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PDB ID	:	70I6
EMDB ID	:	EMD-12919
Title	:	Cryo-EM structure of late human 39S mitoribosome assembly intermediates, state 1
Authors	:	Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2021-05-11
Resolution	:	5.70  Å(reported)

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.

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

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

## 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 5.70 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq=3, 2, 1$  and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq=5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain							
1	D	305	8% 62% 10%	28%						
2	Е	348	73%	9% 18%						
3	F	311	75%	5% 20%						
4	Н	267	<b>33%</b> • 64%							
5	K	178	93%	6% •						
6	L	145	• 72% 70	% 21%						
7	М	296	82%	• 13%						
8	N	251	9% 75%	7% 18%						



Mol	Chain	Length	Quality of chain		
9	Ο	175	84%		• 13%
10	Q	292	69%	5%	26%
11	R	149	91%		• 6%
12	S	205	<b>6</b> 9%	7%	24%
13	Т	206	71%	6%	23%
14	U	153	84%		7% 9%
15	V	216	<b>•</b> 84%		5% 11%
16	Х	256	90%		5% 5%
17	Y	250	69%	•	30%
18	Z	161	72%	•	25%
19	0	188	56% •	43%	
20	2	92	<b>4</b> 5% •	53%	
21	5	423	84%		8% 9%
22	7	338	81%		• 15%
23	9	137	82%		• 15%
24	a	142	57% .	42%	
25	b	215	69%	-	31%
26	с	332	83%		17%
27	d	306	<b>6</b> 9%		31%
28	g	166	78%		22%
29	h	158	63%	37	%
30	i	128	<b>└</b>		24%
31	j	123	<b>6</b> 9%	_	31%
32	0	102	77%		23%
33	р	206	<b>4</b> 9% •	48%	



Mol	Chain	Length	Quality of ch	ain
34	q	222	45%	55%
35	r	196	74%	26%
36	s	439	84%	16%
37	u	234	47%	53%
38	v	70	99%	
39	W	156	6% 51%	49%
40	А	1559	26% 37%	13% 23%
41	х	540	<b>6</b> 9%	• 31%
42	у	387	67%	• 14%
43	1	420	61%	39%
43	Z	420	<u>8%</u> 60%	40%
44	В	69	28% 45%	9% 19%
45	Р	180	<b>6</b> 9%	5% 26%
46	W	148	56%	<b>3%</b> • 34%
47	6	380	82%	• 14%
48	Ι	261	30% 58%	39%
49	J	192	51% 71%	• 27%
50	k	112	34%	• 25%
51	1	138	17% 839	%



## 2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 69386 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 L2, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	D	220	Total 1076	C 636	N 220	O 220	0	0

• Molecule 2 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms			AltConf	Trace	
2	F	285	Total	С	N	Ō	0	0
		200	1399	829	285	285	0	0

• Molecule 3 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms			AltConf	Trace	
3	F	250	Total	С	N	Ō	0	0
J	Г	230	1233	733	250	250	0	U

• Molecule 4 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Н	95	Total 469	C 279	N 95	O 95	0	0

• Molecule 5 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	177	Total 876	C 522	N 177	O 177	0	0

• Molecule 6 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	115	Total 565	C 335	N 115	0 115	0	0



• Molecule 7 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	М	257	Total 1266	C 752	N 257	O 257	0	0

• Molecule 8 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	Ν	205	Total 1006	C 596	N 205	O 205	0	0

• Molecule 9 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Ο	152	Total 749	C 445	N 152	O 152	0	0

• Molecule 10 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Q	217	Total 1075	C 641	N 217	O 217	0	0

• Molecule 11 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	R	140	Total 693	C 413	N 140	O 140	0	0

• Molecule 12 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	S	156	Total 772	C 460	N 156	O 156	0	0

• Molecule 13 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Т	159	Total 788	С 470	N 159	O 159	0	0

• Molecule 14 is a protein called 39S ribosomal protein L23, mitochondrial.



Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace	
14	U	139	Total 686	C 408	N 139	O 139	0	0

• Molecule 15 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
15	V	192	Total 946	C 562	N 192	O 192	0	0

• Molecule 16 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Х	243	Total 1202	C 716	N 243	0 243	0	0

• Molecule 17 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	176	Total 874	C 522	N 176	O 176	0	0

• Molecule 18 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Ζ	120	Total 595	$\begin{array}{c} \mathrm{C} \\ 355 \end{array}$	N 120	O 120	0	0

• Molecule 19 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	0	108	Total	С	Ν	Ο	0	0
19	0	108	534	318	108	108	0	0

• Molecule 20 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	2	43	Total 211	C 125	N 43	0 43	0	0

• Molecule 21 is a protein called 39S ribosomal protein L37, mitochondrial.



Mol	Chain	Residues		Ator	AltConf	Trace		
21	5	387	Total 1916	C 1142	N 387	0 387	0	0

• Molecule 22 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	7	287	Total 1426	C 852	N 287	O 287	0	0

• Molecule 23 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	9	117	Total 575	C 341	N 117	0 117	0	0

• Molecule 24 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	a	82	Total 407	C 243	N 82	O 82	0	0

• Molecule 25 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	b	148	Total 730	C 434	N 148	0 148	0	0

• Molecule 26 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	С	275	Total 1360	C 810	N 275	O 275	0	0

• Molecule 27 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	d	211	Total 1048	C 626	N 211	O 211	0	0

• Molecule 28 is a protein called 39S ribosomal protein L49, mitochondrial.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
28	g	129	Total 638	C 380	N 129	O 129	0	0

• Molecule 29 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	h	100	Total 499	C 299	N 100	O 100	0	0

• Molecule 30 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	i	97	Total 476	C 282	N 97	O 97	0	0

• Molecule 31 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	j	85	Total 417	С 247	N 85	O 85	0	0

• Molecule 32 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	О	79	Total 394	C 236	N 79	O 79	0	0

• Molecule 33 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
99	n	107	Total	С	Ν	Ο	0	0
55	р	107	533	319	107	107	0	0

• Molecule 34 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	q	99	Total 490	C 292	N 99	O 99	0	0

• Molecule 35 is a protein called 39S ribosomal protein S18a, mitochondrial.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
35	r	146	Total 721	C 429	N 146	0 146	0	0

• Molecule 36 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues		Ator	AltConf	Trace		
36	s	370	Total 1838	C 1098	N 370	O 370	0	0

• Molecule 37 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace	
37	u	111	Total 552	C 330	N 111	0 111	0	0

• Molecule 38 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	V	69	Total	С	Ν	0	0	0
	v	00	341	203	69	69	0	0

• Molecule 39 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues		Aton	ıs	AltConf	Trace	
39	W	79	Total 392	$\begin{array}{c} \mathrm{C} \\ 234 \end{array}$	N 79	O 79	0	0

• Molecule 40 is a RNA chain called 16S rRNA.

Mol	Chain	Residues		A	AltConf	Trace			
40	А	1208	Total 25636	C 11507	N 4620	O 8301	Р 1208	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1437	U	UNK	conflict	GB 1025814679

• Molecule 41 is a protein called Probable ATP-dependent RNA helicase DDX28.



Mol	Chain	Residues		Ator	AltConf	Trace		
41	х	374	Total 1843	C 1095	N 374	О 374	0	0

• Molecule 42 is a protein called GTP-binding protein 10.

Mol	Chain	Residues	Atoms			AltConf	Trace	
42	У	331	Total 1621	C 959	N 331	O 331	0	0

• Molecule 43 is a protein called rRNA methyltransferase 3, mitochondrial.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
43	7	253	Total	С	Ν	Ο	0	0
40	Z	200	1242	736	253	253	0	0
43	1	257	Total	С	Ν	Ο	0	0
40	L	201	1262	748	257	257	0	0

• Molecule 44 is a RNA chain called mitochondrial Val tRNA.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
44	В	56	Total 1191	C 534	N 214	0 387	Р 56	0	0

• Molecule 45 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues		Ato	$\mathbf{ms}$		AltConf	Trace
45	Р	133	Total 659	C 393	N 133	0 133	0	0

• Molecule 46 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms			AltConf	Trace	
46	W	08	Total	С	Ν	0	0	0
40	vv	30	481	285	98	98	0	0

• Molecule 47 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
47	6	325	Total 1611	C 961	N 325	O 325	0	0

• Molecule 48 is a protein called 39S ribosomal protein L10, mitochondrial.



Mol	Chain	Residues		Ato	ms		AltConf	Trace
48	Ι	158	Total 785	C 469	N 158	O 158	0	0

• Molecule 49 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms			AltConf	Trace	
49	J	140	Total 686	C 406	N 140	O 140	0	0

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

Mol	Chain	Residues	Atoms			AltConf	Trace	
50	k	84	Total 416	C 248	N 84	O 84	0	0

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

Mol	Chain	Residues	Atoms			AltConf	Trace	
51	1	23	Total	C	N	0	0	0
			115	69	23	23		

• Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
52	F	1	Total Mg 1 1	0
52	g	1	Total Mg 1 1	0
52	А	44	Total Mg 44 44	0
52	х	1	Total Mg 1 1	0
52	W	1	Total Mg 1 1	0

• Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
53	0	1	Total Zn 1 1	0

• Molecule 54 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula:  $C_{11}H_{23}N_2O_7PS$ ).





Mol	Chain	Residues	Atoms				AltConf		
54		1	Total	С	Ν	0	Р	S	0
04	v	1	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 L2, mitochondrial



• Molecule 4: 39S	ribosomal prote	ein L9, mitochond	rial	
Chain H:	33% •		64%	
MET ALA ALA ALA PRO PRO PRO GLY ALA ALA ALA ALA	ARG ALA ALA ALA ALA ALA CLY ARG ARG ARG GLY GLY	VAL VAL GLN GLN GLU LEU ARG ARG ARG ARG ASN ALA	PRO ASP LEU LEU CYS ASN PHE SER FHE SER CLN ABS	617 153 179 197 197
L111 V112 S113 S133 S133 L137 L137 C137 C137 C14 C14 C14 C14 C14	GLU LYS LYS CLN CLN THR THR ALA ALA ALA ALA ALA THR	VAL LYS PHE LEU LEU CYS SER CYS ARG CLU VAL VAL OLV VAL	LYS ASN ASN VAL LYS TRP GLU CLU CLU CLU VAL	ALA ARG PHE PHE LYS ASN LUS OLY GLY
VAL VAL VAL ALA ALA PRO HIS THR THR LEU CVS GLU GLU	THR THR THR GLV GLV TRP GLU CYS GLU VAL	THR VAL ASN GLY CEU ASP VAL ARG VAL PARG VAL PRO RET	VAL VAL ASN ASN PHE GLU CYS LYS LYS LYS ARG TYR TYR	TYR TRP LEU ALA GLN ALA ALA LYS
ALA MET ALA PRO THR SER PRO GLN ILE				
• Molecule 5: 39S	ribosomal prote	ein L13, mitochono	drial	
Chain K:		93%		6% ·
MET S2 Y19 Q29 Q29 A66 A66	R88 194 194 195 195 195 194 196 196 196 197 196 197 196 197 197 197 197 197 197 197 197 197 197	L178		
• Molecule 6: 39S	ribosomal prote	ein L14, mitochone	drial	
Chain L:	729	6	7% 21%	2
MET ALLA PHE PHE THR CLY CLY PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	ARG ARG VAL VAL LEU VAL LEU VAL ARG ARG ARG ARG SER SER SER	THR GLY SER LEU R33 R33 R33 A45 R45 R45 R45	V60 173 1103 1119 1123 1123	0 9 9
• Molecule 7: 39S	ribosomal prote	ein L15, mitochone	drial	
Chain M:		82%	•	13%
MET ALA ALA GLY CLV GLY GLY <b>A</b> 10 <b>A</b> 10 <b>A</b> 10 <b>A</b> 10	H53 CLYS GLV GLV GLU ARG GLU ARG ARG ARC ARC	LEU LEU CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	TILE PRO LYS LYS CLY PHE N84 092 103	L107 Y136 Q138 A145
1167 (172 (172 (173 (173 (173 (173 (173 (173 (173 (173	<b>S296</b>			
• Molecule 8: 39S	ribosomal prote	ein L16, mitochono	drial	
Chain N:	7	5%	7% 18	3%
MET TRP ARG LEU LEU ALA ALA ALA PLO LEU LEU	V ANN V ANN P RAC LEU ASP ASP ALA LEU LEU P RO	ALA SER ALA ALA ALA CLY VAL LEU THR LEU PRO VAL SER SER	PHE GLU ASP VAL SER ILE PRO CLU CLU E54 E54	A56 P57 L58 P60 Y61 Y61 R63 R63 R63 R63 R63



P66 F87 F87 F87 F87 F87 L92 F96 F115 F115 F115 F117	V124 1122 1122 1133 113 1135 1135 1	A187 8191 8192 8192 7215 7215 7219 1226	1230 V261
• Molecule 9: 39S	ribosomal protein L17, mito	chondrial	
Chain O:	84%		• 13%
MET MET ARG SER VAL ALA ALA ALA ALA ALA ALA ALA ALA ALA	1110 A121 A121 A121 A14 A14 A14 A14 A14 A14 A14 A14 A14 A1		
• Molecule 10: 395	5 ribosomal protein L19, mit	ochondrial	
Chain Q:	69%	5%	26%
MET ALA ALA ALA CYS CYS CYS ALA ALA ALA ALA ALA ALA ALA ALA CT V	LEU GLY ARG SER SER SER ALA ALA ALA ALA ALA ALA ALA PRO PRO PRO PRO PRO PRO CYS SER ALA CVS CVS CVS CVS CVS CVS CVS CVS CVS CVS	ARG VAL HIS ALA ALA CLY PRO CLY VAL ARG GLN SER SER THR	GLY PRO PRO GLU PRO GLY ALA ALA ALA ALA PRO PRO PRO PRO PRO
VAL TLE VAL ASP ASP ASP ASC PRO PRO PRO ASC ASC ASC ASC ASC ASC ASC ASC ASC ASC	V119 V119 Q132 Q137 L150 L151 L156 L156 L166 M193 M224	K231 K233 V233 V233 K254 K254 K256 K256 K256 K280 K280	K290 Arg Ser
• Molecule 11: 395	5 ribosomal protein L20, mit	ochondrial	
Chain R:	91%		• 6%
MET VAL PHE LEU LEU ALA ALA ALA ALA CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN			
• Molecule 12: 399	S ribosomal protein L21, mit	ochondrial	
Chain S:	69%	7%	24%
MET ALIA ALIA ALIA ALIA ALIA SER SER LIEU CIV CILU CILU CILU CILU	SER ALA ALA CTS SER HIS SER HIS SER PRO FIC PRO FIC ALA ALA ALA ALA ALA ALA SER TRP FIC SER SER SER	ALA SER ARG ARG PHE ARG CAR GIN SER SER THR SER TYR	LEU PR0 649 649 796 796 796 796 798 798 798 7135 1135 1135 7135 7135 7135 7135 7135
K146 P147 V160 M172 R175 R178 N179 F180			
• Molecule 13: 395	s ribosomal protein L22, mit	ochondrial	
Chain T:	71%	6%	23%
MET ALA ALA ALA ALA ALA CLEU GLN GLN GLN GLN GLN CLEU GLN TRP	HIS ASN LEU ARG ARG GLY GLY CLEU CLEU CLEU CLEU CLEU CLEU CLEU CLEU	THR SER ALA SER LEU LEU ASP S48 S48 A91 R95	<b>G96</b> 199 199 199 103 1106 1106 1142 1142 1142 1142
1156 TYR57 TYR57 TYR57 TYR57 ARG GLY CLS TI66 T166 T166 T166			

• Molecule 14: 39S ribosomal protein L23, mitochondrial



Chain U:	84%		7%	9%
MET A2 L28 139 141 141 142 142 142 142 142 142 142 142	R69 495 796 796 797 799 799 799 610 610 610 610 610 710 710 811	ALA ASP ASP L126 L153		
• Molecule 15: 39S	ribosomal protein L24,	mitochondrial		
Chain V:	84%		5%	11%
MET ARG LEU ALA SER SER LEU LEU LEU LEU LYS VAL YAR	L15 K32 K76 K76 K76 K76 K76 K76 K76 K76 K76 K76	R145 E158 PHE PHE PRO ARC ARA ASP ALA ASP ALA CLU	1169 1186 198	M202
• Molecule 16: 39S	ribosomal protein L28,	mitochondrial		
Chain X:	90%			5% 5%
MET P2 L10 14 186 186 186 089 405 104 104 105	8116 0120 120 120 120 120 120 120 120 120 12	VAL CLN LYS ARG ALA SER GLY GLN		
• Molecule 17: 39S	ribosomal protein L47,	mitochondrial		
Chain Y:	69%	•	30%	
MET ALA ALA ALA ALA ALA CEU CEU CYS CYS CYS CYS CYS CYS SER	SLA ALA LEU LEU LEU LEU SER SER ARG ARG ARG CIN CIN CIN CIN CIN CIN	GLY PHE PHE LEU LEU LEU LEU LEU LRU FRO SER THR ASN	VAL THR SER PHE HIS	TYR ARG LEU LEU LEU THR THR LEU SER
ARG LYS G63 C63 C11 F15 C115 C15 C15 C15 F238 F10 H10 H10 H10	GLU GLU ALA ALA GLN LYS SER SER LEU VAL			
• Molecule 18: 39S	ribosomal protein L30,	mitochondrial		
Chain Z:	72%	•	25%	
MET ALA GLY GLY ILEU ARG ARG ARG ARG CAL ARL ARD GLY PRO PRO PRO	LEU LEU GLN THR VAL THR VAL CYS SER CLY SER LEU CLS CYS SER THR THR THR	ARG K35 S74 1103 N107 V154 CU GLU	LYS ALA HIS GLU SER	
• Molecule 19: 39S	ribosomal protein L32,	mitochondrial		
Chain 0:	56%	• 43	3%	
MET ALA ALA ALA ALA ALA NET LEU VAL VAL VAL VAL SER PRO	ALA ALA ARG CLY VAL LEU ARG CLU ARG CLU CLEU LEU LEU LEU LYS LEU PRO PRO	GLN SER ARG PRO CLY PRO PRO PRO FRO TRP PRO FRO	ALA LEU ALA VAL GLN	PRO PRO ALA MET PHE THR GLU PRO ALA ASN
ASP THR SER GLY GLY GLY GLU GLU CLU LLU LEU LLU LLU LLU LLU SER SER	LLE PLE TRP ANG ANG ANG ANG ANG ANG ANG ANG ANG ANG			
• Molecule 20: 39S	ribosomal protein L34,	mitochondrial		
Chain 2:	45% •	53%		
		W O R L D W I D E		

MET ALA VAL LEU LEU ALA ALA SER ELEU LEU LEU CLY PRO FRO SER SER	ALA ALA ALA ALA ALA CEU CLU CLU CLU CLU CLU CLU CLU CLV CLY CLY CLY CLY CLY CLY	PR0 PR0 PR0 GLN GLN GLN GLN GLN GLY CLY CLY CLY CLY CLY CLY GEC GEC GEC GEC GEC GEC GEC GEC GEC GEC
• Molecule 21: 39S	ribosomal protein L37, mitocho	ondrial
Chain 5:	84%	8% 9%
MET LEU LEU ALA ALA SER PRO PRO PRO ALA ALA ALA ALA ALA CLY	SER GLY GLY GLY GLY GLY GLY GLY ALA ALA ATA ATA ATA ATA ATA ATA ATA	P196 196 196 2007 2207 7208 5209 6221 6223 7223 7223 7223 7223 7223 7223 7224 7223 7223
Y285 T290 L291 L291 L309 L309 A333 A333 A333 A333 A333 A333 A333 A	V351 F352 D363 D363 C380 C380 C381 C381 C381 C381 C381 C381 C381 C382 C481 VAL VAL VAL VAL VAL VAL VAL VAL	ALA
• Molecule 22: 39S	ribosomal protein L39, mitocho	ondrial
Chain 7:	81%	• 15%
MET AGU AGU AGU AGU ALA AGA AGA AGA AGA AGA AGA AGA AGA AGA	LEU VLA ALA ALA ALA CLY CLY CLY CLY TLE TTRE CLY TLE TLE STR STR STR STR STR STR STR STR STR STR	A106 K126 V167 V183 T18 T18 T28 T28 T28 T28 T28 T28 T28 T29 T29 T29 T29 T29 T29 T29 T29 T29 T29
Ka222 WAL VAL THR CLU CLU ALA ALA ALA CLU CLU CLU	THR SER THR	
• Molecule 23: 39S	ribosomal protein L41, mitoche	ondrial
Chain 9:	82%	· 15%
MET VAL VAL LEU LEU ALA ALA ALA ALA CYS CYS CYS CYS CYS CYS CYS CYS CYS	A15 829 640 640 640 640 640 640 833 833 833 833 813 7 813 813 813	
• Molecule 24: 39S	ribosomal protein L42, mitocho	ondrial
Chain a:	57% ·	42%
MET ALA ALA ALA ALA ALA ALA CAL CYS CRA CAL SER SER LIYS SER LIYS SER LIYS SER LIYS SER LIYS	LLE LLEU LLYS HHIS HHIC PHIC PHIC PHIC ASN ASN ASN ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	K77 PRO PRO ASP PRO PRO ASY ASN ASN ASN ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
LYS VAL GLU HIS LEU E104 R142 R142		
• Molecule 25: 39S	ribosomal protein L43, mitoche	ondrial
Chain b:	69%	31%
MET T2 ASP ASP ASP PRO ALA ALA ALA ALA ALA CLY GLY	LEU LEU ALA ALA ALA ALA ALA ALA ALA CLU CLU CLU ASP ASP PRO PRO PRO PRO PRO ASP VAL	ASP PRO TLE SER SER SER SER SER ALA ALA ALA ALA ALA ALA SER SER SER SER SER SER SER SER SER SER



### VAL PRO ALA LEU THR VAL CYS SER ALA

 $\bullet$  Molecule 26: 39S ribosomal protein L44, mitochondrial

Chain c:	83%	17%
MET ALA SER GLY CLEU VAL LEU LEU CLN CLN	GLN GLN ARG ARG CARG CARG CARG ILEU VAL ALA ARG ALA ARG CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	ASN L119 SER PRO PRO PRO PRO ALA ALA ALA ALA ALA ALA ALA TLE SER SER
THR ALA SER		
• Molecule 27:	: 39S ribosomal protein L45, mitochondrial	
Chain d:	69%	31%
MET ALA ALA PRO PRO GLN GLY SER	LEU LEU PHE CLEU CLEU CLEU CLEU CLEU CLEU CLEU CLE	PRO TILE TILE TVN GLN GLN F50 H59 H59 K62 K62 K62 K62 K62 K62 K62 K62 K62 K62
GLY ASP ALA ALA ALA ALA ALA SER SER SER SER LYS	CLU CLU CLEU CLU CLU CLU CLU CLU CLU CLU CLU CLU CL	ALA GLN CLY CLY CLN GLN CLN CLN CLN CLN CLN ALA
• Molecule 28:	: 39S ribosomal protein L49, mitochondrial	
Chain g:	78%	22%
MET ALA ALA ALA MET MET PHE ALA ALA LEU	ARG ARG TRP TRP TRP ARG GLY GLY GLY GLY GLY GLY GLY ARG GLY ARG GLY ARG ASP PRO GLY ARG ASP PRO FRO FRO FRO FRO	
• Molecule 29:	: 39S ribosomal protein L50, mitochondrial	
Chain h:	63%	37%
MET ALA ALA ARG SER VAL SER CLY THR THR	ARG ARG VAL ARG MET TRP TRP SER CYS SER CYS SER ARG CYS SER ARG CVS CYS CYS CVS CVS CVS CVS CVS CVS CVS CVS CVS CV	GLU LYS LYS LYS GLU GLU CVS PRO FTC PRO PRO PRO FTS SER SER SER
SER L82 Y158		
• Molecule 30:	: 39S ribosomal protein L51, mitochondrial	
Chain i:	76%	24%
MET ALA GLY ASN LEU LEU LEU SER GLY GLY	ARG ARG ARG ARG ARG ARD ARD ALA ALA ALA ALA CYS SER ARG CYS SER ARG CLEU CLU CLU CLU CLU CLU CLU CLU ARG ARG ARG ARG ARG ARG ARG ARG ARG ARD ARD ARD ARD ARD ARD ARD ARD ARD ARD	
• Molecule 31:	: 39S ribosomal protein L52, mitochondrial	

WORLDWIDE PROTEIN DATA BANK

Chain j:	69%	31%	
MET ALA ALA LEU GLY VAL LEU PHE PHE	VAL VAL ARG ARG CVS CVS CVS SER CVS SER ALA ALA ALA ALA ALA ALO C ALA ALO C C SER C ALA ALA ALO SER SER SER SER SER SER SER SER SER SER	LEU LYS PRO PRO SER SER GLN GLN	
• Molecule 32	: Ribosomal protein 63, mitochor	ndrial	
Chain o:	77%	23%	
MET PHE LEU LEU ALA LEU LEU TRP ARG GLY	ARG PRID OLY OLY CAN THE THE THE ARG OLY ARG P24 ARG S102		
• Molecule 33	: Peptidyl-tRNA hydrolase ICT1	, mitochondrial	
Chain p:	49% •	48%	
MET ALA ALA ALA ALA ARG CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	SER SER ARG ALA ARG CALY TRP TRP TRP PRO PRO PRO PRO PRO PRO PRO PRO PRO CYS CAS ALA ALA ALA ALA ALA ALA ALA ALA ALA A	ASF GLY THR B38 61 PR0 PR0 PR0 ALA ALA ALA ALA ALA ALA SE8 S83 S83 S83 S83 S81 S81 S82 S81 S81 S81 S81 S81 S81 S81 S81 S81 S81	GLY GLY GLN ASN VAL
ASN LYS N95 897 K98 K98 K142 C143 C143	R145 N146 N146 A143 A143 A143 PR0 CLU CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	ASN MET ASN ARC ARC ARC ARC CLU LEU ARC CLN CLN CLN CLN CLN CLN SER ARC CLN CLN SER ARC SER ARC ARC ARC ARC ARC ARC ARC ARC ARC AR	ARG VAL ASP MET ASP
• Molecule 34	: Growth arrest and DNA damag	ge-inducible proteins-interac	ting protein 1
Chain q:	45%	55%	-
MET ALA ALA ALA SER VAL VAL ARG ALA ALA ALA	LEU LEU ALA ALA ALA ALA ALA ALA ALA ALA ALA CYS CYS CYS ALA ALA ALA ALA ALA CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	ALL VAL ASN TASN TASN TASN GLN GLN GLN GLN ALA ALA ALA ALA ASP ASS	GLU ARG ARG ARG LEU LEU
GLN ALA GLU GLU GLU CLU LEU CLY CLY	GLN ASP ARG SER ARG SER ARG GLU CLU CLU CLU CLU CLU CLU CLU CLU CLU C	CLU CLUS CLUS CLUS CLUS CLUS CLUS CLUS C	ALA GLN ASP PRO ALA ALA
SER GLY ALA PRO SER SER			
• Molecule 35	: 39S ribosomal protein S18a, mi	tochondrial	
Chain r:	74%	26%	
MET ALA ALA ALA LUS LVS LVS LLY VAL SER SER SER SER	CVS CVS CVS LEU LEU LEU ALA ALA ALA ALA ALA ALA ALA ALA ARG CLV ALA ARG CLV ALA	r.35 V39 E40 E40 CLN GLN GLN GLN GLN GLN GLN GLN GLN CLN CLN CLN CLN CLN CLN CLN CLN CLN C	GLY VAL VAL PRO LYS SER LYS
PRO Q146 H196			
• Molecule 36	: 39S ribosomal protein S30, mite	ochondrial	
Chain s:	84%	16%	



### 



• Molecule 37: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u:	47%	53%	

### LLEU CLU V VAL CLU V CLU V CLU V CLU V CLU V VAL V CLU V CLU

### VAL GLU LEU LYS CYS GLU

• Molecule 38: MIEF1 upstream open reading frame protein

Chain v:	99%	·
HI 170		

• Molecule 39: Acyl carrier protein, mitochondrial

	6%				
Chain w:	51%	49%			

MET SSERVAL SS



• Molecule 40: 16S rRNA













Chain B:	28%		45%	-	9%	19%	
C 41603 01604 01606 01606 01606 01609 01609 01609 01609 01610 01612 01612	U1613 U1614 A1615 C C C C A A A1621 A A1621	A1622 G1623 C1624 A1625 C1625 C1626 C1627 C1627 C1628 A1629 A1630	C1631 U1632 U1633 A1640 G1641 G1641	A1643 A1644 A1645 A1645 U U1646 U1648 C1648	A1650 A1651 C U A A	A C U1658 01659 61660 A1661	C 1663 C 1663 C 1666 C 1666 U 1666
G1669 A1670							
• Molecule 45:	39S ribosom	al protein L	18, mitocl	nondrial			
Chain P:		69%		5%	26%	6	
MET ALA ALA ARG SER SER ARG PHE CLEU PHE	VAL VAL CYS ARG ARG ASN PRO GYY CYS ARG	PHE ALA LEU LEU SER SER SER SER SER	PRU ALA LYS PRO GLU VAL	ASP PRO VAL GLU ASN A42 A42	P45 E46	G66 W67 F71 ₽ 06	H114 LEU TYR SER
THR ARG M120 A132 T148 A152 A152 M164	1177 1178 E179						
• Molecule 46:	39S ribosom	al protein L2	27, mitocl	nondrial			
Chain W:		56%	g	9% •	34%		
MET ALA SER SER VAL VAL LEU LEU LEU ALA ARG ARG ARG ARG	THR ALA VAL THR SER LEU LEU SER SER PRO	THR PRO ALA ALA ALA LEU VAL VAL	TYR ALA SER LYS SER GLY	GLY SER SER LYS ASN LEU GLY	GLT SER SER GLY ARC	400 051 153 K54 G58 G58	167 A68
R71 H72 G78 G78 C38 C34 C34 C34 C34 C34 C34 C34 C34 C34 C37 C37 C37 C37 C37 C37 C37 C37 C37 C37	V103 Y104 P121 P121 Y127 Y127	V145 A146 M147 L148					
• Molecule 47:	39S ribosom	al protein L3	38, mitocl	nondrial			
Chain 6:		82%			·	14%	
MET ALA ALA ALA PRO TRP TRP ALA ALA ALA ALA LEU CYS	GLU GLU ARG ARG ARG ARG GLY CLY SER SER	THR ALA VAL LEU GLY K50	G79 GLU LYS THR ASP ASP	LYS CLU LYS LYS ASP ASP CLY CLY	PRO PRO LYS VAL	SEK R99 N116 V117 E118 CTU	E120 R124 LEU
ARG 11.27 61.80 61.80 61.9 61.9 61.9 61.7 55.R	E22 E22 E227 E274 S282	ALU ASP ALA ARG P287 S288 T312 T312	P342 P348 P352 P352	1354 1355 1361 1362	R364	R369 R370 D371 S372 H373 E374 P375	T376
• Molecule 48:	39S ribosom	al protein L	10, mitocl	nondrial			
Chain I:	30% 5	8%	·		39%		
MET ALA ALA ALA ALA ALA ALA ALA GLY CEU ARG GLY GLY	LEU LEU PRO GLN GLN ARG ARG LEU	PRO THR LEU GLN THR VAL ARG TYR GCO	K31 K31 A32 V33 T34 R35	H61 P66 PR0 PR0 SER	PRO PRO GLN GLU GLU	G77 G77 R80 L81 L82	R83 R84 E85 E85 A87 A87 A88



V89 F90 091 N93 N93 N93 N94 N94	A106 E107 L111 H114 Q115 L116 R117 K118 H119 K120 K120	F126 P127 P127 P127 P128 P138 F131 F131 F134 F133 F133 F135 F135 F135 F135 F135 F135	Y140 Q141 N142 L143 P145 V148 N151	V155 8156 E157 E157 E158 V160 V161 K162 E163 E163
R169 1170 1170 1174 1174 1181 1181	1185 1185 1185 1185 1185 1192 1192 1192 1192 1192	PR0 SER SER LEU FR0 FR0 GLY GLY GLY GLY GLY GLY CTS CTS CTS	ALM ALA ALA GLN GLN HIS SER SER LEU LEU CLN HIS GLN PRO	LEU GLN LEU THR THR LEU LEU
ASP GLN TYR ILE ARG GLU GLU GLU CLU CLU SRP SER VAF	MET SER ALA ALA ALA CLYS PRO PRO PRO ASP PRO ASP VAL VAL VAL SER SER			
• Molecule 49: 39	9S ribosomal protein L	11, mitochondrial		
Chain J:	51% 71%		27%	
MET SER LYS LEU LEU GLY ALA ALA ALA ALA ALA ALA ALA ARG CLY CLEU	PR0 CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	P31 632 P33 P34 P34 L35 C40 C40 C41 C41 C43 C43 C43 C43 C43 C43 C43 C43 C43 C43	N47 Q48 F49 C50 K51 F53 F53 F53 F53	Hbe K58 K58 160 K61 E62 G63 G63
P67 T68 K69 L71 L71 V72 K73 P74 P74 P74 R76	T77 F78 E79 E79 K81 K81 K81 A94 A94 A94 A94 A95 C96 C96 C96 C96 C96	K199 6100 6100 8101 R102 8102 6105 6105 8107 8109 8109 6110 6110 1111	L114 K115 H116 V117 V117 T118 E119 L120 A121 R122 R122	K124 A125 Q126 Q126 A131 L132 Q133 Q133 P136 P136 P136 S138 S138
8143 1144 1145 1145 1145 1145 1145 1145 1	ASP ASP SER SER SER SER ALA ALA ALA ALA ALA ALA ALA ALA ALA	PHE LEU ALA ALA ALA GLN CLYS CLU ALA ALA ALA ALA ALA ALA ALA CLU CLU	TYS	
• Molecule 50: $39$	9S ribosomal protein L	53, mitochondrial		
Chain k:	34% 71%		25%	
MET ALA ALA ALA ALA ALA ALA ALA GLY CLEU CLEU ARG PRO	118 118 122 122 122 122 122 123 123 130 130	136 844 844 854 850 850 850 850 850 850 850	81 962 873 174 175 877 877 878	H80 L81 182 A83 A83 E85 E85 S92 H93
194 895 A86 A87 A87 A87 A14 A14 A14 A14 G17 SER SER SER SER SER	PRO GLY ALA ASP ASP GLY GLY ARG			
• Molecule 51: 39	9S ribosomal protein L	54, mitochondrial		
Chain l: 17%		83%		
MET ALA ALA LYS LYS LYS PHE GLY ALA ALA ARG THR THR	ALA GLY GLY GLY ALA ALA ALA CLY GLY ALA ALA ALA ASN ASN ASN ASN ASN ASN ASN ASN ASN AS	LEU ALA ALA ARP ARP ARP CVS PRO PRO PRO PRO CVS CVS CVS CVS CVS CVS CVS CVS CVS CVS	LYS GLY ALA ALA THR SER GLU GLU LEU LEU LYS PRD	ASP
VAL THR ASP ASP ASP ASP CAL CLEU CLEU THR THR THR THR THR THR	GLY GLY ASN TYR ASN TYR CLY GLN GLN CLU PRO FRO FRO ASP	ALA ALA TYR TYR AND AND AND ANN ANN ANN ANN ANN FIR PRO PRO PRO FIR FIR	CLU CLU CLU ASP ASP PRU CLU CLU ASP ARG LEU	



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18134	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 $(e^-/\text{\AA}^2)$	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.478	Depositor
Minimum map value	-0.383	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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: MG, PNS, 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).

Mol	Chain	Bo	ond lengths	Bond angles		
10101	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	D	0.26	0/1074	0.47	0/1486	
2	Е	0.31	0/1397	0.49	0/1937	
3	F	0.33	0/1232	0.50	0/1713	
4	Н	0.26	0/468	0.46	0/650	
5	Κ	0.34	0/875	0.50	0/1218	
6	L	0.27	0/564	0.48	0/782	
7	М	0.31	0/1264	0.48	0/1755	
8	N	0.26	0/1005	0.45	0/1394	
9	0	0.29	0/748	0.45	0/1039	
10	Q	0.28	0/1074	0.45	0/1496	
11	R	0.34	0/692	0.49	0/963	
12	S	0.32	0/771	0.53	0/1073	
13	Т	0.33	0/786	0.51	0/1093	
14	U	0.32	0/684	0.49	0/949	
15	V	0.29	0/944	0.47	0/1310	
16	Х	0.28	0/1201	0.42	0/1672	
17	Y	0.31	0/873	0.41	0/1217	
18	Ζ	0.32	0/594	0.49	0/827	
19	0	0.32	0/533	0.46	0/741	
20	2	0.35	0/210	0.50	0/290	
21	5	0.27	0/1914	0.46	0/2665	
22	7	0.28	0/1425	0.45	0/1988	
23	9	0.30	0/573	0.49	0/793	
24	a	0.33	0/405	0.55	0/562	
25	b	0.38	0/729	0.52	0/1013	
26	с	0.30	0/1358	0.43	0/1889	
27	d	0.27	0/1044	0.48	0/1451	
28	g	0.33	0/637	0.48	0/886	
29	h	0.27	0/497	0.41	0/692	
30	i	0.34	0/475	0.52	0/658	
31	j	0.30	0/416	0.41	0/576	
32	0	0.28	0/393	0.40	0/548	



Mal	Chain	Bo	ond lengths	I	Bond angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
33	р	0.97	4/530~(0.8%)	1.02	7/736~(1.0%)
34	q	0.30	0/489	0.39	0/680
35	r	0.29	0/718	0.45	0/995
36	s	0.29	0/1836	0.46	0/2560
37	u	0.26	0/551	0.42	0/768
38	V	0.23	0/340	0.36	0/472
39	W	0.22	0/391	0.43	0/544
40	А	0.76	11/28659~(0.0%)	1.29	306/44547~(0.7%)
41	Х	0.26	0/1841	0.43	0/2558
42	у	0.30	0/1620	0.51	0/2246
43	1	0.25	0/1259	0.42	0/1744
43	Z	0.25	0/1238	0.43	0/1713
44	В	0.32	0/1328	1.08	5/2056~(0.2%)
45	Р	0.25	0/657	0.45	0/913
46	W	0.25	0/480	0.45	0/665
47	6	0.34	1/1605~(0.1%)	0.66	7/2229~(0.3%)
48	Ι	0.25	0/783	0.41	0/1090
49	J	0.25	0/685	0.41	0/949
50	k	0.23	0/415	0.44	0/577
51	1	0.21	0/114	0.26	0/158
All	All	0.54	16/72394~(0.0%)	0.92	325/105526~(0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1
24	a	0	1
33	р	0	2
42	у	0	3
47	6	0	3
All	All	0	10

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
40	А	1281	А	N9-C4	11.65	1.44	1.37
33	р	145	ARG	C-N	11.26	1.59	1.34
40	А	1281	А	N7-C5	-10.98	1.32	1.39
33	р	146	ASN	N-CA	10.48	1.67	1.46



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	А	1306	G	P-O5'	7.89	1.67	1.59
40	А	148	А	N9-C4	-7.02	1.33	1.37
40	А	1281	А	C8-N7	-6.27	1.27	1.31
40	А	239	А	C6-N1	-6.07	1.31	1.35
40	А	158	А	N9-C4	-6.03	1.34	1.37
47	6	373	HIS	CA-C	5.81	1.68	1.52
33	р	146	ASN	CA-C	5.80	1.68	1.52
40	А	193	А	N9-C4	-5.72	1.34	1.37
40	А	1306	G	C5'-C4'	5.37	1.57	1.51
40	А	340	U	N3-C4	-5.36	1.33	1.38
33	р	145	ARG	N-CA	5.04	1.56	1.46
40	A	476	A	N9-C4	-5.02	1.34	1.37

All (325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
40	А	340	U	C5-C4-O4	20.32	138.09	125.90
40	А	340	U	N3-C4-O4	-18.56	106.41	119.40
40	А	1281	А	C4-C5-C6	16.63	125.32	117.00
40	А	1281	А	N3-C4-N9	13.60	138.28	127.40
40	А	1305	G	O4'-C1'-N9	13.39	118.92	108.20
40	А	1281	А	N3-C4-C5	-13.19	117.57	126.80
40	А	1281	А	C6-C5-N7	-13.00	123.20	132.30
33	р	145	ARG	C-N-CA	11.19	149.67	121.70
40	А	1305	G	N1-C6-O6	-11.03	113.28	119.90
40	А	1281	А	C4-N9-C1'	10.73	145.62	126.30
40	А	239	А	N1-C6-N6	-10.37	112.38	118.60
40	А	1305	G	N9-C4-C5	10.07	109.43	105.40
40	А	1281	А	C8-N9-C4	-9.90	101.84	105.80
40	А	1253	G	C5-C6-O6	9.70	134.42	128.60
40	А	1139	С	C2-N3-C4	-9.69	115.05	119.90
40	А	1315	С	N1-C2-O2	9.62	124.67	118.90
40	А	1279	С	C6-N1-C2	-9.56	116.48	120.30
47	6	373	HIS	N-CA-CB	-9.55	93.41	110.60
40	А	1542	С	C2-N1-C1'	9.21	128.93	118.80
40	А	108	U	C2-N1-C1'	9.15	128.68	117.70
40	А	582	С	N1-C2-O2	9.13	124.38	118.90
40	A	1305	G	C4-C5-N7	-8.98	107.21	110.80
40	А	1303	U	C2-N3-C4	-8.82	121.71	127.00
40	A	1253	G	N1-C6-O6	-8.80	114.62	119.90
40	А	709	С	C6-N1-C2	-8.80	116.78	120.30
40	А	1139	С	N3-C4-C5	8.71	125.39	121.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
40	А	1258	С	N1-C2-O2	8.69	124.11	118.90
40	А	108	U	N3-C2-O2	-8.66	116.14	122.20
47	6	373	HIS	N-CA-C	8.64	134.32	111.00
40	А	118	С	N1-C2-O2	8.60	124.06	118.90
40	А	15	С	N1-C2-O2	8.54	124.02	118.90
40	А	1258	С	C2-N1-C1'	8.52	128.18	118.80
40	А	1279	С	N3-C2-O2	-8.47	115.97	121.90
40	А	23	С	C2-N1-C1'	8.44	128.08	118.80
40	А	1281	А	C8-N9-C1'	-8.43	112.53	127.70
40	А	641	U	C2-N1-C1'	8.43	127.81	117.70
40	А	582	С	C2-N1-C1'	8.38	128.02	118.80
40	А	523	U	C5-C4-O4	8.37	130.92	125.90
40	А	1305	G	C8-N9-C1'	8.33	137.83	127.00
40	А	1228	U	C2-N1-C1'	8.32	127.68	117.70
40	А	1305	G	C5-C6-O6	8.24	133.54	128.60
40	А	1305	G	C6-C5-N7	8.24	135.34	130.40
47	6	373	HIS	C-N-CA	8.08	141.89	121.70
40	А	23	С	N1-C2-O2	8.06	123.74	118.90
40	А	1073	U	C2-N1-C1'	8.05	127.36	117.70
40	А	1281	А	C6-N1-C2	-7.94	113.83	118.60
40	А	423	U	N3-C2-O2	-7.90	116.67	122.20
40	А	709	С	N3-C2-O2	-7.77	116.46	121.90
40	А	195	С	N1-C2-O2	7.75	123.55	118.90
40	А	149	U	O4'-C1'-N1	7.72	114.38	108.20
40	А	1432	U	C2-N1-C1'	7.71	126.96	117.70
40	А	1017	С	C2-N1-C1'	7.68	127.25	118.80
40	А	1138	U	N1-C2-O2	7.64	128.15	122.80
40	А	15	С	N3-C2-O2	-7.63	116.56	121.90
47	6	372	SER	C-N-CA	7.62	140.76	121.70
40	А	161	G	N9-C4-C5	-7.60	102.36	105.40
40	А	55	С	N1-C2-O2	7.59	123.45	118.90
40	А	997	U	N3-C2-O2	-7.57	116.90	122.20
40	А	1522	С	N1-C2-O2	7.47	123.38	118.90
40	А	188	G	C4-N9-C1'	7.47	136.21	126.50
40	А	170	С	C2-N1-C1'	7.46	127.01	118.80
40	А	118	С	N3-C2-O2	-7.44	116.69	121.90
40	A	1487	C	C2-N1-C1'	7.43	126.97	118.80
40	А	12	C	C6-N1-C2	-7.42	117.33	120.30
40	A	423	U	N1-C2-O2	7.42	127.99	122.80
44	В	1627	C	N3-C2-O2	-7.41	116.71	121.90
40	A	195	C	N3-C2-O2	-7.37	$116.7\overline{4}$	121.90
40	A	50	C	N1-C2-O2	7.35	123.31	118.90



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
40	А	24	U	N1-C2-O2	7.31	127.92	122.80
40	А	709	С	N1-C2-O2	7.28	123.27	118.90
40	А	523	U	N3-C4-O4	-7.28	114.31	119.40
40	А	641	U	N1-C2-O2	7.26	127.88	122.80
40	А	169	С	N3-C2-O2	-7.26	116.82	121.90
40	А	108	U	N1-C2-O2	7.25	127.87	122.80
40	А	373	С	C2-N1-C1'	7.24	126.77	118.80
40	А	466	C	N1-C2-O2	7.22	123.23	118.90
40	А	1307	G	O5'-P-OP1	-7.19	99.23	105.70
40	А	582	C	C6-N1-C1'	-7.17	112.19	120.80
40	А	355	C	N1-C2-O2	7.17	123.20	118.90
40	А	108	U	C6-N1-C2	-7.12	116.73	121.00
40	А	423	U	C2-N1-C1'	7.10	126.22	117.70
40	А	188	G	N3-C4-C5	-7.09	125.06	128.60
40	А	1305	G	C4-N9-C1'	-7.06	117.32	126.50
40	А	377	U	C2-N1-C1'	7.05	126.16	117.70
33	р	145	ARG	CA-C-O	-7.04	105.31	120.10
40	А	659	C	C2-N1-C1'	7.03	126.54	118.80
40	А	986	U	N3-C2-O2	-7.03	117.28	122.20
40	А	800	G	N1-C6-O6	-7.03	115.68	119.90
40	А	1306	G	O5'-P-OP1	7.03	119.13	110.70
40	А	1278	C	N1-C2-O2	7.01	123.11	118.90
40	А	1258	С	N3-C2-O2	-7.00	117.00	121.90
40	А	425	U	C5-C6-N1	6.99	126.19	122.70
40	А	377	U	N3-C2-O2	-6.97	117.32	122.20
40	А	1315	С	N3-C2-O2	-6.96	117.03	121.90
40	А	592	С	C6-N1-C2	-6.93	117.53	120.30
40	А	1487	С	N1-C2-O2	6.93	123.06	118.90
40	А	239	A	C5-C6-N6	6.93	129.24	123.70
40	А	1542	С	N1-C2-O2	6.90	123.04	118.90
47	6	373	HIS	CA-C-N	6.89	132.37	117.20
40	A	143	C	C2-N1-C1'	6.86	126.35	118.80
40	A	601	C	N3-C2-O2	-6.85	117.11	121.90
40	A	188	G	N3-C4-N9	6.84	130.10	126.00
40	A	787	A	P-O3'-C3'	6.82	127.88	119.70
40	A	24	U	N3-C2-O2	-6.81	117.44	122.20
40	A	1306	G	O5'-C5'-C4'	6.81	124.64	111.70
40	A	1306	G	C5'-C4'-C3'	6.80	126.88	116.00
40	A	12	C	C2-N1-C1'	6.80	126.28	118.80
40	A	169	C	N1-C2-O2	6.80	122.98	118.90
40	A	705	C	N1-C2-O2	6.78	122.97	118.90
40	A	1315	C	C2-N1-C1'	6.75	126.23	118.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
40	А	161	G	C6-C5-N7	-6.75	126.35	130.40
40	А	377	U	N1-C2-O2	6.72	127.51	122.80
40	А	1434	U	N3-C2-O2	-6.71	117.50	122.20
40	А	23	С	N3-C2-O2	-6.67	117.23	121.90
40	А	1281	А	N7-C8-N9	6.65	117.12	113.80
40	А	1487	С	C6-N1-C1'	-6.65	112.83	120.80
40	А	588	А	N1-C2-N3	6.63	132.62	129.30
40	А	709	С	C2-N1-C1'	6.63	126.10	118.80
40	А	1138	U	N3-C2-O2	-6.63	117.56	122.20
40	А	55	С	N3-C2-O2	-6.62	117.26	121.90
40	А	1531	А	P-O3'-C3'	6.60	127.62	119.70
40	А	641	U	N3-C2-O2	-6.60	117.58	122.20
40	А	161	G	C4-C5-N7	6.59	113.44	110.80
40	А	1542	С	C5-C6-N1	6.58	124.29	121.00
40	А	1138	U	C2-N1-C1'	6.55	125.56	117.70
40	А	1164	С	N1-C2-O2	6.55	122.83	118.90
47	6	373	HIS	O-C-N	-6.53	112.25	122.70
40	А	143	С	N1-C2-O2	6.53	122.82	118.90
40	А	239	А	C8-N9-C1'	-6.53	115.94	127.70
40	А	50	С	C2-N1-C1'	6.52	125.97	118.80
40	А	239	А	C4-N9-C1'	6.51	138.03	126.30
40	А	1542	С	C6-N1-C2	-6.51	117.69	120.30
40	А	1305	G	P-O3'-C3'	6.51	127.51	119.70
40	А	1522	С	N3-C2-O2	-6.50	117.35	121.90
40	А	12	С	N3-C2-O2	-6.48	117.36	121.90
40	А	447	U	N1-C2-O2	6.47	127.33	122.80
40	А	188	G	C8-N9-C1'	-6.45	118.61	127.00
40	А	50	C	N3-C2-O2	-6.42	117.40	121.90
40	А	360	U	P-O3'-C3'	6.42	127.40	119.70
40	А	422	С	C6-N1-C2	-6.42	117.73	120.30
40	А	610	С	N3-C2-O2	-6.42	117.41	121.90
40	А	726	С	N1-C2-O2	6.39	122.73	118.90
40	А	1306	G	C6-C5-N7	-6.39	126.56	130.40
40	А	422	С	N1-C2-O2	6.39	122.73	118.90
40	А	28	С	C6-N1-C2	-6.38	117.75	120.30
40	A	355	C	C2-N1-C1'	6.36	125.80	118.80
40	A	1011	G	C4-C5-N7	6.35	113.34	110.80
40	A	1373	C	N1-C2-O2	6.34	122.70	118.90
44	В	1624	С	N1-C2-O2	6.33	122.70	118.90
40	A	1011	G	N9-C4-C5	-6.32	102.87	105.40
40	A	$14\overline{32}$	U	C5-C6-N1	6.32	125.86	122.70
40	А	192	U	N3-C2-O2	-6.29	117.80	122.20



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
40	А	577	С	N1-C2-O2	6.29	122.67	118.90
40	А	396	С	N1-C2-O2	6.29	122.67	118.90
40	А	1017	С	N1-C2-O2	6.28	122.67	118.90
40	А	670	С	N1-C2-O2	6.27	122.66	118.90
40	А	239	А	N9-C4-C5	-6.26	103.30	105.80
40	А	1283	U	C2-N1-C1'	6.24	125.18	117.70
40	А	459	G	N1-C6-O6	-6.22	116.17	119.90
33	р	146	ASN	O-C-N	-6.21	112.77	122.70
40	А	1542	С	C6-N1-C1'	-6.20	113.36	120.80
40	А	121	G	C6-C5-N7	-6.20	126.68	130.40
40	А	169	С	C2-N1-C1'	6.19	125.61	118.80
40	А	355	С	N3-C2-O2	-6.19	117.57	121.90
40	А	12	С	N1-C2-O2	6.19	122.61	118.90
40	А	1258	С	C6-N1-C1'	-6.18	113.39	120.80
40	А	641	U	C6-N1-C1'	-6.17	112.56	121.20
40	А	161	G	C8-N9-C1'	-6.16	119.00	127.00
40	А	396	С	N3-C2-O2	-6.14	117.60	121.90
40	А	1464	С	N1-C2-O2	6.13	122.58	118.90
40	А	705	С	C2-N1-C1'	6.12	125.54	118.80
40	А	1544	С	N1-C2-O2	6.12	122.57	118.90
40	А	582	С	N3-C2-O2	-6.06	117.66	121.90
40	А	44	С	N1-C2-O2	6.05	122.53	118.90
40	А	153	А	C8-N9-C4	-6.05	103.38	105.80
40	А	1032	G	N3-C4-N9	6.02	129.61	126.00
40	А	176	С	C2-N3-C4	-6.00	116.90	119.90
40	А	330	С	N1-C2-O2	5.99	122.50	118.90
40	А	1228	U	N1-C2-O2	5.98	126.99	122.80
40	А	24	U	C2-N1-C1'	5.98	124.87	117.70
33	р	146	ASN	N-CA-C	5.97	127.11	111.00
40	А	153	А	P-O3'-C3'	5.97	126.86	119.70
40	А	670	С	N3-C2-O2	-5.95	117.73	121.90
40	А	153	А	N7-C8-N9	5.94	116.77	113.80
33	р	144	PHE	C-N-CA	5.94	136.54	121.70
40	А	675	G	N3-C4-N9	5.93	129.56	126.00
40	А	1022	G	N3-C2-N2	-5.91	115.76	119.90
40	А	1038	С	C6-N1-C2	-5.91	117.94	120.30
40	А	447	U	N3-C2-O2	-5.90	118.07	122.20
40	А	23	С	C6-N1-C2	-5.90	117.94	120.30
33	р	143	GLN	C-N-CA	5.90	136.45	121.70
40	A	195	С	C2-N1-C1'	5.89	125.28	118.80
40	A	1432	U	C6-N1-C2	-5.89	117.46	121.00
44	В	1626	С	N1-C2-O2	5.89	122.43	118.90



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
40	А	50	С	C6-N1-C2	-5.88	117.95	120.30
40	А	1552	С	N3-C2-O2	-5.86	117.80	121.90
40	А	997	U	N1-C2-O2	5.86	126.90	122.80
40	А	422	С	N3-C2-O2	-5.86	117.80	121.90
40	А	1017	С	C6-N1-C1'	-5.86	113.77	120.80
40	А	577	С	N3-C2-O2	-5.84	117.81	121.90
40	А	108	U	C5-C6-N1	5.84	125.62	122.70
40	А	1011	G	C8-N9-C1'	-5.82	119.43	127.00
40	А	466	С	N3-C2-O2	-5.81	117.83	121.90
40	А	1228	U	C6-N1-C1'	-5.81	113.07	121.20
40	А	1473	U	N3-C2-O2	-5.78	118.15	122.20
40	А	143	С	N3-C2-O2	-5.76	117.87	121.90
40	А	1291	С	N1-C2-O2	5.74	122.34	118.90
40	А	1032	G	C8-N9-C1'	-5.73	119.55	127.00
33	р	145	ARG	CA-C-N	5.73	129.80	117.20
40	А	1123	С	N1-C2-O2	5.69	122.32	118.90
40	А	628	А	C4-N9-C1'	5.69	136.54	126.30
40	А	23	С	C6-N1-C1'	-5.69	113.98	120.80
40	А	987	С	N1-C2-O2	5.68	122.31	118.90
40	А	379	U	C2-N1-C1'	5.66	124.49	117.70
40	А	73	U	N1-C2-O2	5.65	126.75	122.80
40	А	153	А	C4-N9-C1'	5.64	136.46	126.30
40	А	373	С	N1-C2-O2	5.64	122.28	118.90
40	А	1522	С	C2-N1-C1'	5.64	125.00	118.80
44	В	1627	С	C6-N1-C2	-5.61	118.06	120.30
40	А	1339	С	C2-N1-C1'	5.61	124.97	118.80
40	А	210	С	C2-N1-C1'	5.61	124.97	118.80
40	А	592	С	C5-C6-N1	5.60	123.80	121.00
44	В	1624	С	N3-C2-O2	-5.57	118.00	121.90
40	А	1009	U	N3-C2-O2	-5.57	118.30	122.20
40	А	1073	U	C6-N1-C1'	-5.56	113.42	121.20
40	А	610	С	N1-C2-O2	5.56	122.23	118.90
40	А	19	С	N1-C2-O2	5.55	122.23	118.90
40	А	170	С	N1-C2-O2	5.54	122.22	118.90
40	А	1464	С	C2-N1-C1'	5.54	124.89	118.80
40	А	524	U	N1-C2-O2	5.53	126.67	122.80
40	А	1073	U	N1-C2-O2	5.52	126.67	122.80
40	А	1473	U	$C2-N\overline{1-C1}$	5.52	124.33	117.70
40	A	73	U	$C2-N\overline{1-C1}$	5.52	124.32	117.70
40	A	447	U	$C2-N1-\overline{C1'}$	$5.5\overline{2}$	124.32	117.70
40	А	$14\overline{34}$	U	N1-C2-O2	5.51	126.66	122.80
40	A	1531	A	O4'-C1'-N9	5.50	112.60	108.20



Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^{o})$	$Ideal(^{o})$
40	А	1029	С	C2-N1-C1'	5.48	124.83	118.80
40	А	1315	С	C5-C6-N1	5.48	123.74	121.00
40	А	466	С	C2-N1-C1'	5.44	124.78	118.80
40	А	1011	G	C6-C5-N7	-5.43	127.14	130.40
40	А	19	С	C2-N1-C1'	5.43	124.78	118.80
40	А	248	G	N3-C4-C5	-5.43	125.88	128.60
40	А	1373	С	N3-C2-O2	-5.43	118.10	121.90
40	А	986	U	N1-C2-O2	5.42	126.60	122.80
40	А	675	G	N9-C4-C5	-5.42	103.23	105.40
40	А	118	С	C2-N1-C1'	5.41	124.75	118.80
40	А	1464	С	C6-N1-C2	-5.40	118.14	120.30
40	А	248	G	N3-C4-N9	5.40	129.24	126.00
40	А	170	С	C5-C6-N1	5.38	123.69	121.00
40	А	1011	G	N3-C4-N9	5.38	129.23	126.00
40	А	1004	U	C2-N1-C1'	5.37	124.15	117.70
40	А	609	U	N3-C2-O2	-5.36	118.45	122.20
40	А	44	С	N3-C2-O2	-5.35	118.16	121.90
40	А	210	С	N1-C2-O2	5.34	122.11	118.90
40	А	330	С	C2-N1-C1'	5.34	124.68	118.80
40	А	1032	G	C4-N9-C1'	5.34	133.45	126.50
40	А	1027	G	C8-N9-C1'	-5.34	120.06	127.00
40	А	98	G	N3-C4-N9	5.33	129.20	126.00
40	А	601	С	N1-C2-O2	5.32	122.09	118.90
40	А	1306	G	OP1-P-OP2	-5.32	111.63	119.60
40	А	1489	А	P-O3'-C3'	5.31	126.07	119.70
40	А	1303	U	N3-C4-C5	5.30	117.78	114.60
40	А	628	А	C8-N9-C1'	-5.30	118.17	127.70
40	А	980	С	N1-C2-O2	5.30	122.08	118.90
40	А	239	А	N3-C4-N9	5.29	131.63	127.40
40	А	456	U	N1-C2-O2	5.28	126.49	122.80
40	А	373	С	C5-C6-N1	5.27	123.64	121.00
40	А	573	А	P-O3'-C3'	5.27	126.03	119.70
40	А	659	С	C6-N1-C1'	-5.27	114.48	120.80
40	А	587	С	C2-N1-C1'	5.26	124.59	118.80
40	А	1552	С	N1-C2-O2	5.26	122.06	118.90
40	А	1048	С	C6-N1-C2	-5.25	118.20	120.30
40	А	55	С	C6-N1-C2	-5.25	118.20	120.30
40	А	1238	U	N1-C2-O2	5.25	126.47	122.80
40	А	726	С	N3-C2-O2	-5.24	118.23	121.90
40	А	1228	U	N3-C2-O2	-5.23	118.54	122.20
40	А	216	G	N1-C6-O6	5.23	123.04	119.90
40	А	170	С	C6-N1-C1'	-5.23	114.53	120.80


Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
40	А	1164	С	C2-N1-C1'	5.23	124.55	118.80
40	А	747	С	C2-N1-C1'	5.22	124.54	118.80
40	А	1281	А	C2-N3-C4	5.20	113.20	110.60
40	А	1487	С	O4'-C1'-N1	5.20	112.36	108.20
40	А	396	С	C2-N1-C1'	5.20	124.52	118.80
40	А	1011	G	C4-N9-C1'	5.19	133.25	126.50
40	А	1464	С	N3-C2-O2	-5.19	118.27	121.90
40	А	171	U	N3-C4-O4	5.19	123.03	119.40
40	А	73	U	N3-C2-O2	-5.18	118.58	122.20
47	6	371	ASP	C-N-CA	5.18	134.64	121.70
40	А	349	G	N3-C4-N9	5.17	129.10	126.00
40	А	1164	С	N3-C2-O2	-5.17	118.28	121.90
40	А	1432	U	N3-C2-O2	-5.17	118.58	122.20
40	А	1452	U	C2-N1-C1'	5.17	123.90	117.70
40	А	785	U	N3-C2-O2	-5.16	118.58	122.20
40	А	566	С	P-O3'-C3'	5.16	125.89	119.70
40	А	1279	С	N3-C4-C5	-5.16	119.84	121.90
40	А	640	G	C4-C5-N7	5.14	112.86	110.80
40	А	1306	G	N3-C4-N9	5.14	129.08	126.00
40	А	1434	U	C2-N1-C1'	5.14	123.87	117.70
40	А	687	С	C6-N1-C2	-5.13	118.25	120.30
40	А	726	С	C2-N1-C1'	5.13	124.45	118.80
40	А	670	С	C2-N1-C1'	5.13	124.44	118.80
40	А	8	С	O4'-C1'-N1	-5.11	104.11	108.20
40	А	753	С	C2-N1-C1'	5.11	124.42	118.80
40	А	43	А	P-O3'-C3'	5.11	125.83	119.70
40	А	771	С	C6-N1-C2	-5.10	118.26	120.30
40	А	376	С	N3-C2-O2	-5.10	118.33	121.90
40	А	588	А	C2-N3-C4	-5.09	108.06	110.60
40	А	349	G	N3-C4-C5	-5.09	126.06	128.60
40	А	783	G	C5-C6-N1	5.09	114.04	111.50
40	А	188	G	C6-C5-N7	-5.08	127.35	130.40
40	А	171	U	C2-N1-C1'	5.08	123.80	117.70
40	А	104	U	O4'-C1'-N1	-5.08	104.14	108.20
40	А	1073	U	C5-C6-N1	5.07	125.24	122.70
40	А	170	С	C6-N1-C2	-5.07	118.27	120.30
40	А	98	G	C6-C5-N7	-5.06	127.36	130.40
40	А	705	С	C6-N1-C1'	-5.05	114.74	120.80
40	А	1006	А	C6-N1-C2	-5.05	115.57	118.60
40	А	410	U	N1-C2-O2	5.04	126.33	122.80
40	А	422	С	C2-N1-C1'	5.04	124.34	118.80
40	А	1542	С	O4'-C1'-N1	5.04	112.23	108.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
40	А	56	С	N1-C2-O2	5.03	121.92	118.90
40	А	373	С	C6-N1-C2	-5.02	118.29	120.30
40	А	1305	G	N3-C4-N9	-5.02	122.99	126.00
40	А	705	С	N3-C2-O2	-5.01	118.39	121.90
40	А	575	А	C8-N9-C4	-5.00	103.80	105.80

There are no chirality outliers.

All (10)	planarity	outliers	are listed	below:
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Mol	Chain	Res	Type	Group
47	6	372	SER	Peptide
47	6	373	HIS	Peptide,Mainchain
3	F	151	VAL	Peptide
24	а	40	PRO	Peptide
33	р	145	ARG	Peptide
33	р	148	ALA	Peptide
42	У	127	LEU	Peptide
42	У	130	ASN	Peptide
42	У	131	PHE	Peptide

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1076	0	502	19	0
2	Е	1399	0	611	19	0
3	F	1233	0	543	8	0
4	Н	469	0	199	4	0
5	Κ	876	0	386	6	0
6	L	565	0	252	5	0
7	М	1266	0	559	7	0
8	Ν	1006	0	456	10	0
9	0	749	0	329	3	0
10	Q	1075	0	453	8	0
11	R	693	0	328	2	0
12	S	772	0	330	7	0
13	Т	788	0	344	7	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	U	686	0	292	6	0
15	V	946	0	398	6	0
16	Х	1202	0	513	8	0
17	Y	874	0	383	3	0
18	Ζ	595	0	245	3	0
19	0	534	0	228	2	0
20	2	211	0	90	2	0
21	5	1916	0	819	16	0
22	7	1426	0	610	7	0
23	9	575	0	257	3	0
24	a	407	0	158	0	0
25	b	730	0	320	0	0
26	с	1360	0	604	0	0
27	d	1048	0	442	0	0
28	g	638	0	257	0	0
29	h	499	0	204	0	0
30	i	476	0	203	0	0
31	j	417	0	198	0	0
32	0	394	0	185	0	0
33	р	533	0	234	0	0
34	q	490	0	219	0	0
35	r	721	0	294	0	0
36	s	1838	0	825	0	0
37	u	552	0	229	0	0
38	V	341	0	158	0	0
39	W	392	0	166	0	0
40	А	25636	0	13040	386	0
41	Х	1843	0	825	0	0
42	у	1621	0	735	0	0
43	1	1262	0	579	1	0
43	Z	1242	0	571	0	0
44	В	1191	0	607	19	0
45	Р	659	0	300	6	0
46	W	481	0	221	10	0
47	6	1611	0	701	5	0
48	Ι	785	0	332	3	0
49	J	686	0	323	2	0
50	k	416	0	187	0	0
51	1	115	0	45	0	0
52	А	44	0	0	0	0
52	F	1	0	0	0	0
52	W	1	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
52	g	1	0	0	0	0	
52	Х	1	0	0	0	0	
53	0	1	0	0	0	0	
54	V	21	0	21	0	0	
All	All	69386	0	32310	566	0	

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (566) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
40:A:1446:C:N4	40:A:1470:A:H61	1.50	1.08
40:A:1446:C:H42	40:A:1470:A:N6	1.51	1.07
2:E:106:MET:HA	2:E:119:VAL:O	1.57	1.04
40:A:238:A:H62	40:A:342:A:N6	1.55	1.04
40:A:130:G:N2	40:A:135:A:H62	1.55	1.02
40:A:1454:U:N3	40:A:1463:A:C8	2.26	1.02
40:A:662:C:C2	40:A:774:A:N6	2.26	1.02
40:A:51:C:N4	40:A:60:U:H3	1.57	1.01
40:A:662:C:N4	40:A:772:U:H3	1.58	1.01
40:A:238:A:N6	40:A:342:A:H61	1.63	0.96
22:7:106:ALA:HA	22:7:126:LYS:O	1.64	0.95
40:A:1343:G:H1	40:A:1354:U:H3	1.07	0.94
40:A:1065:G:H1	40:A:1254:U:H3	1.02	0.94
40:A:130:G:H21	40:A:135:A:N6	1.67	0.91
40:A:238:A:H62	40:A:342:A:H61	0.93	0.91
40:A:114:A:H62	40:A:123:G:N2	1.70	0.90
40:A:114:A:H62	40:A:123:G:H21	0.89	0.89
40:A:482:A:H62	40:A:579:G:N2	1.71	0.87
40:A:130:G:H21	40:A:135:A:H62	0.88	0.86
40:A:114:A:N6	40:A:123:G:H21	1.72	0.85
44:B:1607:U:H3	44:B:1664:G:H1	1.22	0.85
1:D:129:VAL:HA	1:D:139:ILE:O	1.78	0.84
12:S:95:LEU:HA	12:S:137:GLY:O	1.78	0.83
40:A:482:A:N6	40:A:579:G:H21	1.78	0.82
16:X:85:TRP:HA	16:X:105:TRP:O	1.80	0.81
2:E:215:PHE:HA	2:E:259:GLY:O	1.80	0.81
40:A:662:C:H42	40:A:772:U:H3	0.84	0.81
40:A:802:A:H62	40:A:984:U:H3	1.27	0.79
2:E:106:MET:CA	2:E:119:VAL:O	2.31	0.78



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
40:A:662:C:N4	40:A:772:U:N3	2.25	0.78	
40:A:482:A:N6	40:A:579:G:N2	2.32	0.78	
40:A:74:A:N6	40:A:84:G:H21	1.81	0.77	
40:A:1371:U:H4'	40:A:1372:U:OP1	1.84	0.77	
40:A:991:U:H2'	40:A:992:A:H8	1.51	0.74	
22:7:183:VAL:O	22:7:294:ILE:HA	1.86	0.74	
12:S:172:MET:HA	12:S:182:LYS:O	1.87	0.74	
44:B:1622:A:N6	44:B:1645:A:C2	2.56	0.74	
40:A:74:A:N6	40:A:84:G:N2	2.36	0.73	
40:A:51:C:N4	40:A:60:U:N3	2.26	0.73	
40:A:74:A:H62	40:A:84:G:N2	1.85	0.73	
40:A:988:U:H3'	40:A:989:C:H2'	1.69	0.72	
8:N:92:LEU:H	8:N:187:ALA:HA	1.55	0.71	
40:A:237:A:C8	40:A:343:U:N3	2.59	0.71	
40:A:51:C:H42	40:A:60:U:H3	1.09	0.71	
40:A:1454:U:C2	40:A:1463:A:N7	2.59	0.71	
40:A:438:G:H21	40:A:442:A:H62	1.37	0.70	
40:A:1139:C:N3	40:A:1254:U:O4	2.25	0.70	
5:K:19:TYR:O	5:K:57:VAL:HA	1.90	0.70	
40:A:1457:G:H2'	40:A:1458:A:H2'	1.73	0.69	
21:5:207:SER:O	21:5:225:SER:HA	1.93	0.68	
40:A:1363:U:H5"	40:A:1364:U:H5'	1.76	0.68	
40:A:111:A:H62	40:A:125:A:H62	1.42	0.67	
40:A:738:U:H2'	40:A:739:A:H8	1.57	0.67	
40:A:73:U:H3	40:A:85:A:H62	1.41	0.67	
40:A:1336:U:O2	40:A:1338:C:N4	2.28	0.67	
40:A:1446:C:N3	40:A:1470:A:N1	2.42	0.67	
40:A:385:U:H2'	40:A:386:G:H8	1.60	0.67	
44:B:1622:A:N6	44:B:1645:A:H2	1.92	0.66	
21:5:196:PRO:O	21:5:199:ALA:HB3	1.95	0.66	
40:A:153:A:H8	40:A:1036:A:HO2'	1.44	0.66	
40:A:1480:U:H2'	40:A:1481:A:H8	1.59	0.66	
44:B:1628:C:H42	44:B:1640:A:H61	1.43	0.66	
1:D:129:VAL:CA	1:D:139:ILE:O	2.44	0.66	
40:A:1454:U:O2	40:A:1463:A:N7	2.28	0.66	
21:5:106:ILE:HA	21:5:221:GLN:O	1.96	0.65	
40:A:113:U:H2'	40:A:114:A:H8	1.61	0.65	
16:X:116:SER:O	16:X:120:ASP:N	2.30	0.65	
40:A:480:U:H2'	40:A:481:A:H8	1.61	0.65	
9:O:9:ILE:N	40:A:788:A:OP1	2.29	0.65	
23:9:40:GLY:O	40:A:35:A:N6	2.30	0.64	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
40:A:1203:A:H5"	46:W:84:GLY:HA3	1.78	0.64	
40:A:647:G:H2'	40:A:648:A:H8	1.63	0.64	
40:A:519:C:H5'	40:A:520:C:H5'	1.78	0.64	
40:A:159:A:H2'	40:A:160:G:H8	1.62	0.63	
40:A:1379:U:O2	40:A:1383:A:N7	2.32	0.63	
21:5:290:THR:HA	21:5:343:GLN:O	1.98	0.63	
40:A:798:A:H61	40:A:989:C:N4	1.96	0.63	
40:A:1446:C:H42	40:A:1470:A:H61	0.73	0.63	
40:A:523:U:C4	40:A:526:A:N1	2.66	0.62	
40:A:662:C:N4	40:A:772:U:C4	2.66	0.62	
40:A:70:A:H3'	40:A:71:A:H2'	1.82	0.62	
40:A:482:A:N6	40:A:579:G:C2	2.67	0.62	
40:A:850:C:O2	40:A:858:G:N2	2.30	0.62	
14:U:69:ARG:O	14:U:95:ALA:HA	1.99	0.62	
21:5:210:SER:HA	21:5:222:VAL:O	2.00	0.62	
40:A:632:U:H2'	40:A:633:A:H8	1.65	0.62	
40:A:1549:G:N2	40:A:1551:A:OP1	2.33	0.61	
40:A:802:A:N6	40:A:984:U:H3	1.97	0.61	
13:T:98:SER:HA	13:T:141:TYR:HA	1.83	0.61	
40:A:1433:C:H2'	40:A:1434:U:H6	1.65	0.61	
40:A:388:C:N3	40:A:411:U:O4	2.34	0.61	
5:K:91:THR:O	5:K:95:LEU:N	2.34	0.60	
40:A:497:A:N6	40:A:542:C:OP2	2.34	0.60	
40:A:1139:C:C4	40:A:1254:U:O4	2.54	0.60	
44:B:1616:A:N6	44:B:1646:U:C2	2.69	0.60	
40:A:241:C:H2'	40:A:242:A:H8	1.67	0.60	
40:A:769:U:H2'	40:A:770:G:H8	1.66	0.60	
40:A:571:A:N6	40:A:572:U:O4	2.34	0.60	
40:A:1398:G:N2	40:A:1398:G:OP2	2.32	0.60	
21:5:391:VAL:O	21:5:398:VAL:N	2.35	0.60	
40:A:256:A:H2	40:A:308:A:H61	1.49	0.60	
2:E:103:LYS:HA	2:E:122:LEU:HA	1.84	0.60	
40:A:118:C:H1'	40:A:248:G:N1	2.17	0.60	
40:A:1160:A:N6	40:A:1167:A:OP2	2.35	0.59	
40:A:391:C:N4	40:A:408:C:O2	2.35	0.59	
40:A:73:U:O4	40:A:85:A:N7	2.36	0.59	
40:A:478:A:H2'	40:A:479:G:H8	1.68	0.59	
40:A:1257:C:H2'	40:A:1258:C:H4	1.85	0.59	
40:A:523:U:O4	40:A:526:A:C6	2.55	0.58	
10:Q:193:ALA:HA	10:Q:224:MET:HA	1.85	0.58	
14:U:39:THR:HA	14:U:98:GLN:HA	1.84	0.58	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:169:ILE:HA	1:D:186:ALA:HB2	1.84	0.58
40:A:180:U:O2'	40:A:464:A:N1	2.37	0.58
40:A:130:G:C2	40:A:135:A:N6	2.72	0.58
40:A:603:A:N1	40:A:623:A:O2'	2.36	0.57
40:A:225:C:H2'	40:A:226:U:H6	1.70	0.57
40:A:53:A:N6	40:A:57:A:OP2	2.37	0.57
11:R:98:ASN:O	11:R:102:LEU:N	2.32	0.57
40:A:632:U:H2'	40:A:633:A:C8	2.40	0.57
2:E:110:TRP:HA	2:E:116:LYS:HA	1.86	0.57
10:Q:250:THR:O	10:Q:254:MET:N	2.36	0.57
13:T:99:ILE:O	13:T:103:LEU:CB	2.53	0.57
40:A:1359:A:H4'	40:A:1360:A:H5'	1.87	0.57
40:A:163:C:N4	40:A:166:A:OP1	2.38	0.56
40:A:802:A:N7	40:A:984:U:O4	2.38	0.56
2:E:134:SER:O	2:E:138:CYS:N	2.37	0.56
40:A:152:U:O2	40:A:1037:A:O2'	2.21	0.56
40:A:160:G:H2'	40:A:161:G:C8	2.39	0.56
40:A:105:A:H2'	40:A:106:G:C8	2.41	0.56
40:A:796:A:O2'	40:A:1485:C:OP2	2.23	0.56
44:B:1611:G:O6	44:B:1644:G:N2	2.22	0.56
40:A:160:G:H2'	40:A:161:G:H8	1.70	0.56
9:O:21:GLY:O	9:O:25:ARG:N	2.37	0.56
5:K:118:ARG:O	5:K:121:MET:N	2.40	0.55
40:A:517:C:O2'	49:J:104:THR:O	2.25	0.55
7:M:92:GLN:O	7:M:136:TYR:N	2.31	0.55
18:Z:35:LYS:N	40:A:433:A:HO2'	2.03	0.55
40:A:747:C:H4'	40:A:748:A:H5'	1.87	0.55
21:5:305:GLN:O	21:5:309:LEU:N	2.35	0.55
40:A:158:A:N6	40:A:1013:C:O2'	2.39	0.55
8:N:132:THR:HA	8:N:148:ASP:H	1.71	0.55
40:A:567:A:H2'	40:A:568:A:C8	2.42	0.55
2:E:203:TYR:HA	2:E:272:LYS:HA	1.88	0.55
40:A:526:A:O2'	40:A:543:A:N1	2.38	0.55
40:A:415:A:H2'	40:A:416:A:H8	1.71	0.55
40:A:1043:C:H2'	40:A:1044:A:C4	2.42	0.55
40:A:1454:U:N3	40:A:1463:A:H8	2.00	0.55
40:A:583:U:H2	40:A:584:C:H6	1.72	0.55
40:A:343:U:N3	40:A:344:A:N7	2.55	0.55
40:A:1040:C:H2	40:A:1041:A:H8	1.72	0.55
7:M:253:PHE:O	7:M:257:CYS:N	2.40	0.54
14:U:61:TYR:O	17:Y:63:GLY:N	2.40	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
40:A:1345:U:OP2	40:A:1347:C:N4	2.41	0.54
40:A:7:C:N3	40:A:128:A:O2'	2.34	0.54
46:W:53:ILE:HA	46:W:68:ALA:HA	1.90	0.54
40:A:774:A:H1'	40:A:775:U:C2	2.42	0.54
22:7:280:VAL:HA	22:7:299:GLY:HA3	1.89	0.54
40:A:583:U:H2'	40:A:584:C:C6	2.43	0.54
40:A:101:C:C4	40:A:102:A:N6	2.75	0.54
40:A:459:G:H2'	40:A:460:A:H8	1.72	0.54
16:X:207:THR:O	16:X:211:ALA:N	2.38	0.54
40:A:130:G:N2	40:A:135:A:N6	2.36	0.54
44:B:1642:G:H2'	44:B:1643:A:H8	1.72	0.54
40:A:998:A:H2'	40:A:999:A:H8	1.72	0.53
40:A:159:A:H2'	40:A:160:G:C8	2.42	0.53
40:A:237:A:N7	40:A:343:U:C2	2.76	0.53
40:A:1139:C:N3	40:A:1254:U:C4	2.77	0.53
3:F:67:GLU:O	3:F:191:ASP:N	2.40	0.53
13:T:48:SER:N	40:A:3:U:OP2	2.41	0.53
40:A:193:A:H2'	40:A:194:A:H8	1.73	0.53
40:A:1338:C:O2'	40:A:1381:A:N3	2.36	0.53
3:F:218:LEU:O	3:F:242:LEU:HA	2.09	0.53
21:5:208:THR:HA	21:5:224:GLY:O	2.08	0.53
40:A:1326:G:H2'	40:A:1327:A:H8	1.73	0.53
44:B:1642:G:H2'	44:B:1643:A:C8	2.44	0.53
40:A:5:A:H3'	40:A:6:A:H8	1.73	0.53
40:A:597:U:H2'	40:A:598:G:H8	1.72	0.53
40:A:113:U:H2'	40:A:114:A:C8	2.43	0.53
8:N:215:PHE:O	8:N:219:ALA:CB	2.57	0.53
40:A:241:C:H2'	40:A:242:A:C8	2.44	0.53
44:B:1609:U:O2	44:B:1616:A:N6	2.41	0.53
40:A:985:G:N2	40:A:989:C:O2	2.42	0.53
1:D:235:GLN:O	1:D:295:TYR:N	2.42	0.53
40:A:105:A:H2'	40:A:106:G:H8	1.73	0.53
40:A:390:A:N6	40:A:408:C:O2'	2.42	0.52
2:E:128:HIS:HA	2:E:192:PRO:HA	1.92	0.52
40:A:1155:G:H1'	40:A:1223:A:H1'	1.91	0.52
2:E:251:VAL:O	40:A:1435:A:O2'	2.27	0.52
44:B:1663:C:N4	44:B:1664:G:O6	2.42	0.52
40:A:97:G:H2'	40:A:98:G:C8	2.44	0.52
40:A:336:C:H2'	40:A:337:U:C6	2.44	0.52
22:7:167:VAL:H	22:7:183:VAL:HA	1.75	0.52
40:A:101:C:N4	40:A:102:A:N6	2.58	0.52



A 4 a 1		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
40:A:1059:U:H2'	40:A:1060:A:C8	2.45	0.52
40:A:79:C:H4'	40:A:80:G:H8	1.74	0.52
40:A:698:C:H2'	40:A:699:A:H8	1.75	0.52
40:A:1074:U:O2	40:A:1075:A:N6	2.37	0.52
46:W:121:PRO:HA	47:6:50:LYS:HA	1.91	0.52
40:A:615:U:H2'	40:A:616:A:H8	1.75	0.51
40:A:459:G:H2'	40:A:460:A:C8	2.46	0.51
2:E:106:MET:CB	2:E:119:VAL:O	2.58	0.51
16:X:10:LEU:O	16:X:14:LEU:N	2.40	0.51
40:A:345:G:N2	40:A:370:G:N3	2.58	0.51
14:U:28:LEU:HA	14:U:42:PHE:HA	1.91	0.51
40:A:647:G:H2'	40:A:648:A:C8	2.43	0.51
40:A:1260:U:H2'	40:A:1261:A:H8	1.75	0.51
40:A:309:U:H2'	40:A:310:A:H8	1.75	0.51
40:A:311:G:H2'	40:A:312:G:H8	1.75	0.51
40:A:841:C:H3'	40:A:842:A:H8	1.76	0.51
8:N:226:ILE:O	8:N:230:LEU:N	2.44	0.51
45:P:132:ALA:HB2	45:P:164:MET:HA	1.93	0.51
7:M:236:LEU:O	7:M:240:TYR:N	2.40	0.51
11:R:82:LYS:O	11:R:85:ALA:N	2.43	0.51
18:Z:103:ILE:O	18:Z:107:ASN:N	2.40	0.51
40:A:751:G:H2'	40:A:752:U:O4'	2.11	0.51
40:A:1380:U:N3	40:A:1383:A:OP2	2.40	0.51
9:O:110:ILE:H	9:O:121:ALA:HA	1.76	0.51
14:U:41:GLN:HA	14:U:96:TYR:HA	1.92	0.51
40:A:607:U:H2'	40:A:608:A:H8	1.76	0.51
40:A:801:G:N2	40:A:985:G:OP2	2.44	0.51
45:P:148:THR:O	45:P:152:ALA:N	2.41	0.50
40:A:618:A:H2'	40:A:619:G:H8	1.77	0.50
40:A:1488:A:H2'	40:A:1489:A:C8	2.46	0.50
40:A:1491:G:N3	40:A:1492:C:O2'	2.43	0.50
12:S:160:VAL:HA	12:S:193:LEU:HA	1.94	0.50
20:2:56:SER:HA	40:A:669:G:H5"	1.92	0.50
12:S:98:VAL:HA	12:S:107:LYS:HA	1.93	0.50
40:A:615:U:H2'	40:A:616:A:C8	2.47	0.50
8:N:96:TYR:HA	8:N:153:PRO:HA	1.94	0.50
40:A:12:C:H1'	40:A:106:G:N2	2.27	0.50
19:0:139:ARG:HA	40:A:651:A:C8	2.47	0.50
40:A:101:C:H2'	40:A:102:A:C8	2.47	0.50
40:A:227:A:H2'	40:A:228:A:H8	1.76	0.50
6:L:123:ILE:O	6:L:145:VAL:N	2.42	0.49



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
10:Q:119:VAL:O	10:Q:132:GLN:HA	2.12	0.49
13:T:102:ALA:O	13:T:106:LEU:CB	2.61	0.49
44:B:1607:U:O2	44:B:1664:G:N2	2.36	0.49
1:D:126:VAL:HA	1:D:142:VAL:HA	1.95	0.49
40:A:220:C:H2'	40:A:221:A:H8	1.76	0.49
40:A:1176:G:H21	40:A:1225:U:H3	1.60	0.49
8:N:86:ASN:O	8:N:192:ARG:N	2.45	0.49
40:A:169:C:H2'	40:A:170:C:C6	2.48	0.49
10:Q:147:ALA:O	10:Q:166:LEU:N	2.43	0.49
40:A:501:U:C2	40:A:503:G:H4'	2.48	0.49
3:F:262:THR:O	3:F:266:VAL:N	2.44	0.49
40:A:53:A:H5"	40:A:54:A:H4'	1.95	0.49
40:A:618:A:H2'	40:A:619:G:C8	2.47	0.49
44:B:1622:A:H2'	44:B:1623:G:C8	2.48	0.49
40:A:430:C:H2'	40:A:431:C:C6	2.47	0.49
40:A:1481:A:N1	40:A:1493:G:O2'	2.36	0.49
40:A:12:C:H1'	40:A:106:G:H21	1.78	0.49
40:A:193:A:H2'	40:A:194:A:C8	2.48	0.49
40:A:991:U:H2'	40:A:992:A:C8	2.40	0.49
40:A:1371:U:O2'	40:A:1372:U:O5'	2.27	0.49
40:A:424:G:H2'	40:A:425:U:C5	2.48	0.49
40:A:1029:C:H2'	40:A:1030:G:H8	1.78	0.49
2:E:158:ALA:O	2:E:162:LEU:N	2.42	0.48
40:A:309:U:H2'	40:A:310:A:C8	2.48	0.48
40:A:70:A:OP2	40:A:71:A:O2'	2.28	0.48
40:A:1330:A:H2'	40:A:1331:G:C8	2.48	0.48
40:A:1364:U:OP2	40:A:1383:A:O2'	2.31	0.48
46:W:58:GLY:N	46:W:97:VAL:O	2.44	0.48
15:V:186:THR:N	17:Y:92:ASN:O	2.45	0.48
46:W:103:VAL:HA	46:W:127:TYR:HA	1.94	0.48
46:W:142:PHE:HA	47:6:344:PHE:H	1.78	0.48
40:A:374:A:H2'	40:A:375:A:C8	2.48	0.48
40:A:402:A:H2'	40:A:403:A:C8	2.49	0.48
40:A:85:A:H2'	40:A:86:A:C8	2.49	0.48
40:A:348:G:H2'	40:A:349:G:H8	1.79	0.48
19:0:166:SER:O	19:0:170:GLN:N	2.47	0.48
21:5:351:VAL:HA	21:5:381:LEU:HA	1.95	0.48
40:A:249:C:H42	40:A:327:C:H4'	1.79	0.48
40:A:381:A:H2'	40:A:382:A:H8	1.79	0.48
40:A:450:G:H2'	40:A:451:G:C8	2.48	0.48
40:A:605:U:H2'	40:A:606:C:H6	1.79	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
40:A:1279:C:H2'	40:A:1280:U:C4	2.48	0.48
3:F:84:PRO:HA	3:F:88:ALA:HB3	1.95	0.48
40:A:478:A:H2'	40:A:479:G:C8	2.49	0.48
40:A:637:U:H2'	40:A:638:A:C8	2.49	0.48
40:A:1488:A:H2'	40:A:1489:A:H8	1.79	0.48
40:A:792:A:H2'	40:A:793:A:H8	1.79	0.47
45:P:71:PHE:N	46:W:105:VAL:O	2.45	0.47
40:A:337:U:H2'	40:A:338:G:C8	2.49	0.47
40:A:371:U:H2'	40:A:372:U:H6	1.78	0.47
40:A:656:C:H2'	40:A:657:U:H6	1.79	0.47
7:M:154:ILE:N	7:M:173:VAL:O	2.47	0.47
40:A:514:A:H2'	40:A:515:G:H8	1.79	0.47
40:A:626:U:H2'	40:A:627:A:C5	2.49	0.47
40:A:1332:G:H2'	40:A:1333:A:C8	2.50	0.47
7:M:167:ILE:O	7:M:172:GLY:N	2.46	0.47
40:A:101:C:N3	40:A:102:A:C6	2.82	0.47
1:D:129:VAL:CB	1:D:139:ILE:O	2.63	0.47
15:V:135:TRP:HA	15:V:145:ARG:HA	1.96	0.47
40:A:377:U:H3'	40:A:378:U:H6	1.79	0.47
10:Q:276:SER:O	10:Q:280:ALA:N	2.46	0.47
18:Z:74:SER:N	40:A:469:U:OP2	2.47	0.47
40:A:208:U:O4	40:A:227:A:N6	2.48	0.47
40:A:783:G:O6	40:A:1002:A:N6	2.48	0.47
40:A:1029:C:H2'	40:A:1030:G:C8	2.49	0.47
40:A:1288:A:H3'	40:A:1289:G:H8	1.79	0.47
44:B:1665:C:H2'	44:B:1666:U:C6	2.49	0.47
8:N:87:PHE:HA	8:N:191:SER:HA	1.97	0.47
16:X:149:PRO:O	16:X:153:LEU:N	2.48	0.47
22:7:180:CYS:HA	22:7:297:PHE:O	2.14	0.47
40:A:998:A:H2'	40:A:999:A:C8	2.49	0.47
40:A:1139:C:N3	40:A:1253:G:C6	2.83	0.47
40:A:1343:G:N2	40:A:1354:U:O2	2.33	0.47
45:P:67:TRP:N	46:W:78:GLY:O	2.47	0.47
3:F:63:GLN:HA	3:F:81:ASP:HA	1.97	0.47
40:A:547:C:OP1	48:I:128:ASN:N	2.47	0.47
40:A:769:U:H2'	40:A:770:G:C8	2.46	0.47
40:A:1019:C:H2'	40:A:1020:G:C8	2.50	0.47
7:M:103:TYR:O	7:M:107:LEU:N	2.34	0.47
16:X:86:ILE:O	16:X:104:VAL:HA	2.15	0.47
21:5:333:ALA:HB1	21:5:363:ASP:HA	1.97	0.47
1:D:145:GLY:H	21:5:259:ILE:HA	1.80	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
45:P:50:ARG:H	47:6:222:ASP:HA	1.80	0.47
2:E:212:GLY:N	40:A:1548:A:OP1	2.47	0.46
5:K:29:GLY:HA3	40:A:569:A:O3'	2.15	0.46
40:A:332:G:C2	40:A:1257:C:N3	2.83	0.46
40:A:993:C:H2'	40:A:994:U:C6	2.50	0.46
40:A:1036:A:O2'	40:A:1037:A:H5'	2.14	0.46
40:A:1139:C:N3	40:A:1254:U:C5	2.83	0.46
13:T:97:MET:O	13:T:142:ILE:N	2.38	0.46
15:V:76:VAL:HA	15:V:87:VAL:O	2.14	0.46
21:5:384:GLN:N	21:5:404:VAL:O	2.46	0.46
40:A:240:C:H2'	40:A:241:C:C6	2.50	0.46
40:A:786:U:H2'	40:A:787:A:H8	1.80	0.46
21:5:352:PHE:O	21:5:380:GLN:N	2.45	0.46
40:A:1450:C:H42	40:A:1466:A:H61	1.64	0.46
13:T:91:ALA:O	13:T:95:ARG:N	2.48	0.46
40:A:220:C:H2'	40:A:221:A:C8	2.51	0.46
40:A:224:G:H2'	40:A:225:C:C6	2.50	0.46
40:A:1306:G:O2'	40:A:1307:G:H5'	2.15	0.46
40:A:1371:U:H6	40:A:1371:U:H5'	1.80	0.46
15:V:76:VAL:HA	15:V:88:VAL:HA	1.97	0.46
40:A:467:C:H2'	40:A:468:U:H6	1.81	0.46
40:A:1078:A:H2'	40:A:1079:A:H8	1.81	0.46
40:A:1332:G:H2'	40:A:1333:A:H8	1.81	0.46
40:A:339:G:C8	40:A:340:U:H2'	2.50	0.46
40:A:510:A:O2'	40:A:536:C:O3'	2.33	0.46
48:I:99:CYS:O	48:I:151:ASN:HA	2.16	0.46
40:A:1065:G:N2	40:A:1254:U:O2	2.31	0.46
21:5:59:THR:HA	21:5:71:ALA:HB3	1.97	0.46
40:A:11:G:N1	40:A:102:A:C2	2.84	0.46
40:A:432:A:N6	40:A:450:G:O6	2.49	0.46
40:A:213:G:H2'	40:A:214:G:H8	1.80	0.46
40:A:332:G:C6	40:A:1257:C:C2	3.03	0.46
40:A:586:U:H2'	40:A:587:C:C6	2.51	0.46
40:A:1259:C:H2'	40:A:1260:U:C6	2.51	0.46
1:D:193:ILE:N	1:D:214:GLY:O	2.44	0.46
6:L:60:VAL:HA	6:L:73:ILE:HA	1.98	0.46
13:T:155:ARG:O	13:T:167:MET:CB	2.64	0.45
40:A:348:G:H2'	40:A:349:G:C8	2.51	0.45
2:E:274:TRP:N	2:E:284:TYR:O	2.42	0.45
40:A:125:A:H2'	40:A:126:A:C4	2.51	0.45
40:A:495:C:H1'	40:A:546:A:H61	1.81	0.45



	lio uo puge	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
44:B:1616:A:C6	44:B:1646:U:N3	2.84	0.45	
40:A:227:A:H2'	40:A:228:A:C8	2.50	0.45	
40:A:450:G:H2'	40:A:451:G:H8	1.81	0.45	
40:A:644:C:H2'	40:A:645:A:C8	2.52	0.45	
1:D:196:VAL:N	1:D:206:TYR:O	2.46	0.45	
40:A:97:G:H2'	40:A:98:G:H8	1.80	0.45	
40:A:521:A:N6	40:A:527:G:OP2	2.38	0.45	
40:A:1078:A:H2'	40:A:1079:A:C8	2.51	0.45	
40:A:100:G:H2'	40:A:101:C:H6	1.81	0.45	
40:A:1379:U:C2	40:A:1383:A:N7	2.85	0.45	
40:A:566:C:O2'	40:A:567:A:O5'	2.31	0.45	
40:A:631:U:H2'	40:A:632:U:C6	2.52	0.45	
40:A:748:A:H2'	40:A:749:C:C6	2.52	0.45	
40:A:1138:U:H1'	40:A:1251:A:H2'	1.99	0.45	
40:A:1470:A:H2'	40:A:1471:A:C8	2.51	0.45	
12:S:146:LYS:HA	12:S:147:PRO:HA	1.78	0.45	
40:A:205:C:H2'	40:A:206:U:C6	2.52	0.45	
40:A:594:A:H2'	40:A:595:A:C8	2.52	0.45	
40:A:696:G:H2'	40:A:697:A:C8	2.52	0.45	
40:A:699:A:H2'	40:A:700:A:H8	1.82	0.45	
40:A:786:U:H2'	40:A:787:A:C8	2.51	0.45	
40:A:1454:U:OP2	40:A:1462:G:N1	2.49	0.45	
40:A:164:U:H2'	40:A:165:A:C8	2.52	0.45	
40:A:225:C:H2'	40:A:226:U:C6	2.51	0.45	
45:P:66:GLY:HA3	46:W:81:VAL:H	1.81	0.45	
1:D:230:SER:N	40:A:849:G:O6	2.50	0.45	
40:A:82:U:H2'	40:A:83:A:C8	2.52	0.45	
40:A:242:A:H2'	40:A:243:G:H8	1.82	0.45	
40:A:429:U:H2'	40:A:430:C:C6	2.51	0.45	
12:S:175:ARG:O	12:S:180:PHE:CB	2.65	0.45	
40:A:21:C:H2'	40:A:22:A:N3	2.32	0.45	
40:A:415:A:H2'	40:A:416:A:C8	2.51	0.45	
40:A:999:A:H2'	40:A:1000:C:C6	2.53	0.45	
40:A:313:U:O2	40:A:318:G:O2'	2.35	0.44	
40:A:1026:A:N7	40:A:1029:C:N4	2.65	0.44	
1:D:196:VAL:O	1:D:206:TYR:N	2.50	0.44	
40:A:457:A:H2'	40:A:458:G:H8	1.82	0.44	
40:A:616:A:H2'	40:A:617:U:C6	2.52	0.44	
40:A:1475:A:H2'	40:A:1476:G:C8	2.52	0.44	
2:E:216:GLN:O	2:E:258:PRO:HA	2.16	0.44	
40:A:1454:U:C4	40:A:1463:A:C8	3.03	0.44	



Atom-1	Atom-2	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
40:A:1481:A:H61	40:A:1493:G:H1'	1.82	0.44	
47:6:274:LYS:N	47:6:312:THR:O	2.47	0.44	
2:E:158:ALA:HB3	2:E:161:ILE:H	1.83	0.44	
3:F:206:LEU:O	3:F:210:ARG:N	2.49	0.44	
40:A:648:A:H2'	40:A:649:A:C8	2.52	0.44	
40:A:850:C:C2	40:A:858:G:N2	2.78	0.44	
1:D:181:ALA:HA	1:D:243:THR:HA	2.00	0.44	
40:A:11:G:C2	40:A:102:A:C2	3.05	0.44	
40:A:51:C:N4	40:A:60:U:C4	2.84	0.44	
40:A:696:G:H2'	40:A:697:A:H8	1.83	0.44	
40:A:258:A:H2'	40:A:259:A:C8	2.53	0.44	
40:A:430:C:H2'	40:A:431:C:H6	1.83	0.44	
8:N:117:ASN:O	8:N:166:ARG:N	2.51	0.44	
22:7:255:HIS:O	22:7:261:ILE:HA	2.17	0.44	
40:A:161:G:N1	40:A:162:A:N3	2.65	0.44	
40:A:993:C:H2'	40:A:994:U:H6	1.82	0.44	
8:N:215:PHE:O	8:N:219:ALA:HB3	2.18	0.44	
20:2:66:TRP:H	40:A:32:A:P	2.41	0.44	
40:A:1139:C:N4	40:A:1253:G:O6	2.50	0.44	
40:A:1389:A:OP1	40:A:1391:G:O2'	2.24	0.44	
40:A:1554:G:H2'	40:A:1555:G:H8	1.83	0.44	
4:H:79:VAL:HA	16:X:89:GLN:H	1.83	0.44	
40:A:460:A:H2'	40:A:463:A:H61	1.82	0.44	
40:A:1446:C:H2'	40:A:1447:C:C6	2.52	0.44	
2:E:208:ALA:O	2:E:265:TYR:HA	2.18	0.43	
6:L:119:ILE:H	6:L:141:ALA:HA	1.83	0.43	
40:A:238:A:N6	40:A:342:A:N6	2.37	0.43	
40:A:672:U:N3	40:A:701:U:O4	2.51	0.43	
40:A:1040:C:H2'	40:A:1041:A:C8	2.51	0.43	
40:A:1197:C:H2'	40:A:1198:C:O4'	2.18	0.43	
22:7:218:THR:HA	22:7:255:HIS:HA	1.99	0.43	
23:9:29:SER:O	23:9:32:GLY:N	2.50	0.43	
40:A:1447:C:H2'	40:A:1448:U:C6	2.53	0.43	
2:E:99:LEU:CB	2:E:299:VAL:O	2.66	0.43	
4:H:94:LEU:O	4:H:113:SER:HA	2.18	0.43	
15:V:93:THR:HA	15:V:112:GLU:HA	2.00	0.43	
16:X:116:SER:O	16:X:120:ASP:CA	2.67	0.43	
40:A:424:G:H2'	40:A:425:U:C6	2.53	0.43	
6:L:39:ARG:N	6:L:103:ASN:O	2.50	0.43	
4:H:133:SER:O	4:H:137:LYS:N	2.49	0.43	
17:Y:155:LEU:HA	17:Y:159:GLY:HA2	2.00	0.43	



	puge	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
40:A:71:A:H4'	40:A:72:G:H4'	2.00	0.43	
40:A:224:G:H2'	40:A:225:C:H6	1.84	0.43	
40:A:699:A:H2'	40:A:700:A:C8	2.53	0.43	
40:A:792:A:H2'	40:A:793:A:C8	2.53	0.43	
40:A:994:U:H2'	40:A:995:U:C6	2.53	0.43	
3:F:222:THR:O	3:F:226:MET:N	2.52	0.43	
40:A:213:G:H2'	40:A:214:G:C8	2.53	0.43	
40:A:228:A:H2'	40:A:229:G:C8	2.53	0.43	
40:A:242:A:H2'	40:A:243:G:C8	2.54	0.43	
40:A:785:U:H2'	40:A:786:U:H6	1.83	0.43	
4:H:97:ILE:HA	4:H:111:LEU:HA	2.00	0.43	
5:K:94:GLN:O	5:K:98:ARG:CB	2.66	0.43	
40:A:512:G:H1'	40:A:529:A:H2'	2.01	0.43	
40:A:862:U:H2'	40:A:863:A:H8	1.82	0.43	
48:I:171:VAL:O	48:I:173:PHE:N	2.51	0.43	
40:A:605:U:H2'	40:A:606:C:C6	2.54	0.43	
1:D:83:GLY:HA2	1:D:97:GLY:HA3	2.01	0.43	
10:Q:137:CYS:HA	10:Q:151:LEU:HA	2.00	0.43	
40:A:1081:G:H2'	40:A:1082:C:C6 2.54		0.43	
40:A:47:U:H2'	40:A:48:A:C8	40:A:48:A:C8 2.54		
40:A:413:U:H2'	40:A:414:A:C8	2.54	0.43	
49:J:104:THR:HA	49:J:105:GLY:HA2	1.58	0.43	
1:D:190:GLY:N	1:D:216:LEU:O	2.49	0.42	
40:A:43:A:H2'	40:A:44:C:C2	2.54	0.42	
40:A:741:U:H2'	40:A:742:A:H8	1.84	0.42	
40:A:1493:G:H2'	40:A:1494:C:H6	1.84	0.42	
40:A:1080:U:H3'	40:A:1081:G:H8	1.84	0.42	
40:A:1474:A:H2'	40:A:1475:A:C8	2.54	0.42	
40:A:467:C:H2'	40:A:468:U:C6	2.54	0.42	
1:D:155:GLU:N	1:D:246:ARG:O	2.53	0.42	
40:A:115:C:H2'	40:A:116:C:C6	2.55	0.42	
40:A:1076:U:H2'	40:A:1077:U:C6	2.54	0.42	
40:A:1476:G:H2'	40:A:1477:G:O4'	2.19	0.42	
5:K:78:SER:HA	5:K:88:ARG:O	2.19	0.42	
40:A:381:A:H2'	40:A:382:A:C8	2.54	0.42	
40:A:431:C:N3	40:A:451:G:N1	2.68	0.42	
40:A:847:U:H2'	40:A:848:A:C8	2.55	0.42	
40:A:1307:G:H4'	40:A:1308:U:H5"	2.01	0.42	
43:1:213:ILE:N	43:1:353:VAL:O	2.43	0.42	
1:D:192:LEU:O	1:D:245:GLY:N	2.44	0.42	
8:N:143:GLY:HA2	40:A:437:G:H4'	2.00	0.42	



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
40:A:610:C:H42	40:A:615:U:H3	1.65	0.42		
40:A:616:A:H2'	40:A:617:U:H6	1.83	0.42		
40:A:768:A:H2'	40:A:769:U:C6	2.54	0.42		
15:V:198:VAL:O	15:V:202:MET:N	2.42	0.42		
40:A:170:C:H2'	40:A:171:U:C6	2.54	0.42		
40:A:258:A:H2'	40:A:259:A:H8	1.84	0.42		
40:A:326:C:H2'	40:A:327:C:C6	2.54	0.42		
40:A:1260:U:H2'	40:A:1261:A:C8	2.53	0.42		
44:B:1609:U:O2'	44:B:1645:A:N3	5:A:N3 2.43			
6:L:45:ALA:O	6:L:49:SER:N	2.52	0.42		
40:A:259:A:H2'	40:A:260:C:C6	2.55	0.42		
40:A:1125:U:H2'	40:A:1126:G:H8	1.85	0.42		
40:A:1289:G:N2	40:A:1296:U:O4	2.52	0.42		
44:B:1661:A:H2'	44:B:1663:C:C6	2.55	0.42		
46:W:54:LYS:N	46:W:67:ILE:O	2.53	0.42		
40:A:337:U:H2'	40:A:338:G:H8	1.84	0.42		
40:A:521:A:N6	40:A:528:A:OP2	2.53	0.42		
40:A:523:U:O4	40:A:526:A:N1	2.51	0.42		
40:A:1436:C:H2'	40:A:1437:U:C6	2.55	0.42		
40:A:1467:G:H2'	40:A:1468:A:C8	2.55	0.42		
40:A:1386:C:H2'	40:A:1387:C:C6	2.54	0.42		
40:A:1448:U:H2'	40:A:1449:C:C6	2.55	0.42		
2:E:151:THR:HA	2:E:173:LYS:HA	2.02	0.41		
40:A:252:C:H2'	40:A:253:C:H6	1.85	0.41		
40:A:1252:A:H2'	40:A:1253:G:H8	1.84	0.41		
40:A:29:C:H5"	40:A:30:U:H5	1.85	0.41		
40:A:533:G:H21	40:A:538:A:H62	1.67	0.41		
40:A:748:A:H2'	40:A:749:C:H6	1.85	0.41		
40:A:1454:U:C4	40:A:1463:A:H8	2.38	0.41		
1:D:85:ARG:HA	1:D:91:ILE:HA	2.01	0.41		
23:9:93:SER:O	23:9:97:ALA:HB2	2.20	0.41		
40:A:119:A:H2'	40:A:120:A:C8	2.55	0.41		
40:A:1374:A:H2'	40:A:1375:A:H8	1.85	0.41		
40:A:201:A:N6	40:A:230:A:H2'	2.35	0.41		
40:A:402:A:H2'	40:A:403:A:H8	1.86	0.41		
40:A:530:A:H2'	40:A:531:G:C8	2.55	0.41		
1:D:121:PRO:HA	1:D:165:ASN:O	2.20	0.41		
10:Q:231:LYS:O	10:Q:233:TRP:N	2.52	0.41		
40:A:317:G:H2'	40:A:318:G:C8	2.55	0.41		
12:S:97:ALA:HA	12:S:135:LEU:O	2.20	0.41		
40:A:212:A:H4'	40:A:213:G:H5'	2.01	0.41		



Atom 1	Atom 2	Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
40:A:620:A:H2'	40:A:621:A:C8	2.56	0.41	
40:A:1140:G:H2'	40:A:1141:G:C8	2.56	0.41	
44:B:1664:G:H2'	44:B:1665:C:C6	2.56	0.41	
3:F:144:PRO:HA	3:F:150:GLY:H	1.86	0.41	
40:A:656:C:H2'	40:A:657:U:C6	2.56	0.41	
40:A:1495:C:H2'	40:A:1496:U:C6	2.56	0.41	
40:A:411:U:H2'	40:A:412:G:C8	2.56	0.41	
40:A:862:U:H2'	40:A:863:A:C8	2.55	0.41	
40:A:1020:G:N1	40:A:1030:G:C6	2.89	0.41	
40:A:1070:A:H2'	40:A:1071:A:C8	2.56	0.41	
40:A:1083:A:H3'	40:A:1084:A:H8	1.86	0.41	
40:A:1249:A:O2'	40:A:1250:C:O4'	2.38	0.41	
40:A:1254:U:H2'	40:A:1255:U:C6	2.55	0.41	
44:B:1615:A:N1	44:B:1621:A:O2'	2.37	0.41	
2:E:146:SER:HA	2:E:178:ILE:HA	2.03	0.41	
40:A:1:G:O2'	40:A:2:C:O4'	2.38	0.41	
40:A:154:U:O2'	40:A:155:A:O5'	2.37	0.41	
40:A:425:U:H2'	40:A:426:U:C6	2.56	0.41	
40:A:570:C:O2'	40:A:572:U:OP2	2.38	0.41	
40:A:586:U:H2'	40:A:587:C:H6	1.86	0.41	
40:A:990:U:H2'	40:A:991:U:C6	2.56	0.41	
40:A:1006:A:H2'	40:A:1007:A:C8	2.56	0.41	
40:A:1494:C:H2'	40:A:1495:C:H6	1.85	0.41	
44:B:1604:G:H2'	44:B:1605:A:C8	2.56	0.41	
21:5:233:LYS:HA	21:5:285:TYR:HA	2.02	0.41	
40:A:366:C:H4'	40:A:367:U:C5	2.56	0.41	
40:A:741:U:H2'	40:A:742:A:C8	2.56	0.41	
40:A:1076:U:H2'	40:A:1077:U:H6	1.86	0.41	
40:A:1263:G:H2'	40:A:1264:G:C8	2.56	0.41	
40:A:1493:G:H2'	40:A:1494:C:C6	2.56	0.41	
40:A:1510:A:H2'	40:A:1511:U:O4'	2.21	0.41	
40:A:1340:G:H1	40:A:1357:U:H3	1.70	0.40	
40:A:83:A:H2'	40:A:84:G:C8	2.57	0.40	
40:A:332:G:H1'	40:A:333:A:C5	2.56	0.40	
40:A:345:G:H21	40:A:370:G:H1'	1.86	0.40	
40:A:421:A:H2'	40:A:422:C:C6	2.56	0.40	
10:Q:150:ILE:HA	10:Q:163:CYS:HA	2.03	0.40	
21:5:291:LEU:O	21:5:344:SER:HA	2.22	0.40	
40:A:662:C:N3	40:A:774:A:C6	2.89	0.40	
1:D:183:PRO:HA	1:D:241:VAL:HA	2.03	0.40	
40:A:729:A:H2'	40:A:730:C:C6	2.57	0.40	



Atom-1	Atom-1 Atom-2		Clash overlap (Å)
40:A:1446:C:H2'	40:A:1447:C:H6	1.85	0.40
7:M:145:ALA:HA	47:6:379:ILE:HA	2.01	0.40
14:U:67:ALA:O	14:U:97:VAL:HA	2.21	0.40
40:A:1445:U:H2'	40:A:1446:C:C6	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	D	216/305~(71%)	204 (94%)	12 (6%)	0	100	100
2	Е	281/348~(81%)	249 (89%)	32 (11%)	0	100	100
3	F	248/311~(80%)	221~(89%)	27 (11%)	0	100	100
4	Н	93/267~(35%)	84 (90%)	9 (10%)	0	100	100
5	K	175/178~(98%)	154 (88%)	21 (12%)	0	100	100
6	L	113/145~(78%)	107~(95%)	6 (5%)	0	100	100
7	М	253/296~(86%)	226 (89%)	27 (11%)	0	100	100
8	Ν	203/251~(81%)	195 (96%)	8 (4%)	0	100	100
9	Ο	150/175~(86%)	138 (92%)	12 (8%)	0	100	100
10	Q	215/292~(74%)	196 (91%)	19 (9%)	0	100	100
11	R	138/149~(93%)	126 (91%)	12 (9%)	0	100	100
12	S	154/205~(75%)	141 (92%)	13 (8%)	0	100	100
13	Т	155/206~(75%)	143 (92%)	12 (8%)	0	100	100
14	U	135/153~(88%)	123 (91%)	12 (9%)	0	100	100
15	V	188/216~(87%)	176 (94%)	12 (6%)	0	100	100
16	Х	241/256~(94%)	227 (94%)	14 (6%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
17	Y	174/250~(70%)	161 (92%)	13 (8%)	0	100	100
18	Z	118/161~(73%)	107 (91%)	11 (9%)	0	100	100
19	0	106/188~(56%)	100 (94%)	6~(6%)	0	100	100
20	2	41/92~(45%)	36~(88%)	5 (12%)	0	100	100
21	5	383/423~(90%)	361 (94%)	21~(6%)	1 (0%)	41	76
22	7	285/338~(84%)	252 (88%)	33 (12%)	0	100	100
23	9	113/137~(82%)	99~(88%)	14 (12%)	0	100	100
24	a	78/142~(55%)	67~(86%)	11 (14%)	0	100	100
25	b	146/215~(68%)	127 (87%)	19 (13%)	0	100	100
26	с	271/332~(82%)	256 (94%)	15 (6%)	0	100	100
27	d	203/306~(66%)	189 (93%)	14 (7%)	0	100	100
28	g	127/166~(76%)	120 (94%)	7 (6%)	0	100	100
29	h	96/158~(61%)	92 (96%)	4 (4%)	0	100	100
30	i	95/128 (74%)	83 (87%)	12 (13%)	0	100	100
31	j	83/123~(68%)	78 (94%)	5 (6%)	0	100	100
32	0	77/102~(76%)	71 (92%)	6 (8%)	0	100	100
33	р	101/206~(49%)	93~(92%)	7 (7%)	1 (1%)	15	54
34	q	97/222~(44%)	93~(96%)	4 (4%)	0	100	100
35	r	140/196~(71%)	129 (92%)	11 (8%)	0	100	100
36	s	366/439~(83%)	341 (93%)	25 (7%)	0	100	100
37	u	109/234~(47%)	100 (92%)	9 (8%)	0	100	100
38	v	67/70~(96%)	64 (96%)	3 (4%)	0	100	100
39	W	77/156~(49%)	73~(95%)	4 (5%)	0	100	100
41	х	370/540~(68%)	351 (95%)	16 (4%)	3 (1%)	19	60
42	У	329/387~(85%)	276 (84%)	49 (15%)	4 (1%)	13	49
43	1	251/420~(60%)	239 (95%)	12 (5%)	0	100	100
43	Z	$\overline{245/420}~(58\%)$	233~(95%)	12 (5%)	0	100	100
45	Р	129/180~(72%)	124 (96%)	4 (3%)	1 (1%)	19	60
46	W	96/148~(65%)	92 (96%)	2 (2%)	2(2%)	7	36
47	6	$\overline{313/380}~(82\%)$	286 (91%)	23 (7%)	4 (1%)	12	48
48	Ι	$\overline{154/261~(59\%)}$	145 (94%)	8 (5%)	1 (1%)	25	65



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
49	J	138/192~(72%)	129~(94%)	8~(6%)	1 (1%)	22 62
50	k	82/112~(73%)	73~(89%)	5~(6%)	4 (5%)	2 20
51	1	21/138~(15%)	21 (100%)	0	0	100 100
All	All	8439/11715 (72%)	7771 (92%)	646 (8%)	22~(0%)	44 76

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	Х	201	ILE
41	Х	347	PRO
42	у	75	SER
47	6	373	HIS
50	k	62	PRO
33	р	142	TYR
42	у	126	LYS
46	W	72	HIS
21	5	216	GLU
42	у	147	LEU
42	у	249	THR
46	W	127	TYR
49	J	70	ILE
50	k	73	ARG
41	Х	397	SER
45	Р	177	ILE
47	6	351	HIS
47	6	375	PRO
48	Ι	61	HIS
50	k	37	VAL
50	k	18	VAL
47	6	288	SER

### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
40	А	1183/1559~(75%)	457~(38%)	20 (1%)



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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	В	51/69~(73%)	18 (35%)	1 (1%)
All	All	1234/1628~(75%)	475 (38%)	21 (1%)

All (475) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
40	А	2	С
40	А	5	А
40	А	6	А
40	А	8	С
40	А	9	U
40	А	10	А
40	А	11	G
40	А	12	С
40	А	14	С
40	А	15	С
40	А	19	С
40	А	22	A
40	А	23	С
40	А	24	U
40	А	29	С
40	А	30	U
40	А	31	U
40	А	32	А
40	А	34	U
40	А	36	С
40	А	37	С
40	А	38	А
40	А	43	А
40	А	44	С
40	А	45	С
40	А	46	U
40	А	47	U
40	А	49	G
40	А	50	С
40	А	52	A
40	А	54	A
40	А	55	С
40	А	57	A
40	А	59	U
40	А	61	A
40	А	68	U



Mol	Chain	Res	Type
40	А	71	А
40	А	73	U
40	А	75	U
40	А	77	G
40	А	78	G
40	А	80	G
40	А	81	А
40	А	99	С
40	А	100	G
40	А	104	U
40	А	105	А
40	А	107	А
40	А	108	U
40	A	109	A
40	А	110	U
40	A	111	A
40	А	112	G
40	А	119	А
40	А	121	G
40	А	123	G
40	А	124	А
40	А	126	А
40	А	133	А
40	А	134	А
40	А	136	U
40	А	142	С
40	А	143	С
40	А	144	А
40	А	149	U
40	А	150	А
40	А	151	А
40	A	152	U
40	А	153	А
40	A	154	U
40	A	155	A
40	A	156	G
40	А	157	С
40	A	158	A
40	А	162	А
40	A	163	С
40	A	167	С
40	А	169	С



Mol	Chain	Res	Type
40	А	170	С
40	А	173	U
40	А	174	А
40	А	175	С
40	А	177	U
40	А	178	U
40	А	179	С
40	А	180	U
40	А	187	U
40	А	192	U
40	А	195	С
40	А	197	А
40	А	198	G
40	A	199	А
40	А	200	А
40	A	201	А
40	А	202	U
40	А	204	А
40	А	205	С
40	А	208	U
40	А	210	С
40	А	212	А
40	А	213	G
40	А	216	G
40	А	217	А
40	А	218	G
40	А	222	А
40	А	223	А
40	A	231	С
40	A	232	С
40	А	233	С
40	A	237	А
40	А	239	A
40	А	244	А
40	A	247	А
40	А	248	G
40	А	303	G
40	A	305	U
40	А	315	G
40	A	316	A
40	А	317	G
40	А	322	С



Mol	Chain	Res	Type
40	А	324	А
40	А	325	А
40	А	328	U
40	А	329	А
40	А	330	С
40	А	332	G
40	А	333	А
40	А	340	U
40	А	341	G
40	А	343	U
40	А	345	G
40	А	346	С
40	А	351	U
40	А	352	G
40	А	358	G
40	А	360	U
40	А	361	А
40	А	366	С
40	А	367	U
40	А	369	А
40	А	374	А
40	А	377	U
40	А	378	U
40	А	379	U
40	А	383	U
40	А	385	U
40	А	386	G
40	А	389	С
40	А	390	А
40	А	391	С
40	А	395	A
40	А	404	A
40	А	409	С
40	А	413	U
40	А	414	A
40	А	415	A
40	А	416	A
40	А	417	U
40	А	418	U
40	А	420	A
40	А	422	С
40	А	423	U



Mol	Chain	Res	Type
40	А	427	А
40	А	432	А
40	А	439	А
40	А	441	C
40	А	443	G
40	А	444	С
40	А	446	С
40	А	447	U
40	А	454	А
40	А	455	С
40	А	456	U
40	А	460	A
40	А	461	А
40	Α	464	A
40	A	465	A
40	A	471	U
40	A	472	A
40	А	473	G
40	А	477	G
40	А	481	А
40	А	483	А
40	А	484	А
40	А	485	А
40	А	487	U
40	А	489	U
40	А	490	А
40	А	495	С
40	А	496	С
40	А	499	А
40	А	500	G
40	A	501	U
40	A	502	A
40	А	503	G
40	A	504	G
40	А	510	A
40	А	511	A
40	А	512	G
40	A	513	C
40	А	514	A
40	A	516	C
40	A	517	C
40	A	522	A



Mol	Chain	Res	Type
40	А	523	U
40	А	524	U
40	А	525	А
40	А	527	G
40	А	528	А
40	А	530	А
40	А	531	G
40	А	532	С
40	А	534	U
40	А	540	C
40	А	541	U
40	А	546	А
40	А	564	С
40	A	565	С
40	А	566	C
40	A	567	A
40	А	571	А
40	А	572	U
40	А	573	А
40	А	574	U
40	А	575	А
40	А	577	С
40	А	580	А
40	А	582	С
40	А	583	U
40	А	587	С
40	А	589	С
40	А	591	С
40	A	592	С
40	A	593	С
40	А	594	A
40	A	599	G
40	A	602	С
40	А	604	А
40	А	609	U
40	A	610	C
40	А	613	С
40	A	614	С
40	A	615	U
40	A	620	A
40	A	622	G
40	А	624	А



Mol	Chain	Res	Type
40	А	626	U
40	А	627	А
40	А	628	А
40	А	629	U
40	А	630	G
40	А	631	U
40	А	639	А
40	А	640	G
40	А	641	U
40	А	642	А
40	А	645	А
40	А	646	U
40	A	647	G
40	A	652	С
40	A	653	A
40	A	654	U
40	A	662	С
40	А	675	G
40	А	679	G
40	А	680	A
40	А	702	U
40	А	703	А
40	А	704	А
40	А	705	С
40	А	709	С
40	А	711	А
40	А	717	U
40	А	718	А
40	А	720	А
40	А	723	C
40	A	724	A
40	A	727	С
40	А	731	A
40	A	734	U
40	A	736	A
40	A	737	U
40	A	744	С
40	A	745	С
40	A	746	U
40	A	748	A
40	A	752	U
40	А	753	С



Mol	Chain	Res	Type
40	А	756	С
40	А	757	С
40	А	758	С
40	А	759	А
40	А	761	С
40	А	765	G
40	А	771	С
40	А	773	C
40	А	774	А
40	А	776	А
40	А	782	A
40	А	788	А
40	А	798	A
40	A	838	С
40	А	841	С
40	А	842	A
40	А	850	С
40	А	851	А
40	А	853	С
40	А	854	А
40	А	856	С
40	А	857	А
40	А	985	G
40	А	986	U
40	А	990	U
40	А	997	U
40	А	1004	U
40	А	1011	G
40	А	1013	С
40	A	1014	C
40	А	1015	U
40	A	1016	G
40	A	1027	G
40	A	1035	U
40	А	1036	A
40	A	1037	A
40	А	1038	С
40	A	1039	A
40	A	1040	С
40	A	1044	A
40	A	1046	G
40	А	1048	С



Mol	Chain	Res	Type
40	А	1049	G
40	А	1055	А
40	А	1061	U
40	А	1069	U
40	А	1070	А
40	А	1071	А
40	А	1073	U
40	А	1075	А
40	А	1078	А
40	А	1080	U
40	А	1081	G
40	А	1083	А
40	А	1084	A
40	A	1085	A
40	А	1129	U
40	А	1131	А
40	А	1134	А
40	А	1138	U
40	А	1140	G
40	А	1155	G
40	А	1161	G
40	А	1162	А
40	А	1163	А
40	А	1167	А
40	А	1168	А
40	А	1169	С
40	А	1174	G
40	А	1177	С
40	А	1184	U
40	А	1187	U
40	А	1189	А
40	А	1194	U
40	A	1195	С
40	А	1200	G
40	A	1201	U
40	A	1222	A
40	А	1224	U
40	А	1226	G
40	А	1227	А
40	А	1230	С
40	А	1231	А
40	А	1236	С



Mol	Chain	Res	Type
40	А	1246	G
40	А	1248	А
40	А	1249	А
40	А	1250	С
40	А	1252	А
40	А	1253	G
40	А	1256	А
40	А	1258	С
40	А	1262	G
40	А	1280	U
40	А	1281	А
40	А	1282	U
40	А	1283	U
40	A	1285	U
40	А	1286	А
40	A	1293	A
40	А	1294	U
40	А	1301	А
40	А	1304	А
40	А	1305	G
40	А	1306	G
40	А	1307	G
40	А	1308	U
40	А	1311	А
40	А	1314	А
40	А	1316	С
40	А	1318	С
40	А	1330	А
40	А	1335	А
40	А	1346	G
40	А	1352	G
40	А	1359	A
40	А	1366	G
40	A	1370	G
40	A	1371	U
40	A	1372	U
40	A	1373	С
40	A	1379	U
40	А	1383	А
40	A	1384	G
40	A	1390	С
40	А	1393	G



Mol	Chain	Res	Type
40	А	1395	U
40	А	1400	G
40	А	1402	U
40	А	1432	U
40	А	1438	U
40	А	1439	U
40	А	1444	U
40	А	1452	U
40	А	1453	G
40	А	1459	А
40	А	1464	С
40	А	1468	А
40	А	1469	G
40	A	1471	A
40	А	1472	А
40	A	1473	U
40	А	1477	G
40	А	1480	U
40	А	1482	С
40	А	1485	С
40	А	1487	С
40	А	1488	А
40	А	1490	А
40	А	1492	С
40	А	1493	G
40	А	1498	С
40	А	1507	А
40	А	1510	А
40	А	1514	С
40	А	1519	С
40	A	1520	A
40	A	1522	С
40	A	1532	U
40	A	1537	А
40	А	1545	С
40	A	1547	A
40	А	1548	А
40	A	1549	G
40	A	1550	А
40	A	1551	A
40	А	1552	С
40	А	1553	А



Mol	Chain	Res	Type
40	А	1558	U
44	В	1607	U
44	В	1608	G
44	В	1609	U
44	В	1611	G
44	В	1613	U
44	В	1614	U
44	В	1615	А
44	В	1629	А
44	В	1630	А
44	В	1631	С
44	В	1632	U
44	В	1633	U
44	В	1641	G
44	В	1644	G
44	В	1645	A
44	В	1650	А
44	В	1659	U
44	В	1669	G

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
40	А	43	А
40	А	135	А
40	А	149	U
40	А	153	А
40	А	173	U
40	А	360	U
40	А	495	С
40	А	516	С
40	А	566	С
40	А	573	А
40	А	628	A
40	А	641	U
40	А	787	А
40	А	837	А
40	А	1235	А
40	A	1249	A
40	A	1371	U
40	А	1443	А
40	A	1489	А



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Mol	Chain	$\mathbf{Res}$	Type
40	А	1531	А
44	В	1607	U

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 50 ligands modelled in this entry, 49 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Bos	Link	Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
54	PNS	v	101	-	13,20,21	2.37	4 (30%)	18,26,29	1.14	1 (5%)

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
54	PNS	v	101	-	-	5/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
54	V	101	PNS	C34-N36	5.40	1.45	1.33
54	V	101	PNS	C39-N41	5.35	1.45	1.33



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
54	V	101	PNS	O40-C39	-2.19	1.18	1.23
54	V	101	PNS	O35-C34	-2.14	1.19	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms Z		$Observed(^{o})$	$Ideal(^{o})$
54	V	101	PNS	C38-C37-N36	-2.93	105.98	111.90

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	V	101	PNS	O33-C32-C34-N36
54	V	101	PNS	O33-C32-C34-O35
54	V	101	PNS	C29-C32-C34-O35
54	V	101	PNS	N41-C42-C43-S44
54	v	101	PNS	O27-C28-C29-C30

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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
40	А	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1182:C	O3'	1183:A	Р	11.06



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12919. 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)

#### 6.1.1 Primary map



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

### 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 180



Y Index: 180



Z Index: 180
The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map



X Index: 196

Y Index: 145

Z Index: 186

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

### 6.4 Orthogonal standard-deviation projections (False-color) (i)

#### 6.4.1 Primary map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



### 6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.6 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  $1540 \text{ nm}^3$ ; this corresponds to an approximate mass of 1391 kDa.

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



## 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.175  $\mathrm{\AA^{-1}}$ 



## 8 Fourier-Shell correlation (i)

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

#### 8.1 FSC (i)



\*Reported resolution corresponds to spatial frequency of 0.175  $\text{\AA}^{-1}$ 



## 8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.58	7.75	5.75
Unmasked-calculated*	-	-	-

\*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-12919 and PDB model 70I6. Per-residue inclusion information can be found in section 3 on page 14.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



### 9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

#### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).



### 9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.9020	0.2800
0	0.9870	0.3990
1	0.8380	0.1160
2	0.9530	0.3520
5	0.9740	0.3200
6	0.9210	0.1630
7	0.9880	0.3370
9	0.9910	0.3940
А	0.9000	0.2670
В	0.8790	0.1270
D	0.8450	0.2270
E	0.9850	0.3670
F	0.9690	0.3770
Н	0.9890	0.3240
Ι	0.5060	0.1080
J	0.2830	0.0330
Κ	0.9750	0.3880
$\mathbf{L}$	0.9660	0.3470
Μ	0.9720	0.3580
Ν	0.8610	0.2230
О	0.9850	0.3580
Р	0.9510	0.1980
$\mathbf{Q}$	0.9830	0.3550
R	0.9640	0.3470
S	0.9740	0.3830
Т	0.9730	0.4000
U	0.9750	0.4030
V	0.9730	0.3530
W	0.9400	0.2100
Х	0.9930	0.3360
Y	0.9790	0.3430
Z	0.9770	0.3820
a	0.9850	0.4090
b	0.9820	0.4060
С	0.9850	0.3380

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Chain	Atom inclusion	Q-score
d	0.9610	0.3390
g	0.9840	0.3690
h	0.9960	0.3500
i	0.9620	0.3810
j	0.9520	0.3340
k	0.5620	0.0720
1	0.9220	0.1080
0	0.9800	0.3540
р	0.9720	0.2790
q	0.9920	0.3330
r	0.9500	0.3200
S	0.9790	0.3600
u	0.9730	0.2860
V	0.9530	0.2500
W	0.8470	0.2180
X	0.9210	0.2530
У	0.2260	0.0440
Z	0.8390	0.1530

