	1786	С	N1-C2-O2	5.79	122.37	118.90
56	AA	1093	С	N3-C2-O2	-5.74	117.89	121.90
56	AA	1413	U	C2-N1-C1'	5.38	124.16	117.70
56	AA	984	С	N1-C2-O2	5.31	122.09	118.90
56	AA	1314	С	C2-N1-C1'	5.27	124.60	118.80
56	AA	1241	С	N3-C2-O2	-5.15	118.29	121.90
1	А	1786	С	N3-C2-O2	-5.11	118.33	121.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.



# 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	Perc	entiles
3	D	234/236~(99%)	200 (86%)	29 (12%)	5 (2%)	7	39
4	Ε	296/304~(97%)	245~(83%)	43~(14%)	8 (3%)	5	35
5	F	248/250~(99%)	206 (83%)	38 (15%)	4 (2%)	9	44
6	Н	93/95~(98%)	79 (85%)	11 (12%)	3 (3%)	4	32
7	Ι	154/168~(92%)	133 (86%)	17 (11%)	4 (3%)	5	35
8	J	138/140~(99%)	115 (83%)	19 (14%)	4 (3%)	4	33
9	K	175/177~(99%)	155 (89%)	16 (9%)	4 (2%)	6	38
10	L	113/115~(98%)	93 (82%)	17 (15%)	3 (3%)	5	35
11	М	285/287~(99%)	238 (84%)	40 (14%)	7 (2%)	5	36
12	Ν	203/205~(99%)	177 (87%)	25 (12%)	1 (0%)	29	67
13	Ο	150/152~(99%)	133 (89%)	16 (11%)	1 (1%)	22	60
14	Р	129/138~(94%)	114 (88%)	14 (11%)	1 (1%)	19	57
15	Q	217/219~(99%)	180 (83%)	31 (14%)	6 (3%)	5	34
16	R	138/140~(99%)	124 (90%)	11 (8%)	3 (2%)	6	38
17	S	154/156~(99%)	134 (87%)	17 (11%)	3 (2%)	8	41
18	Т	164/166~(99%)	145 (88%)	16 (10%)	3 (2%)	8	42
19	U	109/111~(98%)	90 (83%)	17 (16%)	2 (2%)	8	42
20	V	183/202~(91%)	151 (82%)	24 (13%)	8 (4%)	2	25
21	W	113/115~(98%)	97 (86%)	13 (12%)	3 (3%)	5	35
22	Х	241/243~(99%)	207 (86%)	27 (11%)	7 (3%)	4	33
23	Y	174/176~(99%)	154 (88%)	17 (10%)	3 (2%)	9	43
24	Z	118/120 (98%)	106 (90%)	10 (8%)	2 (2%)	9	43
25	0	106/108~(98%)	91 (86%)	13 (12%)	2 (2%)	8	41
26	1	50/52~(96%)	41 (82%)	8 (16%)	1 (2%)	7	40
27	2	44/46~(96%)	42 (96%)	2 (4%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
28	3	93/95~(98%)	85 (91%)	7~(8%)	1 (1%)	14	51
29	4	34/36~(94%)	29~(85%)	5~(15%)	0	100	100
30	5	368/392~(94%)	308 (84%)	49 (13%)	11 (3%)	4	33
31	6	313/354~(88%)	266 (85%)	39~(12%)	8 (3%)	5	35
32	7	258/287~(90%)	227 (88%)	26 (10%)	5 (2%)	8	41
33	8	97/99~(98%)	88 (91%)	7 (7%)	2 (2%)	7	39
34	9	105/123~(85%)	89 (85%)	10 (10%)	6 (6%)	1	21
35	a	78/108~(72%)	75 (96%)	3 (4%)	0	100	100
36	b	146/148~(99%)	126 (86%)	18 (12%)	2 (1%)	11	46
37	с	271/286~(95%)	240 (89%)	25 (9%)	6 (2%)	6	38
38	d	156/171~(91%)	127 (81%)	26 (17%)	3 (2%)	8	41
39	е	211/237~(89%)	177 (84%)	30 (14%)	4 (2%)	8	41
40	f	125/146~(86%)	106 (85%)	19 (15%)	0	100	100
41	g	127/129~(98%)	109 (86%)	12 (9%)	6 (5%)	2	24
42	h	96/103~(93%)	78 (81%)	16 (17%)	2 (2%)	7	39
43	i	95/97~(98%)	84 (88%)	9 (10%)	2 (2%)	7	39
44	j	83/85~(98%)	77 (93%)	4(5%)	2 (2%)	6	37
45	k	82/84~(98%)	62 (76%)	15 (18%)	5 (6%)	1	20
46	1	21/23~(91%)	20 (95%)	1 (5%)	0	100	100
47	m	43/45~(96%)	33 (77%)	8 (19%)	2 (5%)	2	24
48	О	92/94~(98%)	80 (87%)	9 (10%)	3 (3%)	4	31
49	р	119/156~(76%)	109 (92%)	8 (7%)	2 (2%)	9	43
50	q	126/128~(98%)	120 (95%)	4 (3%)	2 (2%)	9	44
51	r	140/162~(86%)	119 (85%)	17~(12%)	4 (3%)	4	33
52	s	366/390~(94%)	318 (87%)	42 (12%)	6 (2%)	9	44
55	Z	202/204~(99%)	176 (87%)	23 (11%)	3 (2%)	10	45
57	AB	215/217~(99%)	186 (86%)	27 (13%)	2 (1%)	17	54
58	AC	$\overline{130/132}$ (98%)	101 (78%)	27 (21%)	2 (2%)	10	45
59	AD	316/343~(92%)	261 (83%)	41 (13%)	14 (4%)	2	25
60	AE	$\overline{120/122}$ (98%)	96 (80%)	22 (18%)	2 (2%)	9	43
61	AF	$197/\overline{208}~(95\%)$	168 (85%)	26 (13%)	3 (2%)	10	45



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	erc	entiles
62	AG	301/326~(92%)	248~(82%)	43~(14%)	10 (3%)		4	31
63	AH	120/122~(98%)	97~(81%)	20~(17%)	3(2%)		5	36
64	AI	134/136~(98%)	102 (76%)	28 (21%)	4 (3%)		4	33
65	AJ	106/108~(98%)	88~(83%)	15 (14%)	3 (3%)		5	34
66	AK	99/101~(98%)	73 (74%)	20 (20%)	6 (6%)		1	20
67	AL	162/164~(99%)	146 (90%)	15 (9%)	1 (1%)		25	63
68	AM	114/116~(98%)	100 (88%)	10 (9%)	4 (4%)		3	30
69	AN	105/107~(98%)	89~(85%)	13 (12%)	3 (3%)		4	33
70	AO	183/185~(99%)	153 (84%)	27 (15%)	3 (2%)		9	44
71	AP	94/96~(98%)	77~(82%)	16 (17%)	1 (1%)		14	51
72	AQ	84/86~(98%)	72 (86%)	10 (12%)	2 (2%)		6	37
73	AR	240/242~(99%)	204 (85%)	27 (11%)	9 (4%)		3	28
74	AS	124/126~(98%)	105 (85%)	17 (14%)	2 (2%)		9	44
75	AT	160/162~(99%)	136 (85%)	21 (13%)	3 (2%)		8	41
76	AU	171/173~(99%)	154 (90%)	12 (7%)	5 (3%)		4	33
77	AV	320/365~(88%)	273~(85%)	40 (12%)	7 (2%)		6	38
78	AW	95/97~(98%)	76~(80%)	16 (17%)	3 (3%)		4	32
79	AX	310/348~(89%)	233~(75%)	56 (18%)	21 (7%)		1	18
80	AY	106/108~(98%)	92~(87%)	10 (9%)	4 (4%)		3	28
81	AZ	85/87~(98%)	75~(88%)	9 (11%)	1 (1%)		13	49
82	A0	197/208~(95%)	162 (82%)	30 (15%)	5 (2%)		5	36
83	A1	252/272~(93%)	197 (78%)	48 (19%)	7 (3%)		5	34
84	A2	114/116~(98%)	95~(83%)	16 (14%)	3(3%)		5	35
85	A3	67/69~(97%)	61 (91%)	5 (8%)	1 (2%)		10	45
86	A4	237/474~(50%)	215 (91%)	20 (8%)	2(1%)		19	57
All	All	12834/13719~(94%)	10913 (85%)	1610 (12%)	311 (2%)		9	37

All (311) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	М	134	ARG
20	V	101	THR
20	V	177	THR

Mol	Chain	Res	Type
30	5	381	LEU
30	5	383	TYR
32	7	308	ALA
36	b	116	ARG
38	d	230	ARG
38	d	231	LEU
58	AC	39	ALA
66	AK	63	LEU
66	AK	82	SER
73	AR	291	ARG
76	AU	34	LEU
77	AV	41	GLU
79	AX	96	GLU
79	AX	156	PRO
79	AX	234	ARG
79	AX	342	PRO
83	A1	243	LYS
4	Е	126	ASP
4	Е	241	GLY
4	Е	317	PRO
5	F	128	TRP
8	J	29	ALA
8	J	125	ALA
10	L	112	GLY
11	М	280	LYS
15	Q	127	SER
16	R	140	GLY
17	S	138	ALA
20	V	99	GLY
20	V	151	GLY
21	W	72	HIS
$\overline{22}$	X	18	GLU
22	X	220	GLU
25	0	116	LEU
31	6	189	CYS
32	7	321	ARG
34	9	34	LYS
34	9	37	GLY
34	9	133	ARG
37	с	183	GLU
37	с	206	SER
39	е	174	PRO



Mol	Chain	Res	Type
41	g	55	THR
41	g	70	SER
41	g	81	ASN
41	g	143	VAL
41	g	145	GLY
42	h	137	ARG
42	h	147	ASN
45	k	36	THR
48	0	61	GLY
49	р	108	ALA
52	s	250	PHE
55	Z	117	ASP
58	AC	125	ARG
59	AD	143	GLY
59	AD	148	LEU
59	AD	193	TRP
59	AD	199	GLY
59	AD	287	ASP
59	AD	299	LYS
59	AD	398	GLU
59	AD	423	SER
62	AG	210	VAL
62	AG	392	THR
64	AI	145	ILE
69	AN	97	GLY
70	AO	221	GLN
72	AQ	81	ALA
73	AR	292	ASP
75	AT	137	ARG
77	AV	119	TYR
77	AV	254	GLY
79	AX	60	GLY
79	AX	270	GLY
$\overline{79}$	AX	325	PRO
83	A1	135	ALA
83	A1	196	GLU
3	D	67	LYS
3	D	167	ASN
3	D	177	ARG
3	D	221	ASN
4	E	215	PHE
4	Е	325	GLU



Mol	Chain	Res	Type
5	F	290	TYR
6	Н	61	LYS
6	Н	103	GLU
7	Ι	61	HIS
8	J	31	PRO
8	J	43	GLY
9	K	4	PHE
9	К	148	PRO
10	L	37	ARG
10	L	103	ASN
11	М	242	TYR
13	0	105	THR
15	Q	76	LEU
15	Q	183	LEU
20	V	125	PRO
21	W	73	PHE
22	Х	175	GLN
22	Х	221	LYS
23	Y	83	ALA
23	Y	162	ARG
24	Z	140	LYS
24	Ζ	143	GLY
25	0	163	GLU
26	1	60	LYS
30	5	70	LEU
30	5	297	ALA
30	5	348	ASP
31	6	50	LYS
31	6	69	HIS
31	6	378	GLY
32	7	121	LYS
34	9	46	SER
37	с	313	PRO
39	е	251	HIS
43	i	127	PHE
44	j	34	ALA
45	k	39	SER
48	0	15	ARG
50	q	42	PRO
50	q	52	LEU
52	S	152	GLN
52	s	272	PRO



Mol	Chain	Res	Type
52	S	408	ASN
59	AD	286	GLU
59	AD	288	HIS
60	AE	116	LYS
61	AF	198	ARG
62	AG	154	GLY
63	AH	147	HIS
63	AH	179	GLN
65	AJ	136	GLN
66	AK	126	ALA
67	AL	194	LEU
68	AM	64	LYS
70	AO	128	CYS
71	AP	131	LYS
73	AR	127	LYS
73	AR	256	ARG
76	AU	30	ARG
76	AU	50	PRO
77	AV	371	ASP
78	AW	146	ASP
79	AX	72	PRO
79	AX	95	SER
79	AX	397	TYR
80	AY	339	GLU
82	A0	108	ASN
82	A0	127	GLU
83	A1	137	LEU
3	D	208	ARG
4	Е	211	ILE
4	Ε	326	GLU
5	F	125	ARG
6	Н	64	LEU
7	Ι	176	LEU
9	K	151	ILE
11	М	47	ARG
11	М	260	LYS
11	М	287	ASP
12	N	174	GLY
16	R	143	SER
18	Т	79	GLN
18	Т	158	TYR
19	U	34	ALA



Mol	Chain	Res	Type
20	V	152	ARG
22	Х	154	CYS
23	Y	183	GLN
28	3	95	THR
30	5	215	ARG
30	5	296	LYS
33	8	91	PRO
34	9	25	ARG
34	9	39	LYS
36	b	50	GLU
37	с	64	PRO
38	d	190	GLU
39	е	264	LEU
43	i	66	PHE
48	0	81	LYS
51	r	55	ALA
52	s	260	GLU
55	Z	112	SER
59	AD	104	ALA
59	AD	138	GLY
60	AE	104	GLU
61	AF	132	GLU
62	AG	232	GLN
62	AG	234	GLY
62	AG	249	THR
62	AG	252	SER
62	AG	261	GLN
65	AJ	130	TYR
66	AK	30	VAL
66	AK	58	ARG
68	AM	15	GLY
69	AN	102	GLY
69	AN	109	PRO
70	AO	53	ASP
73	AR	155	LYS
73	AR	179	GLY
73	AR	267	TYR
75	AT	149	CYS
79	AX	59	HIS
79	AX	131	GLY
79	AX	182	LEU
79	AX	280	SER



Mol	Chain	Res	Type
79	AX	301	TRP
82	A0	194	GLN
83	A1	195	GLY
84	A2	39	GLU
84	A2	41	GLY
84	A2	44	THR
86	A4	620	VAL
9	K	153	LYS
11	М	286	THR
14	Р	173	GLU
15	Q	228	PRO
16	R	138	PRO
18	Т	69	ARG
19	U	11	ARG
20	V	117	HIS
20	V	193	THR
21	W	122	LYS
22	Х	68	PRO
22	Х	155	SER
30	5	272	ASP
30	5	277	THR
30	5	286	PRO
31	6	225	LEU
31	6	359	HIS
37	с	52	ARG
39	е	135	ALA
45	k	58	ASP
45	k	62	PRO
47	m	70	GLU
49	р	122	THR
62	AG	291	GLY
63	AH	127	TYR
64	AI	60	PHE
64	AI	108	ALA
72	AQ	6	LYS
75	AT	132	ARG
76	AU	43	ASN
76	AU	171	GLU
77	AV	253	PRO
79	AX	82	GLY
79	AX	120	PRO
79	AX	133	GLY



Mol	Chain	Res	Type
79	AX	388	PRO
80	AY	319	ALA
82	A0	75	GLY
83	A1	213	PRO
83	A1	306	GLU
85	A3	185	ALA
5	F	91	PRO
7	Ι	178	GLY
30	5	171	PRO
31	6	314	ALA
32	7	213	ASP
33	8	96	ASP
51	r	57	PRO
51	r	64	PRO
57	AB	139	LYS
59	AD	214	THR
59	AD	389	GLY
61	AF	165	GLY
62	AG	289	GLY
65	AJ	54	GLY
73	AR	95	ILE
73	AR	153	THR
77	AV	42	ALA
78	AW	97	ASP
78	AW	117	GLY
79	AX	116	SER
79	AX	235	ASN
4	Е	79	PRO
15	Q	226	PRO
41	g	69	PRO
45	k	64	VAL
81	AZ	90	GLY
7	Ι	102	VAL
15	Q	242	GLY
31	6	351	HIS
32	7	270	PRO
37	с	162	GLY
64	AI	144	VAL
66	AK	123	ILE
68	AM	62	GLY
74	AS	54	GLY
$\overline{74}$	AS	77	VAL



Mol	Chain	Res	Type
77	AV	243	VAL
80	AY	293	PRO
80	AY	325	GLY
47	m	71	PRO
55	Z	183	PRO
68	AM	56	PRO
86	A4	68	VAL
51	r	61	PRO
17	S	168	PRO
44	j	25	GLY
52	s	218	PRO
57	AB	243	PRO
82	A0	143	PRO
17	S	147	PRO

#### 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
3	D	190/190~(100%)	185~(97%)	5(3%)	46 68
4	Ε	255/259~(98%)	253~(99%)	2(1%)	81 89
5	F	217/217~(100%)	210~(97%)	7 (3%)	39 63
6	Η	86/86~(100%)	85~(99%)	1 (1%)	71 83
7	Ι	145/155~(94%)	145 (100%)	0	100 100
8	J	113/113~(100%)	112 (99%)	1 (1%)	78 87
9	Κ	155/155~(100%)	151 (97%)	4 (3%)	46 68
10	L	98/98~(100%)	95~(97%)	3 (3%)	40 64
11	М	245/245~(100%)	240~(98%)	5 (2%)	55 74
12	Ν	172/172~(100%)	170 (99%)	2 (1%)	71 83
13	О	133/133~(100%)	132 (99%)	1 (1%)	81 89
14	Р	115/120~(96%)	113 (98%)	2 (2%)	60 78
15	Q	201/201~(100%)	200 (100%)	1 (0%)	88 93



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
16	R	118/118~(100%)	118 (100%)	0	100	100
17	$\mathbf{S}$	141/141~(100%)	139~(99%)	2(1%)	67	81
18	Т	146/146~(100%)	145 (99%)	1 (1%)	84	90
19	U	99/99~(100%)	97~(98%)	2 (2%)	55	74
20	V	169/180~(94%)	164 (97%)	5 (3%)	41	64
21	W	93/93~(100%)	91 (98%)	2 (2%)	52	71
22	Х	219/219~(100%)	212 (97%)	7 (3%)	39	63
23	Y	159/159~(100%)	158 (99%)	1 (1%)	86	91
24	Z	111/111 (100%)	109 (98%)	2(2%)	59	77
25	0	97/97~(100%)	95~(98%)	2(2%)	53	73
26	1	49/49~(100%)	47 (96%)	2(4%)	30	58
27	2	40/40~(100%)	40 (100%)	0	100	100
28	3	88/88 (100%)	87 (99%)	1 (1%)	73	84
29	4	35/35~(100%)	35 (100%)	0	100	100
30	5	337/353~(96%)	333~(99%)	4 (1%)	71	83
31	6	266/313~(85%)	262 (98%)	4 (2%)	65	80
32	7	242/263~(92%)	237 (98%)	5 (2%)	53	73
33	8	91/91~(100%)	90 (99%)	1 (1%)	73	84
34	9	91/104 (88%)	91 (100%)	0	100	100
35	a	78/104~(75%)	75~(96%)	3 (4%)	33	59
36	b	130/130~(100%)	127 (98%)	3 (2%)	50	71
37	с	241/250~(96%)	241 (100%)	0	100	100
38	d	151/159~(95%)	149 (99%)	2(1%)	69	82
39	е	188/207~(91%)	183 (97%)	5 (3%)	44	67
40	f	117/130~(90%)	116 (99%)	1 (1%)	78	87
41	g	119/119 (100%)	118 (99%)	1 (1%)	81	89
42	h	95/97~(98%)	95 (100%)	0	100	100
43	i	86/86~(100%)	82 (95%)	4 (5%)	26	55
44	j	68/68~(100%)	68 (100%)	0	100	100
45	k	74/74~(100%)	73~(99%)	1 (1%)	67	81
46	l	23/23~(100%)	23 (100%)	0	100	100



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
47	m	40/40~(100%)	39~(98%)	1 (2%)	47	69
48	О	80/80~(100%)	79~(99%)	1 (1%)	69	82
49	р	117/140~(84%)	115 (98%)	2 (2%)	60	78
50	q	110/110~(100%)	107~(97%)	3(3%)	44	67
51	r	133/147~(90%)	131~(98%)	2 (2%)	65	80
52	s	326/344~(95%)	323~(99%)	3 (1%)	78	87
55	Z	179/179~(100%)	176 (98%)	3 (2%)	60	78
57	AB	191/191~(100%)	190 (100%)	1 (0%)	88	93
58	AC	115/115~(100%)	113 (98%)	2 (2%)	60	78
59	AD	269/286~(94%)	263~(98%)	6 (2%)	52	71
60	AE	104/104~(100%)	102 (98%)	2 (2%)	57	75
61	AF	178/185~(96%)	176 (99%)	2 (1%)	73	84
62	AG	265/284~(93%)	256~(97%)	9 (3%)	37	62
63	AH	112/112~(100%)	108 (96%)	4 (4%)	35	61
64	AI	104/104~(100%)	103 (99%)	1 (1%)	76	86
65	AJ	93/93~(100%)	91 (98%)	2 (2%)	52	71
66	AK	91/91~(100%)	89~(98%)	2 (2%)	52	71
67	AL	152/152~(100%)	151 (99%)	1 (1%)	84	90
68	AM	95/95~(100%)	95 (100%)	0	100	100
69	AN	93/93~(100%)	89~(96%)	4 (4%)	29	57
70	AO	166/166~(100%)	158~(95%)	8 (5%)	25	54
71	AP	87/87~(100%)	86~(99%)	1 (1%)	73	84
72	AQ	78/78~(100%)	77~(99%)	1 (1%)	69	82
73	AR	224/224~(100%)	219~(98%)	5 (2%)	52	71
74	AS	109/109~(100%)	108 (99%)	1 (1%)	78	87
75	AT	150/150~(100%)	149 (99%)	1 (1%)	84	90
76	AU	$\overline{149/149}~(100\%)$	146 (98%)	3 (2%)	55	74
77	AV	$\overline{295/327}\ (90\%)$	292 (99%)	3 (1%)	76	86
78	AW	84/84~(100%)	84 (100%)	0	100	100
79	AX	$\overline{275/308~(89\%)}$	272 (99%)	3 (1%)	73	84
80	AY	99/99~(100%)	98~(99%)	1 (1%)	76	86



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
81	AZ	80/80~(100%)	76~(95%)	4 (5%)	24	53
82	A0	176/182~(97%)	173 (98%)	3 (2%)	60	78
83	A1	237/250~(95%)	233~(98%)	4 (2%)	60	78
84	A2	99/99~(100%)	96~(97%)	3(3%)	41	64
85	A3	63/64~(98%)	63~(100%)	0	100	100
86	A4	226/291~(78%)	222~(98%)	4 (2%)	59	77
All	All	11530/11982~(96%)	11339 (98%)	191 (2%)	62	78

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	92	ARG
3	D	113	ARG
3	D	147	ARG
3	D	232	ARG
3	D	274	ARG
4	Е	154	ARG
4	Е	324	ASP
5	F	108	ARG
5	F	125	ARG
5	F	131	LYS
5	F	147	ARG
5	F	170	ARG
5	F	221	LEU
5	F	290	TYR
6	Н	75	ARG
8	J	50	CYS
9	К	95	LEU
9	K	145	LEU
9	K	154	ARG
9	K	168	ARG
10	L	39	ARG
10	L	43	ASN
10	L	78	LYS
11	М	41	ARG
11	М	44	ARG
11	М	109	ARG
11	М	134	ARG
11	М	160	SER
12	N	51	ARG



Mol	Chain	Res	Type
12	Ν	105	MET
13	0	16	ARG
14	Р	50	ARG
14	Р	143	MET
15	Q	102	ARG
17	S	115	LEU
17	S	144	LEU
18	Т	133	ASN
19	U	3	ARG
19	U	71	ARG
20	V	15	LEU
20	V	33	ARG
20	V	143	ARG
20	V	145	ARG
20	V	185	ARG
21	W	70	GLN
21	W	105	VAL
22	Х	23	ARG
22	Х	36	ARG
22	Х	44	ARG
22	Х	59	ARG
22	Х	101	LEU
22	Х	141	LEU
22	Х	216	ARG
23	Y	198	ARG
24	Ζ	73	LYS
24	Ζ	77	ARG
25	0	84	ARG
25	0	179	ARG
26	1	34	ARG
26	1	38	ARG
28	3	167	LYS
30	5	229	ARG
30	5	294	LEU
30	5	373	LEU
30	5	415	LEU
31	6	159	ARG
31	6	173	LEU
31	6	277	GLN
31	6	334	LEU
32	7	64	LYS
32	7	156	ARG



Mol	Chain	Res	Type
32	7	256	ARG
32	7	281	SER
32	7	319	ARG
33	8	101	ARG
35	a	44	ASN
35	a	111	GLN
35	a	122	ARG
36	b	15	LEU
36	b	74	ARG
36	b	144	ARG
38	d	227	ARG
38	d	230	ARG
39	е	55	ARG
39	е	151	ARG
39	е	152	LYS
39	е	171	TRP
39	е	273	ARG
40	f	155	ARG
41	g	121	GLN
43	i	35	ARG
43	i	101	ARG
43	i	107	LEU
43	i	113	ARG
45	k	46	ASN
47	m	42	ARG
48	0	9	ARG
49	р	129	ARG
49	р	191	LYS
50	q	28	ARG
50	q	78	SER
50	q	114	ARG
51	r	36	ARG
51	r	74	ARG
52	S	81	ARG
52	S	230	ARG
52	S	238	ASN
55	Z	65	LYS
55	Z	170	ASN
55	Z	205	LYS
57	AB	169	ARG
58	AC	41	ARG
58	AC	153	LEU



Mol	Chain	Res	Type
59	AD	144	LEU
59	AD	186	LYS
59	AD	234	LYS
59	AD	332	MET
59	AD	341	ASN
59	AD	419	ARG
60	AE	15	ARG
60	AE	105	CYS
61	AF	48	LYS
61	AF	198	ARG
62	AG	106	ARG
62	AG	111	LEU
62	AG	232	GLN
62	AG	243	ARG
62	AG	276	ARG
62	AG	301	GLN
62	AG	310	ARG
62	AG	312	GLN
62	AG	389	ARG
63	AH	92	GLU
63	AH	113	ARG
63	AH	136	MET
63	AH	170	MET
64	AI	189	ARG
65	AJ	43	LYS
65	AJ	129	LYS
66	AK	95	SER
66	AK	102	ARG
67	AL	145	LYS
69	AN	65	LEU
69	AN	73	ARG
69	AN	78	LYS
69	AN	100	CYS
70	AO	94	CYS
70	AO	96	ARG
70	AO	109	ARG
70	AO	136	TYR
70	AO	143	CYS
70	AO	148	LYS
70	AO	163	LEU
70	AO	173	ARG
71	AP	54	MET



Mol	Chain	Res	Type
72	AQ	10	ARG
73	AR	99	LYS
73	AR	116	ARG
73	AR	135	ARG
73	AR	144	GLU
73	AR	258	LYS
74	AS	42	ARG
75	AT	66	MET
76	AU	32	ASP
76	AU	123	ARG
76	AU	155	ARG
77	AV	241	ARG
77	AV	266	VAL
77	AV	380	GLN
79	AX	144	PHE
79	AX	191	PHE
79	AX	397	TYR
80	AY	376	PHE
81	AZ	19	PHE
81	AZ	61	LEU
81	AZ	89	ARG
81	AZ	91	LYS
82	A0	59	ARG
82	A0	60	ARG
82	A0	135	MET
83	A1	110	ASN
83	A1	127	LYS
83	A1	169	ARG
83	A1	312	TYR
84	A2	37	ARG
84	A2	38	ARG
84	A2	68	LYS
86	A4	61	LYS
86	A4	457	TYR
86	A4	478	TYR
86	A4	493	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	205	GLN
3	D	235	GLN



Mol	Chain	Res	Type
5	F	105	ASN
5	F	130	GLN
5	F	276	GLN
6	Н	121	ASN
9	K	48	HIS
12	Ν	173	GLN
13	0	31	ASN
15	Q	158	GLN
16	R	12	ASN
16	R	89	ASN
18	Т	133	ASN
23	Y	73	ASN
23	Y	76	GLN
23	Y	195	ASN
26	1	35	ASN
27	2	64	HIS
28	3	178	GLN
37	с	192	GLN
38	d	149	HIS
41	g	93	ASN
41	g	141	ASN
42	h	151	ASN
49	р	184	ASN
51	r	148	ASN
52	S	238	ASN
55	Z	75	ASN
57	AB	226	ASN
59	AD	341	ASN
60	AE	100	GLN
61	AF	140	ASN
61	AF	147	GLN
64	AI	119	ASN
69	AN	56	GLN
72	AQ	53	GLN
73	AR	214	ASN
74	AS	91	ASN
77	AV	170	GLN
77	AV	224	GLN
79	AX	143	HIS
79	AX	363	ASN
79	AX	367	GLN



# 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	1460/1472~(99%)	373~(25%)	46 (3%)
2	В	52/56~(92%)	12 (23%)	2(3%)
54	u	1/2~(50%)	0	0
56	AA	914/923~(99%)	301 (32%)	22 (2%)
All	All	2427/2453~(98%)	686~(28%)	70 (2%)

All (686) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	А	1672	С
1	А	1674	А
1	А	1679	U
1	А	1680	А
1	А	1685	С
1	А	1689	С
1	А	1693	С
1	А	1694	U
1	А	1695	С
1	А	1696	С
1	А	1697	А
1	А	1699	С
1	А	1700	U
1	А	1704	U
1	А	1705	А
1	А	1708	А
1	А	1713	А
1	А	1714	С
1	А	1715	С
1	А	1717	U
1	А	1722	А
1	А	1724	А
1	А	1732	С
1	А	1741	А
1	А	1748	G
1	А	1750	G
1	А	1751	А
1	А	1773	А
1	А	1777	А
1	А	1782	G
1	А	1794	A
1	А	1795	А



Mol	Chain	Res	Type
1	А	1796	А
1	А	1803	А
1	А	1804	А
1	А	1805	А
1	А	1806	U
1	А	1807	U
1	А	1808	А
1	А	1811	А
1	А	1812	С
1	А	1813	С
1	А	1817	С
1	А	1824	U
1	А	1827	С
1	A	1828	A
1	А	1832	А
1	A	1834	U
1	А	1836	А
1	А	1844	А
1	А	1849	С
1	А	1853	A
1	А	1854	U
1	А	1855	A
1	А	1859	A
1	А	1869	A
1	А	1870	A
1	А	1871	A
1	А	1872	U
1	А	1882	А
1	А	1886	G
1	А	1887	A
1	А	1893	A
1	A	1901	С
1	А	1903	С
1	A	1907	A
1	A	1917	A
1	A	1918	G
1	A	1919	С
1	А	1939	G
1	А	1940	A
1	А	1944	С
1	А	1958	G
1	A	1972	A



Mol	Chain	Res	Type
1	А	1974	А
1	А	1985	G
1	А	1986	А
1	А	1992	С
1	А	1993	А
1	А	1994	А
1	А	1995	А
1	А	2003	A
1	А	2010	U
1	А	2011	G
1	А	2015	G
1	А	2021	U
1	А	2022	G
1	A	2031	A
1	А	2039	А
1	А	2041	U
1	А	2053	U
1	А	2060	А
1	А	2061	С
1	А	2065	А
1	А	2074	А
1	А	2079	С
1	А	2081	U
1	А	2083	U
1	А	2098	G
1	А	2105	G
1	А	2111	С
1	А	2113	G
1	А	2114	С
1	А	2124	А
1	А	2131	А
1	А	2134	А
1	A	2135	А
1	А	2143	G
1	A	2147	G
1	A	$2\overline{159}$	U
1	A	2160	А
1	A	2165	С
1	A	2166	С
1	A	$2\overline{167}$	A
1	A	2168	U
1	А	2171	U



Mol	Chain	Res	Type
1	А	2172	А
1	А	2173	G
1	А	2178	А
1	А	2179	А
1	А	2180	А
1	А	2181	А
1	А	2183	С
1	А	2193	U
1	А	2195	А
1	А	2196	А
1	А	2197	G
1	А	2198	А
1	А	2199	A
1	A	2206	С
1	А	2215	С
1	А	2216	А
1	А	2218	С
1	А	2230	А
1	А	2235	С
1	А	2237	А
1	А	2241	А
1	А	2242	U
1	А	2245	А
1	А	2246	А
1	А	2250	А
1	А	2256	U
1	А	2260	А
1	А	2261	С
1	А	2262	С
1	А	2263	С
1	A	$2\overline{280}$	C
1	A	2281	А
1	А	2282	С
1	A	2283	С
1	A	2284	C
1	A	2293	A
1	А	2295	C
1	A	2296	U
1	A	2299	U
1	A	$2\overline{300}$	G
1	A	2307	U
1	А	2309	А



Mol	Chain	Res	Type
1	А	2313	А
1	А	2315	А
1	А	2332	С
1	А	2345	G
1	А	2350	А
1	А	2358	А
1	А	2359	С
1	А	2364	С
1	А	2366	G
1	А	2369	А
1	А	2372	U
1	А	2373	А
1	А	2384	А
1	А	2385	U
1	А	2386	С
1	А	2387	U
1	А	2388	А
1	А	2389	С
1	А	2390	А
1	А	2393	С
1	А	2395	А
1	А	2398	А
1	А	2404	U
1	А	2406	А
1	А	2407	U
1	А	2415	С
1	А	2417	С
1	А	2433	С
1	А	2434	А
1	А	2435	G
1	A	2442	U
1	А	2443	С
1	A	2444	A
1	Α	2446	A
1	А	2447	А
1	A	2453	G
1	A	2455	U
1	A	2458	A
1	A	2469	A
1	А	2471	G
1	А	2473	A
1	А	2481	А



Mol	Chain	Res	Type
1	А	2493	С
1	А	2499	U
1	А	2511	С
1	А	2512	А
1	А	2520	С
1	А	2522	U
1	А	2523	С
1	А	2524	А
1	А	2525	С
1	А	2526	С
1	А	2527	А
1	А	2530	А
1	А	2531	U
1	А	2532	U
1	А	2540	С
1	А	2546	G
1	А	2556	А
1	А	2557	С
1	А	2558	А
1	А	2559	U
1	А	2564	А
1	А	2570	С
1	А	2583	С
1	А	2585	G
1	А	2586	U
1	А	2592	G
1	А	2593	G
1	А	2594	U
1	А	2599	U
1	А	2600	А
1	А	2604	А
1	А	2605	С
1	А	2606	U
1	А	2614	U
1	A	2618	U
1	А	2623	А
1	А	2624	С
1	A	2625	С
1	А	2627	G
1	А	2629	А
1	А	2630	U
1	А	2632	А



Mol	Chain	Res	Type
1	А	2633	А
1	А	2634	U
1	А	2635	G
1	А	2645	G
1	А	2654	U
1	А	2656	U
1	А	2660	U
1	А	2673	G
1	А	2683	С
1	А	2693	А
1	А	2694	А
1	А	2695	G
1	А	2696	A
1	A	2702	G
1	А	2708	С
1	A	2711	A
1	А	2714	А
1	А	2718	С
1	А	2719	G
1	А	2721	G
1	А	2722	А
1	А	2723	А
1	А	2724	G
1	А	2731	U
1	А	2732	G
1	А	2741	А
1	А	2744	U
1	А	2755	А
1	А	2756	С
1	А	2758	G
1	A	2759	U
1	A	2798	А
1	А	2810	G
1	А	2813	U
1	A	2814	G
1	A	2832	A
1	А	2833	A
1	A	2837	А
1	A	2838	А
1	A	$2\overline{839}$	C
1	A	2847	С
1	А	2849	G



Mol	Chain	Res	Type
1	А	2853	А
1	А	2854	U
1	А	2855	G
1	А	2859	А
1	А	2864	U
1	А	2865	С
1	А	2875	А
1	А	2881	С
1	А	2904	А
1	А	2910	А
1	А	2913	А
1	А	2915	С
1	А	2916	G
1	А	2918	А
1	А	2919	А
1	А	2921	А
1	А	2926	А
1	А	2928	С
1	А	2935	А
1	А	2936	U
1	А	2954	С
1	А	2955	U
1	А	2956	А
1	А	2962	С
1	А	2963	А
1	А	2977	G
1	А	2980	U
1	А	2981	А
1	А	2985	С
1	А	2988	С
1	A	2989	G
1	A	2990	A
1	A	2991	U
1	А	2992	G
1	А	3000	A
1	A	3003	A
1	A	3005	A
1	A	3007	С
1	A	3016	G
1	A	3018	A
1	А	3022	G
1	А	3041	U



Mol	Chain	Res	Type
1	А	3042	U
1	А	3053	А
1	А	3054	G
1	А	3059	А
1	А	3060	С
1	А	3061	G
1	А	3063	G
1	А	3068	G
1	А	3069	А
1	А	3072	U
1	А	3073	С
1	А	3089	А
1	А	3093	С
1	А	3096	U
1	А	3098	U
1	A	3100	U
1	А	3102	U
1	А	3108	U
1	А	3109	U
1	А	3114	U
1	А	3122	U
1	А	3123	G
1	А	3129	А
1	А	3133	А
1	А	3134	С
1	А	3135	А
1	А	3152	С
1	А	3153	U
1	A	3157	С
1	А	3158	А
1	A	3169	С
1	A	3172	C
1	А	3175	А
1	A	3177	A
1	А	3178	U
1	A	3182	A
1	А	3183	U
1	А	3188	U
1	A	3189	С
1	A	3190	А
1	A	3192	C
1	А	3195	А



Mol	Chain	Res	Type
1	А	3202	U
1	А	3206	С
1	А	3217	А
1	А	3218	А
1	А	3228	U
2	В	1604	G
2	В	1609	U
2	В	1611	G
2	В	1631	С
2	В	1637	С
2	В	1638	U
2	В	1644	G
2	В	1645	А
2	В	1646	U
2	В	1651	А
2	В	1667	С
2	В	1670	А
56	AA	650	U
56	AA	651	A
56	AA	656	U
56	AA	673	U
56	AA	674	U
56	AA	675	A
56	AA	680	U
56	AA	685	A
56	AA	688	A
56	AA	689	U
56	AA	690	U
56	AA	691	A
56	AA	694	C
56	AA	696	U
56	AA	704	U
56	AA	706	С
56	AA	710	U
56	AA	711	U
56	AA	712	С
56	AA	715	G
56	AA	718	A
56	AA	721	U
56	AA	722	С
56	AA	723	A
56	AA	732	A



Mol	Chain	Res	Type
56	AA	733	U
56	AA	753	A
56	AA	757	A
56	AA	761	A
56	AA	764	A
56	AA	766	G
56	AA	770	С
56	AA	771	А
56	AA	781	А
56	AA	782	А
56	AA	788	U
56	AA	791	G
56	AA	794	U
56	AA	796	G
56	AA	800	С
56	AA	801	A
56	AA	806	С
56	AA	807	А
56	AA	808	С
56	AA	812	A
56	AA	813	А
56	AA	814	А
56	AA	817	G
56	AA	824	U
56	AA	826	А
56	AA	828	С
56	AA	829	С
56	AA	836	А
56	AA	837	A
56	AA	839	A
56	AA	841	A
56	AA	847	G
56	AA	848	U
56	AA	851	A
56	AA	853	С
56	AA	861	U
56	AA	868	С
56	AA	869	C
56	AA	871	A
56	AA	875	U
56	AA	877	G
56	AA	880	С



Mol	Chain	Res	Type
56	AA	881	А
56	AA	883	U
56	AA	890	С
56	AA	893	G
56	AA	899	G
56	AA	900	С
56	AA	902	G
56	AA	904	С
56	AA	905	А
56	AA	908	С
56	AA	917	С
56	AA	919	А
56	AA	920	G
56	AA	921	U
56	AA	922	С
56	AA	923	А
56	AA	933	G
56	AA	938	А
56	AA	939	А
56	AA	940	А
56	AA	942	А
56	AA	943	G
56	AA	945	G
56	AA	947	U
56	AA	954	С
56	AA	967	А
56	AA	969	А
56	AA	972	G
56	AA	973	С
56	AA	976	A
$\overline{56}$	AA	977	A
56	AA	978	A
56	AA	981	C
$\overline{56}$	AA	987	A
56	AA	992	U
56	AA	995	A
56	AA	997	A
56	AA	1000	U
56	AA	1007	G
56	AA	1010	A
$\overline{56}$	AA	1012	A
56	AA	1013	A



Mol	Chain	Res	Type
56	AA	1014	А
56	AA	1015	А
56	AA	1017	А
56	AA	1022	A
56	AA	1031	G
56	AA	1042	U
56	AA	1044	U
56	AA	1048	С
56	AA	1049	А
56	AA	1052	С
56	AA	1054	А
56	AA	1059	U
56	AA	1063	A
56	AA	1064	C
$\overline{56}$	AA	1065	C
56	AA	1072	G
$\overline{56}$	AA	1080	A
56	AA	1081	U
56	AA	1082	A
56	AA	1089	U
56	AA	1100	С
56	AA	1102	A
56	AA	1105	С
56	AA	1106	С
56	AA	1108	С
56	AA	1109	A
56	AA	1121	A
56	AA	1123	С
56	AA	1125	A
56	AA	1128	C
56	AA	1138	G
56	AA	1142	A
56	AA	1143	C
56	AA	1147	G
56	AA	1151	C
56	AA	1152	A
56	AA	1153	C
56	AA	1154	A
56	AA	1160	A
56	AA	1166	A
56	AA	1167	A
56	AA	1179	G



Mol	Chain	Res	Type
56	AA	1180	U
56	AA	1187	U
56	AA	1188	А
56	AA	1189	U
56	AA	1190	С
56	AA	1191	С
56	AA	1195	U
56	AA	1200	G
56	AA	1202	G
56	AA	1203	С
56	AA	1206	G
56	AA	1211	G
56	AA	1213	A
56	AA	1214	A
56	AA	1215	U
56	AA	1216	С
56	AA	1217	G
56	AA	1219	U
56	AA	1220	А
56	AA	1223	С
56	AA	1225	С
56	AA	1226	С
56	AA	1227	G
56	AA	1228	А
56	AA	1229	U
56	AA	1230	С
56	AA	1231	А
56	AA	1232	А
56	AA	1234	С
56	AA	1235	U
56	AA	1236	С
56	AA	1237	A
56	AA	1245	U
$\overline{56}$	AA	1247	G
56	AA	1248	С
56	AA	$1\overline{250}$	C
56	AA	1251	A
56	AA	1253	С
56	AA	1257	U
56	AA	1258	A
$\overline{56}$	AA	1269	U
56	AA	1270	U



Mol	Chain	Res	Type
56	AA	1271	С
56	AA	1272	А
56	AA	1283	А
56	AA	1284	U
56	AA	1285	G
56	AA	1290	С
56	AA	1292	А
56	AA	1293	С
56	AA	1295	А
56	AA	1296	А
56	AA	1298	U
56	AA	1300	А
56	AA	1309	А
56	AA	1311	С
56	AA	1312	С
56	AA	1314	С
56	AA	1315	G
56	AA	1321	А
56	AA	1326	А
56	AA	1327	G
56	AA	1330	С
56	AA	1331	А
56	AA	1332	А
56	AA	1336	G
56	AA	1342	С
56	AA	1343	А
56	AA	1353	А
56	AA	1354	А
56	AA	1355	G
56	AA	1356	А
56	AA	1357	A
56	AA	1358	A
56	AA	1365	А
56	AA	1371	U
56	AA	1372	С
56	AA	1373	U
56	AA	1376	С
56	AA	1378	С
56	AA	1379	A
56	AA	1382	А
56	AA	1383	А
56	AA	1390	А


Mol	Chain	Res	Type		
56	AA	1393	G		
56	AA	1397	U		
56	AA	1398	U		
56	AA	1399	А		
56	AA	1400	U		
56	AA	1401	G		
56	AA	1402	А		
56	AA	1408	А		
56	AA	1409	A		
56	AA	1410	G		
56	AA	1412	G		
56	AA	1415	G		
56	AA	1416	A		
56	AA	1418	G		
56	AA	1420	U		
56	AA	1422	G		
56	AA	1429	С		
56	AA	1430	А		
56	AA	1431	G		
56	AA	1442	G		
56	AA	1444	A		
56	AA	1446	А		
56	AA	1447	G		
56	AA	1448	U		
56	AA	1451	U		
56	AA	1454	G		
56	AA	1461	A		
56	AA	1466	C		
56	AA	1478	A		
56	AA	1481	C		
56	AA	1482	A		
56	AA	1491	C		
56	AA	1493	C		
56	AA	1495	C		
56	AA	1503	G		
56	AA	1512	A		
56	AA	1516	G		
56	AA	1523	A		
56	AA	1525	C		
56	AA	1526	U		
56	AA	1527	A		
56	AA	1528	A		



Mol	Chain	Res	Type	
56	AA	1531	С	
56	AA	1532	С	
56	AA	1533	С	
56	AA	1535	U	
56	AA	1536	А	
56	AA	1537	С	
56	AA	1538	G	
56	AA	1539	С	
56	AA	1540	А	
56	AA	1549	G	
56	AA	1554	G	
56	AA	1555	А	
56	AA	1556	С	
56	AA	1560	U	
56	AA	1561	С	
56	AA	1562	G	
56	AA	1564	А	
56	AA	1568	U	
56	AA	1582	G	
56	AA	1594	G	
56	AA	1595	G	
56	AA	1598	G	
56	AA	1599	А	
56	AA	1600	A	

All (70) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	А	1713	А
1	А	1731	А
1	А	1794	А
1	А	1795	А
1	А	1807	U
1	А	1810	А
1	А	1848	U
1	А	1870	А
1	А	1871	А
1	А	2040	G
1	А	2052	А
1	А	2080	U
1	А	2179	А
1	А	2205	U



Mol	Chain	Res	Type	
1	А	2245	А	
1	А	2260	А	
1	А	2280	С	
1	А	2349	G	
1	А	2357	С	
1	А	2371	U	
1	А	2384	А	
1	А	2385	U	
1	А	2386	С	
1	А	2387	U	
1	А	2442	U	
1	А	2510	U	
1	А	2511	С	
1	А	2524	А	
1	А	2530	А	
1	А	2558	А	
1	А	2628	U	
1	А	2713	С	
1	А	2721	G	
1	А	2754	А	
1	А	2758	G	
1	А	2838	А	
1	А	2979	U	
1	А	3041	U	
1	А	3058	U	
1	А	3060	С	
1	А	3092	U	
1	А	3113	А	
1	А	3121	С	
1	А	3177	А	
1	A	3201	А	
1	A	3205	C	
2	В	1603	А	
2	В	1637	С	
56	AA	688	A	
56	AA	717	G	
56	AA	793	С	
56	AA	876	U	
56	AA	882	A	
56	AA	920	G	
56	AA	953	U	
56	AA	1012	A	



Mol	Chain	Res	Type
56	AA	1013	А
56	AA	1021	U
56	AA	1062	G
56	AA	1099	С
56	AA	1166	А
56	AA	1213	А
56	AA	1320	G
56	AA	1331	А
56	AA	1415	G
56	AA	1429	С
56	AA	1511	С
56	AA	1515	G
56	AA	1534	С
56	AA	1555	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 134 ligands modelled in this entry, 134 are monoatomic - leaving 0 for Mogul analysis.

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
1	А	14
86	A4	13
56	AA	8
2	В	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	А	2218:C	O3'	2228:A	Р	35.95
1	AA	955:A	O3'	965:C	Р	34.65
1	А	2760:A	O3'	2792:A	Р	26.71
1	А	2881:C	O3'	2889:C	Р	26.07
1	А	1760:G	O3'	1766:U	Р	25.62
1	A4	380:ASP	С	386:UNK	N	24.84
1	A4	399:UNK	С	414:LYS	N	22.74
1	В	1651:A	O3'	1658:U	Р	19.37
1	А	3207:A	O3'	3212:C	Р	19.36
1	A4	345:UNK	С	353:UNK	N	18.19
1	А	2067:C	O3'	2072:A	Р	17.99
1	AA	734:C	O3'	740:G	Р	17.26
1	А	3196:G	O3'	3201:A	Р	16.51
1	AA	1518:C	O3'	1521:U	Р	16.45
1	А	2575:U	O3'	2580:U	Р	15.23
1	A4	250:UNK	С	255:UNK	N	14.86
1	А	1732:C	O3'	1737:A	Р	14.30
1	В	1616:A	O3'	1621:A	Р	14.15
1	A4	326:UNK	С	331:UNK	N	13.54
1	А	2351:U	O3'	2357:C	Р	13.47
1	AA	1383:A	O3'	1388:C	Р	13.43
1	AA	1115:U	O3'	1120:C	Р	12.89
1	A4	300:UNK	С	311:UNK	N	12.39
1	А	3109:U	O3'	3113:A	Р	12.02
1	А	1935:A	O3'	1938:A	Р	11.52
1	A4	362:UNK	С	368:SER	N	11.52
1	AA	1404:A	O3'	1407:U	Р	11.35
1	A4	143:GLU	С	145:UNK	N	10.77
1	A4	173:UNK	С	220:UNK	N	10.76
1	AA	928:A	O3'	931:C	Р	9.54
1	A4	269:UNK	С	272:UNK	N	8.06
1	A4	156:UNK	С	161:UNK	N	7.08



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	1556:C	O3'	1559:G	Р	6.41
1	A4	285:UNK	С	290:UNK	Ν	6.07
1	А	1709:G	O3'	1711:C	Р	5.88
1	A4	232:UNK	С	237:UNK	Ν	4.45
1	В	1661:A	O3'	1663:C	Р	3.29
1	А	2359:C	O3'	2363:A	Р	3.25
1	В	1646:U	O3'	1648:U	Р	3.15

Continued from previous page...



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0514. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

# 6.1 Orthogonal projections (i)

This section was not generated.

#### 6.2 Central slices (i)

This section was not generated.

#### 6.3 Largest variance slices (i)

This section was not generated.

# 6.4 Orthogonal surface views (i)

This section was not generated.

#### 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)

This section was not generated.

#### 7.2 Volume estimate versus contour level (i)

This section was not generated.

### 7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



# 9 Map-model fit (i)

This section was not generated.

