

Jun 24, 2021 – 06:41 PM BST

PDB ID	:	709K
EMDB ID	:	EMD-12763
Title	:	Human mitochondrial ribosome large subunit assembly intermediate with
		MTERF4-NSUN4, MRM2, MTG1, the MALSU module, GTPBP5 and mtEF-
		Tu
Authors	:	Valentin Gese, G.; Hallberg, B.M.
Deposited on	:	2021-04-16
$\operatorname{Resolution}$:	3.10 Å(reported)
Based on initial model	:	500L

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

EMDB validation analysis	:	$0.0.0{ m dev}75$
Mogul	:	1.8.5 (274361), 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)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

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 3.10 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	$egin{array}{llllllllllllllllllllllllllllllllllll$	${f EM} { m structures} \ (\#{ m Entries})$
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% 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	0	188	• 57%	•	43%				
2	a	142	57%	·	42%				
3	1	65	78%		•	20%			
4	2	92	49%		51%				
5	3	188	48% •		49%				
6	4	103	• 34% •	63%					
7	5	423	90%			• 7%			
8	6	380	86%			• 13%			



Mol	Chain	Length	Quality of chain								
9	7	338	•		1494						
	1	000	7%		• 1470						
10	8	206	38% •	59%							
11	9	137	88%		• 10%						
12	А	1559	68%	230	6 8 %						
		1000	6%		• 070						
13	A1	384	88%		• 10%						
14	В	69	58%	29%	13%						
15	A2	381	6 1% ·	3	8%						
16	C	224	66%								
10	U	334	75%	•	24%						
17	D	305	77%	•	22%						
18	Е	348	86%		• 13%						
19	F	311	79%	•	20%						
20	\mathbf{FF}	198	32% 6	5%							
20	t.1	198	18%								
		100	12%								
20	t2	198	15% 85%								
20	t3	198	15% • 85%								
20	+1	108	15%								
	04	130	15% 85%								
20	t5	198	15% 85%								
20	t6	198	14% 86%								
91	G	414			10%						
	u	414		••	19%						
22	Н	267	35% • 6	54%							
23	Ι	261	78%	•	19%						
24	J	192	68%	•	28%						
25	K	178	98%								
26	L	145	74%	5%	21%						
27	М	296	94%								

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Conti	nued fron	n previous	page	
Mol	Chain	Length	Quality of chain	
28	N	251	70% .	29%
29	0	175	82%	5% 13%
30	Р	179	77%	• 21%
31	Q	292	72%	26%
32	R	149	89%	5% 6%
33	S	205	75%	• 24%
34	Т	212	78%	22%
35	U	153	88%	• 9%
36	V	216	91%	• 6%
37	W	148	· · ·	32%
38	X	256	93%	• 5%
39	Y	250	68% •	30%
40	Z	161	72%	25%
41	b	215	64% 5%	31%
42	с	332	80%	• 17%
43	d	306	• 70%	27%
44	е	279	23%	• 22%
45	f	212	5%	42%
46	g	166	76%	• 22%
47	h	158	66%	32%
48	i	128	72%	• 24%
49	j	123	• 67%	31%
50	k	112	• 69% •	29%
51	1	138	5% 30% • 68%	
52	m	128	12% 26% • 73%	



Mol	Chain	Length	Quality of chain		
53	n	246	34%		23%
					2570
54	0	102	86%		• 11%
55	р	206	61%	38%	
56	q	222	- 59% •	39%	
57	r	196	▲ 76%	•	21%
58	S	439	83%		• 16%
59	t	452	31% 84%		16%
60	u	234	5 6% •	43%	
61	v	70	• 90%		7% •
62	W	156	16% 52% •	44%	
63	UNK	28	<u>32%</u> 93%		7%

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2 Entry composition (i)

There are 70 unique types of molecules in this entry. The entry contains 115679 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	0	108	Total 880	C 545	N 172	0 157	S 6	0	0

• Molecule 2 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace	
2	a	82	Total 686	C 434	N 124	O 123	${ m S}{ m 5}$	0	0

• Molecule 3 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1	50	Total	С	Ν	Ο	S	0	0
3	T	52	433	278	83	70	2		0

• Molecule 4 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	45	Total 367	С 227	N 81	O 58	S 1	0	0

• Molecule 5 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	95	Total 831	$ m C \ 539$	N 162	0 127	${ m S} { m 3}$	0	0

• Molecule 6 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
6	4	38	Total 342	С 217	N 72	O 49	$\frac{S}{4}$	0	0



• Molecule 7 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	5	392	Total 3199	C 2067	N 558	O 563	S 11	0	0

• Molecule 8 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
8	6	331	Total 2692	C 1723	N 480	O 480	S 9	0	0

• Molecule 9 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	7	290	Total 2356	C 1509	N 400	O 429	S 18	0	0

• Molecule 10 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
10	8	85	Total 719	С 454	N 129	0 134	${ m S} { m 2}$	0	0

• Molecule 11 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
11	9	123	Total 992	C 642	N 169	0 179	S 2	0	0

• Molecule 12 is a RNA chain called 16S rRNA.

Mol	Chain	Residues		A	toms			AltConf	Trace
12	А	1436	Total 30486	m C 13680	N 5498	O 9872	Р 1436	0	0

• Molecule 13 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues		At	oms			AltConf	Trace
13	A1	344	Total 2731	C 1743	N 476	O 495	S 17	0	0

• Molecule 14 is a RNA chain called MT-TRNAVAL.



Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
14	В	60	Total 1275	C 572	N 230	O 413	Р 60	0	0

• Molecule 15 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
15	A2	238	Total 1942	C 1244	N 336	O 350	S 12	0	0

• Molecule 16 is a protein called Mitochondrial ribosome-associated GTPase 1.

Mol	Chain	Residues		At	AltConf	Trace			
16	С	255	Total 1990	$\begin{array}{c} \mathrm{C} \\ 1267 \end{array}$	N 349	O 360	S 14	0	0

• Molecule 17 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
17	D	237	Total 1851	C 1151	N 375	O 316	S 9	0	0

• Molecule 18 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues		At	AltConf	Trace			
18	Е	304	Total 2396	C 1539	N 416	O 430	S 11	0	0

• Molecule 19 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	250	Total 2013	C 1294	N 365	O 348	S 6	0	0

• Molecule 20 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues		Aton	ns	AltConf	Trace		
20	FF	70	Total	С	Ν	Ο	0	0	
20	T, T,	10	540	348	92	100	0	0	
20	+1	46	Total	С	Ν	Ο	0	0	
20	01	40	354	228	56	70	0	0	
20	+0	20	Total	С	Ν	Ο	0	0	
20	t2	t2 30	238	154	38	46	0	0	



Mol	Chain	Residues	Atoms	AltConf	Trace
20	t3	30	Total C N O	0	0
			238 154 38 46		
20	+1	20	Total C N O	0	0
20	ե	29	229 148 36 45	0	0
20	+5	20	Total C N O	0	0
20	10	29	229 148 36 45	0	0
20	+6	97	Total C N O	0	0
20	ιO	21	214 137 34 43	0	0

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• Molecule 21 is a protein called Mitochondrial ribosome-associated GTPase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	337	Total 2549	C 1608	N 466	O 467	S 8	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	407	ASP	-	expression tag	UNP Q9H4K7
G	408	TYR	-	expression tag	UNP Q9H4K7
G	409	LYS	-	expression tag	UNP Q9H4K7
G	410	ASP	-	expression tag	UNP Q9H4K7
G	411	ASP	-	expression tag	UNP Q9H4K7
G	412	ASP	-	expression tag	UNP Q9H4K7
G	413	ASP	-	expression tag	UNP Q9H4K7
G	414	LYS	-	expression tag	UNP Q9H4K7

• Molecule 22 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
22	Н	95	Total 784	C 498	N 152	О 134	0	0

• Molecule 23 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ι	212	Total 1695	C 1088	N 304	O 292	S 11	0	0

• Molecule 24 is a protein called 39S ribosomal protein L11, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	138	Total 1050	$\begin{array}{c} \mathrm{C} \\ 673 \end{array}$	N 190	O 185	S 2	0	0

• Molecule 25 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	K	177	Total 1451	C 934	N 259	0 251	${ m S}$ 7	0	0

• Molecule 26 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	115	Total 889	$\begin{array}{c} \mathrm{C} \\ 559 \end{array}$	N 171	0 154	${f S}5$	0	0

• Molecule 27 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	М	287	Total 2305	C 1472	N 425	O 402	S 6	0	0

• Molecule 28 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
28	N	179	Total 1457	C 930	N 267	0 251	S 9	0	0

• Molecule 29 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
29	О	152	Total 1245	C 784	N 239	O 215	${ m S} 7$	0	0

• Molecule 30 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues		At	oms			AltConf	Trace
30	Р	141	Total 1148	C 719	N 221	O 203	${ m S}{ m 5}$	0	0

• Molecule 31 is a protein called 39S ribosomal protein L19, mitochondrial.



Mol	Chain	Residues		At	oms			AltConf	Trace
31	Q	217	Total 1805	C 1159	N 317	O 320	S 9	0	0

• Molecule 32 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	R	140	Total 1153	C 732	N 231	O 186	S 4	0	0

• Molecule 33 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
33	S	156	Total 1251	C 806	N 222	O 219	$\frac{S}{4}$	0	0

• Molecule 34 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
34	Т	166	Total 1368	C 875	N 254	O 232	S 7	0	0

• Molecule 35 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
35	U	139	Total 1154	С 734	N 220	0 197	S 3	0	0

• Molecule 36 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
36	V	202	Total 1652	C 1053	N 294	O 297	S 8	0	0

• Molecule 37 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
37	W	101	Total 805	C 520	N 151	0 131	${ m S} { m 3}$	0	0

• Molecule 38 is a protein called 39S ribosomal protein L28, mitochondrial.



Mol	Chain	Residues		Ate	oms			AltConf	Trace
38	Х	243	Total 2035	C 1317	N 351	O 362	${ m S}{ m 5}$	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	Y	176	Total 1517	m C 970	N 291	O 252	$\frac{S}{4}$	0	0

• Molecule 40 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
40	Z	120	Total 978	C 626	N 183	0 166	S 3	0	0

• Molecule 41 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
41	b	148	Total 1178	C 733	N 229	O 213	${ m S} { m 3}$	0	0

• Molecule 42 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
42	С	275	Total 2217	C 1415	N 383	0 410	S 9	0	0

• Molecule 43 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
43	d	223	Total 1847	C 1187	N 317	O 330	S 13	0	0

• Molecule 44 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
44	е	217	Total 1762	C 1124	N 310	O 323	${ m S}{ m 5}$	0	0

• Molecule 45 is a protein called 39S ribosomal protein L48, mitochondrial.



Mol	Chain	Residues		At	oms	AltConf	Trace		
45	f	123	Total 979	$\begin{array}{c} \mathrm{C} \\ 625 \end{array}$	N 164	O 187	${ m S} { m 3}$	0	0

• Molecule 46 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
46	g	129	Total 1067	C 690	N 185	O 190	${ m S} { m 2}$	0	0

• Molecule 47 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
47	h	107	Total 871	$\begin{array}{c} \mathrm{C} \\ 551 \end{array}$	N 153	0 164	${ m S} { m 3}$	0	0

• Molecule 48 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
48	i	97	Total 827	C 532	N 165	O 126	$\frac{S}{4}$	0	0

• Molecule 49 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
49	j	85	Total 684	C 423	N 133	O 126	$\frac{S}{2}$	0	0

• Molecule 50 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
50	k	80	Total 627	C 392	N 116	0 114	${ m S}{ m 5}$	0	0

• Molecule 51 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
51	l	44	Total 395	$\begin{array}{c} \mathrm{C} \\ 251 \end{array}$	N 76	O 67	${ m S}$ 1	0	0

• Molecule 52 is a protein called 39S ribosomal protein L55, mitochondrial.



Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
52	m	35	Total 287	C 180	N 57	O 50	0	0

• Molecule 53 is a protein called rRNA methyltransferase 2, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
53	n	189	Total 1450	$\begin{array}{c} \mathrm{C} \\ 917 \end{array}$	N 259	O 268	S 6	0	0

• Molecule 54 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
54	О	91	Total 771	C 487	N 156	O 125	${ m S} { m 3}$	0	0

• Molecule 55 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
55	р	127	Total 1058	C 661	N 201	O 192	$\frac{S}{4}$	0	0

• Molecule 56 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues		At	oms	AltConf	Trace		
56	q	135	Total 1134	C 705	N 222	O 202	${ m S}{ m 5}$	0	0

• Molecule 57 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues		At	oms	AltConf	Trace		
57	r	155	Total 1268	C 806	N 243	0 211	S 8	0	0

• Molecule 58 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
58	S	370	Total 3036	C 1946	N 542	O 534	S 14	0	0

• Molecule 59 is a protein called Elongation factor Tu, mitochondrial.



Mol	Chain	Residues		At	oms			AltConf	Trace
59	t	381	Total 2939	C 1860	N 519	O 545	${ m S}$ 15	0	0

• Molecule 60 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
60	u	133	Total 1092	C 702	N 181	O 199	S 10	0	0

• Molecule 61 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
61	v	68	Total 584	C 369	N 115	O 100	0	0

• Molecule 62 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues		At	oms			AltConf	Trace
62	W	87	Total 705	C 452	N 103	0 144	S 6	0	0

• Molecule 63 is a protein called UNK.

Mol	Chain	Residues	1	Ator	\mathbf{ns}	AltConf	Trace	
63	UNK	26	Total 130	C 78	N 26	O 26	0	0

• Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
64	0	1	Total Zn 1 1	0
64	4	1	Total Zn 1 1	0

• Molecule 65 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
65	А	85	Total Mg 85 85	0
65	D	1	Total Mg 1 1	0



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Mol	Chain	Residues	Atoms	AltConf
65	Е	1	Total Mg 1 1	0
65	G	2	Total Mg 2 2	0
65	М	1	Total Mg 1 1	0
65	W	1	Total Mg 1 1	0
65	g	1	Total Mg 1 1	0
65	t	1	Total Mg 1 1	0

• Molecule 66 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf
66	A1	1	Total 27	$\begin{array}{c} \mathrm{C} \\ 15 \end{array}$	N 6	O 5	${ m S}$ 1	0

• Molecule 67 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\rm C_{10}H_{15}N_5O_{11}P_2).$





Mol	Chain	Residues		At	oms			AltConf
67	C	1	Total	С	Ν	Ο	Р	0
07	U		28	10	5	11	2	0
67	+	1	Total	С	Ν	Ο	Р	0
07	U	L	28	10	5	11	2	0

• Molecule 68 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $\rm C_{10}H_{16}N_5O_{14}P_3).$



Total C N O P	
$\begin{bmatrix} 68 & G & 1 & 32 & 10 & 5 & 14 & 3 \end{bmatrix}$	0



• Molecule 69 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf
69	n	1	Total	С	Ν	Ο	\mathbf{S}	Ο
05		L	26	14	6	5	1	0

• Molecule 70 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



Mol	Chain	Residues		Α	tom	ıs			AltConf
70		1	Total	С	Ν	Ο	Р	\mathbf{S}	0
10	W	L	21	11	2	6	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 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: 39S ribosomal protein L32, mitochondrial





Chain 3:	48%	·	49%	
MET ALA ALA SER ALA ALA CLY ALA ALA ALA ALA	SER GLY ILE CLEU ARG PRO ASN ILEU LEU LEU SELA	SER THR TYR ANG ASN VAL CYS VAL LYS ALA	SER LIEU TIEU ALLA ALLA LIEU LEU CIEU ARG CIEU ARG CIEU TIE CIEU CIEU VAL VAL SER TER SER TER SER TER SER TER	ARG
특별응급왕호립분은급입분행 • Molecule 6: 395	불법립호확별 설립 불립 물 5 ribosomal prot	ein L36, mitoc	hondrial	
Chain 4:	34% •		63%	
MET ALA ASN LEU LEU PHE TLE ASN VAL ASN PASN LEU	LEU TYR LEU ER ARG HIS THR VAL LYS PRO ARG	LEU THR PHE PHE CLEU CLEU CLEU PHE CLEU CLEU CLEU CLEU CLEU CLEU CLEU CLE	GLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	NAL STH
특물특별 <mark>물 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8</mark>	∳ g 5 ribosomal prot	ein L37, mitoc	hondrial	
Chain 5		90%	. 7%	
별클림클톎블鵳클릴볼볼클림클 • Molecule 8: 395	불통급급급급급급급급급급 5 ribosomal prot	taaasta <mark>s a</mark> an L38, mitoc	60 00 00 00 00 00 00 00 00 00 00 00 00 0	
Chain 6:		86%	• 13%	
MET ALA ALA ALA ALA TRP TRP TRP ALA ALA ALA ALA CYS CYS CYS	ARG ARG TRP ARG ARG GLY CHE SER THE SER SER ALA ALA	617 R27 R47 R47 R52 R47 679	GLU THR THR ASP PRO LYS CLY CLYS CLY CLYS CLY CLYS CLY FRO PRO PRO PRO PRO PRO PRO PRO PRO PRO P	GLU GLU
GLY SER SER SER 2388 7291 7291 1371 1371 1371				
• Molecule 9: 39S	5 ribosomal prot	ein L39, mitoc	hondrial	
Chain 7:		83%	• 14%	
MET GLU GLU ALA ALA MET ALA CLY ALA ALA ALA ALA ALA ALA ALA ALA	TRP ULL VAL VAL ALA ALA ALA CP CP CP CP CP CP CP CP CP CP CP CP CP	PHE PHE ALA ALA TLE SER SER SER CLU LEU	836 1897 1413 1413 1413 1413 1413 1413 1413 141	T325
GLU MET ASP GLU MET OLN ALA SERN ALA LYS ALA ALA GLY TRN GLY GLU SER GLU SER GLU ARG CYS ALA THR LEU TRN LEU TRN LEU	TRP LEU VILL VILL VILL PRO GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	PARA PARA ALA ALA SER SER SER SER CLU	836 1897 1413 1413 1413 1413 1413 1413 1413 1212 1212	T325
탄	불림불길물등등등림을 통 OS ribosomal pro	tein L40, mito	chondrial	1325
	8 ribosomal pro	etein L40, mito	8 8	13.25



• Molecule 11: 39S ribosomal protein L41, mitochondrial

Chain 9:	88%	•	10%
MET VAL VAL LEU ALA ALA ALA ALA ALA ALA ALA CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS			
MI LIDICC DNA			







• Molecule 16: Mitochondrial ribosome-associated GTPase 1





LEU PRO ALA ALA GLN GLN GLN GLN ALA ALA ALA ALA ALA ALA THR THR THR THR THR

• Molecule 20: 39S ribosomal protein L12, mitochondrial

32% Chain FF: 65% 35% PERFORMANCE CONTRACTOR OF CONT 1170 1172 1172 1175 1175 1175 ILE PRO ILE ALA LYS GLU GLU ARG A18 1 E182 E182 I184 K185 K185 A187 L185 E185 E185 E185 A190 V191 • Molecule 20: 39S ribosomal protein L12, mitochondrial 18% Chain t1: 77% • Molecule 20: 39S ribosomal protein L12, mitochondrial 12% Chain t2: 85%

LYS ALA ALA ALA LEU GLU GLY GLY VAL VAL VAL VAL VAL VAL UAL CLU

• Molecule 20: 39S ribosomal protein L12, mitochondrial



Chain t3: 15% . 85%	
NET NET ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
PRI PRI PRI PRI PRI PRI PRI PRI	
TLE ALA ALA ALA ALA ALA ARG GLU VAL CLU CLU CLU ALA ALA ALA ALA ALA ALA ALA ALA ALA A	1
CLU LYS ALA ALA ALA ALA CUU CUU CUU CUU CUU CUU	
• Molecule 20: 39S ribosomal protein L12, mitochondrial	
Chain t4: 15% 85%	
MET ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
PRI 111111111111111111111111111111111111	
TLE MAD ALA ALA ALA ALA ALA ARG ALA ARG ALA ALA ALA ALA ASN ALA ASN ALA ASN ALA ASN ALA ASN ALA ASN ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	
• Molecule 20: 39S ribosomal protein L12, mitochondrial	
Chain t5: 15% 85%	
LIBU ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	
PR0 PR0 PR0 PR0 PR0 PR0 PR0 PR0 PR0 PR0	
TILE TILE ALA ALA ALA TILE TILE TILE TILE TILE TILE TILE TILE	
• Molecule 20: 39S ribosomal protein L12, mitochondrial	
Chain t6: 14% 86%	
MET ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	



PRO PRO R22 Q4 Q4 Q5 Q5 Q5 Q5 Q5 Q5 Q5 Q5 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	L13	K26 K27 T28 ASP ASP ASP AAA AAA MET MET MET MAA MAA AAA AAA	VAL PRO ALA ALA ALA ALA ALA ALA CLU GLU GLU ASP
LLE PRO ALA ALA ALA ALY GLU GLU ARG ARG ARG CLU GLU GLU	ALA LYS PRO VAL VAL CYS LEV LLYS GLU CLYS GLU CLYS ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	GLM TLE LEU VAL VAL CYS CLN ALA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	VAL ALA ALA GLU GLU
ALA GLU CLYS CLYS LLYS LLYS ALA ALA ALA CLU GLU GLU GLU GLY VAL VAL	C LU		
• Molecule 21: Mitoch	 nondrial ribosome-associ	ated GTPase 2	
Chain G:	79%	• 19%	
MET ALA PRO ALA ALA ALA ARG CYS SER ALA ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	GLY VGL GLY HIS HIS HIS TRP TRP SER TRP TRP SER FLY SER FLY SER FLY SER TIS	LEU LEU GLM GLM ALA ALA ALA ALA ALA ALA ALA ALA ALA A	GLU GSD GSD GSD
8 8	Image: second system Image: second system <td>ochondrial</td> <td>ASP</td>	ochondrial	ASP
Chain H: 359	<i>6</i> .	64%	
MET ALA ALA ALA ALA ALA PRO PRO PRO PRO ALA ALA	GLY ALLA GLY GLY GLY CLU CLU GLY GLY GLY CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ALS GLY ASN ASN ASN ASP PRO ASN SER SER SER ASN GLN GLN GLN GLN COM	1145 1146 1147 011 011
GLU GLY GLY LLYS LLYS LLYS GLU GLU GLU GLU ALLA ALLA ALLA ALLA ALL	LYS PHE LLEU LLEU LYS SER CYS CYS CYS GLIY GLIY GLIY GLIY GLIY ASN ASN ASN ASN ASN	LLEU GLU PRO PRO PLU CLU CLU CLU CLU CLU CLU CLU CLU CLU C	HIS LEU LEU LEU
PRO GLU GLU GLU PRO TLE TRF GLU TRP GLU TYP GLU CYS GLU CYS GLU TRP TRP TRP	VAL VAL GJIY CJIY LIEU LIEU VAL VAL VAL VAL VAL VAL VAL VAL VAL VAL	PRO LYS LYS LYS LYS LYS LYS LYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	SER PRO GLN ILE
• Molecule 23: 39S rit	oosomal protein L10, mi	itochondrial	
Chain I:	78%	• 19%	
MET ALA ALA ALA ALA ALA ALA ALA CLA CLA CLA	ALA ALA ARG FRO FRO FRO FRO FRO FRO G29 G29 G29 G29 KST	P69 F71 F72 F72 F73 F74 F75 F75 C77 C78 C77 C78 C77 C78 C78 C77 C78 C78	M152 R169 R189 K196
L197 P198 S199 F201 L200 P201 P201 C205 C205 C205 C205 C205 C205 C205 C205	6210 1211 7212 6213 6213 7215 A216 9217 7215 7216 7216 7216 7216 7221 1222 1222	q223 q225 q225 P226 1227 q228 1223 1223 1223 1233 1233 234 q235 235 q235 1233 1233 1233 1233 1233 1233 1233 1	Q240 ARG GLU LYS ASP ASP VAL MET ASR ASN GLY LYS LYS
THR PRA ASP ASP			
• Molecule 24: 39S rib	oosomal protein L11, mi	itochondrial	
Chain J:	68%	• 28%	



MET SER LYS LYS LEU GLY ALA ALA ALA ALA CLY CLY	ARG ARG ALVS CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	K106 L111 R122 A129 F130
R149 R154 V155 V156 K157 ASP LEU SER	SER GLU GLU GLU ALA ALA ALA ALA ALA ALA ALA ALA ALA A	
• Molecule 25:	39S ribosomal protein L13, mitochondrial	
Chain K:	98% •••	
MET S2 191 L178		
• Molecule 26:	39S ribosomal protein L14, mitochondrial	
Chain L:	74% 5% 21%	
MET ALA PHE TTA CLEU CLEU CLEU CLEU CLEU PHE	THR VAL SER VAL LEU VAL LEU VAL LEU THR TTHR TTHR TTHR TTHR COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS COTS SER RIS	
• Molecule 27:	39S ribosomal protein L15, mitochondrial	
Chain M:	94% • •	
MET ALA GLY PRO FRO CLY GLY GLY GLY	R44 R44 134 R134 R233 R233 R233 R233 R233 R233 R233 R2	
• Molecule 28:	39S ribosomal protein L16, mitochondrial	
Chain N:	70% • 29%	
MET TRP TRP ARG LEU LEU ALA ALA ALA ALA SER ALA SER PRO	LEU VAL PAG PAG PAG PAG PAG PAG PAG PAG PAG PAG	PRO LEU VAL PRO
LYS V62 R63 R64 B34 K116 K134	SER MAR ARG MET MET MELY GLY GLY MELS MELS MELS MELS MELS MELS MELS MELS	
• Molecule 29:	39S ribosomal protein L17, mitochondrial	
Chain O:	82% 5% 13%	
MET ARG LLEU VAL ALA ALA ALA ALA ALA ALA	120 126 126 128 128 128 128 128 128 128 128 128 128	
• Molecule 30:	Mitochondrial ribosomal protein L18, isoform CRA_b	
Chain P:	77% • 21%	
	WORLDWIDE PROTEIN DATA BANK	



Chain W:	66%	·	32%	
MET ALA SIER SIER VAL VAL LEU ARG ARG ARG ARG ARG SIER SIER SIER SIER SIER SIER SIER SIER	ALA THR LEU LEU LEU ALA ALA TYR SER CIY SER SER SER SER SER SER SER SER	SER LYS ASN GLY GLY SER SER	SER 648 R49 C88 C88	V125 L148
• Molecule 38: 39S ribosomal	protein L28, mitocho	ndrial		
Chain X:	93%			• 5%
MET P2 R59 K96 K96 K96 R59 R59 R59 R50 R50 R50 R50 R1A R1A R1A R1A R1A R1A R1A R1A R1A R1A	ALA SER GLY GLN GLN			
• Molecule 39: 39S ribosomal	protein L47, mitochor	ndrial		
Chain Y:	68%	·	30%	_
MET ALA ALA ALA ALA ALA ALA ALA ALA ARG CYS SER ALA ALA ALA ALA SER ALA SER ALA SER ALA SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	LEU LILE THR THR PHC CYS CYS CYS CYS CYS CYS CYS CYS THR CHS CYS CYS LEU	LEU PRO LYS SER THR PRO ASN VAL	THR SER PHE HIS GLN TYR	ARG LEU LEU HIS THR THR LEU SER
ARG 153 053 053 053 053 175 120 120 120 120 120 120 120 120 120 120	TAV TAV SER SER			
• Molecule 40: 39S ribosomal	protein L30, mitochoi	ndrial		
Chain Z:	72%	·	25%	_
	Auto Value Sen Trac Rase Rase Rase Rase Rase Rase Rase Rase	K73 1119 2141 1154 1154 1154	25% 25% SII SII SII SII SII SII	_
Chain Z: 탈클클릭팀팩팀블클클ጀጀጀጀጀጀጀጀጀጀጀጀጀጀ • Molecule 41: 39S ribosomal	72% 日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日	• E E E E	25% SX1 SX1 FTB	_
Chain Z: E3388888888888888888888888888888888888	72% 日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日日	• 8 8 8 8 ndrial	25% TT SI D SI SX T T SI D SI	
Chain Z:	72% 3 3 5 5 5 1 1 5 年 5 年 1 8 1 8 2 1 5 1 protein L43, mitochor 64% 64%	8 11 14 18 19 ndrial 5%	25% NTD SI Y SI ND SI SI Y VI Y SI ND SI 31%	LEU PRO THR VAL ASP PRO TLE SER
Chain Z:	72% 3 1 3 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	• • • • • • • • • • • • • •	25% 1000 St 1 St 10 Es St 1 V Y H H 10 Es 31% 424 00 45 V	LEU PRO THR VAL ASP PRO TIL SER
Chain Z: • Molecule 41: 39S ribosomal Chain b: • Molecule 42: 39S ribosomal	72% 5	· findrial 5% fill fill fill fill fill fill fill fill	25% NTD SX TY SH DD SS 31% 424 084 59	LEU FRO THR VAL ASP PRO TILE SER
Chain Z:	72% 5	ن مطrial ۶% لاه کا کا کا کا مطrial	25% 100 X1 Y1 H H D K 31% 44 K X2 X K X X X X 17%	LEU PRO THR VAL ASP PRO TIL SER
Chain Z:	72% 5 1 3 5 5 5 1 1 2 5 5 5 1 1 2 1 2 2 1 2 1 1 protein L43, mitochor 64% 64% 64% 1 protein L44, mitochor 80% 80%		25% 100 21 1 21 21 21 21 21 21 21 21 21 21 21 2	q193 LEU K246 PR0 K246 VAL K279 ASP L280 111 L280 111 L280 111 E287 SER



• Molecule 43: 39S ribosomal protein L45, mitochondrial



Chain d:	70%		27%	
MET ALA ALA ALA PRO CITY CITY SER SER CITY CITY CITY CITY CITY CITY CITY CITY	PHR PRC PRC PRC PRC PRC PRC PRC PRC VAL PRC VAL	ARC THR LVS LVS LVS RS RS RS RS RS RS RS RS RS RS ALA	LYNS ALA ALA ALA ALA TLE PRO PRO PRO PRO PRO PRO	R74 191
GLU GLY ALSP ALSP ALSP ALSC ALSC CLU CLU CLU CLU CLU CLU CLU CLU CLU CL	R111 R111 1163 1163 1163 1163 1163 10237 10237 10237 10237 10237	62294 611 6114 6114 6114 6114 6114 1175 714 714 6114 6114	ALA	
• Molecule 44: 39S ribos	omal protein L46, mite	ochondrial		
Chain e:	76%	·	22%	
MET ALA ALA ALA ALA PRO PRO PRO ALA CLU CLU CLU CLU CLY CLY CLY ARG ARG	PHE GLU GLU IEU IEU TRP ALA SER SER SER SER SER SER SER SER SER SER	ALA ALA ALA ALA PRO SER SER SER S43 CLY S43	L63 D86 A91 L92 D93 D93 D93	M35 108 108 108 108
K100 K101 K102 K102 K102 LEU LEU LEU ASP GLU GLU GLU GLU GLU ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	A117 0119 0119 1120 1120 1120 1120 0126 7128 1129 1129 1129	F131 K132 G134 G134 G134 T135 F135 F138 F138 F138	D141 E142 K143 V158 G166 D167	P169 P169 A193 F217 PR0 GLN ALA MET
ARG THR GLU SEN SEN ASN ASN 1227 1238 1238 1238 1238 1238 1233 1233 1233	C347 C347 N249 K249 C250 E250 E251 E251 E258 K265 E278 E278			
• Molecule 45: 39S ribos	omal protein L48, mito	ochondrial		
Chain f:	57% •	42%		
MET SER SER GLY TTR GLY CLEU CLEU CLEU CLEU CLEU CYS CLEU CYS CYS CLEU CYS CLEU CYS CLEU CYS CLEU CYS CLEU CLEU CYS CLEA CLEA CLEA CLEA CLEA CLEA CLEA CLEA	ALM ALA SER SER SER LEU LEU LEU ARG PRO GIY CYT TTR TTR TTR	SER VAL CLY CLY CLY CLY CLY CLZ CLZ CLZ CLZ CLZ CLZ CLZ CLZ CLZ CLZ	Add Add GUU Edd CUU CUU CUU CUU CUU CUU CUU CUU CUU C	ТРА 2119 2119
GLU VAL ARG AIA AIA ASN AIA ASN THR ASP TTR ASP TTR GLV TTR GLV TTR T119	1132 ALU VAL LEU CLU CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	NEK VIL 1150 6161 1171 1171 1177 1195 1193	PHE LYS 1996 R101 P201 E206	1208 0000 12010 1211 1211
• Molecule 46: 39S ribos	omal protein L49, mite	ochondrial		
Chain g:	76%	·	22%	
MET ALA ALA ALA ALA ALA ARG ARG ARG ARG GIY TRP ARG GIY VAL CUN	ANG CTS CTS CTS CTS CTS CTS LEU CTS CTS PRO CTT PRO PRO TTS PRO	PANG PANG P43 V143 V143 F147 F166		
• Molecule 47: 39S ribos	omal protein L50, mito	ochondrial		
Chain h:	66%	• 32	2%	
MET ALA ALA ALA ALA ARG SER VAL SER THR VAL THR THR THR THR	CLU CLU CTA CTA CTA CTA CTA CTA CTA CTA CTA CTA	PRD VAL VAL VAL THR CLU CLU CLU CLU CLU	PRO TLE VAL VAL CS2 R56 R75	S84 1158



• Molecule 48:	39S ribosom	nal protein L51,	mitochondrial		
Chain i:		72%		24%	
MET ALA GLY GLY ASN LEU LEU LEU CLE GLY GLY ALA ARG	AKG LEU TRP ASP TRP VAL LEU ALA	CYS ARG SER PHE SER CLEU CLEU CLEU LEU LEU LEU LEU LEU 132	136 137 137 137 130 180 1105 1107 1107 1107		
• Molecule 49:	39S ribosom	nal protein L52,	mitochondrial		
Chain j:		67%	·	31%	
MET ALA ALA ALA LEU CLEU GLY PHE FHE GLY	ARG ARG LLEU HIS CYS SER VAL ALA	ALA TRP ALA A24 K67 L93 L93 A108	LEU LYS PRO PRO PRO LYS SER ALA ALA ALA SER SER SER SER SER SER SER SER SER SER	SER GLN GLN	
• Molecule 50:	39S ribosom	nal protein L53,	mitochondrial		
Chain k:		69%	·	29%	
MET ALA ALA ALA ALA LEU CLEU GLY CLEU GLY ARG	PMU V13 L34 L34 R41 R56 H1S	ASP GUY SER SER AB6 AR6 ASP ALA ALA ALA ALA ALA SER SER	GLY GLY ASP PRO GLY ASP ASP GLY ARG GLY		
• Molecule 51:	39S ribosom	nal protein L54,	mitochondrial		
Chain 1:	30%	•	68%		
MET ALA THR LYS LYS LEU PHE GLY ALA ALA ARG	THR TRP ALA GLY GLY GLY GLU	LEU LEU ASN PRO PRO ALA GLY GLY LEU LEU LEU	ARG ASP TYR ASP ASP ALA LYS CYS CYS GLY ALA ALA	SER GLY GLY GLY ALA VAL THR SER GLU ALA	LEU LYS ASP PRO ASP
VAL CYS CYS ASP ASP ASP ASP AAL GLM LEU THR THR TYR	ALA ALA GLY VAL VAL ASN TSN TYR LYR GLU	GLY GLN ASP ASP PAO FRO LEU FRO ALA ALA ALA TYR	P93 E94 N95 N99 K105 T106 L107 E108 €108	L110 R128 K136 ARG	
• Molecule 52:	39S ribosom	nal protein L55,	mitochondrial		
Chain m:	26%		73%		-
MET ALA ALA ALA ALA ALA CLA CLA CLY CLU CLU LEU LEU	ARG GLN SER THR VAL LYS ALA ALA GLY	PRO ALA LLEU ARG ARG ARG HIS SER THR SER TRP ARG	Data Data Data Data Data Data Data Data	H4-3 H4-4 R4-5 A4-7 A4-7 A4-7 V5-4 V5-4 V5-4	L56 V57 L64 R6 ARG ARG
PRO ARG ARG MET LEU ALA PRO ILE ASP LEU	ASP THR LEU SER PRO GLU GLU ARG	ALA ARG ARG ARG ARG ARG CLY GLU GLU GLU SER SER	ARG LYS CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	VAL GLU GLU GLU ARG GLN GLN GLN TYR THR ARG	THT LYS LYS
• Molecule 53:	rRNA meth 34%	yltransferase 2, :	mitochondrial		
Chain n:		75%	•	23%	
MET ALA GLY CILY LEU LIYS LIYS VAL CYS SER SER	PHE GLN GLN GLN GLY PHE HIS THR VAL	GLY SER ARG CYS CYS CYS ARG ALA GLY HIA GLU	LEU TRP LEU THR THR TRP LEU ARG ARG PRO PRO PRO PRO VAL	ALA ALA LYS VAL GLU GLU S51	E58 E655 N666



R71 L74 L74 K75 V75 L74 K75 V75 K75 K17 K113 K114 K115 K113 K113 K125 K125 K125 K133 K134 K133 K134 </th
V142 P144 P145 P145 R146 R169 R183 R183 R184 R186 R191 R207 R216 R216 R224 R224 R225 R226 R226 R226 R236 R236 R246 R256 R256 R261 R266 R267 R268 R268 <
• Molecule 54: Ribosomal protein 63, mitochondrial
Chain o: 86% · 11%
MET PHE TIRU ARC GIX GIX GI C 102 C 102 C 102 C 102 C 102 C 102 C 102 C 102 C
• Molecule 55: Peptidyl-tRNA hydrolase ICT1, mitochondrial
Chain p: 61% 38%
MET TRP AILA AILA AILA AILA AILA AILA AILA AIL
ASW LLYS VAE PTHR PTHR PTHR PTHR PTHR PTHR PTHR PTHR
\bullet Molecule 56: Growth arrest and DNA damage-inducible proteins-interacting protein 1
Chain q: 59% · 39%
MET ALA ALA SER SER ALA SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
LEU LUN LUN LUN LUN LUN LUN LUN LUN LUN LU
• Molecule 57: 39S ribosomal protein S18a, mitochondrial
Chain r: 76% · 21%
MET LALA ALLA ALLA ALLA ALLA ALLA ALLA AL
• Molecule 58: 39S ribosomal protein S30, mitochondrial
Chain s: 83% · 16%







-	16%				
Chain w:		52%	•	44%	
MET ALA SER ARG VAL LEU SER ALA	TYR VAL SER ARG LEU PRO ALA PHE	PRO LEU PRO PRO ARG ARG ALA ALA ALA ARG	LEU SER THR ALA LEU CYS SER CYS SER GLY GLY THR GLN THR	LEU GLN FIR GLN FRO FRO FRO FIL VAL LEU VAL LEU VAL CLN GLN	VAL PRO GLY ARG
_	••••• •	•• •• • •	** ** * **	• • • • • • •	
VAL THR GLN LEU CYS ARG GLN TYR	SER D70 M71 P72 P73 L75 L75 L75	E77 G78 I79 Q80 Q81 D81 L87 L89 L89 Y90 Y90	E96 K97 N101 S102 S102 F128 F128 F128	D132 K137 1148 1148 D153 D153 V155 K155	
• Molecule	63: UNK				
	32	%			_
Chain UNI	\$:		93%	79	%
	X11 X12 X12 X22 X23 X26	DUK DUK			



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39495	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	49.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.935	Depositor
Minimum map value	-0.278	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	221.34, 280.5, 250.92	wwPDB
Map dimensions	246, 275, 217	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	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: GTP, SAH, OMG, MG, GDP, PNS, SAM, ZN

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	0	0.34	0/895	0.66	0/1201
2	a	0.29	0/709	0.63	0/963
3	1	0.26	0/438	0.69	0/583
4	2	0.33	0/373	0.68	0/496
5	3	0.27	0/852	0.63	0/1136
6	4	0.39	0/350	0.77	1/461~(0.2%)
7	5	0.27	0/3294	0.62	0/4488
8	6	0.27	0/2779	0.62	0/3787
9	7	0.26	0/2413	0.61	0/3264
10	8	0.26	0/734	0.65	0/986
11	9	0.30	0/1020	0.66	0/1374
12	А	0.49	0/34076	0.76	12/53028~(0.0%)
13	A1	0.27	0/2795	0.62	0/3792
14	В	0.46	0/1423	0.72	0/2206
15	A2	0.26	0/1973	0.62	0/2651
16	С	0.35	0/2020	0.55	0/2724
17	D	0.29	0/1888	0.69	0/2538
18	Ε	0.28	0/2465	0.63	0/3344
19	F	0.29	0/2071	0.64	0/2817
20	FF	0.25	0/544	0.66	0/730
20	t1	0.44	0/358	0.54	0/486
20	t2	0.22	0/238	0.36	0/319
20	t3	0.21	0/238	0.35	0/319
20	t4	0.22	0/229	0.34	0/308
20	t5	0.21	0/229	0.41	0/308
20	t6	0.22	0/213	0.39	0/286
21	G	0.28	0/2600	0.63	0/3513
22	Н	0.27	0/798	0.71	0/1073
23	Ι	0.28	0/1731	0.62	0/2345
24	J	0.28	0/1064	0.68	0/1431
25	K	0.28	$0/1\overline{495}$	0.63	$0/2\overline{029}$
26	L	0.28	0/904	0.64	0/1218


Mal	Chain	Bond	i lengths E		ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
27	М	0.28	0/2359	0.66	0/3185
28	N	0.27	0/1494	0.64	0/2010
29	0	0.28	0/1269	0.64	0/1708
30	Р	0.28	0/1173	0.65	0/1588
31	Q	0.27	0/1846	0.64	0/2487
32	R	0.28	0/1174	0.64	0/1572
33	S	0.27	0/1276	0.68	0/1729
34	Т	0.28	0/1402	0.63	0/1886
35	U	0.28	0/1183	0.66	0/1600
36	V	0.27	0/1697	0.64	0/2302
37	W	0.28	0/827	0.65	0/1118
38	Х	0.26	0/2090	0.62	0/2825
39	Y	0.26	0/1552	0.63	0/2079
40	Z	0.28	0/1003	0.66	0/1354
41	b	0.30	0/1202	0.67	0/1626
42	с	0.28	0/2264	0.62	0/3059
43	d	0.27	0/1899	0.64	0/2569
44	е	0.27	0/1797	0.66	0/2422
45	f	0.28	0/994	0.62	0/1336
46	g	0.28	0/1102	0.63	0/1503
47	h	0.29	0/894	0.63	0/1217
48	i	0.29	0/849	0.66	0/1135
49	j	0.32	0/698	0.64	0/940
50	k	0.28	0/635	0.68	0/855
51	1	0.26	0/407	0.62	0/547
52	m	0.28	0/292	0.67	0/394
53	n	0.27	0/1480	0.61	0/2013
54	0	0.26	0/792	0.63	0/1064
55	р	0.28	0/1071	0.64	0/1433
56	q	0.27	0/1165	0.62	0/1575
57	r	0.29	0/1305	0.65	0/1767
58	s	0.27	0/3114	0.62	0/4225
59	t	0.26	0/2992	0.63	0/4047
60	u	0.25	0/1119	0.63	0/1516
61	v	0.25	0/593	0.64	0/788
62	w	0.26	0/717	0.60	0/967
All	All	0.35	0/120935	0.67	13/170645~(0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
12	А	1855	А	C2'-C3'-O3'	7.67	126.38	109.50
12	А	2182	G	C2'-C3'-O3'	7.49	125.97	109.50
12	А	1871	А	C2'-C3'-O3'	6.95	124.82	113.70
12	А	2457	А	C2'-C3'-O3'	6.63	124.31	113.70
12	А	2905	А	C2'-C3'-O3'	6.48	124.07	113.70
12	А	2653	С	C4'-C3'-O3'	6.38	125.75	113.00
6	4	79	CYS	CA-CB-SG	-6.16	102.91	114.00
12	А	2620	G	C2'-C3'-O3'	5.90	123.14	113.70
12	А	2543	С	C2'-C3'-O3'	5.75	122.91	113.70
12	А	2347	С	C2'-C3'-O3'	5.72	122.85	113.70
12	А	1958	G	C1'-O4'-C4'	-5.35	105.62	109.90
12	А	2698	G	O4'-C1'-N9	5.35	112.48	108.20
12	А	1770	G	C4'-C3'-C2'	-5.01	97.59	102.60

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	Percentiles
1	0	106/188~(56%)	103~(97%)	3~(3%)	0	100 100
2	a	78/142~(55%)	75~(96%)	3~(4%)	0	100 100
3	1	50/65~(77%)	50~(100%)	0	0	100 100
4	2	43/92~(47%)	42 (98%)	1 (2%)	0	100 100
5	3	93/188~(50%)	89~(96%)	4 (4%)	0	100 100
6	4	36/103~(35%)	36~(100%)	0	0	100 100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
7	5	390/423~(92%)	376~(96%)	14~(4%)	0	100	100
8	6	323/380~(85%)	310 (96%)	13~(4%)	0	100	100
9	7	288/338~(85%)	274 (95%)	14~(5%)	0	100	100
10	8	83/206~(40%)	75 (90%)	8 (10%)	0	100	100
11	9	121/137~(88%)	117 (97%)	4 (3%)	0	100	100
13	A1	340/384~(88%)	330 (97%)	10 (3%)	0	100	100
15	A2	236/381~(62%)	233 (99%)	3 (1%)	0	100	100
16	С	251/334~(75%)	245 (98%)	6 (2%)	0	100	100
17	D	235/305~(77%)	225 (96%)	10 (4%)	0	100	100
18	Е	302/348~(87%)	288 (95%)	14(5%)	0	100	100
19	F	248/311~(80%)	243 (98%)	5 (2%)	0	100	100
20	FF	68/198~(34%)	65 (96%)	3(4%)	0	100	100
20	t1	44/198~(22%)	38 (86%)	4 (9%)	2(4%)	2	15
20	t2	28/198~(14%)	28 (100%)	0	0	100	100
20	t3	28/198~(14%)	28 (100%)	0	0	100	100
20	t4	27/198~(14%)	27 (100%)	0	0	100	100
20	t5	27/198~(14%)	27 (100%)	0	0	100	100
20	t6	25/198~(13%)	24 (96%)	1 (4%)	0	100	100
21	G	335/414~(81%)	316 (94%)	19~(6%)	0	100	100
22	Н	93/267~(35%)	91 (98%)	2(2%)	0	100	100
23	Ι	210/261~(80%)	207 (99%)	3~(1%)	0	100	100
24	J	134/192~(70%)	127 (95%)	7 (5%)	0	100	100
25	K	175/178~(98%)	173 (99%)	2(1%)	0	100	100
26	L	113/145~(78%)	107 (95%)	6 (5%)	0	100	100
27	М	285/296~(96%)	279 (98%)	6 (2%)	0	100	100
28	N	175/251~(70%)	170 (97%)	5(3%)	0	100	100
29	Ο	150/175~(86%)	144 (96%)	6 (4%)	0	100	100
30	Р	139/179~(78%)	137 (99%)	2 (1%)	0	100	100
31	Q	215/292~(74%)	209 (97%)	6(3%)	0	100	100
32	R	138/149~(93%)	137 (99%)	1 (1%)	0	100	100
33	S	154/205~(75%)	149 (97%)	5 (3%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
34	Т	164/212~(77%)	161~(98%)	3~(2%)	0	100	100
35	U	135/153~(88%)	131~(97%)	4(3%)	0	100	100
36	V	200/216~(93%)	196~(98%)	4 (2%)	0	100	100
37	W	99/148~(67%)	99~(100%)	0	0	100	100
38	Х	241/256~(94%)	239~(99%)	2(1%)	0	100	100
39	Y	174/250~(70%)	170~(98%)	4 (2%)	0	100	100
40	Z	118/161~(73%)	113~(96%)	5(4%)	0	100	100
41	b	146/215~(68%)	138~(94%)	8 (6%)	0	100	100
42	с	271/332~(82%)	267~(98%)	4 (2%)	0	100	100
43	d	217/306~(71%)	207~(95%)	10~(5%)	0	100	100
44	е	211/279~(76%)	202~(96%)	9~(4%)	0	100	100
45	f	115/212~(54%)	107~(93%)	7~(6%)	1 (1%)	17	52
46	g	127/166~(76%)	125~(98%)	2(2%)	0	100	100
47	h	105/158~(66%)	101~(96%)	4 (4%)	0	100	100
48	i	95/128~(74%)	92~(97%)	3~(3%)	0	100	100
49	j	83/123~(68%)	82~(99%)	1 (1%)	0	100	100
50	k	76/112~(68%)	73~(96%)	3~(4%)	0	100	100
51	1	42/138~(30%)	42~(100%)	0	0	100	100
52	m	33/128~(26%)	31~(94%)	2~(6%)	0	100	100
53	n	187/246~(76%)	186~(100%)	1~(0%)	0	100	100
54	О	89/102~(87%)	84~(94%)	5~(6%)	0	100	100
55	р	119/206~(58%)	115~(97%)	4(3%)	0	100	100
56	q	133/222~(60%)	132~(99%)	1 (1%)	0	100	100
57	r	149/196~(76%)	143~(96%)	6~(4%)	0	100	100
58	s	366/439~(83%)	353~(96%)	13~(4%)	0	100	100
59	t	377/452~(83%)	368~(98%)	9(2%)	0	100	100
60	u	131/234~(56%)	124 (95%)	7(5%)	0	100	100
61	v	66/70 (94%)	$61 \ (92\%)$	5 (8%)	0	100	100
62	w	85/156~(54%)	83~(98%)	2(2%)	0	100	100
All	All	$10140/14731~(69\overline{\%})$	9819~(97%)	318 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
20	t1	-3	LYS
45	f	179	PRO
20	t1	1	PRO

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	RotamericOutliersPercent		\mathbf{ntiles}	
1	0	97/164~(59%)	96~(99%)	1 (1%)	76	90
2	a	78/133~(59%)	77~(99%)	1 (1%)	69	87
3	1	49/60~(82%)	48 (98%)	1 (2%)	55	80
4	2	39/72~(54%)	39~(100%)	0	100	100
5	3	88/166~(53%)	84 (96%)	4 (4%)	27	60
6	4	37/89~(42%)	35~(95%)	2(5%)	22	53
7	5	353/368~(96%)	343~(97%)	10~(3%)	43	73
8	6	271/332~(82%)	265~(98%)	6 (2%)	52	78
9	7	266/303~(88%)	257~(97%)	9~(3%)	37	69
10	8	77/190~(40%)	71 (92%)	6 (8%)	12	40
11	9	104/112~(93%)	102~(98%)	2(2%)	57	81
13	A1	297/328~(90%)	292~(98%)	5 (2%)	60	83
15	A2	221/350~(63%)	215~(97%)	6 (3%)	44	74
16	С	224/287~(78%)	219~(98%)	5 (2%)	52	78
17	D	191/245~(78%)	189~(99%)	2(1%)	76	90
18	Ε	259/290~(89%)	255~(98%)	4 (2%)	65	85
19	F	217/262~(83%)	212~(98%)	5(2%)	50	77
20	\mathbf{FF}	58/158~(37%)	58~(100%)	0	100	100
20	t1	40/158~(25%)	38~(95%)	2(5%)	24	57
20	t2	29/158~(18%)	29~(100%)	0	100	100
20	t3	29/158~(18%)	28 (97%)	1 (3%)	37	69
20	t4	28/158~(18%)	28 (100%)	0	100	100



Continued from previous page...

20 t5 28/158 (18%) 28 (100%) 0 100 100 20 t6 26/158 (16%) 26 (100%) 0 100 100 21 G 264/328 (80%) 256 (97%) 8 (3%) 41 71 22 H 86/228 (38%) 185 (95%) 9 (5%) 27 59 23 I 194/323 (84%) 185 (95%) 9 (5%) 27 59 24 J 112/150 (75%) 104 (93%) 8 (7%) 14 44 25 K 155/156 (99%) 152 (98%) 3 (2%) 55 80 26 I 98/124 (79%) 91 (93%) 7 (7%) 14 44 27 M 245/249 (98%) 235 (96%) 10 (4%) 30 64 28 N 152/211 (72%) 149 (98%) 3 (2%) 43 69 30 P 123/154 (80%) 119 (97%) 4 (3%) 38 69 31 Q 199/256 (78%	Mol	Chain	Analysed	Rotameric	Outliers	Perce	\mathbf{ntiles}
20 tic 26/158 (16%) 26 (100%) 0 100 100 21 G 264/328 (80%) 256 (97%) 8 (3%) 41 71 22 H 86/228 (38%) 84 (98%) 2 (2%) 50 77 23 I 194/232 (84%) 185 (95%) 9 (5%) 27 59 24 J 112/150 (75%) 104 (93%) 8 (7%) 14 44 25 K 155/156 (99%) 152 (98%) 3 (2%) 57 81 26 L 98/124 (79%) 91 (93%) 7 (7%) 14 44 27 M 245/249 (98%) 235 (96%) 10 (4%) 30 64 28 N 152/211 (72%) 149 (98%) 3 (2%) 55 80 29 O 133/150 (89%) 124 (93%) 9 (7%) 16 44 20 133/150 (89%) 111 (94%) 7 (6%) 19 50 31 Q 199/256 (78%) <	20	t5	28/158~(18%)	28~(100%)	0	100	100
21 G 264/328 (80%) 256 (97%) 8 (3%) 41 71 22 H 86/228 (38%) 84 (98%) 2 (2%) 50 77 23 I 194/232 (84%) 185 (95%) 9 (5%) 27 59 24 J 112/150 (75%) 104 (93%) 8 (7%) 14 44 25 K 155/156 (99%) 152 (98%) 3 (2%) 57 81 26 L 98/124 (79%) 91 (93%) 7 (7%) 14 44 27 M 245/249 (98%) 235 (96%) 10 (4%) 30 64 28 N 152/211 (72%) 149 (98%) 3 (2%) 38 69 30 P 123/154 (80%) 119 (97%) 4 (3%) 38 69 31 Q 199/256 (78%) 139 (99%) 2 (1%) 84 33 32 R 118/126 (94%) 111 (94%) 7 (6%) 39 69 33 S 141/180	20	t6	26/158~(16%)	26~(100%)	0	100	100
22 H 86/228 (38%) 84 (98%) 2 (2%) 50 77 23 I 194/232 (84%) 185 (95%) 9 (5%) 27 59 24 J 112/150 (75%) 104 (93%) 8 (7%) 14 44 25 K 155/156 (99%) 152 (98%) 3 (2%) 57 81 26 L 98/124 (79%) 91 (93%) 7 (7%) 14 44 27 M 245/249 (98%) 235 (96%) 10 (4%) 30 64 28 N 152/211 (72%) 149 (98%) 3 (2%) 55 80 29 O 133/150 (89%) 124 (93%) 9 (7%) 16 45 30 P 123/154 (80%) 119 (97%) 6 (3%) 41 71 31 Q 199/256 (78%) 139 (99%) 2 (1%) 67 86 33 S 141/180 (78%) 139 (99%) 2 (1%) 63 69 34 T 146/182	21	G	264/328~(80%)	256~(97%)	8 (3%)	41	71
231 $194/232 (84\%)$ $185 (95\%)$ $9 (5\%)$ 27 59 24J $112/150 (75\%)$ $104 (93\%)$ $8 (7\%)$ 14 44 25K $155/156 (99\%)$ $152 (98\%)$ $3 (2\%)$ 57 81 26L $98/124 (79\%)$ $91 (93\%)$ $7 (7\%)$ 14 44 27M $245/249 (98\%)$ $235 (96\%)$ $10 (4\%)$ 30 64 28N $152/211 (72\%)$ $149 (98\%)$ $3 (2\%)$ 55 80 29O $133/150 (89\%)$ $124 (93\%)$ $9 (7\%)$ 16 45 30P $123/154 (80\%)$ $119 (97\%)$ $4 (3\%)$ 38 69 31Q $199/256 (78\%)$ $193 (97\%)$ $6 (3\%)$ 41 71 32R $118/126 (94\%)$ $111 (94\%)$ $7 (6\%)$ 19 50 33S $141/180 (78\%)$ $139 (99\%)$ $2 (1\%)$ 67 86 34 T $146/182 (80\%)$ $145 (99\%)$ $1 (1\%)$ 84 93 35 U $124/135 (92\%)$ $120 (97\%)$ $4 (3\%)$ 39 69 36 V $180/191 (94\%)$ $174 (97\%)$ $6 (3\%)$ 38 69 37 W $83/119 (70\%)$ $80 (96\%)$ $3 (4\%)$ 35 67 39 Y $159/223 (71\%)$ $154 (97\%)$ $5 (3\%)$ 40 70 40 Z $111/147 (76\%)$ $107 (96\%)$ $4 (4\%)$ 35 67 41 b $130/186$	22	Η	86/228~(38%)	84~(98%)	2(2%)	50	77
24J $112/150 (75\%)$ $104 (93\%)$ $8 (7\%)$ 14 44 25K $155/156 (99\%)$ $152 (98\%)$ $3 (2\%)$ 57 81 26L $98/124 (79\%)$ $91 (93\%)$ $7 (7\%)$ 14 44 27M $245/249 (98\%)$ $235 (96\%)$ $10 (4\%)$ 30 64 28N $152/211 (72\%)$ $149 (98\%)$ $3 (2\%)$ 55 80 29O $133/150 (89\%)$ $124 (93\%)$ $9 (7\%)$ 16 45 30P $123/154 (80\%)$ $119 (97\%)$ $4 (3\%)$ 38 69 31Q $199/256 (78\%)$ $193 (97\%)$ $6 (3\%)$ 41 71 32R $118/126 (94\%)$ $111 (94\%)$ $7 (6\%)$ 19 50 33 S $141/180 (78\%)$ $139 (99\%)$ $2 (1\%)$ 67 86 34 T $146/182 (80\%)$ $145 (99\%)$ $1 (1\%)$ 84 93 35 U $124/135 (92\%)$ $120 (97\%)$ $4 (3\%)$ 35 67 38 X $219/229 (96\%)$ $214 (98\%)$ $5 (2\%)$ 50 77 39 Y $159/223 (71\%)$ $154 (97\%)$ $5 (3\%)$ 40 70 41 b $130/186 (70\%)$ $120 (92\%)$ $10 (8\%)$ 38 69 41 b $130/186 (70\%)$ $120 (92\%)$ $10 (8\%)$ 38 69 44 c $241/288 (84\%)$ $233 (97\%)$ $8 (3\%)$ 38 69 44 c	23	Ι	194/232~(84%)	185~(95%)	9~(5%)	27	59
25 K 155/156 (99%) 152 (98%) 3 (2%) 57 81 26 L 98/124 (79%) 91 (93%) 7 (7%) 14 44 27 M 245/249 (98%) 235 (96%) 10 (4%) 30 64 28 N 152/211 (72%) 149 (98%) 3 (2%) 55 80 29 O 133/150 (89%) 124 (93%) 9 (7%) 16 45 30 P 123/154 (80%) 119 (97%) 4 (3%) 38 69 31 Q 199/256 (78%) 193 (97%) 6 (3%) 41 71 32 R 118/126 (94%) 111 (94%) 7 (6%) 19 50 33 S 141/180 (78%) 139 (99%) 2 (1%) 67 86 34 T 146/182 (80%) 145 (99%) 1 (1%) 84 93 35 U 124/135 (92%) 120 (97%) 4 (3%) 35 67 38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 39 Y	24	J	112/150~(75%)	104~(93%)	8 (7%)	14	44
26 L 98/124 (79%) 91 (93%) 7 (7%) 14 44 27 M 245/249 (98%) 235 (96%) 10 (4%) 30 64 28 N 152/211 (72%) 149 (98%) 3 (2%) 55 80 29 O 133/150 (89%) 124 (93%) 9 (7%) 16 45 30 P 123/154 (80%) 119 (97%) 4 (3%) 38 69 31 Q 199/256 (78%) 193 (97%) 6 (3%) 41 71 32 R 118/126 (94%) 111 (94%) 7 (6%) 19 50 33 S 141/180 (78%) 139 (99%) 2 (1%) 67 86 34 T 146/182 (80%) 145 (99%) 1 (1%) 84 93 35 U 124/135 (92%) 120 (97%) 4 (3%) 35 67 38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 39 Y 159/2	25	Κ	155/156~(99%)	152 (98%)	3~(2%)	57	81
27 M 245/249 (98%) 235 (96%) 10 (4%) 30 64 28 N 152/211 (72%) 149 (98%) 3 (2%) 55 80 29 O 133/150 (89%) 124 (93%) 9 (7%) 16 45 30 P 123/154 (80%) 119 (97%) 4 (3%) 38 69 31 Q 199/256 (78%) 193 (97%) 6 (3%) 41 71 32 R 118/126 (94%) 111 (94%) 7 (6%) 19 50 33 S 141/180 (78%) 139 (99%) 2 (1%) 67 86 34 T 146/182 (80%) 145 (99%) 1 (1%) 84 93 35 U 124/135 (92%) 120 (97%) 4 (3%) 39 69 36 V 180/191 (94%) 174 (97%) 6 (3%) 38 69 37 W 83/119 (70%) 80 (96%) 3 (4%) 35 67 39 Y 159/223 (71%) 154 (97%) 5 (3%) 40 70 40 Z	26	L	98/124~(79%)	91~(93%)	7 (7%)	14	44
28 N 152/211 (72%) 149 (98%) 3 (2%) 55 80 29 O 133/150 (89%) 124 (93%) 9 (7%) 16 45 30 P 123/154 (80%) 119 (97%) 4 (3%) 38 69 31 Q 199/256 (78%) 193 (97%) 6 (3%) 41 71 32 R 118/126 (94%) 111 (94%) 7 (6%) 19 50 33 S 141/180 (78%) 139 (99%) 2 (1%) 67 86 34 T 146/182 (80%) 145 (99%) 1 (1%) 84 93 35 U 124/135 (92%) 120 (97%) 4 (3%) 39 69 36 V 180/191 (94%) 174 (97%) 6 (3%) 38 69 37 W 83/119 (70%) 80 (96%) 3 (4%) 35 67 38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 39 Y 159/23	27	М	245/249~(98%)	235~(96%)	10~(4%)	30	64
29O $133/150 (89\%)$ $124 (93\%)$ $9 (7\%)$ 16 45 30P $123/154 (80\%)$ $119 (97\%)$ $4 (3\%)$ 38 69 31Q $199/256 (78\%)$ $193 (97\%)$ $6 (3\%)$ 41 71 32R $118/126 (94\%)$ $111 (94\%)$ $7 (6\%)$ 19 50 33S $141/180 (78\%)$ $139 (99\%)$ $2 (1\%)$ 67 86 34 T $146/182 (80\%)$ $145 (99\%)$ $1 (1\%)$ 84 93 35 U $124/135 (92\%)$ $120 (97\%)$ $4 (3\%)$ 39 69 36 V $180/191 (94\%)$ $174 (97\%)$ $6 (3\%)$ 38 69 37 W $83/119 (70\%)$ $80 (96\%)$ $3 (4\%)$ 35 67 38 X $219/229 (96\%)$ $214 (98\%)$ $5 (2\%)$ 50 77 39 Y $159/223 (71\%)$ $154 (97\%)$ $5 (3\%)$ 40 70 40 Z $111/147 (76\%)$ $107 (96\%)$ $4 (4\%)$ 35 67 41 b $130/186 (70\%)$ $120 (92\%)$ $10 (8\%)$ 13 41 42 c $241/288 (84\%)$ $233 (97\%)$ $8 (3\%)$ 38 69 43 d $207/274 (76\%)$ $197 (95\%)$ $10 (5\%)$ 25 58 44 e $188/236 (80\%)$ $182 (97\%)$ $6 (3\%)$ 39 69 45 f $108/188 (57\%)$ $106 (98\%)$ $2 (2\%)$ 55 80 46 g </td <td>28</td> <td>Ν</td> <td>152/211~(72%)</td> <td>149 (98%)</td> <td>3~(2%)</td> <td>55</td> <td>80</td>	28	Ν	152/211~(72%)	149 (98%)	3~(2%)	55	80
30 P 123/154 (80%) 119 (97%) 4 (3%) 38 69 31 Q 199/256 (78%) 193 (97%) 6 (3%) 41 71 32 R 118/126 (94%) 111 (94%) 7 (6%) 19 50 33 S 141/180 (78%) 139 (99%) 2 (1%) 67 86 34 T 146/182 (80%) 145 (99%) 1 (1%) 84 93 35 U 124/135 (92%) 120 (97%) 4 (3%) 39 69 36 V 180/191 (94%) 174 (97%) 6 (3%) 38 69 37 W 83/119 (70%) 80 (96%) 3 (4%) 35 67 38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 39 Y 159/223 (71%) 154 (97%) 5 (3%) 40 70 41 b 130/186 (70%) 120 (92%) 10 (8%) 38 69 41 b 130/1	29	О	133/150~(89%)	124 (93%)	9~(7%)	16	45
31 Q 199/256 (78%) 193 (97%) 6 (3%) 41 71 32 R 118/126 (94%) 111 (94%) 7 (6%) 19 50 33 S 141/180 (78%) 139 (99%) 2 (1%) 67 86 34 T 146/182 (80%) 145 (99%) 1 (1%) 84 93 35 U 124/135 (92%) 120 (97%) 4 (3%) 39 69 36 V 180/191 (94%) 174 (97%) 6 (3%) 38 69 37 W 83/119 (70%) 80 (96%) 3 (4%) 35 67 38 X 219/229 (96%) 214 (98%) 5 (3%) 40 70 39 Y 159/223 (71%) 154 (97%) 5 (3%) 40 70 41 b 130/186 (70%) 107 (96%) 4 (4%) 35 67 41 b 130/186 (70%) 197 (95%) 10 (5%) 25 58 44 e 188/2	30	Р	123/154~(80%)	119 (97%)	4 (3%)	38	69
32 R 118/126 (94%) 111 (94%) 7 (6%) 19 50 33 S 141/180 (78%) 139 (99%) 2 (1%) 67 86 34 T 146/182 (80%) 145 (99%) 1 (1%) 84 93 69 35 U 124/135 (92%) 120 (97%) 4 (3%) 38 69 69 36 V 180/191 (94%) 174 (97%) 6 (3%) 38 69 63 37 W 83/119 (70%) 80 (96%) 3 (4%) 35 67 6 38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 6 39 Y 159/223 (71%) 154 (97%) 5 (3%) 40 70 70 40 Z 111/147 (76%) 107 (96%) 4 (4%) 35 67 70 41 b 130/186 (70%) 120 (92%) 100 (8%) 133 41 6 42 c 241/288 (84%) 233 (97%) 8 (3%) 38 69 6 43 d	31	Q	199/256~(78%)	193~(97%)	6 (3%)	41	71
33 S 141/180 (78%) 139 (99%) 2 (1%) 67 86 34 T 146/182 (80%) 145 (99%) 1 (1%) 84 93 35 U 124/135 (92%) 120 (97%) 4 (3%) 39 69 36 V 180/191 (94%) 174 (97%) 6 (3%) 38 69 37 W 83/119 (70%) 80 (96%) 3 (4%) 35 67 38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 39 Y 159/223 (71%) 154 (97%) 5 (3%) 40 70 40 Z 111/147 (76%) 107 (96%) 4 (4%) 35 67 41 b 130/186 (70%) 120 (92%) 10 (8%) 13 41 42 c 241/288 (84%) 233 (97%) 8 (3%) 38 69 43 d 207/274 (76%) 197 (95%) 100 (5%) 25 58 44 e 188	32	R	118/126~(94%)	111 (94%)	7 (6%)	19	50
34 T 146/182 (80%) 145 (99%) 1 (1%) 84 93 35 U 124/135 (92%) 120 (97%) 4 (3%) 39 69 36 V 180/191 (94%) 174 (97%) 6 (3%) 38 69 1 37 W 83/119 (70%) 80 (96%) 3 (4%) 35 67 1 38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 1 39 Y 159/223 (71%) 154 (97%) 5 (3%) 40 70 1 40 Z 111/147 (76%) 107 (96%) 4 (4%) 35 67 1 41 b 130/186 (70%) 120 (92%) 10 (8%) 13 41 42 c 241/288 (84%) 233 (97%) 8 (3%) 38 69 1 43 d 207/274 (76%) 197 (95%) 10 (5%) 25 58 1 44 e 188/236 (80%) 182 (97%) 6 (3%) 39 69 1 45 f 108/188 (57%)	33	S	141/180~(78%)	139 (99%)	2(1%)	67	86
35 U 124/135 (92%) 120 (97%) 4 (3%) 39 69 36 V 180/191 (94%) 174 (97%) 6 (3%) 38 69 37 W 83/119 (70%) 80 (96%) 3 (4%) 35 67 38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 39 Y 159/223 (71%) 154 (97%) 5 (3%) 40 70 40 Z 111/147 (76%) 107 (96%) 4 (4%) 35 67 41 b 130/186 (70%) 120 (92%) 10 (8%) 13 41 42 c 241/288 (84%) 233 (97%) 8 (3%) 38 69 43 d 207/274 (76%) 197 (95%) 10 (5%) 25 58 44 e 188/236 (80%) 182 (97%) 6 (3%) 39 69 45 f 108/188 (57%) 106 (98%) 2 (2%) 55 80 45 f 108/188 (67%) 116 (98%) 3 (2%) 47 75 46 g <td>34</td> <td>Т</td> <td>146/182~(80%)</td> <td>145 (99%)</td> <td>1 (1%)</td> <td>84</td> <td>93</td>	34	Т	146/182~(80%)	145 (99%)	1 (1%)	84	93
36 V 180/191 (94%) 174 (97%) 6 (3%) 38 69 37 W 83/119 (70%) 80 (96%) 3 (4%) 35 67 38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 39 Y 159/223 (71%) 154 (97%) 5 (3%) 40 70 40 Z 111/147 (76%) 107 (96%) 4 (4%) 35 67 41 b 130/186 (70%) 120 (92%) 10 (8%) 13 41 42 c 241/288 (84%) 233 (97%) 8 (3%) 38 69 43 d 207/274 (76%) 197 (95%) 10 (5%) 25 58 44 e 188/236 (80%) 182 (97%) 6 (3%) 39 69 45 f 108/188 (57%) 106 (98%) 2 (2%) 57 81 46 g 119/148 (80%) 116 (98%) 3 (2%) 47 75 47 h 101/148 (68%) 99 (98%) 2 (2%) 55 80 48 i	35	U	124/135~(92%)	120 (97%)	4 (3%)	39	69
37W83/119 (70%)80 (96%)3 (4%)356738X219/229 (96%)214 (98%)5 (2%)507739Y159/223 (71%)154 (97%)5 (3%)407040Z111/147 (76%)107 (96%)4 (4%)356741b130/186 (70%)120 (92%)10 (8%)134142c241/288 (84%)233 (97%)8 (3%)386943d207/274 (76%)197 (95%)10 (5%)255844e188/236 (80%)182 (97%)6 (3%)396945f108/188 (57%)106 (98%)2 (2%)578146g119/148 (80%)116 (98%)3 (2%)477547h101/148 (68%)99 (98%)2 (2%)558048i86/110 (78%)81 (94%)5 (6%)205149j68/97 (70%)65 (96%)3 (4%)2861	36	V	180/191~(94%)	174 (97%)	6 (3%)	38	69
38 X 219/229 (96%) 214 (98%) 5 (2%) 50 77 39 Y 159/223 (71%) 154 (97%) 5 (3%) 40 70 40 Z 111/147 (76%) 107 (96%) 4 (4%) 35 67 41 b 130/186 (70%) 120 (92%) 10 (8%) 13 41 42 c 241/288 (84%) 233 (97%) 8 (3%) 38 69 43 d 207/274 (76%) 197 (95%) 10 (5%) 25 58 44 e 188/236 (80%) 182 (97%) 6 (3%) 39 69 45 f 108/188 (57%) 106 (98%) 2 (2%) 57 81 46 g 119/148 (80%) 116 (98%) 3 (2%) 47 75 47 h 101/148 (68%) 99 (98%) 2 (2%) 55 80 48 i 86/110 (78%) 81 (94%) 5 (6%) 20 51 49 j 68/97 (70%) 65 (96%) 3 (4%) 28 61	37	W	83/119~(70%)	80 (96%)	3 (4%)	35	67
39Y159/223 (71%)154 (97%)5 (3%)407040Z111/147 (76%)107 (96%)4 (4%)356741b130/186 (70%)120 (92%)10 (8%)134142c241/288 (84%)233 (97%)8 (3%)386943d207/274 (76%)197 (95%)10 (5%)255844e188/236 (80%)182 (97%)6 (3%)396945f108/188 (57%)106 (98%)2 (2%)578146g119/148 (80%)116 (98%)3 (2%)477547h101/148 (68%)99 (98%)2 (2%)558048i86/110 (78%)81 (94%)5 (6%)205149j68/97 (70%)65 (96%)3 (4%)2861	38	Х	219/229~(96%)	214 (98%)	5 (2%)	50	77
40Z111/147 (76%)107 (96%)4 (4%)356741b130/186 (70%)120 (92%)10 (8%)134142c241/288 (84%)233 (97%)8 (3%)386943d207/274 (76%)197 (95%)10 (5%)255844e188/236 (80%)182 (97%)6 (3%)396945f108/188 (57%)106 (98%)2 (2%)578146g119/148 (80%)116 (98%)3 (2%)477547h101/148 (68%)99 (98%)2 (2%)558048i86/110 (78%)81 (94%)5 (6%)205149j68/97 (70%)65 (96%)3 (4%)2861	39	Y	159/223~(71%)	154 (97%)	5(3%)	40	70
41b130/186 (70%)120 (92%)10 (8%)134142c241/288 (84%)233 (97%)8 (3%)386943d207/274 (76%)197 (95%)10 (5%)255844e188/236 (80%)182 (97%)6 (3%)396945f108/188 (57%)106 (98%)2 (2%)578146g119/148 (80%)116 (98%)3 (2%)477547h101/148 (68%)99 (98%)2 (2%)558048i86/110 (78%)81 (94%)5 (6%)205149j68/97 (70%)65 (96%)3 (4%)2861	40	Ζ	111/147~(76%)	$107 \ (96\%)$	4 (4%)	35	67
42c241/288 (84%)233 (97%)8 (3%)386943d207/274 (76%)197 (95%)10 (5%)255844e188/236 (80%)182 (97%)6 (3%)396945f108/188 (57%)106 (98%)2 (2%)578146g119/148 (80%)116 (98%)3 (2%)477547h101/148 (68%)99 (98%)2 (2%)558048i86/110 (78%)81 (94%)5 (6%)205149j68/97 (70%)65 (96%)3 (4%)2861	41	b	130/186~(70%)	120 (92%)	10 (8%)	13	41
43d207/274 (76%)197 (95%)10 (5%)255844e188/236 (80%)182 (97%)6 (3%)396945f108/188 (57%)106 (98%)2 (2%)578146g119/148 (80%)116 (98%)3 (2%)477547h101/148 (68%)99 (98%)2 (2%)558048i86/110 (78%)81 (94%)5 (6%)205149j68/97 (70%)65 (96%)3 (4%)2861	42	с	241/288~(84%)	233~(97%)	8 (3%)	38	69
44 e 188/236 (80%) 182 (97%) 6 (3%) 39 69 45 f 108/188 (57%) 106 (98%) 2 (2%) 57 81 46 g 119/148 (80%) 116 (98%) 3 (2%) 47 75 47 h 101/148 (68%) 99 (98%) 2 (2%) 55 80 48 i 86/110 (78%) 81 (94%) 5 (6%) 20 51 49 j 68/97 (70%) 65 (96%) 3 (4%) 28 61	43	d	207/274~(76%)	197~(95%)	10 (5%)	25	58
45 f 108/188 (57%) 106 (98%) 2 (2%) 57 81 46 g 119/148 (80%) 116 (98%) 3 (2%) 47 75 47 h 101/148 (68%) 99 (98%) 2 (2%) 55 80 48 i 86/110 (78%) 81 (94%) 5 (6%) 20 51 49 j 68/97 (70%) 65 (96%) 3 (4%) 28 61	44	е	188/236~(80%)	182 (97%)	6 (3%)	39	69
46 g 119/148 (80%) 116 (98%) 3 (2%) 47 75 47 h 101/148 (68%) 99 (98%) 2 (2%) 55 80 48 i 86/110 (78%) 81 (94%) 5 (6%) 20 51 49 j 68/97 (70%) 65 (96%) 3 (4%) 28 61	45	f	108/188~(57%)	106 (98%)	2 (2%)	57	81
47 h 101/148 (68%) 99 (98%) 2 (2%) 55 80 48 i 86/110 (78%) 81 (94%) 5 (6%) 20 51 49 j 68/97 (70%) 65 (96%) 3 (4%) 28 61	46	g	119/148 (80%)	116 (98%)	3 (2%)	47	75
48 i 86/110 (78%) 81 (94%) 5 (6%) 20 51 49 j 68/97 (70%) 65 (96%) 3 (4%) 28 61	47	h	101/148~(68%)	99~(98%)	2(2%)	55	80
49 j 68/97 (70%) 65 (96%) 3 (4%) 28 61	48	i	86/110 (78%)	81 (94%)	5 (6%)	20	51
	49	j	68/97 (70%)	65~(96%)	3 (4%)	28	61



Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
50	k	71/90~(79%)	68~(96%)	3 (4%)	30	62
51	1	43/116~(37%)	41 (95%)	2 (5%)	26	59
52	m	31/113~(27%)	29 (94%)	2 (6%)	17	47
53	n	157/209~(75%)	$152 \ (97\%)$	5 (3%)	39	69
54	0	78/87~(90%)	75~(96%)	3 (4%)	33	66
55	р	117/181~(65%)	116~(99%)	1 (1%)	78	91
56	q	115/178~(65%)	112 (97%)	3 (3%)	46	74
57	r	141/169~(83%)	135~(96%)	6 (4%)	29	62
58	S	326/381~(86%)	319~(98%)	7 (2%)	53	79
59	t	317/371~(85%)	316 (100%)	1 (0%)	92	96
60	u	123/200~(62%)	120 (98%)	3 (2%)	49	76
61	v	59/60~(98%)	54 (92%)	5 (8%)	10	37
62	W	81/136 (60%)	75~(93%)	6 (7%)	13	42
All	All	9055/12593~(72%)	8781 (97%)	274 (3%)	44	71

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	153	THR
2	а	60	CYS
3	1	43	LEU
5	3	103	LYS
5	3	137	THR
5	3	156	LYS
5	3	157	LEU
6	4	76	CYS
6	4	81	LEU
7	5	46	LEU
7	5	55	LEU
7	5	128	LEU
7	5	132	LEU
7	5	280	GLN
7	5	300	ARG
7	5	315	LEU
7	5	316	PHE
7	5	365	ASP
7	5	420	HIS



Mol	Chain	Res	Type
8	6	41	ASP
8	6	52	ARG
8	6	184	LEU
8	6	291	TYR
8	6	371	ASP
8	6	379	ILE
9	7	50	LYS
9	7	97	GLU
9	7	143	TRP
9	7	156	ARG
9	7	196	LYS
9	7	204	LYS
9	7	234	LYS
9	7	272	THR
9	7	321	ARG
10	8	97	LYS
10	8	113	ARG
10	8	117	LEU
10	8	125	LYS
10	8	156	LYS
10	8	163	LYS
11	9	55	GLU
11	9	69	LYS
13	A1	163	LEU
13	A1	189	LEU
13	A1	226	ARG
13	A1	258	CYS
13	A1	275	ARG
15	A2	131	PHE
15	A2	133	LEU
15	A2	134	LEU
15	A2	191	GLN
15	A2	304	ARG
15	A2	319	LEU
16	С	60	ILE
16	С	120	LYS
16	С	216	THR
16	C	317	VAL
16	C	318	MET
17	D	187	LEU
17	D	281	TRP
18	Е	152	VAL



Mol	Chain	Res	Type
18	Е	245	THR
18	Е	303	LYS
18	Е	346	THR
19	F	70	ARG
19	F	130	GLN
19	F	131	LYS
19	F	263	LEU
19	F	291	SER
21	G	63	LEU
21	G	68	LEU
21	G	123	LYS
21	G	168	ARG
21	G	257	THR
21	G	284	ARG
21	G	298	ARG
21	G	300	ILE
22	Н	138	LYS
22	Н	145	LEU
23	Ι	50	VAL
23	Ι	57	LYS
23	Ι	78	LEU
23	Ι	99	CYS
23	Ι	101	ASN
23	Ι	122	LEU
23	Ι	152	MET
23	Ι	169	ARG
23	Ι	197	LEU
24	J	24	VAL
24	J	30	MET
24	J	92	LYS
24	J	102	ARG
24	J	103	GLN
24	J	106	LYS
24	J	111	LEU
24	J	149	ARG
25	K	2	SER
25	K	91	THR
25	K	178	LEU
26	L	35	MET
26	L	37	ARG
26	L	77	ILE
26	L	95	ARG



Mol	Chain	Res	Type
26	L	99	ARG
26	L	101	ASP
26	L	136	LYS
27	М	43	ARG
27	М	44	ARG
27	М	98	LEU
27	М	134	ARG
27	М	146	ASP
27	М	222	TYR
27	М	239	LYS
27	М	269	LEU
27	М	277	MET
27	М	292	LYS
28	N	63	ARG
28	N	208	ASN
28	Ν	238	LYS
29	0	14	VAL
29	0	20	LEU
29	0	26	ILE
29	0	28	LEU
29	0	123	ILE
29	0	144	LEU
29	0	149	LEU
29	0	155	ASP
29	0	156	LEU
30	Р	80	ARG
30	Р	117	TYR
30	Р	120	ARG
30	Р	137	LEU
31	Q	139	GLN
31	Q	214	LYS
31	Q	215	VAL
31	Q	227	LYS
31	Q	247	LEU
31	Q	271	ARG
32	R	11	ARG
32	R	32	ARG
32	R	40	ARG
32	R	82	LYS
32	R	87	ILE
$\overline{32}$	R	104	ASP
32	R	119	LEU



Mol	Chain	Res	Type
33	S	144	LEU
33	S	182	LYS
34	Т	84	LYS
35	U	11	ARG
35	U	12	LEU
35	U	27	GLN
35	U	126	LEU
36	V	40	ARG
36	V	56	LEU
36	V	118	ARG
36	V	186	THR
36	V	202	MET
36	V	213	VAL
37	W	49	ARG
37	W	88	CYS
37	W	125	VAL
38	Х	59	ARG
38	Х	87	LEU
38	Х	96	LYS
38	Х	99	LYS
38	Х	161	LEU
39	Y	121	ARG
39	Y	198	ARG
39	Y	202	LEU
39	Y	226	LEU
39	Y	237	LYS
40	Z	41	ILE
40	Ζ	73	LYS
40	Z	119	ILE
40	Z	141	SER
41	b	4	ARG
41	b	36	ASP
41	b	80	LEU
41	b	86	GLU
41	b	100	LEU
41	b	115	ILE
41	b	119	PHE
41	b	122	ASP
41	b	123	ASN
41	b	141	ARG
42	с	68	TYR
42	с	86	ASP



Mol	Chain	Res	Type
42	с	173	LEU
42	с	193	GLN
42	с	246	LYS
42	с	279	LYS
42	с	280	LEU
42	с	287	GLU
43	d	36	ARG
43	d	74	ARG
43	d	111	ARG
43	d	112	MET
43	d	163	LEU
43	d	194	VAL
43	d	203	MET
43	d	238	VAL
43	d	266	VAL
43	d	287	LEU
44	е	126	GLN
44	е	127	LYS
44	е	133	LEU
44	е	227	LEU
44	e	239	LEU
44	е	243	PHE
45	f	171	LEU
45	f	212	LYS
46	g	43	ASP
46	g	143	VAL
46	g	147	LEU
47	h	56	ARG
47	h	75	LYS
48	i	36	LEU
48	i	37	THR
48	i	80	LEU
48	i	105	ASP
48	i	107	LEU
49	j	67	LYS
49	j	93	LEU
49	j	103	ARG
50	k	34	LEU
50	k	41	LYS
50	k	56	ARG
51	1	110	LEU
51	1	128	ARG



Mol	Chain	Res	Type
52	m	40	LEU
52	m	51	LEU
53	n	55	ARG
53	n	140	LEU
53	n	147	ARG
53	n	155	MET
53	n	224	ARG
54	0	46	HIS
54	0	91	GLN
54	0	98	THR
55	р	179	ARG
56	q	96	LEU
56	q	113	LYS
56	q	150	LYS
57	r	52	ARG
57	r	58	LYS
57	r	70	CYS
57	r	108	CYS
57	r	159	VAL
57	r	164	LYS
58	S	52	THR
58	S	66	TRP
58	s	150	LEU
58	s	200	LEU
58	S	230	ARG
58	s	279	GLU
58	s	379	LEU
59	t	331	ARG
20	t1	-3	LYS
20	t1	3	ILE
20	t3	27	LYS
60	u	92	PHE
60	u	156	HIS
60	u	196	LEU
61	v	16	LEU
61	v	29	ASP
61	v	45	LEU
61	v	47	ASP
61	v	61	PHE
62	W	74	LEU
62	W	75	THR
62	W	88	LYS



Continued from previous page...

Mol	Chain	Res	Type
62	W	89	LEU
62	W	132	ASP
62	W	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
4	2	77	GLN
5	3	154	GLN
7	5	96	HIS
7	5	108	HIS
7	5	165	GLN
7	5	385	HIS
8	6	66	GLN
8	6	354	GLN
9	7	298	GLN
10	8	143	GLN
13	A1	317	ASN
13	A1	367	ASN
15	A2	191	GLN
15	A2	255	GLN
16	С	295	GLN
16	С	297	ASN
19	F	103	GLN
23	Ι	101	ASN
23	Ι	225	GLN
25	K	26	GLN
25	K	126	HIS
25	K	147	GLN
27	М	26	ASN
27	М	30	ASN
27	М	92	GLN
27	М	264	GLN
28	N	210	GLN
29	0	69	ASN
30	Р	147	GLN
32	R	79	HIS
32	R	94	GLN
33	S	84	ASN
34	Т	132	HIS
35	U	103	GLN
35	U	138	GLN



Mol	Chain	Res	Type
38	Х	15	GLN
39	Y	99	HIS
39	Y	183	GLN
41	b	120	HIS
42	с	122	ASN
42	с	172	ASN
42	с	193	GLN
43	d	149	HIS
44	е	175	GLN
45	f	111	HIS
45	f	153	HIS
48	i	59	ASN
49	j	63	GLN
53	n	214	ASN
54	0	33	GLN
54	0	94	HIS
58	s	87	GLN
58	s	101	ASN
58	s	239	ASN
60	u	156	HIS
62	W	103	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	А	1427/1559~(91%)	355~(24%)	54(3%)
14	В	56/69~(81%)	19 (33%)	2(3%)
All	All	1483/1628~(91%)	374 (25%)	56 (3%)

All (374) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	А	1678	С
12	А	1679	U
12	А	1680	А
12	А	1681	G
12	А	1689	С
12	А	1693	С
12	А	1694	U
12	А	1699	С
12	А	1700	U



Mol	Chain	Res	Type
12	А	1704	U
12	А	1707	С
12	А	1708	А
12	А	1714	С
12	А	1715	С
12	А	1724	A
12	А	1728	U
12	А	1733	С
12	А	1734	С
12	А	1735	А
12	А	1736	А
12	А	1743	U
12	А	1748	G
12	А	1750	G
12	А	1751	A
12	А	1769	С
12	А	1770	G
12	А	1780	U
12	А	1794	A
12	А	1795	А
12	А	1798	А
12	А	1804	A
12	А	1805	А
12	А	1812	С
12	А	1817	С
12	А	1824	U
12	А	1827	С
12	А	1828	A
12	А	1829	А
12	А	1832	A
12	А	1836	A
12	А	1844	A
12	А	1849	С
12	А	1852	С
12	А	1853	A
12	А	1854	U
12	А	1855	A
12	А	1856	A
12	А	1867	A
12	А	1869	A
12	А	1872	U
12	А	1878	U



Mol	Chain	Res	Type
12	А	1882	А
12	А	1883	G
12	А	1887	А
12	А	1892	А
12	А	1893	А
12	А	1901	С
12	А	1902	С
12	А	1903	С
12	А	1909	А
12	А	1918	G
12	А	1936	А
12	А	1937	А
12	А	1938	А
12	А	1940	A
12	А	1946	С
12	А	1974	А
12	А	1975	U
12	А	1985	G
12	А	1986	A
12	А	1994	А
12	А	1995	A
12	А	2000	С
12	А	2001	С
12	А	2002	G
12	А	2015	G
12	А	2016	С
12	А	2021	U
12	А	2022	G
12	А	2029	А
12	А	2030	U
12	А	2031	A
12	А	2036	С
12	А	2037	U
12	А	2039	A
12	А	2044	A
12	А	2055	U
12	А	2060	A
12	А	2065	A
12	А	2066	С
12	А	2070	С
12	А	2071	U
12	А	2074	A



Mol	Chain	Res	Type
12	А	2079	С
12	А	2085	А
12	А	2092	С
12	А	2097	А
12	А	2098	G
12	А	2105	G
12	А	2107	G
12	А	2108	G
12	А	2111	С
12	А	2112	A
12	А	2113	G
12	А	2114	С
12	А	2126	U
12	A	2131	A
12	А	2135	А
12	А	2136	С
12	А	2142	А
12	А	2147	G
12	А	2154	А
12	А	2158	U
12	А	2159	U
12	А	2160	A
12	А	2167	А
12	А	2171	U
12	А	2172	А
12	А	2173	G
12	А	2174	G
12	А	2175	С
12	А	2178	А
12	А	2179	А
12	А	2181	A
12	А	2182	G
12	A	2183	С
12	A	2187	С
12	A	2194	U
12	А	2195	A
12	А	2196	A
12	А	2197	G
12	А	2198	A
12	А	2199	A
12	А	2200	A
12	А	2210	С



Mol	Chain	Res	Type
12	А	2211	U
12	А	2228	А
12	А	2229	А
12	А	2230	А
12	А	2233	U
12	А	2237	А
12	А	2241	А
12	А	2243	А
12	А	2245	А
12	А	2246	А
12	А	2250	A
12	А	2251	A
12	А	2257	С
12	А	2262	С
12	А	2263	С
12	А	2264	A
12	А	2284	С
12	А	2285	U
12	А	2297	A
12	А	2300	G
12	A	2321	A
12	А	2322	С
12	A	2324	U
12	А	2332	С
12	А	2345	G
12	А	2348	A
12	А	2350	A
12	А	2351	U
12	А	2358	A
12	А	2359	С
12	А	2360	U
12	А	2361	G
12	A	2362	A
12	А	2363	A
12	A	2374	A
12	А	2381	A
12	А	2390	A
12	А	2394	A
12	А	2401	A
12	A	2404	U
12	А	2406	A
12	A	2407	U



Mol	Chain	Res	Type
12	А	2414	С
12	А	2415	С
12	А	2418	А
12	А	2434	А
12	А	2446	А
12	А	2451	А
12	А	2452	А
12	А	2457	А
12	А	2458	А
12	А	2478	G
12	А	2483	U
12	А	2485	U
12	А	2488	С
12	А	2493	С
12	А	2494	С
12	А	2500	А
12	А	2502	С
12	А	2511	С
12	А	2520	С
12	А	2521	А
12	А	2527	А
12	А	2530	А
12	А	2531	U
12	А	2536	G
12	А	2539	А
12	А	2540	С
12	А	2544	С
12	А	2547	С
12	А	2548	С
12	А	2549	C
12	A	2550	A
12	A	2554	A
12	A	2603	С
12	A	2611	С
12	A	2613	U
$\overline{12}$	A	2617	A
12	A	2618	U
12	A	2619	A
12	A	2620	G
12	A	2621	G
$\overline{12}$	A	2622	G
$1\overline{2}$	А	2623	A



Mol	Chain	\mathbf{Res}	Type
12	А	2626	U
12	А	2627	G
12	А	2628	U
12	А	2629	А
12	А	2630	U
12	А	2633	А
12	А	2634	U
12	А	2645	G
12	А	2654	U
12	А	2655	G
12	А	2656	U
12	А	2660	U
12	А	2670	С
12	A	2683	С
12	А	2684	С
12	А	2686	G
12	А	2693	А
12	А	2694	A
12	А	2695	G
12	А	2696	А
12	А	2698	G
12	А	2699	С
12	А	2706	А
12	А	2709	А
12	А	2719	G
12	А	2722	А
12	А	2723	А
12	А	2724	G
12	А	2725	А
12	А	2732	G
12	А	2739	U
12	А	2740	A
12	А	2743	U
12	А	2756	С
12	А	2810	G
12	А	2815	G
12	А	2816	G
12	А	2819	G
12	А	2828	G
12	А	2831	G
12	А	2832	A
12	А	2833	A



Mol	Chain	Res	Type
12	А	2840	С
12	А	2843	С
12	А	2844	G
12	А	2847	С
12	А	2854	U
12	А	2864	U
12	А	2865	С
12	А	2880	A
12	А	2906	С
12	А	2912	С
12	А	2913	A
12	А	2917	G
12	А	2918	A
12	А	2919	A
12	А	2922	A
12	А	2926	A
12	А	2928	С
12	А	2932	G
12	А	2934	G
12	А	2935	А
12	А	2936	U
12	А	2937	A
12	А	2946	A
12	А	2956	А
12	А	2963	A
12	А	2978	U
12	А	2984	А
12	А	2986	С
12	А	2987	U
12	А	2988	С
12	А	2989	G
12	А	2990	A
12	А	2991	U
12	А	2992	G
12	А	3005	A
12	А	3007	С
12	А	3016	G
12	А	3018	A
12	А	3021	С
12	А	3022	G
12	А	3041	U
12	А	3042	U



Mol	Chain	Res	Type
12	А	3051	А
12	А	3053	А
12	А	3054	G
12	А	3060	С
12	А	3067	U
12	А	3069	А
12	А	3070	G
12	А	3072	U
12	А	3086	U
12	А	3089	A
12	А	3090	G
12	А	3097	U
12	А	3098	U
12	А	3100	U
12	А	3102	U
12	А	3108	U
12	А	3109	U
12	А	3111	A
12	А	3112	А
12	А	3113	А
12	А	3123	G
12	А	3141	A
12	А	3150	U
12	А	3157	С
12	А	3158	А
12	А	3162	С
12	А	3168	С
12	А	3169	С
12	А	3170	С
12	А	3171	С
12	А	3172	С
12	А	3173	G
12	А	3177	A
12	А	3180	A
12	А	3184	C
12	А	3189	С
12	А	3190	A
12	А	3196	G
12	А	3197	U
12	А	3198	A
12	А	3199	U
12	А	3201	A



Mol	Chain	Res	Type
12	А	3202	U
12	А	3207	А
12	А	3208	С
12	А	3209	А
12	А	3211	С
12	А	3212	С
12	А	3217	А
12	А	3218	А
12	А	3220	А
12	А	3228	U
14	В	1604	G
14	В	1608	G
14	В	1609	U
14	В	1610	А
14	В	1611	G
14	В	1614	U
14	В	1615	А
14	В	1617	С
14	В	1618	А
14	В	1620	А
14	В	1621	А
14	В	1622	А
14	В	1628	С
14	В	1632	U
14	В	1633	U
14	В	1644	G
14	В	1645	А
14	В	1646	U
14	В	1670	А

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	А	1727	А
12	А	1749	С
12	А	1772	А
12	А	1811	А
12	А	1823	А
12	А	1824	U
12	А	1853	А
12	А	1854	U
12	А	1855	А



Mol	Chain	Res	Type		
12	А	1871	А		
12	А	1936	A		
12	А	1956	U		
12	А	1974	A		
12	А	1994	A		
12	А	2001	С		
12	А	2015	G		
12	А	2021	U		
12	А	2030	U		
12	А	2065	A		
12	А	2097	A		
12	А	2135	A		
12	А	2158	U		
12	А	2182	G		
12	А	2186	С		
12	А	2245	A		
12	А	2291	A		
12	А	2347	С		
12	А	2361	G		
12	А	2380	С		
12	А	2417	С		
12	А	2457	A		
12	А	2527	A		
12	А	2530	A		
12	А	2543	С		
12	А	2619	A		
12	А	2620	G		
12	А	2628	U		
12	А	2629	A		
12	А	2630	U		
12	А	2653	С		
12	А	2723	A		
12	А	2724	G		
12	А	2739	U		
12	А	2818	C		
12	А	2832	A		
12	А	2846	G		
12	А	2905	A		
12	А	2926	A		
12	А	2935	A		
12	А	2991	U		
12	А	3004	С		



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Mol	Chain	Res	Type
12	А	3041	U
12	А	3068	G
12	А	3206	С
14	В	1607	U
14	В	1614	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	Tuno	Chain	Pog	Tink	Bo	ond leng	\mathbf{ths}	B	ond ang	gles
	Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
12	OMG	А	3040	12	18,26,27	1.44	2 (11%)	$20,\!38,\!41$	2.21	6 (30%)

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
12	OMG	А	3040	12	-	0/5/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
12	А	3040	OMG	C6-C5	4.39	1.48	1.41
12	А	3040	OMG	C5-C4	2.93	1.48	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
12	А	3040	OMG	C2-N3-C4	4.79	120.82	115.36
12	А	3040	OMG	C6-N1-C2	4.19	122.58	115.93
12	А	3040	OMG	C5-C6-N1	-4.13	117.78	123.43



		1	1 5				
Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
12	А	3040	OMG	C6-C5-C4	-3.94	117.03	120.80
12	А	3040	OMG	N3-C2-N1	-3.41	122.67	127.22
12	А	3040	OMG	C4-C5-N7	-2.12	107.19	109.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 101 ligands modelled in this entry, 95 are monoatomic - leaving 6 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).

Mal	Tune	Chain	Dec	Bog Link Bond lengths				Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
67	GDP	C	401	-	$24,\!30,\!30$	1.18	2 (8%)	31,47,47	1.99	8 (25%)
69	SAH	n	301	-	21,28,28	0.64	0	20,40,40	0.82	2 (10%)
70	PNS	W	201	62	13,20,21	0.30	0	$18,\!26,\!29$	0.73	0
66	SAM	A1	401	-	21,29,29	0.64	0	18,42,42	0.96	2(11%)
68	GTP	G	502	65	26,34,34	1.06	1 (3%)	$33,\!54,\!54$	2.04	4 (12%)
67	GDP	t	501	65	24,30,30	1.30	2 (8%)	31,47,47	2.01	8 (25%)

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
67	GDP	С	401	-	-	0/12/32/32	0/3/3/3
69	SAH	n	301	-	-	3/7/31/31	0/3/3/3
70	PNS	W	201	62	-	16/24/26/27	-
66	SAM	A1	401	-	-	3/8/33/33	0/3/3/3
68	GTP	G	502	65	-	2/18/38/38	0/3/3/3
67	GDP	t	501	65	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
67	t	501	GDP	C6-C5	4.65	1.49	1.41
67	С	401	GDP	C6-C5	4.16	1.48	1.41
68	G	502	GTP	C6-N1	4.09	1.40	1.33
67	t	501	GDP	C5-C4	2.69	1.48	1.40
67	С	401	GDP	C5-C4	2.47	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
68	G	502	GTP	C5-C6-N1	-8.69	111.55	123.43
68	G	502	GTP	C6-N1-C2	5.80	125.14	115.93
67	t	501	GDP	C2-N3-C4	5.40	121.52	115.36
67	С	401	GDP	C2-N3-C4	5.07	121.14	115.36
67	С	401	GDP	C5-C6-N1	-4.02	117.93	123.43
67	С	401	GDP	C6-N1-C2	3.99	122.27	115.93
67	t	501	GDP	C6-N1-C2	3.99	122.26	115.93
67	t	501	GDP	C6-C5-C4	-3.95	117.03	120.80
67	t	501	GDP	C5-C6-N1	-3.66	118.43	123.43
67	С	401	GDP	PA-O3A-PB	-3.62	120.40	132.83
67	С	401	GDP	C6-C5-C4	-3.57	117.39	120.80
67	t	501	GDP	N3-C2-N1	-3.56	122.47	127.22
67	С	401	GDP	N3-C2-N1	-3.27	122.86	127.22
67	С	401	GDP	C3'-C2'-C1'	3.15	105.73	100.98
67	t	501	GDP	C3'-C2'-C1'	2.84	105.26	100.98
68	G	502	GTP	N3-C2-N1	-2.84	123.44	127.22
67	t	501	GDP	C4-C5-N7	-2.69	106.60	109.40
67	t	501	GDP	PA-O3A-PB	-2.62	123.83	132.83
67	С	401	GDP	C4-C5-N7	-2.62	106.67	109.40
68	G	502	GTP	C2-N3-C4	-2.49	112.52	115.36
69	n	301	SAH	C3'-C2'-C1'	2.17	104.25	100.98
66	A1	401	SAM	C3'-C2'-C1'	2.10	104.14	100.98
69	n	301	SAH	C5-C6-N6	2.01	123.40	120.35



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Mol	Chain	\mathbf{Res}	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
66	A1	401	SAM	C5-C6-N6	2.00	123.40	120.35

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
66	A1	401	SAM	N-CA-CB-CG
66	A1	401	SAM	C-CA-CB-CG
66	A1	401	SAM	CA-CB-CG-SD
69	n	301	SAH	C-CA-CB-CG
70	W	201	PNS	O27-C28-C29-C31
70	W	201	PNS	O27-C28-C29-C32
70	W	201	PNS	C28-C29-C32-C34
70	W	201	PNS	O33-C32-C34-N36
70	W	201	PNS	C32-C34-N36-C37
70	W	201	PNS	O35-C34-N36-C37
70	W	201	PNS	N36-C37-C38-C39
70	W	201	PNS	O40-C39-N41-C42
70	W	201	PNS	O27-C28-C29-C30
70	W	201	PNS	C38-C39-N41-C42
70	W	201	PNS	O33-C32-C34-O35
70	W	201	PNS	N41-C42-C43-S44
70	W	201	PNS	C30-C29-C32-C34
70	W	201	PNS	C31-C29-C32-C34
69	n	301	SAH	N-CA-CB-CG
69	n	301	SAH	CB-CG-SD-C5'
68	G	502	GTP	O4'-C4'-C5'-O5'
68	G	502	GTP	PA-O3A-PB-O2B
70	W	201	PNS	C37-C38-C39-O40
70	W	201	PNS	C37-C38-C39-N41

There are no ring outliers.

No monomer is involved in short contacts.

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)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12763. 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: 108

6.2.2 Raw map



Y Index: 137



Z Index: 123



X Index: 108

Y Index: 138



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: 106

6.3.2 Raw map



Y Index: 181



Z Index: 113



X Index: 117

Y Index: 182

Z Index: 110

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 0.15. 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 1174 nm^3 ; this corresponds to an approximate mass of 1061 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.



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 0.323 \AA^{-1}



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.91	3.14
Calculated*	3.34	6.43	3.50

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12763 and PDB model 709K. 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 0.15 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 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

