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PDB ID EMDB ID	:	6Z6J EMD-11096
Title	:	Cryo-EM structure of yeast Lso2 bound to 80S ribosomes under native condi-
Authors	:	tion Wells, J.N.; Buschauer, R.; Mackens-Kiani, T.; Best, K.; Kratzat, H.; Bern- inghausen, O.; Becker, T.; Cheng, J.; Beckmann, R.
Deposited on	:	2020-05-28
Resolution	:	3.40 Å(reported)
This is	a I	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. dev 43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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.



Motric	Whole archive	EM structures
WIEUTIC	$(\# {\it Entries})$	$(\# { m Entries})$
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ 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	C2	1800	58%	31%	6% 6%
2	C5	92	52%		14%
3	C1	3396	5%	28%	• 8%
4	C4	121	• 74%		26%
5	C3	158	• 66%	30%	•••
6	SA	252	9%	•	18%
7	SB	255	83%		15%
8	SC	254	• 83%	·	15%

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Conti	nued fron	n previous	page	
Mol	Chain	Length	Quality of chain	
			51%	
9	SD	240	90%	• 7%
10	CE	961	7%	
10	SE	201	96%	•
11	SF	225	900/	. 9%
		220	21%	• 070
12	SG	236	90%	• 8%
			26%	
13	SH	190	91%	5% • •
14	SI	200	0%	60/
14	51	200	94%	6%
15	SJ	197	89%	• • 6%
			63%	
16	SK	105	86%	• 12%
	OT.	1 7 0	11%	
17	SL	156	92%	• 6%
18	SM	1/3	82%	1.20/
10	SM	140	81% 5%	• 13%
19	SN	151	96%	
			6%	
20	SO	137	91%	• 7%
01	CD	140	69%	
	SP	142	80% · ·	16%
22	SQ	143	94%	
	~~~~		29%	
23	SR	136	83%	15%
		1.10	66%	
24	SS	146	96%	• •
25	ST	144	20%	
20	51	144	55%	••
26	SU	121	79% ••	17%
			8%	
27	SV	87	97%	•
	OW	190	·	
28	SW	130	97%	••
29	SX	145	07%	
		110	15%	•••
30	SY	135	96%	• •
	~		42%	
31	SZ	108	63% · 36%	
20	C ₂	110	9%	
32	Sa	119		18%
33	Sb	82	94%	
	~~			

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Mol	Chain	Length	Quality of chain	
34	Sc	67	43%	• 6%
25	Sd	56	34%	
- 55	Su	- 50	30%	5%
36	Se	63	90%	5% 5%
37	Sf	152	22% 78%	
38	Sg	319	88%	
39	LA	254	96%	••
40	LB	387	97%	•
41	LC	362	97%	·
42	LD	297	98%	
43	LE	176	88%	• 11%
44	m LF	244	91%	9%
45	LG	256	8%	• 10%
46	LH	191	98%	••
47	LI	221	94%	• 5%
48	LJ	174	93%	5% •
49	LL	199	90%	6% • •
50	LM	138	9%	••
51	LN	204	97%	•
52	LO	199	97%	••
53	LP	184	5% 93%	• 5%
54	LQ	186	98%	
55	LR	189	89%	• 8%
56	LS	172	<mark>6%</mark> 99%	•
57	LT	160	98%	••
58	LU	121	80%	19%

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Mol	Chain	Length	Quality of chain	
59	LV	137	97%	
60	LW	155	<b>4</b> 0% • 59%	
61	LX	142	<b>8</b> 3% •	15%
62	LY	127	96%	• •
63	LZ	136	98%	•••
64	La	149	97%	••
65	Lb	59	93%	• • •
66	Lc	105	95%	5%
67	Ld	113	9%	• •
68	Le	130	96%	•••
69	Lf	107	98%	••
70	Lg	121	93%	7%
71	Lh	120	98%	•••
72	Li	100	97%	••
73	Lj	88	93%	7%
74	Lk	78	97%	••
75	Ll	51	96%	
76	Lm	128	41% 59%	
77	Ln	25	10%	
78	Lo	106	99%	•
79	Lp	92	97%	••

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## 2 Entry composition (i)

There are 80 unique types of molecules in this entry. The entry contains 196350 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues		1	Atoms			AltConf	Trace
1	C2	1700	Total 36234	C 16201	N 6426	O 11907	Р 1700	0	0

• Molecule 2 is a protein called Protein LSO2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C5	79	Total 633	C 379	N 128	0 125	S 1	0	0

• Molecule 3 is a RNA chain called 25S rRNA.

Mol	Chain	Residues		-	Atoms			AltConf	Trace
3	C1	3127	Total 66891	C 29878	N 12066	O 21820	Р 3127	0	0

• Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues		A	toms			AltConf	Trace
4	C4	121	Total 2579	C 1152	N 461	0 845	Р 121	0	0

• Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues		А	toms			AltConf	Trace
5	C3	157	Total 3333	C 1491	N 584	O 1101	Р 157	0	0

• Molecule 6 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues		Ate	AltConf	Trace			
6	SA	206	Total 1583	C 1017	N 281	0 283	${S \over 2}$	0	0



• Molecule 7 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues		At	AltConf	Trace			
7	SB	216	Total 1722	C 1091	N 312	0 315	${S \atop 4}$	0	0

• Molecule 8 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	$\mathbf{SC}$	217	Total 1635	C 1047	N 289	O 297	${ m S} { m 2}$	0	0

• Molecule 9 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SD	223	Total 1734	C 1101	N 313	0 314	S 6	0	0

• Molecule 10 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
10	SE	260	Total 2068	C 1316	N 389	O 360	${ m S} { m 3}$	0	0

• Molecule 11 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues		Ate		AltConf	Trace		
11	SF	206	Total 1609	C 1007	N 300	0 299	$\frac{S}{3}$	0	0

• Molecule 12 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues		Atoms					Trace
12	SG	218	Total 1751	C 1100	N 337	0 311	$\frac{S}{3}$	0	0

• Molecule 13 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
13	SH	185	Total 1486	C 954	N 266	O 266	0	0

• Molecule 14 is a protein called 40S ribosomal protein S8-A.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	SI	188	Total 1489	C 925	N 298	O 264	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 15 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	SJ	185	Total 1494	C 943	N 289	0 261	S 1	0	0

• Molecule 16 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	SK	92	Total 741	C 478	N 121	0 140	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 17 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
17	$\operatorname{SL}$	146	Total 1168	С 747	N 221	0 197	${ m S} { m 3}$	0	0

• Molecule 18 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	SM	124	Total 890	C 560	N 156	0 172	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 19 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues		At	oms			AltConf	Trace
19	SN	150	Total 1192	C 759	N 224	O 207	${ m S} { m 2}$	0	0

• Molecule 20 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
20	SO	128	Total 949	C 582	N 188	0 176	${ m S} { m 3}$	0	0

• Molecule 21 is a protein called 40S ribosomal protein S15.



Mol	Chain	Residues		At	oms	AltConf	Trace		
21	SP	119	Total 939	$\begin{array}{c} \mathrm{C} \\ 595 \end{array}$	N 176	0 161	${ m S} 7$	0	0

• Molecule 22 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
22	SQ	141	Total 1105	C 708	N 203	0 194	0	0

• Molecule 23 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
23	SR	115	Total 896	C 557	N 172	0 165	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 24 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
24	SS	145	Total 1192	C 743	N 237	0 210	${S \over 2}$	0	0

• Molecule 25 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
25	ST	143	Total 1112	C 694	N 208	O 208	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 26 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues		At	oms	AltConf	Trace		
26	SU	101	Total 805	C 512	N 145	0 147	S 1	0	0

• Molecule 27 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
27	SV	87	Total 684	C 420	N 125	0 137	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 28 is a protein called 40S ribosomal protein S22-A.



Mol	Chain	Residues		At	oms			AltConf	Trace
28	SW	129	Total	С	N	0	S	0	0
			1021	650	188	180	3		

• Molecule 29 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
29	SX	144	Total 1121	C 708	N 220	0 191	${ m S} { m 2}$	0	0

• Molecule 30 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
30	SY	134	Total 1073	C 676	N 208	O 189	0	0

• Molecule 31 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
31	SZ	69	Total 558	C 357	N 103	O 98	0	0

• Molecule 32 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues		At	oms		AltConf	Trace	
32	Sa	97	Total 769	C 475	N 160	0 129	${ m S}{ m 5}$	0	0

• Molecule 33 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues		At	oms			AltConf	Trace
33	$\operatorname{Sb}$	81	Total 610	C 382	N 110	0 113	${ m S}{ m 5}$	0	0

• Molecule 34 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
34	$\operatorname{Sc}$	63	Total 497	C 306	N 99	0 91	S 1	0	0

• Molecule 35 is a protein called 40S ribosomal protein S29-A.



Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
35	Sd	53	Total 442	С 274	N 92	0 72	${f S}$ $4$	0	0

• Molecule 36 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
36	Se	60	Total 475	C 299	N 98	O 77	S 1	0	0

• Molecule 37 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
37	Sf	33	Total 248	C 153	N 46	O 45	${f S}{4}$	0	0

• Molecule 38 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	$\operatorname{Sg}$	313	Total 2403	C 1521	N 411	0 463	S 8	0	0

• Molecule 39 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues		At	oms			AltConf	Trace
39	LA	252	Total 1912	C 1190	N 388	O 333	S 1	0	0

• Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues		At	oms			AltConf	Trace
40	LB	386	Total 3075	C 1950	N 584	O 533	S 8	0	0

• Molecule 41 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
41	LC	361	Total 2748	C 1729	N 522	0 494	${ m S} { m 3}$	0	0

• Molecule 42 is a protein called 60S ribosomal protein L5.



Mol	Chain	Residues		At	AltConf	Trace			
42	LD	294	Total 2359	C 1489	N 412	O 456	${ m S} { m 2}$	0	0

• Molecule 43 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	LE	157	Total 1248	C 806	N 224	0 217	S 1	0	0

• Molecule 44 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues		At	AltConf	Trace			
44	LF	223	Total 1791	C 1155	N 325	O 310	S 1	0	0

• Molecule 45 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues		At	AltConf	Trace			
45	LG	231	Total 1763	C 1130	N 316	0 314	${ m S} { m 3}$	0	0

• Molecule 46 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
46	LH	190	Total 1510	C 957	N 273	O 276	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 47 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues		At	AltConf	Trace			
47	LI	209	Total 1696	C 1077	N 321	O 293	${ m S}{ m 5}$	0	0

• Molecule 48 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
48	LJ	169	Total 1353	C 847	N 253	0 249	${S \atop 4}$	0	0

• Molecule 49 is a protein called 60S ribosomal protein L13-A.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
49	LL	194	Total 1548	C 965	N 316	O 267	0	0

• Molecule 50 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
50	LM	137	Total 1059	C 678	N 200	0 179	${ m S} { m 2}$	0	0

• Molecule 51 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues		Ate	AltConf	Trace			
51	LN	203	Total 1720	C 1077	N 361	0 281	S 1	0	0

• Molecule 52 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues		At	AltConf	Trace			
52	LO	197	Total 1555	C 1003	N 289	O 262	S 1	0	0

• Molecule 53 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
53	LP	175	Total 1378	C 856	N 273	O 249	0	0

• Molecule 54 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
54	LQ	185	Total 1441	C 908	N 290	0 241	${ m S} { m 2}$	0	0

• Molecule 55 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
55	LR	174	Total 1359	C 840	N 283	O 236	0	0

• Molecule 56 is a protein called 60S ribosomal protein L20-A.



Mol	Chain	Residues		At	oms			AltConf	Trace
56	LS	172	Total 1445	C 930	N 267	0 244	$\frac{S}{4}$	0	0

• Molecule 57 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
57	LT	159	Total 1276	C 805	N 246	0 221	${f S}$ $4$	0	0

• Molecule 58 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
58	LU	98	Total 778	C 505	N 127	O 146	0	0

• Molecule 59 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
59	LV	134	Total 993	C 623	N 187	0 176	${ m S} 7$	0	0

• Molecule 60 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
60	LW	63	Total 521	C 336	N 102	O 82	S 1	0	0

• Molecule 61 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues		At	AltConf	Trace			
61	LX	120	Total 959	C 617	N 168	0 172	${S \over 2}$	0	0

• Molecule 62 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
62	LY	124	Total 976	C 614	N 190	0 172	0	0

• Molecule 63 is a protein called 60S ribosomal protein L27-A.



Mol	Chain	Residues		Ato	ms	AltConf	Trace	
63	LZ	135	Total 1092	C 710	N 202	O 180	0	0

• Molecule 64 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues		At	oms	AltConf	Trace		
64	La	148	Total 1173	C 749	N 231	O 190	${ m S} { m 3}$	0	0

• Molecule 65 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
65	Lb	58	Total 462	C 289	N 100	O 73	0	0

• Molecule 66 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues		At	oms	AltConf	Trace		
66	Lc	100	Total 767	C 492	N 128	0 146	S 1	0	0

• Molecule 67 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
67	Ld	109	Total 883	$\begin{array}{c} \mathrm{C} \\ 559 \end{array}$	N 167	0 156	S 1	0	0

• Molecule 68 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues		At	oms	AltConf	Trace		
68	Le	127	Total 1020	С 647	N 205	0 167	S 1	0	0

• Molecule 69 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
69	Lf	106	Total 850	C 540	N 165	0 144	S 1	0	0

• Molecule 70 is a protein called 60S ribosomal protein L34-A.



Mol	Chain	Residues		At	oms	AltConf	Trace		
70	Lg	112	Total 880	$\begin{array}{c} \mathrm{C} \\ 545 \end{array}$	N 179	O 152	$\frac{S}{4}$	0	0

• Molecule 71 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
71	Lh	119	Total 965	C 612	N 185	0 167	S 1	0	0

• Molecule 72 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
72	Li	99	Total 770	C 481	N 156	0 131	${S \atop 2}$	0	0

• Molecule 73 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
73	Lj	82	Total 650	C 396	N 142	O 107	${ m S}{ m 5}$	0	0

• Molecule 74 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
74	Lk	77	Total 608	C 388	N 114	O 106	0	0

• Molecule 75 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace		
75	Ll	50	Total 436	C 272	N 97	O 65	S 2	0	0

• Molecule 76 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
76	Lm	52	Total 417	C 259	N 86	O 67	${f S}{5}$	0	0

• Molecule 77 is a protein called 60S ribosomal protein L41-B.



Mol	Chain	Residues		Atc	$\mathbf{ms}$	AltConf	Trace		
77	Ln	25	Total 233	C 142	N 63	O 27	S 1	0	0

• Molecule 78 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues		At	oms			AltConf	Trace
78	Lo	105	Total 847	C 534	N 170	0 138	${ m S}{ m 5}$	0	0

• Molecule 79 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues		At	oms			AltConf	Trace
79	Lp	91	Total 694	C 429	N 138	0 121	S 6	0	0

• Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
80	C2	1	Total Zn 1 1	0
80	Sa	1	Total Zn 1 1	0
80	$\operatorname{Sb}$	1	Total Zn 1 1	0
80	Sf	1	Total Zn 1 1	0
80	Lg	1	Total Zn 1 1	0
80	Lj	1	Total Zn 1 1	0
80	Lm	1	Total Zn 1 1	0
80	Lo	1	Total Zn 1 1	0
80	Lp	1	Total Zn 1 1	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: 18S rRNA











 $\bullet$  Molecule 3: 25S rRNA











• Molecule 6: 40	)S ribosomal protein	n S0-A			
Chain SA:		79%	• 1	8%	
MET S2 L3 L9 D13 A26	D4-3 04-4 05-1 65-1 65-2 490 19-3 69-4 6100 €100	RI 13 D125 P126 N127 V139 D157	L184 R185 0186 A187 L188 L188 Q193 Q193 R205	P206 P207 GLU GLU CLU CLU GLU GLU GLU GLU GLU	ALA THR THR GJU
GLU ALA GLY GLU GLU GLU GLU GLU GLU GLU CLU CLU CLU CLU CLU	GLU GLU GLN GLN GLU GLU TRP GLU GLU GLU GLU ALA	ASP ASN VAL GLU TRP			
• Molecule 7: 40	)S ribosomal proteir	n S1-A			
Chain SB:	_	83%	·	15%	
MET ALA ALA CLY CLY CLYS ASN ARG LAS SER LAS SER LAS CLYS CLYS	LYS LYS GLY GLN LYS LYS LYS V20 V21 V21 V21 S36	V43 M49 S51 S51 K55 S66 S56 S56 S56 S56	558 D59 G75 D78 G92 G92 G92	1120 1120 1120 1132	A Land
F205 F223 D224 C233 G233 C233 C233	C235 SER SER SER CLY GLU GLU CLYS GLU CLYS CLYS VAL THR THR FHE CLY CLYS CLY CLYS CLY CLYS CLY CLYS CLY CLYS CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	ASP GLU VAL LEU GLU THR VAL			
• Molecule 8: 40	)S ribosomal proteir	n S2			
Chain SC:		83%	·	15%	
MET SER ALA PRO GLU GLU GLN GLN GLN GLN GLY GLY	GLY PHE GLY GLY ASN ASN ASN ASN ASN ASN ASN ASN ASN ASN	PRO ARG ASN THR GLU CJU CJU CJU C34 C34 C34 C34 C34 C34 C34 C34 C34 C34	D70 675 689 190 190 111 1158 1158	Y222 P236 P236 F246 A247 A248 A248 A248 A248 A248 A248 A248 A248	
LYS ARG PHE					
• Molecule 9: 40	)S ribosomal proteir	1 S3			
Chain SD:	51%	90%		• 7%	
MET VAL A3 L4 L5 K8 K3 K10 K10	D14 015 115 116 117 118 112 121 121 121 121 121 121 121	726 126 A30 631 532 535 635 035	E38 V39 N40 V41 P43 P43 E47 E47	149 150 851 A52 A52 T53 R54 C55 Q55 D57	VSS L55 C50 E51 NG2 C53 R64 R65 R65 I65
NG7 E68 L69 L71 L71 L72 K75 K75 K75	K78 480 480 184 184 184 88 88 888 888	R90 V91 092 092 R94 R94 C95 L96 L96 L965	E103 8104 F107 F107 I109 M111 0112 G112 I113	A114 1115 R116 A119 Y120 H124 H124	E128 S129 E135 K141 L142 R143 A144
A145	Q179 G180 K190 K196 K195 G195 F197 F197 F198 K200	A201	E213 E214 E214 E215 P216 P216 A219 P220 S221	V222 V223 V224 V225 ARG ARG ALA GLU GLU THR GLU	ALA GLN ALA ALA PRO VAL VAL GLU
ALA					

 $\bullet$  Molecule 10: 40S ribosomal protein S4-A





• Molecule 15: 40S ribosomal protein S9-A

	I I I I I I I I I I I I I I I I I I I		
Chain SJ:	89%	• • 6%	
MET 72 114 114 114 114 114 114 114 114 114 11	R1 00 R1 00 R1 00 R1 20 R1	S1162 P163 A167 A177 A177 A177 A178 A178 A178 A178 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A183 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181 A181	E186 ALA ALA ASP GLU ALA ALA ASP ASP
GLU ASP GLU GLU GLU			
• Molecule 16: 40S ribos	somal protein S10-A		
Chain SK:	63% 86%	• 12%	
M1 L2 M3 P4 K5 K10 K10 K10 H12 Y14 Y14 V14 L15	F16 q17 E18 C19 V20 V20 V20 V26 V26 V26 V26 V26 V28 V28 C33 C33 C33 C33 C33 C33 C33 C3	135 D36 T37 T37 K38 N39 N41 V42 I43 K44 A45 A45 L46 A45 T50 S51 S51	553 Υ54 Υ55 Κ56 458 462 Υ63 Υ64 Υ65 Υ65 Υ65
T67 E70 E71 E71 E74 Y75 E73 E73 E77 E73 E77 E77 E78 E77 E78 E78 E78 E78 E78 E78	P83 B84 B86 B86 P88 P88 P88 P88 P88 P88 P88 P88 P88 P	ARG TYR	
• Molecule 17: 40S ribos	somal protein S11-A		
Chain SL:	92%	• 6%	
MET S2 E4 E4 E4 L5 E10 M21 K26 K26 K26 K28 K28	R67 F60 F60 F60 F61 F60 F116 A146 A145 A145 A145 A145 A145 A145 A147 A145 A147 A147 A147 A147 A147 A147 A147 A147	OLIN PHE ALA ALA PHE	
• Molecule 18: 40S ribos	somal protein S12		
Chain SM:	82%	5% • 13%	
MET SER ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	THR A20 E21 E21 723 724 E25 625 625 124 K29 V30 V31 128 V31 V31 V31 V33 V33 V33 V33 V31 V31 V31	L36 H38 H38 G40 G40 C41 L41 C41 C44 C44 C44 C44 C44 C44 C44 C44 C	T53 R54 G55 E56 A57 L58 L58 U60 V60 V60
L62 V63 S65 S65 S65 S65 C72 M70 K73 K73 K73 K73 K73 K75	E76 G77 L78 A79 A80 N80 P82 P82 P82 R83 N84 P82 P82 P82 N84 V86 P87 V86 P87 V86 V86 V86 V86 V86 V82 V86 V86 V82 V86 V82 V86 V82 V86 V82 V86 V82 V80 V80 V80 V80 V80 V80 V80 V80 V80 V80	D93 A94 A94 C95 C99 B101 C102 C102 C103 C103 C104 C103 C104 C103 C104 C105 C104 C105 C104 C105 C105 C106 C106 C106 C106 C106 C106 C106 C106	E1100 0111 0111 0111 0111 0111 0117 0117 0117 0117 0117 0117 0117 0117
V122 V123 V123 V125 V126 V126 V126 V126 V126 V126 V123 U131 U131 U131 V133 S134 M135	1136 M137 M137 E138 H139 H139 H139 H139 H139 H139 H139 H139		
• Molecule 19: 40S ribos	somal protein S13		
Chain SN:	96%	<mark>.</mark> .	
MET G2 N21 L28 E31 E31 E31 E31 E31 E31 E31 E31 E31 E31	K140 4 A144 4 T145 4 V150 4 N151 4		

• Molecule 20: 40S r	ibosomal protein S14-A		
Chain SO:	91%	• 7%	
MET SER ASN VAL VAL GLN ASP ASP ASP ASP ASP ASP ASP ASP ASP ASP	143         644         645         A50         A50         B124         C131         C131		
• Molecule 21: 40S r	ibosomal protein S15		
Chain SP:	69% 80%	•• 16%	
MET SER SER ALA ALA ALA LYS LYS LYS LYS LYS TH PHE LYS LYS BHE	S115 Y17 R18 C19 C19 C19 C21 C22 C23 C23 C23 C23 C23 C23 C23 C23 C23	A37 P38 A39 R42 R42 R42 R47 A46 C48 A47 C48 C48 C48 C48 C48 C48 C48 C48 C48 C48	K61
A62 A63 K64 A65 A65 A65 A65 A65 B69 B71 K72 F73	A74 P75 R77 T78 T78 H79 M80 M82 M82 M82 M83 P87 P87 P87 P87 P87 P87 P87 P87 P87 P87	095           196           197           196           197           196           196           196           196           196           196           196           196           196           196           101           101           1014           1107           1107           1108           1109           1111           1111           1111           1115           1116           1116           1117           1118           1116           1116           1116	E118 F119 S120 1121
P125 V126 H127 H128 A131 C132 A131 C132 A131 C132 A13 A13 THR SER A14 A14 A14 A14 A14 A14 A14 A14 A14 A14	PHE PRO LLEU LLYS		
• Molecule 22: 40S r	ibosomal protein S16-A		
Chain SQ:	56% 94%		
MET SER A3 V4 P5 611 K12 A16 A16 A16 A18 V19	A20 H21 V22 K23 A24 A24 C25 C25 C25 C25 C25 C25 C25 C25 C25 C25	144 144 144 144 144 145 145 153 153 153 153 155 155 155 155 155 15	163
R68 V69 S76 Q83 A86 C88 C88 C88 C88 C88 C88 C88 C88 C88 C	A91         Y92         H93         H93         H93         Y96         Y96         Y96         Y97         Y96         Y97         Y96         Y97         Y96         Y97         Y97         Y98         Y112         Y112         Y112	D113 T115 1115 1116 1117 1118 1118 1118 1120 1120 1120 1120 1120	
• Molecule 23: 40S r	ibosomal protein S17-A		
Chain SR:	83%	• 15%	
MET G2 C3 K14 F18 F18 F22 F22 C4	Q28 T300 N31 K32 R33 R33 C37 C38 A38 A38 A38 A38 A44 R44 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C38 C37 C37 C37 C37 C37 C37 C37 C37	R67 R67 C68 C68 C73 C74 C73 C74 C73 C74 C74 C74 C74 C74 C74 C74 C74 C74 C74	66A
L100 N101 V102 N102 D103 0105 C106 V110 K111 K111	K116 L117 P118 L119 ASN VAL ASN ASN ASN ASN ASN ASN ASN ASN		
• Molecule 24: 40S r	ibosomal protein S18-A		
Chain SS:	96%		







Chain SX:	97%	1
MET G2 K39 K39 88 N89 D97	V1 30 A1 34 K1 33 S1 45 S1 45	
• Molecule 30: 4	40S ribosomal protein S24-A	
Chain SY:	96% •	
MET S2 D3 N31 R32 E39 E39	E46 V47 Y48 E51 K52 B53 C53 K52 B53 K52 K52 K52 K129 K124 K102 K124 K102 K124 K102 K124 K102 K124 K102 K124 K102 K125 K124 K102 K125 K124 K125 K125 K125 K125 K125 K125 K125 K125	
• Molecule 31: 4	40S ribosomal protein S25-A	
Chain SZ:	42% 63% • 36%	
	••• • •••••	••••• •
MET PRO PRO CLN CLN CLN CLN CLN CLN SER ALA ALA ALA ALA	ALA ALA ALA ALA ALA ALA ALA ALA ALA CLYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS	E53 V54 P55 T56 Y57 L65 V66
D67 R68 R68 L169 T71 G72 L75 A76 A76	178         A79         B81         B81         B81         B82         B83         E84         B82         E84         B82         E84         B83         B81         B82         B84         B84         B84         B85         B84         B84         B91         B91         B91         B91         B91         B93         A104         A104         A104         A104         A104         A104         A104         GUU	
• Molecule 32: 4	40S ribosomal protein S26-B	
Chain Sa:	<b>78%</b> • 18%	
MET P2 R10 K34 I41 R42	E46 447 47 47 47 47 55 55 46 55 46 55 47 55 75 75 75 75 75 75 75 75 75 75 75 75	
• Molecule 33: 4	40S ribosomal protein S27-A	
Chain Sb:	94% •••	
MET V2 A12 P38 C39 C40 C40 M42	A53 E57 SS8 C59 C59 E75 F79 R81 R81 R81 R81 K82	
• Molecule 34: 4	40S ribosomal protein S28-A	
Chain Sc:	43% 93% • 6%	
MET ASP ASP ASN LYS P6 P6 C1 C9 C1	G20         S21         S21         R22         G24         C25         C25         C25         C25         C23         C23         C33         C34         C35         C35         C36         C37         C38         C40         C40	
• Molecule 35: 4	40S ribosomal protein S29-A	
Chain Sd:	34% 95% 5%	



• Molecule 39: 60S ribosomal p	rotein L2-A	
Chain LA:	96%	
MET MET C2 C3 C3 R23 R23 R23 R246 R193 R193 R246 R246 R246 R246 R246 R246 R247 R246 R237 R237 R237 R237 R237 R237 R237 R237 R236 R237 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R237 R236 R237 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R236 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266 R266	r253 Q253 ASP	
• Molecule 40: 60S ribosomal p	rotein L3	
Chain LB:	97%	
MET S2 D36 D61 M137 A137 A137 A142 C141 A142 C141 A142 C141 A142 C141 C142 C141 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142 C142	E197         €           V205         V205           K248         V260           V280         €           D289         €           R300         €           T372         T372           L387         €	
• Molecule 41: 60S ribosomal p	rotein L4-A	
Chain LC:	97%	<del>.</del>
MET S2 82 489 691 691 691 6147 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H176 H1	A268 S284 S292 S292 S292 S292 S284 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C336 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C3348 C348 C	
• Molecule 42: 60S ribosomal p	rotein L5	
Chain LD:	98%	
MET ALA PHE 0.4 KG A7 A7 A7 C102 E123 E123 E123 E123 E133	E136 D137 G182 G182 E186 E189 E216 E216 E216 E216 E216 E217 M228	1231 1231 1233 4233 1239 1239 1239 8269 8269 8269 8269 8269 8269
A292 4 A294 4 A295 4 Q296 9 Q297 4		
• Molecule 43: 60S ribosomal p	rotein L6-A	
Chain LE:	88%	• 11%
MET 82 A3 A3 A3 A3 A5 A5 V5 V5 C99 E104 E104 E109	LTVS LLEU TTHE LVS CLVS GLV GLV CLV GLV CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	D142 K143 K151 G169 F176
• Molecule 44: 60S ribosomal p	rotein L7-A	
• Molecule 44: 60S ribosomal p Chain LF:	protein L7-A 91%	9%

 $\bullet$  Molecule 45: 60S ribosomal protein L8-A





• Molecule 51: 60S ribosomal protein L15-A Chain LN: 97% • Molecule 52: 60S ribosomal protein L16-A Chain LO: 97% • Molecule 53: 60S ribosomal protein L17-A Chain LP: 93% • 5% A156 VAL ALA ALA ALA ALA ALA GLU CYS LYS R18 I18 • Molecule 54: 60S ribosomal protein L18-A Chain LQ: 98% • Molecule 55: 60S ribosomal protein L19-A Chain LR: 89% 8% . ARG VAL ALA ALA GLU CLYS ARG ASP ASP ALA CLEU LEU LEU LEU LEU CLU SP • Molecule 56: 60S ribosomal protein L20-A 6% Chain LS: 99% • Molecule 57: 60S ribosomal protein L21-A Chain LT: ••• 98%





• Molecule 58: 60S ribosomal protein L22-A

Chain LU:		80%	• 19%	_
MET ALA ASN ASN ASN ASR ASC CLYS GLN LYS GLN E24	N25 026 051 N52 A53 A53 E58 E58 E58 D59	Y108 CAN GLN V108 CAN PRO GLU GLU GLU GLU GLU GLU	GLU	
• Molecule 59: 60S	s ribosomal prot	tein L23-A		
Chain LV:		97%		•••
MET SER GLY G5 A6 V135 V135 V137				
• Molecule 60: 60S	s ribosomal prot	tein L24-A		
Chain LW:	40%	·	59%	_
MI W2 W2 B82 G1U G1U G1U G1U C1U K1A K1A K1A	LYS ARG SER ARG ARG LYS ALA GLN ARG	PR0 THLE THLE THLA ALA ALA ALA ALA ALA CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLU CLYS CLYS CLYS CLYS CLYS CLYS CLYS CLYS	LEU LEU PHO CLU VAL VAL ARG ARG ARG ALU CLU CLU CLU LLU LLU	ALA ASN LYS GLU LYS LYS
LYS ALA GLU CYS ALA ALA ALA CLYS CLYS CLYS CLYS CLYS CLYS CLYS	ALA ALA GLY GLY SER SER SER PHE SER SER LYS SER CLN	GLN ALA LYS GLY ALA PHE PHE CLN VAL LYS VAL ALA ALA ALA ALA ALA ARG		
• Molecule 61: 60S	s ribosomal prot	tein L25		
Chain LX:		83%	• 15%	-
MET ALA PRO PRO ALA ALA ALA ALA LYS LYS LYS VAL	VAL LYS LYS GLY ASN GLY LYS LYS LYS L24 <b>A23</b>	D106		
• Molecule 62: 60S	s ribosomal prot	tein L26-A		
Chain LY:		96%		•
MET A2 121 121 131 6124 6124 6124 150 150 150 510				
• Molecule 63: 60S	s ribosomal prot	tein L27-A		
Chain LZ:		98%		





• Molecule 64: 60S ribosomal protein L28

Chain La:	97%	
MET P2 A17 G18 K47 L78 E84	R87 D88 A94 A149	
• Molecule 65: 60	OS ribosomal protein L29	
Chain Lb:	93%	• • •
MET A2 A2 A2 C2 C2 C2 K22 K23 A56 A57 A57		
• Molecule 66: 60	OS ribosomal protein L30	
Chain Lc:	95%	5%
MET ALA PALA PAL VAL LYS S6 Q7 E8 S9 S9 S9 K19	11104 ← ◆	
• Molecule 67: 60	OS ribosomal protein L31-A	
Chain Ld:	94%	• •
MET ALA GLY L4 K5 T13 V64 V64	E82 E83 E84 F97 V98 A99 A112 A112 A112	
• Molecule 68: 60	OS ribosomal protein L32	
Chain Le:	96%	
MET A2 H6 B81 A127 L128 GLU	ALA	
• Molecule 69: 60	OS ribosomal protein L33-A	
Chain Lf:	98%	
MET A2 137 1107		

• Molecule 70: 60S ribosomal protein L34-A



Chain Lg:	<u>6%</u> 93%	7%
• • •		
MET A2 Q98 E107 E107	H109 E1100 A111 KTH3 CFN GEU CFN CFN CFN CFN CFN CFN CFN CFN CFN CFN	
• Molecule	e 71: 60S ribosomal protein L35-A	
Chain Lh:	<u>5%</u> 98%	
** * *		
MET A2 G3 E15 E15		
• Molecule	e 72: 60S ribosomal protein L36-A	
Chain Li:	97%	••
MET T2 V3 K38 M63	■ 181 182 8 183 9 190 9 1	
• Molecule	e 73: 60S ribosomal protein L37-A	
Chain Lj:	93%	7%
MET G2 SER LYS ALA SER SER	ALA	
• Molecule	e 74: 60S ribosomal protein L38	
Chain Lk [.]	14%	
MET A2 D7 R17	N32 K33 D58 A59 A59 A59 A59 L73 L73 L73 L73 L73	
• Molecule	e 75: 60S ribosomal protein L39	
Chain Ll:	<b>9</b> 6%	•••
MET A2 L23 N32		
• Molecule	e 76: Ubiquitin-60S ribosomal protein L40	
Chain Lm:	÷ 41% 59%	
MET GLN ILE PHE VAL LYS THR LEU	THR THR THR THR THR THR THR THR THR THR	ARG THR LEU SER ASP TYR ASN






## 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	34951	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II $(4k \times 4k)$	Depositor
Maximum map value	0.865	Depositor
Minimum map value	-0.566	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	433.6, 433.6, 433.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	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: ZN

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

Mal	Chain	B	ond lengths	Bond angles		
NIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	C2	1.06	19/40528~(0.0%)	1.42	623/63141~(1.0%)	
2	C5	0.37	0/636	0.51	0/837	
3	C1	1.34	50/74873~(0.1%)	1.37	901/116727~(0.8%)	
4	C4	1.14	0/2883	1.28	18/4491~(0.4%)	
5	C3	1.31	3/3724~(0.1%)	1.28	34/5798~(0.6%)	
6	SA	0.51	0/1623	0.71	0/2222	
7	SB	0.52	0/1748	0.70	2/2352~(0.1%)	
8	SC	0.55	0/1665	0.70	0/2263	
9	SD	0.41	0/1759	0.68	1/2368~(0.0%)	
10	SE	0.55	0/2109	0.70	1/2839~(0.0%)	
11	SF	0.40	0/1629	0.66	0/2202	
12	SG	0.45	0/1775	0.68	2/2374~(0.1%)	
13	SH	0.50	0/1511	0.76	2/2036~(0.1%)	
14	SI	0.62	0/1514	0.66	0/2021	
15	SJ	0.49	0/1519	0.65	0/2035	
16	SK	0.40	0/757	0.64	0/1022	
17	SL	0.64	0/1194	0.63	0/1610	
18	SM	0.36	0/898	0.84	1/1220~(0.1%)	
19	SN	0.54	0/1215	0.69	1/1638~(0.1%)	
20	SO	0.56	0/960	0.70	0/1290	
21	SP	0.44	0/959	0.74	1/1288~(0.1%)	
22	SQ	0.42	0/1125	0.71	1/1510~(0.1%)	
23	SR	0.41	0/904	0.62	0/1210	
24	$\mathbf{SS}$	0.39	0/1211	0.64	0/1628	
25	ST	0.40	0/1130	0.62	1/1517~(0.1%)	
26	SU	0.42	0/815	0.69	0/1102	
27	SV	0.55	0/693	0.67	1/935~(0.1%)	
28	SW	0.63	0/1038	0.67	0/1395	
29	SX	0.58	0/1139	0.67	0/1518	
30	SY	0.48	0/1087	0.67	0/1449	
31	SZ	0.38	0/566	0.71	0/761	
32	Sa	0.56	0/782	0.68	0/1047	



Mal	Bond lengths		Bond angles		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
33	$\operatorname{Sb}$	0.49	0/620	0.73	2/838~(0.2%)
34	Sc	0.40	0/499	0.73	0/670
35	Sd	0.42	0/452	0.65	0/600
36	Se	0.46	0/483	0.62	0/643
37	Sf	0.40	0/253	0.70	0/340
38	Sg	0.37	0/2456	0.69	1/3343~(0.0%)
39	LA	0.72	0/1946	0.74	1/2614~(0.0%)
40	LB	0.69	0/3146	0.67	0/4228
41	LC	0.66	0/2800	0.71	1/3790~(0.0%)
42	LD	0.54	0/2408	0.62	1/3248~(0.0%)
43	LE	0.57	0/1269	0.65	0/1705
44	m LF	0.66	0/1828	0.70	3/2461~(0.1%)
45	LG	0.62	0/1795	0.71	0/2429
46	LH	0.54	0/1531	0.64	0/2062
47	LI	0.57	0/1732	0.63	0/2323
48	LJ	0.52	0/1374	0.77	0/1842
49	LL	0.63	0/1573	0.78	3/2113~(0.1%)
50	LM	0.57	0/1074	0.63	0/1446
51	LN	0.75	0/1757	0.72	2/2354~(0.1%)
52	LO	0.63	0/1585	0.67	1/2128~(0.0%)
53	LP	0.69	0/1400	0.67	0/1882
54	LQ	0.60	1/1465~(0.1%)	0.69	0/1965
55	LR	0.66	1/1376~(0.1%)	0.64	0/1842
56	LS	0.66	0/1481	0.65	0/1990
57	LT	0.66	0/1300	0.65	0/1743
58	LU	0.56	0/794	0.60	0/1076
59	LV	0.62	0/1008	0.70	0/1356
60	LW	0.64	0/533	0.64	0/707
61	LX	0.62	0/974	0.69	0/1314
62	LY	0.54	0/987	0.62	0/1318
63	LZ	0.64	0/1118	0.63	0/1497
64	La	0.66	0/1204	0.70	1/1612~(0.1%)
65	Lb	0.47	0/473	0.70	0/629
66	Lc	0.60	0/775	0.67	0/1040
67	Ld	0.66	0/897	0.66	0/1205
68	Le	0.63	0/1041	0.68	0/1394
69	Lf	0.77	0/868	0.67	0/1168
70	Lg	0.65	0/890	0.67	0/1189
71	Lh	0.56	0/974	0.61	0/1297
72	Li	0.51	0/777	0.62	0/1033
73	Lj	0.79	0/665	0.69	0/882
74	Lk	0.53	0/614	0.70	0/822
75	Ll	0.65	0/443	0.68	0/588



Mal	Chain	В	ond lengths	Bond angles	
INIOI		RMSZ	# Z  > 5	RMSZ	# Z  > 5
76	Lm	0.62	0/423	0.62	0/562
77	Ln	0.49	0/234	0.55	0/300
78	Lo	0.57	0/860	0.60	0/1136
79	Lp	0.70	0/701	0.70	0/934
All	All	1.02	74/210825~(0.0%)	1.16	1606/309504~(0.5%)

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
6	SA	0	4
7	SB	0	1
8	SC	0	1
10	SE	0	3
12	SG	0	1
13	SH	0	5
15	SJ	0	1
16	SK	0	2
18	SM	0	3
19	SN	0	2
20	SO	0	2
21	SP	0	2
22	SQ	0	2
24	SS	0	1
26	SU	0	3
28	SW	0	1
30	SY	0	2
31	SZ	0	1
32	Sa	0	2
33	Sb	0	2
36	Se	0	3
39	LA	0	4
40	LB	0	2
41	LC	0	4
45	LG	0	1
48	LJ	0	1
49	LL	0	4
51	LN	0	1
54	LQ	0	1
56	LS	0	1



Mol	Chain	#Chirality outliers	#Planarity outliers
58	LU	0	1
63	LZ	0	2
64	La	0	1
65	Lb	0	2
67	Ld	0	1
71	Lh	0	2
72	Li	0	1
79	Lp	0	1
All	All	0	74

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C2	853	G	N1-C2	-7.62	1.31	1.37
1	C2	818	С	N3-C4	-7.37	1.28	1.33
3	C1	2149	А	N9-C4	-6.94	1.33	1.37
1	C2	163	G	N9-C4	-6.62	1.32	1.38
3	C1	340	С	N1-C6	-6.59	1.33	1.37
5	C3	12	А	N9-C4	-6.36	1.34	1.37
3	C1	936	А	N9-C4	-6.31	1.34	1.37
3	C1	1506	А	N9-C4	-6.14	1.34	1.37
55	LR	58	HIS	CA-CB	-6.12	1.40	1.53
3	C1	920	А	N9-C4	-6.08	1.34	1.37
1	C2	1141	G	N3-C4	-6.05	1.31	1.35
1	C2	853	G	N9-C4	6.04	1.42	1.38
1	C2	14	С	C2-O2	-5.87	1.19	1.24
1	C2	621	А	N9-C4	-5.85	1.34	1.37
3	C1	57	А	N9-C4	-5.83	1.34	1.37
1	C2	118	U	C2-N3	-5.74	1.33	1.37
3	C1	2338	С	N1-C6	-5.73	1.33	1.37
3	C1	914	А	N7-C5	-5.68	1.35	1.39
3	C1	647	А	N7-C5	-5.66	1.35	1.39
3	C1	346	С	N1-C6	-5.65	1.33	1.37
3	C1	75	G	C2-N2	-5.63	1.28	1.34
1	C2	853	G	C5-C6	5.61	1.48	1.42
3	C1	2131	А	C5-C4	-5.58	1.34	1.38
1	C2	1141	G	C2-N2	-5.53	1.29	1.34
3	C1	2149	А	N3-C4	-5.52	1.31	1.34
3	C1	656	А	N7-C5	-5.52	1.35	1.39
1	C2	872	G	N7-C5	-5.47	1.35	1.39
5	C3	61	А	N9-C4	-5.47	1.34	1.37
3	C1	75	G	C2-N3	-5.46	1.28	1.32



Contre	naca jion	i preute	, us puye.	••			
Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C1	2130	G	N7-C5	-5.45	1.35	1.39
3	C1	2947	G	C5-C4	-5.41	1.34	1.38
3	C1	3310	А	N7-C5	-5.40	1.36	1.39
3	C1	920	А	C5-C6	-5.39	1.36	1.41
1	C2	350	U	C2-N3	-5.36	1.33	1.37
3	C1	875	G	N7-C5	-5.35	1.36	1.39
3	C1	2957	G	C5-C4	-5.35	1.34	1.38
3	C1	1152	G	N9-C4	-5.34	1.33	1.38
3	C1	2982	А	C5-C4	-5.34	1.35	1.38
3	C1	438	А	N9-C4	5.32	1.41	1.37
3	C1	1158	А	N9-C4	-5.31	1.34	1.37
3	C1	2967	А	N7-C5	-5.30	1.36	1.39
3	C1	1515	А	C6-N1	-5.28	1.31	1.35
3	C1	2702	А	N9-C4	-5.27	1.34	1.37
1	C2	394	С	N1-C6	-5.26	1.33	1.37
3	C1	1161	G	N3-C4	-5.23	1.31	1.35
3	C1	2689	А	N7-C5	-5.23	1.36	1.39
3	C1	1857	С	N1-C6	-5.22	1.34	1.37
1	C2	474	А	N9-C4	-5.21	1.34	1.37
3	C1	1195	А	N9-C4	-5.21	1.34	1.37
3	C1	2323	G	C5-C4	-5.21	1.34	1.38
3	C1	88	А	N9-C4	-5.20	1.34	1.37
3	C1	1799	А	N9-C4	-5.18	1.34	1.37
54	LQ	172	PHE	CA-CB	-5.18	1.42	1.53
3	C1	2946	А	N9-C4	-5.15	1.34	1.37
3	C1	2424	А	N7-C5	-5.15	1.36	1.39
3	C1	820	A	N7-C5	-5.14	1.36	1.39
3	C1	2352	A	N7-C5	-5.14	1.36	1.39
3	C1	2182	A	N9-C4	-5.12	1.34	1.37
3	C1	1199	C	N3-C4	-5.11	1.30	1.33
3	C1	1385	C	N1-C6	-5.11	1.34	1.37
5	C3	24	G	C5-C4	-5.10	1.34	1.38
1	C2	1728	A	N9-C4	-5.08	1.34	1.37
3	C1	2407	С	C4-C5	-5.07	1.38	1.43
3	C1	2270	A	N9-C4	-5.05	1.34	1.37
3	C1	650	С	C4-C5	-5.04	1.39	1.43
3	C1	1145	G	N7-C5	-5.04	1.36	1.39
1	C2	1455	G	N9-C4	-5.03	1.33	1.38
1	C2	1787	С	N1-C6	-5.02	1.34	1.37
3	C1	1605	A	N9-C4	-5.02	1.34	1.37
3	C1	807	А	N7-C5	-5.02	1.36	1.39
1	C2	247	A	N9-C4	-5.01	1.34	1.37



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C1	1381	А	N9-C4	-5.01	1.34	1.37
3	C1	2610	G	N7-C5	-5.01	1.36	1.39
1	C2	1137	А	N9-C4	-5.01	1.34	1.37

All (1606) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	853	G	C2-N3-C4	27.75	125.78	111.90
1	C2	853	G	N1-C6-O6	-24.59	105.14	119.90
1	C2	853	G	N3-C4-C5	-19.87	118.66	128.60
1	C2	853	G	N9-C4-C5	19.21	113.08	105.40
1	C2	818	С	N1-C2-O2	17.25	129.25	118.90
1	C2	853	G	C5-C6-N1	16.90	119.95	111.50
3	C1	1152	G	N1-C6-O6	-16.66	109.90	119.90
1	C2	853	G	O4'-C1'-N9	16.01	121.01	108.20
1	C2	853	G	C8-N9-C4	-14.84	100.46	106.40
1	C2	853	G	C4-C5-N7	-14.77	104.89	110.80
1	C2	818	C	N3-C2-O2	-13.95	112.14	121.90
1	C2	854	U	O4'-C1'-N1	13.41	118.93	108.20
1	C2	453	U	C2-N1-C1'	13.12	133.44	117.70
1	C2	818	С	O4'-C1'-N1	13.12	118.69	108.20
1	C2	853	G	C6-C5-N7	13.07	138.25	130.40
1	C2	818	C	C2-N1-C1'	12.81	132.89	118.80
1	C2	1	U	N1-C2-O2	12.79	131.75	122.80
1	C2	853	G	C6-N1-C2	-12.63	117.52	125.10
3	C1	2572	С	N1-C2-O2	11.75	125.95	118.90
1	C2	1	U	C2-N1-C1'	11.71	131.75	117.70
1	C2	1	U	N3-C2-O2	-11.62	114.06	122.20
1	C2	453	U	N1-C2-O2	11.52	130.87	122.80
1	C2	830	U	C5-C4-O4	-11.14	119.22	125.90
3	C1	2209	U	N1-C2-O2	11.05	130.53	122.80
3	C1	3235	C	N3-C2-O2	-10.89	114.28	121.90
1	C2	1454	G	N1-C6-O6	-10.83	113.40	119.90
3	C1	1495	U	C2-N1-C1'	10.71	130.56	117.70
1	C2	818	C	C6-N1-C1'	-10.70	107.96	120.80
1	C2	35	U	N3-C2-O2	-10.64	114.75	122.20
12	SG	69	LEU	CA-CB-CG	10.58	139.63	115.30
1	C2	1440	С	N3-C2-O2	-10.55	114.52	121.90
1	C2	854	U	C5'-C4'-O4'	10.54	121.75	109.10
1	C2	1389	С	C2-N1-C1'	10.52	130.37	118.80
1	C2	853	G	C5-C6-O6	10.50	134.90	128.60
1	C2	1473	U	C2-N1-C1'	10.49	130.29	117.70



Ζ

Observed(°)

Ideal(°)

Continued from previous page										
Mol	Chain	Res	Type	Atoms						
3	C1	2209	U	N3-C2-O2						
3	C1	3235	С	N1-C2-O2						
1	CO	007	α	M1 CO OO						

114.88 -10.46 122.20 10.39 125.13 118.90 10.38 125.12 118.90 N1-C2-O2 T C2697 C 3 C12553U 117.70 C2-N1-C1' 10.26130.01 3  $\overline{\mathrm{C1}}$ 525 C N1-C2-O2 10.16 124.99 118.90 C11228С N3-C2-O2 -10.15114.79 3 121.90 3  $\overline{\mathrm{C1}}$ 2209 U C2-N1-C1' 10.13 129.86 117.70 3  $\overline{\mathrm{C1}}$ 758  $\overline{\mathbf{C}}$ N3-C2-O2 -10.13 114.81 121.90 1 C21246 С N1-C2-O2 10.13124.98 118.90 С 3 C18 C5-C6-N1 10.03 126.01 121.00 3 C12263 С C2-N1-C1' 10.01 129.81 118.80 3 C11501 U N3-C2-O2 -9.98 115.21 122.20 C2453 U 1 N3-C2-O2 -9.98115.21 122.20C2194 U 9.85 129.70 1 N1-C2-O2 122.80 C21210 С 1 N3-C2-O2 -9.85 115.00 121.90 3 C11515N1-C6-N6 -9.81112.71 А 118.603 C1 С C5-C6-N1 23669.80 125.90 121.00 С 3 C1 8 C6-N1-C2 -9.76 116.40 120.30 3 C11152G C5-C6-O6 9.73 134.44128.60 3 С C1102 N1-C2-O2 9.72 124.73 118.90 N3-C2-O2 3  $\overline{\mathrm{C1}}$ 175 C -9.71115.10 121.90 1 C21338 С C2-N1-C1' 9.70 129.47 118.80 3 C12263 С N1-C2-O2 9.66 124.70 118.90 5C3C 21 C2-N1-C1' 9.61 129.37 118.80 3  $\overline{\mathrm{C1}}$ 915 А 9.52 C2-N3-C4 115.36 110.60 C2650 U N3-C2-O2 -9.50115.55122.20 1 3  $\overline{\mathrm{C1}}$ 1437 С C6-N1-C2 -9.50 116.50 120.30 1 C2194 U N3-C2-O2 -9.49 115.56 122.20 1 C21209 С N3-C2-O2 -9.45115.29 121.90 1 C2697 С C2-N1-C1' 9.43 129.18 118.80 1 C21455G N3-C4-N9 -9.38 120.38 126.00 1  $\overline{\mathrm{C2}}$ 35 U N1-C2-O2 9.37 129.36 122.80 1 C2194U C2-N1-C1' 9.36 128.93117.70 C3U  $\overline{5}$ 82 C5-C6-N1 9.30 127.35 122.70 3 102 С C1N3-C2-O2 -9.28115.41 121.90 3 C11280 С -9.25 N3-C2-O2 115.42 121.90 С C2189 C6-N1-C2 -9.25 116.60 120.30 1 2537 U 3 C1N1-C2-O2 9.23 129.26 122.80 3 C12545С C2-N1-C1' 9.23 128.95 118.80 1 C2190 С N3-C2-O2 -9.23 115.44121.90 3 С C11199 N3-C4-N4 -9.20 111.56 118.00 3 C11283 С N1-C2-O2 9.18 124.41 118.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	453	U	C6-N1-C1'	-9.16	108.37	121.20
1	C2	583	С	C2-N1-C1'	9.16	128.87	118.80
1	C2	850	А	N7-C8-N9	9.16	118.38	113.80
1	C2	1454	G	C5-C6-O6	9.15	134.09	128.60
3	C1	729	С	C5-C6-N1	9.14	125.57	121.00
1	C2	1501	С	N3-C2-O2	-9.13	115.51	121.90
1	C2	1056	U	C5-C6-N1	9.10	127.25	122.70
1	C2	160	С	N1-C2-O2	9.09	124.35	118.90
3	C1	1283	С	N3-C2-O2	-9.09	115.54	121.90
3	C1	1907	С	N1-C2-O2	9.07	124.34	118.90
3	C1	525	С	N3-C2-O2	-9.01	115.59	121.90
1	C2	1591	С	C6-N1-C2	-8.93	116.73	120.30
1	C2	1473	U	N1-C2-O2	8.91	129.04	122.80
3	C1	75	G	N3-C2-N2	-8.88	113.68	119.90
1	C2	1501	С	C6-N1-C2	-8.86	116.76	120.30
1	C2	163	G	N3-C4-N9	-8.85	120.69	126.00
3	C1	2263	С	C5-C6-N1	8.80	125.40	121.00
3	C1	2237	С	N1-C2-O2	8.79	124.17	118.90
3	C1	2366	С	C6-N1-C2	-8.76	116.80	120.30
1	C2	614	С	C6-N1-C2	-8.69	116.82	120.30
3	C1	2572	С	N3-C2-O2	-8.65	115.85	121.90
3	C1	1819	U	N1-C2-O2	8.63	128.84	122.80
3	C1	2553	U	N1-C2-O2	8.63	128.84	122.80
3	C1	1878	G	C4-N9-C1'	8.62	137.71	126.50
3	C1	1228	С	C6-N1-C2	-8.62	116.85	120.30
1	C2	280	U	C2-N1-C1'	8.60	128.02	117.70
3	C1	935	U	C5-C6-N1	8.55	126.98	122.70
3	C1	2537	U	N3-C2-O2	-8.53	116.23	122.20
3	C1	2572	С	C2-N1-C1'	8.49	128.13	118.80
3	C1	1118	С	C6-N1-C2	-8.45	116.92	120.30
1	C2	1148	С	C6-N1-C2	-8.44	116.92	120.30
3	C1	1604	G	C2-N3-C4	8.43	116.11	111.90
1	C2	54	С	C6-N1-C2	-8.43	116.93	120.30
3	C1	2237	С	N3-C2-O2	-8.41	116.01	121.90
4	C4	105	С	N1-C2-O2	8.41	123.95	118.90
3	C1	113	C	C6-N1-C2	-8.41	116.94	120.30
1	C2	1440	C	C6-N1-C2	-8.39	116.94	120.30
3	C1	3357	U	C5-C6-N1	8.38	126.89	122.70
1	C2	191	C	C6-N1-C1'	8.36	130.83	120.80
1	C2	1560	U	C2-N1-C1'	8.35	127.72	117.70
1	C2	697	C	C5-C6-N1	8.33	$125.1\overline{7}$	121.00
1	C2	1214	U	C5-C6-N1	8.32	126.86	122.70



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	1309	U	N1-C2-O2	8.31	128.62	122.80
3	C1	758	С	C6-N1-C2	-8.29	116.99	120.30
1	C2	1185	U	C2-N1-C1'	8.28	127.64	117.70
1	C2	583	С	C6-N1-C2	-8.27	116.99	120.30
1	C2	1637	С	N1-C2-O2	8.25	123.85	118.90
1	C2	1000	С	C2-N1-C1'	8.21	127.83	118.80
3	C1	1817	G	O4'-C1'-N9	8.21	114.77	108.20
3	C1	1496	С	C2-N1-C1'	8.20	127.83	118.80
1	C2	850	А	C5-N7-C8	-8.20	99.80	103.90
1	C2	1440	С	N1-C2-O2	8.19	123.82	118.90
1	C2	1389	С	N1-C2-O2	8.18	123.81	118.90
1	C2	427	С	C6-N1-C2	-8.16	117.04	120.30
1	C2	853	G	N9-C1'-C2'	8.15	124.60	114.00
3	C1	2274	U	C2-N1-C1'	8.14	127.47	117.70
1	C2	697	С	C6-N1-C2	-8.14	117.05	120.30
1	C2	1274	С	N1-C2-O2	8.13	123.78	118.90
5	C3	64	U	N3-C2-O2	-8.13	116.51	122.20
1	C2	1252	С	C5-C6-N1	8.11	125.06	121.00
1	C2	1258	U	N3-C2-O2	-8.11	116.53	122.20
3	C1	1032	С	C6-N1-C2	-8.10	117.06	120.30
3	C1	986	U	N3-C2-O2	-8.09	116.54	122.20
1	C2	1246	С	C2-N1-C1'	8.08	127.69	118.80
1	C2	160	С	N3-C2-O2	-8.07	116.25	121.90
1	C2	1021	С	C2-N1-C1'	8.07	127.67	118.80
1	C2	163	G	N3-C4-C5	8.06	132.63	128.60
3	C1	113	С	C5-C6-N1	8.06	125.03	121.00
3	C1	2550	U	N3-C2-O2	-8.06	116.56	122.20
3	C1	1756	С	N3-C2-O2	-8.04	116.27	121.90
3	C1	3131	U	C2-N1-C1'	8.04	127.35	117.70
3	C1	113	С	C2-N1-C1'	8.04	127.64	118.80
3	C1	2594	С	C6-N1-C2	-8.04	117.08	120.30
1	C2	1248	С	C2-N1-C1'	8.03	127.63	118.80
3	C1	379	С	C6-N1-C2	-8.02	117.09	120.30
3	C1	3058	U	C2-N1-C1'	8.02	127.32	117.70
3	C1	715	А	C8-N9-C4	-8.01	102.60	105.80
1	C2	189	С	C5-C6-N1	8.00	125.00	121.00
3	C1	1495	U	N3-C2-O2	-7.99	116.61	122.20
1	C2	1185	U	N1-C2-O2	7.98	128.39	122.80
1	C2	848	C	N1-C2-O2	7.98	123.69	118.90
3	C1	1604	G	N3-C4-N9	7.97	130.78	126.00
1	C2	184	C	N1-C2-O2	7.97	123.68	118.90
3	C1	1819	U	N3-C2-O2	-7.97	116.62	122.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	C3	11	С	C6-N1-C2	-7.96	117.11	120.30
3	C1	1597	С	C5-C6-N1	7.96	124.98	121.00
3	C1	2406	С	C6-N1-C2	-7.94	117.12	120.30
1	C2	1389	С	C6-N1-C2	-7.94	117.12	120.30
1	C2	1473	U	C5-C6-N1	7.93	126.66	122.70
3	C1	69	С	N3-C2-O2	-7.92	116.35	121.90
3	C1	1437	С	C5-C6-N1	7.90	124.95	121.00
5	C3	11	С	C5-C6-N1	7.89	124.95	121.00
3	C1	2553	U	C6-N1-C1'	-7.89	110.16	121.20
3	C1	3252	G	N3-C4-N9	7.89	130.73	126.00
3	C1	729	С	C6-N1-C2	-7.87	117.15	120.30
3	C1	2545	С	N1-C2-O2	7.85	123.61	118.90
1	C2	614	С	C5-C6-N1	7.84	124.92	121.00
3	C1	2571	U	C2-N1-C1'	7.83	127.10	117.70
1	C2	855	А	O4'-C1'-N9	7.83	114.47	108.20
3	C1	2274	U	N1-C2-O2	7.83	128.28	122.80
1	C2	1060	U	N1-C2-O2	7.83	128.28	122.80
1	C2	1596	С	N1-C2-O2	7.82	123.59	118.90
1	C2	1674	С	C6-N1-C2	-7.80	117.18	120.30
1	C2	275	С	C2-N1-C1'	7.80	127.38	118.80
3	C1	2708	С	C5-C6-N1	7.78	124.89	121.00
3	C1	2594	С	C5-C6-N1	7.78	124.89	121.00
1	C2	1274	С	N3-C2-O2	-7.78	116.46	121.90
3	C1	2600	С	C5-C6-N1	7.76	124.88	121.00
3	C1	2646	С	C6-N1-C2	-7.76	117.20	120.30
1	C2	1141	G	N3-C2-N2	-7.75	114.47	119.90
3	C1	2513	U	OP1-P-O3'	7.75	122.25	105.20
1	C2	1214	U	N1-C2-O2	7.75	128.22	122.80
51	LN	124	ASP	CB-CG-OD1	7.75	125.27	118.30
1	C2	830	U	N3-C4-O4	7.73	124.81	119.40
3	C1	753	С	C6-N1-C2	-7.72	117.21	120.30
1	C2	1246	С	N3-C2-O2	-7.71	116.50	121.90
1	C2	184	С	C2-N1-C1'	7.71	127.28	118.80
3	C1	702	С	C6-N1-C2	-7.71	117.22	120.30
4	C4	68	С	C6-N1-C2	-7.70	117.22	120.30
1	C2	1455	G	N3-C4-C5	7.70	132.45	128.60
3	C1	982	С	C6-N1-C2	-7.70	117.22	120.30
1	C2	697	С	N3-C2-O2	-7.69	116.52	121.90
3	C1	1495	U	N1-C2-O2	7.68	128.18	122.80
3	C1	1832	С	C5-C6-N1	7.68	124.84	121.00
3	C1	638	С	C5-C6-N1	7.68	124.84	121.00
1	C2	14	С	N3-C2-O2	-7.68	116.52	121.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	853	G	C8-N9-C1'	7.67	136.98	127.00
3	C1	2199	G	C6-C5-N7	-7.67	125.80	130.40
3	C1	69	С	C6-N1-C2	-7.67	117.23	120.30
3	C1	2405	С	C6-N1-C2	-7.66	117.23	120.30
1	C2	1216	С	N3-C2-O2	-7.65	116.55	121.90
3	C1	745	С	C6-N1-C2	-7.63	117.25	120.30
3	C1	1338	С	C6-N1-C2	-7.63	117.25	120.30
3	C1	379	С	C5-C6-N1	7.63	124.81	121.00
3	C1	2844	С	C6-N1-C2	-7.62	117.25	120.30
5	C3	82	U	C6-N1-C2	-7.62	116.43	121.00
1	C2	1458	G	C4-N9-C1'	7.62	136.40	126.50
1	C2	1473	U	C6-N1-C1'	-7.61	110.55	121.20
1	C2	54	С	N3-C2-O2	-7.61	116.57	121.90
1	C2	1674	С	C5-C6-N1	7.60	124.80	121.00
3	C1	2407	С	C5-C6-N1	7.60	124.80	121.00
3	C1	1368	U	C2-N1-C1'	7.60	126.82	117.70
3	C1	1578	С	N1-C2-O2	7.58	123.45	118.90
1	C2	1458	G	N3-C4-C5	-7.58	124.81	128.60
3	C1	243	G	N3-C4-N9	7.58	130.55	126.00
3	C1	1222	G	O4'-C1'-N9	7.57	114.26	108.20
3	C1	1309	U	N3-C2-O2	-7.57	116.90	122.20
3	C1	2708	С	C6-N1-C2	-7.56	117.28	120.30
5	C3	21	С	C6-N1-C1'	-7.56	111.73	120.80
1	C2	583	С	C5-C6-N1	7.55	124.78	121.00
3	C1	2407	С	C6-N1-C2	-7.54	117.28	120.30
3	C1	2537	U	C2-N1-C1'	7.54	126.75	117.70
3	C1	1333	С	C5-C6-N1	7.53	124.77	121.00
3	C1	1878	G	C8-N9-C1'	-7.52	117.22	127.00
1	C2	427	С	C5-C6-N1	7.52	124.76	121.00
3	C1	174	С	N1-C2-O2	7.52	123.41	118.90
3	C1	2832	С	C6-N1-C2	-7.50	117.30	120.30
1	C2	1537	С	N3-C2-O2	-7.49	116.66	121.90
3	C1	500	С	C6-N1-C2	-7.49	117.31	120.30
1	C2	190	С	N1-C2-O2	7.48	123.39	118.90
3	C1	638	C	C6-N1-C2	-7.48	117.31	120.30
3	C1	1333	С	C6-N1-C2	-7.47	117.31	120.30
1	C2	1	U	C5-C6-N1	7.47	126.43	122.70
1	C2	14	C	C6-N1-C2	-7.46	117.32	120.30
1	C2	1	U	C6-N1-C1'	-7.46	110.76	121.20
3	C1	2204	C	N3-C2-O2	-7.45	116.68	121.90
3	C1	2336	U	N3-C2-O2	-7.45	116.99	122.20
3	C1	1145	G	C5-C6-O6	-7.44	124.13	128.60



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	2585	G	N3-C4-C5	-7.44	124.88	128.60
3	C1	1941	С	C6-N1-C2	-7.44	117.32	120.30
3	C1	2585	G	N3-C4-N9	7.43	130.46	126.00
3	C1	2263	С	C6-N1-C2	-7.41	117.33	120.30
3	C1	1307	G	P-O3'-C3'	7.40	128.58	119.70
3	C1	2652	U	N3-C2-O2	-7.40	117.02	122.20
3	C1	1496	С	C6-N1-C2	-7.39	117.34	120.30
3	C1	1907	С	N3-C2-O2	-7.39	116.72	121.90
3	C1	2108	С	C6-N1-C2	-7.39	117.34	120.30
1	C2	818	С	N1-C1'-C2'	7.39	123.60	114.00
3	C1	2638	С	C6-N1-C2	-7.39	117.35	120.30
1	C2	191	С	C2-N1-C1'	-7.38	110.68	118.80
3	C1	3042	U	C5-C6-N1	7.38	126.39	122.70
3	C1	2550	U	N1-C2-O2	7.37	127.96	122.80
3	C1	1320	С	C6-N1-C2	-7.34	117.36	120.30
1	C2	517	U	N3-C2-O2	-7.34	117.06	122.20
3	C1	1872	С	N1-C2-O2	7.34	123.30	118.90
1	C2	861	U	C2-N1-C1'	7.33	126.49	117.70
3	C1	2329	С	C5-C6-N1	7.32	124.66	121.00
5	C3	82	U	N1-C2-O2	7.31	127.92	122.80
3	C1	1815	U	P-O3'-C3'	7.31	128.47	119.70
1	C2	1255	G	OP1-P-O3'	7.27	121.20	105.20
1	C2	1389	С	C5-C6-N1	7.27	124.63	121.00
3	C1	102	С	C6-N1-C2	-7.27	117.39	120.30
1	C2	1007	С	C6-N1-C2	-7.25	117.40	120.30
3	C1	2132	С	C6-N1-C2	-7.25	117.40	120.30
1	C2	758	U	N1-C2-O2	7.25	127.87	122.80
1	C2	1141	G	C5-C6-O6	7.24	132.94	128.60
1	C2	462	G	O5'-P-OP1	-7.24	99.19	105.70
3	C1	1358	С	C5-C6-N1	7.24	124.62	121.00
1	C2	818	С	N3-C4-C5	7.23	124.79	121.90
1	C2	650	U	N1-C2-O2	7.22	127.86	122.80
1	C2	1455	G	C4-N9-C1'	-7.22	117.11	126.50
1	C2	1141	G	N9-C4-C5	7.22	108.29	105.40
3	C1	1525	G	C4-N9-C1'	7.22	135.88	126.50
3	C1	1579	С	N1-C2-O2	7.22	123.23	118.90
3	C1	3163	А	C5-C6-N6	-7.22	117.92	123.70
3	C1	650	С	C5-C6-N1	7.21	124.61	121.00
1	C2	1214	U	C2-N1-C1'	7.21	126.35	117.70
3	C1	1134	G	N9-C4-C5	7.20	108.28	105.40
3	C1	1844	С	C6-N1-C2	-7.18	117.43	120.30
1	C2	229	U	C5-C6-N1	7.18	126.29	122.70



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U

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	782	U	N1-C2-O2	7.18	127.83	122.80
1	C2	854	U	N3-C2-O2	-7.17	117.18	122.20
1	C2	111	U	N3-C2-O2	-7.16	117.19	122.20
3	C1	1338	С	C5-C6-N1	7.16	124.58	121.00
3	C1	1579	С	N3-C2-O2	-7.16	116.89	121.90
3	C1	2154	U	N3-C2-O2	-7.16	117.19	122.20
3	C1	325	А	C2-N3-C4	7.15	114.18	110.60
3	C1	2571	U	N1-C2-O2	7.15	127.80	122.80
5	C3	38	U	N3-C2-O2	-7.15	117.19	122.20
1	C2	1338	С	N1-C2-O2	7.15	123.19	118.90
3	C1	438	А	C2-N3-C4	7.15	114.17	110.60
3	C1	700	С	C6-N1-C2	-7.15	117.44	120.30
3	C1	1032	С	C5-C6-N1	7.15	124.57	121.00
1	C2	639	U	N3-C2-O2	-7.14	117.20	122.20
1	C2	864	U	C2-N1-C1'	7.14	126.26	117.70
3	C1	3231	U	C5-C6-N1	7.14	126.27	122.70
1	C2	1097	U	P-O3'-C3'	7.13	128.26	119.70
3	C1	881	С	C6-N1-C2	-7.13	117.45	120.30
3	C1	1095	U	C2-N1-C1'	7.13	126.26	117.70
3	C1	2552	С	C2-N1-C1'	7.13	126.64	118.80
1	C2	1497	U	C5-C6-N1	7.12	126.26	122.70
1	C2	1239	U	C5-C6-N1	7.12	126.26	122.70
3	C1	1115	G	C4-N9-C1'	7.12	135.76	126.50
3	C1	2513	U	P-O3'-C3'	7.12	128.24	119.70
1	C2	1527	С	C5-C6-N1	7.11	124.56	121.00
1	C2	747	С	C5-C6-N1	7.11	124.55	121.00
1	C2	21	U	N3-C2-O2	-7.11	117.23	122.20
3	C1	1145	G	C4-C5-N7	7.11	113.64	110.80
1	C2	758	U	N3-C2-O2	-7.10	117.23	122.20
3	C1	2894	С	C6-N1-C2	-7.10	117.46	120.30
3	C1	327	А	N1-C6-N6	-7.10	114.34	118.60
3	C1	2199	G	C4-N9-C1'	7.09	135.72	126.50
1	C2	1514	U	N1-C2-O2	7.09	127.76	122.80
1	C2	280	U	N1-C2-O2	7.07	127.75	122.80
3	C1	713	U	N3-C2-O2	-7.07	117.25	122.20
1	C2	1060	U	C2-N1-C1'	7.06	126.17	117.70
3	C1	1095	U	N1-C2-O2	7.06	127.74	122.80
3	C1	2199	G	N3-C4-N9	7.06	130.23	126.00
3	C1	1241	U	P-O3'-C3'	7.05	128.16	119.70
1	C2	1210	С	N1-C2-N3	7.05	124.13	119.20
1	C2	1455	G	C8-N9-C1'	7.04	136.16	127.00

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122.20

117.27



-7.04

N3-C2-O2

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	1437	С	C2-N1-C1'	7.04	126.55	118.80
4	C4	96	U	C5-C6-N1	7.04	126.22	122.70
3	C1	2329	С	C6-N1-C2	-7.02	117.49	120.30
1	C2	116	U	N3-C2-O2	-7.02	117.29	122.20
1	C2	1161	С	C6-N1-C2	-7.02	117.49	120.30
3	C1	2928	С	C6-N1-C2	-7.02	117.49	120.30
1	C2	1637	С	C2-N1-C1'	7.01	126.52	118.80
3	C1	1031	С	C5-C6-N1	7.00	124.50	121.00
5	C3	21	С	C5-C6-N1	7.00	124.50	121.00
5	C3	82	U	N3-C2-O2	-7.00	117.30	122.20
3	C1	1856	С	C5-C6-N1	7.00	124.50	121.00
1	C2	54	С	N1-C2-O2	6.99	123.09	118.90
1	C2	1458	G	N3-C4-N9	6.99	130.19	126.00
1	C2	542	А	P-O3'-C3'	6.98	128.08	119.70
3	C1	427	С	C6-N1-C2	-6.98	117.51	120.30
3	C1	2773	С	C6-N1-C2	-6.98	117.51	120.30
3	C1	180	С	C6-N1-C2	-6.97	117.51	120.30
3	C1	2683	U	C5-C6-N1	6.97	126.19	122.70
3	C1	3301	U	N3-C2-O2	-6.97	117.32	122.20
1	C2	1580	С	C5-C6-N1	6.97	124.49	121.00
3	C1	2389	С	C5-C6-N1	6.97	124.48	121.00
3	C1	1081	U	P-O3'-C3'	6.96	128.05	119.70
1	C2	795	U	C2-N1-C1'	6.96	126.05	117.70
3	C1	1501	U	C2-N3-C4	-6.96	122.83	127.00
3	C1	1495	U	C6-N1-C1'	-6.95	111.47	121.20
1	C2	686	С	C6-N1-C2	-6.95	117.52	120.30
1	C2	1338	С	C5-C6-N1	6.95	124.47	121.00
3	C1	995	U	N1-C2-O2	6.95	127.67	122.80
3	C1	776	U	C5-C6-N1	-6.94	119.23	122.70
3	C1	1496	С	N1-C2-O2	6.94	123.06	118.90
3	C1	3190	С	C6-N1-C2	-6.93	117.53	120.30
1	C2	853	G	C5-N7-C8	6.93	107.77	104.30
1	C2	1389	С	C6-N1-C1'	-6.93	112.48	120.80
1	C2	854	U	N1-C2-N3	6.93	119.06	114.90
3	C1	1716	U	P-O3'-C3'	6.92	128.01	119.70
1	C2	1620	С	P-O3'-C3'	6.92	128.01	119.70
3	C1	1763	U	N1-C2-O2	6.92	127.64	122.80
3	C1	886	С	C5-C6-N1	6.92	124.46	121.00
3	C1	1199	C	C5-C4-N4	6.92	125.04	120.20
1	C2	1560	U	N3-C2-O2	-6.92	117.36	122.20
1	C2	795	U	N3-C2-O2	-6.91	117.36	122.20
3	C1	3105	U	N3-C2-O2	-6.91	117.36	122.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	C3	76	С	C6-N1-C2	-6.91	117.54	120.30
3	C1	2383	С	N3-C2-O2	-6.90	117.07	121.90
1	C2	817	А	C5-C6-N1	6.89	121.15	117.70
3	C1	283	G	N3-C4-N9	6.89	130.14	126.00
18	SM	62	LEU	CA-CB-CG	6.89	131.15	115.30
3	C1	2772	С	P-O3'-C3'	6.88	127.96	119.70
3	C1	3058	U	N1-C2-O2	6.88	127.62	122.80
3	C1	985	U	N3-C2-O2	-6.88	117.38	122.20
1	C2	136	С	N1-C2-O2	6.88	123.03	118.90
1	C2	1596	С	C2-N1-C1'	6.88	126.36	118.80
1	C2	854	U	C6-N1-C2	-6.88	116.88	121.00
1	C2	1596	С	N3-C2-O2	-6.88	117.09	121.90
1	C2	817	А	N3-C4-N9	6.87	132.89	127.40
3	C1	1604	G	C4-N9-C1'	6.86	135.42	126.50
1	C2	1185	U	N3-C2-O2	-6.86	117.40	122.20
3	C1	220	G	N3-C4-N9	6.86	130.12	126.00
1	C2	1637	С	C5-C6-N1	6.86	124.43	121.00
1	C2	139	С	P-O3'-C3'	6.85	127.92	119.70
1	C2	1560	U	N1-C2-O2	6.85	127.60	122.80
1	C2	120	U	N3-C2-O2	-6.84	117.41	122.20
1	C2	532	U	N3-C2-O2	-6.84	117.42	122.20
1	C2	320	U	O5'-P-OP1	-6.83	99.55	105.70
3	C1	2707	С	C5-C6-N1	6.83	124.41	121.00
3	C1	1118	С	C5-C6-N1	6.83	124.41	121.00
1	C2	1429	G	N3-C4-N9	6.82	130.09	126.00
1	C2	1514	U	N3-C2-O2	-6.82	117.43	122.20
3	C1	524	U	N1-C2-O2	6.82	127.57	122.80
1	C2	1081	А	N7-C8-N9	6.81	117.20	113.80
3	C1	2708	С	C2-N1-C1'	6.81	126.29	118.80
1	C2	1506	G	N3-C4-N9	6.81	130.08	126.00
1	C2	1591	С	C5-C6-N1	6.81	124.40	121.00
3	C1	2652	U	N1-C2-O2	6.80	127.56	122.80
3	C1	2274	U	N3-C2-O2	-6.80	117.44	122.20
1	C2	695	U	N3-C2-O2	-6.79	117.45	122.20
1	C2	1389	С	N3-C2-O2	-6.79	117.15	121.90
3	C1	496	C	C5-C6-N1	6.79	124.39	121.00
3	C1	3039	C	C6-N1-C2	-6.79	117.59	120.30
3	C1	1052	U	N3-C2-O2	-6.78	117.46	122.20
1	C2	1248	C	C6-N1-C2	-6.78	117.59	120.30
1	C2	163	G	C8-N9-C1'	6.77	135.81	127.00
3	C1	1024	G	O4'-C1'-N9	6.77	113.62	108.20
3	C1	1577	G	N3-C2-N2	6.77	124.64	119.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	1448	G	N1-C2-N2	-6.76	110.11	116.20
3	C1	927	С	C6-N1-C2	-6.76	117.59	120.30
1	C2	1210	С	C6-N1-C2	-6.76	117.59	120.30
3	C1	2568	С	N3-C2-O2	-6.75	117.17	121.90
3	C1	427	С	C5-C6-N1	6.75	124.37	121.00
1	C2	817	А	C6-N1-C2	-6.74	114.56	118.60
1	C2	1340	U	N3-C2-O2	-6.74	117.48	122.20
1	C2	1527	С	C2-N1-C1'	6.74	126.21	118.80
1	C2	1338	С	C6-N1-C1'	-6.74	112.71	120.80
3	C1	663	С	C6-N1-C2	-6.74	117.61	120.30
1	C2	161	U	N3-C2-O2	-6.73	117.49	122.20
3	C1	679	U	C5-C6-N1	6.73	126.06	122.70
3	C1	1589	А	N1-C6-N6	-6.73	114.56	118.60
3	C1	2836	С	N1-C2-O2	6.73	122.94	118.90
3	C1	283	G	C4-C5-N7	6.73	113.49	110.80
3	C1	3214	U	C2-N1-C1'	6.73	125.77	117.70
3	C1	2263	С	C6-N1-C1'	-6.73	112.73	120.80
3	C1	2405	С	C2-N1-C1'	6.72	126.20	118.80
1	C2	453	U	C5-C6-N1	6.72	126.06	122.70
3	C1	111	С	C6-N1-C2	-6.72	117.61	120.30
3	C1	1320	С	C5-C6-N1	6.72	124.36	121.00
3	C1	1134	G	N1-C6-O6	-6.72	115.87	119.90
3	C1	2094	С	C6-N1-C2	-6.72	117.61	120.30
1	C2	864	U	N1-C2-O2	6.71	127.50	122.80
3	C1	803	С	C5-C6-N1	6.71	124.35	121.00
1	C2	975	С	C6-N1-C2	-6.71	117.62	120.30
5	C3	21	С	N1-C2-O2	6.71	122.92	118.90
3	C1	243	G	N3-C4-C5	-6.70	125.25	128.60
3	C1	1115	G	C8-N9-C1'	-6.70	118.29	127.00
1	C2	14	С	N1-C2-N3	6.70	123.89	119.20
3	C1	524	U	N3-C2-O2	-6.69	117.51	122.20
3	C1	2118	С	N1-C2-O2	6.69	122.92	118.90
3	C1	2548	С	C2-N1-C1'	6.69	126.16	118.80
1	C2	272	U	P-O3'-C3'	6.69	127.72	119.70
1	C2	229	U	C2-N1-C1'	6.68	125.72	117.70
1	C2	1338	C	C6-N1-C2	-6.68	117.63	120.30
3	C1	753	С	C5-C6-N1	6.67	124.34	121.00
3	C1	1597	C	C6-N1-C2	-6.67	117.63	120.30
3	C1	2612	U	N3-C4-O4	6.67	124.07	119.40
1	C2	1209	С	N1-C2-O2	6.67	122.90	118.90
1	C2	120	U	N1-C2-O2	6.67	127.47	122.80
3	C1	1638	A	C8-N9-C4	-6.67	103.13	105.80



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	1097	U	OP2-P-O3'	6.66	119.86	105.20
3	C1	2545	С	C6-N1-C1'	-6.66	112.81	120.80
3	C1	193	С	C5-C6-N1	6.66	124.33	121.00
3	C1	27	С	C6-N1-C2	-6.65	117.64	120.30
3	C1	2683	U	C2-N1-C1'	6.65	125.67	117.70
3	C1	439	С	C6-N1-C2	-6.64	117.64	120.30
1	C2	1246	С	C6-N1-C2	-6.64	117.64	120.30
1	C2	160	С	C6-N1-C2	-6.64	117.64	120.30
1	C2	1021	С	N1-C2-O2	6.64	122.88	118.90
3	C1	2199	G	C8-N9-C1'	-6.63	118.38	127.00
3	C1	1706	С	N1-C2-O2	6.63	122.88	118.90
3	C1	3116	G	N1-C6-O6	-6.63	115.92	119.90
1	C2	1270	G	N3-C4-N9	6.63	129.98	126.00
3	C1	561	С	C6-N1-C2	-6.63	117.65	120.30
3	C1	2988	C	C6-N1-C2	-6.63	117.65	120.30
1	C2	1060	U	N3-C2-O2	-6.62	117.57	122.20
1	C2	1248	С	C5-C6-N1	6.61	124.30	121.00
3	C1	1878	G	N3-C4-N9	6.60	129.96	126.00
3	C1	3252	G	N3-C4-C5	-6.60	125.30	128.60
3	C1	325	A	C5-C6-N1	6.60	121.00	117.70
3	C1	561	С	C2-N1-C1'	6.60	126.06	118.80
1	C2	1115	U	N1-C2-O2	6.59	127.41	122.80
3	C1	286	U	C5-C6-N1	6.58	125.99	122.70
1	C2	1249	U	C5-C6-N1	6.58	125.99	122.70
5	C3	100	U	C2-N1-C1'	6.57	125.59	117.70
3	C1	2571	U	N3-C2-O2	-6.57	117.60	122.20
3	C1	544	С	C6-N1-C1'	6.57	128.68	120.80
1	C2	196	G	N3-C4-N9	-6.56	122.06	126.00
3	C1	2572	С	C6-N1-C1'	-6.56	112.93	120.80
3	C1	2843	U	N3-C2-O2	-6.56	117.61	122.20
1	C2	101	U	N1-C2-O2	6.56	127.39	122.80
3	C1	1843	C	C5-C6-N1	6.56	124.28	121.00
3	C1	3163	A	N1-C6-N6	6.56	122.54	118.60
1	C2	916	U	N3-C2-O2	-6.56	117.61	122.20
3	C1	2181	С	C5-C6-N1	6.56	124.28	121.00
1	C2	1216	С	C6-N1-C2	-6.55	117.68	120.30
1	C2	101	U	N3-C2-O2	-6.55	117.62	122.20
3	C1	645	A	C2-N3-C4	6.54	113.87	110.60
3	C1	2553	U	N3-C2-O2	-6.54	117.62	122.20
3	C1	2612	U	C5-C4-O4	-6.54	121.98	125.90
3	C1	2889	C	C5-C6-N1	6.54	$1\overline{24.2}\overline{7}$	121.00
44	LF	229	PHE	CB-CG-CD1	6.54	125.37	120.80



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C1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C3	100	U	C5-C6-N1	6.53	125.97	122.70
1	C2	767	U	C2-N1-C1'	6.53	125.53	117.70
1	C2	223	U	N1-C2-O2	6.53	127.37	122.80
3	C1	1368	U	N1-C2-O2	6.53	127.37	122.80
1	C2	1573	A	P-O3'-C3'	6.52	127.53	119.70
3	C1	2266	U	N3-C2-O2	-6.52	117.64	122.20
3	C1	2146	С	C6-N1-C2	-6.52	117.69	120.30
3	C1	101	G	C8-N9-C1'	-6.52	118.53	127.00
3	C1	1869	С	C5-C6-N1	6.52	124.26	121.00
1	C2	874	С	N3-C2-O2	-6.52	117.34	121.90
1	C2	743	U	C5-C6-N1	6.51	125.96	122.70
3	C1	1496	С	C5-C6-N1	6.51	124.26	121.00
3	C1	1589	А	C5-C6-N1	6.51	120.95	117.70
1	C2	189	С	N1-C2-O2	6.51	122.81	118.90
1	C2	1000	С	C6-N1-C1'	-6.50	113.00	120.80
3	C1	2585	G	C4-N9-C1'	6.50	134.94	126.50
3	C1	3357	U	N1-C2-O2	6.50	127.35	122.80
3	C1	1525	G	C8-N9-C1'	-6.50	118.56	127.00
1	C2	1537	С	C6-N1-C2	-6.49	117.70	120.30
1	C2	189	С	N3-C2-O2	-6.49	117.36	121.90
3	C1	3163	А	C4-C5-N7	6.49	113.94	110.70
3	C1	2206	G	N3-C4-C5	-6.48	125.36	128.60
3	C1	3111	U	C5-C6-N1	6.48	125.94	122.70
3	C1	270	U	N3-C2-O2	-6.48	117.66	122.20
3	C1	1878	G	N3-C4-C5	-6.48	125.36	128.60
3	C1	945	С	C6-N1-C2	-6.48	117.71	120.30
3	C1	2353	G	N3-C4-N9	6.48	129.89	126.00
3	C1	2434	U	C2-N1-C1'	6.48	125.47	117.70
3	C1	3235	С	C6-N1-C2	-6.48	117.71	120.30
1	C2	816	G	N1-C6-O6	-6.47	116.02	119.90
3	C1	283	G	C4-N9-C1'	6.47	134.92	126.50
3	C1	577	С	C6-N1-C2	-6.47	117.71	120.30
3	C1	1312	С	C6-N1-C2	-6.47	117.71	120.30
3	C1	2112	U	P-O3'-C3'	6.47	127.47	119.70
3	C1	1377	G	C5-C6-O6	6.47	132.48	128.60
3	C1	2928	C	C5-C6-N1	6.46	124.23	121.00
1	C2	144	U	C2-N1-C1'	6.46	125.45	117.70
3	C1	1175	C	C6-N1-C2	-6.45	117.72	120.30
3	C1	1579	C	C6-N1-C2	-6.45	117.72	120.30
1	C2	842	C	N1-C2-O2	6.45	122.77	118.90
3	C1	3023	U	N3-C2-O2	-6.45	117.69	$12\overline{2.20}$

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122.20

117.69



N3-C2-O2

-6.45

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	196	G	N3-C4-C5	6.45	131.82	128.60
3	C1	1701	С	C5-C6-N1	6.45	124.22	121.00
3	C1	2970	С	C5-C6-N1	6.45	124.22	121.00
3	C1	1273	А	C5-C6-N6	-6.44	118.55	123.70
3	C1	3084	С	C6-N1-C2	-6.44	117.72	120.30
3	C1	2546	С	C2-N1-C1'	6.44	125.88	118.80
5	C3	4	С	C6-N1-C2	-6.44	117.72	120.30
1	C2	382	С	C5-C6-N1	6.43	124.22	121.00
1	C2	644	С	N1-C2-O2	6.43	122.76	118.90
1	C2	1058	U	P-O3'-C3'	6.43	127.42	119.70
3	C1	946	U	C5-C6-N1	6.43	125.91	122.70
3	C1	2431	С	C6-N1-C2	-6.43	117.73	120.30
3	C1	927	С	C5-C6-N1	6.42	124.21	121.00
3	C1	2101	С	C6-N1-C2	-6.42	117.73	120.30
3	C1	1578	С	N3-C2-O2	-6.42	117.41	121.90
3	C1	315	С	C2-N1-C1'	6.42	125.86	118.80
1	C2	587	С	C6-N1-C2	-6.41	117.74	120.30
3	C1	142	С	C6-N1-C2	-6.41	117.74	120.30
3	C1	1604	G	C8-N9-C1'	-6.41	118.67	127.00
4	C4	113	С	C5-C6-N1	6.41	124.20	121.00
3	C1	2389	С	C6-N1-C2	-6.40	117.74	120.30
3	C1	1604	G	N3-C4-C5	-6.40	125.40	128.60
3	C1	1478	С	C6-N1-C2	-6.40	117.74	120.30
3	C1	1219	С	N1-C2-O2	6.40	122.74	118.90
3	C1	1092	С	C6-N1-C2	-6.39	117.75	120.30
3	C1	220	G	N9-C4-C5	-6.37	102.85	105.40
1	C2	1077	С	N3-C2-O2	-6.36	117.45	121.90
5	C3	143	U	C5-C6-N1	6.36	125.88	122.70
5	C3	4	С	C5-C6-N1	6.36	124.18	121.00
1	C2	1456	С	N1-C2-O2	6.35	122.71	118.90
3	C1	2204	С	C6-N1-C2	-6.35	117.76	120.30
1	C2	1332	С	C6-N1-C2	-6.35	117.76	120.30
3	C1	1448	U	N1-C2-O2	6.35	127.25	122.80
38	Sg	23	LEU	CA-CB-CG	6.34	129.89	115.30
1	C2	118	U	N3-C4-O4	-6.34	114.96	119.40
1	C2	184	С	N3-C2-O2	-6.34	117.46	121.90
3	C1	2827	U	C2-N1-C1'	6.34	125.31	117.70
1	C2	1458	G	C8-N9-C1'	-6.34	118.76	127.00
1	C2	176	С	C5-C6-N1	6.34	124.17	121.00
3	C1	1819	U	C2-N1-C1'	6.34	125.30	117.70
3	C1	2405	С	C5-C6-N1	6.34	124.17	121.00
49	LL	140	SER	C-N-CA	6.34	137.54	121.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	548	G	C5-C6-O6	6.33	132.40	128.60
3	C1	1916	U	C5-C6-N1	6.33	125.87	122.70
41	LC	91	GLY	N-CA-C	-6.33	97.27	113.10
1	C2	745	U	C5-C6-N1	6.33	125.87	122.70
3	C1	3007	U	C5-C6-N1	6.33	125.86	122.70
3	C1	2986	U	C5-C6-N1	6.33	125.86	122.70
3	C1	3231	U	N1-C2-O2	6.33	127.23	122.80
1	C2	644	С	C2-N1-C1'	6.33	125.76	118.80
3	C1	1155	С	C6-N1-C2	-6.31	117.77	120.30
1	C2	1053	G	N3-C4-C5	-6.31	125.44	128.60
1	C2	848	С	N3-C2-O2	-6.31	117.48	121.90
3	C1	1155	С	C2-N1-C1'	6.31	125.74	118.80
3	C1	1273	А	C4-C5-N7	6.31	113.85	110.70
3	C1	1671	С	C6-N1-C2	-6.30	117.78	120.30
3	C1	3043	С	C6-N1-C2	-6.30	117.78	120.30
5	C3	113	U	C2-N1-C1'	6.30	125.26	117.70
3	C1	3357	U	C6-N1-C2	-6.30	117.22	121.00
3	C1	2836	С	C2-N1-C1'	6.29	125.72	118.80
3	C1	3383	G	C4-N9-C1'	6.29	134.68	126.50
3	C1	404	G	C4-C5-N7	6.29	113.32	110.80
3	C1	2209	U	C6-N1-C1'	-6.29	112.40	121.20
1	C2	1613	U	C5-C6-N1	6.29	125.84	122.70
3	C1	1448	U	C2-N1-C1'	6.28	125.24	117.70
1	C2	558	U	P-O3'-C3'	6.28	127.23	119.70
1	C2	975	С	C5-C6-N1	6.27	124.14	121.00
1	C2	1506	G	C4-N9-C1'	6.27	134.65	126.50
1	C2	1527	С	C6-N1-C2	-6.27	117.79	120.30
3	C1	3317	U	P-O3'-C3'	6.26	127.22	119.70
3	C1	1190	А	C4-N9-C1'	6.26	137.57	126.30
3	C1	2844	С	C5-C6-N1	6.26	124.13	121.00
3	C1	3228	С	P-O3'-C3'	6.26	127.21	119.70
1	C2	417	А	P-O3'-C3'	6.26	127.21	119.70
1	C2	1777	G	N3-C4-C5	-6.26	125.47	128.60
1	C2	1148	С	C5-C6-N1	6.25	124.13	121.00
3	C1	184	U	N1-C2-O2	6.25	127.18	122.80
3	C1	543	С	N1-C2-O2	6.25	122.65	118.90
1	C2	35	U	C2-N1-C1'	6.25	125.20	117.70
1	C2	965	U	C2-N1-C1'	6.25	125.20	117.70
3	C1	663	C	C5-C6-N1	6.25	124.12	121.00
3	C1	1152	G	C5-N7-C8	-6.24	101.18	104.30
3	C1	2274	U	C5-C6-N1	6.24	125.82	122.70
3	C1	3269	U	P-O3'-C3'	6.24	127.19	119.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	548	G	N3-C4-N9	-6.24	122.26	126.00
3	C1	1582	С	C6-N1-C2	-6.24	117.81	120.30
4	C4	105	С	N3-C2-O2	-6.23	117.54	121.90
3	C1	700	С	C5-C6-N1	6.23	124.11	121.00
5	C3	80	А	P-O3'-C3'	6.23	127.17	119.70
1	C2	1141	G	N1-C6-O6	-6.22	116.17	119.90
1	C2	1439	С	N1-C2-O2	6.22	122.63	118.90
3	C1	1152	G	C4-C5-N7	6.22	113.29	110.80
1	C2	185	U	N3-C2-O2	-6.22	117.84	122.20
1	C2	1034	С	C6-N1-C2	-6.22	117.81	120.30
3	C1	354	U	N1-C2-O2	6.22	127.16	122.80
1	C2	1572	G	C4-N9-C1'	6.22	134.59	126.50
3	C1	3058	U	N3-C2-O2	-6.22	117.85	122.20
42	LD	179	ARG	C-N-CA	6.22	137.25	121.70
3	C1	356	С	C5-C6-N1	6.22	124.11	121.00
3	C1	1901	А	C8-N9-C4	-6.22	103.31	105.80
3	C1	2905	U	C5-C6-N1	6.22	125.81	122.70
44	m LF	179	LEU	CA-CB-CG	6.22	129.60	115.30
1	C2	1058	U	OP1-P-O3'	6.21	118.86	105.20
3	C1	1219	С	C6-N1-C2	-6.21	117.81	120.30
3	C1	2731	U	C5-C6-N1	6.21	125.81	122.70
1	C2	1024	U	N3-C2-O2	-6.21	117.86	122.20
1	C2	1053	G	N3-C4-N9	6.21	129.72	126.00
1	C2	1077	С	N1-C2-O2	6.21	122.62	118.90
1	C2	834	G	C4-N9-C1'	6.21	134.57	126.50
1	C2	1255	G	P-O3'-C3'	6.20	127.14	119.70
3	C1	42	С	C6-N1-C2	-6.20	117.82	120.30
3	C1	1064	А	P-O3'-C3'	6.20	127.14	119.70
3	C1	283	G	C8-N9-C1'	-6.20	118.94	127.00
3	C1	502	U	C5-C6-N1	6.20	125.80	122.70
1	C2	1258	U	C2-N1-C1'	6.20	125.14	117.70
4	C4	68	С	C5-C6-N1	6.20	124.10	121.00
1	C2	1448	G	N3-C2-N2	6.19	124.24	119.90
3	C1	1175	С	C5-C6-N1	6.19	124.10	121.00
3	C1	1140	G	C4-N9-C1'	6.19	134.55	126.50
1	C2	1473	U	N3-C2-O2	-6.19	117.87	122.20
1	C2	782	U	N3-C2-O2	-6.19	117.87	122.20
3	C1	3118	С	N1-C2-O2	6.18	122.61	118.90
1	C2	382	С	C6-N1-C2	-6.18	117.83	120.30
1	C2	1220	С	C2-N1-C1'	6.18	125.60	118.80
1	C2	449	С	C6-N1-C2	-6.18	117.83	120.30
1	C2	842	С	N3-C2-O2	-6.17	117.58	121.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	2610	G	C6-C5-N7	-6.17	126.70	130.40
3	C1	142	С	C5-C6-N1	6.17	124.08	121.00
3	C1	161	G	C6-C5-N7	-6.17	126.70	130.40
3	C1	803	С	C6-N1-C2	-6.17	117.83	120.30
3	C1	406	G	O4'-C1'-N9	6.16	113.13	108.20
3	C1	1515	А	C5-C6-N6	6.16	128.63	123.70
3	C1	2610	G	N7-C8-N9	6.16	116.18	113.10
3	C1	823	С	C6-N1-C2	-6.16	117.84	120.30
3	C1	949	С	C5-C6-N1	6.15	124.08	121.00
3	C1	512	U	N3-C2-O2	-6.15	117.89	122.20
3	C1	2199	G	C4-C5-N7	6.15	113.26	110.80
3	C1	881	С	N3-C2-O2	-6.15	117.60	121.90
3	C1	2190	U	C5-C6-N1	6.15	125.77	122.70
1	C2	1098	U	O5'-P-OP2	-6.14	100.17	105.70
3	C1	1669	С	C5-C6-N1	6.14	124.07	121.00
33	$\operatorname{Sb}$	59	CYS	CA-CB-SG	6.14	125.05	114.00
1	C2	163	G	C4-N9-C1'	-6.14	118.52	126.50
3	C1	3190	С	C5-C6-N1	6.14	124.07	121.00
5	C3	82	U	C2-N1-C1'	6.14	125.06	117.70
1	C2	191	С	C5-C4-N4	6.13	124.49	120.20
1	C2	1119	G	N3-C4-C5	-6.13	125.53	128.60
7	SB	54	LEU	CA-CB-CG	6.13	129.40	115.30
3	C1	2263	С	N3-C2-O2	-6.13	117.61	121.90
3	C1	2788	С	C5-C6-N1	6.12	124.06	121.00
1	C2	587	С	C5-C6-N1	6.12	124.06	121.00
3	C1	881	С	C2-N1-C1'	6.11	125.52	118.80
1	C2	144	U	C5-C4-O4	-6.11	122.23	125.90
1	C2	4	С	C6-N1-C2	-6.11	117.86	120.30
3	C1	2638	С	C5-C6-N1	6.11	124.05	121.00
3	C1	65	А	P-O3'-C3'	6.11	127.03	119.70
3	C1	2304	С	N1-C2-O2	6.10	122.56	118.90
1	C2	852	С	N3-C2-O2	-6.10	117.63	121.90
3	C1	1134	G	C4-C5-N7	-6.10	108.36	110.80
3	C1	2843	U	C2-N1-C1'	6.10	125.02	117.70
3	C1	655	С	C6-N1-C2	-6.10	117.86	120.30
3	C1	794	U	C5-C6-N1	6.10	125.75	122.70
3	C1	2189	U	N3-C2-O2	-6.09	117.94	122.20
3	C1	3321	C	C6-N1-C2	-6.09	117.86	120.30
3	C1	1282	G	N1-C6-O6	-6.09	116.25	119.90
3	C1	421	G	N3-C4-N9	6.09	129.65	126.00
1	C2	194	U	$C6-N1-\overline{C1'}$	-6.08	112.68	121.20
3	C1	2337	С	C6-N1-C2	-6.08	117.87	120.30



 $Ideal(^{o})$ 

119.70

128.60 120.30

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$
3	C1	735	А	P-O3'-C3'	6.08	127.00
3	C1	1237	G	N3-C4-C5	-6.08	125.56
3	C1	2711	С	C6-N1-C2	-6.08	117.87
3	C1	2953	U	C5-C6-N1	6.07	125.74
3	C1	3350	С	C2-N1-C1'	6.07	125.48
3	C1	2546	С	N1-C2-O2	6.07	122.54
3	C1	151	А	P-O3'-C3'	6.07	126.98
3	C1	297	G	O4'-C1'-N9	6.07	113.06
3	C1	1356	U	N3-C2-O2	-6.07	117.95
1	C2	610	G	C4-N9-C1'	6.07	134.38
1	C2	1196	А	P-O3'-C3'	6.07	126.98
3	C1	576	С	C6-N1-C2	-6.07	117.87
1	C2	1620	С	C6-N1-C2	-6.06	117.88
3	C1	4	U	C5-C6-N1	6.06	125.73
3	C1	1309	U	C2-N1-C1'	6.06	124.97
3	C1	2582	С	C5-C6-N1	6.06	124.03
3	C1	1854	С	C6-N1-C2	-6.06	117.88
3	C1	2190	U	C2-N1-C1'	6.06	124.97
3	C1	2550	U	C2-N1-C1'	6.05	124.97
3	C1	3023	U	C2-N1-C1'	6.05	124.97
1	C2	687	G	N3-C2-N2	-6.05	115.67
3	C1	78	U	C2-N3-C4	-6.05	123.37
3	C1	1579	С	C2-N1-C1'	6.05	125.45
1	C2	916	U	N1-C2-O2	6.04	127.03
1	C2	1342	C	C2-N1-C1'	6.04	125.44
3	C1	969	C	C6-N1-C2	-6.04	117.89
3	C1	2548	C	C5-C6-N1	6.03	124.02
19	SN	80	LEU	CA-CB-CG	6.03	129.17
3	C1	1495	U	C5-C6-N1	6.03	125.72

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3	C1	2953	U	C5-C6-N1	6.07	125.74	122.70
3	C1	3350	С	C2-N1-C1'	6.07	125.48	118.80
3	C1	2546	С	N1-C2-O2	6.07	122.54	118.90
3	C1	151	А	P-O3'-C3'	6.07	126.98	119.70
3	C1	297	G	O4'-C1'-N9	6.07	113.06	108.20
3	C1	1356	U	N3-C2-O2	-6.07	117.95	122.20
1	C2	610	G	C4-N9-C1'	6.07	134.38	126.50
1	C2	1196	А	P-O3'-C3'	6.07	126.98	119.70
3	C1	576	С	C6-N1-C2	-6.07	117.87	120.30
1	C2	1620	С	C6-N1-C2	-6.06	117.88	120.30
3	C1	4	U	C5-C6-N1	6.06	125.73	122.70
3	C1	1309	U	C2-N1-C1'	6.06	124.97	117.70
3	C1	2582	С	C5-C6-N1	6.06	124.03	121.00
3	C1	1854	С	C6-N1-C2	-6.06	117.88	120.30
3	C1	2190	U	C2-N1-C1'	6.06	124.97	117.70
3	C1	2550	U	C2-N1-C1'	6.05	124.97	117.70
3	C1	3023	U	C2-N1-C1'	6.05	124.97	117.70
1	C2	687	G	N3-C2-N2	-6.05	115.67	119.90
3	C1	78	U	C2-N3-C4	-6.05	123.37	127.00
3	C1	1579	С	C2-N1-C1'	6.05	125.45	118.80
1	C2	916	U	N1-C2-O2	6.04	127.03	122.80
1	C2	1342	С	C2-N1-C1'	6.04	125.44	118.80
3	C1	969	С	C6-N1-C2	-6.04	117.89	120.30
3	C1	2548	С	C5-C6-N1	6.03	124.02	121.00
19	SN	80	LEU	CA-CB-CG	6.03	129.17	115.30
3	C1	1495	U	C5-C6-N1	6.03	125.72	122.70
1	C2	1185	U	C6-N1-C1'	-6.03	112.76	121.20
3	C1	1356	U	N1-C2-O2	6.03	127.02	122.80
1	C2	131	С	C6-N1-C2	-6.02	117.89	120.30
3	C1	3089	С	C6-N1-C2	-6.02	117.89	120.30
1	C2	280	U	N3-C2-O2	-6.02	117.99	122.20
1	C2	852	С	P-O3'-C3'	6.02	126.92	119.70
3	C1	2204	С	OP1-P-O3'	6.01	118.43	105.20
1	C2	954	G	C5-C6-O6	6.01	132.21	128.60
1	C2	161	U	N1-C2-O2	6.01	127.00	122.80
1	C2	1585	U	N1-C2-O2	6.01	127.00	122.80
1	C2	191	С	O4'-C1'-N1	6.00	113.00	108.20
1	C2	1718	G	C4-N9-C1'	6.00	134.30	126.50
1	C2	280	U	C6-N1-C1'	-6.00	112.80	121.20
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	3159	С	N1-C2-O2	6.00	122.50	118.90
3	C1	880	G	N1-C6-O6	-6.00	116.30	119.90
3	C1	102	С	C2-N1-C1'	5.99	125.39	118.80
3	C1	864	G	N3-C4-N9	5.99	129.59	126.00
3	C1	1417	G	N1-C6-O6	5.99	123.50	119.90
3	C1	496	С	C6-N1-C2	-5.99	117.90	120.30
1	C2	1227	А	OP2-P-O3'	5.99	118.37	105.20
3	C1	916	G	P-O3'-C3'	5.99	126.89	119.70
3	C1	2600	С	C6-N1-C2	-5.99	117.91	120.30
3	C1	3067	С	C6-N1-C2	-5.99	117.91	120.30
3	C1	1763	U	C2-N1-C1'	5.99	124.88	117.70
3	C1	2340	U	C5-C6-N1	5.98	125.69	122.70
3	C1	3058	U	C6-N1-C1'	-5.98	112.82	121.20
3	C1	2889	С	C6-N1-C2	-5.98	117.91	120.30
3	C1	3118	С	C6-N1-C2	-5.98	117.91	120.30
1	C2	650	U	C6-N1-C2	-5.97	117.42	121.00
3	C1	1292	С	C6-N1-C2	-5.97	117.91	120.30
3	C1	101	G	O4'-C1'-N9	5.96	112.97	108.20
1	C2	853	G	N3-C2-N2	5.96	124.07	119.90
1	C2	854	U	N1-C1'-C2'	-5.96	105.44	112.00
3	C1	1705	U	N3-C2-O2	-5.96	118.03	122.20
3	C1	1872	С	N3-C2-O2	-5.96	117.73	121.90
1	C2	1456	С	C2-N1-C1'	5.96	125.35	118.80
3	C1	2663	G	C4-C5-N7	5.96	113.18	110.80
3	C1	3383	G	N3-C4-C5	-5.96	125.62	128.60
3	C1	2209	U	C5-C6-N1	5.95	125.68	122.70
3	C1	1095	U	N3-C2-O2	-5.95	118.03	122.20
3	C1	2843	U	N1-C2-O2	5.95	126.97	122.80
1	C2	1	U	C6-N1-C2	-5.95	117.43	121.00
3	C1	1032	С	C2-N1-C1'	5.95	125.35	118.80
3	C1	1725	С	C5-C6-N1	5.95	123.97	121.00
1	C2	637	С	C6-N1-C2	-5.95	117.92	120.30
1	C2	519	С	N1-C2-O2	5.94	122.47	118.90
1	C2	1506	G	C8-N9-C1'	-5.94	119.27	127.00
3	C1	2822	U	N1-C2-O2	5.94	126.96	122.80
3	C1	609	G	N3-C4-N9	5.94	129.56	126.00
1	C2	146	U	C2-N1-C1'	5.94	124.83	117.70
3	C1	1501	U	N1-C2-N3	5.94	118.46	114.90
3	C1	297	G	C4-N9-C1'	5.93	134.22	126.50
3	C1	1589	A	C4-C5-C6	-5.93	114.03	117.00
3	C1	2836	C	N3-C2-O2	-5.93	117.75	121.90
3	C1	750	G	C4-C5-N7	5.93	113.17	110.80



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	223	U	N3-C2-O2	-5.93	118.05	122.20
3	C1	1015	U	P-O3'-C3'	5.93	126.82	119.70
3	C1	2132	С	N3-C2-O2	-5.93	117.75	121.90
3	C1	1172	G	C4-N9-C1'	5.92	134.20	126.50
3	C1	2266	U	N1-C2-O2	5.92	126.94	122.80
3	C1	750	G	C5-C6-O6	-5.92	125.05	128.60
3	C1	1756	С	C6-N1-C2	-5.92	117.93	120.30
3	C1	180	C	C5-C6-N1	5.92	123.96	121.00
3	C1	37	U	N1-C2-O2	5.91	126.94	122.80
3	C1	1832	C	C6-N1-C2	-5.91	117.94	120.30
3	C1	2835	U	C5-C4-O4	-5.91	122.36	125.90
1	C2	120	U	C2-N1-C1'	5.91	124.79	117.70
1	C2	354	C	C6-N1-C2	-5.91	117.94	120.30
1	C2	1454	G	N1-C2-N3	5.91	127.44	123.90
1	C2	855	A	C5-C6-N6	-5.90	118.98	123.70
1	C2	1536	G	C8-N9-C4	-5.90	104.04	106.40
3	C1	561	С	N1-C2-O2	5.90	122.44	118.90
1	C2	1248	С	N1-C2-O2	5.89	122.44	118.90
3	C1	1283	С	C6-N1-C2	-5.89	117.94	120.30
1	C2	855	A	N7-C8-N9	5.89	116.75	113.80
1	C2	79	С	N1-C2-O2	5.89	122.43	118.90
3	C1	524	U	C2-N1-C1'	5.89	124.77	117.70
3	C1	37	U	N3-C2-O2	-5.89	118.08	122.20
3	C1	995	U	N3-C2-O2	-5.89	118.08	122.20
3	C1	2726	C	C2-N1-C1'	5.88	125.27	118.80
3	C1	3275	U	OP1-P-O3'	5.88	118.14	105.20
1	C2	191	C	N3-C2-O2	-5.88	117.78	121.90
3	C1	1889	G	C4-N9-C1'	5.88	134.14	126.50
3	C1	3201	С	N1-C2-O2	5.88	122.43	118.90
1	C2	1482	С	O4'-C1'-N1	5.88	112.90	108.20
3	C1	1870	C	C6-N1-C2	-5.88	117.95	120.30
3	C1	1022	U	C5-C6-N1	5.88	125.64	122.70
1	C2	422	G	C4-N9-C1'	-5.88	118.86	126.50
1	C2	767	U	N3-C2-O2	-5.87	118.09	122.20
3	C1	438	A	N3-C4-N9	5.87	132.10	127.40
52	LO	84	LEU	CB-CG-CD1	-5.87	101.02	111.00
1	C2	162	A	C8-N9-C4	-5.87	103.45	105.80
1	C2	697	C	C6-N1-C1'	-5.87	113.75	120.80
1	C2	25	C	P-O3'-C3'	5.87	126.74	119.70
1	C2	949	C	C5-C6-N1	5.87	123.94	121.00
3	C1	544	C	C2-N1-C1'	-5.86	112.35	118.80
3	C1	2512	C	C6-N1-C2	-5.86	117.95	120.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	2336	U	N1-C2-O2	5.86	126.90	122.80
3	C1	2118	С	N3-C2-O2	-5.86	117.80	121.90
3	C1	2373	А	O5'-P-OP1	-5.86	100.43	105.70
3	C1	267	G	O4'-C1'-N9	-5.86	103.52	108.20
1	C2	29	U	C5-C6-N1	5.85	125.62	122.70
1	C2	305	С	C5-C6-N1	5.85	123.92	121.00
3	C1	1377	G	C8-N9-C4	-5.85	104.06	106.40
13	SH	41	LEU	CA-CB-CG	5.84	128.73	115.30
3	C1	297	G	C6-C5-N7	-5.84	126.90	130.40
1	C2	1209	С	C6-N1-C2	-5.84	117.97	120.30
3	C1	327	А	C5-C6-N6	5.84	128.37	123.70
1	C2	1501	С	N1-C2-O2	5.83	122.40	118.90
1	C2	609	U	N3-C2-O2	-5.83	118.12	122.20
1	C2	1007	С	C5-C6-N1	5.83	123.92	121.00
3	C1	730	С	C6-N1-C2	-5.83	117.97	120.30
3	C1	1390	А	N1-C6-N6	-5.83	115.10	118.60
1	C2	1053	G	C4-N9-C1'	5.83	134.08	126.50
3	C1	921	А	O4'-C1'-N9	-5.83	103.54	108.20
3	C1	2764	С	C6-N1-C2	-5.83	117.97	120.30
3	C1	3275	U	C5-C6-N1	5.83	125.61	122.70
3	C1	1145	G	C6-C5-N7	-5.82	126.91	130.40
1	C2	1342	С	C5-C6-N1	5.82	123.91	121.00
3	C1	2350	С	C5-C6-N1	5.82	123.91	121.00
3	C1	1669	С	C6-N1-C2	-5.81	117.97	120.30
1	C2	855	А	C5-C6-N1	5.81	120.61	117.70
1	C2	1173	С	C6-N1-C2	-5.81	117.98	120.30
3	C1	1763	U	N3-C2-O2	-5.80	118.14	122.20
1	C2	1000	С	N1-C2-O2	5.80	122.38	118.90
1	C2	1258	U	N1-C2-O2	5.80	126.86	122.80
3	C1	3201	С	N3-C2-O2	-5.80	117.84	121.90
3	C1	101	G	C4-N9-C1'	5.80	134.04	126.50
1	C2	442	С	C5-C6-N1	5.80	123.90	121.00
3	C1	175	С	C6-N1-C2	-5.80	117.98	120.30
3	C1	2101	С	P-O3'-C3'	5.80	126.66	119.70
3	C1	3116	G	C5-C6-O6	5.80	132.08	128.60
3	C1	2610	G	C4-C5-N7	5.79	113.12	110.80
1	C2	850	А	C4-C5-N7	5.79	113.60	110.70
3	C1	1501	U	C5-C4-O4	-5.79	122.43	125.90
1	C2	111	U	N1-C2-O2	5.78	126.85	122.80
3	C1	1578	C	C2-N1-C1'	5.78	$1\overline{25.16}$	118.80
3	C1	2707	C	C6-N1-C2	-5.78	117.99	120.30
1	C2	854	U	C6-N1-C1'	5.78	129.29	121.20



$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	1155	С	C5-C6-N1	5.78	123.89	121.00
1	C2	270	С	C6-N1-C2	-5.78	117.99	120.30
3	C1	2235	С	C2-N1-C1'	5.77	125.15	118.80
3	C1	969	С	C5-C6-N1	5.77	123.88	121.00
3	C1	2135	U	C5-C6-N1	5.77	125.58	122.70
3	C1	3357	U	N3-C2-O2	-5.77	118.16	122.20
1	C2	1771	U	C5-C6-N1	5.77	125.58	122.70
1	C2	54	С	C2-N1-C1'	5.76	125.14	118.80
3	C1	1872	С	C2-N1-C1'	5.76	125.14	118.80
1	C2	302	U	N1-C2-O2	5.76	126.83	122.80
1	C2	1210	С	C5-C4-N4	5.76	124.23	120.20
1	C2	1246	С	C5-C6-N1	5.76	123.88	121.00
3	C1	179	С	C6-N1-C2	-5.76	118.00	120.30
5	C3	28	С	C6-N1-C2	-5.76	118.00	120.30
1	C2	1021	С	C6-N1-C1'	-5.76	113.89	120.80
3	C1	3337	G	N3-C4-C5	-5.76	125.72	128.60
1	C2	1141	G	N1-C2-N3	5.75	127.35	123.90
1	C2	1614	А	O4'-C1'-N9	5.75	112.80	108.20
3	C1	3163	А	C5-N7-C8	-5.75	101.02	103.90
1	C2	873	U	C5-C6-N1	5.75	125.58	122.70
3	C1	916	G	OP1-P-O3'	5.75	117.85	105.20
1	C2	1214	U	N3-C2-O2	-5.75	118.17	122.20
3	C1	42	С	C5-C6-N1	5.75	123.88	121.00
1	C2	449	С	C5-C6-N1	5.75	123.87	121.00
1	C2	848	С	C2-N1-C1'	5.75	125.12	118.80
3	C1	2277	С	C6-N1-C2	-5.75	118.00	120.30
3	C1	2512	С	C2-N1-C1'	5.75	125.12	118.80
3	C1	2899	С	C2-N1-C1'	5.75	125.12	118.80
1	C2	504	U	C5-C6-N1	5.75	125.57	122.70
1	C2	270	С	C5-C6-N1	5.74	123.87	121.00
3	C1	2546	С	C5-C6-N1	5.74	123.87	121.00
1	C2	1174	С	C6-N1-C2	-5.74	118.00	120.30
3	C1	27	С	C5-C6-N1	5.74	123.87	121.00
1	C2	1082	С	C5-C4-N4	5.74	124.21	120.20
3	C1	713	U	C6-N1-C2	-5.74	117.56	121.00
1	C2	146	U	N1-C2-O2	5.73	126.81	122.80
3	C1	2951	G	C4-C5-N7	5.73	113.09	110.80
1	C2	1081	А	OP1-P-O3'	5.73	117.81	105.20
3	C1	28	С	C6-N1-C2	-5.73	118.01	120.30
3	C1	940	G	C4-C5-N7	5.73	113.09	110.80
3	C1	404	G	C5-C6-O6	-5.73	125.16	128.60
3	C1	3023	U	N1-C2-O2	5.73	126.81	122.80
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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	3378	С	N1-C2-O2	5.73	122.34	118.90
1	C2	853	G	P-O3'-C3'	5.73	126.57	119.70
3	C1	220	G	C4-C5-N7	5.72	113.09	110.80
3	C1	2209	U	C6-N1-C2	-5.72	117.57	121.00
1	C2	442	С	C6-N1-C2	-5.72	118.01	120.30
3	C1	3159	С	C2-N1-C1'	5.72	125.09	118.80
3	C1	1292	С	N1-C2-O2	5.72	122.33	118.90
1	C2	393	С	C6-N1-C2	-5.71	118.01	120.30
3	C1	2954	U	C2-N1-C1'	5.71	124.55	117.70
1	C2	610	G	C8-N9-C1'	-5.71	119.58	127.00
1	C2	1454	G	N1-C2-N2	-5.71	111.06	116.20
3	C1	986	U	C6-N1-C2	-5.71	117.57	121.00
3	C1	1818	U	N3-C2-O2	-5.71	118.20	122.20
1	C2	934	С	C2-N1-C1'	5.71	125.08	118.80
1	C2	1560	U	C6-N1-C1'	-5.71	113.21	121.20
3	C1	311	С	C6-N1-C2	-5.71	118.02	120.30
3	C1	1560	G	P-O3'-C3'	5.70	126.54	119.70
5	C3	18	U	C5-C6-N1	5.70	125.55	122.70
1	C2	1081	А	C8-N9-C4	-5.70	103.52	105.80
3	C1	2204	С	P-O3'-C3'	5.70	126.54	119.70
3	C1	2440	G	C4-C5-N7	5.70	113.08	110.80
1	C2	1777	G	N3-C4-N9	5.70	129.42	126.00
3	C1	2112	U	OP2-P-O3'	5.70	117.73	105.20
3	C1	1560	G	OP1-P-O3'	5.69	117.73	105.20
3	C1	982	С	C5-C6-N1	5.69	123.85	121.00
3	C1	1227	С	C6-N1-C2	-5.69	118.02	120.30
3	C1	1856	С	C6-N1-C2	-5.69	118.02	120.30
5	C3	118	С	C6-N1-C2	-5.69	118.02	120.30
1	C2	874	С	N1-C2-O2	5.69	122.31	118.90
3	C1	821	U	N3-C2-O2	-5.69	118.22	122.20
3	C1	1604	G	C5-C6-N1	5.69	114.34	111.50
3	C1	868	С	C5-C6-N1	5.69	123.84	121.00
1	C2	1568	С	P-O3'-C3'	5.68	126.52	119.70
3	C1	184	U	N3-C2-O2	-5.68	118.22	122.20
3	C1	320	G	N1-C6-O6	-5.68	116.49	119.90
3	C1	1872	С	C6-N1-C2	-5.68	118.03	120.30
1	C2	103	A	P-O3'-C3'	5.68	126.52	119.70
1	C2	$11\overline{29}$	U	N3-C2-O2	-5.68	118.22	122.20
3	C1	$23\overline{53}$	G	N3-C4-C5	-5.68	125.76	128.60
1	C2	146	U	N3-C2-O2	-5.68	118.22	122.20
1	C2	$58\overline{3}$	C	$C6-N1-\overline{C1'}$	-5.68	113.98	120.80
1	C2	1307	U	N3-C2-O2	-5.68	118.22	122.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	2406	С	C5-C6-N1	5.68	123.84	121.00
1	C2	1274	С	C2-N1-C1'	5.68	125.04	118.80
1	C2	1733	С	C6-N1-C2	-5.68	118.03	120.30
3	C1	853	G	C4-C5-N7	5.68	113.07	110.80
3	C1	1368	U	C5-C6-N1	5.68	125.54	122.70
3	C1	2378	С	C5-C6-N1	5.68	123.84	121.00
1	C2	426	G	C4-N9-C1'	5.67	133.88	126.50
3	C1	2431	С	C5-C6-N1	5.67	123.83	121.00
3	C1	1579	С	C5-C6-N1	5.67	123.83	121.00
1	C2	118	U	N3-C2-O2	-5.66	118.24	122.20
1	C2	1315	U	C5-C6-N1	5.66	125.53	122.70
3	C1	1227	С	C5-C6-N1	5.66	123.83	121.00
3	C1	1023	С	N1-C2-O2	5.66	122.30	118.90
1	C2	1536	G	C4-N9-C1'	5.66	133.85	126.50
3	C1	2545	С	N3-C2-O2	-5.66	117.94	121.90
1	C2	1601	G	N3-C4-N9	-5.65	122.61	126.00
3	C1	1237	G	N3-C4-N9	5.65	129.39	126.00
3	C1	3218	А	P-O3'-C3'	5.65	126.48	119.70
3	C1	915	А	C4-N9-C1'	5.65	136.47	126.30
1	C2	1536	G	N3-C4-C5	-5.65	125.78	128.60
3	C1	804	С	C6-N1-C2	-5.65	118.04	120.30
3	C1	1249	G	N3-C4-N9	5.64	129.38	126.00
1	C2	1342	С	C6-N1-C2	-5.64	118.04	120.30
1	C2	1375	A	N9-C4-C5	-5.64	103.54	105.80
1	C2	872	G	N7-C8-N9	5.63	115.92	113.10
3	C1	1577	G	N1-C2-N2	-5.63	111.13	116.20
1	C2	559	C	C5-C6-N1	5.63	123.81	121.00
1	C2	1470	С	N3-C2-O2	-5.63	117.96	121.90
1	C2	1307	U	N1-C2-O2	5.62	126.74	122.80
1	C2	35	U	C6-N1-C2	-5.62	117.63	121.00
1	C2	219	A	O4'-C1'-N9	5.62	112.70	108.20
3	C1	2397	А	N1-C2-N3	-5.62	126.49	129.30
39	LA	246	LEU	CA-CB-CG	5.62	128.22	115.30
1	C2	1454	G	C4-C5-N7	-5.61	108.56	110.80
3	C1	577	С	C5-C6-N1	5.61	123.81	121.00
3	C1	1072	G	C4-N9-C1'	5.61	133.79	126.50
1	C2	354	С	C5-C6-N1	5.61	123.80	121.00
3	C1	1248	C	O4'-C1'-N1	5.61	112.69	108.20
3	C1	2537	U	C5-C6-N1	5.61	125.50	122.70
1	C2	907	A	C8-N9-C4	-5.61	103.56	105.80
3	C1	503	C	C6-N1-C2	-5.61	118.06	120.30
3	C1	1917	C	C6-N1-C2	-5.61	118.06	120.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	1152	G	C5-C6-N1	5.60	114.30	111.50
3	C1	864	G	C6-C5-N7	-5.60	127.04	130.40
1	C2	761	G	C6-C5-N7	-5.60	127.04	130.40
3	C1	1119	С	C5-C6-N1	5.60	123.80	121.00
4	C4	105	С	C5-C6-N1	5.60	123.80	121.00
3	C1	2288	G	C4-N9-C1'	5.59	133.77	126.50
1	C2	1455	G	C6-C5-N7	5.59	133.76	130.40
3	C1	3118	С	N3-C2-O2	-5.59	117.98	121.90
3	C1	2184	U	C5-C6-N1	5.59	125.50	122.70
3	C1	2548	С	N1-C2-O2	5.59	122.25	118.90
1	C2	191	С	C6-N1-C2	-5.59	118.06	120.30
1	C2	1274	С	C6-N1-C2	-5.59	118.06	120.30
3	C1	263	С	C6-N1-C2	-5.59	118.06	120.30
1	C2	1501	С	C5-C6-N1	5.58	123.79	121.00
3	C1	3357	U	P-O3'-C3'	5.58	126.40	119.70
3	C1	1684	U	N3-C2-O2	-5.58	118.29	122.20
1	C2	831	U	C5-C4-O4	-5.58	122.55	125.90
1	C2	1720	G	C6-C5-N7	-5.58	127.05	130.40
1	C2	850	А	N1-C6-N6	5.58	121.95	118.60
1	C2	632	U	C6-N1-C2	-5.58	117.65	121.00
1	C2	1572	G	N3-C2-N2	5.58	123.81	119.90
3	C1	180	С	C2-N1-C1'	5.58	124.94	118.80
3	C1	497	С	C6-N1-C2	-5.58	118.07	120.30
3	C1	1296	С	C6-N1-C2	-5.58	118.07	120.30
1	C2	184	С	C6-N1-C1'	-5.58	114.11	120.80
3	C1	1368	U	C6-N1-C1'	-5.58	113.39	121.20
3	C1	113	С	N1-C2-O2	5.57	122.24	118.90
3	C1	1219	С	N3-C2-O2	-5.57	118.00	121.90
3	C1	2610	G	C8-N9-C4	-5.57	104.17	106.40
3	C1	1587	А	N1-C6-N6	-5.57	115.26	118.60
3	C1	1134	G	C5-C6-O6	5.57	131.94	128.60
1	C2	76	А	C2-N3-C4	5.57	113.38	110.60
1	C2	1796	С	C2-N1-C1'	5.57	124.92	118.80
3	C1	715	А	N7-C8-N9	5.57	116.58	113.80
3	C1	421	G	C4-N9-C1'	5.56	133.73	126.50
10	SE	38	LEU	CA-CB-CG	5.56	$1\overline{28.10}$	115.30
1	C2	536	C	C5-C6-N1	5.56	123.78	121.00
1	C2	531	C	N3-C2-O2	-5.56	118.01	121.90
3	C1	732	C	C6-N1-C2	-5.56	118.08	120.30
3	C1	2137	U	$C2-N1-\overline{C1'}$	5.56	124.37	117.70
3	C1	2872	A	C5-N7-C8	-5.56	101.12	103.90
1	C2	519	C	N3-C2-O2	-5.56	118.01	121.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	1021	С	C5-C6-N1	5.56	123.78	121.00
3	C1	1339	С	C5-C6-N1	5.56	123.78	121.00
3	C1	2189	U	N1-C2-O2	5.55	126.69	122.80
3	C1	430	U	N1-C2-O2	5.55	126.69	122.80
1	C2	1344	А	P-O3'-C3'	5.55	126.36	119.70
3	C1	3317	U	C2-N1-C1'	5.55	124.36	117.70
3	C1	1705	U	N1-C2-O2	5.55	126.68	122.80
3	C1	2336	U	C2-N1-C1'	5.55	124.36	117.70
3	C1	2878	G	C4-C5-N7	5.55	113.02	110.80
1	C2	1332	С	C2-N1-C1'	5.54	124.90	118.80
3	C1	79	U	N3-C2-O2	-5.54	118.32	122.20
3	C1	2616	С	C5-C6-N1	5.54	123.77	121.00
1	C2	834	G	N3-C4-C5	-5.54	125.83	128.60
3	C1	1249	G	C4-N9-C1'	5.54	133.71	126.50
1	C2	1485	С	N1-C2-O2	5.54	122.22	118.90
3	C1	2876	С	C6-N1-C2	-5.54	118.08	120.30
1	C2	1063	U	C5-C6-N1	5.54	125.47	122.70
1	C2	1141	G	N3-C4-N9	-5.54	122.68	126.00
1	C2	1506	G	C6-C5-N7	-5.54	127.08	130.40
3	C1	1763	U	C5-C6-N1	5.54	125.47	122.70
1	C2	58	U	N3-C2-O2	-5.53	118.33	122.20
3	C1	2763	U	N3-C2-O2	-5.53	118.33	122.20
3	C1	500	С	C5-C6-N1	5.53	123.77	121.00
3	C1	930	U	C5-C6-N1	5.53	125.47	122.70
3	C1	977	С	C6-N1-C2	-5.53	118.09	120.30
3	C1	2206	G	C2-N3-C4	5.53	114.67	111.90
3	C1	1299	U	N1-C2-O2	5.53	126.67	122.80
3	C1	1367	G	C6-C5-N7	-5.53	127.08	130.40
3	C1	3282	U	C5-C6-N1	5.53	125.46	122.70
3	C1	3362	А	N7-C8-N9	5.52	116.56	113.80
3	C1	2585	G	C8-N9-C1'	-5.52	119.82	127.00
5	C3	76	С	C5-C6-N1	5.52	123.76	121.00
3	C1	2132	С	C5-C6-N1	5.52	123.76	121.00
3	C1	543	С	C5-C6-N1	5.52	123.76	121.00
1	C2	1454	G	N9-C4-C5	5.52	107.61	105.40
1	C2	76	А	N3-C4-N9	5.51	131.81	127.40
3	C1	1685	С	C6-N1-C2	-5.51	118.09	120.30
3	C1	180	С	N1-C2-O2	5.51	122.21	118.90
1	C2	853	G	C1'-O4'-C4'	-5.51	105.49	109.90
3	C1	1230	G	C5-C6-O6	5.51	131.91	128.60
1	C2	149	С	C5-C6-N1	5.51	123.75	121.00
1	C2	858	G	O4'-C1'-N9	5.51	112.61	108.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	1773	С	C6-N1-C2	-5.51	118.10	120.30
25	ST	28	LEU	CA-CB-CG	5.50	127.96	115.30
1	C2	1676	U	C5-C6-N1	5.50	125.45	122.70
1	C2	1789	G	C4-C5-N7	5.50	113.00	110.80
3	C1	3067	С	C5-C6-N1	5.50	123.75	121.00
1	C2	947	U	C5-C6-N1	5.50	125.45	122.70
3	C1	2883	U	C5-C6-N1	5.50	125.45	122.70
1	C2	1129	U	N1-C2-O2	5.50	126.65	122.80
3	C1	2517	U	N3-C2-O2	-5.50	118.35	122.20
3	C1	1732	U	N1-C2-O2	5.49	126.65	122.80
3	C1	69	С	C6-N1-C1'	5.49	127.39	120.80
1	C2	934	С	C5-C6-N1	5.49	123.74	121.00
33	Sb	41	LEU	CA-CB-CG	5.49	127.92	115.30
3	C1	1764	U	OP1-P-O3'	5.49	117.27	105.20
1	C2	115	G	C8-N9-C4	-5.49	104.21	106.40
1	C2	854	U	C5'-C4'-C3'	5.49	124.78	116.00
3	C1	1780	G	C4-N9-C1'	5.49	133.63	126.50
3	C1	1103	А	OP2-P-O3'	5.48	117.26	105.20
3	C1	2652	U	C2-N1-C1'	5.48	124.28	117.70
1	C2	1247	U	N3-C2-O2	-5.48	118.37	122.20
1	C2	426	G	O5'-P-OP1	-5.47	100.77	105.70
3	C1	1033	U	N3-C2-O2	-5.47	118.37	122.20
3	C1	1608	С	C2-N1-C1'	5.47	124.82	118.80
27	SV	10	GLU	CA-CB-CG	5.47	125.43	113.40
3	C1	886	С	C6-N1-C2	-5.47	118.11	120.30
3	C1	1208	U	N1-C2-O2	5.47	126.63	122.80
3	C1	931	С	C6-N1-C2	-5.46	118.11	120.30
3	C1	3279	А	N9-C4-C5	-5.46	103.61	105.80
1	C2	893	U	C5-C6-N1	5.46	125.43	122.70
1	C2	1560	U	O4'-C1'-N1	5.46	112.57	108.20
1	C2	184	С	C5-C6-N1	5.46	123.73	121.00
3	C1	79	U	N3-C4-O4	5.46	123.22	119.40
1	C2	21	U	N1-C2-O2	5.46	126.62	122.80
1	C2	1639	С	C6-N1-C2	-5.46	118.12	120.30
3	C1	853	G	N9-C4-C5	-5.45	103.22	105.40
3	C1	2181	С	C6-N1-C2	-5.45	118.12	120.30
1	C2	1246	С	C2-N3-C4	5.45	122.62	119.90
3	C1	1904	С	C5-C6-N1	5.45	123.72	121.00
1	C2	1637	С	N3-C2-O2	-5.45	118.09	121.90
5	C3	46	G	C4-N9-C1'	5.45	133.58	126.50
1	C2	536	С	C6-N1-C2	-5.45	118.12	120.30
3	C1	327	А	N9-C4-C5	5.45	107.98	105.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	3214	U	O4'-C1'-N1	5.45	112.56	108.20
1	C2	1600	А	C2-N3-C4	5.44	113.32	110.60
1	C2	1012	U	C5-C6-N1	5.44	125.42	122.70
3	C1	2683	U	C6-N1-C2	-5.44	117.73	121.00
3	C1	1033	U	N1-C2-O2	5.44	126.61	122.80
3	C1	1267	U	N1-C2-O2	5.44	126.61	122.80
3	C1	2716	U	N3-C2-O2	-5.44	118.39	122.20
3	C1	3212	С	C6-N1-C2	-5.44	118.12	120.30
3	C1	544	С	C5-C4-N4	5.43	124.00	120.20
1	C2	381	С	C6-N1-C2	-5.43	118.13	120.30
1	C2	54	С	C5-C6-N1	5.43	123.72	121.00
1	C2	275	С	C6-N1-C1'	-5.43	114.28	120.80
3	C1	1706	С	C2-N1-C1'	5.43	124.77	118.80
3	C1	2638	С	N1-C2-O2	5.43	122.16	118.90
3	C1	90	С	C5-C6-N1	5.42	123.71	121.00
3	C1	2893	С	C5-C6-N1	5.42	123.71	121.00
4	C4	49	G	N1-C6-O6	-5.42	116.64	119.90
3	C1	315	С	C5-C6-N1	5.42	123.71	121.00
1	C2	798	С	C6-N1-C2	-5.42	118.13	120.30
5	C3	45	С	C5-C6-N1	5.42	123.71	121.00
1	C2	1170	G	C6-N1-C2	-5.42	121.85	125.10
3	C1	184	U	C5-C6-N1	5.42	125.41	122.70
3	C1	653	А	C5-N7-C8	-5.42	101.19	103.90
1	C2	115	G	C6-C5-N7	-5.41	127.15	130.40
1	C2	650	U	C5-C6-N1	5.41	125.41	122.70
1	C2	136	С	C2-N1-C1'	5.41	124.75	118.80
3	C1	777	U	C5-C6-N1	5.41	125.41	122.70
3	C1	1238	С	P-O3'-C3'	5.41	126.19	119.70
1	C2	394	С	C5-C6-N1	5.40	123.70	121.00
1	C2	1161	С	C5-C6-N1	5.40	123.70	121.00
1	C2	615	А	C8-N9-C4	-5.40	103.64	105.80
3	C1	1228	С	N1-C2-N3	5.40	122.98	119.20
3	C1	3120	С	C5-C6-N1	5.40	123.70	121.00
3	C1	288	С	C5-C6-N1	5.40	123.70	121.00
3	C1	429	U	C5-C6-N1	5.40	125.40	122.70
3	C1	1273	A	N9-C4-C5	-5.40	103.64	105.80
3	C1	2663	G	N7-C8-N9	5.40	115.80	113.10
3	C1	245	U	N1-C2-O2	5.40	126.58	122.80
1	C2	1332	C	$C5-C6-\overline{N1}$	5.39	$123.7\overline{0}$	121.00
3	C1	2763	U	N1-C2-O2	5.39	126.58	122.80
3	C1	3158	G	C8-N9-C1'	-5.39	119.99	127.00
1	C2	953	G	N3-C4-N9	5.39	129.24	126.00



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	1716	U	OP1-P-O3'	5.39	117.06	105.20
3	C1	915	А	N1-C2-N3	-5.39	126.61	129.30
3	C1	1006	А	N1-C6-N6	-5.39	115.37	118.60
44	LF	229	PHE	CB-CG-CD2	-5.39	117.03	120.80
1	C2	196	G	C2-N3-C4	-5.38	109.21	111.90
3	C1	2706	G	C4-N9-C1'	5.38	133.50	126.50
1	C2	76	А	C4-N9-C1'	5.38	135.99	126.30
3	C1	1280	С	N1-C2-O2	5.38	122.13	118.90
3	C1	1448	U	N3-C2-O2	-5.38	118.43	122.20
3	C1	2545	С	C6-N1-C2	-5.38	118.15	120.30
5	C3	26	U	C5-C6-N1	5.38	125.39	122.70
1	C2	94	U	N3-C2-O2	-5.38	118.43	122.20
3	C1	2980	U	N3-C2-O2	-5.38	118.43	122.20
1	C2	361	С	C6-N1-C2	-5.38	118.15	120.30
3	C1	702	С	C5-C6-N1	5.38	123.69	121.00
3	C1	245	U	C5-C6-N1	5.38	125.39	122.70
3	C1	2783	U	N3-C2-O2	-5.38	118.44	122.20
3	C1	2825	С	N1-C2-O2	5.38	122.13	118.90
4	C4	105	С	C6-N1-C2	-5.38	118.15	120.30
1	C2	1003	А	O4'-C1'-N9	5.38	112.50	108.20
3	C1	497	С	C5-C6-N1	5.37	123.69	121.00
3	C1	881	С	N1-C2-O2	5.37	122.12	118.90
1	C2	778	G	N3-C4-C5	-5.37	125.91	128.60
1	C2	1497	U	C2-N1-C1'	5.37	124.14	117.70
3	C1	174	С	N3-C2-O2	-5.37	118.14	121.90
3	C1	971	G	C5-C6-N1	5.37	114.18	111.50
3	C1	297	G	C8-N9-C1'	-5.36	120.03	127.00
3	C1	1578	С	C6-N1-C2	-5.36	118.16	120.30
5	C3	112	U	O4'-C1'-N1	5.36	112.49	108.20
3	C1	3131	U	C6-N1-C1'	-5.36	113.69	121.20
12	SG	24	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	C2	798	С	N3-C2-O2	-5.36	118.15	121.90
1	C2	1373	С	C6-N1-C2	-5.36	118.16	120.30
3	C1	430	U	N3-C2-O2	-5.36	118.45	122.20
1	C2	275	С	C6-N1-C2	-5.35	118.16	120.30
1	C2	275	C	N1-C2-O2	5.35	122.11	118.90
3	C1	1190	A	C8-N9-C1'	-5.35	118.07	127.70
4	C4	39	C	C2-N1-C1'	5.35	124.68	118.80
3	C1	1732	U	N3-C2-O2	-5.35	118.46	122.20
1	C2	302	U	$C2-N1-\overline{C1'}$	$5.3\overline{4}$	124.11	117.70
3	C1	315	C	C6-N1-C2	-5.34	118.16	120.30
3	C1	404	G	N9-C4-C5	-5.34	103.26	105.40



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	645	А	N1-C6-N6	-5.34	115.39	118.60
3	C1	2646	С	C5-C6-N1	5.34	123.67	121.00
4	C4	78	U	N1-C2-O2	5.34	126.54	122.80
1	C2	1397	U	N3-C2-O2	-5.34	118.46	122.20
3	C1	1185	С	C6-N1-C2	-5.34	118.16	120.30
1	C2	136	С	N3-C2-O2	-5.34	118.16	121.90
1	C2	1119	G	N3-C4-N9	5.34	129.20	126.00
3	C1	609	G	C4-N9-C1'	5.34	133.44	126.50
3	C1	1327	С	C6-N1-C2	-5.34	118.17	120.30
1	C2	4	С	C2-N1-C1'	5.34	124.67	118.80
1	C2	1640	С	C5-C6-N1	5.34	123.67	121.00
3	C1	1831	U	C5-C6-N1	5.34	125.37	122.70
3	C1	2273	G	C8-N9-C1'	5.34	133.94	127.00
3	C1	2986	U	C6-N1-C2	-5.34	117.80	121.00
1	C2	1000	С	N3-C2-O2	-5.33	118.17	121.90
1	C2	1072	С	C6-N1-C2	-5.33	118.17	120.30
1	C2	1718	G	C8-N9-C1'	-5.33	120.06	127.00
1	C2	571	G	N7-C8-N9	5.33	115.77	113.10
1	C2	889	U	C5-C4-O4	-5.33	122.70	125.90
1	C2	1509	С	C6-N1-C2	-5.33	118.17	120.30
3	C1	78	U	N1-C2-N3	5.33	118.10	114.90
1	C2	1252	С	C6-N1-C2	-5.33	118.17	120.30
4	C4	116	С	C5-C6-N1	5.32	123.66	121.00
3	C1	713	U	C5-C6-N1	5.32	125.36	122.70
3	C1	911	С	C6-N1-C2	-5.32	118.17	120.30
3	C1	2380	U	C5-C6-N1	5.32	125.36	122.70
1	C2	814	А	N1-C2-N3	-5.32	126.64	129.30
1	C2	1227	А	P-O3'-C3'	5.32	126.08	119.70
3	C1	302	U	C5-C6-N1	5.32	125.36	122.70
3	C1	2832	С	C5-C6-N1	5.32	123.66	121.00
3	C1	3158	G	C4-N9-C1'	5.32	133.41	126.50
1	C2	361	С	N1-C2-O2	5.31	122.09	118.90
3	C1	2984	С	C5-C6-N1	5.31	123.66	121.00
1	C2	1718	G	C6-C5-N7	-5.31	127.21	130.40
3	C1	413	U	C5-C6-N1	5.31	125.36	122.70
3	C1	776	U	C4-C5-C6	5.31	122.89	119.70
3	C1	1137	С	C2-N3-C4	-5.31	117.25	119.90
4	C4	49	G	N9-C4-C5	5.31	107.52	105.40
1	C2	864	U	C5-C6-N1	5.31	125.35	122.70
7	SB	120	LEU	CA-CB-CG	5.31	127.50	115.30
49	LL	27	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C2	1220	C	C6-N1-C2	-5.31	118.18	120.30


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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	907	А	N7-C8-N9	5.30	116.45	113.80
3	C1	1273	А	N3-C4-N9	5.30	131.64	127.40
3	C1	3053	G	N3-C4-N9	5.30	129.18	126.00
1	C2	1415	U	N3-C2-O2	-5.30	118.49	122.20
3	C1	3357	U	C2-N1-C1'	5.30	124.06	117.70
1	C2	501	U	N1-C2-O2	5.30	126.51	122.80
3	C1	1515	А	N1-C2-N3	-5.30	126.65	129.30
3	C1	3042	U	C6-N1-C2	-5.30	117.82	121.00
1	C2	1251	U	O4'-C1'-N1	5.29	112.43	108.20
1	C2	542	А	C8-N9-C4	-5.29	103.68	105.80
1	C2	1456	С	O4'-C1'-N1	5.29	112.43	108.20
1	C2	1796	С	N3-C2-O2	-5.29	118.20	121.90
3	C1	404	G	C6-C5-N7	-5.29	127.22	130.40
3	C1	1140	G	C8-N9-C1'	-5.29	120.12	127.00
3	C1	2239	G	N3-C4-N9	-5.29	122.83	126.00
3	C1	2905	U	C6-N1-C2	-5.29	117.83	121.00
5	C3	64	U	N1-C2-O2	5.29	126.50	122.80
3	C1	1230	G	N3-C4-N9	-5.29	122.83	126.00
1	C2	1429	G	C6-C5-N7	-5.29	127.23	130.40
3	C1	238	А	C8-N9-C4	-5.29	103.69	105.80
3	C1	1358	С	C6-N1-C2	-5.29	118.19	120.30
1	C2	1056	U	C6-N1-C2	-5.28	117.83	121.00
3	C1	2960	С	C6-N1-C2	-5.28	118.19	120.30
1	C2	319	U	OP1-P-O3'	5.28	116.82	105.20
3	C1	2666	С	C2-N1-C1'	5.28	124.61	118.80
3	C1	2364	G	O4'-C1'-N9	5.28	112.42	108.20
3	C1	3235	С	C2-N1-C1'	5.28	124.61	118.80
4	C4	39	С	N3-C2-O2	-5.28	118.21	121.90
1	C2	1461	С	C6-N1-C2	-5.28	118.19	120.30
3	C1	1533	U	N3-C2-O2	-5.28	118.51	122.20
3	C1	3300	U	N3-C2-O2	-5.28	118.51	122.20
3	C1	2304	С	N3-C2-O2	-5.27	118.21	121.90
3	C1	2675	С	C6-N1-C2	-5.27	118.19	120.30
1	C2	927	С	C6-N1-C2	-5.27	118.19	120.30
1	C2	818	С	C6-N1-C2	-5.26	118.19	120.30
1	C2	1458	G	C2-N3-C4	5.26	114.53	111.90
3	C1	306	A	N9-C4-C5	-5.26	103.69	105.80
3	C1	982	С	C2-N1-C1'	5.26	124.59	118.80
1	C2	583	С	N1-C2-O2	5.26	122.06	118.90
3	C1	1049	C	C5-C6-N1	5.26	123.63	121.00
1	C2	873	U	C2-N1-C1'	5.26	124.02	117.70
3	C1	864	G	N3-C4-C5	-5.26	$1\overline{25.97}$	128.60



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Mol	Chain	Res	Type	Aton

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	Ideal(°)
1	C2	337	G	C5-N7-C8	-5.26	101.67	104.30
3	C1	1439	U	C5-C6-N1	5.26	125.33	122.70
3	C1	1728	G	C4-C5-N7	5.26	112.90	110.80
3	C1	3086	А	C5-N7-C8	-5.26	101.27	103.90
3	C1	1172	G	C8-N9-C1'	-5.26	120.16	127.00
1	C2	1111	G	N3-C4-N9	5.26	129.15	126.00
1	C2	542	А	C6-C5-N7	-5.25	128.62	132.30
1	C2	816	G	C5-C6-O6	5.25	131.75	128.60
3	C1	210	U	C5-C6-N1	5.25	125.33	122.70
3	C1	1706	С	N3-C2-O2	-5.25	118.22	121.90
3	C1	2552	С	C6-N1-C1'	-5.25	114.50	120.80
1	C2	1773	С	C5-C6-N1	5.25	123.62	121.00
3	C1	1685	С	C5-C6-N1	5.25	123.62	121.00
1	C2	342	С	C5-C6-N1	5.25	123.62	121.00
1	C2	1796	С	C6-N1-C2	-5.25	118.20	120.30
3	C1	421	G	C8-N9-C1'	-5.25	120.18	127.00
3	C1	2894	С	C5-C6-N1	5.25	123.62	121.00
1	C2	1340	U	N1-C2-O2	5.25	126.47	122.80
3	C1	2190	U	C6-N1-C2	-5.25	117.85	121.00
3	C1	2663	G	C5-N7-C8	-5.25	101.68	104.30
1	C2	532	U	N1-C2-N3	5.25	118.05	114.90
3	C1	3023	U	C5-C6-N1	5.25	125.32	122.70
3	C1	1299	U	N3-C2-O2	-5.24	118.53	122.20
3	C1	1878	G	C6-C5-N7	-5.24	127.26	130.40
3	C1	2098	С	C6-N1-C2	-5.24	118.20	120.30
3	C1	2827	U	N1-C2-O2	5.24	126.47	122.80
49	LL	48	PRO	N-CA-C	5.24	125.72	112.10
1	C2	323	A	C8-N9-C4	-5.24	103.70	105.80
1	C2	543	С	C6-N1-C2	5.23	122.39	120.30
1	C2	559	С	C6-N1-C2	-5.23	118.21	120.30
1	C2	1438	G	N3-C4-C5	-5.23	125.98	128.60
3	C1	1081	U	OP2-P-O3'	5.23	116.71	105.20
3	C1	3383	G	N3-C4-N9	5.23	129.14	126.00
1	C2	872	G	C8-N9-C4	-5.23	104.31	106.40
1	C2	1530	С	C6-N1-C2	-5.23	118.21	120.30
3	C1	149	U	C6-N1-C2	-5.23	117.86	121.00
3	C1	2422	С	C6-N1-C2	-5.23	118.21	120.30
3	C1	2638	C	N3-C2-O2	-5.23	118.24	121.90
1	C2	1509	C	C5-C6-N1	5.23	123.61	121.00
3	C1	$2\overline{153}$	U	N3-C2-O2	-5.23	118.54	122.20
1	C2	584	С	C6-N1-C2	-5.22	118.21	120.30
1	C2	1681	A	O4'-C1'-N9	5.22	112.38	108.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	3253	G	C5-C6-O6	5.22	131.74	128.60
1	C2	1439	С	N3-C2-O2	-5.22	118.25	121.90
1	C2	160	С	C2-N1-C1'	5.22	124.54	118.80
1	C2	691	С	C5-C6-N1	5.22	123.61	121.00
3	C1	2350	С	C6-N1-C2	-5.22	118.21	120.30
3	C1	687	U	N3-C2-O2	-5.22	118.55	122.20
3	C1	1609	С	C5-C6-N1	5.22	123.61	121.00
3	C1	1152	G	C4-C5-C6	-5.22	115.67	118.80
3	C1	3257	С	C5-C6-N1	5.22	123.61	121.00
3	C1	3283	U	N3-C2-O2	-5.22	118.55	122.20
3	C1	2273	G	C4-N9-C1'	-5.21	119.72	126.50
3	C1	3039	С	C5-C6-N1	5.21	123.61	121.00
1	C2	1123	С	N1-C2-O2	5.21	122.03	118.90
3	C1	1818	U	N1-C2-O2	5.21	126.45	122.80
3	C1	2199	G	N9-C4-C5	-5.21	103.32	105.40
1	C2	1244	А	C2-N3-C4	5.21	113.20	110.60
3	C1	2582	С	C6-N1-C2	-5.21	118.22	120.30
3	C1	3086	A	N7-C8-N9	5.21	116.40	113.80
1	C2	422	G	O4'-C1'-N9	5.20	112.36	108.20
1	C2	1354	G	N3-C4-N9	5.20	129.12	126.00
1	C2	1572	G	N3-C4-N9	5.20	129.12	126.00
1	C2	826	U	C5-C6-N1	5.20	125.30	122.70
3	C1	900	G	C5-C6-O6	-5.20	125.48	128.60
1	C2	512	А	P-O3'-C3'	5.20	125.94	119.70
3	C1	1561	G	O4'-C1'-N9	5.20	112.36	108.20
3	C1	3104	U	N3-C2-O2	-5.20	118.56	122.20
1	C2	870	С	C6-N1-C2	-5.20	118.22	120.30
3	C1	45	А	C2-N3-C4	5.19	113.20	110.60
3	C1	1283	С	C2-N1-C1'	5.19	124.51	118.80
1	C2	160	С	C5-C6-N1	5.19	123.59	121.00
1	C2	1078	С	C6-N1-C2	-5.19	118.22	120.30
1	C2	1527	С	N1-C2-O2	5.19	122.02	118.90
3	C1	438	А	C4-N9-C1'	5.19	135.64	126.30
3	C1	661	G	N1-C6-O6	-5.19	116.79	119.90
3	C1	1145	G	N3-C4-N9	5.19	129.11	126.00
3	C1	1872	С	C5-C6-N1	5.19	123.59	121.00
3	C1	1531	C	C6-N1-C2	-5.19	118.23	120.30
3	C1	3076	С	C6-N1-C2	-5.19	118.23	120.30
1	C2	1392	U	C5-C6-N1	5.18	125.29	122.70
3	C1	412	G	N3-C4-C5	-5.18	126.01	128.60
22	SQ	117	LEU	CA-CB-CG	5.18	$1\overline{27.22}$	115.30
1	C2	1107	G	N3-C4-N9	5.18	129.11	126.00



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	175	С	N1-C2-N3	5.18	122.83	119.20
3	C1	2405	С	N1-C2-O2	5.18	122.01	118.90
3	C1	548	G	N1-C6-O6	-5.18	116.79	119.90
1	C2	1340	U	C2-N1-C1'	5.18	123.91	117.70
1	C2	795	U	N1-C2-O2	5.17	126.42	122.80
1	C2	1354	G	C4-N9-C1'	5.17	133.23	126.50
3	C1	1102	А	C6-C5-N7	5.17	135.92	132.30
3	C1	1168	U	C6-N1-C2	-5.17	117.89	121.00
3	C1	2560	С	N1-C2-O2	5.17	122.00	118.90
1	C2	1269	U	C2-N1-C1'	5.17	123.91	117.70
1	C2	1024	U	N1-C2-O2	5.17	126.42	122.80
3	C1	125	С	N1-C2-O2	5.17	122.00	118.90
1	C2	142	G	C4-N9-C1'	5.17	133.22	126.50
1	C2	1063	U	N1-C2-O2	5.17	126.42	122.80
3	C1	1843	С	C6-N1-C2	-5.17	118.23	120.30
3	C1	1854	С	C5-C6-N1	5.17	123.58	121.00
3	C1	1900	А	C5-C6-N1	5.17	120.28	117.70
1	C2	747	С	C6-N1-C2	-5.17	118.23	120.30
1	C2	1278	G	N3-C4-N9	5.17	129.10	126.00
1	C2	1500	С	N3-C2-O2	-5.17	118.28	121.90
3	C1	1425	U	N3-C2-O2	-5.17	118.58	122.20
3	C1	1816	А	P-O3'-C3'	5.17	125.90	119.70
3	C1	1869	С	C6-N1-C2	-5.17	118.23	120.30
1	C2	18	С	C5-C6-N1	5.16	123.58	121.00
1	C2	1271	G	C5-C6-O6	5.16	131.70	128.60
3	C1	2585	G	C2-N3-C4	5.16	114.48	111.90
3	C1	1284	С	P-O3'-C3'	5.16	125.89	119.70
1	C2	542	A	N7-C8-N9	5.16	116.38	113.80
4	C4	35	С	C6-N1-C2	-5.16	118.24	120.30
1	C2	1720	G	C8-N9-C1'	-5.16	120.30	127.00
3	C1	141	С	C6-N1-C2	-5.16	118.24	120.30
3	C1	3043	С	C5-C6-N1	5.16	123.58	121.00
1	C2	162	А	N7-C8-N9	5.15	116.38	113.80
1	C2	834	G	C8-N9-C1'	-5.15	120.30	127.00
3	C1	15	С	N1-C2-O2	5.15	121.99	118.90
3	C1	851	С	C5-C6-N1	5.15	123.58	121.00
3	C1	404	G	N3-C4-N9	5.15	129.09	126.00
3	C1	1448	U	C5-C6-N1	5.15	125.28	122.70
1	C2	339	С	C6-N1-C2	-5.15	118.24	120.30
3	C1	2984	С	C2-N1-C1'	5.15	124.46	118.80
1	C2	1246	С	C6-N1-C1'	-5.14	114.63	120.80
3	C1	327	А	C8-N9-C4	-5.14	103.74	105.80



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Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	1173	U	C5-C6-N1	5.14	125.27	122.70
4	C4	58	С	C5-C6-N1	5.14	123.57	121.00
51	LN	183	THR	CA-CB-CG2	5.14	119.60	112.40
1	C2	424	С	C5-C6-N1	5.14	123.57	121.00
1	C2	1053	G	C2-N3-C4	5.14	114.47	111.90
1	C2	1115	U	C2-N1-C1'	5.14	123.87	117.70
3	C1	1316	С	OP1-P-O3'	5.14	116.51	105.20
3	C1	2988	С	C5-C6-N1	5.14	123.57	121.00
3	C1	3214	U	C6-N1-C1'	-5.14	114.00	121.20
1	C2	956	С	C6-N1-C2	-5.14	118.25	120.30
1	C2	1210	С	C6-N1-C1'	5.14	126.97	120.80
1	C2	1415	U	N1-C2-O2	5.14	126.40	122.80
13	SH	38	LEU	CA-CB-CG	5.14	127.12	115.30
3	C1	1466	G	C6-C5-N7	-5.14	127.32	130.40
3	C1	2918	G	C8-N9-C4	-5.14	104.34	106.40
3	C1	1711	С	C5-C6-N1	5.14	123.57	121.00
3	C1	2571	U	C6-N1-C1'	-5.14	114.01	121.20
3	C1	2227	С	C6-N1-C2	-5.13	118.25	120.30
1	C2	1455	G	C5-C6-O6	5.13	131.68	128.60
3	C1	573	С	C5-C6-N1	5.13	123.56	121.00
1	C2	945	U	C5-C6-N1	5.13	125.26	122.70
3	C1	2137	U	N3-C2-O2	-5.13	118.61	122.20
3	C1	2935	U	N3-C2-O2	-5.13	118.61	122.20
3	C1	3137	С	C6-N1-C2	-5.13	118.25	120.30
5	C3	38	U	N1-C2-O2	5.13	126.39	122.80
3	C1	1063	G	C4-C5-N7	5.13	112.85	110.80
3	C1	3105	U	C6-N1-C2	-5.13	117.92	121.00
3	C1	3362	А	C4-N9-C1'	5.13	135.53	126.30
3	C1	2359	С	C5-C6-N1	5.12	123.56	121.00
3	C1	3289	G	P-O3'-C3'	5.12	125.85	119.70
1	C2	270	С	C2-N1-C1'	5.12	124.43	118.80
3	C1	1041	U	N3-C2-O2	-5.12	118.61	122.20
3	C1	1115	G	N3-C4-C5	-5.12	126.04	128.60
1	C2	350	U	C2-N3-C4	-5.12	123.93	127.00
4	C4	39	С	C6-N1-C2	-5.12	118.25	120.30
9	SD	218	LEU	CA-CB-CG	5.11	127.06	115.30
3	C1	2553	U	C5-C6-N1	5.11	125.26	122.70
1	C2	873	U	N1-C2-O2	5.11	126.38	122.80
1	C2	$16\overline{37}$	C	C6-N1-C2	-5.11	118.26	120.30
3	C1	2638	C	C2-N1-C1'	5.11	124.42	118.80
1	C2	$17\overline{1}$	A	C6-N1-C2	-5.11	$115.5\overline{3}$	118.60
1	C2	638	U	OP2-P-O3'	5.11	116.44	105.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	1059	U	OP1-P-OP2	-5.11	111.94	119.60
1	C2	1572	G	C8-N9-C1'	-5.11	120.36	127.00
3	C1	1115	G	N3-C4-N9	5.11	129.06	126.00
1	C2	422	G	C8-N9-C1'	5.11	133.64	127.00
3	C1	124	U	N3-C2-O2	-5.11	118.63	122.20
3	C1	1144	U	N3-C4-O4	5.11	122.97	119.40
3	C1	2818	U	O5'-P-OP2	-5.11	101.11	105.70
3	C1	3174	А	N9-C4-C5	-5.10	103.76	105.80
1	C2	110	U	C5-C6-N1	5.10	125.25	122.70
3	C1	817	А	C5-C6-N1	5.10	120.25	117.70
3	C1	1377	G	N1-C6-O6	-5.10	116.84	119.90
3	C1	2379	U	N1-C2-N3	5.10	117.96	114.90
3	C1	2405	С	N3-C2-O2	-5.10	118.33	121.90
3	C1	2545	С	C5-C6-N1	5.10	123.55	121.00
1	C2	1214	U	C6-N1-C2	-5.10	117.94	121.00
3	C1	178	U	C2-N1-C1'	5.10	123.82	117.70
3	C1	2383	С	N1-C2-O2	5.10	121.96	118.90
3	C1	3205	G	O4'-C1'-N9	5.10	112.28	108.20
1	C2	1596	С	C6-N1-C1'	-5.10	114.69	120.80
3	C1	292	U	C5-C6-N1	5.09	125.25	122.70
1	C2	1643	U	N1-C2-O2	5.09	126.36	122.80
5	C3	112	U	C2-N1-C1'	-5.09	111.59	117.70
1	C2	390	G	C8-N9-C4	-5.09	104.36	106.40
3	C1	1889	G	C8-N9-C1'	-5.09	120.39	127.00
64	La	47	LYS	C-N-CA	5.09	134.42	121.70
3	C1	220	G	C5-C6-O6	-5.08	125.55	128.60
1	C2	187	G	P-O3'-C3'	5.08	125.80	119.70
3	C1	297	G	C4-C5-N7	5.08	112.83	110.80
3	C1	1156	С	C5-C6-N1	5.08	123.54	121.00
1	C2	176	С	C6-N1-C2	-5.08	118.27	120.30
1	C2	1390	U	C2-N1-C1'	5.08	123.80	117.70
3	C1	817	А	C2-N3-C4	5.08	113.14	110.60
1	C2	272	U	OP2-P-O3'	5.08	116.38	105.20
1	C2	1485	С	N3-C2-O2	-5.08	118.34	121.90
3	C1	945	С	C5-C6-N1	5.08	123.54	121.00
3	C1	868	С	C6-N1-C2	-5.08	118.27	120.30
3	C1	3231	U	N3-C2-O2	-5.08	118.65	122.20
3	C1	3363	U	N3-C2-O2	-5.08	118.65	122.20
1	C2	1506	G	N3-C4-C5	-5.08	126.06	128.60
1	C2	1720	G	C4-N9-C1'	5.08	133.10	126.50
1	C2	302	U	N3-C2-O2	-5.07	118.65	122.20
1	C2	960	U	N3-C2-O2	-5.07	118.65	122.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	C2	1115	U	N3-C2-O2	-5.07	118.65	122.20
3	C1	1267	U	N3-C2-O2	-5.07	118.65	122.20
3	C1	1417	G	C5-C6-O6	-5.07	125.56	128.60
3	C1	2225	U	C5-C6-N1	5.07	125.24	122.70
3	C1	3165	А	N1-C6-N6	-5.07	115.56	118.60
5	C3	46	G	C8-N9-C4	-5.07	104.37	106.40
1	C2	230	С	C5-C6-N1	5.07	123.53	121.00
1	C2	1021	С	C6-N1-C2	-5.07	118.27	120.30
1	C2	981	U	N3-C2-O2	-5.07	118.65	122.20
3	C1	1312	С	C5-C6-N1	5.07	123.53	121.00
1	C2	21	U	C6-N1-C2	-5.06	117.96	121.00
1	C2	1248	С	C6-N1-C1'	-5.06	114.72	120.80
3	C1	283	G	N9-C4-C5	-5.06	103.38	105.40
3	C1	3362	А	O4'-C1'-N9	5.06	112.25	108.20
5	C3	113	U	N1-C2-O2	5.06	126.34	122.80
3	C1	107	А	C8-N9-C4	-5.06	103.78	105.80
3	C1	126	U	N1-C2-O2	5.06	126.34	122.80
3	C1	271	С	N3-C2-O2	-5.06	118.36	121.90
3	C1	1145	G	N9-C4-C5	-5.06	103.38	105.40
3	C1	1409	G	C8-N9-C4	-5.06	104.38	106.40
3	C1	2415	С	C6-N1-C2	-5.06	118.28	120.30
3	C1	3255	U	N3-C2-O2	-5.06	118.66	122.20
3	C1	3301	U	N1-C2-O2	5.06	126.34	122.80
3	C1	3382	U	C2-N1-C1'	5.06	123.77	117.70
1	C2	1500	С	N1-C2-O2	5.06	121.93	118.90
3	C1	512	U	N1-C2-O2	5.06	126.34	122.80
3	C1	1496	С	N3-C2-O2	-5.06	118.36	121.90
3	C1	1604	G	C4-C5-N7	5.06	112.82	110.80
1	C2	1240	U	C2-N1-C1'	5.05	123.77	117.70
3	C1	1273	А	C2-N3-C4	5.05	113.13	110.60
3	C1	2822	U	N3-C2-O2	-5.05	118.66	122.20
4	C4	58	С	C6-N1-C2	-5.05	118.28	120.30
3	C1	3105	U	C2-N1-C1'	5.05	123.76	117.70
3	C1	1496	С	C6-N1-C1'	-5.05	114.74	120.80
3	C1	3321	С	C5-C6-N1	5.05	123.53	121.00
3	C1	1901	A	C4-N9-C1'	5.05	135.39	126.30
3	C1	2829	U	N1-C2-O2	5.05	126.33	122.80
1	C2	1514	U	C2-N1-C1'	5.05	123.76	117.70
1	C2	$17\overline{23}$	U	N3-C2-O2	-5.05	118.67	122.20
3	C1	561	C	N3-C2-O2	-5.05	118.37	121.90
3	C1	1022	U	C5-C4-O4	-5.05	122.87	125.90
3	C1	2815	G	N1-C6-O6	-5.05	116.87	119.90



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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
3	C1	2925	С	C6-N1-C2	-5.05	118.28	120.30
1	C2	1601	G	C4-N9-C1'	-5.04	119.94	126.50
21	SP	71	GLU	C-N-CA	5.04	134.31	121.70
3	C1	2558	U	N3-C2-O2	-5.04	118.67	122.20
1	C2	196	G	C4-N9-C1'	-5.04	119.95	126.50
1	C2	828	U	C2-N1-C1'	5.04	123.75	117.70
1	C2	1285	U	C2-N1-C1'	5.04	123.75	117.70
3	C1	1478	С	C5-C6-N1	5.04	123.52	121.00
3	C1	1495	U	C6-N1-C2	-5.04	117.98	121.00
3	C1	3262	U	N3-C2-O2	-5.04	118.67	122.20
1	C2	691	С	C2-N1-C1'	5.04	124.34	118.80
1	C2	968	U	C5-C6-N1	5.04	125.22	122.70
1	C2	1601	G	C6-C5-N7	5.04	133.42	130.40
3	C1	1725	С	C6-N1-C2	-5.04	118.29	120.30
3	C1	2366	С	C2-N3-C4	5.04	122.42	119.90
1	C2	949	С	C6-N1-C2	-5.03	118.29	120.30
3	C1	1501	U	N1-C2-O2	5.03	126.32	122.80
3	C1	3166	С	C6-N1-C2	-5.03	118.29	120.30
1	C2	120	U	C5-C6-N1	5.03	125.22	122.70
3	C1	503	С	C5-C6-N1	5.03	123.52	121.00
3	C1	609	G	C8-N9-C1'	-5.03	120.46	127.00
3	C1	2961	G	C4-N9-C1'	5.03	133.04	126.50
3	C1	1241	U	OP1-P-O3'	5.03	116.26	105.20
1	C2	484	С	C2-N1-C1'	5.03	124.33	118.80
1	C2	852	С	C2-N1-C1'	5.03	124.33	118.80
1	C2	917	U	N3-C2-O2	-5.03	118.68	122.20
3	C1	1730	G	C5-C6-N1	5.03	114.01	111.50
3	C1	2872	A	C4-C5-N7	5.03	113.21	110.70
1	C2	644	С	C6-N1-C2	-5.03	118.29	120.30
1	C2	1278	G	C6-C5-N7	-5.02	127.39	130.40
3	C1	1923	С	C6-N1-C2	-5.02	118.29	120.30
3	C1	2274	U	C6-N1-C1'	-5.02	114.17	121.20
3	C1	2788	С	C2-N1-C1'	5.02	124.32	118.80
3	C1	354	U	C2-N1-C1'	5.02	123.72	117.70
1	C2	230	С	C6-N1-C2	-5.02	118.29	120.30
1	C2	559	C	C2-N1-C1'	5.02	124.32	118.80
3	C1	1907	C	C2-N1-C1'	5.02	124.32	118.80
1	C2	131	C	C5-C6-N1	5.01	123.51	121.00
1	C2	854	U	C2-N3-C4	-5.01	123.99	127.00
3	C1	126	U	N3-C2-O2	-5.01	118.69	122.20
3	C1	1027	A	P-O3'-C3'	5.01	$125.7\overline{2}$	119.70
3	C1	2889	C	N1-C2-O2	5.01	121.91	118.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	C1	2369	G	N3-C4-C5	-5.01	126.09	128.60
3	C1	312	С	C6-N1-C2	-5.01	118.30	120.30
1	C2	115	G	N7-C8-N9	5.01	115.61	113.10
1	C2	337	G	O4'-C1'-N9	-5.01	104.19	108.20
3	C1	768	С	C2-N1-C1'	5.01	124.31	118.80
3	C1	2379	U	N3-C2-O2	-5.01	118.69	122.20
1	C2	1049	U	C5-C6-N1	5.01	125.20	122.70
3	C1	412	G	C2-N3-C4	5.01	114.40	111.90
3	C1	1292	С	C5-C6-N1	5.01	123.50	121.00
3	C1	1337	А	N1-C2-N3	-5.01	126.80	129.30
3	C1	3105	U	N1-C2-O2	5.01	126.31	122.80
3	C1	3111	U	C5-C4-O4	-5.01	122.90	125.90
1	C2	817	A	N9-C4-C5	-5.00	103.80	105.80
3	C1	191	U	N1-C2-O2	5.00	126.30	122.80
3	C1	938	С	C6-N1-C2	-5.00	118.30	120.30
3	C1	1190	A	C2-N3-C4	5.00	113.10	110.60
3	C1	2546	С	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (74) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
39	LA	13	GLY	Peptide
39	LA	237	LEU	Peptide
39	LA	249	SER	Peptide
39	LA	55	GLY	Peptide
40	LB	2	SER	Peptide
40	LB	248	LYS	Peptide
41	LC	144	LYS	Peptide
41	LC	268	ALA	Peptide
41	LC	338	LYS	Peptide
41	LC	89	ALA	Peptide
45	LG	221	ASN	Peptide
48	LJ	94	ARG	Peptide
49	LL	135	ALA	Peptide
49	LL	46	ILE	Peptide
49	LL	47	ALA	Peptide
49	LL	61	PRO	Peptide
51	LN	146	ALA	Peptide
54	LQ	98	LYS	Peptide
56	LS	171	PHE	Peptide
58	LU	25	ASN	Peptide



Mol	Chain	Res	Type	Group
63	LZ	102	GLU	Peptide
63	LZ	125	GLY	Peptide
64	La	17	ALA	Peptide
65	Lb	20	GLY	Peptide
65	Lb	21	ILE	Peptide
67	Ld	90	PHE	Peptide
71	Lh	118	ILE	Peptide
71	Lh	83	LYS	Peptide
72	Li	63	ASN	Peptide
79	Lp	51	ALA	Peptide
6	SA	184	LEU	Peptide
6	SA	186	GLY	Peptide
6	SA	43	ASP	Peptide
6	SA	94	GLY	Peptide
7	SB	105	PHE	Peptide
8	SC	236	PRO	Peptide
10	SE	118	GLU	Peptide
10	SE	195	ILE	Peptide
10	SE	89	VAL	Peptide
12	SG	68	LEU	Peptide
13	SH	110	GLN	Peptide
13	SH	130	VAL	Peptide
13	SH	31	SER	Peptide
13	SH	64	VAL	Peptide
13	SH	9	LEU	Peptide
15	SJ	162	SER	Peptide
16	SK	23	ALA	Peptide
16	SK	86	ILE	Peptide
18	SM	102	GLY	Peptide
18	SM	110	GLY	Peptide
18	SM	130	THR	Peptide
19	SN	21	ASN	Peptide
19	SN	28	LEU	Peptide
20	SO	131	GLY	Peptide
20	SO	90	ARG	Peptide
21	SP	124	THR	Peptide
21	SP	127	ARG	Peptide
22	SQ	112	TYR	Peptide
22	SQ	113	ASP	Peptide
24	SS	101	LEU	Peptide
26	SU	50	LEU	Peptide
26	SU	51	VAL	Peptide

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Mol	Chain	Res	Type	Group
26	SU	72	ASN	Peptide
28	SW	54	ASP	Peptide
30	SY	32	ARG	Peptide
30	SY	51	GLU	Peptide
31	SZ	86	GLU	Peptide
32	Sa	10	ARG	Peptide
32	Sa	46	GLU	Peptide
33	Sb	59	CYS	Peptide
33	Sb	75	GLU	Peptide
36	Se	4	VAL	Peptide
36	Se	44	PHE	Peptide
36	Se	47	VAL	Peptide

## 5.2 Too-close contacts (i)

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

# 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	C5	77/92~(84%)	73~(95%)	4 (5%)	0	100	100
6	SA	204/252~(81%)	175 (86%)	29~(14%)	0	100	100
7	SB	214/255~(84%)	190 (89%)	24 (11%)	0	100	100
8	SC	215/254~(85%)	195 (91%)	19 (9%)	1 (0%)	29	61
9	SD	221/240~(92%)	196 (89%)	25~(11%)	0	100	100
10	SE	258/261~(99%)	233 (90%)	24 (9%)	1 (0%)	34	67
11	SF	204/225~(91%)	177 (87%)	26~(13%)	1 (0%)	29	61
12	SG	216/236~(92%)	201 (93%)	15 (7%)	0	100	100
13	SH	183/190~(96%)	156 (85%)	24~(13%)	3 (2%)	9	34



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
14	SI	184/200~(92%)	173~(94%)	11 (6%)	0	100	100
15	SJ	183/197~(93%)	166 (91%)	15 (8%)	2(1%)	14	44
16	SK	90/105~(86%)	70 (78%)	20~(22%)	0	100	100
17	$\operatorname{SL}$	144/156~(92%)	123~(85%)	21~(15%)	0	100	100
18	SM	122/143~(85%)	83~(68%)	36~(30%)	3~(2%)	5	26
19	SN	148/151~(98%)	135~(91%)	13~(9%)	0	100	100
20	SO	126/137~(92%)	109 (86%)	17~(14%)	0	100	100
21	SP	117/142~(82%)	95 (81%)	20~(17%)	2 (2%)	9	34
22	SQ	139/143~(97%)	126 (91%)	12 (9%)	1 (1%)	22	55
23	SR	111/136~(82%)	96 (86%)	15~(14%)	0	100	100
24	SS	143/146~(98%)	123 (86%)	20 (14%)	0	100	100
25	ST	141/144~(98%)	127 (90%)	14 (10%)	0	100	100
26	SU	99/121~(82%)	91 (92%)	7~(7%)	1 (1%)	15	46
27	SV	85/87~(98%)	72 (85%)	12~(14%)	1 (1%)	13	41
28	SW	127/130~(98%)	119 (94%)	8~(6%)	0	100	100
29	SX	142/145~(98%)	128 (90%)	12 (8%)	2(1%)	11	37
30	SY	132/135~(98%)	113 (86%)	17~(13%)	2(2%)	10	36
31	SZ	67/108~(62%)	61 (91%)	6~(9%)	0	100	100
32	Sa	95/119~(80%)	80 (84%)	14~(15%)	1 (1%)	14	44
33	$\operatorname{Sb}$	79/82~(96%)	64 (81%)	14 (18%)	1 (1%)	12	39
34	$\operatorname{Sc}$	61/67~(91%)	53 (87%)	8 (13%)	0	100	100
35	Sd	51/56~(91%)	46 (90%)	5 (10%)	0	100	100
36	Se	58/63~(92%)	46 (79%)	12 (21%)	0	100	100
37	Sf	31/152~(20%)	23~(74%)	8~(26%)	0	100	100
38	$\operatorname{Sg}$	311/319~(98%)	275~(88%)	36~(12%)	0	100	100
39	LA	250/254~(98%)	213 (85%)	37~(15%)	0	100	100
40	LB	384/387~(99%)	352 (92%)	32 (8%)	0	100	100
41	LC	$359/362~(\overline{99\%})$	314 (88%)	44~(12%)	1 (0%)	41	72
42	LD	292/297~(98%)	273 (94%)	19~(6%)	0	100	100
43	LE	153/176~(87%)	132 (86%)	21 (14%)	0	100	100
44	m LF	221/244~(91%)	207 (94%)	14~(6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
45	LG	229/256~(90%)	199~(87%)	30~(13%)	0	100	100
46	LH	188/191~(98%)	178~(95%)	10~(5%)	0	100	100
47	$\operatorname{LI}$	205/221~(93%)	189 (92%)	15 (7%)	1 (0%)	29	61
48	LJ	167/174~(96%)	139~(83%)	25~(15%)	3 (2%)	8	32
49	LL	192/199~(96%)	164 (85%)	19~(10%)	9~(5%)	2	15
50	LM	135/138~(98%)	126~(93%)	9~(7%)	0	100	100
51	LN	201/204~(98%)	180 (90%)	20~(10%)	1 (0%)	29	61
52	LO	195/199~(98%)	188 (96%)	6~(3%)	1 (0%)	29	61
53	LP	171/184~(93%)	159~(93%)	12 (7%)	0	100	100
54	LQ	183/186~(98%)	172 (94%)	11 (6%)	0	100	100
55	LR	172/189~(91%)	161 (94%)	11 (6%)	0	100	100
56	LS	170/172~(99%)	157~(92%)	13 (8%)	0	100	100
57	LT	157/160~(98%)	145~(92%)	12 (8%)	0	100	100
58	LU	96/121~(79%)	91~(95%)	5~(5%)	0	100	100
59	LV	132/137~(96%)	122 (92%)	10 (8%)	0	100	100
60	LW	61/155~(39%)	58~(95%)	3~(5%)	0	100	100
61	LX	118/142~(83%)	109 (92%)	9~(8%)	0	100	100
62	LY	122/127~(96%)	114 (93%)	8~(7%)	0	100	100
63	LZ	133/136~(98%)	114 (86%)	18 (14%)	1 (1%)	19	51
64	La	146/149~(98%)	130 (89%)	14 (10%)	2 (1%)	11	37
65	Lb	56/59~(95%)	46 (82%)	9~(16%)	1 (2%)	8	32
66	Lc	98/105~(93%)	89 (91%)	9  (9%)	0	100	100
67	Ld	107/113~(95%)	99~(92%)	8 (8%)	0	100	100
68	Le	125/130~(96%)	115~(92%)	9~(7%)	1 (1%)	19	51
69	$\mathrm{Lf}$	104/107~(97%)	91~(88%)	13~(12%)	0	100	100
70	Lg	110/121~(91%)	107~(97%)	3~(3%)	0	100	100
71	Lh	117/120~(98%)	109 (93%)	8 (7%)	0	100	100
72	Li	97/100~(97%)	89 (92%)	8 (8%)	0	100	100
73	Lj	80/88~(91%)	76 (95%)	4(5%)	0	100	100
74	Lk	75/78~(96%)	69 (92%)	5(7%)	1 (1%)	12	39
75	Ll	48/51~(94%)	42 (88%)	6~(12%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
76	Lm	50/128~(39%)	48 (96%)	2~(4%)	0	100	100
77	Ln	23/25~(92%)	22 (96%)	1 (4%)	0	100	100
78	Lo	103/106~(97%)	98~(95%)	5 (5%)	0	100	100
79	Lp	89/92~(97%)	81 (91%)	8~(9%)	0	100	100
All	All	10892/11972~(91%)	9760 (90%)	1088 (10%)	44 (0%)	38	67

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	SQ	116	LEU
41	LC	339	LEU
48	LJ	95	ASN
49	LL	48	PRO
49	LL	62	THR
51	LN	147	ARG
64	La	78	LEU
74	Lk	17	ARG
11	SF	101	GLY
18	SM	109	GLU
18	SM	131	ASP
30	SY	52	LYS
49	LL	76	THR
49	LL	77	LEU
10	SE	196	VAL
13	SH	74	GLN
13	SH	111	LYS
21	SP	68	PRO
21	SP	71	GLU
48	LJ	109	HIS
49	LL	140	SER
15	SJ	163	PRO
18	SM	130	THR
27	SV	11	LEU
29	SX	89	ASN
47	LI	175	ASN
48	LJ	115	LYS
49	LL	47	ALA
63	LZ	102	GLU
13	SH	10	SER
26	SU	71	PRO
29	SX	88	PRO



Mol	Chain	Res	Type
32	Sa	34	LYS
49	LL	5	LYS
49	LL	60	ALA
49	LL	61	PRO
65	Lb	20	GLY
68	Le	6	HIS
52	LO	5	PRO
64	La	18	GLY
15	SJ	162	SER
30	SY	79	VAL
33	Sb	76	GLY
8	SC	236	PRO

### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	C5	60/70~(86%)	60 (100%)	0	100 100
6	SA	165/210~(79%)	163~(99%)	2(1%)	71 85
7	SB	192/224~(86%)	190 (99%)	2(1%)	76 88
8	$\mathbf{SC}$	176/205~(86%)	170 (97%)	6 (3%)	37 65
9	SD	182/195~(93%)	176~(97%)	6 (3%)	38 66
10	SE	221/222 (100%)	217~(98%)	4 (2%)	59 79
11	$\mathbf{SF}$	173/191~(91%)	167~(96%)	6 (4%)	36 65
12	$\operatorname{SG}$	186/201~(92%)	183~(98%)	3~(2%)	62 81
13	SH	165/170~(97%)	161 (98%)	4 (2%)	49 74
14	SI	150/161~(93%)	149 (99%)	1 (1%)	84 92
15	SJ	158/166~(95%)	151 (96%)	7 (4%)	28 58
16	SK	73/98~(74%)	73~(100%)	0	100 100
17	SL	129/137~(94%)	126 (98%)	3(2%)	50 74
18	SM	88/119 (74%)	86 (98%)	2 (2%)	50 74



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
19	SN	127/128~(99%)	125~(98%)	2(2%)	62	81
20	SO	97/105~(92%)	95~(98%)	2(2%)	53	76
21	SP	98/118~(83%)	95~(97%)	3(3%)	40	68
22	SQ	117/119~(98%)	115 (98%)	2(2%)	60	80
23	SR	92/124~(74%)	90~(98%)	2(2%)	52	75
24	SS	128/129~(99%)	124 (97%)	4 (3%)	40	68
25	ST	115/116~(99%)	114 (99%)	1 (1%)	78	90
26	SU	94/114 (82%)	92~(98%)	2 (2%)	53	76
27	SV	74/74~(100%)	73~(99%)	1 (1%)	67	83
28	SW	110/111~(99%)	108 (98%)	2(2%)	59	79
29	SX	119/120~(99%)	116 (98%)	3 (2%)	47	72
30	SY	112/113~(99%)	111 (99%)	1 (1%)	78	90
31	SZ	61/89~(68%)	61 (100%)	0	100	100
32	Sa	83/100 (83%)	82 (99%)	1 (1%)	71	85
33	Sb	70/71~(99%)	70 (100%)	0	100	100
34	Sc	56/60~(93%)	55~(98%)	1 (2%)	59	79
35	Sd	47/49~(96%)	47 (100%)	0	100	100
36	Se	51/54~(94%)	51 (100%)	0	100	100
37	Sf	27/135~(20%)	27~(100%)	0	100	100
38	$\operatorname{Sg}$	255/262~(97%)	253~(99%)	2(1%)	81	91
39	LA	192/196~(98%)	187 (97%)	5(3%)	46	72
40	LB	318/323~(98%)	311 (98%)	7 (2%)	52	75
41	LC	288/289~(100%)	285~(99%)	3 (1%)	76	88
42	LD	243/245~(99%)	242 (100%)	1 (0%)	91	95
43	LE	135/153~(88%)	133 (98%)	2 (2%)	65	82
44	LF	187/205~(91%)	186 (100%)	1 (0%)	88	94
45	LG	177/208~(85%)	175 (99%)	2 (1%)	73	86
46	LH	170/171~(99%)	168 (99%)	2 (1%)	71	85
47	LI	177/187 (95%)	176 (99%)	1 (1%)	86	94
48	LJ	147/150 (98%)	143 (97%)	4 (3%)	44	70
49	LL	154/159~(97%)	151 (98%)	3 (2%)	57	78



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
50	LM	108/109~(99%)	106~(98%)	2(2%)	57	78
51	LN	175/176~(99%)	174~(99%)	1 (1%)	86	94
52	LO	160/162~(99%)	159~(99%)	1 (1%)	86	94
53	LP	139/146~(95%)	136~(98%)	3(2%)	52	75
54	LQ	150/151~(99%)	150 (100%)	0	100	100
55	LR	132/154~(86%)	128 (97%)	4 (3%)	41	68
56	LS	156/156~(100%)	155~(99%)	1 (1%)	86	94
57	LT	136/137~(99%)	133~(98%)	3 (2%)	52	75
58	LU	85/107~(79%)	85 (100%)	0	100	100
59	LV	103/105~(98%)	102 (99%)	1 (1%)	76	88
60	LW	55/129~(43%)	54 (98%)	1 (2%)	59	79
61	LX	104/118 (88%)	102 (98%)	2 (2%)	57	78
62	LY	107/110~(97%)	105~(98%)	2 (2%)	57	78
63	LZ	115/116~(99%)	115 (100%)	0	100	100
64	La	118/119~(99%)	118 (100%)	0	100	100
65	Lb	46/47~(98%)	45 (98%)	1 (2%)	52	75
66	Lc	84/88~(96%)	84 (100%)	0	100	100
67	Ld	94/97~(97%)	92~(98%)	2(2%)	53	76
68	Le	109/111~(98%)	108~(99%)	1 (1%)	78	90
69	$\mathbf{L}\mathbf{f}$	90/91~(99%)	89~(99%)	1 (1%)	73	86
70	Lg	95/103~(92%)	95 (100%)	0	100	100
71	Lh	103/105~(98%)	103 (100%)	0	100	100
72	Li	80/82~(98%)	79~(99%)	1 (1%)	69	84
73	Lj	67/71~(94%)	67~(100%)	0	100	100
74	Lk	67/69~(97%)	67~(100%)	0	100	100
75	Ll	45/46~(98%)	44 (98%)	1 (2%)	52	75
76	Lm	47/116 (40%)	47 (100%)	0	100	100
77	Ln	23/23~(100%)	23 (100%)	0	100	100
78	Lo	90/91~(99%)	90 (100%)	0	100	100
79	Lp	71/72~(99%)	70~(99%)	1 (1%)	67	83
All	All	9193/10053~(91%)	9058~(98%)	135 (2%)	66	82



Mol	Chain	Res	Type
6	SA	93	THR
6	SA	139	VAL
7	SB	144	ARG
7	SB	205	PHE
8	SC	69	ILE
8	SC	89	GLN
8	SC	91	ARG
8	SC	111	VAL
8	SC	158	THR
8	SC	222	TYR
9	SD	17	PHE
9	SD	48	VAL
9	SD	94	ARG
9	SD	163	PRO
9	SD	168	ILE
9	SD	196	ARG
10	SE	96	ASN
10	SE	158	ASP
10	SE	202	ASP
10	SE	240	LYS
11	SF	23	VAL
11	SF	52	GLU
11	SF	73	THR
11	SF	90	ILE
11	SF	143	ARG
11	SF	148	ARG
12	SG	69	LEU
12	SG	71	THR
12	SG	98	ARG
13	SH	5	GLN
13	SH	9	LEU
13	SH	41	LEU
13	SH	47	ARG
14	SI	76	THR
15	SJ	3	ARG
15	SJ	14	THR
15	SJ	41	GLU
15	SJ	140	ILE
15	SJ	151	ASP
15	SJ	161	THR
15	SJ	168	ARG
17	$\overline{\mathrm{SL}}$	35	TYR

All (135) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
17	SL	60	PHE
17	SL	67	ARG
18	SM	43	ARG
18	SM	63	VAL
19	SN	46	THR
19	SN	87	ASP
20	SO	26	THR
20	SO	43	THR
21	SP	52	LYS
21	SP	71	GLU
21	SP	105	VAL
22	SQ	69	VAL
22	SQ	97	VAL
23	SR	9	VAL
23	SR	106	THR
24	SS	62	THR
24	SS	111	ASP
24	SS	116	LEU
24	SS	140	THR
25	ST	28	LEU
26	SU	51	VAL
26	SU	81	THR
27	SV	17	CYS
28	SW	103	ILE
28	SW	106	THR
29	SX	89	ASN
29	SX	107	PHE
29	SX	130	VAL
30	SY	38	ASP
32	Sa	15	ARG
34	Sc	56	LEU
38	Sg	115	ILE
38	Sg	229	LYS
39	LA	23	ARG
39	LA	112	ILE
39	LA	193	ARG
39	LA	246	LEU
39	LA	247	ARG
40	LB	114	VAL
40	LB	137	TYR
40	LB	205	VAL
40	LB	260	VAL



Mol	Chain	Res	Type
40	LB	332	ARG
40	LB	361	THR
40	LB	372	THR
41	LC	197	ARG
41	LC	230	VAL
41	LC	292	SER
42	LD	271	LYS
43	LE	51	ARG
43	LE	52	VAL
44	LF	229	PHE
45	LG	79	GLN
45	LG	197	VAL
46	LH	17	THR
46	LH	59	ASN
47	LI	177	ASP
48	LJ	12	LEU
48	LJ	65	ILE
48	LJ	130	VAL
48	LJ	152	HIS
49	LL	21	ARG
49	LL	58	VAL
49	LL	100	ARG
50	LM	66	THR
50	LM	113	THR
51	LN	167	THR
52	LO	189	ASP
53	LP	79	THR
53	LP	113	TYR
53	LP	120	ASN
55	LR	151	ARG
55	LR	156	ASN
55	LR	158	GLU
55	LR	160	GLU
$5\overline{6}$	LS	172	TYR
57	LT	18	ASP
57	LT	82	ASN
57	LT	130	ARG
59	LV	135	VAL
60	LW	19	THR
61	LX	106	ASP
61	LX	127	THR
62	LY	21	THR



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Mol	Chain	Res	Type	
62	LY	31	LEU	
65	Lb	14	ARG	
67	Ld	13	THR	
67	Ld	64	VAL	
68	Le	91	THR	
69	Lf	37	THR	
72	Li	81	THR	
75	Ll	23	LEU	
79	Lp	73	THR	

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
2	C5	33	GLN
2	C5	58	GLN
6	SA	28	ASN
6	SA	33	GLN
7	SB	148	ASN
8	SC	201	ASN
9	SD	62	ASN
9	SD	101	GLN
9	SD	174	HIS
10	SE	36	HIS
10	SE	57	ASN
11	SF	37	GLN
11	SF	103	ASN
11	SF	127	GLN
12	SG	22	HIS
12	SG	190	GLN
12	SG	210	GLN
13	SH	71	HIS
13	SH	170	GLN
14	SI	32	GLN
14	SI	88	ASN
15	SJ	48	GLN
16	SK	29	GLN
17	SL	14	GLN
19	SN	49	GLN
23	SR	31	ASN
24	SS	75	ASN
24	$\mathbf{SS}$	104	ASN
25	ST	64	HIS



Mol	Chain	Res	Type
25	ST	129	GLN
26	SU	36	ASN
28	SW	80	ASN
29	SX	27	ASN
29	SX	63	GLN
31	SZ	82	HIS
32	Sa	25	ASN
32	Sa	94	ASN
33	Sb	42	ASN
35	Sd	27	HIS
35	Sd	48	ASN
36	Se	17	GLN
37	Sf	123	ASN
38	Sg	106	HIS
38	Sg	153	GLN
38	Sg	196	ASN
38	Sg	299	GLN
39	LA	38	HIS
39	LA	50	HIS
39	LA	79	ASN
39	LA	97	ASN
40	LB	165	GLN
40	LB	279	ASN
41	LC	48	GLN
41	LC	59	GLN
41	LC	175	HIS
41	LC	196	ASN
41	LC	213	ASN
41	LC	320	ASN
42	LD	40	HIS
42	LD	274	GLN
45	LG	33	ASN
45	LG	38	GLN
45	LG	41	GLN
45	LG	77	GLN
45	LG	145	ASN
45	LG	240	ASN
45	LG	243	GLN
46	LH	51	GLN
46	LH	157	ASN
47	LI	59	GLN
47	LI	144	ASN



Mol	Chain	Res	Type
47	LI	163	GLN
47	LI	209	ASN
48	LJ	20	ASN
48	LJ	150	ASN
48	LJ	152	HIS
49	LL	149	GLN
51	LN	11	GLN
51	LN	15	GLN
51	LN	175	ASN
52	LO	29	ASN
53	LP	55	GLN
53	LP	96	GLN
53	LP	116	HIS
53	LP	172	GLN
54	LQ	58	ASN
54	LQ	73	GLN
54	LQ	145	ASN
55	LR	7	GLN
55	LR	34	GLN
56	LS	142	GLN
60	LW	32	GLN
61	LX	55	ASN
62	LY	120	GLN
64	La	44	ASN
67	Ld	43	HIS
69	Lf	24	ASN
69	Lf	26	ASN
70	Lg	33	GLN
71	Lh	34	GLN
73	Lj	28	HIS
74	Lk	10	GLN
76	Lm	90	ASN
76	Lm	109	ASN
78	Lo	22	GLN

## 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C2	1693/1800~(94%)	472~(27%)	31 (1%)
3	C1	3120/3396~(91%)	699~(22%)	39~(1%)
4	C4	120/121~(99%)	21~(17%)	0



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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	C3	156/158~(98%)	37~(23%)	2 (1%)
All	All	5089/5475~(92%)	1229 (24%)	72 (1%)

All (1229) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C2	2	А
1	C2	4	С
1	C2	25	С
1	C2	26	А
1	C2	27	U
1	C2	34	G
1	C2	35	U
1	C2	43	А
1	C2	45	U
1	C2	46	А
1	C2	47	A
1	C2	57	G
1	C2	60	U
1	C2	63	G
1	C2	67	А
1	C2	68	А
1	C2	69	G
1	C2	72	А
1	C2	77	U
1	C2	81	G
1	C2	101	U
1	C2	104	А
1	C2	105	А
1	C2	111	U
1	C2	114	С
1	C2	115	G
1	C2	127	G
1	C2	128	U
1	C2	130	С
1	C2	132	U
1	C2	137	U
1	C2	138	А
1	C2	140	A
1	C2	141	U
1	C2	145	A
1	C2	146	U



Mol	Chain	Res	Type
1	C2	148	А
1	C2	153	G
1	C2	156	A
1	C2	158	U
1	C2	161	U
1	C2	166	С
1	C2	168	А
1	C2	174	U
1	C2	176	С
1	C2	178	U
1	C2	187	G
1	C2	188	А
1	C2	191	С
1	C2	192	U
1	C2	193	U
1	C2	194	U
1	C2	195	G
1	C2	196	G
1	C2	197	A
1	C2	198	А
1	C2	200	A
1	C2	207	U
1	C2	216	U
1	C2	217	А
1	C2	218	А
1	C2	219	А
1	C2	220	А
1	C2	230	С
1	C2	233	С
1	C2	237	С
1	C2	239	С
1	C2	240	U
1	C2	241	U
1	C2	250	С
1	C2	261	U
1	C2	265	А
1	C2	266	A
1	C2	270	С
1	C2	271	A
1	C2	272	U
1	C2	273	G
1	C2	276	С



Mol	Chain	Res	Type
1	C2	278	U
1	C2	280	U
1	C2	290	G
1	C2	299	А
1	C2	302	U
1	C2	309	С
1	C2	314	С
1	C2	316	A
1	C2	319	U
1	C2	320	U
1	C2	333	А
1	C2	337	G
1	C2	338	С
1	C2	339	С
1	C2	343	С
1	C2	344	А
1	C2	350	U
1	C2	352	A
1	C2	359	А
1	C2	360	A
1	C2	361	С
1	C2	369	А
1	C2	399	А
1	C2	400	A
1	C2	401	А
1	C2	402	С
1	C2	404	G
1	C2	416	А
1	C2	417	A
1	C2	418	G
1	C2	419	G
1	C2	421	А
1	C2	423	G
1	C2	424	C
1	C2	425	A
1	C2	426	G
1	C2	428	A
1	C2	434	G
1	C2	436	A
1	C2	439	U
1	C2	444	C
1	C2	445	A



Mol	Chain	Res	Type
1	C2	448	С
1	C2	454	U
1	C2	455	С
1	C2	459	G
1	C2	464	А
1	C2	468	А
1	C2	475	А
1	C2	477	A
1	C2	480	G
1	C2	486	G
1	C2	488	G
1	C2	500	С
1	C2	501	U
1	C2	505	A
1	C2	506	A
1	C2	510	G
1	C2	511	A
1	C2	512	A
1	C2	513	U
1	C2	515	A
1	C2	518	А
1	C2	519	С
1	C2	525	А
1	C2	526	A
1	C2	527	A
1	C2	534	A
1	C2	536	С
1	C2	538	А
1	C2	539	G
1	C2	540	G
1	C2	541	A
1	C2	542	A
1	C2	543	С
1	C2	545	A
1	C2	548	G
1	C2	549	G
1	C2	551	G
1	C2	554	С
1	C2	555	A
1	C2	556	A
1	C2	557	G
1	C2	558	U



Mol	Chain	Res	Type
1	C2	559	С
1	C2	561	G
1	C2	565	С
1	C2	568	G
1	C2	570	А
1	C2	574	G
1	C2	578	U
1	C2	579	A
1	C2	580	А
1	C2	581	U
1	C2	583	С
1	C2	594	А
1	C2	595	G
1	C2	606	A
1	C2	611	U
1	C2	613	G
1	C2	619	A
1	C2	620	A
1	C2	622	А
1	C2	623	A
1	C2	624	G
1	C2	630	A
1	C2	634	G
1	C2	635	A
1	C2	639	U
1	C2	640	U
1	C2	641	G
1	C2	644	С
1	C2	647	G
1	C2	648	G
1	C2	688	G
1	C2	691	C
1	C2	696	С
1	C2	698	U
1	C2	701	U
1	C2	741	C
1	C2	742	U
1	C2	743	U
1	C2	754	A
1	C2	755	A
1	C2	756	A
1	C2	765	G



Mol	Chain	Res	Type
1	C2	766	U
1	C2	767	U
1	C2	773	С
1	C2	774	А
1	C2	775	G
1	C2	781	U
1	C2	782	U
1	C2	783	G
1	C2	789	А
1	C2	793	А
1	C2	794	U
1	C2	803	A
1	C2	807	А
1	C2	811	A
1	C2	812	A
1	C2	813	U
1	C2	815	G
1	C2	816	G
1	C2	817	A
1	C2	818	С
1	C2	819	G
1	C2	820	U
1	C2	823	G
1	C2	825	U
1	C2	826	U
1	C2	829	А
1	C2	831	U
1	C2	833	U
1	C2	834	G
1	C2	835	U
1	C2	839	U
1	C2	848	C
1	C2	849	C
1	C2	852	С
1	C2	853	G
1	C2	854	U
1	C2	855	А
1	C2	856	A
1	C2	861	U
1	C2	862	A
1	C2	863	A
1	C2	873	U



Mol	Chain	Res	Type
1	C2	886	U
1	C2	898	А
1	C2	906	A
1	C2	913	G
1	C2	914	G
1	C2	921	U
1	C2	926	А
1	C2	931	С
1	C2	932	U
1	C2	933	A
1	C2	934	С
1	C2	935	U
1	C2	940	A
1	C2	942	G
1	C2	945	U
1	C2	951	A
1	C2	959	U
1	C2	960	U
1	C2	966	A
1	C2	969	С
1	C2	970	А
1	C2	992	А
1	C2	993	А
1	C2	997	G
1	C2	1004	U
1	C2	1005	А
1	C2	1020	А
1	C2	1021	C
1	C2	1025	А
1	C2	1026	А
1	C2	1028	С
1	C2	1029	U
1	C2	1030	A
1	C2	1039	A
1	C2	1040	G
1	C2	1052	U
1	C2	1053	G
1	C2	1054	U
1	C2	1056	U
1	C2	1057	U
1	C2	1058	U
1	C2	1059	U



Mol	Chain	Res	Type
1	C2	1060	U
1	C2	1062	А
1	C2	1082	С
1	C2	1083	G
1	C2	1092	А
1	C2	1093	А
1	C2	1096	С
1	C2	1097	U
1	C2	1098	U
1	C2	1099	U
1	C2	1100	G
1	C2	1109	G
1	C2	1113	A
1	C2	1143	A
1	C2	1150	G
1	C2	1154	G
1	C2	1155	G
1	C2	1158	С
1	C2	1159	С
1	C2	1160	А
1	C2	1167	G
1	C2	1185	U
1	C2	1190	С
1	C2	1193	А
1	C2	1194	А
1	C2	1196	А
1	C2	1197	С
1	C2	1199	G
1	C2	1200	G
1	C2	1201	G
1	C2	1202	А
1	C2	1207	С
1	C2	1212	G
1	C2	1217	A
1	C2	1218	G
1	C2	1220	С
1	C2	1221	А
1	C2	1225	U
1	C2	1228	G
1	C2	1229	G
1	C2	1231	U
1	C2	1240	U



Mol	Chain	Res	Type
1	C2	1243	G
1	C2	1244	А
1	C2	1245	G
1	C2	1252	С
1	C2	1255	G
1	C2	1256	А
1	C2	1257	U
1	C2	1258	U
1	C2	1259	U
1	C2	1260	U
1	C2	1261	G
1	C2	1264	G
1	C2	1274	С
1	C2	1276	U
1	C2	1284	С
1	C2	1285	U
1	C2	1286	U
1	C2	1293	U
1	C2	1299	G
1	C2	1300	А
1	C2	1305	U
1	C2	1307	U
1	C2	1314	U
1	C2	1315	U
1	C2	1316	G
1	C2	1321	А
1	C2	1325	А
1	C2	1337	А
1	C2	1338	С
1	C2	1341	А
1	C2	1345	A
1	C2	1347	U
1	C2	1349	G
1	C2	1354	G
1	C2	1360	А
1	C2	1361	U
1	C2	1363	U
1	C2	1364	G
1	C2	1365	С
1	C2	1367	G
1	C2	1370	U
1	C2	1371	А



Mol	Chain	Res	Type
1	C2	1388	А
1	C2	1390	U
1	C2	1398	U
1	C2	1399	С
1	C2	1402	G
1	C2	1407	U
1	C2	1413	U
1	C2	1414	U
1	C2	1415	U
1	C2	1425	А
1	C2	1426	С
1	C2	1427	А
1	C2	1428	G
1	C2	1436	А
1	C2	1438	G
1	C2	1440	С
1	C2	1444	А
1	C2	1445	G
1	C2	1446	А
1	C2	1448	G
1	C2	1449	U
1	C2	1451	С
1	C2	1458	G
1	C2	1459	С
1	C2	1460	А
1	C2	1461	С
1	C2	1469	А
1	C2	1471	A
1	C2	1473	U
1	C2	1474	G
1	C2	1481	С
1	C2	1482	С
1	C2	1483	A
1	C2	1486	G
1	C2	1490	С
1	C2	1492	A
1	C2	1493	A
1	C2	1496	U
1	C2	1501	С
1	C2	1506	G
1	C2	1516	A
1	C2	1521	G



Mol	Chain	Res	Type
1	C2	1523	G
1	C2	1524	А
1	C2	1530	С
1	C2	1535	U
1	C2	1536	G
1	C2	1537	С
1	C2	1540	G
1	C2	1543	A
1	C2	1548	G
1	C2	1555	А
1	C2	1557	U
1	C2	1559	А
1	C2	1565	С
1	C2	1568	С
1	C2	1569	А
1	C2	1573	А
1	C2	1574	G
1	C2	1575	G
1	C2	1583	А
1	C2	1584	G
1	C2	1590	G
1	C2	1595	U
1	C2	1596	С
1	C2	1601	G
1	C2	1607	G
1	C2	1616	G
1	C2	1618	С
1	C2	1621	U
1	C2	1658	G
1	C2	1663	G
1	C2	1665	U
1	C2	1680	G
1	C2	1682	U
1	C2	1685	G
1	C2	$1\overline{686}$	С
1	C2	1713	G
1	C2	1717	G
1	C2	1720	G
1	C2	1736	G
1	C2	1744	А
1	C2	1750	A
1	C2	1754	А



Mol	Chain	Res	Type
1	C2	1755	А
1	C2	1756	А
1	C2	1757	G
1	C2	1766	А
1	C2	1767	G
1	C2	1769	U
1	C2	1780	G
1	C2	1783	С
1	C2	1790	А
1	C2	1792	G
1	C2	1793	G
1	C2	1794	А
1	C2	1795	U
1	C2	1796	С
1	C2	1799	U
1	C2	1800	А
3	C1	18	G
3	C1	26	А
3	C1	40	А
3	C1	43	А
3	C1	45	А
3	C1	49	А
3	C1	57	А
3	C1	59	G
3	C1	60	А
3	C1	65	А
3	C1	66	А
3	C1	85	А
3	C1	89	А
3	C1	92	G
3	C1	96	G
3	C1	99	A
3	C1	105	С
3	C1	109	A
3	C1	110	G
3	C1	111	С
3	C1	116	A
3	C1	118	U
3	C1	121	A
3	C1	122	A
3	C1	134	U
3	C1	135	С



Mol	Chain	Res	Type
3	C1	136	G
3	C1	146	U
3	C1	147	U
3	C1	150	А
3	C1	152	U
3	C1	156	G
3	C1	157	А
3	C1	161	G
3	C1	169	U
3	C1	171	G
3	C1	182	U
3	C1	184	U
3	C1	187	A
3	C1	190	U
3	C1	191	U
3	C1	200	С
3	C1	210	U
3	C1	211	A
3	C1	212	G
3	C1	213	А
3	C1	218	G
3	C1	219	А
3	C1	231	G
3	C1	239	G
3	C1	240	U
3	C1	241	G
3	C1	251	G
3	C1	252	U
3	C1	253	А
3	C1	254	A
3	C1	263	C
3	C1	269	G
3	C1	283	G
3	C1	284	A
3	C1	286	U
3	C1	295	A
3	C1	314	U
3	C1	315	С
3	C1	323	A
3	C1	329	U
3	C1	339	C
3	C1	349	A


Mol	Chain	Res	Type
3	C1	350	С
3	C1	352	А
3	C1	359	U
3	C1	372	А
3	C1	376	G
3	C1	385	А
3	C1	395	А
3	C1	398	А
3	C1	399	A
3	C1	401	U
3	C1	402	A
3	C1	403	С
3	C1	404	G
3	C1	421	G
3	C1	422	A
3	C1	438	A
3	C1	439	С
3	C1	440	А
3	C1	498	A
3	C1	503	C
3	C1	521	A
3	C1	523	A
3	C1	535	G
3	C1	543	С
3	C1	544	С
3	C1	545	U
3	C1	546	С
3	C1	547	G
3	C1	548	G
3	C1	549	U
3	C1	550	A
3	C1	551	A
3	C1	552	G
3	C1	555	U
3	C1	557	A
3	C1	558	U
3	C1	559	A
3	C1	569	A
3	C1	570	A
3	C1	578	A
3	C1	579	G
3	C1	592	A



Mol	Chain	Res	Type
3	C1	604	G
3	C1	609	G
3	C1	611	A
3	C1	619	A
3	C1	620	U
3	C1	621	А
3	C1	622	А
3	C1	636	С
3	C1	647	А
3	C1	649	A
3	C1	667	С
3	C1	677	А
3	C1	681	U
3	C1	683	U
3	C1	690	А
3	C1	691	A
3	C1	705	А
3	C1	712	G
3	C1	715	А
3	C1	716	А
3	C1	719	U
3	C1	720	А
3	C1	725	G
3	C1	736	A
3	C1	737	G
3	C1	739	G
3	C1	742	G
3	C1	758	С
3	C1	766	U
3	C1	767	U
3	C1	771	A
3	C1	774	G
3	C1	776	U
3	C1	777	U
3	C1	780	A
3	C1	781	G
3	C1	785	G
3	C1	786	A
3	C1	801	A
3	C1	806	A
3	C1	817	A
3	C1	830	A



Mol	Chain	Res	Type
3	C1	861	С
3	C1	865	U
3	C1	869	G
3	C1	874	U
3	C1	879	U
3	C1	880	G
3	C1	886	С
3	C1	888	А
3	C1	890	С
3	C1	896	А
3	C1	897	U
3	C1	907	G
3	C1	908	G
3	C1	914	А
3	C1	915	А
3	C1	916	G
3	C1	924	G
3	C1	925	А
3	C1	932	U
3	C1	933	A
3	C1	937	G
3	C1	943	U
3	C1	944	С
3	C1	953	G
3	C1	959	С
3	C1	960	U
3	C1	961	С
3	C1	974	G
3	C1	979	U
3	C1	984	G
3	C1	994	G
3	C1	1000	С
3	C1	1001	G
3	C1	1002	А
3	C1	1010	G
3	C1	1015	U
3	C1	1016	С
3	C1	1017	С
3	C1	1018	G
3	C1	1019	G
3	C1	1020	G
3	C1	1021	G



Mol	Chain	Res	Type
3	C1	1024	G
3	C1	1025	А
3	C1	1026	А
3	C1	1027	А
3	C1	1028	U
3	C1	1029	G
3	C1	1032	С
3	C1	1035	G
3	C1	1047	А
3	C1	1049	С
3	C1	1051	U
3	C1	1052	U
3	C1	1063	G
3	C1	1064	A
3	C1	1065	А
3	C1	1071	U
3	C1	1072	G
3	C1	1075	А
3	C1	1079	А
3	C1	1081	U
3	C1	1082	U
3	C1	1085	А
3	C1	1087	G
3	C1	1093	А
3	C1	1094	U
3	C1	1095	U
3	C1	1096	U
3	C1	1097	G
3	C1	1098	А
3	C1	1103	А
3	C1	1104	G
3	C1	1117	G
3	C1	1131	G
3	C1	1143	A
3	C1	1144	U
3	C1	1151	U
3	C1	1152	G
3	C1	1159	А
3	C1	1160	C
3	C1	1170	А
3	C1	1172	G
3	C1	1178	G



Mol	Chain	Res	Type
3	C1	1180	А
3	C1	1181	U
3	C1	1182	А
3	C1	1191	U
3	C1	1193	А
3	C1	1196	С
3	C1	1201	С
3	C1	1208	U
3	C1	1221	А
3	C1	1222	G
3	C1	1228	С
3	C1	1232	С
3	C1	1235	U
3	C1	1236	G
3	C1	1237	G
3	C1	1238	С
3	C1	1239	С
3	C1	1241	U
3	C1	1242	G
3	C1	1243	G
3	C1	1245	А
3	C1	1246	G
3	C1	1248	С
3	C1	1262	G
3	C1	1263	А
3	C1	1264	G
3	C1	1265	U
3	C1	1266	G
3	C1	1272	С
3	C1	1285	G
3	C1	1286	А
3	C1	1287	А
3	C1	1301	А
3	C1	1307	G
3	C1	1308	A
3	C1	1309	U
3	C1	1313	G
3	C1	1330	A
3	C1	1348	U
3	C1	1354	G
3	C1	1355	А
3	C1	1357	G



Mol	Chain	Res	Type
3	C1	1386	А
3	C1	1399	А
3	C1	1400	G
3	C1	1406	А
3	C1	1419	А
3	C1	1421	G
3	C1	1427	U
3	C1	1433	А
3	C1	1434	G
3	C1	1437	С
3	C1	1443	G
3	C1	1446	А
3	C1	1449	А
3	C1	1450	G
3	C1	1475	A
3	C1	1481	А
3	C1	1482	А
3	C1	1484	U
3	C1	1487	G
3	C1	1488	G
3	C1	1494	U
3	C1	1495	U
3	C1	1496	C
3	C1	1508	C
3	C1	1512	U
3	C1	1526	U
3	C1	1527	C
3	C1	1533	U
3	C1	1535	A
3	C1	1536	G
3	C1	1539	A
3	C1	1546	A
3	C1	1547	G
3	C1	1554	U
3	C1	1555	U
3	C1	1560	G
3	C1	1561	G
3	C1	1562	C
3	C1	1574	C
3	C1	1575	A
3	C1	1576	G
3	C1	1577	G



Mol	Chain	Res	Type
3	C1	1578	С
3	C1	1580	А
3	C1	1581	С
3	C1	1582	С
3	C1	1583	А
3	C1	1584	U
3	C1	1587	А
3	C1	1589	А
3	C1	1593	А
3	C1	1596	С
3	C1	1605	А
3	C1	1619	А
3	C1	1620	U
3	C1	1629	U
3	C1	1630	U
3	C1	1639	С
3	C1	1643	A
3	C1	1644	С
3	C1	1645	U
3	C1	1656	А
3	C1	1657	С
3	C1	1677	G
3	C1	1683	A
3	C1	1696	A
3	C1	1701	С
3	C1	1705	U
3	C1	1716	U
3	C1	1717	U
3	C1	1724	U
3	C1	1730	G
3	C1	1736	G
3	C1	1749	A
3	C1	1750	A
3	C1	1751	G
3	C1	1756	C
3	C1	1759	C
3	C1	1760	A
3	C1	1761	C
3	C1	1762	С
3	C1	1765	U
3	C1	1770	G
3	C1	1778	G



Mol	Chain	Res	Type
3	C1	1780	G
3	C1	1793	С
3	C1	1797	А
3	C1	1812	G
3	C1	1815	U
3	C1	1816	А
3	C1	1817	G
3	C1	1818	U
3	C1	1821	U
3	C1	1839	А
3	C1	1841	А
3	C1	1842	А
3	C1	1846	С
3	C1	1849	С
3	C1	1850	А
3	C1	1858	А
3	C1	1866	С
3	C1	1867	А
3	C1	1878	G
3	C1	1879	А
3	C1	1880	U
3	C1	1881	А
3	C1	1886	А
3	C1	1892	G
3	C1	1893	А
3	C1	1900	А
3	C1	1901	А
3	C1	1904	С
3	C1	1906	G
3	C1	1926	C
3	C1	1930	A
3	C1	1952	G
3	C1	1953	G
3	C1	$21\overline{00}$	A
3	C1	2101	C
3	C1	2102	U
3	C1	2110	G
3	C1	2111	G
3	C1	2113	A
3	C1	2114	C
3	C1	2121	G
3	C1	2122	G



Mol	Chain	Res	Type
3	C1	2131	А
3	C1	2134	G
3	C1	2140	U
3	C1	2144	А
3	C1	2145	А
3	C1	2155	G
3	C1	2158	А
3	C1	2169	G
3	C1	2174	G
3	C1	2175	U
3	C1	2176	U
3	C1	2179	С
3	C1	2180	G
3	C1	2187	G
3	C1	2192	С
3	C1	2205	U
3	C1	2207	А
3	C1	2208	А
3	C1	2209	U
3	C1	2223	А
3	C1	2225	U
3	C1	2229	A
3	C1	2244	A
3	C1	2245	C
3	C1	2246	G
3	C1	2249	G
3	C1	2250	G
3	C1	2255	A
3	C1	2256	A
3	C1	2257	C
3	C1	2262	A
3	C1	2265	C
3	C1	2272	G
3	C1	2273	G
3	C1	2279	A
3		2281	A
3	Cl	2288	G
3	Cl	2295	A
3	CI	2306	C
3	CI	2307	G
3	CI	2309	A
3	C1	2310	U



Mol	Chain	Res	Type
3	C1	2313	A
3	C1	2315	G
3	C1	2318	U
3	C1	2325	G
3	C1	2334	U
3	C1	2336	U
3	C1	2347	U
3	C1	2356	А
3	C1	2373	А
3	C1	2374	С
3	C1	2375	G
3	C1	2383	С
3	C1	2385	G
3	C1	2388	U
3	C1	2393	G
3	C1	2397	А
3	C1	2398	A
3	C1	2400	G
3	C1	2401	А
3	C1	2402	А
3	C1	2403	G
3	C1	2404	А
3	C1	2405	С
3	C1	2411	U
3	C1	2412	G
3	C1	2418	G
3	C1	2419	А
3	C1	2435	G
3	C1	2440	G
3	C1	2506	U
3	C1	2510	U
3	C1	2511	A
3	C1	2514	U
3	C1	2515	A
3	C1	2522	G
3	C1	2523	A
3	C1	2524	A
3	C1	2526	C
3	C1	2530	G
3	C1	2535	A
3	C1	2537	U
3	C1	2538	U



Mol	Chain	Res	Type
3	C1	2539	С
3	C1	2540	А
3	C1	2541	U
3	C1	2542	U
3	C1	2543	U
3	C1	2544	U
3	C1	2549	G
3	C1	2551	U
3	C1	2552	С
3	C1	2555	G
3	C1	2561	А
3	C1	2567	С
3	C1	2569	А
3	C1	2571	U
3	C1	2572	С
3	C1	2573	G
3	C1	2574	G
3	C1	2585	G
3	C1	2586	G
3	C1	2593	А
3	C1	2594	С
3	C1	2595	А
3	C1	2606	G
3	C1	2607	G
3	C1	2610	G
3	C1	2614	G
3	C1	2620	G
3	C1	2629	U
3	C1	2635	А
3	C1	2636	А
3	C1	2652	U
3	C1	2656	А
3	C1	2657	A
3	C1	2663	G
3	C1	2667	A
3	C1	2674	A
3	C1	2677	G
3	C1	2678	А
3	C1	2688	U
3	C1	2689	А
3	C1	2691	А
3	C1	2694	А



Mol	Chain	Res	Type
3	C1	2696	А
3	C1	2703	A
3	C1	2705	А
3	C1	2713	U
3	C1	2714	G
3	C1	2719	U
3	C1	2726	С
3	C1	2727	А
3	C1	2728	G
3	C1	2729	U
3	C1	2747	А
3	C1	2752	U
3	C1	2753	G
3	C1	2755	С
3	C1	2762	A
3	C1	2771	U
3	C1	2772	С
3	C1	2773	С
3	C1	2777	G
3	C1	2778	G
3	C1	2779	А
3	C1	2782	U
3	C1	2796	G
3	C1	2799	А
3	C1	2800	G
3	C1	2801	А
3	C1	2802	А
3	C1	2803	A
3	C1	2810	С
3	C1	2814	G
3	C1	2816	G
3	C1	2817	A
3	C1	2818	U
3	C1	2819	A
3	C1	2821	С
3	C1	2834	G
3	C1	2843	U
3	C1	2845	A
3	C1	2847	А
3	C1	2849	С
3	C1	2853	A
3	C1	2856	G



Mol	Chain	Res	Type
3	C1	2860	U
3	C1	2861	U
3	C1	2863	G
3	C1	2867	С
3	C1	2871	G
3	C1	2872	А
3	C1	2875	U
3	C1	2887	А
3	C1	2889	С
3	C1	2899	С
3	C1	2911	А
3	C1	2912	G
3	C1	2918	G
3	C1	2922	G
3	C1	2923	U
3	C1	2928	С
3	C1	2933	А
3	C1	2935	U
3	C1	2936	А
3	C1	2938	G
3	C1	2941	А
3	C1	2942	С
3	C1	2945	G
3	C1	2947	G
3	C1	2951	G
3	C1	2954	U
3	C1	2971	А
3	C1	2983	С
3	C1	2996	U
3	C1	2997	G
3	C1	3012	A
3	C1	3021	A
3	C1	3049	A
3	C1	3059	G
3	C1	3074	G
3	C1	3078	U
3	C1	3079	U
3	C1	3086	A
3	C1	3092	С
3	C1	3101	G
3	C1	3104	U
3	C1	3109	G



Mol	Chain	Res	Type
3	C1	3116	G
3	C1	3127	А
3	C1	3129	А
3	C1	3131	U
3	C1	3142	А
3	C1	3143	С
3	C1	3153	U
3	C1	3158	G
3	C1	3159	С
3	C1	3165	А
3	C1	3171	U
3	C1	3172	А
3	C1	3173	G
3	C1	3174	А
3	C1	3175	U
3	C1	3176	G
3	C1	3179	U
3	C1	3180	А
3	C1	3181	С
3	C1	3186	А
3	C1	3187	А
3	C1	3188	G
3	C1	3194	С
3	C1	3196	U
3	C1	3197	G
3	C1	3206	С
3	C1	3207	U
3	C1	3210	А
3	C1	3217	С
3	C1	3218	А
3	C1	3219	G
3	C1	3224	G
3	C1	3227	А
3	C1	3229	G
3	C1	3238	G
3	C1	3239	G
3	C1	3242	G
3	C1	3243	A
3	C1	3245	А
3	C1	3247	G
3	C1	3259	U
3	C1	3260	G



Mol	Chain	Res	Type
3	C1	3263	G
3	C1	3268	А
3	C1	3269	U
3	C1	3270	U
3	C1	3271	G
3	C1	3273	А
3	C1	3276	G
3	C1	3279	А
3	C1	3280	U
3	C1	3281	U
3	C1	3282	U
3	C1	3287	U
3	C1	3288	G
3	C1	3289	G
3	C1	3290	G
3	C1	3294	А
3	C1	3304	U
3	C1	3313	U
3	C1	3318	G
3	C1	3320	А
3	C1	3331	U
3	C1	3340	G
3	C1	3341	U
3	C1	3342	А
3	C1	3345	G
3	C1	3348	G
3	C1	3349	С
3	C1	3351	U
3	C1	3352	U
3	C1	3354	U
3	C1	3355	U
3	C1	3356	G
3	C1	3357	U
3	C1	3358	U
3	C1	3362	А
3	C1	3368	U
3	C1	3369	G
3	C1	3375	А
3	C1	3378	С
3	C1	3382	U
3	C1	3386	G
3	C1	3389	U



Mol	Chain	Res	Type
3	C1	3396	U
4	C4	7	G
4	C4	11	А
4	C4	22	А
4	C4	29	С
4	C4	33	U
4	C4	38	U
4	C4	41	G
4	C4	52	G
4	C4	54	U
4	C4	55	А
4	C4	65	G
4	C4	73	С
4	C4	74	С
4	C4	76	A
4	C4	91	G
4	C4	93	С
4	C4	99	G
4	C4	102	А
4	C4	103	А
4	C4	112	G
4	C4	121	U
5	C3	13	А
5	C3	21	С
5	C3	23	U
5	C3	34	U
5	C3	35	С
5	C3	48	А
5	C3	51	G
5	C3	52	А
5	C3	59	A
5	C3	62	C
5	C3	63	G
5	C3	75	G
5	C3	80	A
5	C3	81	U
5	C3	82	U
5	C3	83	С
5	C3	84	С
5	C3	85	G
5	C3	87	G
5	C3	90	U



Mol	Chain	Res	
- F	Cham	1005	
5	C3	92	A
5	C3	95	G
5	C3	104	A
5	C3	106	С
5	C3	111	А
5	C3	112	U
5	C3	113	U
5	C3	116	G
5	C3	124	G
5	C3	125	U
5	C3	126	А
5	C3	127	U
5	C3	131	А
5	C3	138	А
5	C3	148	G
5	C3	152	G
5	C3	157	U

All (72) RNA pucker outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	C2	25	С
1	C2	103	А
1	C2	114	С
1	C2	139	С
1	C2	187	G
1	C2	272	U
1	C2	319	U
1	C2	417	А
1	C2	422	G
1	C2	512	А
1	C2	542	А
1	C2	555	А
1	C2	558	U
1	C2	755	А
1	C2	818	С
1	C2	853	G
1	C2	854	U
1	C2	1051	G
1	C2	1058	U
1	C2	1097	U
1	C2	1098	U



Mol	Chain	Res	Type
1	C2	1196	А
1	C2	1227	А
1	C2	1244	А
1	C2	1255	G
1	C2	1344	А
1	C2	1481	С
1	C2	1568	С
1	C2	1572	G
1	C2	1573	А
1	C2	1620	С
3	C1	65	А
3	C1	151	А
3	C1	170	G
3	C1	210	U
3	C1	282	G
3	C1	715	А
3	C1	735	А
3	C1	1015	U
3	C1	1027	А
3	C1	1062	А
3	C1	1064	А
3	C1	1081	U
3	C1	1238	С
3	C1	1241	U
3	C1	1284	С
3	C1	1307	G
3	C1	1560	G
3	C1	1582	C
3	C1	1716	U
3	C1	1815	U
3	C1	1816	A
3	C1	1878	G
3	C1	2101	C
3	C1	2112	U
3	C1	2204	С
3	C1	$2\overline{513}$	U
3	C1	2522	G
3	C1	2662	G
3	C1	2714	G
3	C1	2772	С
3	C1	2801	A
3	C1	3055	U



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Mol	Chain	Res	Type
3	C1	3218	А
3	C1	3228	С
3	C1	3269	U
3	C1	3276	G
3	C1	3289	G
3	C1	3317	U
3	C1	3357	U
5	C3	80	А
5	C3	106	С

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

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

### 5.5Carbohydrates (i)

There are no monosaccharides in this entry.

### Ligand geometry (i) 5.6

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### Other polymers (i) 5.7

There are no such residues in this entry.

#### Polymer linkage issues (i) 5.8

There are no chain breaks in this entry.



### 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11096. 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.

### Orthogonal projections (i) 6.1

#### 6.1.1Primary map



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

### 6.2Central slices (i)

#### 6.2.1Primary map



X Index: 200

Y Index: 200

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: 198

Y Index: 227

Z Index: 181

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



# 6.5 Mask visualisation (i)

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



# 7 Map analysis (i)

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

# 7.1 Map-value distribution (i)



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



# 7.2 Volume estimate (i)



The volume at the recommended contour level is  $1042 \text{ nm}^3$ ; this corresponds to an approximate mass of 941 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 0.294  $\mathrm{\AA^{-1}}$ 



# 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 0.294  $\text{\AA}^{-1}$ 



# 8.2 Resolution estimates (i)

$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.34	4.05	3.42
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-11096 and PDB model 6Z6J. Per-residue inclusion information can be found in section 3 on page 18.

# 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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 (0.1).



## 9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 73% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7250	0.4820
C1	0.8264	0.4970
C2	0.7009	0.4390
C3	0.8494	0.5050
C4	0.8488	0.4930
C5	0.3880	0.4340
LA	0.7905	0.5480
LB	0.7779	0.5390
LC	0.7640	0.5270
LD	0.6611	0.4830
LE	0.6727	0.4960
m LF	0.7444	0.5260
LG	0.7023	0.4990
LH	0.7085	0.5130
LI	0.7152	0.5200
LJ	0.6129	0.4620
LL	0.7245	0.5060
LM	0.7054	0.5090
LN	0.8082	0.5530
LO	0.7814	0.5350
LP	0.7819	0.5400
LQ	0.7663	0.5310
LR	0.7723	0.5400
LS	0.7611	0.5390
LT	0.7589	0.5310
LU	0.6924	0.4920
LV	0.7595	0.5480
LW	0.7545	0.5370
LX	0.7353	0.5240
LY	0.7471	0.5260
LZ	0.7330	0.5200
La	0.7942	0.5450
Lb	0.6991	0.4940
Lc	0.7232	0.5170
Ld	0.7351	0.5260



Chain	Atom inclusion	Q-score
Le	0.7807	0.5440
Lf	0.8161	0.5600
Lg	0.7535	0.5370
Lh	0.7114	0.5220
Li	0.7056	0.5040
Lj	0.8496	0.5630
Lk	0.6202	0.4840
Ll	0.7928	0.5470
Lm	0.7376	0.5310
Ln	0.6415	0.5120
Lo	0.7527	0.5380
Lp	0.7209	0.5370
SA	0.6606	0.4790
SB	0.6324	0.4930
SC	0.7102	0.5160
SD	0.3831	0.3800
SE	0.6971	0.5080
SF	0.3743	0.3930
SG	0.5795	0.4690
SH	0.5580	0.4420
SI	0.7208	0.5260
SJ	0.6623	0.4960
SK	0.2847	0.3240
SL	0.7265	0.5260
SM	0.1057	0.2230
SN	0.7299	0.5180
SO	0.6834	0.5080
SP	0.2525	0.2970
SQ	0.3735	0.3740
SR	0.5103	0.4320
SS	0.3111	0.3330
ST	0.3858	0.3700
SU	0.3152	0.3560
SV	0.6928	0.4930
SW	0.7555	0.5400
SX	0.7203	0.5290
SY	0.6215	0.4690
SZ	0.3137	0.3300
Sa	0.7068	0.5170
Sb	0.6395	0.4950
Sc	0.4172	0.4190
Sd	0.4941	0.4340



Chain	Atom inclusion	Q-score
Se	0.5468	0.4430
Sf	0.1388	0.2310
Sg	0.1996	0.3160

