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PDB ID	:	6SPC
EMDB ID	:	EMD-10281
Title	:	Pseudomonas aeruginosa 30s ribosome from an aminoglycoside resistant clini-
		cal isolate
Authors	:	Halfon, Y.; Jimenez-Fernande, A.; La Ros, R.; Espinos, R.; Krogh Johansen,
		H.; Matzov, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Belousoff, M.; Molin,
		S.; Yonath, A.
Deposited on	:	2019-09-01
Resolution	:	2.95  Å(reported)

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

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

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

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

:	0.0.1. dev 43
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber $(2001)$
:	Parkinson et al. (1996)
:	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 2.95 Å.

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



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain	Quality of chain							
1	a	1519	<b>4</b> 7% 44%		10%						
2	b	221	68%	31%							
3	С	203	37% 97%		•						
4	d	205	95%		5%						
5	е	149	90%		9% •						
6	f	100	92%		7% •						
7	g	154	62%	38%							



Mol	Chain	Length	Quality of chain	
8	h	125	<b>•</b> 75% 17%	6% •
9	i	126	98%	·
10	j	96	97%	•
11	k	115	95%	5%
12	1	120	84% 9%	• 6%
13	m	109	94%	6%
14	n	98	97%	•
15	0	87	97%	
16	р	78	94%	6%
17	q	76	97%	•
18	r	56	96%	•
19	s	80	94%	6%
20	t	86	97%	••
21	u	34	100%	

Continued from previous page...



### 2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 50569 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1519	Total 32595	C 14540	N 5985	O 10552	Р 1518	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	2	А	-	conflict	GB 1359201046
a	?	-	С	deletion	GB 1359201046
a	?	-	G	deletion	GB 1359201046
a	72	А	G	conflict	GB 1359201046
a	101	А	G	conflict	GB 1359201046

• Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	221	Total 1728	C 1088	N 316	0 314	S 10	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	?	-	THR	deletion	UNP A0A072ZPV8
b	?	-	PHE	deletion	UNP A0A072ZPV8
b	?	-	ASP	deletion	UNP A0A072ZPV8
b	?	-	LYS	deletion	UNP A0A072ZPV8
b	?	-	LEU	deletion	UNP A0A072ZPV8

• Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	с	203	Total 1609	C 1017	N 303	0 284	${S \atop 5}$	0	0



• Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total 1600	C 991	N 310	0 294	${f S}{5}$	0	0

• Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms				AltConf	Trace	
5	е	149	Total 1092	C 687	N 202	0 197	S 6	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
е	?	-	ALA	deletion	UNP A0A241XG65

• Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total 802	C 497	N 152	0 149	$\frac{S}{4}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	80	ALA	TYR	$\operatorname{conflict}$	UNP A0A069Q263

• Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	154	Total 1190	С 747	N 227	0 211	${ m S}{ m 5}$	0	0

• Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	123	Total 915	C 575	N 161	0 174	${S \atop 5}$	0	0

There are 2 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
h	94	ALA	LYS	conflict	UNP E2RXT9
h	129	VAL	LEU	conflict	UNP E2RXT9

• Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	126	Total 994	C 616	N 198	0 179	S 1	0	0

• Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	96	Total 763	C 479	N 143	0 140	S 1	0	0

• Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	115	Total 828	C 511	N 159	0 156	${ m S} { m 2}$	0	0

• Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	113	Total 893	C 547	N 184	0 158	$\frac{S}{4}$	0	0

• Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	109	Total 847	C 515	N 173	0 155	$\frac{S}{4}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	?	-	TYR	deletion	UNP E2RXU3

• Molecule 14 is a protein called 30S ribosomal protein S14.



Mol	Chain	Residues	Atoms				AltConf	Trace	
14	n	98	Total 776	$\begin{array}{c} \mathrm{C} \\ 479 \end{array}$	N 163	0 131	${ m S} { m 3}$	0	0

• Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace	
15	О	86	Total 686	C 425	N 134	O 126	S 1	0	0

• Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues		Ato	$\mathbf{ms}$		AltConf	Trace
16	р	78	Total 606	C 379	N 120	O 107	0	0

• Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace	
17	q	76	Total 619	C 387	N 120	0 110	${ m S} { m 2}$	0	0

• Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms			AltConf	Trace	
18	r	56	Total 443	C 283	N 79	0 81	0	0

• Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms				AltConf	Trace	
19	s	80	Total 635	C 405	N 121	O 106	${ m S} { m 3}$	0	0

• Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace	
20	t	85	Total 653	C 404	N 135	0 112	${S \over 2}$	0	0

• Molecule 21 is a protein called 30S ribosomal protein S21.



Mol	Chain	Residues	Atoms			AltConf	Trace	
21	u	34	Total 295	C 178	N 70	O 47	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	46	ARG	LYS	conflict	UNP A0A069QC99



## 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.

- Chain a: 47% 44% 10%
- $\bullet$  Molecule 1: 16S rRNA









V5 P1 P1 N8 V15 E117 H18 T19 D31	V39 V42 A50 A50 B56 A61 A61 A61 A61 A64	R65 166 167 167 71 77 777 773 774 773 774 775 775 777 777 777 777 778 778	681 882 883 886 885 885 988 988 998 1101
1103 E104 E105 E105 N107 Y108 E110 E110 D112 M113 S119 S119	q122 • q124 • q1	A156	V200
• Molecule 4: 30S ribose	omal protein S4		
Chain d:	95%	5%	
A2 C9 A27 A27 C32 C32 C32 C32 C32 C32 C32 C32 C32 C32	H41 849 1110 1110 8205 8205 1146 1146		
• Molecule 5: 30S ribose	omal protein S5		
Chain e:	90%	9% •	
<b>G11</b> E14 Q18 V19 R11 R51 K53 K53 K53 K53 K53 K53 K53	1107 1107 11107 1113 1113 1125 1125 1133 1133 1133 1133		
• Molecule 6: 30S ribose	omal protein S6		
Chain f:	92%	7% •	
R2 19 19 19 19 10 10 10 10 10 10 10			
• Molecule 7: 30S ribose	omal protein S7		
Chain g:	62%	38%	
R3 R5 R5 R5 R5 R10 R10 R10 B11 P16 R14 R17 P12 R21 S20 S20 S20 S20 S20 S21	K25 M27 M27 M28 M28 S33 C34 C34 C34 C34 C34 C34 C34 C34 C34 C	K51 E52 R53 R53 A56 A56 L66 L66 L66 L66 L72	577 577 R78 R78 V80 C81
T84 V87 V88 P88 V89 B90 V91 K102 K102 M102	6 112 6 112 6 112 6 113 8 114 8 114 8 114 1120 1120 1120 1120 1120 1120 1120 1	R143 M144 A145 E146 A147 K148 K148 S152 S152 H153 F156 F156	
• Molecule 8: 30S ribose	omal protein S8		
Chain h:	75%	17% 6% •	
S2 L7 S29 S30 K31 L32 K31 L33 A34 A34 F43 F43 F43	L59 F66 K69 K69 B81 P81 C432 L83 C432 L83 C432 C432 C432 C432 C432 C432 C432 C43	ALA V95 V95 C100 V101 V104 V104 V106 N106 M105 M116 A115 A118	V128
• Molecule 9: 30S riboso	omal protein S9		



Chain i:	98% .
A3 T14 N32 R41 R106	
• Molecule 1	0: 30S ribosomal protein S10
Chain j:	18% . 97% ·
18 F13 R16 K30 R31	133 434 435 435 435 779 779 779 778 780 180 180 1931 433 433 433 433 433 433 433 433 433 4
• Molecule 1	1: 30S ribosomal protein S11
Chain k:	95% 5%
K14 R37 S55 R56 R56 L100	
• Molecule 1	2: 30S ribosomal protein S12
Chain l:	84% 9% • 6%
ALA THR ILE N5 K10 C25 Q25	L81 1104 1104 1104 110 1115 1115 1115 1115
• Molecule 1	3: 30S ribosomal protein S13
Chain m:	19% 94% 6%
R3 122 C26 A30	931         133         133         133         133         133         133         133         133         133         133         133         133         133         140         155         165         165         165         165         165         165         165         165         165         165         165         165         165         165         165         165         165         112         112
• Molecule 1	4: 30S ribosomal protein S14
Chain n:	28% 97%
K3 M6 K7 K12 K13	Q14         T15         V17         A25         A25         A25         A26         A27         A28         A29         A44         A44         A44         A38         A44         A44         A99         S100         S100
• Molecule 1	5: 30S ribosomal protein S15
Chain o:	97%
ALA L3 E19 R68 R88	



• Molecule 16: 30S ribosomal protein S16 Chain p: 94% 6% • Molecule 17: 30S ribosomal protein S17 Chain q: 97% • Molecule 18: 30S ribosomal protein S18 Chain r: 96% • Molecule 19: 30S ribosomal protein S19 10% Chain s: 94% 6% • Molecule 20: 30S ribosomal protein S20 Chain t: . . 97% ALA • Molecule 21: 30S ribosomal protein S21 21% Chain u: 100%



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	319022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.603	Depositor
Minimum map value	-0.352	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.00936	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor



## 5 Model quality (i)

#### 5.1 Standard geometry (i)

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

Mol Chain		Bo	ond lengths	Bond angles		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	a	1.40	78/36497~(0.2%)	1.83	689/56927~(1.2%)	
2	b	0.35	0/1754	0.57	0/2355	
3	с	0.30	0/1638	0.60	0/2209	
4	d	0.48	1/1619~(0.1%)	0.76	1/2168~(0.0%)	
5	е	0.53	0/1106	0.72	0/1488	
6	f	0.49	0/815	0.71	1/1098~(0.1%)	
7	g	0.24	0/1207	0.50	0/1616	
8	h	0.73	1/924~(0.1%)	1.14	6/1243~(0.5%)	
9	i	0.32	0/1006	0.68	0/1347	
10	j	0.29	0/773	0.63	0/1045	
11	k	0.47	0/844	0.66	1/1148~(0.1%)	
12	1	0.57	0/906	0.91	2/1215~(0.2%)	
13	m	0.31	0/853	0.71	0/1144	
14	n	0.31	0/786	0.68	0/1047	
15	0	0.61	0/693	0.75	0/926	
16	р	0.77	0/617	0.89	2/832~(0.2%)	
17	q	0.59	0/627	0.67	0/844	
18	r	0.62	0/450	0.76	1/608~(0.2%)	
19	S	4.73	1/649~(0.2%)	0.75	1/874~(0.1%)	
20	t	0.56	0/660	0.67	0/880	
21	u	0.43	0/298	0.60	0/391	
All	All	1.28	81/54722~(0.1%)	1.58	704/81405~(0.9%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	с	0	2
4	d	0	2
8	h	0	15
11	k	0	2



Mol	Chain	#Chirality outliers	<b>#Planarity outliers</b>
12	1	0	6
13	m	0	4
14	n	0	2
16	р	0	1
All	All	0	34

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	s	3	ARG	CB-CG	120.10	4.76	1.52
1	a	1313	А	N3-C4	57.70	1.69	1.34
1	a	1313	А	C6-N1	51.87	1.71	1.35
1	a	1219	А	N9-C4	44.11	1.64	1.37
1	a	1313	А	C5-C4	41.51	1.67	1.38
1	a	1313	А	N1-C2	37.98	1.68	1.34
1	a	1313	А	C2-N3	36.86	1.66	1.33
1	a	1313	А	C5-C6	35.36	1.72	1.41
1	a	1219	А	N9-C8	-26.48	1.16	1.37
1	a	1219	A	N3-C4	20.53	1.47	1.34
1	a	1219	А	C8-N7	14.52	1.41	1.31
1	a	636	A	N9-C4	14.44	1.46	1.37
1	a	446	А	N9-C4	-11.06	1.31	1.37
1	a	103	А	N9-C4	-10.87	1.31	1.37
1	a	61	G	N3-C4	-10.78	1.27	1.35
1	a	61	G	N9-C4	-10.60	1.29	1.38
1	a	61	G	C2-N3	-9.25	1.25	1.32
1	a	51	А	N9-C4	-7.77	1.33	1.37
1	a	475	G	C2-N3	-7.63	1.26	1.32
1	a	1219	А	N7-C5	-7.02	1.35	1.39
1	a	761	А	N3-C4	-6.96	1.30	1.34
8	h	104	VAL	CB-CG1	-6.89	1.38	1.52
4	d	32	CYS	CB-SG	6.85	1.93	1.82
1	a	446	А	C6-N6	-6.81	1.28	1.33
1	a	475	G	N9-C4	-6.79	1.32	1.38
1	a	446	А	C5-C6	-6.79	1.34	1.41
1	a	1518	С	N3-C4	-6.78	1.29	1.33
1	a	372	G	C5-C4	-6.57	1.33	1.38
1	a	871	G	C5-C4	-6.50	1.33	1.38
1	a	99	G	N1-C2	-6.48	1.32	1.37
1	a	60	A	C5-C4	-6.35	1.34	1.38
1	a	722	A	N9-C4	-6.33	1.34	1.37
1	a	426	A	N9-C4	6.25	1.41	1.37



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1505	G	C6-N1	-6.24	1.35	1.39
1	a	61	G	C2-N2	-6.24	1.28	1.34
1	a	101	А	C5-C4	-6.22	1.34	1.38
1	a	475	G	N3-C4	-6.16	1.31	1.35
1	a	759	G	N7-C5	-6.07	1.35	1.39
1	a	369	U	N3-C4	-6.07	1.32	1.38
1	a	1505	G	C8-N7	-5.98	1.27	1.30
1	a	726	С	N1-C6	-5.98	1.33	1.37
1	a	308	С	N3-C4	-5.95	1.29	1.33
1	a	761	А	C5-C6	-5.94	1.35	1.41
1	a	61	G	N7-C5	-5.90	1.35	1.39
1	a	761	А	N9-C4	-5.84	1.34	1.37
1	a	1505	G	N1-C2	-5.82	1.33	1.37
1	a	380	С	N3-C4	-5.81	1.29	1.33
1	a	1058	G	N9-C4	5.71	1.42	1.38
1	a	808	А	N7-C5	-5.70	1.35	1.39
1	a	636	А	N1-C2	-5.68	1.29	1.34
1	a	60	А	C5-C6	-5.65	1.35	1.41
1	a	106	G	C2-N3	-5.61	1.28	1.32
1	a	726	С	N3-C4	-5.61	1.30	1.33
1	a	303	А	N9-C4	-5.58	1.34	1.37
1	a	799	С	N3-C4	-5.56	1.30	1.33
1	a	532	А	N9-C4	5.53	1.41	1.37
1	a	576	U	N3-C4	-5.45	1.33	1.38
1	a	307	A	N7-C5	-5.43	1.35	1.39
1	a	1343	A	N9-C4	5.43	1.41	1.37
1	a	724	G	N7-C5	-5.42	1.35	1.39
1	a	273	А	N9-C4	-5.41	1.34	1.37
1	a	806	G	C5-C4	-5.41	1.34	1.38
1	a	34	С	N3-C4	-5.38	1.30	1.33
1	a	720	С	N3-C4	-5.38	1.30	1.33
1	a	721	G	N7-C5	-5.33	1.36	1.39
1	a	34	С	N1-C6	-5.19	1.34	1.37
1	a	110	A	N7-C5	-5.18	1.36	1.39
1	a	118	С	N3-C4	-5.18	1.30	1.33
1	a	575	G	C6-N1	-5.17	1.35	1.39
1	a	1219	A	C5-C4	-5.15	1.35	1.38
1	a	383	A	C6-N1	-5.12	1.31	1.35
1	a	99	G	N9-C4	-5.11	1.33	1.38
1	a	366	C	N3-C4	-5.10	1.30	1.33
1	a	379	C	N3-C4	-5.09	1.30	1.33
1	a	575	G G	N1-C2	-5.08	1.33	1.37

Continued from previous page...



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	a	579	G	C5-C4	-5.08	1.34	1.38
1	а	867	А	N7-C5	-5.08	1.36	1.39
1	a	384	U	C2-N3	-5.07	1.34	1.37
1	a	761	А	N7-C5	-5.05	1.36	1.39
1	a	750	С	N3-C4	-5.04	1.30	1.33
1	a	325	G	C2-N3	-5.02	1.28	1.32

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All (704) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	1219	A	N7-C8-N9	-144.78	41.41	113.80
1	a	1219	А	C4-C5-N7	-137.11	42.15	110.70
1	a	1219	А	C8-N9-C4	-133.34	52.46	105.80
1	a	1219	А	C5-N7-C8	57.27	132.53	103.90
1	a	1219	А	C6-C5-N7	38.34	159.14	132.30
1	a	1313	А	N1-C2-N3	-35.45	111.57	129.30
1	a	1313	A	C2-N3-C4	30.09	125.64	110.60
1	a	636	А	C8-N9-C4	-26.12	95.35	105.80
1	a	636	А	C2-N3-C4	23.10	122.15	110.60
1	a	1219	А	N3-C4-N9	20.52	143.81	127.40
1	a	1219	А	C2-N3-C4	17.55	119.37	110.60
1	a	636	A	N3-C4-C5	-16.95	114.94	126.80
1	a	1219	А	C8-N9-C1'	-16.65	97.72	127.70
1	a	1219	A	N9-C4-C5	-16.55	99.18	105.80
1	a	61	G	N3-C4-N9	-16.54	116.08	126.00
1	a	636	А	N9-C4-C5	16.33	112.33	105.80
1	a	636	А	N1-C6-N6	-16.02	108.99	118.60
1	a	1219	А	C5-C6-N1	15.39	125.39	117.70
1	a	1106	С	N1-C2-O2	15.24	128.04	118.90
1	a	61	G	N3-C2-N2	-15.10	109.33	119.90
1	a	1313	A	C6-N1-C2	14.89	127.53	118.60
1	a	1313	A	N7-C8-N9	14.76	121.18	113.80
1	a	1219	А	N3-C4-C5	-13.99	117.00	126.80
1	a	1316	С	N1-C2-O2	13.83	127.20	118.90
1	a	636	A	N7-C8-N9	13.55	120.57	113.80
1	a	1219	A	C4-N9-C1'	13.27	150.19	126.30
1	a	475	G	N3-C2-N2	-13.08	110.75	119.90
1	a	1316	С	C2-N1-C1'	12.99	133.09	118.80
1	a	176	С	C5-C6-N1	12.94	127.47	121.00
1	a	61	G	N3-C4-C5	12.76	134.98	128.60
1	a	475	G	N3-C4-N9	-12.29	118.63	126.00
1	a	1518	С	N3-C2-O2	-12.02	113.49	121.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	1106	С	C2-N1-C1'	11.90	131.89	118.80
1	a	1106	С	N3-C2-O2	-11.68	113.72	121.90
1	a	638	U	N1-C2-O2	11.48	130.84	122.80
1	a	720	С	C6-N1-C2	-11.31	115.78	120.30
1	a	761	А	C5-N7-C8	-11.27	98.27	103.90
1	a	1313	А	N3-C4-N9	11.27	136.41	127.40
1	a	799	С	N3-C2-O2	-11.24	114.03	121.90
1	a	576	U	N3-C2-O2	-11.22	114.34	122.20
1	a	726	C	N3-C2-O2	-11.12	114.11	121.90
1	a	1316	C	N3-C2-O2	-11.01	114.19	121.90
1	a	379	С	C6-N1-C2	-10.95	115.92	120.30
1	a	103	A	C2-N3-C4	-10.86	105.17	110.60
1	a	131	U	N3-C2-O2	-10.80	114.64	122.20
1	a	61	G	C2-N3-C4	-10.71	106.55	111.90
1	a	1058	G	N3-C4-C5	-10.55	123.33	128.60
1	a	799	С	N1-C2-O2	10.29	125.07	118.90
1	a	726	С	C2-N1-C1'	10.24	130.06	118.80
1	a	373	С	C6-N1-C2	-10.16	116.23	120.30
1	a	761	A	N7-C8-N9	10.14	118.87	113.80
1	a	636	А	O4'-C1'-N9	9.94	116.16	108.20
1	a	34	С	C2-N1-C1'	9.86	129.65	118.80
1	a	176	С	C2-N1-C1'	9.81	129.59	118.80
1	a	726	С	N1-C2-O2	9.79	124.78	118.90
1	a	1058	G	C2-N3-C4	9.76	116.78	111.90
1	a	725	G	C4-C5-N7	9.75	114.70	110.80
12	1	24	LEU	CA-CB-CG	9.75	137.73	115.30
1	a	475	G	N1-C2-N2	9.73	124.96	116.20
1	a	546	U	C5-C6-N1	9.71	127.56	122.70
1	a	638	U	N3-C2-O2	-9.69	115.42	122.20
1	a	790	C	N3-C2-O2	-9.62	115.17	121.90
1	a	176	C	C4-C5-C6	-9.52	112.64	117.40
1	a	34	С	N3-C2-O2	-9.52	115.24	121.90
1	a	502	U	N1-C2-O2	9.47	129.43	122.80
1	a	373	C	C5-C6-N1	9.42	125.71	121.00
1	a	771	А	N7-C8-N9	9.40	118.50	113.80
1	a	1518	С	N1-C2-O2	9.30	124.48	118.90
1	a	423	U	C4-C5-C6	9.30	125.28	119.70
1	a	1058	G	N3-C4-N9	9.29	131.58	126.00
1	a	1057	С	C2-N1-C1'	9.26	128.98	118.80
1	a	1309	U	C2-N1-C1'	9.19	128.73	117.70
1	a	1061	A	O4'-C1'-N9	9.14	115.51	108.20
1	a	725	G	C5-N7-C8	-9.09	99.76	104.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	1057	С	C5-C6-N1	9.07	125.54	121.00
1	a	759	G	C8-N9-C4	-9.07	102.77	106.40
1	a	860	С	C6-N1-C2	-9.04	116.69	120.30
1	a	1316	С	C6-N1-C1'	-8.97	110.04	120.80
1	a	636	А	C5-C6-N1	8.95	122.17	117.70
1	a	369	U	N3-C2-O2	-8.92	115.96	122.20
1	a	1313	А	C4-C5-N7	-8.91	106.25	110.70
1	a	502	U	C2-N1-C1'	8.89	128.37	117.70
1	a	572	С	C6-N1-C2	-8.87	116.75	120.30
1	a	59	А	C8-N9-C4	-8.87	102.25	105.80
1	a	61	G	N9-C4-C5	8.84	108.94	105.40
1	a	402	G	C8-N9-C4	-8.82	102.87	106.40
1	a	446	А	C5-N7-C8	-8.80	99.50	103.90
1	a	720	С	C5-C6-N1	8.74	125.37	121.00
1	a	807	U	N3-C2-O2	-8.68	116.12	122.20
1	a	771	А	C5-N7-C8	-8.65	99.58	103.90
1	a	799	С	C2-N1-C1'	8.63	128.29	118.80
1	a	1316	С	C6-N1-C2	-8.59	116.86	120.30
1	a	374	G	O4'-C1'-N9	8.57	115.05	108.20
1	a	1057	С	N1-C2-O2	8.56	124.03	118.90
1	a	807	U	N1-C2-O2	8.55	128.79	122.80
1	a	380	С	C6-N1-C2	-8.54	116.88	120.30
1	a	701	U	N3-C2-O2	-8.53	116.23	122.20
1	a	759	G	C4-C5-N7	8.53	114.21	110.80
1	a	60	А	O4'-C1'-N9	8.51	115.01	108.20
1	a	860	С	C5-C6-N1	8.51	125.25	121.00
1	a	374	G	N7-C8-N9	8.49	117.34	113.10
1	a	795	U	C2-N1-C1'	8.48	127.88	117.70
1	a	677	G	N3-C4-N9	8.48	131.09	126.00
1	a	759	G	C5-N7-C8	-8.46	100.07	104.30
1	a	465	U	N1-C2-O2	8.46	128.72	122.80
1	a	790	С	N1-C2-O2	8.44	123.97	118.90
1	a	1313	А	N3-C4-C5	-8.43	120.90	126.80
1	a	465	U	N3-C2-O2	-8.38	116.33	122.20
1	a	475	G	N3-C4-C5	8.36	132.78	128.60
1	a	782	U	N3-C2-O2	-8.35	116.36	122.20
1	a	1106	С	C6-N1-C1'	-8.35	110.78	120.80
1	a	477	C	N3-C2-O2	-8.34	116.06	121.90
1	a	1454	С	C5-C6-N1	8.34	125.17	121.00
1	a	176	С	N1-C2-O2	8.33	123.90	118.90
1	a	1075	G	C4-C5-N7	8.31	114.12	110.80
1	a	759	G	N7-C8-N9	8.31	117.25	113.10



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	761	А	O4'-C1'-N9	8.28	114.82	108.20
1	a	725	G	N7-C8-N9	8.27	117.24	113.10
1	a	1020	G	C4-N9-C1'	8.26	137.24	126.50
1	a	67	С	N3-C2-O2	-8.25	116.13	121.90
1	a	761	А	C4-C5-N7	8.19	114.79	110.70
1	a	479	U	N1-C1'-C2'	8.16	124.61	114.00
1	a	790	С	C6-N1-C2	-8.14	117.04	120.30
1	a	103	А	N3-C4-C5	8.11	132.47	126.80
1	a	60	А	N9-C4-C5	-8.10	102.56	105.80
1	a	1345	U	C2-N1-C1'	8.10	127.41	117.70
1	a	394	С	C6-N1-C2	-8.08	117.07	120.30
1	a	638	U	C2-N1-C1'	8.08	127.40	117.70
1	a	356	G	C8-N9-C4	-8.07	103.17	106.40
1	a	636	А	N9-C1'-C2'	8.06	124.48	114.00
1	a	369	U	C2-N1-C1'	8.02	127.32	117.70
1	a	1353	С	N1-C2-O2	8.00	123.70	118.90
1	a	636	А	C4-C5-N7	-7.97	106.72	110.70
1	a	1343	А	C2-N3-C4	7.96	114.58	110.60
1	a	636	А	C4-N9-C1'	7.95	140.61	126.30
1	a	725	G	C6-C5-N7	-7.94	125.64	130.40
1	a	446	А	C4-C5-N7	7.94	114.67	110.70
1	a	59	А	N9-C4-C5	7.91	108.96	105.80
1	a	423	U	N3-C2-O2	-7.90	116.67	122.20
1	a	475	G	C8-N9-C1'	7.86	137.21	127.00
1	a	580	U	N3-C2-O2	-7.84	116.71	122.20
1	a	748	С	C2-N1-C1'	7.84	127.42	118.80
1	a	325	G	C8-N9-C4	-7.84	103.27	106.40
1	a	726	С	C6-N1-C1'	-7.82	111.42	120.80
1	a	34	С	C6-N1-C2	-7.81	117.17	120.30
1	a	465	U	C2-N1-C1'	7.81	127.07	117.70
1	a	1313	A	N9-C4-C5	-7.80	102.68	105.80
1	a	423	U	O4'-C1'-N1	7.80	114.44	108.20
1	a	446	A	C4-C5-C6	-7.79	113.11	117.00
1	a	475	G	N9-C4-C5	7.78	108.51	105.40
1	a	131	U	N1-C2-O2	7.76	128.23	122.80
1	a	576	U	N1-C2-O2	7.75	128.22	122.80
1	a	761	A	N1-C6-N6	7.74	123.24	118.60
1	a	1215	G	C4-N9-C1'	7.73	136.55	126.50
1	a	176	C	C6-N1-C2	-7.73	117.21	120.30
1	a	192	G	N7-C8-N9	7.72	116.96	113.10
1	a	539	C	04'-C1'-N1	7.70	114.36	108.20
1	a	60	A	N1-C2-N3	-7.70	125.45	129.30

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	673	U	C2-N1-C1'	7.69	126.93	117.70
1	a	1054	U	N1-C2-O2	7.69	128.18	122.80
1	a	677	G	N3-C4-C5	-7.67	124.77	128.60
1	a	434	А	C8-N9-C4	-7.67	102.73	105.80
1	a	61	G	N1-C2-N3	7.65	128.49	123.90
1	a	964	C	C6-N1-C2	-7.65	117.24	120.30
1	a	131	U	C2-N1-C1'	7.62	126.85	117.70
1	a	373	C	N1-C2-O2	7.62	123.47	118.90
4	d	32	CYS	CA-CB-SG	7.61	127.70	114.00
1	a	434	А	N7-C8-N9	7.59	117.59	113.80
1	a	683	C	C6-N1-C2	7.59	123.33	120.30
1	a	192	G	C5-N7-C8	-7.59	100.51	104.30
1	a	94	С	C6-N1-C2	-7.58	117.27	120.30
1	a	1106	С	C6-N1-C2	-7.56	117.28	120.30
1	a	536	G	OP1-P-O3'	7.55	121.82	105.20
1	a	324	С	N1-C2-O2	7.55	123.43	118.90
1	a	178	U	O5'-P-OP1	-7.55	98.91	105.70
1	a	677	G	C4-N9-C1'	7.54	136.30	126.50
1	a	956	С	N1-C2-O2	7.54	123.42	118.90
1	a	96	G	C4-N9-C1'	7.53	136.29	126.50
1	a	1009	G	N3-C4-C5	-7.50	124.85	128.60
1	a	956	С	C6-N1-C2	-7.50	117.30	120.30
16	р	19	LEU	CA-CB-CG	7.50	132.54	115.30
1	a	374	G	C8-N9-C4	-7.49	103.40	106.40
1	a	701	U	C2-N1-C1'	7.49	126.68	117.70
1	a	99	G	C6-N1-C2	7.47	129.58	125.10
1	a	103	A	C5-N7-C8	-7.45	100.17	103.90
1	a	1439	U	P-O3'-C3'	7.45	128.64	119.70
1	a	1345	U	N1-C2-O2	7.41	127.99	122.80
1	a	502	U	C6-N1-C1'	-7.41	110.83	121.20
1	a	374	G	C4-N9-C1'	7.40	136.13	126.50
1	a	701	U	N1-C2-O2	7.38	127.97	122.80
1	a	475	G	C4-N9-C1'	-7.38	116.91	126.50
1	a	505	C	C6-N1-C2	-7.38	117.35	120.30
1	a	1219	A	N1-C2-N3	-7.35	125.62	129.30
1	a	973	C	N1-C2-O2	7.34	123.31	118.90
1	a	542	G	C4-C5-N7	7.33	113.73	110.80
1	a	790	C	C2-N1-C1'	7.33	126.86	118.80
1	a	101	A	C2-N3-C4	7.32	114.26	110.60
1	a	748	C	C6-N1-C1'	-7.32	112.02	120.80
1	a	446	A	N3-C4-C5	7.30	131.91	126.80
1	a	256	A	C5-N7-C8	-7.30	100.25	103.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	1234	U	C2-N1-C1'	7.28	126.44	117.70
1	a	498	С	C2-N1-C1'	7.28	126.81	118.80
1	a	20	U	C5-C6-N1	7.28	126.34	122.70
1	a	325	G	C5-N7-C8	-7.28	100.66	104.30
1	a	1436	G	C4-C5-N7	7.26	113.70	110.80
1	a	1435	А	C2-N3-C4	7.21	114.21	110.60
1	a	380	С	N3-C2-O2	-7.16	116.89	121.90
1	a	1055	G	N3-C4-C5	-7.15	125.02	128.60
1	a	699	U	C5-C4-O4	-7.12	121.62	125.90
1	a	370	G	C5-N7-C8	-7.12	100.74	104.30
1	a	325	G	C4-C5-N7	7.12	113.65	110.80
1	a	673	U	N3-C2-O2	-7.11	117.23	122.20
1	a	762	А	C8-N9-C4	-7.10	102.96	105.80
1	a	1454	С	C6-N1-C2	-7.10	117.46	120.30
1	a	96	G	C4-C5-N7	7.09	113.64	110.80
1	a	60	А	C8-N9-C4	7.09	108.64	105.80
1	a	677	G	C8-N9-C1'	-7.08	117.80	127.00
1	a	18	C	C6-N1-C2	-7.08	117.47	120.30
1	a	402	G	N7-C8-N9	7.05	116.62	113.10
1	a	370	G	N7-C8-N9	7.04	116.62	113.10
16	р	6	LEU	CA-CB-CG	7.03	131.47	115.30
1	a	1309	U	N1-C2-O2	7.00	127.70	122.80
1	a	786	А	O4'-C1'-N9	6.99	113.80	108.20
1	a	1089	U	C5-C6-N1	6.99	126.19	122.70
1	a	96	G	C6-C5-N7	-6.98	126.21	130.40
1	a	94	С	C5-C6-N1	6.98	124.49	121.00
1	a	347	A	O4'-C1'-N9	6.97	113.78	108.20
1	a	536	G	P-O3'-C3'	6.95	128.04	119.70
1	a	403	U	OP1-P-OP2	-6.95	109.17	119.60
1	a	479	U	P-O3'-C3'	6.95	128.04	119.70
1	a	585	С	C6-N1-C2	-6.95	117.52	120.30
1	a	1020	G	C8-N9-C1'	-6.94	117.97	127.00
1	a	939	G	N3-C4-C5	-6.94	125.13	128.60
1	a	543	С	C6-N1-C2	-6.93	117.53	120.30
1	a	1060	C	C6-N1-C2	-6.90	117.54	120.30
1	a	347	A	C5-N7-C8	-6.90	100.45	103.90
1	a	227	C	C6-N1-C2	-6.90	117.54	120.30
1	a	102	G	C5-N7-C8	-6.90	100.85	104.30
1	a	95	A	N1-C6-N6	-6.89	114.46	118.60
1	a	374	G	C5-N7-C8	-6.89	100.85	104.30
1	a	433	U	P-O3'-C3'	6.89	127.97	119.70
1	a	450	C	C6-N1-C2	-6.89	117.55	120.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	1436	G	C6-C5-N7	-6.88	126.27	130.40
1	a	101	А	N1-C2-N3	-6.85	125.88	129.30
1	a	782	U	C2-N1-C1'	6.85	125.92	117.70
1	a	325	G	N7-C8-N9	6.84	116.52	113.10
1	a	771	А	C4-C5-N7	6.84	114.12	110.70
1	a	1234	U	N1-C2-O2	6.83	127.58	122.80
1	a	1515	С	N1-C2-O2	6.83	123.00	118.90
1	a	1353	С	C2-N1-C1'	6.82	126.30	118.80
1	a	402	G	O5'-P-OP1	-6.81	99.57	105.70
1	a	58	С	C6-N1-C2	-6.80	117.58	120.30
1	a	211	С	C6-N1-C2	-6.80	117.58	120.30
1	a	576	U	C2-N1-C1'	6.80	125.86	117.70
1	a	939	G	C4-N9-C1'	6.80	135.34	126.50
1	a	34	С	C6-N1-C1'	-6.79	112.66	120.80
1	a	1061	А	N9-C1'-C2'	6.79	122.82	114.00
1	a	725	G	C8-N9-C4	-6.77	103.69	106.40
1	a	492	А	C8-N9-C4	-6.76	103.09	105.80
1	a	1009	G	N3-C4-N9	6.76	130.06	126.00
1	a	720	С	N3-C2-O2	-6.76	117.17	121.90
1	a	374	G	C4-C5-N7	6.75	113.50	110.80
1	a	1227	G	C4-N9-C1'	6.75	135.28	126.50
1	a	256	А	N7-C8-N9	6.75	117.17	113.80
1	a	771	А	C8-N9-C4	-6.74	103.10	105.80
1	a	873	С	C6-N1-C2	-6.74	117.60	120.30
1	a	574	С	N3-C2-O2	-6.74	117.18	121.90
1	a	759	G	C6-C5-N7	-6.74	126.36	130.40
1	a	1054	U	N3-C2-O2	-6.72	117.50	122.20
1	a	159	G	P-O3'-C3'	6.71	127.75	119.70
1	a	1309	U	N3-C2-O2	-6.70	117.51	122.20
1	a	1142	U	C2-N1-C1'	6.70	125.74	117.70
1	a	817	С	C6-N1-C2	-6.70	117.62	120.30
1	a	761	A	C8-N9-C4	-6.69	103.12	105.80
1	a	192	G	C4-C5-N7	6.68	113.47	110.80
1	a	876	C	C6-N1-C2	-6.67	117.63	120.30
1	a	177	G	OP1-P-O3'	6.67	119.88	105.20
1	a	266	C	C6-N1-C2	-6.66	117.64	120.30
1	a	532	A	C2-N3-C4	6.65	113.93	110.60
1	a	370	G	C8-N9-C4	-6.63	103.75	106.40
1	a	423	U	N1-C2-N3	6.62	118.87	114.90
1	a	748	C	N1-C2-O2	6.61	122.87	118.90
1	a	1020	G	N3-C4-N9	6.61	129.97	126.00
1	a	542	G	C5-N7-C8	-6.60	101.00	104.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	256	A	O4'-C1'-N9	6.59	113.47	108.20
1	a	1142	U	N1-C2-O2	6.59	127.41	122.80
1	a	1215	G	N3-C4-C5	-6.58	125.31	128.60
1	a	795	U	N3-C2-O2	-6.58	117.60	122.20
1	a	574	С	N1-C2-O2	6.57	122.84	118.90
1	a	675	С	C5-C6-N1	6.57	124.29	121.00
1	a	1057	С	C6-N1-C2	-6.55	117.68	120.30
1	a	379	С	N3-C2-O2	-6.55	117.32	121.90
1	a	1514	С	N1-C2-O2	6.54	122.83	118.90
1	a	347	А	C4-C5-N7	6.53	113.97	110.70
1	a	636	А	C6-N1-C2	-6.52	114.69	118.60
1	a	887	С	C5-C6-N1	6.52	124.26	121.00
1	a	862	С	C6-N1-C2	-6.51	117.69	120.30
1	a	964	С	N1-C2-O2	6.51	122.81	118.90
1	a	1055	G	N3-C4-N9	6.51	129.91	126.00
1	a	637	С	C5-C6-N1	6.51	124.25	121.00
1	a	673	U	N1-C2-O2	6.50	127.35	122.80
1	a	956	С	N3-C2-O2	-6.50	117.35	121.90
1	a	374	G	C6-C5-N7	-6.49	126.51	130.40
1	a	101	A	C5-C6-N1	6.47	120.94	117.70
1	a	36	C	C5-C6-N1	6.46	124.23	121.00
1	a	33	A	C5-N7-C8	-6.46	100.67	103.90
1	a	1316	С	C5-C6-N1	6.46	124.23	121.00
1	a	126	C	C6-N1-C2	-6.45	117.72	120.30
1	a	373	C	N3-C2-O2	-6.45	117.39	121.90
1	a	1518	C	C6-N1-C2	-6.44	117.72	120.30
1	a	504	A	N7-C8-N9	6.41	117.00	113.80
1	a	1110	U	C5-C4-O4	-6.41	122.05	125.90
1	a	795	U	C6-N1-C1'	-6.41	112.23	121.20
1	a	1075	G	C5-N7-C8	-6.41	101.10	104.30
1	a	477	С	N1-C2-O2	6.41	122.74	118.90
1	a	1106	C	C5-C6-N1	6.40	124.20	121.00
1	a	1488	G	N3-C4-N9	6.39	129.84	126.00
1	a	290	U	N3-C2-O2	-6.39	117.73	122.20
1	a	61	G	N1-C2-N2	6.39	121.95	116.20
1	a	271	C	C6-N1-C2	-6.39	117.75	120.30
1	a	939	G	N3-C4-N9	6.39	129.83	126.00
1	a	607	C	C6-N1-C2	-6.38	117.75	120.30
1	a	1215	G	N3-C4-N9	6.38	129.83	126.00
1	a	636	A	C5-C6-N6	6.38	128.81	123.70
1	a	444	G	C5-C6-O6	-6.38	$124.7\overline{7}$	128.60
1	a	60	A	C4-C5-N7	6.38	113.89	110.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	66	G	N3-C2-N2	6.36	124.35	119.90
1	a	1309	U	C5-C6-N1	6.36	125.88	122.70
1	a	103	А	C4-C5-N7	6.36	113.88	110.70
1	a	956	С	C2-N1-C1'	6.35	125.79	118.80
1	a	176	С	C6-N1-C1'	-6.35	113.18	120.80
1	a	61	G	C8-N9-C4	-6.35	103.86	106.40
1	a	799	С	C6-N1-C2	-6.34	117.76	120.30
1	a	1253	С	N3-C2-O2	-6.33	117.47	121.90
1	a	215	С	N1-C2-O2	6.32	122.69	118.90
1	a	265	С	C6-N1-C2	-6.32	117.77	120.30
8	h	113	ASP	CB-CG-OD1	6.31	123.98	118.30
1	a	761	А	C6-C5-N7	-6.30	127.89	132.30
1	a	744	С	N1-C2-O2	6.30	122.68	118.90
8	h	7	LEU	CA-CB-CG	6.29	129.78	115.30
1	a	391	А	C2-N3-C4	6.29	113.74	110.60
1	a	1253	С	N1-C2-O2	6.28	122.67	118.90
1	a	1488	G	C4-N9-C1'	6.28	134.66	126.50
1	a	84	С	C6-N1-C2	-6.27	117.79	120.30
1	a	1057	С	C6-N1-C1'	-6.23	113.32	120.80
1	a	245	G	N7-C8-N9	6.23	116.22	113.10
1	a	400	G	N9-C4-C5	-6.22	102.91	105.40
1	a	399	U	C5-C6-N1	6.22	125.81	122.70
1	a	86	С	C5-C6-N1	6.21	124.11	121.00
1	a	771	A	C6-C5-N7	-6.20	127.96	132.30
1	a	502	U	N3-C2-O2	-6.20	117.86	122.20
1	a	227	С	N1-C2-O2	6.19	122.62	118.90
1	a	504	A	C8-N9-C4	-6.19	103.33	105.80
1	a	96	G	C8-N9-C1'	-6.18	118.97	127.00
1	a	285	U	N3-C2-O2	-6.18	117.88	122.20
1	a	1345	U	C5-C6-N1	6.17	125.79	122.70
1	a	96	G	N7-C8-N9	6.17	116.19	113.10
1	a	324	С	N3-C2-O2	-6.17	117.58	121.90
1	a	973	С	C2-N1-C1'	6.17	125.58	118.80
1	a	782	U	N1-C2-O2	6.16	127.11	122.80
1	a	380	С	N1-C2-O2	6.15	122.59	118.90
1	a	572	C	N3-C2-O2	-6.14	117.60	121.90
1	a	33	A	N7-C8-N9	6.14	116.87	113.80
1	a	1009	G	C4-N9-C1'	6.13	134.47	126.50
1	a	37	U	O4'-C1'-N1	6.13	113.10	108.20
1	a	426	A	C4-N9-C1'	6.13	137.33	126.30
1	a	$75\overline{2}$	G	C6-C5-N7	-6.11	$126.7\overline{3}$	130.40
1	a	733	C	C6-N1-C2	-6.11	117.86	120.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	245	G	C5-N7-C8	-6.11	101.25	104.30
1	a	1388	А	O4'-C1'-N9	6.11	113.08	108.20
1	a	887	С	C6-N1-C2	-6.10	117.86	120.30
1	a	1141	С	N1-C2-O2	6.10	122.56	118.90
1	a	1215	G	C8-N9-C1'	-6.10	119.07	127.00
1	a	1227	G	N3-C4-N9	6.10	129.66	126.00
1	a	1488	G	C8-N9-C1'	-6.09	119.08	127.00
1	a	227	С	N3-C2-O2	-6.09	117.64	121.90
1	a	1392	А	C5-N7-C8	-6.09	100.86	103.90
1	a	492	А	N7-C8-N9	6.08	116.84	113.80
1	a	771	А	O4'-C1'-N9	6.07	113.06	108.20
1	a	636	А	N3-C4-N9	6.06	132.25	127.40
1	a	1518	С	C2-N1-C1'	6.05	125.46	118.80
1	a	1020	G	N3-C4-C5	-6.05	125.58	128.60
1	a	356	G	O4'-C1'-N9	6.03	113.03	108.20
1	a	775	А	C5-N7-C8	-6.03	100.88	103.90
1	a	290	U	N1-C2-O2	6.03	127.02	122.80
1	a	876	С	C5-C6-N1	6.03	124.01	121.00
1	a	893	С	C6-N1-C2	-6.02	117.89	120.30
1	a	60	А	C5-C6-N1	6.02	120.71	117.70
1	a	1345	U	N3-C2-O2	-6.02	117.99	122.20
1	a	1525	А	O4'-C1'-N9	6.01	113.01	108.20
1	a	1009	G	C2-N3-C4	6.01	114.91	111.90
1	a	1058	G	C4-N9-C1'	6.00	134.30	126.50
1	a	1358	U	C2-N1-C1'	5.99	124.89	117.70
1	a	1061	А	C8-N9-C4	-5.99	103.40	105.80
1	a	66	G	C4-C5-N7	5.98	113.19	110.80
1	a	543	С	C5-C6-N1	5.98	123.99	121.00
1	a	34	С	N1-C2-O2	5.97	122.48	118.90
1	а	423	U	C6-N1-C2	-5.97	117.42	121.00
1	a	964	С	N3-C2-O2	-5.97	117.72	121.90
1	a	862	С	C5-C6-N1	5.96	123.98	121.00
1	a	58	С	O4'-C1'-N1	5.96	112.97	108.20
1	a	245	G	C4-C5-N7	5.95	113.18	110.80
1	a	498	С	N1-C2-O2	5.95	122.47	118.90
1	a	368	А	N9-C4-C5	-5.93	103.43	105.80
1	a	1248	G	C4-N9-C1'	5.92	134.20	126.50
1	a	346	C	N1-C2-O2	5.92	122.45	118.90
1	a	673	U	C6-N1-C1'	-5.92	112.92	121.20
1	a	804	С	N3-C2-O2	-5.92	117.76	121.90
1	a	866	A	N9-C4-C5	-5.91	103.44	105.80
1	a	479	U	OP1-P-O3'	5.91	118.20	105.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	h	92	LEU	CA-CB-CG	5.91	128.89	115.30
1	a	192	G	O4'-C1'-N9	5.91	112.93	108.20
1	a	1343	А	N3-C4-N9	5.89	132.11	127.40
1	a	675	С	C6-N1-C2	-5.88	117.95	120.30
1	a	1227	G	C8-N9-C1'	-5.88	119.35	127.00
1	a	422	G	P-O3'-C3'	5.88	126.75	119.70
1	a	699	U	C2-N1-C1'	5.87	124.75	117.70
1	a	1514	С	C6-N1-C2	-5.86	117.95	120.30
1	a	256	А	C4-C5-N7	5.86	113.63	110.70
1	a	532	А	N7-C8-N9	5.85	116.72	113.80
1	a	685	G	C5-C6-O6	-5.85	125.09	128.60
1	a	192	G	C8-N9-C4	-5.84	104.06	106.40
1	a	379	С	C5-C6-N1	5.84	123.92	121.00
1	a	1008	А	C8-N9-C4	-5.84	103.47	105.80
1	a	1209	G	C4-N9-C1'	5.83	134.08	126.50
1	a	426	А	C2-N3-C4	5.83	113.51	110.60
1	a	308	С	N1-C2-O2	5.82	122.39	118.90
1	a	530	С	N1-C2-O2	5.82	122.39	118.90
1	a	60	А	C4-C5-C6	-5.81	114.09	117.00
1	a	394	С	P-O3'-C3'	5.81	126.68	119.70
1	a	305	U	N3-C2-O2	-5.81	118.13	122.20
1	a	391	А	C8-N9-C4	-5.80	103.48	105.80
1	a	546	U	C6-N1-C2	-5.80	117.52	121.00
1	a	58	С	N3-C4-C5	-5.79	119.58	121.90
1	a	813	А	O4'-C1'-N9	-5.79	103.57	108.20
1	a	1142	U	N3-C2-O2	-5.79	118.15	122.20
1	a	102	G	C4-N9-C1'	5.79	134.02	126.50
1	a	102	G	N7-C8-N9	5.78	115.99	113.10
1	a	1234	U	N3-C2-O2	-5.78	118.15	122.20
1	a	1343	А	N3-C4-C5	-5.78	122.75	126.80
1	a	177	G	C4-C5-N7	5.78	113.11	110.80
1	a	308	С	N3-C2-O2	-5.77	117.86	121.90
1	a	512	С	P-O3'-C3'	5.77	126.63	119.70
1	a	61	G	C8-N9-C1'	5.75	134.48	127.00
1	a	874	С	C6-N1-C2	-5.74	118.00	120.30
1	a	103	A	O4'-C1'-N9	-5.74	103.61	108.20
1	a	239	U	N1-C2-O2	5.74	126.82	122.80
1	a	67	С	N1-C2-O2	5.74	122.34	118.90
1	a	1183	U	N1-C2-O2	5.74	126.81	122.80
1	a	51	А	C5-N7-C8	-5.73	101.03	103.90
1	a	1505	G	N9-C4-C5	-5.73	103.11	105.40
1	a	211	С	N3-C2-O2	-5.73	117.89	121.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	310	С	N1-C2-O2	5.72	122.33	118.90
1	a	864	А	C5-N7-C8	-5.72	101.04	103.90
1	a	799	С	C6-N1-C1'	-5.72	113.94	120.80
1	a	33	А	O4'-C1'-N9	5.72	112.77	108.20
1	a	423	U	N3-C4-C5	-5.71	111.17	114.60
1	a	970	G	N3-C4-N9	5.71	129.43	126.00
1	a	800	С	C6-N1-C2	-5.70	118.02	120.30
1	a	34	С	O4'-C1'-N1	5.70	112.76	108.20
1	a	403	U	C6-N1-C1'	5.69	129.16	121.20
8	h	118	ALA	N-CA-C	5.69	126.36	111.00
1	a	403	U	N1-C1'-C2'	5.68	121.38	114.00
1	a	239	U	N3-C2-O2	-5.68	118.23	122.20
1	a	915	U	C5-C6-N1	5.67	125.53	122.70
1	a	1183	U	N3-C2-O2	-5.67	118.23	122.20
1	a	131	U	C4-C5-C6	5.66	123.10	119.70
1	a	535	G	P-O3'-C3'	5.66	126.49	119.70
1	a	550	С	C6-N1-C2	-5.65	118.04	120.30
1	a	356	G	C8-N9-C1'	5.65	134.34	127.00
1	a	383	А	N1-C2-N3	-5.65	126.47	129.30
1	a	612	С	N3-C2-O2	-5.64	117.95	121.90
1	a	1504	С	N3-C2-O2	-5.64	117.95	121.90
1	a	1516	U	N3-C2-O2	-5.64	118.25	122.20
1	a	1248	G	N3-C4-C5	-5.64	125.78	128.60
1	a	59	А	O4'-C1'-N9	5.64	112.71	108.20
1	a	837	U	P-O3'-C3'	5.64	126.47	119.70
1	a	400	G	C8-N9-C1'	-5.63	119.68	127.00
1	a	1504	С	N1-C2-O2	5.63	122.28	118.90
1	a	356	G	N9-C4-C5	5.63	107.65	105.40
1	a	369	U	C4-C5-C6	5.63	123.08	119.70
1	a	265	С	C5-C6-N1	5.62	123.81	121.00
1	a	284	С	C6-N1-C2	-5.62	118.05	120.30
1	a	1107	С	C6-N1-C2	-5.62	118.05	120.30
1	a	1514	С	C2-N1-C1'	5.62	124.98	118.80
1	a	945	G	C4-N9-C1'	5.62	133.80	126.50
1	a	1406	С	C6-N1-C2	-5.62	118.05	120.30
1	a	613	U	P-O3'-C3'	5.62	126.44	119.70
1	a	102	G	C4-C5-N7	5.61	113.05	110.80
1	a	400	G	N3-C4-N9	5.61	129.37	126.00
1	a	752	G	C4-C5-N7	5.61	113.05	110.80
1	a	794	G	C8-N9-C4	-5.61	104.16	106.40
1	a	956	C	C5-C6-N1	5.61	$1\overline{23.80}$	121.00
1	a	1115	U	N1-C2-O2	5.61	$126.7\overline{2}$	122.80



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	102	G	O4'-C1'-N9	5.60	112.68	108.20
1	a	248	G	O5'-P-OP1	-5.60	100.66	105.70
1	a	369	U	C6-N1-C2	-5.60	117.64	121.00
1	a	1505	G	C4-C5-N7	5.60	113.04	110.80
1	a	23	С	N1-C2-O2	5.59	122.25	118.90
1	a	383	А	C6-N1-C2	5.59	121.95	118.60
1	a	385	С	C4-C5-C6	-5.59	114.61	117.40
1	a	1185	А	N1-C6-N6	-5.59	115.25	118.60
1	a	426	А	N3-C4-N9	5.58	131.87	127.40
1	a	369	U	N1-C2-N3	5.58	118.25	114.90
1	a	794	G	N3-C4-C5	-5.58	125.81	128.60
1	a	1309	U	C6-N1-C1'	-5.58	113.39	121.20
1	a	325	G	N3-C2-N2	-5.57	116.00	119.90
1	a	1472	U	C5-C6-N1	5.56	125.48	122.70
1	a	349	С	O5'-P-OP1	-5.54	100.71	105.70
1	a	541	А	OP1-P-O3'	5.54	117.39	105.20
1	a	353	G	C8-N9-C4	-5.54	104.19	106.40
1	a	1219	А	C5-C6-N6	-5.53	119.28	123.70
1	a	370	G	C4-C5-N7	5.52	113.01	110.80
1	a	608	С	C6-N1-C2	-5.52	118.09	120.30
1	a	203	U	C2-N1-C1'	5.52	124.33	117.70
19	s	68	GLY	N-CA-C	5.52	126.90	113.10
1	a	16	А	N1-C2-N3	-5.51	126.54	129.30
1	a	368	А	C4-C5-N7	5.51	113.46	110.70
1	a	95	А	C6-C5-N7	5.51	136.16	132.30
1	a	177	G	C6-C5-N7	-5.51	127.09	130.40
1	a	61	G	C5-N7-C8	-5.50	101.55	104.30
1	a	463	С	N3-C2-O2	-5.50	118.05	121.90
1	a	709	A	P-O3'-C3'	5.49	126.29	119.70
1	a	399	U	C5-C4-O4	-5.49	122.61	125.90
1	a	1219	А	N1-C6-N6	-5.49	115.31	118.60
1	a	18	С	C5-C6-N1	5.48	123.74	121.00
1	a	369	U	C5-C4-O4	5.48	129.19	125.90
1	a	684	G	C8-N9-C4	-5.48	104.21	106.40
1	a	50	А	P-O3'-C3'	5.47	126.27	119.70
1	a	374	G	C8-N9-C1'	-5.47	119.88	127.00
1	a	1515	С	N3-C2-O2	-5.47	118.07	121.90
1	a	179	С	C5-C6-N1	5.47	123.73	121.00
1	a	532	А	C4-N9-C1'	5.46	136.14	126.30
1	a	226	G	C2-N3-C4	5.46	114.63	111.90
1	a	117	С	N1-C2-O2	5.46	122.18	118.90
1	a	1313	А	C6-C5-N7	5.46	136.12	132.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	534	G	N3-C4-C5	-5.46	125.87	128.60
1	a	1379	G	P-O3'-C3'	5.46	126.25	119.70
1	a	535	G	OP1-P-O3'	5.46	117.20	105.20
1	a	891	С	N3-C2-O2	-5.46	118.08	121.90
1	a	1221	А	C2-N3-C4	5.46	113.33	110.60
1	a	363	G	C8-N9-C4	-5.45	104.22	106.40
1	a	637	С	C6-N1-C2	-5.44	118.12	120.30
8	h	119	ALA	C-N-CA	5.44	133.72	122.30
1	a	97	С	C6-N1-C2	-5.43	118.13	120.30
1	a	771	А	C4-N9-C1'	5.43	136.07	126.30
1	a	1455	G	O5'-P-OP2	-5.43	100.81	105.70
1	a	318	G	N1-C2-N3	5.43	127.16	123.90
1	a	103	А	N9-C4-C5	-5.42	103.63	105.80
1	a	874	С	C5-C6-N1	5.42	123.71	121.00
1	a	893	С	P-O3'-C3'	5.42	126.21	119.70
8	h	118	ALA	CB-CA-C	-5.42	101.97	110.10
1	a	1250	U	C2-N1-C1'	5.41	124.20	117.70
1	a	1253	С	C6-N1-C2	-5.41	118.14	120.30
1	a	202	U	C5-C6-N1	5.40	125.40	122.70
1	a	937	U	N1-C2-O2	5.40	126.58	122.80
1	a	33	А	C8-N9-C4	-5.40	103.64	105.80
1	a	532	А	N3-C4-N9	5.40	131.72	127.40
1	a	1077	U	N3-C2-O2	-5.40	118.42	122.20
1	a	444	G	C4-C5-N7	5.39	112.96	110.80
1	a	446	А	N3-C4-N9	-5.39	123.09	127.40
1	a	550	С	N3-C2-O2	-5.39	118.13	121.90
1	a	762	А	P-O3'-C3'	5.39	126.17	119.70
1	a	446	A	C8-N9-C1'	5.38	137.39	127.70
1	a	970	G	N3-C4-C5	-5.38	125.91	128.60
1	a	266	С	C5-C6-N1	5.37	123.69	121.00
1	a	777	C	C6-N1-C2	-5.37	118.15	120.30
1	a	702	A	C8-N9-C4	-5.37	103.65	105.80
1	a	906	C	C6-N1-C2	-5.37	118.15	120.30
1	a	380	С	C5-C6-N1	5.36	123.68	121.00
1	a	479	U	O4'-C1'-N1	5.35	112.48	108.20
1	a	34	C	C4-C5-C6	5.35	120.08	117.40
1	a	471	U	N3-C2-O2	-5.35	118.46	122.20
1	a	744	С	N3-C2-O2	-5.35	118.16	121.90
1	a	1358	U	N1-C2-O2	5.34	126.54	122.80
1	a	446	A	C4-N9-C1'	-5.34	116.68	126.30
1	a	873	C	C5-C6-N1	5.34	123.67	121.00
1	a	1122	С	C6-N1-C2	-5.33	118.17	120.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	720	С	N1-C2-O2	5.32	122.09	118.90
1	a	1141	С	C6-N1-C2	-5.32	118.17	120.30
1	a	1075	G	C6-C5-N7	-5.31	127.22	130.40
1	a	179	С	C6-N1-C2	-5.31	118.18	120.30
1	a	638	U	C6-N1-C1'	-5.30	113.77	121.20
1	a	542	G	O4'-C1'-N9	5.30	112.44	108.20
1	a	1455	G	C6-C5-N7	-5.30	127.22	130.40
1	a	1209	G	N3-C4-N9	5.29	129.18	126.00
1	a	852	G	C4-C5-N7	5.29	112.92	110.80
1	a	475	G	C6-C5-N7	5.29	133.57	130.40
1	a	614	C	C6-N1-C2	-5.29	118.19	120.30
1	a	714	С	N3-C4-C5	5.29	124.02	121.90
1	a	1115	U	C2-N1-C1'	5.28	124.04	117.70
1	a	542	G	N7-C8-N9	5.28	115.74	113.10
1	a	964	C	C5-C6-N1	5.28	123.64	121.00
1	a	534	G	N3-C4-N9	5.28	129.17	126.00
6	f	9	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	a	765	G	C6-C5-N7	-5.27	127.24	130.40
1	a	1309	U	C6-N1-C2	-5.27	117.84	121.00
1	a	370	G	O4'-C1'-N9	5.26	112.41	108.20
1	a	498	С	C6-N1-C1'	-5.26	114.48	120.80
1	a	318	G	N7-C8-N9	5.26	115.73	113.10
1	a	1248	G	N3-C4-N9	5.26	129.16	126.00
1	a	356	G	P-O3'-C3'	5.26	126.01	119.70
1	a	576	U	C6-N1-C2	-5.25	117.85	121.00
1	a	1057	С	C2-N3-C4	5.25	122.52	119.90
12	1	81	LEU	CA-CB-CG	5.25	127.37	115.30
1	a	1455	G	O5'-P-OP1	5.25	117.00	110.70
1	a	413	С	C6-N1-C2	-5.25	118.20	120.30
1	a	333	С	N1-C2-O2	5.24	122.05	118.90
1	a	939	G	C2-N3-C4	5.24	114.52	111.90
1	a	378	G	P-O3'-C3'	5.24	125.98	119.70
1	a	397	С	N3-C2-O2	-5.24	118.23	121.90
1	a	1141	С	C5-C6-N1	5.24	123.62	121.00
1	a	1343	A	C4-N9-C1'	5.23	135.72	126.30
1	a	462	A	O4'-C1'-N9	5.23	112.39	108.20
1	a	23	C	N3-C2-O2	-5.23	118.24	121.90
1	a	1392	A	N7-C8-N9	5.23	116.41	113.80
1	a	468	C	N1-C2-O2	5.22	122.03	118.90
1	a	465	U	C6-N1-C1'	-5.22	113.89	121.20
1	a	1461	C	N3-C2-02	-5.22	$118.2\overline{4}$	121.90
1	a	612	C	N1-C2-O2	5.22	122.03	118.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	209	С	N1-C2-O2	5.22	122.03	118.90
1	a	569	G	O4'-C1'-N9	-5.22	104.03	108.20
1	a	316	С	C5-C6-N1	5.22	123.61	121.00
1	a	1008	А	N7-C8-N9	5.21	116.41	113.80
1	a	1115	U	N3-C2-O2	-5.21	118.55	122.20
1	a	1055	G	C2-N3-C4	5.21	114.51	111.90
1	a	426	А	C8-N9-C1'	-5.21	118.32	127.70
1	a	871	G	N7-C8-N9	-5.21	110.50	113.10
1	a	474	U	P-O3'-C3'	5.21	125.94	119.70
1	a	532	А	C8-N9-C4	-5.21	103.72	105.80
1	a	36	С	C6-N1-C2	-5.20	118.22	120.30
1	a	177	G	C4-N9-C1'	5.20	133.26	126.50
1	a	637	С	N1-C2-O2	5.19	122.01	118.90
1	a	318	G	C8-N9-C4	-5.19	104.33	106.40
1	a	1345	U	C6-N1-C1'	-5.18	113.94	121.20
1	a	99	G	C5-N7-C8	-5.18	101.71	104.30
1	a	750	С	N1-C2-O2	5.18	122.01	118.90
1	a	86	С	N1-C2-O2	5.18	122.01	118.90
1	a	599	U	N3-C2-O2	-5.18	118.58	122.20
1	a	777	С	P-O3'-C3'	5.18	125.91	119.70
1	a	653	С	C6-N1-C2	-5.17	118.23	120.30
1	a	939	G	C8-N9-C1'	-5.17	120.27	127.00
1	a	825	С	C6-N1-C2	-5.16	118.24	120.30
1	a	1209	G	C8-N9-C1'	-5.16	120.29	127.00
1	a	1009	G	C8-N9-C4	-5.16	104.34	106.40
1	a	1353	С	N3-C2-O2	-5.16	118.29	121.90
1	a	532	А	N3-C4-C5	-5.16	123.19	126.80
1	a	1227	G	N3-C4-C5	-5.15	126.02	128.60
1	a	691	U	C5-C6-N1	5.15	125.27	122.70
1	a	730	С	C6-N1-C2	-5.15	118.24	120.30
1	a	820	С	N1-C2-O2	5.15	121.99	118.90
1	a	945	G	N3-C4-C5	-5.15	126.03	128.60
1	a	1250	U	N1-C2-O2	5.14	126.40	122.80
1	a	23	С	C6-N1-C2	-5.14	118.24	120.30
1	a	1055	G	C4-N9-C1'	5.14	133.18	126.50
1	a	682	G	N1-C6-O6	5.13	122.98	119.90
1	a	538	G	C8-N9-C1'	-5.13	120.33	127.00
1	a	480	U	C2-N1-C1'	5.13	123.86	117.70
1	a	1357	Α	C2-N3-C4	5.12	113.16	110.60
1	a	773	С	C6-N1-C2	-5.12	118.25	120.30
1	a	1089	U	C2-N1-C1'	5.12	123.85	117.70
1	a	20	U	C2-N1-C1'	5.11	123.84	117.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	a	37	U	C6-N1-C2	-5.11	117.93	121.00
1	a	248	G	OP1-P-OP2	5.11	127.27	119.60
18	r	55	LEU	CA-CB-CG	5.11	127.06	115.30
1	a	1505	G	N3-C2-N2	5.11	123.48	119.90
1	a	471	U	N1-C2-O2	5.11	126.37	122.80
1	a	1431	A	P-O3'-C3'	5.11	125.83	119.70
1	a	444	G	N1-C6-O6	5.09	122.96	119.90
1	a	423	U	O5'-P-OP1	-5.08	101.12	105.70
1	a	426	A	N3-C4-C5	-5.08	123.24	126.80
1	a	762	A	C2'-C3'-O3'	5.08	121.83	113.70
1	a	1215	G	C8-N9-C4	-5.08	104.37	106.40
1	a	1219	A	C6-N1-C2	-5.08	115.55	118.60
1	a	1514	С	C5-C6-N1	5.08	123.54	121.00
1	a	66	G	N9-C4-C5	-5.08	103.37	105.40
1	a	672	U	N3-C2-O2	-5.08	118.65	122.20
1	a	576	U	C5-C4-O4	5.07	128.94	125.90
1	a	775	A	N7-C8-N9	5.07	116.34	113.80
1	a	1234	U	C6-N1-C1'	-5.06	114.11	121.20
1	a	939	G	C8-N9-C4	-5.06	104.38	106.40
1	a	1436	G	N1-C6-O6	5.06	122.94	119.90
1	a	761	A	C5-C6-N6	-5.06	119.66	123.70
11	k	121	CYS	C-N-CA	-5.06	109.06	121.70
1	a	284	С	C5-C6-N1	5.05	123.53	121.00
1	a	171	G	C4-N9-C1'	5.05	133.07	126.50
1	a	215	С	N3-C2-O2	-5.05	118.36	121.90
1	a	1514	С	N3-C2-O2	-5.05	118.36	121.90
1	a	1101	С	C6-N1-C2	-5.05	118.28	120.30
1	a	1354	A	C2-N3-C4	5.05	113.12	110.60
1	a	51	A	N1-C6-N6	5.04	121.63	118.60
1	a	645	С	C6-N1-C2	-5.04	118.28	120.30
1	a	810	A	N1-C2-N3	-5.04	126.78	129.30
1	a	1454	С	C2-N1-C1'	5.04	124.35	118.80
1	a	636	A	N1-C2-N3	-5.04	126.78	129.30
1	a	245	G	C6-C5-N7	-5.04	127.38	130.40
1	a	1488	G	C6-C5-N7	-5.04	127.38	130.40
1	a	86	C	C6-N1-C2	-5.03	118.29	120.30
1	a	970	G	C4-N9-C1'	5.03	133.04	126.50
1	a	837	U	C2-N1-C1'	5.02	123.72	117.70
1	a	271	C	C5-C6-N1	5.01	123.51	121.00
1	a	675	C	N1-C2-O2	5.01	121.91	118.90
1	a	96	G	C5-N7-C8	-5.00	101.80	104.30
1	a	607	C	C5-C6-N1	5.00	123.50	121.00



There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	с	12	LEU	Peptide
3	с	176	HIS	Peptide
4	d	205	SER	Peptide
4	d	49	SER	Peptide
8	h	100	GLY	Peptide
8	h	104	VAL	Peptide
8	h	29	SER	Peptide
8	h	31	LYS	Peptide
8	h	33	LYS	Peptide
8	h	34	ALA	Peptide
8	h	41	LYS	Peptide
8	h	43	GLU	Peptide
8	h	49	PHE	Peptide
8	h	66	PHE	Peptide
8	h	75	VAL	Peptide
8	h	79	SER	Peptide
8	h	80	ARG	Peptide
8	h	83	LEU	Peptide
8	h	88	SER	Peptide
11	k	118	HIS	Peptide
11	k	55	SER	Peptide
12	1	104	THR	Peptide
12	l	107	VAL	Peptide
12	1	110	ARG	Peptide
12	1	111	LYS	Peptide
12	1	113	ARG	Peptide
12	1	115	LYS	Peptide
13	m	101	ARG	Peptide
13	m	106	ALA	Peptide
13	m	22	ILE	Peptide
13	m	26	GLY	Peptide
14	n	50	LYS	Peptide
14	n	51	GLN	Peptide
16	р	51	SER	Peptide

#### 5.2 Too-close contacts (i)

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32595	0	16400	0	0
2	b	1728	0	1766	0	0
3	с	1609	0	1636	0	0
4	d	1600	0	1620	0	0
5	е	1092	0	1139	0	0
6	f	802	0	769	0	0
7	g	1190	0	1227	0	0
8	h	915	0	952	0	0
9	i	994	0	1031	0	0
10	j	763	0	801	0	0
11	k	828	0	808	0	0
12	1	893	0	932	0	0
13	m	847	0	888	0	0
14	n	776	0	818	0	0
15	0	686	0	709	0	0
16	р	606	0	606	0	0
17	q	619	0	659	0	0
18	r	443	0	460	0	0
19	S	635	0	662	0	0
20	t	653	0	699	0	0
21	u	295	0	313	0	0
All	All	50569	0	34895	0	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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


Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	b	217/221~(98%)	179~(82%)	34~(16%)	4 (2%)	8	33
3	с	201/203~(99%)	170 (85%)	29~(14%)	2 (1%)	15	48
4	d	203/205~(99%)	161 (79%)	39 (19%)	3 (2%)	10	38
5	е	147/149~(99%)	130 (88%)	15~(10%)	2 (1%)	11	39
6	f	98/100~(98%)	86~(88%)	10 (10%)	2 (2%)	7	30
7	g	152/154~(99%)	115 (76%)	27~(18%)	10 (7%)	1	5
8	h	121/125~(97%)	84 (69%)	29 (24%)	8 (7%)	1	5
9	i	124/126~(98%)	104 (84%)	20 (16%)	0	100	100
10	j	94/96~(98%)	82 (87%)	12 (13%)	0	100	100
11	k	113/115~(98%)	93~(82%)	20 (18%)	0	100	100
12	1	111/120 (92%)	91 (82%)	18 (16%)	2 (2%)	8	33
13	m	105/109~(96%)	86 (82%)	19 (18%)	0	100	100
14	n	96/98~(98%)	80~(83%)	16 (17%)	0	100	100
15	О	84/87~(97%)	79~(94%)	4(5%)	1 (1%)	13	43
16	р	76/78~(97%)	64 (84%)	12 (16%)	0	100	100
17	q	74/76~(97%)	71 (96%)	3 (4%)	0	100	100
18	r	54/56~(96%)	52 (96%)	2(4%)	0	100	100
19	S	78/80~(98%)	63~(81%)	15 (19%)	0	100	100
20	t	83/86~(96%)	83 (100%)	0	0	100	100
21	u	$3\overline{2}/34~(94\%)$	25 (78%)	7(22%)	0	100	100
All	All	2263/2318 (98%)	1898 (84%)	331 (15%)	34 (2%)	14	38

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	с	8	ASN
4	d	14	ARG
4	d	33	LYS
5	е	14	GLU
6	f	86	ARG
7	g	32	GLU
8	h	32	LEU
8	h	106	THR
12	1	111	LYS
8	h	89	VAL
12	1	112	GLN



Mol	Chain	Res	Type
2	b	14	VAL
3	с	7	PRO
7	g	81	GLY
7	g	112	GLY
15	0	19	GLU
2	b	78	LYS
4	d	27	ALA
5	е	102	GLU
6	f	67	SER
7	g	27	MET
7	g	28	ASN
7	g	88	PRO
7	g	115	SER
7	g	128	ALA
8	h	118	ALA
8	h	113	ASP
8	h	115	ALA
2	b	71	GLY
2	b	95	ARG
7	g	34	GLY
7	g	152	SER
8	h	101	VAL
8	h	81	PRO

#### 5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	b	182/183~(100%)	114 (63%)	68~(37%)	0 0
3	с	163/169~(96%)	161 (99%)	2 (1%)	71 88
4	d	166/173~(96%)	162 (98%)	4 (2%)	49 77
5	е	108/109~(99%)	94 (87%)	14 (13%)	4 16
6	f	81/85~(95%)	75~(93%)	6 (7%)	13 41
7	g	116/120~(97%)	66 (57%)	50 (43%)	0 0



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
8	h	98/103~(95%)	90~(92%)	8 (8%)	11	36
9	i	102/102~(100%)	99~(97%)	3~(3%)	42	73
10	j	85/85~(100%)	82~(96%)	3(4%)	36	68
11	k	82/87~(94%)	79~(96%)	3 (4%)	34	66
12	1	100/104~(96%)	97~(97%)	3(3%)	41	72
13	m	91/91 (100%)	89~(98%)	2(2%)	52	79
14	n	78/80~(98%)	77~(99%)	1 (1%)	69	87
15	О	73/73~(100%)	72~(99%)	1 (1%)	67	86
16	р	60/63~(95%)	58~(97%)	2 (3%)	38	70
17	q	70/70~(100%)	68~(97%)	2(3%)	42	73
18	r	46/48~(96%)	45 (98%)	1 (2%)	52	79
19	S	69/71~(97%)	66~(96%)	3~(4%)	29	62
20	t	67/68~(98%)	65~(97%)	2(3%)	41	72
21	u	28/28~(100%)	28 (100%)	0	100	100
All	All	1865/1912 (98%)	1687 (90%)	178 (10%)	12	29

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	3	GLN
2	b	5	ASN
2	b	7	ARG
2	b	8	ASP
2	b	9	MET
2	b	10	LEU
2	b	21	ARG
2	b	23	TRP
2	b	24	ASN
2	b	29	LYS
2	b	31	ILE
2	b	38	ILE
2	b	42	ASN
2	b	43	LEU
2	b	47	LEU
2	b	50	PHE
2	b	52	GLU
2	b	58	GLU



Mol	Chain	Res	Type
2	b	59	ARG
2	b	60	LEU
2	b	64	LYS
2	b	66	LYS
2	b	67	ILE
2	b	68	LEU
2	b	74	ARG
2	b	75	SER
2	b	78	LYS
2	b	83	GLU
2	b	86	ARG
2	b	92	VAL
2	b	95	ARG
2	b	100	MET
2	b	101	LEU
2	b	102	THR
2	b	105	LYS
2	b	107	ILE
2	b	108	ARG
2	b	112	LYS
2	b	113	ARG
2	b	114	LEU
2	b	117	LEU
2	b	130	THR
2	b	131	LYS
2	b	132	LYS
2	b	136	MET
2	b	139	ARG
2	b	141	LEU
2	b	143	LYS
2	b	152	LYS
2	b	154	MET
2	b	164	ILE
2	b	167	ASP
2	b	171	ILE
2	b	177	ASN
2	b	178	LYS
2	b	181	ILE
2	b	190	ASN
2	b	192	SER
2	b	197	ASP
2	b	199	VAL



Mol	Chain	Res	Type
2	b	205	ASP
2	b	207	ILE
2	b	212	LEU
2	b	214	LEU
2	b	219	GLU
2	b	222	ILE
2	b	225	LYS
2	b	226	GLN
3	с	5	VAL
3	с	6	HIS
4	d	9	CYS
4	d	17	THR
4	d	110	THR
4	d	146	ARG
5	е	18	GLN
5	е	20	ASN
5	е	21	ARG
5	е	46	ARG
5	е	51	ARG
5	е	53	LYS
5	е	62	GLN
5	е	77	LEU
5	е	102	GLU
5	е	107	ILE
5	е	113	ARG
5	е	125	LEU
5	е	133	ASN
5	е	149	GLN
6	f	2	ARG
6	f	7	VAL
6	f	21	MET
6	f	24	ARG
6	f	78	PHE
6	f	86	ARG
7	g	5	ARG
7	g	9	LYS
7	g	11	GLU
7	g	13	LEU
7	g	15	ASP
7	g	17	LYS
7	g	20	SER
7	g	22	ILE



Mol	Chain	Res	Type
7	g	25	LYS
7	g	26	PHE
7	g	35	LYS
7	g	38	VAL
7	g	41	ARG
7	g	42	ILE
7	g	47	LEU
7	g	48	ASP
7	g	49	LYS
7	g	51	LYS
7	g	52	GLU
7	g	53	ARG
7	g	57	ASP
7	g	61	THR
7	g	64	LYS
7	g	66	LEU
7	g	72	LEU
7	g	75	VAL
7	g	77	SER
7	g	79	ARG
7	g	84	THR
7	g	87	VAL
7	g	89	VAL
7	g	91	VAL
7	g	96	ARG
7	g	99	LEU
7	g	102	ARG
7	g	111	ARG
7	g	113	GLU
7	g	115	SER
7	g	116	MET
7	g	118	LEU
7	g	119	ARG
7	g	120	LEU
7	g	125	LEU
7	g	131	LYS
7	g	136	LYS
7	g	137	LYS
$7^{-}$	g	146	GLU
7	g	148	ASN
7	g	149	LYS
7	g	154	TYR



Mol	Chain	Res	Type
8	h	7	LEU
8	h	31	LYS
8	h	33	LYS
8	h	49	PHE
8	h	59	LEU
8	h	69	LYS
8	h	106	THR
8	h	108	LYS
9	i	41	ARG
9	i	106	ARG
9	i	113	ARG
10	j	13	PHE
10	j	16	ARG
10	j	82	LYS
11	k	37	ARG
11	k	56	ARG
11	k	100	LEU
12	1	5	ASN
12	1	10	LYS
12	1	25	GLN
13	m	40	ASN
13	m	105	ASN
14	n	75	ARG
15	0	58	ARG
16	р	21	VAL
16	р	28	ARG
17	q	54	ASN
17	q	68	ARG
18	r	70	TYR
19	s	29	LYS
19	S	55	ARG
19	s	78	ARG
20	t	27	MET
20	t	29	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	19	GLN
2	b	36	ASN
2	b	39	HIS
2	b	42	ASN



Mol	Chain	Res	Type
2	b	65	ASN
2	b	177	ASN
2	b	190	ASN
4	d	43	GLN
5	е	18	GLN
5	е	20	ASN
5	е	83	GLN
5	е	90	HIS
5	е	123	ASN
5	е	133	ASN
6	f	3	HIS
6	f	55	HIS
6	f	63	ASN
7	g	97	ASN
7	g	148	ASN
9	i	6	ASN
9	i	50	GLN
11	k	38	GLN
11	k	81	ASN
12	1	72	HIS
13	m	40	ASN
13	m	91	HIS
13	m	105	ASN
14	n	8	ASN
14	n	71	HIS
15	0	42	HIS
17	q	34	HIS
17	q	54	ASN
19	S	14	HIS
20	t	68	HIS

$\alpha$ $\cdots$ 1	e		
Continued	trom	nremous	naae
Contentaca	<i>J</i> 10110	preciouo	pago

### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1514/1519~(99%)	677~(44%)	0

All (677) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	а	9	G
1	a	15	G



1       a       32       A         1       a       33       A         1       a       33       A         1       a       34       C         1       a       35       G         1       a       36       C         1       a       39       G         1       a       39       G         1       a       47       C         1       a       47       C         1       a       50       A         1       a       52       C         1       a       59       A         1       a       66       G         1       a       72       A         1       a       73       A         1       a       78       A         1       a       93       U         1       a       94       C         1       a       94       C         1       a       10       A         1       a       124       A         1       a       125       U <tr< th=""><th>Mol</th><th>Chain</th><th>Res</th><th>Type</th></tr<>	Mol	Chain	Res	Type
1       a       32       A         1       a       33       A         1       a       35       G         1       a       36       C         1       a       38       G         1       a       39       G         1       a       39       G         1       a       47       C         1       a       50       A         1       a       52       C         1       a       59       A         1       a       59       A         1       a       66       G         1       a       72       A         1       a       73       A         1       a       78       A         1       a       93       U         1       a       94       C         1       a       94       C         1       a       95       A         1       a       10       A         1       a       124       A         1       a       125       U <tr< td=""><td>1</td><td>a</td><td>22</td><td>G</td></tr<>	1	a	22	G
1       a       33       A         1       a       34       C         1       a       35       G         1       a       36       C         1       a       38       G         1       a       39       G         1       a       50       A         1       a       52       C         1       a       59       A         1       a       59       A         1       a       60       A         1       a       72       A         1       a       78       A         1       a       93       U         1       a       94       C         1       a       94       C         1       a       10       A         1       a       122       G         1       a       124       A <tr< td=""><td>1</td><td>a</td><td>32</td><td>А</td></tr<>	1	a	32	А
1       a $34$ C         1       a $35$ G         1       a $36$ C         1       a $38$ G         1       a $39$ G         1       a $39$ G         1       a $47$ C         1       a $47$ C         1       a $50$ A         1       a $52$ C         1       a $53$ A         1       a $59$ A         1       a $72$ A         1       a $72$ A         1       a $78$ A         1       a $91$ A         1       a $94$ C         1       a $95$ A         1       a	1	a	33	А
1       a       35       G         1       a       36       C         1       a       39       G         1       a       39       G         1       a       39       G         1       a       47       C         1       a       48       C         1       a       50       A         1       a       52       C         1       a       59       A         1       a       59       A         1       a       60       A         1       a       66       G         1       a       72       A         1       a       73       A         1       a       73       A         1       a       93       U         1       a       94       C         1       a       95       A         1       a       96       G         1       a       122       G         1       a       124       A         1       a       124       A <t< td=""><td>1</td><td>a</td><td>34</td><td>С</td></t<>	1	a	34	С
1       a $36$ C         1       a $38$ G         1       a $39$ G         1       a $47$ C         1       a $47$ C         1       a $50$ A         1       a $50$ A         1       a $52$ C         1       a $53$ A         1       a $59$ A         1       a $66$ G         1       a $72$ A         1       a $73$ A         1       a $78$ A         1       a $78$ A         1       a $91$ A         1       a $92$ G         1       a $10$ A         1       a	1	a	35	G
1       a       38       G         1       a       39       G         1       a       47       C         1       a       50       A         1       a       52       C         1       a       53       A         1       a       59       A         1       a       60       A         1       a       66       G         1       a       72       A         1       a       73       A         1       a       78       A         1       a       93       U         1       a       93       U         1       a       94       C         1       a       95       A         1       a       97       C         1       a       10       A         1       a       122       G         1       a       124       A         1       a       122       G         1       a       124       A         1       a       124       A	1	a	36	С
1       a       39       G         1       a       47       C         1       a       50       A         1       a       52       C         1       a       53       A         1       a       59       A         1       a       59       A         1       a       60       A         1       a       66       G         1       a       72       A         1       a       73       A         1       a       78       A         1       a       82       U         1       a       93       U         1       a       94       C         1       a       95       A         1       a       96       G         1       a       10       A         1       a       122       G         1       a       124       A         1       a       125       U         1       a       133       G         1       a       136       G	1	a	38	G
1       a       47       C         1       a       50       A         1       a       52       C         1       a       53       A         1       a       59       A         1       a       60       A         1       a       66       G         1       a       72       A         1       a       73       A         1       a       73       A         1       a       78       A         1       a       82       U         1       a       93       U         1       a       94       C         1       a       95       A         1       a       96       G         1       a       10       A         1       a       122       G         1       a       124       A         1       a       125       U         1       a       126       C         1       a       133       G         1       a       136       G	1	a	39	G
1a48C1a50A1a52C1a53A1a59A1a60A1a71U1a72A1a73A1a78A1a82U1a93U1a93U1a94C1a95A1a97C1a122G1a124A1a125U1a132G1a133G1a136G1a136G1a136G1a136G1a136G1a136G1a136G1a136G1a136G1a156A1a156A1a160G1a163C	1	a	47	С
1       a       50       A         1       a       53       A         1       a       59       A         1       a       60       A         1       a       66       G         1       a       71       U         1       a       72       A         1       a       73       A         1       a       78       A         1       a       78       A         1       a       82       U         1       a       93       U         1       a       94       C         1       a       95       A         1       a       96       G         1       a       15       U         1       a       122       G         1       a       125       U         1       a       126       C         1       a       133       G         1       a       136       G         1       a       136       G         1       a       136       G	1	a	48	С
1       a       52       C         1       a       53       A         1       a       59       A         1       a       60       A         1       a       66       G         1       a       71       U         1       a       72       A         1       a       73       A         1       a       78       A         1       a       78       A         1       a       82       U         1       a       91       A         1       a       93       U         1       a       94       C         1       a       95       A         1       a       96       G         1       a       10       A         1       a       122       G         1       a       125       U         1       a       125       U         1       a       133       G         1       a       136       G         1       a       136       G	1	a	50	А
1       a       53       A         1       a       59       A         1       a       60       A         1       a       66       G         1       a       71       U         1       a       72       A         1       a       73       A         1       a       78       A         1       a       82       U         1       a       91       A         1       a       93       U         1       a       94       C         1       a       95       A         1       a       95       A         1       a       96       G         1       a       10       A         1       a       122       G         1       a       125       U         1       a       126       C         1       a       133       G         1       a       136       G         1       a       136       G         1       a       156       A	1	a	52	С
1       a       59       A         1       a       60       A         1       a       66       G         1       a       71       U         1       a       72       A         1       a       73       A         1       a       73       A         1       a       78       A         1       a       82       U         1       a       93       U         1       a       93       U         1       a       93       U         1       a       94       C         1       a       95       A         1       a       95       A         1       a       96       G         1       a       110       A         1       a       115       U         1       a       122       G         1       a       125       U         1       a       132       G         1       a       133       G         1       a       136       G	1	a	53	А
1       a       60       A         1       a       76       G         1       a       71       U         1       a       72       A         1       a       73       A         1       a       73       A         1       a       78       A         1       a       82       U         1       a       88       U         1       a       93       U         1       a       94       C         1       a       95       A         1       a       96       G         1       a       97       C         1       a       110       A         1       a       122       G         1       a       124       A         1       a       125       U         1       a       132       G         1       a       133       G         1       a       136       G         1       a       136       G         1       a       156       A	1	a	59	А
1a $66$ G1a $71$ U1a $72$ A1a $73$ A1a $73$ A1a $78$ A1a $82$ U1a $82$ U1a $91$ A1a $91$ A1a $93$ U1a $94$ C1a $95$ A1a $96$ G1a $10$ A1a $122$ G1a $124$ A1a $125$ U1a $126$ C1a $133$ G1a $136$ G1a $156$ A1a $156$ A1a $157$ C1a $163$ C	1	a	60	А
1       a       71       U         1       a       72       A         1       a       73       A         1       a       78       A         1       a       78       A         1       a       78       A         1       a       82       U         1       a       82       U         1       a       91       A         1       a       93       U         1       a       93       U         1       a       94       C         1       a       95       A         1       a       96       G         1       a       10       A         1       a       115       U         1       a       122       G         1       a       125       U         1       a       132       G         1       a       133       G         1       a       136       G         1       a       136       A         1       a       156       A	1	a	66	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	71	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	72	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	73	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	78	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	82	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	88	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	91	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	93	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	94	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	95	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	96	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	97	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	110	А
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	1	a	115	U
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	122	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	124	А
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	125	U
1     a     132     G       1     a     133     G       1     a     136     G       1     a     140     G       1     a     156     A       1     a     157     C       1     a     160     G       1     a     163     C	1	a	126	С
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	132	G
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	133	G
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	136	G
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	140	G
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	a	156	A
1         a         160         G           1         a         163         C	1	a	157	С
1 a 163 C	1	a	160	G
	1	a	163	С



Mol	Chain	Res	Type
1	a	167	U
1	a	171	G
1	a	176	С
1	a	177	G
1	a	178	U
1	a	182	G
1	a	183	А
1	a	184	G
1	a	185	G
1	a	186	G
1	a	191	А
1	a	197	G
1	a	198	G
1	a	199	A
1	a	201	С
1	a	202	U
1	a	204	С
1	a	205	G
1	a	206	G
1	a	214	G
1	a	227	С
1	a	239	U
1	a	241	G
1	a	245	G
1	a	248	G
1	a	250	U
1	a	252	G
1	a	256	А
1	a	260	G
1	a	261	С
1	a	266	С
1	a	274	С
1	a	275	G
1	a	283	A
1	a	287	G
1	a	292	A
1	a	299	G
1	a	300	A
1	a	310	С
1	a	312	G
1	a	314	A
1	a	315	A



Mol	Chain	Res	Type
1	a	322	С
1	a	323	А
1	a	325	G
1	a	326	G
1	a	338	А
1	a	339	С
1	a	340	G
1	a	341	G
1	a	342	G
1	a	346	C
1	a	347	А
1	a	348	G
1	a	352	U
1	a	353	G
1	a	357	А
1	a	361	U
1	a	362	U
1	a	363	G
1	a	366	С
1	a	370	G
1	a	373	С
1	a	375	A
1	a	378	G
1	a	379	С
1	a	382	G
1	a	384	U
1	a	386	C
1	a	387	А
1	a	388	G
1	a	391	А
1	a	392	U
1	a	394	С
1	a	395	С
1	a	399	U
1	a	400	G
1	a	401	U
1	a	402	G
1	a	403	U
1	a	404	G
1	a	405	A
1	a	406	A
1	a	407	G



Mol	Chain	Res	Type
1	a	409	А
1	a	410	G
1	a	411	G
1	a	412	U
1	a	414	U
1	a	415	U
1	a	416	С
1	a	417	G
1	a	418	G
1	a	419	А
1	a	421	U
1	a	422	G
1	a	423	U
1	a	424	А
1	a	426	А
1	a	427	G
1	a	428	С
1	a	429	А
1	a	430	С
1	a	432	U
1	a	433	U
1	a	434	А
1	a	445	А
1	a	446	А
1	a	449	G
1	a	451	А
1	a	452	G
1	a	456	G
1	a	457	U
1	a	459	A
1	a	460	A
1	a	461	U
1	a	462	A
1	a	463	С
1	a	470	G
1	a	475	G
1	a	479	U
1	a	480	U
1	a	490	A
1	a	491	U
1	a	492	A
1	a	493	А



Mol	Chain	Res	Type
1	a	500	G
1	a	501	С
1	a	502	U
1	a	503	A
1	a	504	A
1	a	505	С
1	a	506	U
1	a	512	С
1	a	513	С
1	a	519	С
1	a	521	G
1	a	525	U
1	a	526	A
1	a	527	A
1	a	528	U
1	a	530	C
1	a	533	А
1	a	534	G
1	a	535	G
1	a	536	G
1	a	537	U
1	a	538	G
1	a	539	С
1	a	541	А
1	a	542	G
1	a	546	U
1	a	552	G
1	a	553	А
1	a	556	U
1	a	558	С
1	a	560	G
1	a	566	A
1	a	567	A
1	a	570	C
1	a	571	G
1	a	573	G
1	a	575	G
1	a	576	U
1	a	601	А
1	a	602	A
1	a	612	С
1	a	613	U



Mol	Chain	Res	Type
1	a	614	С
1	a	627	G
1	a	635	А
1	a	636	A
1	a	643	A
1	a	647	A
1	a	650	G
1	a	654	G
1	a	656	U
1	a	659	А
1	a	660	G
1	a	664	G
1	a	675	С
1	a	676	U
1	a	677	G
1	a	678	U
1	a	679	G
1	a	680	U
1	a	681	А
1	a	682	G
1	a	683	С
1	a	684	G
1	a	685	G
1	a	687	G
1	a	688	A
1	a	689	A
1	a	691	U
1	a	692	G
1	a	693	С
1	a	694	G
1	a	695	U
1	a	696	А
1	a	698	A
1	a	700	А
1	a	701	U
1	a	702	A
1	a	703	G
1	a	708	G
1	a	709	A
1	a	710	A
1	a	711	С
1	a	712	А



Mol	Chain	Res	Type
1	a	714	С
1	a	715	А
1	a	717	U
1	a	718	G
1	a	727	G
1	a	741	А
1	a	749	A
1	a	753	A
1	a	754	G
1	a	755	G
1	a	757	G
1	a	759	G
1	a	760	A
1	a	763	G
1	a	765	G
1	a	771	A
1	a	775	A
1	a	776	A
1	a	778	A
1	a	779	G
1	a	787	U
1	a	788	A
1	a	792	U
1	a	795	U
1	a	808	А
1	a	809	A
1	a	810	A
1	a	811	C
1	a	815	G
1	a	822	А
1	a	830	G
1	a	835	С
1	a	838	G
1	a	839	А
1	a	840	G
1	a	843	С
1	a	847	G
1	a	858	A
1	a	861	G
1	a	864	A
1	a	865	U
1	a	866	А



1         a         868         G           1         a         870         C           1         a         878         U           1         a         879         G           1         a         881         C	
1         a         870         C           1         a         878         U           1         a         879         G           1         a         881         C	
1         a         878         U           1         a         879         G           1         a         881         C	
1 a 879 G	
1 a 881 C	
1 a 883 A	
1 a 884 G	
1 a 885 U	
1 a 886 A	
1 a 894 A	
1 a 896 G	
1 a 902 A	
1 a 906 C	
1 a 908 A	
1 a 909 A	
1 a 913 A	
1 a 916 G	
1 a 921 G	
1 a 928 C	
1 a 929 A	
1 a 931 A	
1 a 932 A	
1 a 933 G	
1 a 934 C	
1 a 935 G	
1 a 937 U	
1 a 938 G	
1 a 939 G	
1 a 940 A	
1 a 941 G	
1 a 942 C	
1 a 943 A	
1 a 945 G	
1 a 946 U	
1 a 953 A	
1 a 954 U	
1 a 956 C	
1 a 957 G	
1 a 958 A	
1 a 959 A	
1 a 960 G	
1 a 961 C	



Mol	Chain	Res	Type
1	a	962	А
1	a	963	А
1	a	964	С
1	a	965	G
1	a	966	С
1	a	967	G
1	a	968	А
1	a	969	А
1	a	970	G
1	a	971	А
1	a	972	А
1	a	973	С
1	a	974	С
1	a	975	U
1	a	976	U
1	a	977	А
1	a	978	С
1	a	979	С
1	a	981	G
1	a	982	G
1	a	983	С
1	a	984	С
1	a	985	U
1	a	986	U
1	a	987	G
1	a	988	А
1	a	989	С
1	a	990	А
1	a	998	А
1	a	1002	U
1	a	1004	С
1	a	1005	С
1	a	1007	G
1	a	1008	А
1	a	1009	G
1	a	1011	U
1	a	1012	G
1	a	1013	G
1	a	1014	A
1	a	1015	U
1	a	1017	G
1	a	1019	U



Mol	Chain	Res	Type
1	a	1020	G
1	a	1023	U
1	a	1025	С
1	a	1026	G
1	a	1030	А
1	a	1032	U
1	a	1036	А
1	a	1038	А
1	a	1039	С
1	a	1040	А
1	a	1043	U
1	a	1044	G
1	a	1047	G
1	a	1048	С
1	a	1049	А
1	a	1050	U
1	a	1051	G
1	a	1052	G
1	a	1054	U
1	a	1055	G
1	a	1056	U
1	a	1057	С
1	a	1058	G
1	a	1060	С
1	a	1062	G
1	a	1063	С
1	a	1075	G
1	a	1077	U
1	a	1078	G
1	a	1079	U
1	a	1082	G
1	a	1088	G
1	a	1089	U
1	a	1090	С
1	a	1095	А
1	a	1101	С
1	a	1102	G
1	a	1104	А
1	a	1105	A
1	a	1106	С
1	a	1108	С
1	a	1110	U



Mol	Chain	Res Type	
1	a	1111	G
1	a	1112	U
1	a	1113	С
1	a	1115	U
1	a	1116	U
1	a	1117	А
1	a	1118	G
1	a	1119	U
1	a	1120	U
1	a	1121	А
1	a	1122	С
1	a	1123	С
1	a	1125	G
1	a	1126	С
1	a	1127	А
1	a	1129	С
1	a	1130	U
1	a	1132	G
1	a	1133	G
1	a	1134	G
1	a	1135	U
1	a	1137	G
1	a	1139	С
1	a	1140	А
1	a	1141	С
1	a	1142	U
1	a	1143	С
1	a	1145	А
1	a	1146	А
1	a	$1\overline{149}$	A
1	a	1150	G
1	a	1151	A
1	a	1152	С
1	a	1153	U
1	a	1154	G
1	a	1155	С
1	a	1162	С
1	a	1163	A
1	a	1164	A
1	a	1170	A
1	a	1171	G
1	a	1172	G



Mol	Chain	Res	Type
1	a	1173	А
1	a	1174	А
1	a	1175	G
1	a	1176	G
1	a	1177	U
1	a	1178	G
1	a	1179	G
1	a	1180	G
1	a	1181	G
1	a	1182	А
1	a	1183	U
1	a	1184	G
1	a	1185	A
1	a	1188	U
1	a	1189	C
1	a	1190	A
1	a	1191	A
1	a	1192	G
1	a	1194	С
1	a	1195	А
1	a	1196	U
1	a	1197	С
1	a	1199	U
1	a	1200	G
1	a	1201	G
1	a	1205	U
1	a	1206	U
1	a	1207	А
1	a	1208	С
1	a	1209	G
1	a	1210	G
1	a	1211	С
1	a	1212	С
1	a	1213	A
1	a	1214	G
1	a	1217	С
1	a	1218	U
1	a	1219	A
1	a	1221	A
1	a	1223	A
1	a	1225	G
1	a	1226	U



Mol	Chain	Res Type	
1	a	1227	G
1	a	1228	С
1	a	1229	U
1	a	1230	А
1	a	1231	С
1	a	1232	А
1	a	1233	А
1	a	1234	U
1	a	1235	G
1	a	1236	G
1	a	1237	U
1	a	1238	С
1	a	1239	G
1	a	1240	G
1	a	1242	А
1	a	1244	А
1	a	1245	А
1	a	1246	А
1	a	1247	G
1	a	1250	U
1	a	1251	U
1	a	1252	G
1	a	1254	С
1	a	1255	А
1	a	1257	G
1	a	1258	С
1	a	1259	С
1	a	1260	G
1	a	1262	G
1	a	1263	А
1	a	1264	G
1	a	1265	G
1	a	1266	U
1	a	1267	G
1	a	1268	G
1	a	1273	A
1	a	1274	A
1	a	1275	U
1	a	1276	С
1	a	1277	С
1	a	1279	A
1	a	1281	A



Mol	Chain	Res Type	
1	a	1282	А
1	a	1285	С
1	a	1286	С
1	a	1287	G
1	a	1289	U
1	a	1291	G
1	a	1292	U
1	a	1293	А
1	a	1294	G
1	a	1295	U
1	a	1296	С
1	a	1297	С
1	a	1298	G
1	a	1299	G
1	a	1300	А
1	a	1301	U
1	a	1302	С
1	a	1303	G
1	a	1304	С
1	a	1305	А
1	a	1307	U
1	a	1308	С
1	a	1309	U
1	a	1310	G
1	a	1311	С
1	a	1312	А
1	a	1313	А
1	a	1314	С
1	a	1315	U
1	a	1316	С
1	a	1317	G
1	a	1318	A
1	a	1319	С
1	a	1320	U
1	a	1321	G
1	a	1323	G
1	a	1324	U
1	a	1325	G
1	a	1327	A
1	a	1330	C
1	a	1331	G
1	a	1332	G



Mol	Chain	Res	Type
1	a	1333	А
1	a	1334	А
1	a	1336	С
1	a	1337	G
1	a	1338	С
1	a	1339	U
1	a	1340	А
1	a	1341	G
1	a	1342	U
1	a	1344	А
1	a	1345	U
1	a	1346	С
1	a	1347	G
1	a	1348	U
1	a	1349	G
1	a	1351	А
1	a	1352	U
1	a	1353	С
1	a	1354	А
1	a	1355	G
1	a	1356	А
1	a	1357	А
1	a	1358	U
1	a	1359	G
1	a	1361	С
1	a	1362	А
1	a	1363	С
1	a	1364	G
1	a	1365	G
1	a	1366	U
1	a	1367	G
1	a	1368	A
1	a	1369	А
1	a	1370	U
1	a	1371	A
1	a	1372	С
1	a	1373	G
1	a	1374	U
1	a	1375	U
1	a	1378	С
1	a	1379	G
1	a	1380	G



Mol	Chain	Res	Type
1	a	1382	С
1	a	1388	А
1	a	1392	А
1	a	1394	С
1	a	1395	G
1	a	1398	С
1	a	1404	А
1	a	1405	С
1	a	1413	G
1	a	1420	G
1	a	1428	А
1	a	1432	G
1	a	1435	А
1	a	1436	G
1	a	1438	С
1	a	1439	U
1	a	1440	А
1	a	1441	А
1	a	1445	С
1	a	1446	А
1	a	1447	А
1	a	1448	G
1	a	1454	С
1	a	1455	G
1	a	1458	U
1	a	1461	С
1	a	1466	А
1	a	1469	G
1	a	1471	U
1	a	1481	G
1	a	1486	А
1	a	1487	А
1	a	1488	G
1	a	1497	A
1	a	1500	U
1	a	1502	G
1	a	1511	G
1	a	1513	A
1	a	1514	С
1	a	1515	С
1	a	1522	U
1	a	1523	G



 $Continued \ from \ previous \ page...$ 

Mol	Chain	Res	Type
1	a	1524	G
1	а	1525	А
1	а	1526	U

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

# 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	а	4
2	b	1
13	m	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	2:A	O3'	7:A	Р	21.37
1	a	63:C	O3'	65:A	Р	7.46
1	b	124:GLY	С	130:THR	Ν	5.42
1	m	20:THR	С	22:ILE	Ν	3.27



	J $I$	I J				
Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1376:C	O3'	1377:C	Р	3.24
1	a	53:A	O3'	55:A	Р	3.13



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10281. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

## 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



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

## 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 200

Y Index: 200



Z 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: 218

Y Index: 207

Z Index: 268

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 0.00936. 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 868  $\rm nm^3;$  this corresponds to an approximate mass of 784 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 0.339  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

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



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10281 and PDB model 6SPC. Per-residue inclusion information can be found in section 3 on page 9.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.00936 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 (0.00936).



### 9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 91% 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 (0.00936) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9146	0.4440
a	0.9445	0.4710
b	0.9769	0.5140
с	0.5423	0.1890
d	0.9276	0.4220
е	0.9729	0.5630
f	0.9820	0.5190
g	0.8147	0.3130
h	0.8831	0.4250
i	0.8249	0.1150
j	0.7151	0.2080
k	0.9679	0.4590
1	0.9406	0.5120
m	0.7197	0.1780
n	0.6121	0.2090
0	0.9955	0.5860
р	0.9880	0.5980
q	0.9766	0.5740
r	0.9860	0.5670
S	0.7617	0.2050
t	0.9890	0.5810
u	0.7283	0.4130

