

Mar 10, 2024 – 11:47 AM EDT

PDB ID	:	6OIG
EMDB ID	:	EMD-20077
Title	:	Subunit joining exposes nascent pre-40S rRNA for processing and quality con-
		trol
Authors	:	Rai, J.; Parker, M.D.; Ghalei, H.; Johnson, M.C.; Karbstein, K.; Stroupe,
		M.E.
Deposited on	:	2019-04-09
Resolution	:	3.80 Å(reported)
This is		wwPDB FM Validation Report for a publicly released PDB entry

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

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

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

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

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	EM structures (#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	Z	204	28%	8%
2	А	252	98%	•
3	В	386	98%	•
4	С	361	95%	5%•
5	D	296	• 99%	
6	Е	175	86%	• 11%
7	F	222	97%	·
8	G	233	98%	·



Continued from previous page... Chain Length Quality of chain Mol i 9 Η 19196% • İ. 10 Ι 220• 92% • 11 J 169. . 97% 10% •• 12 \mathbf{S} 15594% i 13L 193. . 95% 14М 13699% . 25% Ν 1520398% • 16Ο 197. 99% Р 183 17••• 98% 18Q 18597% • 19% 19R 18895% 5% \mathbf{S} 20172... 98% i. 21Т 15996% • 22U 10099% • V 2313699% 53% 24W 1355% 95% Х 25121• 97% ÷ Y 126268% 92% 27Ζ 135• 98% i. 28148 \mathbf{a} 95% 5% 29 \mathbf{b} 5890% 10% 30 97 ... \mathbf{c} 98% 31 109d 100% 32127е 97% • 33 f 106 5% 95%



Mol	Chain	Length		Quality of chain							
34	g	112	•	98%	••						
35	h	119		98%	•						
36	i	99	•	97%	•						
37	j	87	ė	93%	7%						
38	k	77	•	97%							
39	1	50		94%							
40	m	52	98%								
41	0	105	•								
42	р	91	•	98%	••						
43	q	219	19%		35%						
44	5	3394	36%	45%	15% •						
45	8	158	28%	55%	16%						
46	7	121	41%	49%	10%						
47	x	47	51%	100%							
48	у	46	74	1%							



2 Entry composition (i)

There are 48 unique types of molecules in this entry. The entry contains 129140 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues		Ate		AltConf	Trace		
1	Z	204	Total 1602	C 1026	N 277	O 290	S 9	0	0

• Molecule 2 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues		At	AltConf	Trace			
2	А	252	Total 1918	C 1193	N 389	O 335	S 1	0	0

• Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues		Ate	AltConf	Trace			
3	В	386	Total 3082	C 1956	N 584	0 534	S 8	0	0

• Molecule 4 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues		Ate	AltConf	Trace			
4	С	361	Total 2750	C 1730	N 522	0 495	${ m S} { m 3}$	0	0

• Molecule 5 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	296	Total 2376	C 1501	N 414	0 459	${ m S} { m 2}$	0	0

• Molecule 6 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
6	Е	156	Total 1240	C 800	N 222	0 217	S 1	0	0



• Molecule 7 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues		Ate	AltConf	Trace			
7	F	222	Total 1785	C 1151	N 324	O 309	S 1	0	0

• Molecule 8 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues		Ate		AltConf	Trace		
8	G	233	Total 1818	C 1159	N 326	O 330	${ m S} { m 3}$	0	0

• Molecule 9 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
9	Н	191	Total 1519	C 963	N 274	0 278	$\frac{S}{4}$	0	0

• Molecule 10 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues		Ate	AltConf	Trace			
10	Ι	211	Total 1718	C 1089	N 325	O 298	S 6	0	0

• Molecule 11 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues		At	oms		AltConf	Trace	
11	J	169	Total 1354	C 847	N 253	O 250	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 12 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
12	S	150	Total 737	C 437	N 150	O 150	0	0

• Molecule 13 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
13	L	193	Total 1543	C 962	N 315	O 266	0	0

• Molecule 14 is a protein called 60S ribosomal protein L14-A.



Mol	Chain	Residues		At	oms			AltConf	Trace
14	М	136	Total 1054	C 675	N 199	0 178	S 2	0	0

• Molecule 15 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues		Ate	AltConf	Trace			
15	N	203	Total 1721	C 1077	N 361	O 282	S 1	0	0

• Molecule 16 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues		Ate	AltConf	Trace			
16	0	197	Total 1556	C 1003	N 289	O 263	S 1	0	0

• Molecule 17 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
17	D	192	Total	С	Ν	Ο	0	0
11	1	165	1443	896	287	260	0	0

• Molecule 18 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	Q	185	Total 1442	C 908	N 290	O 242	S 2	0	0

• Molecule 19 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
19	R	188	Total 1522	C 935	N 326	O 261	0	0

• Molecule 20 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues		At	AltConf	Trace			
20	S	172	Total 1446	C 930	N 267	0 245	${S \atop 4}$	0	0

• Molecule 21 is a protein called 60S ribosomal protein L21-A.



Mol	Chain	Residues		At	oms			AltConf	Trace
21	Т	159	Total 1277	C 805	N 246	O 222	$\frac{S}{4}$	0	0

• Molecule 22 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
22	U	100	Total 796	C 516	N 131	0 149	0	0

• Molecule 23 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues		At	AltConf	Trace			
23	V	136	Total 1004	C 628	N 189	0 180	${f S}{7}$	0	0

• Molecule 24 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
24	W	135	Total 1089	C 682	N 219	0 187	S 1	0	0

• Molecule 25 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	Х	121	Total 969	C 623	N 170	0 174	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 26 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace	
26	Y	126	Total 994	C 625	N 192	O 177	0	0

• Molecule 27 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
27	Ζ	135	Total 1093	C 710	N 202	O 181	0	0

• Molecule 28 is a protein called 60S ribosomal protein L28.



Mol	Chain	Residues		At	oms			AltConf	Trace
28	a	148	Total 1174	C 749	N 231	O 191	${ m S} { m 3}$	0	0

• Molecule 29 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues		Ator	ns	AltConf	Trace	
29	b	58	Total 463	C 289	N 100	О 74	0	0

• Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	с	97	Total 743	C 479	N 124	0 139	S 1	0	0

• Molecule 31 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues		At	oms			AltConf	Trace
31	d	109	Total 890	C 565	N 168	0 156	S 1	0	0

• Molecule 32 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues		At	oms	AltConf	Trace		
32	е	127	Total 1020	C 647	N 205	O 167	S 1	0	0

• Molecule 33 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
33	f	106	Total 851	$\begin{array}{c} \mathrm{C} \\ 540 \end{array}$	N 165	0 145	S 1	0	0

• Molecule 34 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
34	g	112	Total 881	C 546	N 179	0 152	${S \atop 4}$	0	0

• Molecule 35 is a protein called 60S ribosomal protein L35-A.



Mol	Chain	Residues		At	oms	AltConf	Trace		
35	h	119	Total 970	C 615	N 186	0 168	S 1	0	0

• Molecule 36 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
36	i	99	Total 772	C 481	N 156	0 133	${ m S} { m 2}$	0	0

• Molecule 37 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues		At	AltConf	Trace			
37	j	87	Total 682	C 414	N 148	0 115	${ m S}{ m 5}$	0	0

• Molecule 38 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
38	k	77	Total 613	C 391	N 115	O 107	0	0

• Molecule 39 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
39	1	50	Total 437	С 272	N 97	O 66	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 40 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
40	m	52	Total	С	Ν	0	S	0	0
40	111	52	418	259	86	68	5	0	0

• Molecule 41 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues		At	AltConf	Trace			
41	О	105	Total 848	C 534	N 170	0 139	${f S}{5}$	0	0

• Molecule 42 is a protein called 60S ribosomal protein L43-A.



Mol	Chain	Residues		At	oms	AltConf	Trace		
42	р	91	Total 695	C 429	N 138	0 122	S 6	0	0

• Molecule 43 is a protein called 60S acidic ribosomal protein P0,60S acidic ribosomal protein P0,AO, L1OE.

Mol	Chain	Residues		At	oms	Atoms					
43	q	143	Total 1077	C 687	N 192	O 195	${ m S} { m 3}$	0	0		

• Molecule 44 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	5	3243	Total 69359	C 30981	N 12493	O 22643	Р 3242	0	0

• Molecule 45 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
45	8	158	Total 3354	C 1500	N 586	O 1110	Р 158	0	0

• Molecule 46 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
46	7	121	Total 2580	C 1152	N 461	0 846	Р 121	0	0

• Molecule 47 is a protein called P1.

Mol	Chain	Residues		Aton	ıs		AltConf	Trace
47	х	47	Total 235	C 141	N 47	O 47	0	0

• Molecule 48 is a protein called P2.

Mol	Chain	Residues		Aton	ns		AltConf	Trace
48	У	46	Total 230	C 138	N 46	O 46	0	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: 60S ribosomal protein L1-A





• Molecule 6: 60S ribosomal protein L6-A

Chain E:	86%	• 11%
226 A227 P231 R255 E283 V303	E333 LYS LYS LYS LYS LYS CLU CYS CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	
• Molecule 7:	60S ribosomal protein L7-A	
Chain F:	97%	•
A233 1302 1366 1366 1366 1368 1369 1370 1426		
• Molecule 8:	60S ribosomal protein L8-A	
Chain G:	98%	
N188 R221 A240 K286 K286 R368	₩ <mark>450</mark>	
• Molecule 9:	60S ribosomal protein L9-A	
Chain H:	96%	•
M201 Y203 S222 S222 R265 R265	N316 N357 A358 A388 A358 A358 A A358 A A A A A A A A A A A A A	
• Molecule 10:	60S ribosomal protein L10	
Chain I:	92%	
A187 R192 R209 A249	N254 N254 N287 N287 N287 SER SER CYS SER CYS ASP ASP	
• Molecule 11:	60S ribosomal protein L11-B	
Chain J:	97%	••
Q97 R101 D102 R183 R183 R183 R192		

• Molecule 12: 60S ribosomal protein L12-A



Chain s:	0.40/	_
◆ ◆ ◆ ◆	94%	•••
E146 G160 ALA ALA ALA K165 K165	P171 L172 C173 C173 P176 P176 P176 P16 P16 P16 P16 P260 P260 P260 P260 P260 P260 P260 P26	
• Molecule 13: 60	0S ribosomal protein L13-A	
Chain L:	95%	•••
A2 A47 L54 T62 T62 T62	110-4 11152 11152 11152	
• Molecule 14: 6	0S ribosomal protein L14-A	
Chain M:	99%	
T152 K157 U161 L214 K276		
• Molecule 15: 60	0S ribosomal protein L15-A	
Chain N:	98%	. .
C2 E29 652 652 763 763 764 763 764	K72 479 479 479 486 479 486 4985 897 4985 897 4985 8118 8118 8118 8118 8118 8113 8113 81	A141 A141 A146 A146 A146 A147 Y148 M150 H156 A151 A159
R162 4 1167	N182 + R187 + R187 + R193 - R193 - R193 - R193 - R193 - R195 - R199 - R199 - R203 - R203 - R204 - R2	
• Molecule 16: 60	0S ribosomal protein L16-A	
Chain O:	99%	.
V3 A24 R59 R117 Y199		
• Molecule 17: 60	0S ribosomal protein L17-A	
Chain P:	98%	
A2 830 6103 A104 A156 A156 A156	K154 A184 A184	
• Molecule 18: 60	0S ribosomal protein L18-A	
Chain Q:	97%	·

PROT

R L D W I D E PDB TEIN DATA BANK

G127 Q134 K145 K145 F231 F231 F231 F231 Y311

 \bullet Molecule 19: 60S ribosomal protein L19-A

19%			
Chain R:	95%	5%	
A137 N174 R177 R220 R220 R239 C264 N265 N266	Q285 R286 E292 E293 A294 E295 A296 R298 R298 R298 R298 R298 R299 R300 R301 R301 R303 R304 R303	R307 R309 A309 A309 Q310 R311 V312 A313 R315 R315 R315 R315 R315 A315 A313 C319 C319 C319 C319 C319 C320	A324
• Molecule 20: 60S	ribosomal protein L20-A		
Chain S:	98%		
M12 R13 P22 F163 V172			
• Molecule 21: 60S	ribosomal protein L21-A		
Chain T:	96%		•
G2 R17 R12 R92 A115 A119 ↓126 Q127 L128	R139		
• Molecule 22: 60S	ribosomal protein L22-A		
Chain U:	99%		
Q88 R89 ¥183 ¥187			
• Molecule 23: 60S	ribosomal protein L23-A		
Chain V:	99%		
s131 6132 6133 6134 A135 0136 A135 0136 C132 S173	N267		
• Molecule 24: 60S	ribosomal protein L24-A		
Chain W:	53% 95%	5%	<i>∕</i> ₀
M146 S171 K189 K206 6207 1208 V212	A213 K216 R216 S217 S217 Y219 Y221 Y220 A223 A223 P226 T220 T220 C225 A223 A223 A223 A223 A223	S231 4 L232 4 D233 4 L234 4 L234 6 L234 6 S240 6 S240 6 S240 6 R238 8 R238 8 R238 6 R234 6 F241 6 F243 6 F243 6 F244 6 F246 6 F246 6 F246 6 F246 6 F246 6 F246 6 F246 6 F246 6 F246 6 F2	V245 + R246 + R246 + R246 + R246 + R247 + R247 + R248 + R250 + R250 + E251 + E252 + R256 + R256 + R256 + R256 + R256 + R258 + R256 + R258 + R2



K261 K262 K262 F264 K265 K265 K266 K266 K266 K270 K272 K274 K276 K277 K	8275 A276 G277 Q279 Q279 S280	
• Molecule 25: 60S ribos	somal protein L25	
Chain X:	97%	·
K136 R147 Q179 Q179 Q268 Y755 I256		
• Molecule 26: 60S ribos	somal protein L26-A	
Chain Y:	92%	8%
A2 810 011 812 810 812 825 825 825 825 825 825 825 825 825 82	D114 K125 L126 E127	
• Molecule 27: 60S ribos	somal protein L27-A	
Chain Z:	98%	·
A1 V13 S32 F135 F135		
• Molecule 28: 60S ribos	somal protein L28	
Chain a:	95%	5%
883 884 885 M15 H120 H120 H121 H121 H121 H121 H121 C197 C197 C197 C197		
• Molecule 29: 60S ribos	somal protein L29	
Chain b:	90%	10%
A68 H83 H84 H84 H84 H84 H84 H85 H84 H89 H116 H116 H116 H116 H116		
• Molecule 30: 60S ribos	somal protein L30	
Chain c:	98%	••
S9 116 116 1105 ◆		

 \bullet Molecule 31: 60S ribosomal protein L31-A



Chain d:	100%	
L62 N114		
• Molecule 32: 60S ribos	somal protein L32	
Chain e:	97%	.
A153	6 <i>12</i> 71	
• Molecule 33: 60S ribos	somal protein L33-A	
Chain f:	95%	5%
A320 D368 A369 F361 F361 R391 N405 N424 1425		
• Molecule 34: 60S ribos	somal protein L34-A	
Chain g:	98%	
Q 2 2 4 2 4 1 5 4 6 3 4 6 3 4 6 3 4 1 3 8 4 8 13		
• Molecule 35: 60S ribos	somal protein L35-A	
Chain h:	98%	
A2 K49 A120		
• Molecule 36: 60S ribos	somal protein L36-A	
Chain i:	97%	·
128 836 157 118 1000		
• Molecule 37: 60S ribos	somal protein L37-A	
Chain j:	93%	7%
8 <mark>2 7 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 </mark>		
688 888 888 888 888 888 888 888 888 888		
	PROTEIN DATA BANK	

• Molecule 38: 60S ribos	somal protein L38	
Chain k:	97%	
A2 R1 6 L78		
• Molecule 39: 60S ribos	somal protein L39	
Chain l:	94%	6%
A2 K6 N43 151		
• Molecule 40: Ubiquitir	n-60S ribosomal protein L40	
Chain m:	98%	.
177 185 1128 1128		
• Molecule 41: 60S ribos	somal protein L42-A	
Chain o:	99%	
V2 C12 0105		
• Molecule 42: 60S ribos	somal protein L43-A	
Chain p:	98%	
A2 Y17 A92		
• Molecule 43: 60S acidi	c ribosomal protein P0,60S acidic ribo	somal protein P0,AO, L1OE
Chain q:	63% · 3	5%
G3 E10 Y11 S24 N32 L55 M53 C54 M53 C54 C54	S68 K77 K77 F78 F78 F78 F78 F78 F78 F78 F78 F78 F	GLU GLU ASP ASP VAL ARG ALA ASA ASA ASA ASA ASA ASA ASA ASA ASA
SER PHE PHE PHE LEU ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	111E VAL VAL VAL VAL VAL VAL VAL ASP ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	PR0 PHE C1184 C1185 C1186 C1186 C1185 C1185 C1185 C1185 C1185 C1190 C1190 C1192 C1192 C1192 C1192 C1192 C1193 C119



 \bullet Molecule 44: 25S ribosomal RNA

Chain 5:	36%	45%	15% •
<mark>U3</mark> G5 C4 C8 C8 U9	C10 A12 A13 A13 A14 A14 A14 A14 A14 A24 A23 A23 A23 A23 A23 A23 A23 A23 A23 A23	G30 G31 C31 C35 C35 A40 C42 C42 C42 C42 C42 C42 C42 C42 C42 C42	G53 G54 G55 G55 G55 G55 G58 A 61 A 61 A 61 A 61 A 65 A 65 A 65 A 65 A 65 A 65 A 65 A 65
C68 C69 A70 A71 C72 C73 C73	A77 U78 U78 U79 C82 U83 U83 C89 C91 C93 C93 C93 C94 C94 C94 C94 C97 C97 C97 C94 C94 C97 C97 C97 C97 C97 C97 C97 C97 C97 C97	C102 C103 C103 C104 C104 A109 A109 C110 C111 A116 A116 A116 U112 A116 U112 U112 U112 A116 U112 A116 U117 A116 A116 A116 A116 A116 A116 A116 A	M122 M123 U124 U126 U126 U128 U128 U128 U128 U133 U133 U133 U133 U133 U133 U133 U13
G137 U138 G139 C140 C141 C141 C142 C142 G143	A144 A145 C145 C145 C146 C146 A160 C156 C156 C156 C156 C156 C156 C156 C156	6162 A164 A164 A164 A165 C166 0168 0168 0170 0177 0177 0177 0177 0177 0177 017	0182 0184 0184 0188 0188 0188 0188 0188 0188
A199 C200 A201 G202 G203 A204	C205 C205 C206 C208 C208 C210 C211 C210 C214 C214 C214 C214 C214 C215 C214 C215 C216 C215 C216 C216 C216 C216 C216 C216 C216 C216	U223 0224 0224 0228 0228 0229 0229 0229 0229 0235 0235 0235 0235 0235 02241 02242 02242 02242 02242 02242 02242	C247 C247 U249 U249 U250 U255 A253 A253 A255 C255 C255 C256 C256
U261 U262 C263 A265 A265 A266 G267	A268 0270 0271 0271 0271 0274 0284 A286 A284 A286 A286 A286 A286 A286 A286	(1299) 1306 1306 1306 1308 1308 1308 1308 1308 1319 1319 1319 1319 1319 1319 1319 131	A325 A325 A325 A326 C330 C332 C333 A336 A336 A336 A336 A336 C333 A336 C339 C339 C339
C340 C341 A342 U343 A344 A344 C347	A348 A349 C3550 A351 A351 A355 C355 C355 C355 C355 C355 C355 C355	A374 A375 G375 G376 C379 U381 U382 A386 A386 A386 A386 A386 A386 A386 A386	6400 6401 A401 C403 C403 C403 C406 6406 A405 A408 A408 A408 A408 C411 C411 C412 C412 C412 C412 C412
6415 6420 6421 6422 6422	4427 4427 1428 1429 1430 4433 4433 4433 6433 6443 6443 6443 6	и 446 1447 1447 1449 1449 1449 1449 1449 1449	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
и А486 1489	0000 0000 0000 0000 0000 0000 0000 0000 0000	6515 6515 6515 6516 6516 6518 6518 4521 4522 4522 4522 4522 4522 4533 4533 4533	6535 0536 0536 0538 0539 0539 0539 0539 0539 0534 0544 0544 0544 0544 0546 0546 0546 054
4550 4551 4552 4552 4554 U555 U556	4557 4559 4559 4559 6564 4569 4568 4568 4578 6579 6579 6579 6579 4578 4578 4578 4578 4578 4578 4578 4578	G582 A585 A585 C586 C586 C586 C586 C586 C596 C596 C596 C596 C596 C596 C596 C59	6600 6610 6611 1613 0613 0614 0614 0614 0614 0614 0614 0618 0616 0618 0620 A622 A622 A622
G624 G625 U626 U627 A628 U629 A630	0631 0632 0638 0638 0644 0644 0644 0644 0644 0644 0644 064	A663 C654 C654 C654 C655 A655 A655 G658 C663 C663 A666 A665 A666 A666 A666 A666 A677 A666	U679 U680 U682 U682 U682 A691 A691 A692 A695 A695 A695 A695 A695 A695 A695
A699 C700 A705 A711 G712	7713 7715 7715 7716 7716 7717 7718 7718 7720 7720 7723 7725 7725 7725 7725 7725 7725 7725	C732 C733 C733 C734 A735 A735 G739 G739 G739 G740 C743 C743 C743 C743 C743 C752 C752 C752	UT56 UT56 CT58 CT58 CT58 UT64 UT64 UT64 UT64 UT64 UT66 UT64 UT66 UT67 UT66 UT70
U772 G773 G774 A775 U776 U777	77/3 77/3 77/3 77/3 77/5 77/5 77/5 77/5	6800 6800 6803 6803 6803 6813 6813 6813 6813 6813 6813 6833 683	6835 6835 6835 6835 6835 6835 6835 6835
U355 (3856 (3857 (3857 (3858 (3859 (3860 (3860	00000000000000000000000000000000000000	A884 A884 A886 A896 A997 A914 A914 A914 A915 A914 A915 A915 A917 A915 A917 A915 A917 A917 A917	C318 U319 A921 A921 A922 C923 C924 A926 A926 A926 A926 A926 A926 A926 A926
C938 U939 U943 C944 C945 U946	C949 1954 1955 1955 1955 1955 1955 1956 1956 1956	69.74 69.75 69.75 19.79 19.98 19.98 19.98 19.98 19.98 19.98 19.98 19.99 19.99 19.99 19.99 19.99 19.99 19.99 19.99 19.99 19.99 19.99 19.99 19.99 19.99 19.99 10.99	A998 A998 G999 G1001 G1001 A1002 A1003 U1004 A1009 G1010 A1001 G1011 G1012 G1012 G1012 G1012

U1014	U1015 C1016	C1017	G1019 G1020	G1021	G1024	A1025	A1026 A1027	U1028	G1029	C1032	U1033	01034 G1035	A1036	C1037 C1038	U1039	A1040	01042	C1043	C1045	A1046 A1047	A1048 C1049	01010	01056 A1057	U1058 C1059	U1060	A1061 A1062	G1063	A1065	G1066	C1069	U1071	G1072	01073 01074	A1075	C1076	01010 01028	U1081 U1082
G1083	A1084 A1085	C1086	01088 01088 01089		U1094	01095 01096	G1097 A1098	00014	A1103	A1105		01109 01110	-	G1113 11111	61115 G1115	G1116 61117	C1118	0	01124 01125	G1126 G1127	U1128	A1129 A1130	G1131	A1135	C1137		C1141	G1142 A1143	U1144 C1145		G1148 G1149	A1150	U1151 C1152	A1153	A1154	C1155 C1156	A1159
C1160	G1161 U1162	A1163 C1164	A1165	U1168	A1170	G1171 G1172	01173 61174	C1175	C1176 C1177	G1178	A1179	A1180 U1181	A1182	C1183	LOTTY	C1189	01191 01191	10	A1195 C1196	A1197 C1198	C1199	C1201	G1206	G1207	G1209	U1210 111211		01214 01215	C1216 A1217	U1218	01219 01220	A1221	G1222 A1223	C1224	A1225	G1226 C1227	C1228 G1229
G1230	A1231 C1232	G1233	01235 01236 01236	G1237	C1 239 C1 239	A1240 U1241	G1242	A1244	A1245 61246	U1247	C1248	G1249 G1250	A1251	A1252	C1254	C1255	C1257	U1258	A1260	G1261 G1262	A1263	U1265	G1266 U1267	G1268	01203 A1270	A1271		C17/9	A1278 C1279	C1280	G1281 G1282	C1283	C1284	41286 A1286	A1287	01788	C1292 U1293
A1294	G1295 C1296	C1297	01299 01299	A1301	A1303	A1304 U1305	G1306 C1307	A1308	U1309 61310	G1311	C1312	01315	C1316	A1317 A1318	G1319	C1320	U1322	G1323	01324 01325	C1328	U1329 A1320	N1331	A1332 C1333	U1334	00010	U1341		G1345 G1346	U1347 111348	G1349	A1350 U1351	A1352	U1353	A1355	U1356	G1358 C1358	C1359
A1363	<mark>C1364</mark> G1365	A1366	G1370 C1371	C1372	CLOTH	C1376	A1381	G1383	A1386	G1387		A1390 C1391	G1392	A1393	C1396	41300 41300	G1400	2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	01405	A1406 A1407	G1408	01410	C1411 G1412	G1413	G1417	A1418 A1A10	C1420	G1421 G1422	C1423 C1424	U1425	01426 01427	A1428	G1429 111430	G1431	C1432	A1433 G1434	A1435 U1436
C1437	G1440	G1441	A1446 C1447	U1448	G1450	C1451 A1452	111 AGG	A1456	U1457 111458	C1459	A1460	A1461 A1462	U1463	G1464	G1466	A1467	A1400 C1469	U1470	G1473	A1474 A1475	G1476	01479	G1480 A1481	A1482	01484	G1485	G1487	61488 A1489	C1492		C1496 C1497	A1498	C1499 C1500	U1501	C1502	A1503 A1504	C1508
_	U1511 U1512	G1513 G1514	1515 1516	517 517	19	53	24 25	26	27 28	Q.	32	22	36	0	43	44	<u>47</u>	48	10 10	51 52	53	55	56 57	220	60 09	61 67	233	22 22	20	- 00 0	"		0 0	74		78	80
<mark>C1581</mark>			D A C	5 <u>5</u> 5	G15	U15	A15	U15	C15		C15:	A153	G15	u U U	G15	G15.	G15	C15	C151	C15 G15	U15	015 U15	C15 A15	A 1	G15	G15 C15	C15	0156 G156	A156	0156 0156	U156	A157	U157 C157	C15	2	615 C15	C1E A1E
	C1582 A1583	01584		31590 G1	31592 G15	A1593 A1594 U15	01595 A15	C1597 U15	31598 C15	U1601	A1602 C15	A1603 31604 A153	A1605 G15	01606 11607	C1608 G15	G15	41619 G15	01620 C15	A1021 0150 01622 C150	G1623 C15 G1624 G15	A1625 U15		C1628 C15 U1629 A15	U1630 A1	A1632 G15 G15	C1633 G15 C1633 G15	C1034	A1638 G156	C1639 A156	U1641 U156	A1642 0156 A1643 0157	C1644 A157	01645 0157	A1647 C15	A1648	01649 615 31650 C15	01651 C16 31652 A15
1653	1657 C1582	01584 01584 01585	1661 11589 C	1663 G1590 G1	1666 G1592 G15	1667 A1593 A1594 U15	1671 U1595 A15		1675 G1598 C15 1676 G1598 C15	1677 U1601	A1602 C15:	1680 A1603 A1503 A153 A153	1683 A1605 G15	1684 U1606 C15		1687 G15.	1689 A1619 G15	1690 U1620 C15	1692 U1622 C15	1693 G1623 C15 1694 G1624 G1524	1695 A1625 U15	1697 U1627 U15	C1628 C15 1700 U1629 A15	1701 U1630 A1		1705 C1633 G15 1706 C1634 C15		1709 A1638 G156	1710 C1639 A156	1712 U1641 U156	1/13 A1642 U156 1714 A1643 U157	1715 C1644 A157	1716 U1645 U157 1717 C1646 C157	1718 A1647 C15	A1648	1/22 01049 G15 1723 G1650 C15	1724 01651 C15 1725 G1652 A15
726 G1653	727 C1582 728 C1657 A1583	729 C1 660 C1 686	20 C1000 C1000 C1000 C	33 C1663 G1590 G1 733 73 74 11	735 G1666 G1592 G16 100 G1666 G1592 G15	736 A1667 A1593 737 A1594 U15	C1671 U1595 A15	742 C1597 U15	G1675 G1598 C15 745 A1676 G1598 C15	746 G1677 U1601	747 A1602 C15	749 G1680 A1603 A1503 A150 749 G1604 A155	750 A1683 A1605 G15	751 U1684 U1606 753 C1685 II1607 C15	753 U1686 C1608 G15	754 U1687 G15.	756 U1689 A1619 G15	757 C1690 U1620 C15	759 U1692 U1622 C15	760 C1693 G1623 C15 761 U1694 G1624 G15	762 U1695 A1625 U15 763 A1606 11626 116	764 A1090 01020 010	765 C1628 C15 766 G1700 U1629 A15	767 C1701 U1630 A1	769 01/02 01/02 01631 016	770 U1705 C1633 G15 771 C1706 C1634 C15		7/3 C1/08 A1637 U156 774 C1709 A1638 G156	75 C1710 C1639 A156	77 G1712 U1641 U156	7/8 G1/13 A1642 U156 779 A1714 A1643 U157	780 A1715 C1644 A157	0157 01645 0157 284 11217 01646 0157	785 G1718 A1647 C15	A1648	78/ 01/22 01649 G15 788 A1723 G1650 C15	789 U1724 U1651 C16 790 C1725 G1652 A15
91 C1726 G1653	92 G1727 C1682 93 G1728 C1657 A1583	94 A1729 U1584 DE C1730 C1660 C1584	30 41731 C1661 41661 A 96 A1731 C1661 A A A	01212121111111111111111111111111111111		03 G1736 A1667 A1593 04 U1737 A1694 U15	05 C1671 U1595 A15 Die A1771 II1672 C1506 C15	OC A171 OLO 2 OLO	08 G1675 G1598 C15 30 C1776 A1676 G1598 C15	U1746 G1677 U1601	12 G1747 A1602 C15	13 G1/48 G1680 A1603 14 A1749 G1680 G1604 A155	15 A1750 A1683 A1605 G15	16 G1751 U1684 U1606 17 A1752 C1685 T1607 C15	16 01753 01686 01608 015	19 G1754 U1687 G15	20 01756 01669 A1619 G15	22 A1757 C1690 U1620 C15	23 010 010 010 010 010 010 010 010 010 01	25 A1760 C1693 G1623 C15 26 C1761 U1694 G1624 G15	C1762 U1695 A1625 U15 30 H1763 A1606 H1626 U15	29 01/05 A1090 01020 010 30 01764 A1697 01627 015	U1765 C16 C1628 C15 35 G1766 G1700 U1629 A15	36 C1767 C1701 U1630 A1	38 G1769 01702 01632 G15	39 G1770 U1705 C1633 G15 10 C1771 C1706 C1633 C15	10 01/11 01/00 01/00 01/00 010	42 C1//3 C1/08 A153/ U105 C1774 C1709 A1638 G156	46 G1775 C1710 C1639 A156 17 G1776 C1711 G1840 1156	48 U1777 G1712 U1641 U156	49 G1/78 G1/13 A1642 U156 50 C1779 A1714 A1643 U157	51 G1780 A1715 C1644 A157	U1716 U1645 U157 54 017284 01717 01646 0157	01785 G1718 A1647 C15	57 G1786 A1648	58 A1/6/ U1/22 U1049 G15 59 C1788 A1723 G1650 C15	G1789 U1724 U1661 C18 56 G1790 C1725 G1652 A18
7 C1791 C1726 G1653	8 C1792 G1727 C1682 9 C1793 G1728 C1667 A1683	G1794 A1729 U1584 U1584 U1584 U1584 U1584 U1584 U1584	2 01796 01700 0160 0160 01700 0	4 (1733 (1733 (1663 (1590 (1	G1735 G1666 G1592 G15	7 C1803 G1736 A1667 A1593 8 A1804 U1737 A1694 U1	9 C1805 1 C1671 U1595 A15 0 0.1806 0.1741 11.672 61.606 61.5	Image: Number of the state of the	2 G1808 G1675 G1598 C15 2 A1800 C1745 A1676 G1598 C15	4 N1009 01746 01677 U1601	G1812 G1747 A1602 C15	6 A1813 G1/48 G1680 A1603 A1503 A151 A151 A151 A151 A151 A151 A151 A15	8 U1815 A1750 A1683 A1605 G15	B A1816 G1751 U1684 U1606 1 C1817 A17E0 C1685 D1607 C15	U1818 01753 U1686 C1608 015	3 U1819 G1754 U1687 G15.	± 0.0220 0.1750 0.1960 0.1010 5 01821 01756 01689 A1619 G15	6 C1822 A1757 C1690 U1620 C15	A1023 U103 U1091 A1021 U10 3 U1824 C1759 U1692 U1622 C15	9 61825 A1760 C1693 61623 C15 0 C1826 C1761 U1694 C1624 C15	1 C1762 U1695 A1625 U15 C1900 11723 A1606 11626 114	4 G1830 U1764 A1697 U1627 U1627	U1765 U1765 C1628 C15 A1835 G1766 G1770 U1629 A15	7 C1836 C1767 C1701 U1630 A1	2 G1838 G1769 U1/02 G1632 G15	A1839 G1770 U1705 C1633 G15 C1721 C1706 C1633 C15 C1706 C1634 C15	1 01640 01772 01707 0100 01004 0100	2 A1842 C1//3 C1/08 A153/ U155 3 C1774 C1709 A1638 G156	4 C1846 G1775 C1710 C1639 A156 4 A1847 G1776 C1711 C1840 I1156	G1848 U1777 G1712 U1641 U156	/ C1849 G1/78 G1/13 A1642 U156 A1850 C1779 A1714 A1643 U157	0 G1851 G1780 A1715 C1644 A157	1 U157 U157 U157 U157 C1546 U157	2 01001 01/17 01/17 01010 01010	4 C1857 G1786 A1648 A1648	A1859 A1.87 U1.722 U1099 G15 A1859 C1788 A1723 G1650 C15	9 C186 G1790 C1725 C1652 A15
A1867 C1791 C1726 G1653	G1868 C1792 G1727 C1582 C1869 C1793 G1728 C1657 A1563	C1870 C1794 A1729 U1884 U188	0 0101 01100 01100 01100 01000 0 0 01172 011796 01731 01661 01680 0 111872 011727 11173 01660 01680 0	A1874 A160 C1733 C1663 C1590 C1 A1874 A160 C1733 C1663 C1590 C1 A1675 A160 C1734 C1564 C1590 C1	U1876 01736 01666 01592 016	01877 C1803 G1736 A1667 A1593 C1736 C1878 A1894 U15	A1879 C1805 C1671 U1695 A15 11880 A1906 A1741 11.672 C1506 C15	A1881 G1807 U1742 C1597 U15	G1882 G1808 G1675 G1598 C15 A1883 A1800 G17745 A1875 G1598 C15	A1884 A1876 C167 U1601	U1885 G1812 G1747 A1602 C151	A1886 A1813 G1/48 G1680 A1603 A1503 A1503 A1503 A1503 A1514 A15144 A1514 A15144 A1514 A1514 A1514 A1514 A1514 A1514 A1514 A15	U1888 U1815 A1750 A1683 A1605 G15	G1889 A1816 G1751 U1684 U1606 114800 G1817 A1752 G185 G15	U1818 01753 U1686 01608 015	A1893 U1819 G1754 U1687 G16 114000 114000 A1755 114600 A1610	A1895 U1821 C1756 U1689 A1619 C15	A1896 C1822 A1757 C1690 U1620 C15	G1898 U1824 C1759 U1692 U1622 C15	G1899 G1825 A1760 C1693 G1623 C15 A1900 C1826 C1761 U1694 G1624 G15	A1901 C1762 U1695 A1625 U15 C1990 11723 A1606 11626 U15	C1904 C1830 U1764 A1697 U1627 U15	G1905 U1765 C1628 C16 G1906 A1835 G1766 G1766 A15	C1907 C1836 C1767 C1701 U1630 A1	U1912 01838 01769 01/02 01631 A12	A1839 G1770 U1706 C1633 G15 11900 H1800 C1776 C1634 C15	41921 01640 01772 0170 0100 0100 0100 0100 0100 01	A1922 A1842 C1//3 C1/08 A163/ U15 C1923 C1774 C1709 A1638 G156	U1924 C1846 G1775 C1710 C1639 A156 11425 A1847 C1776 C1711 C1840 11166	C1926 G1848 U1777 G1712 U1641 U156	G1927 C1849 G1779 G1713 A1642 U156 A1850 C1779 A1714 A1643 U157	A1930 G1861 G1780 A1715 C1644 A157	U1931 U1931 U1645 U157 U157 U157 U157 U157 U157 U157 U15	A1933 01078 01718 01647 015	G1934 C1857 G1786 A1648	G1355 A1856 A1787 U1722 U1649 G15 A1859 C1788 A1723 G1650 C15	G1339 G1789 U1724 U1661 C18 G1940 C1866 G1790 C1725 G1652 A18
C1941 A1867 C1791 C1726 G1653	U1942 C1868 C1792 G1727 C1863 C1657 A1563 C1943 C1869 C1793 C1728 C1657 A1563	C1870 C1794 A1729 U1584 U1584 C1877 C1877 C1877 C1877 C1877 C1877 C1877 C18787 C17787 C18787 C18787 C1888	diametric diametric <thditric< th=""> <thditri< th=""> diametr</thditri<></thditric<>	U1960 A1874 G1733 C1663 G1590 G1 11960 A1874 G1733 C1663 G1590 G1 11054 A1955 A1955 G1590 G1	G1952 U1876 G1735 G1666 G1592 G16	G1953 U1877 C1803 G1736 A1667 A1593 G1954 G1878 A1804 U1737 A1594 U16	U1955 A1879 C1805 C1671 U1595 A15 A1566 A1879 A1506 A1741 I1672 C155 C15	A1000 A1000 A1010 A10100 A1010 A1010 <t< td=""><td>U1958 G1882 G1808 G1675 G1598 C15 C1650 A1883 A1800 C1746 A1876 C15</td><td>41950 A1884 A1003 U1746 G1677 U1601</td><td>C1961 U1885 C1812 C1747 A1602 C151</td><td>G1962 A1886 A1813 G1/48 G1680 A1803 A1503 G A1887 A1814 A1749 G1664 A155</td><td>C U1888 U1815 A1750 A1683 A1605 G15</td><td>C G1889 A1816 G1751 U1684 U1606 II I1800 G1817 A1750 C1885 II1 607 G15</td><td>U U1866 C1608 G1753 U1686 C1608 G15</td><td>G A1893 U1819 G1754 U1687 G15 C 1160A 1140A 01265 71640</td><td>U A1895 U1821 C1756 U1689 A1619 C15</td><td>C A1896 C1822 A1757 C1690 U1620 C15</td><td>G G1898 U1824 C1759 U1692 U1622 C15</td><td>A G1899 G1825 A1760 C1693 G1623 C15 C A1900 C1826 C1761 D1694 G1624 G15</td><td>G A1901 C1762 U1695 A1626 U15 C A1606 T1606 T1606 T1606</td><td>A C1904 C1830 U1764 A1697 U1627 U15</td><td>G G1905 U1765 C1628 C15 C G1906 A1835 G1766 G1700 U1629 A15</td><td>G C1907 C1836 C1767 C1701 U1630 A1</td><td>G U1912 G1838 G1769 U1/02 C1031 A10</td><td>C A1839 G1770 U1705 C1633 G15 C 119000 HI 840 C1774 C1706 C1633 C15</td><td>U U172 1100 01034 010</td><td>G A1922 A1842 C1//3 C1/08 A163/ UDF C C1923 C1774 C1709 A1638 G156</td><td>U U1924 C1846 G1775 C1710 C1639 A156 II I1955 A1847 C1776 C1711 C1640 I1166</td><td>G C1926 G1848 U1777 G1712 U1641 U156</td><td>U G192/ C1849 G1/78 G1/13 A1642 U156 G A1714 A1643 U157</td><td>G A1930 G1861 G1780 A1715 C1644 A157</td><td>A U1931 U157 U154 U154 U1545 U157 C A1932 C185A C178A U1717 C18A6 C157</td><td>U A1933 U1785 G1718 A1647 C15</td><td>G G1934 C1857 G1786 A1648</td><td>U G1355 A1888 A1/6/ U1/22 U1549 G15 U A1859 C1788 A1723 G1650 C15</td><td>U G1939 G1789 U161 C18 G G1940 C1866 G1790 C1725 G1652 A15</td></t<>	U1958 G1882 G1808 G1675 G1598 C15 C1650 A1883 A1800 C1746 A1876 C15	41950 A1884 A1003 U1746 G1677 U1601	C1961 U1885 C1812 C1747 A1602 C151	G1962 A1886 A1813 G1/48 G1680 A1803 A1503 G A1887 A1814 A1749 G1664 A155	C U1888 U1815 A1750 A1683 A1605 G15	C G1889 A1816 G1751 U1684 U1606 II I1800 G1817 A1750 C1885 II 1 607 G15	U U1866 C1608 G1753 U1686 C1608 G15	G A1893 U1819 G1754 U1687 G15 C 1160A 1140A 01265 71640	U A1895 U1821 C1756 U1689 A1619 C15	C A1896 C1822 A1757 C1690 U1620 C15	G G1898 U1824 C1759 U1692 U1622 C15	A G1899 G1825 A1760 C1693 G1623 C15 C A1900 C1826 C1761 D1694 G1624 G15	G A1901 C1762 U1695 A1626 U15 C A1606 T1606 T1606 T1606	A C1904 C1830 U1764 A1697 U1627 U15	G G1905 U1765 C1628 C15 C G1906 A1835 G1766 G1700 U1629 A15	G C1907 C1836 C1767 C1701 U1630 A1	G U1912 G1838 G1769 U1/02 C1031 A10	C A1839 G1770 U1705 C1633 G15 C 119000 HI 840 C1774 C1706 C1633 C15	U U172 1100 01034 010	G A1922 A1842 C1//3 C1/08 A163/ UDF C C1923 C1774 C1709 A1638 G156	U U1924 C1846 G1775 C1710 C1639 A156 II I1955 A1847 C1776 C1711 C1640 I1166	G C1926 G1848 U1777 G1712 U1641 U156	U G192/ C1849 G1/78 G1/13 A1642 U156 G A1714 A1643 U157	G A1930 G1861 G1780 A1715 C1644 A157	A U1931 U157 U154 U154 U1545 U157 C A1932 C185A C178A U1717 C18A6 C157	U A1933 U1785 G1718 A1647 C15	G G1934 C1857 G1786 A1648	U G1355 A1888 A1/6/ U1/22 U1549 G15 U A1859 C1788 A1723 G1650 C15	U G1939 G1789 U161 C18 G G1940 C1866 G1790 C1725 G1652 A15



טמ	C C	n	IJ	U A	C.	с D	С С2076	U2077	C2078	G2079	U2081	U2082	G2083 C2084	U2085	A2086	42088	А	D II	A	A2093	C2094 G2095	A2096	U2097 C2098	A2099	A2100	U2102	C0105	A2106	A2107 C2108	U2109	G21110 G2111	U2112	A2113 C2114	G2115	G2116 A2117	C2118	A2119 A2120	G2121	G2122	ı
U2129 G2130	A2131 C2132	U2133 G2134		U2137 A2138	A2139	A2142	A2143 A2144	A2145 A2145	C2146	A2147 U2148	A2149	G2150 C2151	A2152	U2153	02154	A2158	U2159	G2161	U2162	C2163 A2164		A2167	A2168 G2169	U2170	1/175	U2175 110176	02170 G2177	A2178	C2181	A2182 A2183	U2184	G2185 112186	G2187	A2188	U2190	U2191	C2192 U2193	G2194 C2195	C2196	
C2197 A2198	<mark>G2199</mark> U2200	G2201 C2202	U2203	C2204 U2205	G2206 47207	A2208	U2209	01775	A2213	G2216	U2217	(1000)	A2222	A2223	A2224	C2227	A2228	C2231	A2232	A2233 G2234	C2235	G2236	G2236 G2238	G2239	P2240	A2243	AZ244 C2245	G2246	G2253	02254 472555	A2256	112260	G2261	A2262	C2263	F0770	G2273	A2279	A2280 A2281	
U2282 G2283	C2284 C2285	U2286 C2287	G2288	U2289 C2290	A2291	C2293	U2294 A 2295	A2296	U2297	U2298 A2299	G2300	U2301	A2303	C2304	G2306 C2306	G2307	C2308	A 2309 U 2310	G2311	A2312 A2313	U2314	G2315	U2319		0 2322	G2325	A2332	CODO E	U2336	C2337 C2337	C2339	C0343		C2346 117247	02347 A2348	U2349	C2350 U2351	A2352	C2354	
G2355	A2358	A2361	C2365	C2366 A2367	40370	A2373	C2374 C2375	G2376	G2377	C2378	G2381	CJ3RE	A2386		C2389 A2390	G2391	C2392	G2394	G2395	G2396 A2397	A2398	A2399	G2400 A2401	A2402	42405 A2404	C2405	0.2400	U2411	U2416	U2417 G2418	A2419	C2420	U2427		A 2430 C 2431	A2432	U2433 U2434	G2435 112436	62437	
A2438 A2439	G2440 A2441	G2442 A2443		A2447 G2448	A2449 C2450	G2451	G2452	U2453	42404	02455 A2456	G2457	A2458 A2459	U2460	A2461	A 24 02 G 24 63	U2464	G2465 C2466	G2467	A2468	G2469 C2470	U2471	U2472	C2473	G2474	62475 C2476	G2477	C2479 C2479	A2480	U2482	G2483 47484	A2485	A2486 112487	A2488	C2489	A 24 91	C2492	U2493 A2464	C2495	C2496 U2497	U2498 U2499
A2500 U2501	A2502 G2503	U2504 U2505	U2506	C2507 U2508	U2509 112510		U2513	A2515	U2516	U2517 C2518	A2519	A2520 112521	G2522	A2523	A2524 G2525	C2526		G2530	C2531	U2532 G2533	G2534	A2535	A2536 U2537	U2538	02033 A2540	U2541	02542 U2543	U2544	C2546	A2547 C2548	G2549	U2550 112551	C2552	U2553	A 2004 G 2555	C2556	A2557 U2558	A 76.61	A2562	
G2563	C2566 C2567	C2568 A2569	U2570	U2571 C2572	G2573	G2576	C2577	U2581	C2582	C2583 G2584	G2585	G2586	A2590	A2591	G2592 A2593	C2594	A2595 117506	06270	G2603	U2604 G2605	G2606	G2607	G2609 A2609	G2610	U2612	U2613	G2615	C2616	G2618	G2619 C2620	G2621	C2622 C2623	G2624	C2625	A2020 C2627	A2628	U2629 C2630	10637	C2638	
G2639 A2640	A2643	C2644 G2645	C2646	A2647	G2651 117652		A2656	G2662		C2666 A2667	U2668	A 7671	G2672	A2673	A 2674 C 2675	A2676	G2677	A 2010 A 2679	A2680	U2681 C2682	U2683	C2684	G2687	U2688	A 2009 G 2690	1 000 000	A 2034 A 2695	A2696	<mark>G2699</mark>	G2700	A2702	A2703	A2705	G2706	C2709	C2710	C2711 U2712	U2713 62714		
G2720 A2721	U2722	C2726 A2727	G2728	U2729 G2730	U2731	A2736	C2737	A2740	C2741	C2742 A2743	U2744	40748	G2749	U2750	G2751 U2752	G2753	G2754	02100	C2760	G2761 A2762	U2763	C2764	U2766	U2767	02769 A2769	02200	C2/12 C2773	<u></u>	G2778	A2779 A2780	U2781	U2782 112783	00170	G2786	G2788	U2789	A2790 G2791	A2792	G2794	
U2795 G2796	C2797 C2798	A2799 G2800	A2801	A2802 A2803	A2804 C2805	U2806	C1810		A2813	G2814 G2815	G2816	A2817 112818	A2819	A2820	C2821 U2822		C2825	G2828	<mark>U2829</mark>	G2830 G2831		G2834	02836 C2836	A2837	A2030 G2839	C2840	42041 U2842	U2843	A2845	U2846 47847	G2848	C2849	U2854	U2855	U2858	U2859	U2860 U2861	U2862	42864	
<mark>U2865</mark> U2866	C2867 U2868	G2871	A2872	U2873 G2874	C3870	U2880	C2881	C2884	C2885	U2886 A2887	U2888	C2889	G2895	A2896	C2899	A2900	G2901	C2906	G2907	A 2910		C2913	U2916	G2917	42910 A2919	U2920	G2922	U2923	C2927	C2928 C2929		U2932 47933	A2934	U2935	A 29 30	A2941	C2942 G2943	U2944 C2045	A2946	
<mark>G2947</mark> C2948	U2949 G2950	G2951 G2952	U2953	U2954 U2955	Cooper-	G2961	U2962	U2965	G2966	A2967 G2968	A2969	C2970	G2972	G2973	0.2974	G2977	U2978 112070	U2980	U2981	A2982 C2983	C2984		U2989 U2989		76670	A2995 10006	02997 G2997	U2998	C3002	G3003 C3004	A3005	A3006 113007		A3011	ZIOCH	A3016	A3017 C3018	U3019	A3021	

W O R L D W I D E PROTEIN DATA BANK

A3029 G3030 G3030 A3032 A3033 A3033 A3033 A3033 C3039 C3039 C3039 A3049 U3042 U3042 U3042 U3042 U3042 U3042 U3056 U3056 U3056 C30560 C3

G3022 U3023

<mark>C3025</mark> G3026 U3068 U3070 U3071 U3071 C3072 C3075 C3082 C3082 C3082 C3082 C3082 C3083 C3075 C3075 C3075 C3075 C3077 C3082




Chain y:

Cł	nai	n	у																		-	100)%													
	•	•	•	•	•	•	•	•	•	•	•	•		•	•	•	•	•	•	•	•	•	•	•	•	•	••	•	•	••	•••	••	••	••	٠	
Y	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	X21	X22	X 23	X24	X27	X 28	X 29	X 30	X31	X32	Х 33	Х34	X35	Х36	X37	Х38	X 39	X40	X41	X42	X43	X44	X45	X46	

74%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83558	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 $(e^-/\text{\AA}^2)$	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	476.16, 476.16, 476.16	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	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).

Mal	Chain	B	ond lengths		Bond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Z	0.46	0/1620	0.88	2/2164~(0.1%)
2	А	0.44	0/1952	0.69	0/2622
3	В	0.43	0/3153	0.71	1/4239~(0.0%)
4	С	0.44	1/2802~(0.0%)	0.73	1/3792~(0.0%)
5	D	0.50	0/2426	0.67	1/3271~(0.0%)
6	Е	0.47	0/1261	0.74	0/1694
7	F	0.52	0/1822	0.71	0/2451
8	G	0.46	0/1850	0.69	0/2495
9	Н	0.54	0/1540	0.78	2/2073~(0.1%)
10	Ι	0.51	0/1754	0.72	0/2350
11	J	0.48	0/1375	0.78	0/1842
12	s	0.34	0/734	0.71	1/1015~(0.1%)
13	L	0.45	0/1568	0.73	0/2106
14	М	0.47	0/1069	0.70	0/1438
15	Ν	0.41	0/1758	0.68	0/2354
16	0	0.46	0/1586	0.67	0/2128
17	Р	0.46	0/1466	0.70	0/1968
18	Q	0.44	0/1466	0.74	1/1965~(0.1%)
19	R	0.95	2/1539~(0.1%)	0.91	5/2050~(0.2%)
20	S	0.47	0/1482	0.69	0/1990
21	Т	0.47	0/1301	0.69	0/1743
22	U	0.46	0/812	0.71	0/1099
23	V	0.43	0/1019	0.68	0/1369
24	W	0.48	0/1099	0.74	0/1446
25	Х	0.45	0/984	0.74	0/1325
26	Υ	0.46	0/1005	0.82	1/1341~(0.1%)
27	Ζ	0.49	0/1119	0.71	0/1497
28	a	0.41	0/1205	0.74	3/1612~(0.2%)
29	b	0.46	0/474	0.83	1/629~(0.2%)
30	с	0.49	0/751	0.75	2/1008~(0.2%)
31	d	0.46	0/904	0.66	0/1213
32	е	0.46	0/1041	0.79	1/1394~(0.1%)
33	f	0.42	0/869	0.68	0/1168
34	g	0.43	0/891	0.69	0/1191



Mal	Chain	E	ond lengths		Bond angles
INIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
35	h	0.49	0/979	0.70	0/1301
36	i	0.50	0/779	0.73	0/1034
37	j	0.47	0/697	0.76	0/923
38	k	0.42	0/619	0.78	2/826~(0.2%)
39	1	0.44	0/444	0.73	0/588
40	m	0.47	0/424	0.76	1/562~(0.2%)
41	0	0.53	1/861~(0.1%)	0.75	0/1136
42	р	0.50	0/702	0.73	0/934
43	q	0.51	0/977	0.88	1/1313~(0.1%)
44	5	1.16	111/77625~(0.1%)	1.70	2290/121004~(1.9%)
45	8	1.20	12/3747~(0.3%)	1.69	115/5832~(2.0%)
46	7	1.22	5/2884~(0.2%)	1.74	93/4491~(2.1%)
All	All	0.96	132/138435~(0.1%)	1.43	2524/203986~(1.2%)

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
1	Z	0	8
2	А	0	2
4	С	0	11
5	D	0	2
6	Е	0	4
7	F	0	4
8	G	0	1
9	Н	0	2
10	Ι	0	1
11	J	0	2
12	s	0	4
13	L	0	3
14	М	0	1
15	Ν	0	1
17	Р	0	2
18	Q	0	2
19	R	0	3
20	S	0	3
21	Т	0	4
24	W	0	3
25	Х	0	2
26	Y	0	6



Mol	Chain	#Chirality outliers	#Planarity outliers
27	Ζ	0	1
28	а	0	1
29	b	0	2
32	е	0	2
33	f	0	1
34	g	0	1
37	j	0	2
42	р	0	1
43	q	0	3
All	All	0	85

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	5	2263	С	O3'-P	-83.01	0.61	1.61
19	R	312	VAL	CA-C	31.59	2.35	1.52
44	5	2279	А	O3'-P	29.63	1.96	1.61
44	5	1749	А	N9-C4	-10.94	1.31	1.37
46	7	1	G	OP3-P	-10.82	1.48	1.61
45	8	1	А	OP3-P	-10.69	1.48	1.61
44	5	307	А	N9-C4	-9.10	1.32	1.37
44	5	12	А	N9-C4	-8.13	1.32	1.37
41	0	12	CYS	CA-CB	-8.01	1.36	1.53
44	5	374	А	N9-C4	-7.66	1.33	1.37
44	5	1260	А	N9-C4	-7.51	1.33	1.37
44	5	170	G	C2-N3	-7.40	1.26	1.32
45	8	71	А	N9-C4	-7.35	1.33	1.37
44	5	1566	А	N7-C5	-7.19	1.34	1.39
44	5	170	G	N9-C4	-7.19	1.32	1.38
44	5	786	А	N9-C4	-7.14	1.33	1.37
45	8	149	А	N9-C4	-7.04	1.33	1.37
44	5	1266	G	C8-N7	-7.00	1.26	1.30
46	7	63	А	N9-C4	-6.91	1.33	1.37
19	R	312	VAL	C-N	6.89	1.50	1.34
44	5	211	А	N9-C4	-6.88	1.33	1.37
45	8	96	А	N9-C4	-6.84	1.33	1.37
44	5	492	С	C5-C6	-6.73	1.28	1.34
44	5	59	G	N9-C4	-6.61	1.32	1.38
44	5	3005	А	N9-C4	-6.59	1.33	1.37
44	5	677	А	N9-C4	-6.57	1.33	1.37
44	5	1392	G	N9-C4	-6.51	1.32	1.38
44	5	547	G	N9-C4	-6.46	1.32	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	5	3234	A	N9-C4	-6.43	1.33	1.37
44	5	532	A	N9-C4	-6.41	1.34	1.37
44	5	1714	A	N9-C4	-6.39	1.34	1.37
44	5	2253	G	O3'-P	6.35	1.68	1.61
45	8	88	A	N7-C5	-6.35	1.35	1.39
44	5	2208	A	N9-C4	-6.34	1.34	1.37
45	8	61	А	N9-C4	-6.25	1.34	1.37
44	5	559	А	N9-C4	-6.21	1.34	1.37
44	5	1266	G	N7-C5	-6.18	1.35	1.39
44	5	517	G	N9-C4	-6.10	1.33	1.38
44	5	137	G	N9-C4	-6.07	1.33	1.38
44	5	170	G	N3-C4	-6.07	1.31	1.35
44	5	2702	А	N9-C4	-6.07	1.34	1.37
44	5	308	А	N7-C5	-6.06	1.35	1.39
44	5	775	А	N9-C4	-6.04	1.34	1.37
44	5	1259	А	N9-C4	-6.04	1.34	1.37
44	5	48	А	N9-C4	-6.03	1.34	1.37
44	5	693	А	N9-C4	-6.01	1.34	1.37
44	5	1519	G	C2-N3	-5.95	1.27	1.32
44	5	1018	G	N9-C4	-5.95	1.33	1.38
44	5	3256	G	N9-C4	-5.91	1.33	1.38
45	8	24	G	C8-N7	-5.89	1.27	1.30
44	5	442	G	N7-C5	-5.87	1.35	1.39
44	5	209	А	N7-C5	-5.87	1.35	1.39
44	5	319	A	N9-C4	-5.86	1.34	1.37
44	5	2541	U	C4-O4	-5.85	1.19	1.23
44	5	551	A	N9-C4	-5.84	1.34	1.37
44	5	1637	А	N7-C5	-5.82	1.35	1.39
44	5	353	G	N9-C4	-5.80	1.33	1.38
44	5	3274	A	C6-N6	-5.78	1.29	1.33
45	8	33	A	N9-C4	-5.76	1.34	1.37
44	5	1544	G	C2-N3	-5.76	1.28	1.32
45	8	17	A	N7-C5	-5.75	1.35	1.39
44	5	67	А	N9-C4	-5.72	1.34	1.37
44	5	3230	G	N9-C4	-5.71	1.33	1.38
44	5	2524	A	N9-C4	-5.69	1.34	1.37
44	5	3219	G	N9-C4	-5.69	1.33	1.38
44	5	342	A	C6-N1	-5.67	1.31	1.35
44	5	1346	G	C2-N3	-5.65	1.28	1.32
44	5	123	A	N7-C5	-5.65	1.35	1.39
44	5	907	G	N9-C4	-5.65	1.33	1.38
44	5	1804	A	$N9-\overline{C4}$	-5.64	1.34	1.37



Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(Å)	Ideal(Å)
44	5	516	А	N9-C4	-5.64	1.34	1.37
45	8	148	G	N9-C4	-5.59	1.33	1.38
44	5	2844	С	C4-N4	-5.57	1.28	1.33
44	5	2206	G	C2-N3	-5.57	1.28	1.32
4	С	250	TRP	CB-CG	-5.52	1.40	1.50
44	5	1940	G	C2-N3	-5.51	1.28	1.32
44	5	1638	А	N9-C4	-5.48	1.34	1.37
44	5	59	G	C2-N3	-5.46	1.28	1.32
44	5	660	А	N9-C4	-5.46	1.34	1.37
44	5	552	G	C2-N3	-5.45	1.28	1.32
44	5	2831	G	C2-N3	-5.43	1.28	1.32
44	5	1318	А	N9-C4	-5.43	1.34	1.37
44	5	3320	А	N9-C4	-5.42	1.34	1.37
44	5	1577	G	N9-C4	-5.42	1.33	1.38
44	5	611	А	N9-C4	-5.40	1.34	1.37
44	5	1637	А	C8-N7	-5.40	1.27	1.31
44	5	2149	А	C6-N6	-5.39	1.29	1.33
44	5	3197	G	N9-C4	-5.39	1.33	1.38
44	5	352	А	N9-C4	-5.38	1.34	1.37
44	5	2863	G	C2-N3	-5.38	1.28	1.32
44	5	1747	G	C2-N3	-5.36	1.28	1.32
44	5	3305	А	N9-C4	-5.36	1.34	1.37
44	5	1760	А	N9-C4	-5.35	1.34	1.37
44	5	1800	А	N9-C4	-5.34	1.34	1.37
44	5	18	G	N1-C2	-5.34	1.33	1.37
44	5	1231	А	N7-C5	-5.33	1.36	1.39
44	5	783	А	N9-C4	-5.32	1.34	1.37
46	7	13	А	N9-C4	-5.31	1.34	1.37
44	5	1085	А	N9-C4	-5.28	1.34	1.37
44	5	3279	А	N9-C4	-5.28	1.34	1.37
44	5	3121	U	C5-C6	-5.26	1.29	1.34
44	5	1960	А	N9-C4	5.24	1.41	1.37
44	5	2534	G	N9-C4	-5.24	1.33	1.38
44	5	3094	А	N9-C4	-5.24	1.34	1.37
44	5	2520	А	N9-C4	-5.23	1.34	1.37
44	5	17	G	C2-N3	-5.22	1.28	1.32
44	5	2966	G	N9-C4	-5.22	1.33	1.38
44	5	1806	A	N7-C5	-5.21	1.36	1.39
44	5	1084	A	N9-C4	-5.20	1.34	1.37
46	7	120	C	C4-C5	-5.20	1.38	1.43
44	5	107	A	N9-C4	-5.18	1.34	1.37
44	5	2171	l G	C2-N3	-5.17	1.28	1.32



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
44	5	2787	G	C2-N3	-5.17	1.28	1.32
44	5	122	А	N9-C4	-5.17	1.34	1.37
44	5	333	G	C2-N3	-5.17	1.28	1.32
44	5	3239	G	C2-N3	-5.16	1.28	1.32
44	5	2591	А	N9-C4	-5.11	1.34	1.37
44	5	743	C	N1-C6	-5.11	1.34	1.37
44	5	3200	G	N9-C4	-5.11	1.33	1.38
46	7	74	C	N1-C6	-5.11	1.34	1.37
44	5	537	А	C6-N6	-5.10	1.29	1.33
44	5	3165	A	N9-C4	-5.09	1.34	1.37
44	5	1789	G	C2-N3	-5.08	1.28	1.32
44	5	1898	G	C2-N3	-5.07	1.28	1.32
44	5	2706	G	N9-C4	-5.07	1.33	1.38
44	5	3288	G	N9-C4	-5.04	1.33	1.38
44	5	20	A	N9-C4	-5.03	1.34	1.37
44	5	1246	G	C2-N3	-5.03	1.28	1.32
44	5	2593	A	C8-N7	-5.03	1.28	1.31
44	5	1566	A	C8-N7	-5.02	1.28	1.31
45	8	87	G	C2-N3	-5.02	1.28	1.32
45	8	70	G	C8-N7	-5.00	1.27	1.30

All (2524) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2279	А	P-O3'-C3'	35.94	162.82	119.70
44	5	2263	С	P-O3'-C3'	32.49	158.69	119.70
44	5	2279	А	O3'-P-O5'	-30.93	45.23	104.00
44	5	2263	С	OP1-P-O3'	24.51	159.12	105.20
44	5	2263	С	OP2-P-O3'	-22.12	56.55	105.20
44	5	2279	А	OP2-P-O3'	20.85	151.07	105.20
44	5	1231	А	N7-C8-N9	14.56	121.08	113.80
19	R	312	VAL	CB-CA-C	14.33	138.62	111.40
44	5	78	U	N3-C2-O2	-13.89	112.47	122.20
44	5	170	G	N3-C2-N2	-13.62	110.37	119.90
44	5	163	С	N1-C2-O2	13.09	126.75	118.90
44	5	788	С	C5-C6-N1	12.90	127.45	121.00
44	5	170	G	N3-C4-N9	-12.42	118.55	126.00
44	5	2844	С	N3-C4-C5	12.35	126.84	121.90
44	5	163	С	C5-C6-N1	12.32	127.16	121.00
44	5	2467	G	N7-C8-N9	12.18	119.19	113.10
44	5	1231	А	C8-N9-C4	-11.79	101.08	105.80
44	5	2434	U	N1-C2-O2	11.66	130.97	122.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	788	С	C6-N1-C2	-11.62	115.65	120.30
44	5	78	U	N1-C2-O2	11.55	130.89	122.80
44	5	3288	G	C4-N9-C1'	-11.54	111.49	126.50
44	5	1742	U	C5-C6-N1	11.50	128.45	122.70
44	5	581	U	N1-C2-O2	11.42	130.79	122.80
44	5	2867	С	N1-C2-O2	11.37	125.72	118.90
44	5	2899	С	N1-C2-O2	11.36	125.72	118.90
44	5	2195	С	C6-N1-C2	-11.32	115.77	120.30
44	5	3304	U	OP1-P-O3'	-11.30	80.35	105.20
44	5	524	U	C5-C6-N1	11.23	128.32	122.70
44	5	192	С	N1-C2-O2	11.19	125.61	118.90
45	8	152	G	N1-C6-O6	-11.18	113.19	119.90
19	R	312	VAL	O-C-N	-11.15	104.86	122.70
44	5	1283	С	N1-C2-O2	11.14	125.58	118.90
45	8	28	С	N1-C2-O2	11.13	125.58	118.90
44	5	59	G	N3-C2-N2	-11.09	112.14	119.90
44	5	2469	G	C8-N9-C4	-11.08	101.97	106.40
44	5	163	С	C6-N1-C2	-11.07	115.87	120.30
44	5	881	С	N1-C2-O2	10.98	125.49	118.90
44	5	1228	С	N1-C2-O2	10.98	125.49	118.90
44	5	263	С	N1-C2-O2	10.93	125.46	118.90
44	5	2467	G	C8-N9-C4	-10.83	102.07	106.40
44	5	2764	С	C5-C6-N1	10.76	126.38	121.00
44	5	2469	G	N7-C8-N9	10.73	118.46	113.10
44	5	1923	С	C5-C6-N1	10.69	126.34	121.00
44	5	1224	С	C5-C6-N1	10.68	126.34	121.00
44	5	2996	U	C2-N1-C1'	10.66	130.50	117.70
44	5	2867	С	N3-C2-O2	-10.64	114.45	121.90
44	5	3031	G	N7-C8-N9	10.64	118.42	113.10
44	5	1283	С	N3-C2-O2	-10.63	114.46	121.90
44	5	2476	С	N1-C2-O2	10.59	125.25	118.90
44	5	2476	С	N3-C2-O2	-10.51	114.54	121.90
44	5	2447	А	N1-C6-N6	10.50	124.90	118.60
44	5	922	U	N1-C2-O2	10.46	130.12	122.80
44	5	1254	С	C6-N1-C2	-10.36	116.16	120.30
44	5	163	C	N3-C2-O2	-10.34	114.66	121.90
44	5	170	G	N1-C2-N2	10.28	125.45	116.20
44	5	18	G	N1-C6-O6	-10.28	113.73	119.90
45	8	23	U	C2-N3-C4	-10.27	120.84	127.00
44	5	1231	А	C5-N7-C8	-10.26	98.77	103.90
44	5	547	G	N3-C2-N2	-10.21	112.75	119.90
44	5	3288	G	O4'-C1'-N9	10.21	116.37	108.20



α \cdot 1	C		
Continued	trom	previous	page
	J	1	r J

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2196	С	C5-C6-N1	10.20	126.10	121.00
44	5	1328	С	N3-C2-O2	-10.15	114.79	121.90
44	5	1806	А	N7-C8-N9	10.13	118.87	113.80
44	5	2983	С	N1-C2-O2	10.09	124.95	118.90
46	7	120	С	C5-C6-N1	10.06	126.03	121.00
44	5	263	С	N3-C2-O2	-10.05	114.86	121.90
44	5	1759	С	N1-C2-O2	10.02	124.91	118.90
44	5	435	С	C5-C6-N1	10.02	126.01	121.00
44	5	2764	С	C6-N1-C2	-10.01	116.29	120.30
44	5	3214	U	N3-C2-O2	-10.01	115.19	122.20
44	5	581	U	N3-C2-O2	-9.96	115.23	122.20
44	5	1759	С	C2-N1-C1'	9.95	129.75	118.80
44	5	881	С	C6-N1-C2	-9.90	116.34	120.30
44	5	339	С	N1-C2-O2	9.88	124.83	118.90
44	5	1718	G	C4-C5-N7	9.82	114.73	110.80
44	5	2279	А	OP1-P-O3'	-9.75	83.74	105.20
46	7	29	С	N1-C2-O2	9.74	124.74	118.90
44	5	1574	С	N3-C2-O2	-9.71	115.11	121.90
44	5	1392	G	N3-C4-C5	9.70	133.45	128.60
44	5	36	С	N1-C2-O2	9.69	124.71	118.90
44	5	1155	С	N1-C2-O2	9.68	124.70	118.90
44	5	2195	С	C5-C6-N1	9.62	125.81	121.00
44	5	149	U	N3-C2-O2	-9.61	115.47	122.20
44	5	308	А	N7-C8-N9	9.60	118.60	113.80
44	5	717	С	N1-C2-O2	9.59	124.66	118.90
45	8	87	G	C4-N9-C1'	-9.53	114.11	126.50
44	5	1218	U	N1-C2-O2	9.49	129.44	122.80
44	5	230	U	N1-C2-O2	9.49	129.44	122.80
45	8	87	G	N3-C4-N9	-9.48	120.31	126.00
44	5	2447	А	C5-C6-N6	-9.45	116.14	123.70
44	5	435	С	C6-N1-C2	-9.42	116.53	120.30
44	5	3304	U	OP2-P-O3'	-9.42	84.48	105.20
44	5	441	U	O4'-C1'-N1	9.41	115.73	108.20
44	5	3034	С	N1-C2-O2	9.40	124.54	118.90
19	R	312	VAL	CA-CB-CG1	9.39	124.99	110.90
44	5	1752	А	C5-N7-C8	-9.37	99.21	103.90
44	5	1283	C	C6-N1-C2	-9.36	116.56	120.30
44	5	547	G	C4-N9-C1'	-9.35	114.35	126.50
44	5	3269	U	N1-C2-O2	9.34	129.34	122.80
45	8	120	С	C5-C6-N1	9.34	125.67	121.00
46	7	35	С	C6-N1-C2	-9.33	116.57	120.30
44	5	986	U	N1-C2-O2	9.31	129.32	122.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1878	G	N3-C4-N9	9.30	131.58	126.00
44	5	192	С	C2-N1-C1'	9.28	129.00	118.80
44	5	538	G	N7-C8-N9	9.26	117.73	113.10
44	5	1749	А	C4-C5-C6	-9.24	112.38	117.00
44	5	51	A	C5-C6-N6	-9.24	116.31	123.70
44	5	2366	С	N1-C2-O2	9.24	124.44	118.90
45	8	152	G	C5-C6-O6	9.23	134.14	128.60
44	5	1218	U	N3-C2-O2	-9.22	115.74	122.20
44	5	729	С	C5-C6-N1	9.22	125.61	121.00
44	5	1749	А	N3-C4-C5	9.21	133.25	126.80
44	5	547	G	N3-C4-N9	-9.20	120.48	126.00
44	5	3038	U	N3-C2-O2	-9.19	115.77	122.20
44	5	10	С	C6-N1-C2	-9.17	116.63	120.30
44	5	1752	A	N7-C8-N9	9.17	118.38	113.80
44	5	3334	U	C6-N1-C2	9.16	126.49	121.00
44	5	3025	C	C5-C6-N1	9.15	125.58	121.00
44	5	675	C	C5-C6-N1	9.14	125.57	121.00
44	5	503	C	C2-N1-C1'	9.12	128.83	118.80
44	5	1759	C	C5-C6-N1	9.09	125.54	121.00
44	5	1727	G	C5-C6-O6	-9.07	123.16	128.60
44	5	2568	C	C6-N1-C2	9.06	123.92	120.30
44	5	1625	A	N7-C8-N9	9.06	118.33	113.80
45	8	87	G	C8-N9-C1'	9.05	138.77	127.00
44	5	881	С	C5-C6-N1	9.05	125.53	121.00
44	5	3288	G	C8-N9-C1'	9.05	138.77	127.00
44	5	2684	С	C5-C6-N1	9.05	125.52	121.00
44	5	170	G	N3-C4-C5	9.00	133.10	128.60
44	5	3165	A	C6-N1-C2	8.96	123.97	118.60
44	5	1351	U	C2-N1-C1'	8.95	128.44	117.70
44	5	515	C	N1-C2-O2	8.94	124.26	118.90
44	5	1597	С	C6-N1-C2	-8.94	116.72	120.30
44	5	3123	A	N1-C6-N6	-8.92	113.25	118.60
44	5	1392	G	C8-N9-C4	8.89	109.96	106.40
44	5	2763	U	N1-C2-O2	8.89	129.03	122.80
44	5	1922	A	C5-N7-C8	-8.89	99.46	103.90
45	8	23	U	N1-C2-N3	8.88	120.23	114.90
44	5	434	U	C5-C6-N1	8.88	127.14	122.70
44	5	3262	U	N1-C2-O2	8.87	129.01	122.80
43	q	52	LEU	CA-CB-CG	8.84	135.64	115.30
44	5	170	G	C4-N9-C1'	-8.84	115.01	126.50
44	5	321	C	N1-C2-O2	8.84	124.20	118.90
44	5	2513	U	N1-C2-O2	8.83	128.98	122.80



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	3344	А	C5-N7-C8	-8.82	99.49	103.90
46	7	29	С	N3-C2-O2	-8.82	115.72	121.90
44	5	2496	С	N3-C2-O2	-8.82	115.73	121.90
44	5	1922	А	N1-C6-N6	8.82	123.89	118.60
44	5	493	U	C5-C6-N1	8.81	127.11	122.70
44	5	2899	С	C2-N1-C1'	8.80	128.48	118.80
44	5	1018	G	N3-C4-N9	-8.79	120.72	126.00
44	5	2148	U	C5-C6-N1	8.79	127.09	122.70
44	5	1279	С	N1-C2-O2	8.78	124.17	118.90
44	5	3300	U	N3-C2-O2	-8.76	116.07	122.20
44	5	1351	U	N1-C2-O2	8.76	128.93	122.80
44	5	2901	G	C6-C5-N7	-8.75	125.15	130.40
44	5	51	А	N1-C6-N6	8.73	123.84	118.60
44	5	3158	G	C5-C6-O6	-8.72	123.37	128.60
44	5	1800	А	C5-N7-C8	-8.72	99.54	103.90
44	5	2509	U	N1-C2-O2	8.72	128.90	122.80
44	5	2531	С	N1-C2-O2	8.71	124.13	118.90
44	5	3214	U	N1-C2-O2	8.68	128.88	122.80
44	5	157	А	O5'-P-OP1	8.68	121.12	110.70
44	5	1566	А	N7-C8-N9	8.67	118.14	113.80
44	5	638	С	C5-C6-N1	8.67	125.33	121.00
44	5	1501	U	N1-C2-O2	8.66	128.86	122.80
44	5	2118	С	N1-C2-O2	8.66	124.10	118.90
44	5	1556	С	N1-C2-O2	8.65	124.09	118.90
44	5	2496	С	N1-C2-O2	8.63	124.08	118.90
44	5	743	С	C6-N1-C2	-8.63	116.85	120.30
44	5	1328	С	N1-C2-O2	8.61	124.06	118.90
44	5	170	G	C8-N9-C1'	8.61	138.19	127.00
44	5	308	А	C8-N9-C4	-8.60	102.36	105.80
44	5	2378	С	N3-C2-O2	-8.59	115.89	121.90
44	5	2836	С	N1-C2-O2	8.59	124.05	118.90
44	5	3181	С	C2-N1-C1'	8.58	128.24	118.80
44	5	1239	С	C6-N1-C2	-8.57	116.87	120.30
44	5	3230	G	N3-C4-N9	-8.56	120.86	126.00
44	5	27	C	N1-C2-O2	8.56	124.04	118.90
44	5	3181	C	N1-C2-O2	8.56	124.04	118.90
44	5	380	U	N1-C2-O2	8.55	128.79	122.80
44	5	881	C	N3-C2-O2	-8.55	115.91	121.90
44	5	1597	C	C5-C6-N1	8.55	125.27	121.00
44	5	3350	C	C6-N1-C2	-8.55	116.88	120.30
44	5	2452	G	C5-C6-O6	-8.54	123.48	128.60
46	7	39		C2-N1-C1'	8.51	128.16	118.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1749	А	C8-N9-C4	8.51	109.20	105.80
44	5	3131	U	N3-C2-O2	-8.50	116.25	122.20
44	5	1359	С	N1-C2-O2	8.49	124.00	118.90
44	5	1824	U	N1-C2-O2	8.48	128.74	122.80
44	5	306	А	N1-C6-N6	8.46	123.68	118.60
44	5	2562	А	N9-C4-C5	-8.46	102.42	105.80
44	5	3344	А	N7-C8-N9	8.46	118.03	113.80
44	5	339	С	N3-C2-O2	-8.46	115.98	121.90
44	5	922	U	C2-N1-C1'	8.45	127.84	117.70
44	5	2545	С	C6-N1-C2	-8.44	116.93	120.30
44	5	335	G	C4-C5-N7	8.42	114.17	110.80
44	5	3153	U	N1-C2-N3	-8.42	109.85	114.90
44	5	1190	А	N9-C4-C5	-8.41	102.43	105.80
44	5	2466	G	O5'-P-OP1	-8.41	98.13	105.70
44	5	1342	С	C5-C6-N1	8.41	125.21	121.00
46	7	35	С	N3-C2-O2	-8.41	116.01	121.90
44	5	493	U	C6-N1-C2	-8.41	115.96	121.00
46	7	26	С	N3-C2-O2	-8.40	116.02	121.90
44	5	2629	U	N1-C2-O2	8.40	128.68	122.80
44	5	2996	U	N1-C2-O2	8.40	128.68	122.80
44	5	192	С	N3-C2-O2	-8.39	116.03	121.90
44	5	2645	G	N3-C2-N2	-8.39	114.03	119.90
44	5	547	G	C8-N9-C1'	8.38	137.90	127.00
44	5	3057	U	N3-C2-O2	-8.38	116.33	122.20
44	5	621	A	C5-N7-C8	-8.37	99.72	103.90
44	5	2836	C	C2-N1-C1'	8.37	128.01	118.80
44	5	1411	С	N1-C2-O2	8.36	123.92	118.90
46	7	39	С	N1-C2-O2	8.36	123.92	118.90
44	5	3344	A	C5-C6-N6	-8.36	117.02	123.70
44	5	2711	С	C2-N1-C1'	8.35	127.99	118.80
44	5	51	A	C4-C5-N7	8.35	114.88	110.70
44	5	2629	U	N3-C2-O2	-8.34	116.36	122.20
44	5	235	А	N7-C8-N9	8.32	117.96	113.80
44	5	2901	G	N7-C8-N9	8.32	117.26	113.10
44	5	2789	U	N3-C2-O2	-8.31	116.38	122.20
46	7	26	C	C6-N1-C2	-8.31	116.98	120.30
44	5	1224	С	C4-C5-C6	-8.30	113.25	117.40
44	5	1359	C	C2-N1-C1'	8.31	127.94	118.80
44	5	1574	C	N1-C2-O2	8.29	123.88	118.90
44	5	2983	C	C2-N1-C1'	8.29	127.92	118.80
44	5	1018	G	N3-C2-N2	-8.28	114.10	119.90
44	5	1718	G	C6-C5-N7	-8.28	125.43	130.40



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1355	A	N1-C6-N6	8.28	123.56	118.60
44	5	522	A	N1-C6-N6	-8.27	113.64	118.60
44	5	2132	С	C2-N1-C1'	8.27	127.89	118.80
44	5	1718	G	N9-C4-C5	-8.26	102.10	105.40
44	5	3031	G	C5-N7-C8	-8.25	100.18	104.30
44	5	2118	С	C2-N1-C1'	8.24	127.87	118.80
44	5	1263	A	C5-C6-N6	-8.24	117.11	123.70
44	5	1246	G	N7-C8-N9	8.24	117.22	113.10
44	5	79	U	N3-C2-O2	-8.22	116.44	122.20
44	5	2515	A	N9-C4-C5	-8.21	102.51	105.80
44	5	3305	A	OP1-P-OP2	8.21	131.92	119.60
45	8	72	A	C2-N3-C4	8.21	114.71	110.60
44	5	1574	С	C6-N1-C2	-8.20	117.02	120.30
44	5	1018	G	N3-C4-C5	8.19	132.70	128.60
44	5	130	A	C5-N7-C8	-8.19	99.80	103.90
46	7	26	С	N1-C2-O2	8.17	123.80	118.90
44	5	946	U	C5-C6-N1	8.15	126.78	122.70
44	5	1425	U	N1-C2-O2	8.14	128.50	122.80
44	5	2434	U	C2-N1-C1'	8.14	127.47	117.70
44	5	1355	A	C5-C6-N6	-8.14	117.19	123.70
44	5	3166	С	C5-C6-N1	8.13	125.06	121.00
44	5	1805	С	C6-N1-C2	-8.12	117.05	120.30
46	7	34	С	C6-N1-C2	-8.12	117.05	120.30
44	5	2526	С	C5-C6-N1	8.12	125.06	121.00
44	5	1717	U	C5-C4-O4	-8.11	121.03	125.90
44	5	1223	A	N7-C8-N9	8.11	117.85	113.80
44	5	11	А	O4'-C1'-N9	8.10	114.68	108.20
44	5	1566	A	C8-N9-C4	-8.10	102.56	105.80
44	5	2789	U	N1-C2-O2	8.09	128.47	122.80
44	5	1923	С	C6-N1-C2	-8.09	117.06	120.30
44	5	3300	U	N1-C2-O2	8.09	128.46	122.80
44	5	1927	G	C5-C6-O6	-8.09	123.75	128.60
44	5	2582	С	N1-C2-O2	8.09	123.75	118.90
44	5	3068	U	N3-C2-O2	-8.07	116.55	122.20
44	5	564	G	N1-C6-O6	8.06	124.74	119.90
44	5	1227	C	N1-C2-O2	8.06	$1\overline{23.74}$	118.90
46	7	6	C	C5-C6-N1	8.06	125.03	121.00
44	5	180	C	C5-C6-N1	8.05	125.03	121.00
44	5	2216	G	N3-C2-N2	-8.05	114.27	119.90
44	5	1878	G	N3-C4-C5	-8.04	$124.5\overline{8}$	128.60
44	5	3038	U	N1-C2-O2	8.04	128.43	122.80
44	5	2492	C	C6-N1-C2	-8.02	117.09	120.30


Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	3133	С	C5-C6-N1	8.02	125.01	121.00
44	5	335	G	N3-C4-N9	8.02	130.81	126.00
44	5	1086	С	C6-N1-C2	-8.02	117.09	120.30
46	7	58	С	C5-C6-N1	8.00	125.00	121.00
44	5	3253	G	C5-C6-O6	-7.99	123.80	128.60
44	5	1087	G	N9-C4-C5	-7.99	102.20	105.40
44	5	547	G	N3-C4-C5	7.98	132.59	128.60
44	5	1246	G	C8-N9-C4	-7.98	103.21	106.40
46	7	58	С	C6-N1-C2	-7.98	117.11	120.30
44	5	335	G	N9-C4-C5	-7.96	102.22	105.40
44	5	2200	U	C5-C4-O4	-7.95	121.13	125.90
44	5	1010	G	N1-C6-O6	7.95	124.67	119.90
44	5	168	U	O4'-C1'-N1	7.94	114.55	108.20
44	5	564	G	C5-C6-O6	-7.93	123.84	128.60
44	5	1876	U	N1-C2-O2	7.93	128.35	122.80
44	5	3089	С	C5-C6-N1	7.93	124.96	121.00
44	5	437	G	N7-C8-N9	7.92	117.06	113.10
44	5	2996	U	N3-C2-O2	-7.92	116.66	122.20
44	5	1904	С	C2-N1-C1'	7.92	127.51	118.80
44	5	2863	G	N3-C2-N2	-7.92	114.36	119.90
44	5	1752	А	C4-C5-N7	7.92	114.66	110.70
44	5	161	G	C8-N9-C1'	7.91	137.29	127.00
45	8	104	А	N1-C2-N3	-7.91	125.34	129.30
44	5	1922	А	N7-C8-N9	7.91	117.75	113.80
44	5	489	U	C2-N1-C1'	7.90	127.19	117.70
44	5	1766	G	C4-C5-N7	7.90	113.96	110.80
44	5	27	С	N3-C2-O2	-7.90	116.37	121.90
44	5	1266	G	C6-C5-N7	-7.89	125.66	130.40
44	5	2836	С	N3-C2-O2	-7.89	116.37	121.90
44	5	3219	G	C8-N9-C4	7.89	109.56	106.40
44	5	3273	А	N1-C6-N6	7.89	123.33	118.60
44	5	911	С	C5-C6-N1	7.88	124.94	121.00
45	8	120	С	N1-C2-O2	7.88	123.63	118.90
44	5	2838	А	C5-C6-N6	-7.88	117.40	123.70
44	5	3058	U	C2-N1-C1'	7.88	127.15	117.70
44	5	10	С	C6-N1-C1'	7.87	130.25	120.80
45	8	41	A	C5-C6-N6	-7.87	117.41	123.70
44	5	97	U	N3-C2-O2	-7.85	116.70	122.20
44	5	2434	U	N3-C2-O2	-7.85	116.70	122.20
44	5	1296	С	C5-C6-N1	7.85	124.93	121.00
46	7	68	С	C6-N1-C2	-7.85	117.16	120.30
44	5	568	G	C4-C5-N7	7.85	113.94	110.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1808	G	O4'-C1'-N9	7.85	114.48	108.20
44	5	1800	А	N7-C8-N9	7.84	117.72	113.80
44	5	51	А	N9-C4-C5	-7.84	102.66	105.80
44	5	2470	С	C4-C5-C6	7.84	121.32	117.40
44	5	3354	U	C2-N1-C1'	7.84	127.11	117.70
44	5	1155	С	C2-N1-C1'	7.84	127.42	118.80
44	5	1591	G	C6-C5-N7	-7.84	125.70	130.40
44	5	31	С	C2-N1-C1'	7.83	127.41	118.80
44	5	2534	G	N3-C4-N9	-7.83	121.31	126.00
44	5	2825	С	N1-C2-O2	7.83	123.59	118.90
44	5	1280	С	O4'-C1'-N1	7.82	114.45	108.20
46	7	63	А	C8-N9-C4	7.81	108.92	105.80
44	5	1249	G	C5-C6-O6	7.81	133.29	128.60
44	5	1284	С	C5-C6-N1	7.81	124.91	121.00
44	5	2196	С	C6-N1-C2	-7.80	117.18	120.30
44	5	2513	U	C5-C6-N1	7.80	126.60	122.70
44	5	2585	G	N3-C4-C5	-7.79	124.70	128.60
44	5	1876	U	N3-C2-O2	-7.78	116.75	122.20
44	5	677	А	C2-N3-C4	-7.78	106.71	110.60
44	5	137	G	N3-C4-C5	7.77	132.49	128.60
44	5	3111	U	C5-C6-N1	7.77	126.59	122.70
45	8	41	А	C4-C5-N7	7.77	114.58	110.70
46	7	105	С	C5-C6-N1	7.77	124.88	121.00
44	5	2171	G	N1-C6-O6	-7.77	115.24	119.90
44	5	12	A	N3-C4-N9	-7.76	121.19	127.40
44	5	1238	C	O5'-P-OP1	-7.76	98.72	105.70
44	5	3068	U	N1-C2-O2	7.76	128.23	122.80
44	5	90	С	C5-C6-N1	7.75	124.88	121.00
44	5	59	G	N3-C4-C5	7.75	132.47	128.60
44	5	631	U	N3-C2-O2	-7.75	116.78	122.20
44	5	729	С	C6-N1-C2	-7.75	117.20	120.30
44	5	1263	A	N3-C4-N9	7.74	133.59	127.40
44	5	3306	U	C2-N1-C1'	7.74	126.98	117.70
44	5	987	U	C5-C6-N1	7.73	126.57	122.70
44	5	851	С	N1-C2-O2	7.73	123.54	118.90
44	5	2189	U	C5-C6-N1	7.72	126.56	122.70
44	5	2585	G	N3-C4-N9	7.72	130.63	126.00
44	5	539	C	C5-C6-N1	7.72	124.86	121.00
44	5	1010	G	C5-C6-O6	-7.71	123.97	128.60
44	5	2596	U	C5-C6-N1	7.70	126.55	122.70
44	5	3350	C	C5-C6-N1	7.70	124.85	121.00
44	5	353	G	N3-C4-C5	7.70	132.45	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1171	G	N1-C6-O6	-7.69	115.28	119.90
44	5	2772	С	N1-C2-O2	7.69	123.51	118.90
44	5	397	А	N9-C4-C5	-7.69	102.72	105.80
44	5	717	С	N3-C2-O2	-7.69	116.52	121.90
44	5	22	G	N7-C8-N9	7.68	116.94	113.10
44	5	217	U	N1-C2-O2	7.68	128.18	122.80
44	5	2996	U	C6-N1-C1'	-7.68	110.44	121.20
44	5	1292	С	N1-C2-O2	7.68	123.51	118.90
44	5	211	А	C8-N9-C4	7.67	108.87	105.80
44	5	3031	G	C8-N9-C4	-7.67	103.33	106.40
44	5	2467	G	C5-N7-C8	-7.67	100.46	104.30
44	5	59	G	N1-C2-N2	7.67	123.10	116.20
44	5	1159	А	C2-N3-C4	7.67	114.43	110.60
44	5	1577	G	N3-C4-N9	-7.66	121.40	126.00
44	5	155	G	O4'-C1'-N9	7.66	114.32	108.20
44	5	2132	С	C6-N1-C2	-7.64	117.24	120.30
44	5	18	G	C5-C6-O6	7.64	133.19	128.60
44	5	2217	U	N1-C2-O2	7.64	128.15	122.80
44	5	539	С	C6-N1-C2	-7.63	117.25	120.30
44	5	659	G	N7-C8-N9	7.63	116.91	113.10
44	5	1088	U	N1-C2-O2	7.63	128.14	122.80
46	7	44	С	C5-C6-N1	7.63	124.81	121.00
44	5	3360	С	C2-N1-C1'	7.62	127.19	118.80
44	5	517	G	N3-C4-C5	7.62	132.41	128.60
44	5	2509	U	N3-C2-O2	-7.62	116.86	122.20
46	7	120	С	C4-C5-C6	-7.62	113.59	117.40
44	5	3219	G	N3-C4-C5	7.61	132.41	128.60
44	5	3256	G	N3-C4-N9	-7.61	121.43	126.00
44	5	163	С	C4-C5-C6	-7.61	113.59	117.40
44	5	22	G	C5-N7-C8	-7.61	100.50	104.30
44	5	2193	U	C2-N1-C1'	7.61	126.83	117.70
44	5	181	U	C5-C6-N1	7.60	126.50	122.70
44	5	2935	U	C2-N1-C1'	7.60	126.82	117.70
44	5	522	А	C4-C5-C6	-7.59	113.21	117.00
44	5	2205	U	N1-C2-O2	7.59	128.11	122.80
44	5	3025	С	C6-N1-C2	-7.58	117.27	120.30
44	5	2861	U	C2-N1-C1'	-7.58	108.60	117.70
44	5	59	G	N3-C4-N9	-7.58	121.45	126.00
44	5	785	G	N3-C2-N2	-7.58	114.59	119.90
44	5	386	A	N7-C8-N9	7.57	117.59	113.80
44	5	3099	C	N1-C2-O2	7.57	123.44	118.90
44	5	3266	G	N3-C2-N2	-7.57	114.60	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	3109	G	N9-C4-C5	-7.56	102.38	105.40
44	5	621	А	N1-C6-N6	7.55	123.13	118.60
44	5	3230	G	N3-C4-C5	7.55	132.38	128.60
44	5	306	А	C4-C5-N7	7.54	114.47	110.70
44	5	1496	С	C6-N1-C2	-7.54	117.28	120.30
44	5	299	G	N7-C8-N9	7.54	116.87	113.10
44	5	3288	G	N3-C4-C5	7.54	132.37	128.60
44	5	758	С	N1-C2-O2	7.53	123.42	118.90
44	5	3131	U	N1-C2-O2	7.53	128.07	122.80
44	5	1648	A	C5-N7-C8	-7.53	100.14	103.90
44	5	986	U	N3-C2-O2	-7.53	116.93	122.20
44	5	1958	U	P-O3'-C3'	7.53	128.73	119.70
44	5	2541	U	P-O3'-C3'	7.53	128.73	119.70
45	8	148	G	C4-N9-C1'	-7.52	116.72	126.50
44	5	1033	U	C6-N1-C2	-7.52	116.49	121.00
44	5	3076	С	C5-C6-N1	7.52	124.76	121.00
44	5	613	G	N9-C4-C5	-7.52	102.39	105.40
44	5	3105	U	N3-C2-O2	-7.52	116.94	122.20
44	5	3253	G	N1-C6-O6	7.52	124.41	119.90
44	5	711	А	N7-C8-N9	7.52	117.56	113.80
44	5	734	С	N1-C2-O2	7.51	123.41	118.90
44	5	149	U	C2-N1-C1'	7.51	126.71	117.70
44	5	336	А	C2-N3-C4	7.51	114.36	110.60
44	5	7	С	N3-C2-O2	-7.50	116.65	121.90
44	5	2768	U	N1-C2-O2	7.50	128.05	122.80
44	5	897	U	N1-C2-O2	7.50	128.05	122.80
44	5	1280	С	N3-C2-O2	-7.50	116.65	121.90
44	5	2983	С	N3-C2-O2	-7.50	116.65	121.90
44	5	1547	G	C4-N9-C1'	-7.49	116.76	126.50
44	5	1239	С	N3-C2-O2	-7.49	116.66	121.90
44	5	2393	G	O5'-P-OP1	-7.49	98.96	105.70
45	8	35	С	N1-C2-O2	7.49	123.39	118.90
44	5	1018	G	C8-N9-C1'	7.48	136.73	127.00
44	5	1190	А	N3-C4-N9	7.48	133.38	127.40
44	5	3192	U	C5-C6-N1	7.48	126.44	122.70
44	5	3325	G	N3-C4-N9	7.48	130.49	126.00
44	5	1224	C	C5-C4-N4	-7.47	114.97	120.20
45	8	32	C	N1-C2-O2	7.47	123.38	118.90
44	5	170	G	C6-C5-N7	7.46	134.88	130.40
44	5	3325	G	N9-C4-C5	-7.46	102.41	105.40
44	5	3256	G	N3-C4-C5	7.46	132.33	128.60
44	5	218	G	C2-N3-C4	-7.46	108.17	111.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1806	А	C8-N9-C4	-7.46	102.82	105.80
44	5	1228	С	N3-C2-O2	-7.45	116.68	121.90
44	5	3132	С	C5-C6-N1	7.45	124.73	121.00
44	5	1283	С	C2-N1-C1'	7.45	127.00	118.80
45	8	41	А	C5-N7-C8	-7.45	100.18	103.90
44	5	2656	А	N1-C2-N3	-7.45	125.58	129.30
44	5	1268	G	C2-N3-C4	-7.44	108.18	111.90
44	5	492	С	C4-C5-C6	7.44	121.12	117.40
45	8	37	А	N1-C6-N6	7.44	123.06	118.60
44	5	2132	С	N1-C2-O2	7.44	123.36	118.90
44	5	3262	U	N3-C2-O2	-7.44	116.99	122.20
44	5	2217	U	N3-C2-O2	-7.43	117.00	122.20
19	R	312	VAL	N-CA-CB	-7.43	95.15	111.50
44	5	306	А	N9-C4-C5	-7.42	102.83	105.80
46	7	1	G	C4-C5-N7	7.42	113.77	110.80
44	5	1311	G	N7-C8-N9	7.42	116.81	113.10
44	5	1922	А	C4-C5-N7	7.42	114.41	110.70
45	8	8	С	C5-C6-N1	7.41	124.70	121.00
44	5	122	А	O5'-P-OP2	-7.41	99.03	105.70
44	5	945	С	N1-C2-O2	7.41	123.34	118.90
44	5	1333	С	N1-C2-O2	7.41	123.34	118.90
44	5	2899	С	C6-N1-C1'	-7.41	111.91	120.80
44	5	3274	A	C5-C6-N1	7.41	121.40	117.70
44	5	2884	С	C6-N1-C2	-7.40	117.34	120.30
44	5	537	A	C5-C6-N1	7.40	121.40	117.70
44	5	621	А	N7-C8-N9	7.40	117.50	113.80
44	5	1275	С	C5-C6-N1	7.40	124.70	121.00
44	5	299	G	C5-N7-C8	-7.39	100.60	104.30
44	5	400	G	C5-C6-O6	-7.39	124.17	128.60
44	5	621	А	C5-C6-N6	-7.38	117.79	123.70
44	5	180	С	C6-N1-C2	-7.38	117.35	120.30
44	5	179	С	C5-C6-N1	7.38	124.69	121.00
44	5	1684	U	C5-C6-N1	7.38	126.39	122.70
44	5	38	U	N1-C2-O2	7.38	127.97	122.80
44	5	1248	С	N1-C2-O2	7.38	123.33	118.90
44	5	3360	C	C5-C6-N1	7.38	124.69	121.00
44	5	3039	C	N1-C2-O2	7.38	123.33	118.90
45	8	148	G	N3-C4-C5	7.38	132.29	128.60
44	5	1041	U	N1-C2-O2	7.38	127.96	122.80
44	5	1018	G	C4-N9-C1'	-7.37	116.92	126.50
44	5	1392	G	C4-N9-C1'	-7.37	116.92	126.50
45	8	8	C	N1-C2-O2	7.37	123.32	118.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	306	А	C5-N7-C8	-7.37	100.22	103.90
44	5	1227	С	N3-C2-O2	-7.37	116.74	121.90
44	5	1228	С	C5-C6-N1	7.37	124.68	121.00
44	5	137	G	N3-C4-N9	-7.37	121.58	126.00
44	5	192	С	C6-N1-C2	-7.37	117.35	120.30
44	5	3344	А	C4-C5-N7	7.37	114.38	110.70
44	5	678	G	C2-N3-C4	-7.36	108.22	111.90
44	5	770	G	C4-N9-C1'	-7.36	116.93	126.50
44	5	95	A	N7-C8-N9	7.36	117.48	113.80
44	5	1071	U	O4'-C1'-N1	7.36	114.09	108.20
44	5	551	A	O4'-C1'-N9	7.36	114.09	108.20
44	5	158	G	N9-C4-C5	-7.35	102.46	105.40
44	5	2358	A	C5-C6-N6	-7.35	117.82	123.70
44	5	922	U	N3-C2-O2	-7.34	117.06	122.20
44	5	2913	С	C2-N3-C4	7.34	123.57	119.90
44	5	3385	U	C5-C6-N1	7.34	126.37	122.70
44	5	2467	G	C6-C5-N7	-7.33	126.00	130.40
44	5	3146	G	C8-N9-C4	7.33	109.33	106.40
44	5	3163	А	C5-C6-N6	-7.33	117.84	123.70
44	5	2794	G	N3-C4-C5	7.32	132.26	128.60
44	5	2889	С	C6-N1-C2	-7.32	117.37	120.30
44	5	170	G	N9-C4-C5	7.32	108.33	105.40
44	5	1238	С	N1-C2-O2	7.32	123.29	118.90
44	5	2831	G	N3-C2-N2	-7.31	114.78	119.90
44	5	1307	G	P-O3'-C3'	7.31	128.47	119.70
44	5	1922	А	C5-C6-N6	-7.31	117.85	123.70
44	5	175	С	N1-C2-O2	7.29	123.28	118.90
44	5	1501	U	C5-C6-N1	7.29	126.35	122.70
44	5	681	U	C2-N1-C1'	7.29	126.45	117.70
44	5	2780	A	N9-C4-C5	-7.29	102.89	105.80
44	5	1364	С	N3-C2-O2	-7.29	116.80	121.90
44	5	2507	С	C5-C6-N1	7.29	124.64	121.00
44	5	149	U	N1-C2-O2	7.28	127.90	122.80
44	5	1280	С	N1-C2-O2	7.28	123.27	118.90
44	5	1239	С	N1-C2-O2	7.28	123.27	118.90
44	5	1904	C	N1-C2-O2	7.28	123.27	118.90
44	5	1759	C	C6-N1-C1'	-7.28	112.07	120.80
44	5	3256	G	N3-C2-N2	-7.28	114.81	119.90
44	5	492	C	N3-C4-N4	7.28	123.09	118.00
44	5	770	G	N3-C4-C5	7.27	132.24	128.60
44	5	3165	A	N1-C2-N3	-7.27	125.67	129.30
44	5	1246	G	N3-C2-N2	-7.27	114.81	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2829	U	N3-C2-O2	-7.27	117.11	122.20
44	5	79	U	N1-C2-O2	7.27	127.89	122.80
44	5	1342	С	C6-N1-C2	-7.26	117.40	120.30
44	5	1508	С	N3-C2-O2	-7.26	116.82	121.90
44	5	2192	С	C5-C6-N1	7.25	124.62	121.00
44	5	3071	U	C5-C6-N1	7.24	126.32	122.70
44	5	3158	G	N1-C6-O6	7.24	124.25	119.90
44	5	1018	G	N1-C2-N2	7.24	122.71	116.20
44	5	235	A	C5-N7-C8	-7.24	100.28	103.90
44	5	3230	G	C8-N9-C1'	7.24	136.41	127.00
44	5	3370	А	N9-C4-C5	-7.24	102.91	105.80
44	5	1496	С	C2-N1-C1'	7.23	126.76	118.80
44	5	2948	С	O5'-P-OP2	-7.23	99.19	105.70
44	5	3349	С	C5-C6-N1	7.23	124.61	121.00
44	5	2928	С	N1-C2-O2	7.23	123.24	118.90
44	5	1633	С	N1-C2-O2	7.22	123.23	118.90
44	5	307	A	C8-N9-C4	7.22	108.69	105.80
44	5	2358	А	C5-N7-C8	-7.21	100.29	103.90
44	5	59	G	N1-C6-O6	7.21	124.23	119.90
44	5	2606	G	N3-C4-C5	-7.21	125.00	128.60
44	5	178	U	C5-C6-N1	7.21	126.30	122.70
44	5	998	A	N7-C8-N9	7.21	117.40	113.80
44	5	1268	G	C5-N7-C8	-7.21	100.70	104.30
45	8	120	С	C2-N1-C1'	7.21	126.73	118.80
44	5	374	А	C8-N9-C4	7.20	108.68	105.80
44	5	3248	С	C6-N1-C2	-7.20	117.42	120.30
44	5	2358	A	C4-C5-N7	7.20	114.30	110.70
44	5	3197	G	N3-C4-N9	-7.20	121.68	126.00
44	5	1878	G	C4-N9-C1'	7.20	135.86	126.50
44	5	2358	A	N1-C6-N6	7.20	122.92	118.60
44	5	3306	U	N1-C2-O2	7.20	127.84	122.80
44	5	2197	C	N3-C4-C5	7.20	124.78	121.90
44	5	575	G	C4-C5-N7	7.19	113.68	110.80
44	5	786	А	N1-C2-N3	-7.19	125.71	129.30
44	5	1078	U	N3-C2-O2	-7.18	117.17	122.20
44	5	161	G	O4'-C1'-N9	7.18	113.94	108.20
44	5	3383	G	N3-C2-N2	-7.18	114.88	119.90
44	5	142	C	N1-C2-O2	7.17	123.20	118.90
44	5	2901	G	C5-N7-C8	-7.17	100.72	104.30
44	5	3119	U	C5-C6-N1	7.16	126.28	122.70
44	5	3325	G	C5-C6-O6	-7.16	124.31	128.60
44	5	786	A	C4-C5-C6	-7.16	113.42	117.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2582	С	C2-N1-C1'	7.16	126.67	118.80
44	5	1904	С	C6-N1-C2	-7.15	117.44	120.30
44	5	1260	А	C6-N1-C2	7.15	122.89	118.60
44	5	2283	G	C4-N9-C1'	-7.15	117.21	126.50
44	5	3269	U	C2-N1-C1'	7.15	126.28	117.70
44	5	2867	С	C6-N1-C2	-7.15	117.44	120.30
44	5	1279	С	N3-C2-O2	-7.14	116.90	121.90
44	5	517	G	C2-N3-C4	-7.14	108.33	111.90
44	5	2447	А	C4-C5-N7	7.14	114.27	110.70
44	5	353	G	C4-N9-C1'	-7.13	117.23	126.50
44	5	1826	С	N1-C2-O2	7.13	123.18	118.90
44	5	955	U	N1-C2-O2	7.12	127.79	122.80
44	5	1349	G	N3-C4-N9	7.12	130.27	126.00
46	7	78	U	C5-C6-N1	7.12	126.26	122.70
44	5	2932	U	C5-C6-N1	7.12	126.26	122.70
44	5	680	G	C4-N9-C1'	-7.12	117.25	126.50
44	5	3266	G	N3-C4-N9	-7.12	121.73	126.00
44	5	353	G	N3-C4-N9	-7.11	121.73	126.00
44	5	12	А	N3-C4-C5	7.11	131.78	126.80
44	5	2534	G	C5-C6-O6	7.11	132.87	128.60
44	5	881	С	C2-N1-C1'	7.10	126.61	118.80
44	5	82	С	C6-N1-C2	7.10	123.14	120.30
44	5	51	A	C5-N7-C8	-7.10	100.35	103.90
44	5	1404	G	N9-C4-C5	-7.10	102.56	105.40
44	5	2235	C	N3-C2-O2	-7.10	116.93	121.90
44	5	3260	G	N3-C4-N9	7.10	130.26	126.00
44	5	2992	U	N3-C2-O2	-7.09	117.24	122.20
28	a	197	GLY	N-CA-C	7.08	130.81	113.10
46	7	36	С	C6-N1-C2	-7.08	117.47	120.30
44	5	545	U	N1-C2-O2	7.08	127.75	122.80
44	5	1263	А	N9-C4-C5	-7.08	102.97	105.80
44	5	2983	С	C6-N1-C1'	-7.07	112.31	120.80
44	5	1303	A	C8-N9-C4	7.07	108.63	105.80
44	5	743	С	C5-C6-N1	7.07	124.53	121.00
44	5	2901	G	C4-C5-N7	7.07	113.63	110.80
44	5	680	G	C6-C5-N7	7.06	134.64	130.40
44	5	2594	C	N1-C2-O2	7.06	123.14	118.90
44	5	1421	G	N1-C6-O6	-7.06	115.66	119.90
44	5	1648	A	N7-C8-N9	7.06	117.33	113.80
45	8	118	C	N1-C2-O2	7.06	123.14	118.90
44	5	1604	G	C4-N9-C1'	7.06	135.68	126.50
46	7	31	U	N1-C2-O2	7.06	127.74	122.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	561	С	C5-C6-N1	7.05	124.53	121.00
46	7	105	С	N1-C2-O2	7.05	123.13	118.90
44	5	38	U	N3-C2-O2	-7.05	117.27	122.20
44	5	613	G	C4-C5-N7	7.04	113.62	110.80
44	5	449	U	C5-C6-N1	7.04	126.22	122.70
44	5	3135	U	N3-C2-O2	-7.04	117.27	122.20
44	5	2171	G	C5-C6-O6	7.04	132.82	128.60
44	5	492	С	C5-C4-N4	-7.03	115.28	120.20
44	5	1251	А	N1-C6-N6	-7.03	114.38	118.60
44	5	3058	U	N1-C2-O2	7.03	127.72	122.80
44	5	1238	С	OP1-P-OP2	-7.02	109.06	119.60
44	5	1714	А	C2-N3-C4	-7.02	107.09	110.60
44	5	3104	U	C5-C4-O4	-7.02	121.69	125.90
44	5	374	А	N3-C4-C5	7.01	131.71	126.80
44	5	3360	С	N1-C2-O2	7.01	123.11	118.90
44	5	140	С	C5-C6-N1	7.01	124.50	121.00
44	5	659	G	C5-N7-C8	-7.01	100.80	104.30
44	5	680	G	O4'-C1'-N9	7.01	113.81	108.20
44	5	1282	G	N1-C6-O6	-7.01	115.69	119.90
44	5	2572	С	C6-N1-C2	-7.01	117.50	120.30
44	5	2195	С	N1-C2-O2	7.00	123.10	118.90
44	5	3313	U	N1-C2-O2	7.00	127.70	122.80
44	5	678	G	C4-C5-N7	7.00	113.60	110.80
44	5	1301	А	O4'-C1'-N9	-7.00	102.60	108.20
44	5	2545	С	C5-C6-N1	7.00	124.50	121.00
44	5	113	С	C2-N1-C1'	7.00	126.49	118.80
45	8	140	G	N1-C6-O6	6.99	124.10	119.90
44	5	2726	С	N3-C2-O2	-6.99	117.01	121.90
44	5	643	U	N1-C2-O2	6.98	127.69	122.80
44	5	1497	С	C5-C6-N1	6.98	124.49	121.00
44	5	1806	А	C5-N7-C8	-6.98	100.41	103.90
44	5	2562	А	C4-C5-N7	6.98	114.19	110.70
44	5	12	А	C2-N3-C4	-6.97	107.11	110.60
44	5	2582	С	C5-C6-N1	6.97	124.49	121.00
44	5	561	С	N1-C2-O2	6.97	123.08	118.90
44	5	2478	C	OP1-P-OP2	6.97	130.05	119.60
44	5	397	A	C4-C5-N7	6.97	114.18	110.70
44	5	1824	U	N3-C2-O2	-6.96	117.33	122.20
44	5	2619	G	N3-C4-N9	6.96	130.18	126.00
44	5	1718	G	N1-C6-O6	6.96	124.08	119.90
44	5	$25\overline{34}$	G	N1-C6-O6	-6.96	115.72	119.90
44	5	3030	G	N3-C2-N2	-6.96	115.03	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1249	G	N1-C6-O6	-6.96	115.72	119.90
46	7	1	G	C2-N3-C4	6.96	115.38	111.90
44	5	897	U	N3-C2-O2	-6.96	117.33	122.20
44	5	126	U	N1-C2-O2	6.96	127.67	122.80
44	5	538	G	C8-N9-C4	-6.95	103.62	106.40
44	5	1266	G	C4-C5-N7	6.95	113.58	110.80
44	5	2452	G	N1-C6-O6	6.95	124.07	119.90
44	5	1641	U	C5-C4-O4	-6.95	121.73	125.90
44	5	2235	С	N1-C2-O2	6.94	123.06	118.90
45	8	77	А	C5-C6-N1	6.94	121.17	117.70
46	7	35	С	N1-C2-O2	6.94	123.06	118.90
44	5	1087	G	C4-C5-N7	6.94	113.58	110.80
44	5	2619	G	C4-N9-C1'	6.94	135.52	126.50
44	5	1201	С	N1-C2-O2	6.94	123.06	118.90
44	5	1508	C	N1-C2-O2	6.94	123.06	118.90
44	5	2552	C	N1-C2-O2	6.94	123.06	118.90
44	5	2726	С	C6-N1-C2	-6.94	117.53	120.30
44	5	82	С	N1-C2-O2	6.93	123.06	118.90
44	5	1633	С	N3-C2-O2	-6.92	117.05	121.90
44	5	500	С	N1-C2-O2	6.92	123.05	118.90
44	5	538	G	C5-N7-C8	-6.92	100.84	104.30
44	5	524	U	C4-C5-C6	-6.92	115.55	119.70
44	5	1591	G	C4-N9-C1'	6.92	135.49	126.50
44	5	2358	A	N9-C4-C5	-6.92	103.03	105.80
44	5	82	С	N3-C4-C5	6.92	124.67	121.90
45	8	102	U	N3-C2-O2	-6.91	117.36	122.20
44	5	95	A	C5-N7-C8	-6.91	100.44	103.90
44	5	2195	C	N3-C2-O2	-6.91	117.06	121.90
44	5	2726	C	C2-N1-C1'	6.91	126.40	118.80
46	7	64	A	N1-C6-N6	-6.91	114.46	118.60
44	5	328	U	C5-C6-N1	6.90	126.15	122.70
44	5	1573	G	C5-N7-C8	-6.90	100.85	104.30
44	5	1785	U	N3-C2-O2	-6.90	117.37	122.20
45	8	28	C	N3-C2-O2	-6.89	117.07	121.90
44	5	752	C	N1-C2-O2	6.89	123.03	118.90
44	5	2863	G	C8-N9-C4	-6.89	103.64	106.40
45	8	41	A	NI-C6-N6	6.89	122.73	118.60
44	5	2531		N3-C2-O2	-6.88	117.08	121.90
46	<u>'</u> (G	N3-C4-N9	6.88	130.13	126.00
44	5	120	G	N3-C4-C5	6.88	132.04	128.60
44	5	907	G	N3-C4-C5	6.88	132.04	128.60
44	5	- 77	A	N9-C4-C5	-6.87	103.05	105.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	3308	С	C5-C6-N1	6.87	124.43	121.00
44	5	1206	G	N9-C4-C5	-6.87	102.65	105.40
44	5	1018	G	N1-C6-O6	6.87	124.02	119.90
44	5	1645	U	N3-C2-O2	-6.87	117.39	122.20
44	5	130	А	C4-C5-N7	6.86	114.13	110.70
44	5	1082	U	N1-C2-O2	6.86	127.60	122.80
44	5	1535	А	C5-N7-C8	-6.86	100.47	103.90
44	5	299	G	C4-C5-N7	6.86	113.54	110.80
44	5	127	G	N7-C8-N9	6.85	116.53	113.10
44	5	173	G	N3-C2-N2	-6.85	115.10	119.90
44	5	1547	G	N3-C4-N9	-6.85	121.89	126.00
44	5	1550	С	C5-C6-N1	6.85	124.43	121.00
44	5	1130	А	N7-C8-N9	6.85	117.22	113.80
46	7	43	U	N3-C2-O2	-6.85	117.41	122.20
44	5	793	С	N1-C2-O2	6.85	123.01	118.90
44	5	2684	С	C6-N1-C2	-6.84	117.56	120.30
44	5	1351	U	N3-C2-O2	-6.84	117.41	122.20
44	5	2928	С	C2-N1-C1'	6.84	126.33	118.80
44	5	400	G	C4-C5-N7	6.84	113.53	110.80
44	5	1260	А	N1-C2-N3	-6.83	125.88	129.30
44	5	851	С	C2-N1-C1'	6.83	126.31	118.80
44	5	1717	U	C5-C6-N1	6.83	126.12	122.70
44	5	489	U	C5-C6-N1	6.82	126.11	122.70
44	5	196	G	N3-C2-N2	6.82	124.67	119.90
44	5	1190	А	N1-C2-N3	-6.82	125.89	129.30
44	5	1752	А	N1-C6-N6	6.82	122.69	118.60
44	5	443	G	C8-N9-C1'	6.81	135.86	127.00
44	5	500	С	C2-N1-C1'	6.81	126.29	118.80
44	5	2238	G	C4-C5-N7	6.81	113.53	110.80
44	5	1258	U	C6-N1-C2	-6.81	116.91	121.00
44	5	2149	А	C5-C6-N1	6.81	121.10	117.70
44	5	3269	U	N3-C2-O2	-6.81	117.43	122.20
44	5	2585	G	C4-N9-C1'	6.80	135.34	126.50
44	5	2766	U	N1-C2-O2	6.80	127.56	122.80
44	5	2763	U	N3-C2-O2	-6.80	117.44	122.20
45	8	87	G	N3-C4-C5	6.80	132.00	128.60
44	5	149	U	C6-N1-C2	-6.80	116.92	121.00
44	5	3265	C	C2-N1-C1	6.80	126.28	118.80
45	8	140	G	$C5-C6-\overline{O6}$	-6.80	$124.5\overline{2}$	128.60
44	5	3034	C	N3-C2-O2	-6.79	117.15	121.90
44	5	2619	G	C8-N9-C1	-6.78	118.19	127.00
44	5	545	U	C2-N1-C1'	6.78	125.83	117.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	3181	С	C6-N1-C1'	-6.78	112.67	120.80
44	5	3334	U	N1-C2-N3	-6.78	110.83	114.90
44	5	1224	С	N3-C4-C5	6.77	124.61	121.90
44	5	172	G	N3-C2-N2	-6.77	115.16	119.90
44	5	2534	G	C4-N9-C1'	-6.77	117.70	126.50
44	5	1181	U	C5-C4-O4	-6.76	121.84	125.90
44	5	2603	G	N3-C2-N2	-6.76	115.17	119.90
44	5	1871	U	N3-C2-O2	-6.76	117.47	122.20
44	5	1223	А	C5-N7-C8	-6.75	100.52	103.90
44	5	1077	U	C5-C6-N1	6.75	126.08	122.70
44	5	545	U	N3-C2-O2	-6.75	117.48	122.20
44	5	437	G	C5-N7-C8	-6.74	100.93	104.30
44	5	998	А	C5-N7-C8	-6.74	100.53	103.90
44	5	1951	С	C5-C6-N1	6.74	124.37	121.00
44	5	168	U	C2-N1-C1'	-6.74	109.61	117.70
44	5	1767	С	N1-C2-O2	6.74	122.94	118.90
44	5	3197	G	C2-N3-C4	-6.74	108.53	111.90
44	5	1228	С	C6-N1-C2	-6.73	117.61	120.30
44	5	3153	U	C6-N1-C1'	-6.73	111.77	121.20
44	5	2884	C	C5-C6-N1	6.73	124.37	121.00
44	5	2550	U	N3-C2-O2	-6.73	117.49	122.20
46	7	120	С	N1-C2-O2	6.73	122.94	118.90
44	5	3265	С	N1-C2-O2	6.72	122.93	118.90
44	5	1638	A	C8-N9-C4	6.72	108.49	105.80
44	5	411	U	N1-C2-O2	6.71	127.50	122.80
44	5	2541	U	N3-C4-C5	6.71	118.63	114.60
44	5	1251	A	N1-C2-N3	6.71	132.66	129.30
44	5	3238	G	N3-C2-N2	-6.71	115.20	119.90
45	8	149	A	C2-N3-C4	-6.71	107.25	110.60
44	5	1082	U	N3-C2-O2	-6.70	117.51	122.20
44	5	230	U	N3-C2-O2	-6.70	117.51	122.20
44	5	1396	С	C5-C6-N1	6.70	124.35	121.00
44	5	1556	С	N3-C2-O2	-6.70	117.21	121.90
44	5	3230	G	C4-N9-C1'	-6.70	117.79	126.50
44	5	321	С	C2-N1-C1'	6.70	126.17	118.80
44	5	1046	A	N1-C2-N3	-6.70	125.95	129.30
44	5	1263	A	N1-C6-N6	6.70	122.62	118.60
44	5	1960	A	C2-N3-C4	6.70	113.95	110.60
44	5	2960	C	C5-C6-N1	6.70	124.35	121.00
44	5	2434	U	C6-N1-C1'	-6.70	111.82	121.20
44	5	3187	A	C8-N9-C4	-6.70	103.12	105.80
44	5	340	C	C4-C5-C6	-6.69	114.05	117.40



Continued from previous page									
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$		
44	5	1625	А	C8-N9-C4	-6.69	103.12	105.80		
45	8	46	G	C2-N3-C4	6.69	115.25	111.90		
44	5	638	С	C6-N1-C2	-6.69	117.62	120.30		
44	5	855	U	C2-N1-C1'	6.68	125.72	117.70		
44	5	2819	А	C6-N1-C2	6.68	122.61	118.60		
44	5	1805	С	N3-C2-O2	-6.68	117.22	121.90		
44	5	162	G	C4-C5-N7	6.68	113.47	110.80		
44	5	173	G	N1-C2-N2	6.68	122.21	116.20		
46	7	44	С	C6-N1-C2	-6.68	117.63	120.30		
44	5	1479	U	N1-C2-O2	6.68	127.47	122.80		
44	5	2726	С	N1-C2-O2	6.68	122.91	118.90		
44	5	2656	А	N9-C4-C5	-6.67	103.13	105.80		
44	5	529	А	C4-C5-N7	6.67	114.04	110.70		
44	5	1266	G	N1-C6-O6	6.67	123.90	119.90		
44	5	1168	U	N1-C2-O2	6.67	127.47	122.80		
44	5	2652	U	N3-C2-O2	-6.67	117.53	122.20		
44	5	2469	G	C6-C5-N7	-6.67	126.40	130.40		
44	5	2526	С	N1-C2-O2	6.67	122.90	118.90		
46	7	27	А	N7-C8-N9	6.67	117.13	113.80		
44	5	492	С	C2-N1-C1'	6.67	126.13	118.80		
44	5	2867	С	C2-N1-C1'	6.66	126.13	118.80		
44	5	382	U	C5-C6-N1	6.66	126.03	122.70		
44	5	406	G	N3-C4-C5	6.66	131.93	128.60		
44	5	675	С	C2-N1-C1'	6.66	126.12	118.80		
44	5	271	С	N3-C2-O2	-6.65	117.24	121.90		
44	5	54	С	N1-C2-O2	6.65	122.89	118.90		
44	5	397	А	C5-C6-N6	-6.65	118.38	123.70		
44	5	2263	С	O3'-P-O5'	-6.65	91.37	104.00		
44	5	307	А	N3-C4-C5	6.64	131.45	126.80		
44	5	2381	G	N9-C4-C5	-6.64	102.74	105.40		
44	5	126	U	N3-C2-O2	-6.64	117.55	122.20		
44	5	1854	С	C5-C6-N1	6.64	124.32	121.00		
44	5	2576	G	C5-C6-O6	-6.64	124.62	128.60		
44	5	3153	U	N1-C2-O2	6.64	127.45	122.80		
44	5	179	С	C6-N1-C2	-6.63	117.65	120.30		
44	5	1037	С	C6-N1-C2	-6.63	117.65	120.30		
44	5	380	U	N3-C2-O2	-6.63	117.56	122.20		
44	5	1448	U	N1-C2-O2	6.62	127.44	122.80		
44	5	2134	G	C2-N3-C4	6.62	115.21	111.90		
44	5	2187	G	C8-N9-C4	6.62	109.05	106.40		
44	5	1637	A	C8-N9-C4	-6.62	103.15	105.80		
46	7	38	U	N1-C2-O2	6.62	127.43	122.80		



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
44	5	1573	G	C4-C5-N7	6.61	113.45	110.80
44	5	1501	U	C2-N1-C1'	6.61	125.64	117.70
46	7	36	С	C5-C6-N1	6.61	124.31	121.00
44	5	1170	А	C5-N7-C8	-6.61	100.59	103.90
44	5	1404	G	C8-N9-C4	6.61	109.04	106.40
44	5	3354	U	N1-C2-O2	6.61	127.43	122.80
44	5	234	G	C4-C5-N7	6.61	113.44	110.80
44	5	3260	G	N9-C4-C5	-6.61	102.76	105.40
4	С	299	ILE	C-N-CA	-6.61	105.19	121.70
44	5	406	G	C8-N9-C4	6.61	109.04	106.40
44	5	2353	G	N1-C6-O6	6.61	123.86	119.90
44	5	549	U	C5-C6-N1	6.60	126.00	122.70
44	5	307	А	C2-N3-C4	-6.60	107.30	110.60
44	5	1254	С	C5-C6-N1	6.60	124.30	121.00
44	5	3312	U	N1-C2-O2	6.60	127.42	122.80
45	8	28	С	C5-C6-N1	6.60	124.30	121.00
44	5	1577	G	N3-C4-C5	6.59	131.90	128.60
44	5	1878	G	C8-N9-C1'	-6.58	118.44	127.00
44	5	2532	U	C5-C6-N1	6.58	125.99	122.70
44	5	945	С	C2-N1-C1'	6.58	126.04	118.80
44	5	3057	U	N1-C2-O2	6.58	127.41	122.80
44	5	17	G	N3-C2-N2	-6.58	115.30	119.90
44	5	31	С	N1-C2-O2	6.58	122.84	118.90
44	5	59	G	C5-C6-O6	-6.58	124.66	128.60
44	5	433	А	N7-C8-N9	6.57	117.09	113.80
44	5	1236	G	N1-C2-N2	-6.57	110.29	116.20
44	5	2486	А	C8-N9-C4	6.57	108.43	105.80
44	5	855	U	N1-C2-O2	6.56	127.39	122.80
44	5	1170	А	N7-C8-N9	6.56	117.08	113.80
45	8	55	U	N3-C2-O2	-6.56	117.61	122.20
44	5	175	С	C2-N1-C1'	6.56	126.02	118.80
44	5	680	G	C8-N9-C1'	6.56	135.53	127.00
44	5	1239	С	C5-C4-N4	6.56	124.79	120.20
44	5	8	С	N3-C4-N4	-6.56	113.41	118.00
44	5	3278	С	C2-N1-C1'	6.56	126.01	118.80
44	5	1591	G	C8-N9-C1'	-6.55	118.48	127.00
44	5	1392	G	N3-C4-N9	-6.55	$1\overline{22.07}$	126.00
44	5	1873	U	N1-C2-O2	6.55	$1\overline{27.38}$	122.80
45	8	8	C	C6-N1-C2	-6.55	117.68	120.30
44	5	2516	U	C5-C6-N1	6.54	125.97	122.70
44	5	342	A	N1-C6-N6	-6.54	114.68	118.60
12	S	260	ARG	C-N-CA	6.53	138.03	121.70



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1825	G	N3-C4-N9	6.53	129.92	126.00
44	5	547	G	N1-C2-N2	6.53	122.08	116.20
44	5	1155	С	N3-C2-O2	-6.53	117.33	121.90
44	5	1392	G	C2-N3-C4	-6.53	108.64	111.90
44	5	175	С	C5-C6-N1	6.53	124.26	121.00
44	5	2188	А	N9-C4-C5	-6.52	103.19	105.80
44	5	2298	U	N1-C2-O2	6.52	127.37	122.80
44	5	2971	A	C2-N3-C4	6.52	113.86	110.60
44	5	525	C	N1-C2-O2	6.52	122.81	118.90
44	5	1497	C	C6-N1-C2	-6.52	117.69	120.30
44	5	2534	G	N3-C4-C5	6.52	131.86	128.60
44	5	1349	G	C4-N9-C1'	6.51	134.97	126.50
44	5	3313	U	N3-C2-O2	-6.51	117.64	122.20
44	5	503	С	C6-N1-C2	-6.51	117.69	120.30
44	5	1705	U	C5-C6-N1	6.51	125.96	122.70
44	5	1306	G	N9-C4-C5	-6.51	102.80	105.40
44	5	2354	С	C6-N1-C2	-6.50	117.70	120.30
44	5	2780	A	C8-N9-C4	6.50	108.40	105.80
44	5	3124	G	N1-C6-O6	-6.50	116.00	119.90
44	5	1078	U	N1-C2-O2	6.50	127.35	122.80
44	5	1086	С	N3-C2-O2	-6.50	117.35	121.90
44	5	142	С	C6-N1-C2	-6.49	117.70	120.30
44	5	400	G	N1-C6-O6	6.49	123.80	119.90
44	5	2468	A	N1-C2-N3	-6.49	126.05	129.30
45	8	32	С	N3-C2-O2	-6.49	117.36	121.90
44	5	3346	U	C5-C6-N1	6.49	125.95	122.70
45	8	87	G	O4'-C1'-N9	6.49	113.39	108.20
44	5	851	С	C5-C6-N1	6.49	124.24	121.00
44	5	3058	U	N3-C2-O2	-6.49	117.66	122.20
44	5	1427	U	N1-C2-O2	6.49	127.34	122.80
44	5	2562	A	C5-C6-N6	-6.49	118.51	123.70
44	5	2617	U	N3-C2-O2	-6.49	117.66	122.20
44	5	2901	G	C2-N3-C4	-6.48	108.66	111.90
44	5	1501	U	N3-C2-O2	-6.48	117.67	122.20
46	7	39	С	N3-C2-O2	-6.48	117.37	121.90
44	5	2355	G	C8-N9-C4	6.47	108.99	106.40
44	5	2899	C	N3-C2-O2	-6.47	117.37	121.90
44	5	3309	G	C8-N9-C1'	-6.47	118.58	127.00
44	5	2205	U	N3-C2-O2	-6.47	117.67	122.20
44	5	835	G	C4-N9-C1'	-6.47	118.09	126.50
44	5	1950	U	N1-C2-O2	6.47	127.33	122.80
44	5	3102	G G	C4-C5-N7	6.47	113.39	110.80



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
44	5	2819	А	N1-C2-N3	-6.47	126.06	129.30
44	5	3110	С	N1-C2-O2	6.47	122.78	118.90
45	8	8	С	C2-N3-C4	6.46	123.13	119.90
44	5	621	А	C4-C5-N7	6.46	113.93	110.70
44	5	614	С	N1-C2-O2	6.46	122.78	118.90
44	5	1211	U	C5-C6-N1	6.46	125.93	122.70
44	5	352	А	C8-N9-C4	6.46	108.38	105.80
44	5	1447	G	N3-C4-N9	-6.46	122.13	126.00
44	5	1514	G	C4-N9-C1'	6.46	134.89	126.50
44	5	529	А	C5-N7-C8	-6.45	100.67	103.90
44	5	862	U	N1-C2-O2	6.45	127.32	122.80
44	5	2355	G	N9-C4-C5	-6.45	102.82	105.40
44	5	3312	U	N3-C2-O2	-6.45	117.68	122.20
44	5	2469	G	C5-N7-C8	-6.45	101.08	104.30
44	5	3200	G	N3-C2-N2	-6.45	115.39	119.90
44	5	1246	G	C5-N7-C8	-6.45	101.08	104.30
44	5	1907	С	C6-N1-C2	-6.45	117.72	120.30
44	5	2477	G	C8-N9-C1'	-6.45	118.62	127.00
44	5	1220	U	O4'-C1'-N1	-6.44	103.05	108.20
45	8	49	G	C4-C5-N7	6.44	113.38	110.80
44	5	1645	U	N1-C2-O2	6.44	127.31	122.80
44	5	2486	А	OP1-P-OP2	-6.44	109.94	119.60
44	5	207	U	C5-C6-N1	6.44	125.92	122.70
44	5	3031	G	C6-C5-N7	-6.44	126.53	130.40
44	5	400	G	N9-C4-C5	-6.44	102.82	105.40
44	5	362	U	N1-C2-O2	6.43	127.31	122.80
44	5	2515	А	N1-C6-N6	6.43	122.46	118.60
44	5	1662	G	N1-C6-O6	6.43	123.76	119.90
44	5	2189	U	N1-C2-O2	6.43	127.30	122.80
44	5	2836	С	C6-N1-C1'	-6.43	113.09	120.80
44	5	1718	G	C5-N7-C8	-6.42	101.09	104.30
46	7	45	А	N9-C4-C5	-6.42	103.23	105.80
44	5	16	А	N9-C4-C5	-6.42	103.23	105.80
44	5	1021	G	C5-C6-O6	6.42	132.45	128.60
44	5	3109	G	N3-C4-N9	6.42	129.85	126.00
44	5	2720	G	C8-N9-C4	-6.42	103.83	106.40
44	5	2842	U	N1-C2-O2	6.42	127.29	122.80
44	5	2378	С	N1-C2-O2	6.41	122.75	118.90
44	5	111	С	N1-C2-O2	6.41	122.75	118.90
44	5	1078	U	C2-N1-C1'	6.41	125.39	117.70
44	5	2935	U	C6-N1-C1'	-6.41	112.23	121.20

5

44

517

G

Continued on next page...

104.30

101.10



-6.40

C5-N7-C8

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	786	А	C6-C5-N7	6.40	136.78	132.30
44	5	524	U	C5-C4-O4	-6.40	122.06	125.90
44	5	1547	G	C8-N9-C1'	6.40	135.32	127.00
44	5	3089	С	C6-N1-C2	-6.40	117.74	120.30
44	5	3325	G	C4-C5-N7	6.40	113.36	110.80
44	5	1591	G	C4-C5-N7	6.40	113.36	110.80
44	5	1396	С	C6-N1-C2	-6.39	117.74	120.30
44	5	2204	С	C5-C6-N1	6.39	124.20	121.00
44	5	2928	С	C5-C6-N1	6.39	124.20	121.00
44	5	714	G	OP2-P-O3'	6.39	119.26	105.20
44	5	2343	С	C5-C6-N1	6.39	124.20	121.00
44	5	192	С	C5-C6-N1	6.38	124.19	121.00
44	5	3091	A	C5-N7-C8	-6.38	100.71	103.90
44	5	2992	U	N1-C2-O2	6.38	127.27	122.80
44	5	681	U	N1-C2-O2	6.38	127.26	122.80
44	5	1268	G	N7-C8-N9	6.38	116.29	113.10
44	5	1229	G	N9-C4-C5	-6.37	102.85	105.40
44	5	54	С	N3-C2-O2	-6.37	117.44	121.90
44	5	2101	С	P-O3'-C3'	6.37	127.34	119.70
44	5	3344	A	C5-C6-N1	6.37	120.89	117.70
44	5	1037	С	C5-C6-N1	6.37	124.18	121.00
44	5	1283	С	C5-C6-N1	6.37	124.19	121.00
44	5	2846	U	C2-N1-C1'	6.37	125.34	117.70
44	5	2285	С	C6-N1-C2	-6.37	117.75	120.30
44	5	3007	U	C5-C6-N1	6.37	125.88	122.70
44	5	162	G	C5-N7-C8	-6.37	101.12	104.30
44	5	2966	G	N3-C4-C5	6.37	131.78	128.60
44	5	1898	G	N3-C2-N2	-6.36	115.44	119.90
44	5	2622	C	C6-N1-C2	-6.36	117.75	120.30
44	5	2638	C	N1-C2-O2	6.36	122.72	118.90
44	5	2821	С	N1-C2-O2	6.36	122.72	118.90
44	5	2351	U	N1-C2-O2	6.36	127.25	122.80
44	5	3234	A	C2-N3-C4	-6.36	107.42	110.60
44	5	437	G	N1-C6-O6	6.36	123.71	119.90
44	5	1637	A	C2-N3-C4	6.36	113.78	110.60
44	5	1749	A	N1-C2-N3	-6.36	126.12	129.30
44	5	437	G	C4-C5-N7	6.36	113.34	110.80
44	5	717	C	C2-N1-C1	6.35	125.79	118.80
44	5	2768	U	N3-C2-O2	-6.35	117.75	122.20
44	5	1359	C	C6-N1-C1'	-6.35	113.18	120.80
44	5	1514	G	N3-C4-N9	6.35	129.81	126.00
44	5	2844	C	C2-N3-C4	-6.35	116.73	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	544	С	C5-C6-N1	6.35	124.17	121.00
44	5	155	G	C8-N9-C1'	6.34	135.25	127.00
44	5	2118	С	N3-C2-O2	-6.34	117.46	121.90
44	5	2576	G	N1-C6-O6	6.34	123.71	119.90
44	5	1591	G	N3-C4-N9	6.34	129.81	126.00
44	5	1727	G	C4-C5-N7	6.34	113.34	110.80
44	5	3371	G	C8-N9-C4	-6.34	103.86	106.40
44	5	2709	С	N1-C2-O2	6.34	122.70	118.90
44	5	2889	С	C5-C6-N1	6.34	124.17	121.00
44	5	331	G	C4-N9-C1'	-6.33	118.27	126.50
44	5	2772	С	N3-C2-O2	-6.33	117.47	121.90
46	7	39	С	C5-C6-N1	6.33	124.17	121.00
44	5	3200	G	N3-C4-C5	6.33	131.76	128.60
46	7	31	U	N3-C2-O2	-6.33	117.77	122.20
44	5	212	G	C5-C6-O6	6.33	132.40	128.60
44	5	437	G	C6-C5-N7	-6.33	126.60	130.40
44	5	3349	С	C6-N1-C2	-6.33	117.77	120.30
44	5	3354	U	N3-C2-O2	-6.33	117.77	122.20
44	5	3306	U	N3-C2-O2	-6.33	117.77	122.20
44	5	3161	С	N1-C2-O2	6.33	122.69	118.90
44	5	3298	С	C5-C6-N1	6.33	124.16	121.00
44	5	735	А	N7-C8-N9	6.32	116.96	113.80
44	5	2307	G	N3-C4-C5	6.32	131.76	128.60
44	5	1033	U	N1-C2-N3	6.32	118.69	114.90
44	5	3288	G	N3-C4-N9	-6.32	122.21	126.00
44	5	618	С	C6-N1-C2	-6.32	117.77	120.30
44	5	1577	G	N3-C2-N2	-6.31	115.48	119.90
44	5	443	G	N3-C4-N9	-6.31	122.21	126.00
44	5	543	С	C6-N1-C2	-6.31	117.78	120.30
44	5	1640	G	N3-C4-C5	6.31	131.75	128.60
44	5	786	А	C8-N9-C4	6.30	108.32	105.80
46	7	60	G	C2-N3-C4	6.30	115.05	111.90
44	5	36	С	N3-C2-O2	-6.30	117.49	121.90
44	5	1278	A	C2-N3-C4	6.30	113.75	110.60
44	5	2195	С	C2-N1-C1'	6.30	125.73	118.80
44	5	3145	C	N1-C2-O2	6.30	122.68	118.90
44	5	2381	G	C8-N9-C4	6.30	108.92	106.40
44	5	2783	U	C5-C6-N1	6.30	125.85	122.70
44	5	1535	A	N7-C8-N9	6.29	116.95	113.80
44	5	922	U	C6-N1-C1'	-6.29	112.39	121.20
44	5	1785	U	N1-C2-O2	6.29	127.21	122.80
45	8	17	A	N1-C6-N6	6.29	122.38	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	3106	A	N7-C8-N9	6.29	116.94	113.80
44	5	254	A	C5-N7-C8	-6.29	100.75	103.90
44	5	2351	U	N3-C2-O2	-6.29	117.80	122.20
44	5	142	С	C5-C6-N1	6.29	124.14	121.00
44	5	218	G	N1-C2-N3	6.29	127.67	123.90
44	5	388	G	N3-C2-N2	-6.29	115.50	119.90
44	5	2825	С	N3-C2-O2	-6.29	117.50	121.90
44	5	492	С	C6-N1-C1'	-6.28	113.26	120.80
44	5	1224	С	C6-N1-C2	-6.28	117.79	120.30
46	7	43	U	N1-C2-O2	6.28	127.20	122.80
44	5	131	С	C5-C6-N1	6.28	124.14	121.00
44	5	155	G	C4-N9-C1'	-6.28	118.34	126.50
44	5	313	А	N9-C4-C5	-6.28	103.29	105.80
44	5	629	U	C5-C6-N1	6.28	125.84	122.70
44	5	1238	С	C5-C6-N1	6.28	124.14	121.00
44	5	532	A	C2-N3-C4	-6.28	107.46	110.60
44	5	1349	G	N1-C6-O6	-6.28	116.14	119.90
44	5	3383	G	C8-N9-C4	-6.28	103.89	106.40
44	5	978	G	N9-C4-C5	-6.27	102.89	105.40
44	5	3371	G	N7-C8-N9	6.27	116.23	113.10
44	5	1854	С	C6-N1-C2	-6.26	117.79	120.30
44	5	3083	G	N9-C4-C5	-6.26	102.89	105.40
45	8	25	G	C4-C5-N7	6.26	113.30	110.80
44	5	699	А	N7-C8-N9	6.26	116.93	113.80
44	5	2576	G	C4-C5-N7	6.26	113.30	110.80
44	5	27	С	C6-N1-C2	-6.26	117.80	120.30
44	5	2187	G	N7-C8-N9	-6.26	109.97	113.10
44	5	2132	С	N3-C2-O2	-6.25	117.52	121.90
44	5	3197	G	N3-C4-C5	6.25	131.72	128.60
44	5	96	G	C8-N9-C4	6.25	108.90	106.40
44	5	3333	G	N3-C4-C5	6.25	131.72	128.60
44	5	77	А	C4-C5-N7	6.25	113.82	110.70
44	5	219	A	N9-C4-C5	-6.24	103.30	105.80
44	5	503	С	C6-N1-C1'	-6.24	113.31	120.80
44	5	254	А	N7-C8-N9	6.24	116.92	113.80
44	5	1625	А	C5-N7-C8	-6.24	100.78	103.90
44	5	443	G	C4-N9-C1'	-6.24	118.39	126.50
44	5	1752	A	C6-C5-N7	-6.24	127.93	132.30
44	5	1800	A	C4-C5-N7	6.24	113.82	110.70
44	5	2285	С	C5-C6-N1	6.24	124.12	121.00
44	5	16	A	C4-C5-N7	6.24	113.82	110.70
44	5	429	U	N1-C2-O2	6.24	127.16	122.80



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
44	5	2711	С	C6-N1-C2	-6.24	117.81	120.30
44	5	2711	С	N1-C2-O2	6.24	122.64	118.90
45	8	148	G	N3-C4-N9	-6.23	122.26	126.00
44	5	1662	G	C5-C6-O6	-6.23	124.86	128.60
44	5	275	U	C5-C6-N1	6.23	125.81	122.70
44	5	124	U	N3-C2-O2	-6.23	117.84	122.20
44	5	1573	G	N1-C6-O6	6.23	123.64	119.90
44	5	1724	U	O4'-C1'-N1	6.22	113.18	108.20
44	5	2822	U	N3-C2-O2	-6.22	117.84	122.20
44	5	97	U	N1-C2-O2	6.22	127.15	122.80
44	5	1246	G	N3-C4-N9	-6.22	122.27	126.00
44	5	3105	U	N1-C2-O2	6.22	127.15	122.80
44	5	852	U	N3-C2-O2	-6.22	117.85	122.20
44	5	1260	А	N3-C4-C5	6.22	131.15	126.80
44	5	2224	А	C5-N7-C8	-6.22	100.79	103.90
44	5	386	А	C8-N9-C4	-6.22	103.31	105.80
44	5	434	U	C6-N1-C2	-6.21	117.27	121.00
44	5	2227	С	C5-C6-N1	6.21	124.11	121.00
44	5	2626	А	C5-C6-N6	-6.21	118.73	123.70
44	5	3273	А	N9-C4-C5	-6.21	103.31	105.80
46	7	44	С	C5-C4-N4	-6.21	115.85	120.20
46	7	27	А	C5-N7-C8	-6.21	100.80	103.90
44	5	1826	С	C2-N1-C1'	6.21	125.63	118.80
44	5	142	С	N3-C2-O2	-6.21	117.55	121.90
44	5	735	А	C5-N7-C8	-6.21	100.80	103.90
46	7	39	С	C6-N1-C2	-6.21	117.82	120.30
44	5	1260	А	C5-N7-C8	-6.21	100.80	103.90
46	7	112	G	C4-C5-N7	6.21	113.28	110.80
44	5	881	С	C2-N3-C4	6.20	123.00	119.90
44	5	1299	U	N3-C2-O2	-6.20	117.86	122.20
44	5	3029	A	N7-C8-N9	6.20	116.90	113.80
44	5	1005	G	N3-C4-N9	-6.20	122.28	126.00
44	5	1806	A	C4-N9-C1'	6.20	137.46	126.30
44	5	2948	С	C5-C6-N1	6.20	124.10	121.00
44	5	3253	G	N3-C2-N2	-6.20	115.56	119.90
44	5	1800	A	N1-C6-N6	6.19	122.32	118.60
45	8	129	С	C6-N1-C2	-6.19	117.82	120.30
44	5	1278	A	N1-C2-N3	-6.19	126.20	129.30
44	5	3191	G	C4-C5-N7	6.19	113.28	110.80
44	5	1766	G	N9-C4-C5	-6.19	102.92	105.40
44	5	1904	С	N3-C2-O2	-6.19	117.57	121.90
44	5	1222	G	O4'-C1'-N9	6.19	113.15	108.20



$\alpha \cdots $	c		
Continued	from	previous	page

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
44	5	2652	U	N1-C2-O2	6.18	127.13	122.80
44	5	3005	А	C8-N9-C4	6.18	108.27	105.80
44	5	1042	U	N3-C2-O2	-6.18	117.88	122.20
44	5	1473	G	C4-C5-N7	6.18	113.27	110.80
44	5	2132	С	C5-C6-N1	6.18	124.09	121.00
44	5	2353	G	C6-C5-N7	-6.18	126.69	130.40
9	Н	346	LEU	CA-CB-CG	6.17	129.49	115.30
44	5	2815	G	N1-C6-O6	-6.17	116.20	119.90
44	5	1066	G	C4-C5-N7	6.17	113.27	110.80
44	5	3212	С	C5-C6-N1	6.17	124.08	121.00
44	5	163	С	C2-N1-C1'	6.17	125.58	118.80
44	5	1057	А	C6-N1-C2	6.17	122.30	118.60
44	5	3018	С	N1-C2-O2	6.17	122.60	118.90
44	5	1920	U	N1-C2-O2	-6.16	118.49	122.80
44	5	3362	А	C5-N7-C8	-6.16	100.82	103.90
44	5	602	А	N7-C8-N9	6.16	116.88	113.80
44	5	1128	U	N1-C2-O2	6.16	127.11	122.80
44	5	204	А	C8-N9-C4	6.16	108.26	105.80
44	5	3163	А	N1-C6-N6	6.16	122.30	118.60
44	5	1351	U	C5-C6-N1	6.16	125.78	122.70
44	5	161	G	C4-N9-C1'	-6.15	118.50	126.50
44	5	422	А	N1-C2-N3	-6.15	126.22	129.30
44	5	2838	А	N1-C6-N6	6.15	122.29	118.60
44	5	3161	С	C2-N1-C1'	6.15	125.56	118.80
44	5	1427	U	N3-C2-O2	-6.15	117.90	122.20
44	5	2134	G	N3-C4-C5	-6.15	125.53	128.60
44	5	1322	U	N3-C2-O2	-6.15	117.90	122.20
44	5	1566	А	N1-C6-N6	6.15	122.29	118.60
44	5	3297	U	N1-C2-O2	6.14	127.10	122.80
44	5	121	А	N1-C6-N6	-6.14	114.91	118.60
44	5	3005	А	C4-C5-C6	-6.14	113.93	117.00
44	5	1222	G	C2-N3-C4	-6.14	108.83	111.90
30	с	16	LEU	CA-CB-CG	6.14	129.42	115.30
44	5	3110	С	C2-N1-C1'	6.14	125.55	118.80
44	5	308	А	O4'-C1'-N9	6.13	113.11	108.20
44	5	1272	С	N1-C2-O2	6.13	122.58	118.90
45	8	70	G	N1-C6-O6	-6.13	116.22	119.90
44	5	2515	А	C4-C5-N7	6.13	113.77	110.70
44	5	90	С	C6-N1-C2	-6.13	117.85	120.30
44	5	1604	G	C8-N9-C1'	-6.13	119.03	127.00
45	8	83	С	C5-C4-N4	-6.12	115.91	120.20
46	7	68	С	C5-C6-N1	6.12	124.06	121.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	838	G	C5-C6-O6	-6.12	124.93	128.60
44	5	2447	А	C5-N7-C8	-6.12	100.84	103.90
45	8	152	G	O5'-P-OP1	-6.12	100.19	105.70
44	5	680	G	N1-C6-O6	-6.12	116.23	119.90
44	5	1279	С	C2-N1-C1'	6.12	125.53	118.80
44	5	1805	С	C6-N1-C1'	6.11	128.14	120.80
44	5	2960	С	C6-N1-C2	-6.11	117.86	120.30
46	7	98	С	N3-C2-O2	-6.11	117.62	121.90
44	5	1437	С	N1-C2-O2	6.11	122.57	118.90
44	5	77	А	C5-C6-N6	-6.11	118.82	123.70
44	5	6	А	O4'-C1'-N9	6.10	113.08	108.20
44	5	3002	С	N1-C2-O2	6.10	122.56	118.90
44	5	130	А	N7-C8-N9	6.10	116.85	113.80
44	5	191	U	N3-C2-O2	-6.10	117.93	122.20
44	5	410	U	C5-C6-N1	6.10	125.75	122.70
44	5	1035	G	C4-C5-N7	6.10	113.24	110.80
44	5	406	G	C2-N3-C4	-6.09	108.85	111.90
44	5	1278	А	N1-C6-N6	-6.09	114.94	118.60
44	5	3122	А	C5-C6-N6	-6.09	118.83	123.70
44	5	335	G	C6-C5-N7	-6.09	126.75	130.40
44	5	1349	G	N3-C4-C5	-6.09	125.55	128.60
44	5	3273	А	C5-C6-N6	-6.09	118.83	123.70
44	5	271	С	N1-C2-O2	6.09	122.55	118.90
44	5	185	С	C5-C6-N1	6.09	124.04	121.00
44	5	551	А	C4-N9-C1'	-6.09	115.34	126.30
44	5	1425	U	N3-C2-O2	-6.09	117.94	122.20
44	5	2706	G	N3-C4-C5	6.09	131.64	128.60
44	5	1220	U	OP2-P-O3'	6.08	118.58	105.20
44	5	2093	А	C2-N3-C4	6.08	113.64	110.60
44	5	518	G	C8-N9-C1'	-6.08	119.09	127.00
44	5	2711	С	C5-C6-N1	6.08	124.04	121.00
44	5	1227	С	C6-N1-C2	-6.08	117.87	120.30
44	5	1697	А	C5-N7-C8	-6.08	100.86	103.90
44	5	16	А	N1-C6-N6	6.08	122.25	118.60
44	5	380	U	C2-N1-C1'	6.08	124.99	117.70
44	5	3217	С	N1-C2-O2	6.08	122.55	118.90
44	5	1042	U	C5-C6-N1	6.08	125.74	122.70
44	5	1640	G	N1-C6-O6	-6.08	116.25	119.90
44	5	374	А	C4-C5-C6	-6.08	113.96	117.00
44	5	3378	С	N3-C2-O2	-6.08	117.65	121.90
46	7	112	G	C6-C5-N7	-6.08	126.75	130.40

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

Continued on next page...

113.10

116.14



6.07

N7-C8-N9

1035

G

44

5

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2935	U	C5-C4-O4	-6.07	122.26	125.90
44	5	1547	G	N3-C4-C5	6.07	131.64	128.60
44	5	2769	А	N7-C8-N9	6.07	116.83	113.80
44	5	960	U	C5-C6-N1	-6.07	119.67	122.70
44	5	556	U	C5-C4-O4	-6.07	122.26	125.90
44	5	1005	G	N3-C2-N2	-6.07	115.65	119.90
44	5	1033	U	C6-N1-C1'	6.07	129.69	121.20
44	5	643	U	N3-C2-O2	-6.06	117.96	122.20
44	5	1282	G	C5-C6-O6	6.06	132.24	128.60
44	5	1267	U	C5-C6-N1	6.06	125.73	122.70
44	5	3118	С	N1-C2-O2	6.06	122.53	118.90
44	5	787	G	C6-C5-N7	-6.06	126.77	130.40
44	5	526	С	C5-C6-N1	6.05	124.03	121.00
44	5	2233	A	N7-C8-N9	6.05	116.83	113.80
45	8	120	С	C6-N1-C2	-6.05	117.88	120.30
44	5	177	U	C5-C6-N1	6.05	125.72	122.70
44	5	723	U	N3-C2-O2	-6.05	117.97	122.20
44	5	3157	U	N1-C2-O2	6.05	127.03	122.80
44	5	2416	U	N1-C2-O2	6.05	127.03	122.80
44	5	1248	C	N3-C4-C5	6.05	124.32	121.90
44	5	1311	G	C8-N9-C4	-6.05	103.98	106.40
44	5	1876	U	C2-N1-C1'	6.05	124.96	117.70
44	5	2291	A	N9-C4-C5	-6.05	103.38	105.80
44	5	3109	G	C8-N9-C4	6.05	108.82	106.40
44	5	2202	С	C5-C6-N1	6.04	124.02	121.00
44	5	2821	С	C6-N1-C2	-6.04	117.88	120.30
44	5	2822	U	N1-C2-O2	6.04	127.03	122.80
44	5	2668	U	C5-C6-N1	6.04	125.72	122.70
46	7	26	С	C5-C6-N1	6.04	124.02	121.00
44	5	575	G	N9-C4-C5	-6.04	102.98	105.40
44	5	907	G	N3-C4-N9	-6.04	122.38	126.00
44	5	1749	A	C6-N1-C2	6.04	122.22	118.60
44	5	2507	С	C6-N1-C2	-6.04	117.88	120.30
44	5	2684	C	C2-N1-C1'	6.04	125.45	118.80
44	5	3064	U	N3-C2-O2	-6.04	117.97	122.20
44	5	2961	G	C4-C5-N7	6.04	113.22	110.80
44	5	3362	A	C4-C5-N7	6.04	113.72	110.70
44	5	441	U	C5'-C4'-O4'	6.04	116.35	109.10
44	5	1951	C	C6-N1-C2	-6.04	117.88	120.30
45	8	148	G	C8-N9-C1'	6.04	134.85	127.00
46	7	6	C	C6-N1-C2	-6.04	117.89	120.30
44	5	1040	A	C5-N7-C8	-6.03	100.88	103.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1235	U	C6-N1-C2	6.03	124.62	121.00
44	5	3072	С	C5-C6-N1	6.03	124.02	121.00
44	5	2510	U	N3-C2-O2	-6.03	117.98	122.20
44	5	2863	G	N7-C8-N9	6.03	116.12	113.10
44	5	1556	С	C2-N1-C1'	6.03	125.43	118.80
44	5	816	А	C5-C6-N1	6.02	120.71	117.70
44	5	803	С	C6-N1-C2	-6.02	117.89	120.30
44	5	429	U	N3-C2-O2	-6.02	117.99	122.20
44	5	1904	С	C5-C6-N1	6.02	124.01	121.00
44	5	2110	G	O4'-C1'-N9	6.02	113.02	108.20
45	8	8	С	C2-N1-C1'	6.02	125.42	118.80
44	5	838	G	N1-C6-O6	6.01	123.51	119.90
44	5	3223	А	N9-C4-C5	-6.01	103.39	105.80
44	5	3306	U	C6-N1-C1'	-6.01	112.78	121.20
44	5	141	С	C6-N1-C2	-6.01	117.90	120.30
44	5	500	С	C6-N1-C1'	-6.01	113.59	120.80
44	5	3057	U	C2-N1-C1'	6.01	124.91	117.70
44	5	306	А	C5-C6-N6	-6.01	118.89	123.70
44	5	568	G	N9-C4-C5	-6.01	103.00	105.40
44	5	736	А	N7-C8-N9	6.01	116.81	113.80
44	5	1168	U	N3-C2-O2	-6.00	118.00	122.20
44	5	354	U	C5-C6-N1	6.00	125.70	122.70
44	5	679	U	O4'-C1'-N1	6.00	113.00	108.20
46	7	19	С	C6-N1-C2	-6.00	117.90	120.30
44	5	1766	G	N1-C6-O6	6.00	123.50	119.90
44	5	737	G	C4-C5-N7	6.00	113.20	110.80
44	5	1303	А	N7-C8-N9	-6.00	110.80	113.80
44	5	590	G	N1-C6-O6	5.99	123.50	119.90
44	5	3249	С	C6-N1-C2	-5.99	117.90	120.30
45	8	41	А	N9-C4-C5	-5.99	103.40	105.80
44	5	1351	U	C6-N1-C1'	-5.99	112.82	121.20
44	5	3122	А	C5-N7-C8	-5.99	100.91	103.90
44	5	547	G	C5-C6-O6	-5.99	125.01	128.60
44	5	3099	С	N3-C2-O2	-5.99	117.71	121.90
44	5	3200	G	N1-C2-N2	5.99	121.59	116.20
45	8	69	U	O4'-C1'-N1	5.98	112.99	108.20
44	5	93	С	C5-C6-N1	-5.98	118.01	121.00
44	5	1355	A	N9-C4-C5	-5.98	103.41	105.80
44	5	3121	U	C6-N1-C1'	-5.98	112.83	121.20
44	5	234	G	C6-C5-N7	-5.98	126.81	130.40
44	5	258	G	N9-C4-C5	-5.98	103.01	105.40
44	5	1717	U	N3-C4-O4	5.98	123.58	119.40



α \cdot 1	C		
Continued	trom	previous	page
0010000000	J. 00	proceed as	P~90

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
44	5	3260	G	C6-C5-N7	-5.98	126.81	130.40
44	5	736	А	C5-N7-C8	-5.98	100.91	103.90
44	5	1038	С	C6-N1-C2	-5.98	117.91	120.30
19	R	312	VAL	CA-C-O	5.97	132.64	120.10
40	m	85	LEU	CA-CB-CG	5.97	129.04	115.30
44	5	2476	С	N3-C4-N4	-5.97	113.82	118.00
44	5	2496	С	N3-C4-N4	-5.97	113.82	118.00
44	5	3292	А	N7-C8-N9	5.97	116.78	113.80
44	5	397	А	N1-C6-N6	5.97	122.18	118.60
44	5	3318	G	N3-C4-C5	5.97	131.58	128.60
44	5	192	С	C6-N1-C1'	-5.97	113.64	120.80
44	5	1373	А	N9-C4-C5	-5.97	103.41	105.80
44	5	164	А	C4-C5-C6	-5.96	114.02	117.00
44	5	756	U	N1-C2-O2	5.96	126.98	122.80
44	5	1752	А	N9-C4-C5	-5.96	103.41	105.80
44	5	1961	G	N3-C4-N9	5.96	129.58	126.00
44	5	538	G	C6-C5-N7	-5.96	126.82	130.40
45	8	15	G	C4-N9-C1'	-5.96	118.75	126.50
44	5	1346	G	N3-C4-N9	-5.96	122.43	126.00
44	5	2294	U	N1-C2-O2	5.96	126.97	122.80
44	5	217	U	N3-C2-O2	-5.95	118.03	122.20
46	7	63	А	N3-C4-C5	5.95	130.97	126.80
44	5	3106	А	C5-N7-C8	-5.95	100.93	103.90
44	5	3174	А	O4'-C1'-N9	5.95	112.96	108.20
44	5	2196	С	C4-C5-C6	-5.95	114.43	117.40
44	5	1420	С	N1-C2-O2	5.95	122.47	118.90
44	5	1457	U	N3-C2-O2	-5.95	118.04	122.20
44	5	2151	С	C6-N1-C2	-5.95	117.92	120.30
44	5	103	G	N9-C4-C5	-5.94	103.02	105.40
44	5	767	U	O4'-C1'-N1	5.94	112.95	108.20
44	5	138	U	C5-C6-N1	5.94	125.67	122.70
44	5	1627	U	C5-C6-N1	5.94	125.67	122.70
45	8	66	A	N9-C4-C5	-5.94	103.42	105.80
30	с	41	LEU	CA-CB-CG	5.94	128.96	115.30
44	5	680	G	C4-C5-N7	-5.94	108.42	110.80
44	5	835	G	C8-N9-C4	5.94	108.78	106.40
44	5	955	U	N3-C2-O2	-5.94	118.04	122.20
44	5	1311	G	O5'-P-OP1	-5.94	100.36	105.70
44	5	93	С	C6-N1-C2	5.93	122.67	120.30
44	5	2913	C	N1-C2-O2	5.93	122.46	118.90
44	5	1591	G	N9-C4-C5	-5.93	103.03	105.40
44	5	2375	G	N3-C4-C5	5.93	131.57	128.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1254	С	N3-C4-C5	-5.93	119.53	121.90
44	5	2353	G	C4-C5-N7	5.93	113.17	110.80
44	5	3317	U	N1-C2-O2	5.93	126.95	122.80
44	5	1604	G	N3-C4-C5	-5.93	125.64	128.60
44	5	284	А	C5-C6-N1	5.93	120.66	117.70
44	5	837	А	C5-C6-N1	5.93	120.66	117.70
44	5	2702	А	C4-C5-C6	-5.93	114.04	117.00
44	5	3269	U	C6-N1-C1'	-5.93	112.90	121.20
44	5	3337	G	C5-N7-C8	-5.92	101.34	104.30
44	5	2492	С	N3-C4-C5	-5.92	119.53	121.90
45	8	87	G	C6-C5-N7	5.92	133.95	130.40
44	5	307	А	C4-C5-C6	-5.92	114.04	117.00
38	k	16	ARG	NE-CZ-NH2	5.92	123.26	120.30
44	5	315	С	C6-N1-C2	-5.92	117.93	120.30
44	5	1544	G	C2-N3-C4	5.92	114.86	111.90
44	5	1098	А	N9-C4-C5	-5.91	103.44	105.80
44	5	1155	С	C6-N1-C1'	-5.91	113.71	120.80
44	5	1956	А	C2-N3-C4	5.91	113.56	110.60
44	5	2283	G	C8-N9-C4	5.91	108.76	106.40
44	5	201	А	C5-N7-C8	-5.91	100.95	103.90
44	5	1742	U	C2-N3-C4	5.91	130.54	127.00
44	5	3369	G	C4-N9-C1'	5.91	134.18	126.50
44	5	2189	U	C2-N1-C1'	5.91	124.79	117.70
44	5	2234	G	N7-C8-N9	5.91	116.05	113.10
44	5	631	U	N1-C2-O2	5.90	126.93	122.80
44	5	1923	С	C4-C5-C6	-5.90	114.45	117.40
44	5	1943	С	C5-C6-N1	5.90	123.95	121.00
44	5	3309	G	C4-N9-C1'	5.90	134.18	126.50
44	5	430	U	N3-C2-O2	-5.90	118.07	122.20
46	7	75	G	N7-C8-N9	5.90	116.05	113.10
46	7	120	С	C5-C4-N4	-5.90	116.07	120.20
44	5	283	G	C4-N9-C1'	5.90	134.17	126.50
44	5	1128	U	N3-C2-O2	-5.90	118.07	122.20
44	5	2562	А	C6-C5-N7	-5.90	128.17	132.30
44	5	2534	G	C8-N9-C1'	5.90	134.67	127.00
44	5	3325	G	C8-N9-C1'	-5.90	119.33	127.00
44	5	748	U	N3-C2-O2	-5.90	118.07	122.20
44	5	1246	G	N1-C2-N2	5.90	121.51	116.20
44	5	1230	G	N1-C2-N2	-5.90	110.89	116.20

С

G

U

1854

2467

3104

C2-N1-C1'

N1-C2-N3

C2-N1-C1'

44

44

44

5

5

5

Continued from previous page...

Continued on next page...

118.80

123.90

117.70

125.29

127.44

124.78



5.90

5.90

5.90

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	518	G	C4-N9-C1'	5.89	134.16	126.50
44	5	787	G	N1-C6-O6	5.89	123.44	119.90
44	5	120	G	C8-N9-C4	5.89	108.76	106.40
44	5	191	U	N1-C2-O2	5.89	126.92	122.80
44	5	322	U	N3-C2-O2	-5.89	118.08	122.20
44	5	1604	G	N3-C4-N9	5.89	129.54	126.00
44	5	2584	G	C4-C5-N7	5.89	113.16	110.80
44	5	161	G	N3-C4-N9	-5.89	122.47	126.00
44	5	193	С	N1-C2-O2	5.89	122.43	118.90
44	5	2647	А	C8-N9-C4	5.89	108.16	105.80
44	5	1372	С	N1-C2-O2	5.88	122.43	118.90
44	5	65	А	C5-C6-N6	-5.88	119.00	123.70
44	5	2477	G	C4-N9-C1'	5.88	134.15	126.50
44	5	1035	G	C6-C5-N7	-5.88	126.87	130.40
44	5	1254	С	C2-N1-C1'	5.88	125.27	118.80
44	5	2197	С	C6-N1-C2	5.88	122.65	120.30
44	5	575	G	C5-N7-C8	-5.88	101.36	104.30
44	5	1035	G	C5-C6-O6	-5.88	125.07	128.60
44	5	2913	С	C5-C6-N1	5.88	123.94	121.00
44	5	615	U	N1-C2-O2	5.88	126.91	122.80
44	5	1573	G	N7-C8-N9	5.87	116.04	113.10
44	5	2769	А	C5-N7-C8	-5.87	100.96	103.90
44	5	172	G	N1-C2-N2	5.87	121.48	116.20
44	5	2534	G	C6-C5-N7	5.87	133.92	130.40
45	8	19	С	C6-N1-C2	-5.87	117.95	120.30
44	5	168	U	C6-N1-C1'	5.87	129.41	121.20
26	Y	126	LEU	CA-CB-CG	5.87	128.79	115.30
44	5	1646	G	N3-C4-N9	-5.87	122.48	126.00
45	8	37	А	N9-C4-C5	-5.87	103.45	105.80
44	5	3214	U	C2-N1-C1'	5.86	124.73	117.70
46	7	39	С	C6-N1-C1'	-5.86	113.76	120.80
44	5	1742	U	C6-N1-C2	-5.86	117.48	121.00
44	5	1184	A	C8-N9-C4	5.86	108.14	105.80
45	8	24	G	C6-C5-N7	-5.86	126.88	130.40
44	5	1448	U	N3-C2-O2	-5.86	118.10	122.20
44	5	$\overline{59}$	G	C4-N9-C1'	-5.86	118.89	126.50
44	5	202	G	N3-C4-N9	5.86	129.51	126.00
44	5	623	U	N1-C2-O2	5.86	126.90	122.80
44	5	1278	A	C5-C6-N1	5.86	120.63	117.70
44	5	1563	C	C6-N1-C1	5.86	127.83	120.80
44	5	$21\overline{81}$	C	C6-N1-C2	-5.85	117.96	120.30
44	5	3292	A	C5-N7-C8	-5.85	100.97	103.90



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	308	А	C4-N9-C1'	5.85	136.83	126.30
44	5	812	G	C2-N3-C4	5.85	114.83	111.90
44	5	3031	G	C4-C5-N7	5.85	113.14	110.80
44	5	1201	С	N3-C2-O2	-5.85	117.81	121.90
44	5	3225	С	C5-C6-N1	5.85	123.92	121.00
46	7	19	С	C5-C6-N1	5.85	123.92	121.00
44	5	1288	U	N1-C2-O2	5.84	126.89	122.80
44	5	247	С	N1-C2-O2	5.84	122.41	118.90
44	5	1376	С	N3-C2-O2	-5.84	117.81	121.90
44	5	1706	С	N1-C2-O2	5.84	122.40	118.90
44	5	3362	А	N9-C4-C5	-5.84	103.47	105.80
44	5	446	U	N3-C4-C5	5.84	118.10	114.60
44	5	1355	А	C8-N9-C4	5.83	108.13	105.80
44	5	1475	А	N9-C4-C5	-5.83	103.47	105.80
44	5	528	U	C5-C6-N1	5.83	125.62	122.70
44	5	1077	U	N1-C2-O2	5.83	126.88	122.80
44	5	1174	G	C4-N9-C1'	5.83	134.08	126.50
44	5	1190	А	C6-C5-N7	-5.83	128.22	132.30
44	5	3378	С	N1-C2-O2	5.83	122.40	118.90
45	8	55	U	N1-C2-O2	5.83	126.88	122.80
44	5	835	G	O4'-C1'-N9	5.83	112.86	108.20
44	5	1376	С	N1-C2-O2	5.83	122.40	118.90
44	5	2488	А	C4-N9-C1'	5.83	136.79	126.30
44	5	3201	С	C5-C6-N1	5.83	123.92	121.00
44	5	743	С	C2-N1-C1'	5.83	125.21	118.80
45	8	96	А	N3-C4-C5	5.83	130.88	126.80
44	5	433	А	C8-N9-C4	-5.83	103.47	105.80
44	5	1035	G	C5-N7-C8	-5.83	101.39	104.30
44	5	1775	G	N9-C4-C5	-5.83	103.07	105.40
44	5	2844	С	C4-C5-C6	-5.83	114.49	117.40
44	5	2900	А	C5-C6-N6	-5.83	119.04	123.70
44	5	2355	G	C4-C5-N7	5.83	113.13	110.80
44	5	1750	А	N9-C4-C5	-5.83	103.47	105.80
44	5	3266	G	C8-N9-C1'	5.83	134.57	127.00
46	7	64	А	C4-C5-C6	-5.83	114.09	117.00
44	5	679	U	N3-C2-O2	-5.82	118.12	122.20
44	5	681	U	C5-C6-N1	5.82	125.61	122.70
44	5	2118	C	C6-N1-C1'	-5.81	113.82	120.80
44	5	2790	A	N9-C4-C5	-5.81	103.47	105.80
44	5	18	G	N1-C2-N2	-5.81	110.97	116.20
44	5	1867	А	C5-C6-N6	-5.81	119.05	123.70
44	5	2171	G	N3-C2-N2	-5.81	115.83	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2585	G	C8-N9-C1'	-5.81	119.45	127.00
44	5	3111	U	N1-C2-O2	5.81	126.87	122.80
44	5	55	G	C4-N9-C1'	-5.81	118.95	126.50
44	5	536	U	N1-C2-O2	5.81	126.86	122.80
44	5	1130	А	C8-N9-C4	-5.81	103.48	105.80
44	5	1706	С	N3-C2-O2	-5.81	117.83	121.90
44	5	818	С	N1-C2-O2	5.80	122.38	118.90
44	5	1447	G	O4'-C1'-N9	5.80	112.84	108.20
44	5	2506	U	N1-C2-O2	5.80	126.86	122.80
44	5	321	С	C5-C6-N1	5.80	123.90	121.00
44	5	1009	A	N1-C2-N3	-5.80	126.40	129.30
44	5	770	G	C8-N9-C1'	5.80	134.54	127.00
44	5	3005	А	N3-C4-C5	5.80	130.86	126.80
44	5	368	G	C2-N3-C4	5.80	114.80	111.90
44	5	399	А	C5-N7-C8	-5.80	101.00	103.90
44	5	3272	С	N3-C2-O2	-5.80	117.84	121.90
1	Z	345	ASP	CB-CG-OD1	5.80	123.52	118.30
44	5	988	U	C5-C6-N1	5.80	125.60	122.70
44	5	1872	С	N1-C2-O2	5.80	122.38	118.90
44	5	175	С	C2-N3-C4	5.79	122.80	119.90
44	5	1226	G	N3-C4-N9	-5.79	122.52	126.00
44	5	1306	G	C5-C6-O6	-5.79	125.12	128.60
44	5	213	А	C8-N9-C4	5.79	108.12	105.80
44	5	758	С	C2-N1-C1'	5.79	125.17	118.80
44	5	2506	U	C5-C6-N1	5.79	125.59	122.70
46	7	70	U	N3-C2-O2	-5.79	118.15	122.20
44	5	515	С	C2-N1-C1'	5.79	125.17	118.80
44	5	3344	A	N1-C6-N6	5.79	122.07	118.60
46	7	70	U	N1-C2-O2	5.79	126.85	122.80
44	5	2537	U	C5-C6-N1	-5.79	119.81	122.70
44	5	3153	U	C6-N1-C2	5.79	124.47	121.00
44	5	1238	C	O5'-P-OP2	5.79	117.64	110.70
44	5	1299	U	N1-C2-O2	5.79	126.85	122.80
44	5	705	A	N1-C6-N6	5.78	122.07	118.60
44	5	1060	U	N3-C2-O2	-5.78	118.15	122.20
44	5	569	A	N9-C4-C5	-5.78	103.49	105.80
44	5	1316	C	C6-N1-C2	-5.78	117.99	120.30
44	5	2604	U	N3-C2-O2	-5.78	118.15	122.20
44	5	777	U	N3-C2-O2	-5.78	118.16	122.20
44	5	621	A	N9-C4-C5	-5.77	103.49	105.80
44	5	3293	U	O4'-C1'-N1	-5.77	103.58	108.20
46	7	28	l C	C5-C6-N1	5.77	123.89	121.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1392	G	N7-C8-N9	-5.77	110.21	113.10
44	5	16	А	C5-C6-N6	-5.77	119.08	123.70
44	5	1727	G	N9-C4-C5	-5.77	103.09	105.40
44	5	2972	G	C4-C5-N7	5.77	113.11	110.80
44	5	8	С	C4-C5-C6	-5.77	114.52	117.40
44	5	838	G	N9-C4-C5	-5.77	103.09	105.40
44	5	2197	С	O4'-C1'-N1	-5.77	103.59	108.20
44	5	177	U	C6-N1-C2	-5.76	117.54	121.00
44	5	812	G	N1-C6-O6	-5.76	116.44	119.90
44	5	729	С	C2-N1-C1'	5.76	125.14	118.80
44	5	1242	G	C2-N3-C4	5.76	114.78	111.90
44	5	1958	U	OP1-P-O3'	5.76	117.87	105.20
44	5	568	G	C5-C6-O6	-5.75	125.15	128.60
44	5	1042	U	N1-C2-O2	5.75	126.83	122.80
44	5	680	G	N3-C4-N9	-5.75	122.55	126.00
44	5	2184	U	N3-C2-O2	-5.75	118.17	122.20
44	5	2452	G	C4-C5-N7	5.75	113.10	110.80
44	5	2585	G	C2-N3-C4	5.75	114.78	111.90
44	5	340	С	C5-C6-N1	5.75	123.88	121.00
44	5	1312	С	N1-C2-O2	5.75	122.35	118.90
44	5	1411	С	C5-C6-N1	5.75	123.88	121.00
44	5	1867	А	N9-C4-C5	-5.75	103.50	105.80
44	5	1306	G	C4-C5-N7	5.75	113.10	110.80
44	5	2622	С	C5-C6-N1	5.75	123.88	121.00
44	5	786	А	N7-C8-N9	-5.75	110.92	113.80
44	5	2353	G	C5-C6-O6	-5.75	125.15	128.60
44	5	380	U	C5-C6-N1	5.75	125.57	122.70
44	5	1806	А	C6-C5-N7	-5.75	128.28	132.30
44	5	758	С	C6-N1-C2	-5.74	118.00	120.30
44	5	201	А	C4-C5-N7	5.74	113.57	110.70
44	5	1736	G	N3-C4-N9	5.74	129.44	126.00
44	5	150	А	N9-C4-C5	-5.74	103.50	105.80
44	5	3003	G	N9-C4-C5	-5.74	103.11	105.40
44	5	665	А	C5-N7-C8	-5.74	101.03	103.90
44	5	1263	А	C2-N3-C4	5.74	113.47	110.60
44	5	1514	G	N3-C4-C5	-5.74	125.73	128.60
44	5	2146	С	C5-C6-N1	5.74	123.87	121.00
44	5	1421	G	C5-C6-O6	5.73	132.04	128.60
44	5	2533	G	N3-C4-C5	5.73	131.47	128.60
44	5	3288	G	C8-N9-C4	5.73	108.69	106.40
45	8	146	U	C2-N1-C1'	-5.73	110.82	117.70
44	5	414	U	N3-C2-O2	-5.73	118.19	122.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	502	U	N1-C2-O2	5.73	126.81	122.80
44	5	1096	U	C2-N3-C4	5.73	130.44	127.00
44	5	2932	U	N1-C2-O2	5.73	126.81	122.80
44	5	650	С	N3-C2-O2	-5.73	117.89	121.90
44	5	1392	G	O4'-C1'-N9	5.72	112.78	108.20
44	5	386	A	C5-N7-C8	-5.72	101.04	103.90
44	5	1381	A	N1-C2-N3	-5.72	126.44	129.30
44	5	1907	С	N3-C2-O2	-5.72	117.89	121.90
44	5	1697	A	N7-C8-N9	5.72	116.66	113.80
44	5	2231	С	C6-N1-C2	-5.72	118.01	120.30
44	5	2389	С	C5-C6-N1	5.72	123.86	121.00
44	5	3253	G	N1-C2-N2	5.72	121.35	116.20
45	8	72	A	N3-C4-C5	-5.72	122.80	126.80
44	5	400	G	C6-C5-N7	-5.72	126.97	130.40
44	5	1170	А	O5'-P-OP1	-5.72	100.56	105.70
44	5	2961	G	C5-N7-C8	-5.72	101.44	104.30
44	5	2821	C	C5-C6-N1	5.71	123.86	121.00
44	5	3383	G	N7-C8-N9	5.71	115.96	113.10
44	5	373	A	C5-N7-C8	-5.71	101.04	103.90
44	5	3385	U	C6-N1-C2	-5.71	117.57	121.00
44	5	803	C	C5-C6-N1	5.71	123.86	121.00
44	5	1082	U	C2-N1-C1'	5.71	124.55	117.70
44	5	1206	G	N3-C4-N9	5.71	129.43	126.00
44	5	2748	A	N1-C6-N6	5.71	122.03	118.60
44	5	748	U	N1-C2-O2	5.71	126.80	122.80
44	5	596	C	N3-C2-O2	-5.71	117.91	121.90
44	5	758	C	N3-C2-O2	-5.71	117.91	121.90
44	5	3388	C	C6-N1-C1'	5.71	127.65	120.80
44	5	31	С	C6-N1-C2	-5.70	118.02	120.30
44	5	374	A	N3-C4-N9	-5.70	122.84	127.40
44	5	1766	G	C5-C6-O6	-5.70	125.18	128.60
44	5	3121	U	OP1-P-O3'	5.70	117.75	105.20
44	5	2750	U	N3-C2-O2	-5.70	118.21	122.20
44	5	547	G	N1-C6-O6	5.70	123.32	119.90
44	5	2603	G	N1-C2-N2	5.70	121.33	116.20
44	5	54	C	C6-N1-C2	-5.70	118.02	120.30
44	5	679	U	N1-C2-O2	5.70	126.79	122.80
44	5	2846	U	N3-C2-O2	-5.70	118.21	122.20
46	7	45	A	N1-C2-N3	-5.70	126.45	129.30
44	5	1255	C	C2-N1-C1'	5.70	125.06	118.80
44	5	137	G	C4-N9-C1'	-5.69	119.10	126.50
44	5	1059	G	N3-C2-N2	-5.69	115.92	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2711	С	C6-N1-C1'	-5.69	113.97	120.80
44	5	430	U	N1-C2-O2	5.69	126.78	122.80
44	5	752	С	C5-C6-N1	5.69	123.85	121.00
45	8	39	G	C8-N9-C4	5.69	108.68	106.40
44	5	1088	U	N3-C2-O2	-5.69	118.22	122.20
44	5	1496	С	N1-C2-O2	5.69	122.31	118.90
46	7	63	А	N9-C4-C5	-5.69	103.53	105.80
44	5	1483	G	N3-C4-C5	5.69	131.44	128.60
44	5	321	С	N3-C2-O2	-5.68	117.92	121.90
44	5	1960	А	N3-C4-N9	5.68	131.95	127.40
45	8	87	G	N9-C4-C5	5.68	107.67	105.40
45	8	120	С	C4-C5-C6	-5.68	114.56	117.40
44	5	207	U	C2-N3-C4	5.68	130.41	127.00
44	5	2907	G	N3-C2-N2	-5.68	115.92	119.90
44	5	3223	А	C4-C5-N7	5.68	113.54	110.70
44	5	2188	А	C4-C5-N7	5.68	113.54	110.70
44	5	2606	G	C2-N3-C4	5.68	114.74	111.90
44	5	3345	G	C4-C5-N7	5.68	113.07	110.80
44	5	1174	G	C8-N9-C1'	-5.68	119.62	127.00
45	8	25	G	C6-C5-N7	-5.68	126.99	130.40
46	7	24	А	C5-N7-C8	-5.68	101.06	103.90
44	5	1057	А	C4-C5-N7	5.68	113.54	110.70
44	5	2193	U	N1-C2-O2	5.68	126.77	122.80
45	8	83	С	N3-C4-C5	5.68	124.17	121.90
18	Q	151	LEU	CA-CB-CG	5.67	128.35	115.30
44	5	339	С	C2-N1-C1'	5.67	125.04	118.80
44	5	613	G	N3-C4-N9	5.67	129.41	126.00
44	5	12	A	C4-N9-C1'	-5.67	116.09	126.30
44	5	2794	G	N3-C4-N9	-5.67	122.60	126.00
44	5	3353	G	N3-C2-N2	-5.67	115.93	119.90
44	5	353	G	C8-N9-C1'	5.67	134.37	127.00
44	5	788	С	C4-C5-C6	-5.67	114.56	117.40
44	5	2995	A	C5-N7-C8	-5.67	101.07	103.90
44	5	2449	A	C5-N7-C8	-5.67	101.07	103.90
44	5	3072	С	C6-N1-C2	-5.67	118.03	120.30
44	5	2204	C	C4-C5-C6	-5.66	114.57	117.40
44	5	1315	U	C2-N3-C4	-5.66	123.60	127.00
44	5	406	G	C4-N9-C1'	-5.66	119.14	126.50
44	5	1057	A	C5-N7-C8	-5.66	101.07	103.90
44	5	1871	U	N1-C2-O2	5.66	126.76	122.80
44	5	1567	U	N1-C2-O2	5.66	126.76	122.80
45	8	102	U	N1-C2-O2	5.66	126.76	122.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	162	G	N7-C8-N9	5.66	115.93	113.10
44	5	230	U	C2-N3-C4	5.66	130.39	127.00
44	5	1870	С	C5-C6-N1	5.66	123.83	121.00
44	5	540	U	N1-C2-O2	5.66	126.76	122.80
44	5	1242	G	N3-C4-C5	-5.66	125.77	128.60
44	5	2612	U	C5-C4-O4	-5.66	122.51	125.90
44	5	308	А	C5-N7-C8	-5.65	101.07	103.90
44	5	627	U	C6-N1-C2	-5.65	117.61	121.00
44	5	2213	А	N1-C6-N6	5.65	121.99	118.60
44	5	2689	А	N7-C8-N9	5.65	116.62	113.80
45	8	118	С	C5-C6-N1	5.65	123.82	121.00
44	5	1321	G	C8-N9-C4	5.65	108.66	106.40
44	5	2366	С	N3-C2-O2	-5.65	117.95	121.90
44	5	561	С	C2-N3-C4	5.64	122.72	119.90
44	5	2477	G	N3-C4-N9	5.64	129.39	126.00
44	5	1040	А	C2-N3-C4	-5.64	107.78	110.60
44	5	1057	А	N1-C2-N3	-5.64	126.48	129.30
44	5	3166	С	C4-C5-C6	-5.64	114.58	117.40
44	5	2118	С	C5-C6-N1	5.64	123.82	121.00
44	5	2514	U	C2-N1-C1'	-5.64	110.93	117.70
44	5	1951	С	N1-C2-O2	5.64	122.28	118.90
44	5	50	U	C5-C6-N1	5.64	125.52	122.70
44	5	1229	G	N3-C4-N9	5.64	129.38	126.00
44	5	336	А	N3-C4-N9	5.63	131.91	127.40
44	5	1941	С	C4-C5-C6	-5.63	114.58	117.40
44	5	2515	А	C5-C6-N6	-5.63	119.20	123.70
44	5	2550	U	C2-N1-C1'	5.63	124.45	117.70
44	5	778	U	N1-C2-O2	5.63	126.74	122.80
44	5	1411	С	N3-C2-O2	-5.63	117.96	121.90
44	5	330	G	N3-C4-C5	5.62	131.41	128.60
44	5	352	А	C4-N9-C1'	-5.62	116.18	126.30
44	5	2208	А	N3-C4-C5	5.62	130.74	126.80
44	5	3091	А	C4-C5-N7	5.62	113.51	110.70
44	5	3285	С	C5-C6-N1	5.62	123.81	121.00
44	5	3305	А	C8-N9-C4	5.62	108.05	105.80
44	5	$1\overline{279}$	C	C6-N1-C2	-5.62	118.05	120.30
44	5	1749	A	N9-C4-C5	-5.62	103.55	105.80
44	5	3161	C	C5-C6-N1	5.62	123.81	121.00
44	5	3224	G	N3-C4-N9	5.62	129.37	126.00
44	5	551	А	C8-N9-C4	5.62	108.05	105.80
44	5	615	U	N1-C2-N3	-5.61	111.53	114.90
44	5	3345	G	N1-C6-O6	5.61	123.27	119.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
46	7	80	G	N7-C8-N9	5.61	115.91	113.10
44	5	65	А	N1-C6-N6	5.61	121.97	118.60
44	5	149	U	C5-C6-N1	5.61	125.51	122.70
46	7	75	G	C8-N9-C4	-5.61	104.16	106.40
44	5	176	G	C4-N9-C1'	5.61	133.79	126.50
44	5	518	G	N3-C4-N9	5.61	129.37	126.00
44	5	2553	U	N1-C2-O2	5.61	126.73	122.80
44	5	2576	G	N9-C4-C5	-5.61	103.16	105.40
44	5	2967	А	N7-C8-N9	5.61	116.61	113.80
46	7	1	G	N9-C4-C5	-5.61	103.16	105.40
46	7	28	С	N1-C2-O2	5.61	122.27	118.90
44	5	299	G	C6-C5-N7	-5.61	127.03	130.40
44	5	3181	С	N3-C2-O2	-5.61	117.97	121.90
44	5	1854	С	N1-C2-O2	5.61	122.26	118.90
44	5	1927	G	N9-C4-C5	-5.61	103.16	105.40
44	5	2307	G	C2-N3-C4	-5.61	109.10	111.90
44	5	1473	G	C6-C5-N7	-5.60	127.04	130.40
44	5	3333	G	C4-N9-C1'	-5.60	119.22	126.50
46	7	64	А	C6-C5-N7	5.60	136.22	132.30
44	5	77	А	C5-C6-N1	5.60	120.50	117.70
45	8	24	G	C2-N3-C4	-5.60	109.10	111.90
44	5	3121	U	O4'-C1'-N1	-5.60	103.72	108.20
44	5	5	G	N3-C4-C5	5.60	131.40	128.60
44	5	607	А	C4-N9-C1'	5.60	136.38	126.30
44	5	2531	С	C2-N1-C1'	5.60	124.96	118.80
44	5	3228	С	P-O3'-C3'	5.60	126.42	119.70
44	5	2427	U	C5-C6-N1	5.60	125.50	122.70
44	5	3145	С	N3-C2-O2	-5.60	117.98	121.90
45	8	4	С	C5-C6-N1	5.60	123.80	121.00
44	5	1087	G	N1-C6-O6	5.59	123.26	119.90
44	5	1280	С	C2-N1-C1'	-5.59	112.65	118.80
44	5	1826	С	C5-C6-N1	5.59	123.80	121.00
44	5	1934	G	N3-C2-N2	-5.59	115.98	119.90
44	5	2337	C	C5-C4-N4	5.59	124.12	120.20
44	5	2794	G	C2-N3-C4	-5.59	109.10	111.90
44	5	2861	U	<u>C6-N1-C1</u> '	5.59	129.02	121.20
44	5	3342	A	N1-C2-N3	5.59	132.09	129.30
44	5	3334	U	N3-C4-C5	5.59	117.95	114.60
44	5	529	A	N9-C4-C5	-5.59	103.56	105.80
44	5	1311	G	C5-N7-C8	-5.59	101.51	104.30
44	5	1125	U	N1-C2-O2	5.58	126.71	122.80
44	5	128	G	N7-C8-N9	5.58	115.89	113.10



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	356	С	C6-N1-C2	-5.58	118.07	120.30
44	5	1018	G	C5-C6-O6	-5.58	125.25	128.60
44	5	2244	А	N1-C2-N3	-5.58	126.51	129.30
44	5	5	G	C5-C6-N1	-5.58	108.71	111.50
44	5	59	G	C8-N9-C1'	5.58	134.25	127.00
44	5	2114	С	C6-N1-C2	-5.58	118.07	120.30
44	5	2838	А	N9-C4-C5	-5.58	103.57	105.80
38	k	16	ARG	NE-CZ-NH1	-5.58	117.51	120.30
44	5	954	U	N3-C2-O2	-5.58	118.30	122.20
44	5	1312	С	N3-C2-O2	-5.58	118.00	121.90
44	5	2416	U	N3-C2-O2	-5.58	118.30	122.20
44	5	178	U	N1-C2-O2	5.58	126.70	122.80
44	5	286	U	N1-C2-O2	5.58	126.70	122.80
44	5	536	U	N3-C2-O2	-5.57	118.30	122.20
44	5	51	А	C6-C5-N7	-5.57	128.40	132.30
44	5	786	А	N3-C4-C5	5.57	130.70	126.80
44	5	2950	G	N3-C4-C5	-5.56	125.82	128.60
44	5	966	U	C5-C6-N1	5.56	125.48	122.70
44	5	1927	G	N1-C6-O6	5.56	123.24	119.90
44	5	2203	U	N1-C2-O2	5.56	126.69	122.80
44	5	2666	С	C5-C6-N1	5.56	123.78	121.00
45	8	24	G	C4-C5-N7	5.56	113.03	110.80
44	5	3083	G	C4-C5-N7	5.56	113.03	110.80
44	5	2901	G	C4-N9-C1'	5.56	133.73	126.50
44	5	3326	G	N3-C2-N2	-5.56	116.01	119.90
44	5	2296	А	N1-C2-N3	5.56	132.08	129.30
44	5	612	U	N1-C2-O2	5.56	126.69	122.80
44	5	2981	U	N3-C2-O2	-5.56	118.31	122.20
44	5	705	A	C5-C6-N6	-5.55	119.26	123.70
44	5	3122	А	C4-C5-N7	5.55	113.48	110.70
44	5	3161	С	C6-N1-C2	-5.55	118.08	120.30
44	5	3266	G	N1-C2-N2	5.55	121.20	116.20
45	8	153	U	N3-C2-O2	-5.55	118.31	122.20
44	5	1514	G	C8-N9-C1'	-5.55	119.78	127.00
44	5	1544	G	N1-C2-N2	5.55	121.20	116.20
44	5	551	A	N3-C4-C5	$5.5\overline{5}$	130.69	126.80
44	5	862	U	N3-C2-O2	-5.55	118.31	122.20
44	5	664	U	N3-C2-O2	-5.55	118.32	122.20
44	5	1231	A	C6-C5-N7	-5.55	128.42	132.30
44	5	12	A	C4-C5-C6	-5.55	114.23	117.00
44	5	161	G	C8-N9-C4	-5.55	104.18	106.40
44	5	1349	G	C8-N9-C1'	-5.55	119.79	127.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1424	С	C5-C6-N1	5.55	123.77	121.00
44	5	2593	А	N9-C4-C5	-5.55	103.58	105.80
44	5	2720	G	N7-C8-N9	5.55	115.87	113.10
44	5	2920	U	N1-C2-O2	5.55	126.68	122.80
45	8	140	G	N9-C4-C5	-5.55	103.18	105.40
44	5	2684	С	C2-N3-C4	5.54	122.67	119.90
44	5	3200	G	N3-C4-N9	-5.54	122.67	126.00
44	5	860	G	O5'-P-OP1	-5.54	100.71	105.70
44	5	1266	G	N7-C8-N9	5.54	115.87	113.10
44	5	2788	С	N1-C2-O2	5.54	122.23	118.90
45	8	87	G	N3-C2-N2	-5.54	116.02	119.90
44	5	688	G	N7-C8-N9	5.54	115.87	113.10
44	5	915	А	C2-N3-C4	5.54	113.37	110.60
44	5	2766	U	N3-C2-O2	-5.54	118.32	122.20
44	5	1577	G	C2-N3-C4	-5.54	109.13	111.90
44	5	1252	А	N7-C8-N9	5.53	116.57	113.80
44	5	2792	A	N9-C4-C5	-5.53	103.59	105.80
44	5	1805	С	N1-C2-N3	5.53	123.07	119.20
44	5	30	G	N3-C4-N9	5.53	129.32	126.00
44	5	376	G	O4'-C1'-N9	5.53	112.62	108.20
44	5	1228	С	C2-N3-C4	5.53	122.66	119.90
44	5	3239	G	N3-C2-N2	-5.53	116.03	119.90
44	5	1040	А	N7-C8-N9	5.53	116.56	113.80
44	5	1700	G	N3-C4-C5	5.53	131.36	128.60
45	8	118	C	C2-N1-C1'	5.52	124.88	118.80
44	5	1515	A	N9-C4-C5	-5.52	103.59	105.80
44	5	331	G	C8-N9-C1'	5.52	134.18	127.00
44	5	3219	G	C4-N9-C1'	-5.52	119.32	126.50
44	5	3373	U	C5-C6-N1	5.52	125.46	122.70
45	8	37	A	C5-C6-N6	-5.52	119.28	123.70
44	5	675	С	C6-N1-C2	-5.52	118.09	120.30
44	5	1010	G	N3-C2-N2	-5.52	116.04	119.90
44	5	3317	U	N3-C2-O2	-5.52	118.34	122.20
44	5	560	G	C5-C6-O6	-5.52	125.29	128.60
45	8	30	С	N3-C2-O2	-5.52	118.04	121.90
46	7	17	A	C5-N7-C8	-5.52	101.14	103.90
44	5	517	G	N3-C4-N9	-5.51	122.69	126.00
44	5	27	C	C5-C6-N1	5.51	123.76	121.00
44	5	2988	C	N3-C4-N4	-5.51	114.14	118.00
44	5	436	A	C4-C5-C6	-5.51	114.25	117.00
44	5	2205	U	C5-C6-N1	5.51	125.45	122.70
44	5	3058	U	C6-N1-C1'	-5.51	113.49	121.20


$Ideal(^{o})$

119.90

126.50

123.90

126.00

122.20

122.70

Mol	Chain	Res	Type	Atoms	Z	Observed(°)
44	5	55	G	N3-C2-N2	-5.51	116.05
44	5	1565	G	C4-N9-C1'	5.51	133.66
46	7	1	G	N1-C2-N3	-5.51	120.60
44	5	1113	G	N3-C4-N9	-5.50	122.70
44	5	2513	U	N3-C2-O2	-5.50	118.35
44	5	698	U	C5-C6-N1	5.50	125.45
44	5	1447	G	C4-N9-C1'	-5.50	119.35
44	5	1640	G	C4-N9-C1'	-5.50	119.35
44	5	1701	С	N1-C2-O2	5.50	122.20
44	5	2966	G	C4-N9-C1'	-5.49	119.36
44	5	3360	С	C6-N1-C1'	-5.49	114.21
44	5	2626	А	C4-C5-N7	5.49	113.45
44	5	3197	G	C8-N9-C1'	5.49	134.14
44	5	1660	С	C5-C6-N1	5.49	123.75
46	7	44	С	N3-C4-N4	5.49	121.84
44	5	69	С	N1-C2-O2	5.49	122.19
44	5	110	G	C2-N3-C4	-5.49	109.16
44	5	1525	G	C4-N9-C1'	5.49	133.63
44	5	2568	С	C2-N1-C1'	-5.49	112.76
44	5	1869	С	C6-N1-C2	-5.49	118.11
44	5	922	U	C2-N3-C4	5.49	130.29
44	5	1097	G	N3-C4-C5	-5.49	125.86
44	5	561	С	C2-N1-C1'	5.48	124.83
44	5	3311	С	N1-C2-O2	5.48	122.19
44	5	1275	С	C6-N1-C2	-5.48	118.11

Continued from previous page.

44	5	1447	G	C4-N9-C1'	-5.50	119.35	126.50
44	5	1640	G	C4-N9-C1'	-5.50	119.35	126.50
44	5	1701	С	N1-C2-O2	5.50	122.20	118.90
44	5	2966	G	C4-N9-C1'	-5.49	119.36	126.50
44	5	3360	С	C6-N1-C1'	-5.49	114.21	120.80
44	5	2626	А	C4-C5-N7	5.49	113.45	110.70
44	5	3197	G	C8-N9-C1'	5.49	134.14	127.00
44	5	1660	С	C5-C6-N1	5.49	123.75	121.00
46	7	44	С	N3-C4-N4	5.49	121.84	118.00
44	5	69	С	N1-C2-O2	5.49	122.19	118.90
44	5	110	G	C2-N3-C4	-5.49	109.16	111.90
44	5	1525	G	C4-N9-C1'	5.49	133.63	126.50
44	5	2568	С	C2-N1-C1'	-5.49	112.76	118.80
44	5	1869	С	C6-N1-C2	-5.49	118.11	120.30
44	5	922	U	C2-N3-C4	5.49	130.29	127.00
44	5	1097	G	N3-C4-C5	-5.49	125.86	128.60
44	5	561	С	C2-N1-C1'	5.48	124.83	118.80
44	5	3311	С	N1-C2-O2	5.48	122.19	118.90
44	5	1275	С	C6-N1-C2	-5.48	118.11	120.30
44	5	2572	С	C2-N1-C1'	5.48	124.83	118.80
44	5	2594	С	N3-C4-C5	5.48	124.09	121.90
44	5	1060	U	N1-C2-O2	5.48	126.64	122.80
44	5	3234	А	N3-C4-C5	5.48	130.63	126.80
44	5	1417	G	O4'-C1'-N9	5.48	112.58	108.20
44	5	336	А	N1-C2-N3	-5.47	126.56	129.30
44	5	1086	С	C6-N1-C1'	5.47	127.37	120.80
44	5	3383	G	N1-C2-N3	5.47	127.19	123.90
44	5	137	G	C2-N3-C4	-5.47	109.16	111.90
44	5	2953	U	C5-C6-N1	5.47	125.44	122.70
45	8	135	G	N9-C4-C5	-5.47	103.21	105.40
44	5	283	G	N3-C4-N9	5.47	129.28	126.00
9	Н	291	ARG	NE-CZ-NH1	5.47	123.03	120.30
44	5	2206	G	N3-C2-N2	-5.47	116.07	119.90
44	5	2606	G	C4-N9-C1'	5.47	133.61	126.50
44	5	1527	С	P-O3'-C3'	5.47	126.26	119.70
44	5	3039	С	C2-N1-C1'	5.47	124.81	118.80
						Continued on n	ext page



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	3278	С	C6-N1-C2	-5.47	118.11	120.30
45	8	96	А	N3-C4-N9	-5.47	123.03	127.40
44	5	2786	G	N3-C2-N2	-5.47	116.07	119.90
44	5	2544	U	N1-C2-O2	5.46	126.62	122.80
44	5	1595	U	C5-C6-N1	-5.46	119.97	122.70
44	5	2562	А	N1-C6-N6	5.46	121.88	118.60
44	5	2838	А	C4-C5-N7	5.46	113.43	110.70
44	5	12	А	C6-C5-N7	5.46	136.12	132.30
44	5	499	G	C8-N9-C4	5.46	108.58	106.40
44	5	518	G	C6-C5-N7	-5.46	127.12	130.40
44	5	527	А	C5-N7-C8	-5.46	101.17	103.90
44	5	1565	G	C8-N9-C4	-5.46	104.22	106.40
44	5	2118	С	C6-N1-C2	-5.46	118.11	120.30
44	5	2711	С	N3-C2-O2	-5.46	118.08	121.90
44	5	3217	С	C2-N1-C1'	5.46	124.81	118.80
45	8	49	G	N9-C4-C5	-5.46	103.22	105.40
44	5	140	С	C6-N1-C2	-5.46	118.12	120.30
44	5	1663	С	C6-N1-C2	-5.46	118.12	120.30
44	5	1223	А	C4-C5-N7	5.46	113.43	110.70
44	5	1296	С	C4-C5-C6	-5.46	114.67	117.40
44	5	2337	С	C6-N1-C2	-5.46	118.12	120.30
44	5	2714	G	N3-C4-C5	5.46	131.33	128.60
44	5	3199	G	C6-C5-N7	-5.46	127.12	130.40
45	8	72	А	N3-C4-N9	5.46	131.77	127.40
44	5	130	A	N9-C4-C5	-5.46	103.62	105.80
44	5	1672	U	N1-C2-O2	5.46	126.62	122.80
44	5	335	G	C8-N9-C1'	-5.46	119.91	127.00
44	5	62	А	P-O3'-C3'	5.45	126.24	119.70
44	5	1837	U	N1-C2-O2	5.45	126.62	122.80
44	5	3158	G	N9-C4-C5	-5.45	103.22	105.40
45	8	23	U	C5-C4-O4	-5.45	122.63	125.90
44	5	1404	G	O5'-P-OP2	-5.45	100.79	105.70
44	5	1824	U	C5-C6-N1	5.45	125.42	122.70
45	8	155	A	N1-C6-N6	-5.45	115.33	118.60
3	В	351	LEU	CA-CB-CG	5.45	127.83	115.30
44	5	158	G	C4-C5-N7	5.45	112.98	110.80
44	5	2531	С	C6-N1-C2	-5.45	118.12	120.30
44	5	2553	U	N3-C2-O2	-5.45	118.39	122.20
44	5	1281	G	N3-C4-N9	5.45	129.27	126.00
44	5	955	U	C2-N1-C1'	5.45	124.23	117.70
44	5	1592	G	N3-C2-N2	-5.45	116.09	119.90
44	5	1064	A	N7-C8-N9	-5.44	111.08	113.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	3173	G	N3-C4-N9	5.44	129.27	126.00
44	5	602	А	C5-N7-C8	-5.44	101.18	103.90
44	5	1759	С	C2-N3-C4	5.44	122.62	119.90
44	5	2656	А	C6-N1-C2	5.44	121.86	118.60
44	5	1061	А	C5-N7-C8	-5.44	101.18	103.90
44	5	1087	G	C8-N9-C4	5.44	108.58	106.40
46	7	87	G	C2-N3-C4	5.44	114.62	111.90
44	5	185	С	C4-C5-C6	-5.43	114.68	117.40
44	5	2283	G	N3-C4-C5	5.43	131.32	128.60
46	7	40	С	C6-N1-C2	-5.43	118.13	120.30
44	5	11	А	N9-C4-C5	-5.43	103.63	105.80
44	5	137	G	C8-N9-C1'	5.43	134.06	127.00
44	5	283	G	C8-N9-C1'	-5.43	119.94	127.00
44	5	340	С	C2-N3-C4	5.43	122.62	119.90
44	5	2499	U	N3-C2-O2	-5.43	118.40	122.20
44	5	235	А	C8-N9-C4	-5.43	103.63	105.80
44	5	1750	A	O4'-C1'-N9	5.43	112.54	108.20
44	5	546	С	C6-N1-C2	5.43	122.47	120.30
44	5	3123	А	C4-C5-C6	-5.43	114.28	117.00
45	8	26	U	C5-C6-N1	-5.43	119.98	122.70
44	5	1262	G	N3-C4-C5	5.43	131.31	128.60
44	5	2523	А	C8-N9-C4	5.43	107.97	105.80
44	5	3308	С	C6-N1-C2	-5.43	118.13	120.30
44	5	143	G	N3-C2-N2	-5.43	116.10	119.90
44	5	242	С	N3-C4-C5	5.43	124.07	121.90
44	5	2962	U	N1-C2-O2	5.43	126.60	122.80
44	5	1298	С	N1-C2-O2	5.42	122.15	118.90
44	5	2209	U	C5-C6-N1	-5.42	119.99	122.70
45	8	149	A	N3-C4-C5	5.42	130.60	126.80
44	5	1676	A	N9-C4-C5	-5.42	103.63	105.80
44	5	1766	G	C6-C5-N7	-5.42	127.15	130.40
44	5	2470	С	C5-C6-N1	-5.42	118.29	121.00
44	5	3289	G	N3-C2-N2	-5.42	116.11	119.90
44	5	2101	С	OP1-P-O3'	5.42	117.12	105.20
44	5	3254	G	N3-C4-C5	5.42	131.31	128.60
44	5	1464	G	C5-N7-C8	-5.42	101.59	104.30
44	5	2541	U	C5-C4-O4	-5.42	122.65	125.90
44	5	1259	A	C8-N9-C4	5.42	107.97	105.80
45	8	69	U	N3-C2-O2	-5.42	118.41	122.20
44	5	439	C	N1-C2-O2	5.41	122.15	118.90
44	5	1759	C	C6-N1-C2	-5.41	118.13	120.30
32	e	226	LEU	CA-CB-CG	5.41	127.75	115.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	233	С	C6-N1-C2	-5.41	118.14	120.30
44	5	2196	С	N1-C2-O2	5.41	122.15	118.90
44	5	2299	А	C5-C6-N6	-5.41	119.37	123.70
46	7	100	С	C5-C6-N1	5.41	123.70	121.00
44	5	627	U	C5-C6-N1	5.41	125.40	122.70
44	5	793	С	N3-C2-O2	-5.41	118.11	121.90
44	5	1907	С	N1-C2-O2	5.41	122.14	118.90
44	5	2299	А	N1-C6-N6	5.41	121.84	118.60
44	5	311	С	N1-C2-O2	5.41	122.14	118.90
44	5	1087	G	C5-C6-O6	-5.41	125.36	128.60
44	5	1483	G	C4-N9-C1'	-5.41	119.47	126.50
44	5	2195	С	C2-N3-C4	5.41	122.60	119.90
44	5	2947	G	N1-C6-O6	-5.41	116.66	119.90
44	5	1061	А	N1-C6-N6	5.40	121.84	118.60
44	5	2687	G	N9-C4-C5	-5.40	103.24	105.40
44	5	3263	G	N1-C6-O6	5.40	123.14	119.90
44	5	852	U	N1-C2-O2	5.40	126.58	122.80
44	5	2810	С	N1-C2-O2	5.40	122.14	118.90
44	5	3147	G	C8-N9-C4	5.40	108.56	106.40
44	5	3161	С	C2-N3-C4	5.40	122.60	119.90
44	5	3163	А	N9-C4-C5	-5.40	103.64	105.80
44	5	127	G	C5-N7-C8	-5.40	101.60	104.30
44	5	373	А	N7-C8-N9	5.40	116.50	113.80
44	5	1306	G	C8-N9-C4	5.40	108.56	106.40
44	5	1409	G	C8-N9-C4	5.40	108.56	106.40
44	5	2283	G	C8-N9-C1'	5.40	134.02	127.00
44	5	1922	А	C6-C5-N7	-5.40	128.52	132.30
44	5	2353	G	N9-C4-C5	-5.40	103.24	105.40
44	5	2790	А	N1-C2-N3	-5.40	126.60	129.30
44	5	2855	U	C5-C6-N1	5.40	125.40	122.70
46	7	106	U	N1-C2-O2	5.40	126.58	122.80
44	5	3041	U	N3-C2-O2	-5.39	118.42	122.20
44	5	120	G	C2-N3-C4	-5.39	109.20	111.90
44	5	525	С	C5-C6-N1	5.39	123.69	121.00
44	5	2488	А	C8-N9-C1'	-5.39	118.00	127.70
44	5	3007	U	C2-N1-C1'	5.39	124.17	117.70
44	5	3273	A	C4-C5-N7	5.39	113.39	110.70
44	5	2234	G	C8-N9-C4	-5.39	104.25	106.40
44	5	446	U	C4-C5-C6	-5.38	116.47	119.70
44	5	1262	G	C4-N9-C1'	-5.38	119.50	126.50
44	5	1544	G	N3-C2-N2	-5.38	116.13	119.90
44	5	2490	C	C5-C6-N1	5.38	123.69	121.00

Continued on next page...



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2899	С	C2-N3-C4	5.38	122.59	119.90
44	5	1532	С	N1-C2-O2	5.38	122.13	118.90
44	5	1881	А	N9-C4-C5	-5.38	103.65	105.80
44	5	2486	А	N7-C8-N9	-5.38	111.11	113.80
44	5	2606	G	N3-C4-N9	5.38	129.23	126.00
44	5	2748	А	C5-N7-C8	-5.38	101.21	103.90
44	5	3016	А	N1-C2-N3	-5.38	126.61	129.30
44	5	3016	А	N9-C4-C5	-5.38	103.65	105.80
44	5	446	U	N3-C4-O4	-5.38	115.63	119.40
44	5	3133	С	C4-C5-C6	-5.38	114.71	117.40
44	5	1346	G	C6-C5-N7	5.38	133.63	130.40
44	5	1594	А	O4'-C1'-N9	5.38	112.50	108.20
44	5	2494	A	N1-C2-N3	-5.38	126.61	129.30
44	5	2626	А	N1-C6-N6	5.38	121.83	118.60
44	5	569	А	C4-C5-N7	5.38	113.39	110.70
44	5	1321	G	N9-C4-C5	-5.38	103.25	105.40
44	5	3233	С	C6-N1-C2	-5.38	118.15	120.30
44	5	529	А	N1-C6-N6	5.38	121.83	118.60
44	5	2291	А	C4-C5-N7	5.38	113.39	110.70
44	5	1222	G	N3-C4-C5	5.37	131.29	128.60
44	5	1266	G	N9-C4-C5	-5.37	103.25	105.40
44	5	2513	U	C4-C5-C6	-5.37	116.47	119.70
44	5	3278	С	N3-C2-O2	-5.37	118.14	121.90
44	5	613	G	C5-C6-O6	-5.37	125.38	128.60
44	5	946	U	N1-C2-O2	5.37	126.56	122.80
44	5	2706	G	C8-N9-C4	5.37	108.55	106.40
44	5	3242	G	C5-C6-O6	-5.37	125.38	128.60
44	5	568	G	C5-N7-C8	-5.37	101.61	104.30
44	5	2167	A	C5-N7-C8	-5.37	101.22	103.90
44	5	1483	G	N3-C4-N9	-5.37	122.78	126.00
44	5	3076	C	C6-N1-C2	-5.37	118.15	120.30
44	5	861	С	C5-C6-N1	5.37	123.68	121.00
44	5	1288	U	N3-C2-O2	-5.37	118.44	122.20
44	5	1595	U	C2-N1-C1'	-5.37	111.26	117.70
44	5	2337	C	N3-C4-N4	-5.37	114.25	118.00
44	5	3278	C	N1-C2-O2	5.37	122.12	118.90
46	7	8	G	N3-C4-C5	5.37	131.28	128.60
44	5	150	A	C8-N9-C4	5.36	107.95	105.80
44	5	678	G	C5-N7-C8	-5.36	101.62	104.30
44	5	1817	G	C4-N9-C1'	-5.36	119.53	126.50
44	5	2582	C	C6-N1-C2	-5.36	118.16	120.30
44	5	3228	I C	OP2-P-O3'	5.36	117.00	105.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	581	U	C2-N1-C1'	5.36	124.13	117.70
44	5	654	С	N1-C2-O2	5.36	122.12	118.90
44	5	1268	G	C4-C5-N7	5.36	112.94	110.80
44	5	2098	С	C5-C6-N1	5.36	123.68	121.00
44	5	2346	С	C5-C6-N1	5.36	123.68	121.00
44	5	3202	G	N3-C4-N9	5.36	129.22	126.00
44	5	1671	С	N1-C2-O2	5.36	122.11	118.90
44	5	2149	А	C5-C6-N6	-5.36	119.42	123.70
1	Z	399	LEU	CA-CB-CG	5.35	127.61	115.30
44	5	141	С	C5-C6-N1	5.35	123.68	121.00
44	5	660	А	N3-C4-N9	-5.35	123.12	127.40
45	8	94	С	C5-C6-N1	5.35	123.68	121.00
44	5	1061	А	C4-C5-N7	5.35	113.38	110.70
44	5	1685	С	C5-C6-N1	5.35	123.67	121.00
44	5	3146	G	N9-C4-C5	-5.35	103.26	105.40
44	5	1346	G	N1-C6-O6	-5.35	116.69	119.90
44	5	3110	С	N3-C2-O2	-5.35	118.16	121.90
44	5	437	G	C5-C6-O6	-5.35	125.39	128.60
44	5	3260	G	C4-C5-N7	5.35	112.94	110.80
44	5	2200	U	C5-C6-N1	5.34	125.37	122.70
44	5	2436	U	C5-C6-N1	5.34	125.37	122.70
44	5	2148	U	N1-C2-O2	5.34	126.54	122.80
44	5	243	G	C4-C5-N7	5.34	112.94	110.80
44	5	1836	С	N3-C2-O2	-5.34	118.16	121.90
44	5	1238	С	C2-N3-C4	5.34	122.57	119.90
44	5	1422	G	C8-N9-C4	5.34	108.54	106.40
44	5	1953	G	O5'-P-OP1	-5.34	100.89	105.70
44	5	2146	С	C6-N1-C2	-5.34	118.16	120.30
44	5	3023	U	N3-C2-O2	-5.34	118.46	122.20
44	5	1268	G	N1-C6-O6	5.34	123.10	119.90
44	5	3112	G	C4-C5-N7	5.34	112.94	110.80
44	5	234	G	N9-C4-C5	-5.34	103.27	105.40
44	5	374	А	C4-N9-C1'	-5.34	116.69	126.30
44	5	1141	С	C6-N1-C2	-5.34	118.17	120.30
44	5	2638	С	N3-C2-O2	-5.34	118.17	121.90
44	5	3135	U	N1-C2-O2	5.34	126.54	122.80
44	5	3248	С	C5-C6-N1	5.33	123.67	121.00
44	5	677	A	C5-N7-C8	-5.33	101.23	103.90
44	5	2354	C	C5-C6-N1	5.33	123.67	121.00
44	5	2969	A	C8-N9-C4	5.33	107.93	105.80
44	5	1756	C	N1-C2-O2	$5.3\overline{3}$	$122.1\overline{0}$	118.90
44	5	3023	U	C6-N1-C2	-5.33	117.80	121.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1231	А	C4-C5-N7	5.33	113.36	110.70
44	5	224	С	C2-N1-C1'	5.33	124.66	118.80
44	5	537	А	C5-N7-C8	-5.33	101.24	103.90
44	5	2928	С	C6-N1-C1'	-5.33	114.41	120.80
44	5	31	С	C6-N1-C1'	-5.33	114.41	120.80
44	5	1227	С	N3-C4-N4	-5.33	114.27	118.00
44	5	1750	A	C4-C5-N7	5.33	113.36	110.70
45	8	149	A	N3-C4-N9	-5.33	123.14	127.40
44	5	1358	С	C6-N1-C2	-5.32	118.17	120.30
44	5	1057	A	N9-C4-C5	-5.32	103.67	105.80
44	5	175	C	C6-N1-C2	-5.32	118.17	120.30
44	5	600	G	N9-C4-C5	-5.32	103.27	105.40
44	5	1922	A	N9-C4-C5	-5.32	103.67	105.80
44	5	2596	U	C5-C4-O4	-5.32	122.71	125.90
44	5	1039	U	N1-C2-O2	5.32	126.52	122.80
46	7	35	C	C5-C6-N1	5.32	123.66	121.00
44	5	55	G	C8-N9-C1'	5.32	133.91	127.00
44	5	1566	A	C6-C5-N7	-5.32	128.58	132.30
44	5	3017	A	C5-N7-C8	-5.32	101.24	103.90
44	5	1816	А	P-O3'-C3'	5.32	126.08	119.70
44	5	2375	G	C8-N9-C4	5.32	108.53	106.40
44	5	3191	G	C6-C5-N7	-5.32	127.21	130.40
44	5	555	U	N3-C2-O2	5.31	125.92	122.20
44	5	1874	A	N9-C4-C5	-5.31	103.67	105.80
45	8	77	A	C2-N3-C4	5.31	113.25	110.60
44	5	393	U	N1-C2-O2	5.31	126.52	122.80
44	5	949	С	N1-C2-O2	5.31	122.08	118.90
44	5	1646	G	N3-C4-C5	5.31	131.25	128.60
44	5	2238	G	C5-N7-C8	-5.31	101.65	104.30
44	5	3153	U	O4'-C1'-N1	5.31	112.45	108.20
28	a	159	LEU	CA-CB-CG	5.30	127.50	115.30
44	5	31	С	C5-C6-N1	5.30	123.65	121.00
44	5	121	A	C4-C5-C6	-5.30	114.35	117.00
44	5	242	С	C4-C5-C6	-5.30	114.75	117.40
44	5	120	G	C4-N9-C1'	-5.30	119.61	126.50
44	5	200	C	N3-C4-C5	5.30	124.02	121.90
45	8	15	G	C8-N9-C4	5.30	108.52	106.40
44	5	397	A	C5-N7-C8	-5.30	101.25	103.90
44	5	919	U	N3-C2-O2	-5.30	118.49	122.20
44	5	1190	A	C4-C5-N7	5.30	113.35	110.70
44	5	3337	G	C4-C5-N7	5.30	112.92	110.80
44	5	445	G	N3-C4-N9	5.30	129.18	126.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1901	А	C4-N9-C1'	5.30	135.84	126.30
44	5	2550	U	N1-C2-O2	5.30	126.51	122.80
44	5	433	А	C5-N7-C8	-5.29	101.25	103.90
44	5	638	С	C2-N1-C1'	5.29	124.62	118.80
44	5	1447	G	N3-C4-C5	5.29	131.25	128.60
44	5	1825	G	N3-C4-C5	-5.29	125.96	128.60
44	5	2556	С	C5-C6-N1	5.29	123.64	121.00
44	5	732	С	C6-N1-C2	-5.29	118.19	120.30
44	5	2995	A	C4-C5-N7	5.29	113.34	110.70
44	5	835	G	N3-C4-C5	5.29	131.24	128.60
44	5	1292	С	C2-N1-C1'	5.29	124.61	118.80
44	5	1898	G	N1-C6-O6	-5.29	116.73	119.90
44	5	2683	U	C5-C6-N1	-5.29	120.06	122.70
44	5	637	С	P-O3'-C3'	5.28	126.04	119.70
44	5	855	U	N3-C2-O2	-5.28	118.50	122.20
44	5	130	А	N1-C6-N6	5.28	121.77	118.60
44	5	390	G	C4-C5-N7	5.28	112.91	110.80
44	5	998	А	C4-C5-N7	5.28	113.34	110.70
44	5	1190	A	C8-N9-C1'	-5.28	118.20	127.70
44	5	3005	А	C4-N9-C1'	-5.28	116.80	126.30
44	5	1145	G	N9-C4-C5	-5.28	103.29	105.40
44	5	2981	U	N1-C2-O2	5.28	126.50	122.80
45	8	93	U	N3-C2-O2	-5.27	118.51	122.20
46	7	79	A	C5-N7-C8	-5.27	101.26	103.90
44	5	1005	G	C6-C5-N7	5.27	133.56	130.40
44	5	1888	U	N3-C2-O2	-5.27	118.51	122.20
44	5	2129	U	N1-C2-O2	5.27	126.49	122.80
44	5	2492	С	P-O3'-C3'	5.27	126.03	119.70
44	5	3369	G	C2-N3-C4	5.27	114.54	111.90
45	8	140	G	C8-N9-C4	5.27	108.51	106.40
44	5	975	C	C6-N1-C2	-5.27	118.19	120.30
44	5	1432	C	N3-C4-C5	5.27	124.01	121.90
44	5	2529	A	N7-C8-N9	5.27	116.44	113.80
44	5	3193	C	C5-C6-N1	5.27	123.64	121.00
44	5	1301	A	N1-C6-N6	-5.27	115.44	118.60
44	5	1464	G	C4-C5-N7	5.27	112.91	110.80
44	5	289	A	N7-C8-N9	5.27	116.43	113.80
44	5	772	U	C5-C6-N1	5.27	125.33	122.70
44	5	1817	G	C8-N9-C1'	5.27	133.85	127.00
44	5	2731	U	N3-C2-O2	-5.27	118.51	122.20
44	5	564	G	N9-C4-C5	-5.26	103.30	105.40
44	5	949	C	C5-C6-N1	5.26	123.63	121.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1145	G	C4-C5-N7	5.26	112.91	110.80
44	5	1280	С	C6-N1-C1'	5.26	127.12	120.80
44	5	1535	А	C4-C5-N7	5.26	113.33	110.70
44	5	3200	G	C4-N9-C1'	-5.26	119.66	126.50
44	5	3121	U	C2-N1-C1'	5.26	124.02	117.70
44	5	501	А	N9-C4-C5	-5.26	103.70	105.80
44	5	1849	С	N3-C4-C5	5.26	124.00	121.90
44	5	1924	U	N1-C2-O2	5.26	126.48	122.80
44	5	103	G	N3-C4-N9	5.26	129.16	126.00
44	5	414	U	N1-C2-O2	5.26	126.48	122.80
46	7	80	G	C8-N9-C4	-5.26	104.30	106.40
44	5	1749	А	N3-C4-N9	-5.26	123.19	127.40
44	5	786	А	N3-C4-N9	-5.26	123.19	127.40
44	5	1242	G	C4-N9-C1'	5.26	133.33	126.50
44	5	1742	U	N1-C2-O2	5.26	126.48	122.80
46	7	26	С	C2-N1-C1'	5.26	124.58	118.80
44	5	352	А	N7-C8-N9	-5.25	111.17	113.80
44	5	352	А	O4'-C1'-N9	5.25	112.40	108.20
44	5	2720	G	N3-C4-C5	-5.25	125.97	128.60
44	5	202	G	C2-N3-C4	5.25	114.53	111.90
44	5	1066	G	C5-N7-C8	-5.25	101.67	104.30
44	5	1759	С	C5-C4-N4	-5.25	116.52	120.20
44	5	3029	А	C5-N7-C8	-5.25	101.28	103.90
44	5	1239	С	N3-C4-N4	-5.25	114.33	118.00
44	5	1947	G	N3-C2-N2	-5.25	116.22	119.90
44	5	2096	А	N9-C4-C5	-5.25	103.70	105.80
44	5	2541	U	C6-N1-C2	5.25	124.15	121.00
44	5	2562	A	C5-N7-C8	-5.25	101.28	103.90
44	5	258	G	C4-C5-N7	5.25	112.90	110.80
44	5	2096	A	C4-C5-N7	5.24	113.32	110.70
44	5	129	U	C5-C6-N1	5.24	125.32	122.70
44	5	3185	U	N3-C2-O2	5.24	125.87	122.20
44	5	1869	С	C5-C6-N1	5.24	123.62	121.00
44	5	120	G	N3-C4-N9	-5.24	122.86	126.00
44	5	1873	U	C5-C6-N1	5.24	125.32	122.70
44	5	3230	G	C2-N3-C4	-5.24	109.28	111.90
44	5	2253	G	P-O3'-C3'	5.24	125.98	119.70
44	5	308	A	C6-C5-N7	-5.24	128.63	132.30
44	5	909	G	P-O3'-C3'	5.24	125.98	119.70
44	5	3158	G	C4-C5-N7	5.24	112.89	110.80
44	5	3193	C	C4-C5-C6	-5.24	114.78	117.40
44	5	439		C2-N1-C1'	5.23	124.56	118.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1961	G	C4-N9-C1'	5.23	133.30	126.50
46	7	17	A	N9-C4-C5	-5.23	103.71	105.80
44	5	2748	A	N7-C8-N9	5.23	116.42	113.80
44	5	3023	U	C5-C6-N1	5.23	125.32	122.70
44	5	3191	G	C5-N7-C8	-5.23	101.69	104.30
44	5	2391	G	N1-C6-O6	-5.23	116.76	119.90
44	5	2848	G	N3-C2-N2	-5.23	116.24	119.90
44	5	64	G	N1-C6-O6	5.23	123.04	119.90
44	5	445	G	C4-N9-C1'	5.23	133.30	126.50
44	5	607	A	C8-N9-C1'	-5.23	118.29	127.70
44	5	2841	G	N7-C8-N9	5.23	115.71	113.10
45	8	148	G	N1-C2-N2	5.23	120.90	116.20
44	5	353	G	N3-C2-N2	-5.23	116.24	119.90
44	5	2221	G	N3-C4-C5	5.23	131.21	128.60
44	5	2948	С	C6-N1-C2	-5.23	118.21	120.30
44	5	123	A	N3-C4-N9	5.22	131.58	127.40
44	5	920	A	C8-N9-C4	5.22	107.89	105.80
44	5	1563	С	C2-N1-C1'	-5.22	113.05	118.80
44	5	1590	G	C4-C5-N7	5.22	112.89	110.80
45	8	4	С	C6-N1-C2	-5.22	118.21	120.30
46	7	59	U	C5-C6-N1	5.22	125.31	122.70
44	5	2114	С	C5-C6-N1	5.22	123.61	121.00
44	5	64	G	C5-C6-O6	-5.22	125.47	128.60
44	5	1216	С	C6-N1-C2	-5.22	118.21	120.30
44	5	2965	U	O4'-C1'-N1	5.22	112.38	108.20
44	5	3326	G	N1-C2-N2	5.22	120.90	116.20
44	5	2193	U	C6-N1-C1'	-5.22	113.89	121.20
44	5	1263	A	C6-C5-N7	-5.22	128.65	132.30
44	5	2552	С	N3-C2-O2	-5.22	118.25	121.90
44	5	1066	G	N9-C4-C5	-5.21	103.31	105.40
44	5	1487	G	N9-C4-C5	-5.21	103.31	105.40
44	5	1825	G	C4-N9-C1'	5.21	133.28	126.50
46	7	17	A	C4-C5-N7	5.21	113.31	110.70
44	5	3354	U	C6-N1-C1'	-5.21	113.90	121.20
44	5	3365	U	N1-C2-O2	5.21	126.45	122.80
44	5	526	C	C6-N1-C2	-5.21	118.22	120.30
44	5	665	A	C4-C5-N7	5.21	113.31	110.70
44	5	1345	G	C2-N3-C4	5.21	114.50	111.90
44	5	660	A	C2-N3-C4	-5.21	108.00	110.60
44	5	1376	C	O4'-C1'-N1	5.21	112.37	108.20
44	5	342	A	C5-C6-N6	5.21	127.87	123.70
44	5	542	G	C4-C5-N7	5.21	112.88	110.80



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	863	С	C2-N1-C1'	5.21	124.53	118.80
44	5	1878	G	C2-N3-C4	5.21	114.50	111.90
44	5	2078	С	C6-N1-C2	-5.21	118.22	120.30
45	8	154	С	C6-N1-C1'	5.21	127.05	120.80
44	5	3033	А	C5-C6-N1	5.21	120.30	117.70
44	5	347	G	C2-N3-C4	5.20	114.50	111.90
44	5	113	С	N1-C2-O2	5.20	122.02	118.90
44	5	428	А	N9-C4-C5	-5.20	103.72	105.80
44	5	55	G	C6-C5-N7	5.20	133.52	130.40
44	5	390	G	N3-C4-N9	5.20	129.12	126.00
44	5	518	G	C4-C5-N7	5.20	112.88	110.80
44	5	656	A	N7-C8-N9	5.20	116.40	113.80
44	5	2322	С	N1-C2-O2	5.20	122.02	118.90
44	5	2577	С	C5-C6-N1	5.20	123.60	121.00
44	5	2782	U	C2-N3-C4	5.20	130.12	127.00
44	5	2868	U	N1-C2-O2	5.20	126.44	122.80
28	a	214	LEU	CA-CB-CG	5.20	127.25	115.30
44	5	1420	С	N3-C2-O2	-5.20	118.26	121.90
44	5	859	G	N7-C8-N9	5.20	115.70	113.10
44	5	2531	С	C5-C6-N1	5.20	123.60	121.00
44	5	2918	G	C2-N3-C4	5.20	114.50	111.90
45	8	92	A	N9-C4-C5	-5.20	103.72	105.80
44	5	1749	A	C4-N9-C1'	-5.19	116.95	126.30
44	5	3272	С	C5'-C4'-O4'	5.19	115.33	109.10
44	5	333	G	O5'-P-OP2	-5.19	101.03	105.70
44	5	1126	G	N1-C6-O6	-5.19	116.78	119.90
44	5	1046	А	C4-C5-N7	5.19	113.30	110.70
44	5	1718	G	C5-C6-O6	-5.19	125.49	128.60
44	5	1736	G	C2-N3-C4	5.19	114.49	111.90
44	5	623	U	N3-C4-C5	5.19	117.71	114.60
44	5	3303	G	C4-C5-N7	5.19	112.88	110.80
46	7	77	G	N3-C4-C5	5.19	131.19	128.60
44	5	3388	C	C2-N1-C1'	-5.19	113.10	118.80
44	5	540	U	C5-C6-N1	5.18	125.29	122.70
44	5	1245	A	N9-C4-C5	-5.18	103.73	105.80
44	5	2439	A	N7-C8-N9	5.18	116.39	113.80
44	5	781	G	C4-C5-N7	5.18	112.87	110.80
44	5	1310	G	OP1-P-O3'	5.18	116.60	105.20
45	8	35	C	N3-C2-O2	-5.18	118.27	121.90
44	5	978	G	C4-C5-N7	5.18	112.87	110.80
44	5	1733	G	N1-C6-O6	-5.18	116.79	119.90
44	5	1953	G	C2-N3-C4	5.18	114.49	111.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2584	G	N9-C4-C5	-5.18	103.33	105.40
44	5	2873	U	N1-C2-O2	5.18	126.43	122.80
44	5	110	G	N3-C4-C5	5.18	131.19	128.60
44	5	1217	А	C4-C5-N7	5.18	113.29	110.70
44	5	1263	А	C8-N9-C1'	-5.18	118.38	127.70
44	5	1877	U	C5-C6-N1	5.18	125.29	122.70
44	5	2483	G	C8-N9-C4	-5.18	104.33	106.40
44	5	3034	С	C5-C6-N1	5.18	123.59	121.00
44	5	439	C	C6-N1-C1'	-5.18	114.59	120.80
44	5	551	A	C4-C5-C6	-5.18	114.41	117.00
44	5	1838	G	C8-N9-C4	5.18	108.47	106.40
44	5	2779	А	C2-N3-C4	5.18	113.19	110.60
44	5	10	С	C2-N1-C1'	-5.17	113.11	118.80
44	5	677	А	N3-C4-C5	5.17	130.42	126.80
44	5	3199	G	C4-C5-N7	5.17	112.87	110.80
5	D	553	LEU	CA-CB-CG	5.17	127.20	115.30
44	5	196	G	N1-C2-N2	-5.17	111.55	116.20
44	5	1400	G	C4-C5-N7	5.17	112.87	110.80
44	5	1960	A	N3-C4-C5	-5.17	123.18	126.80
44	5	2447	А	N9-C4-C5	-5.17	103.73	105.80
44	5	2545	С	N3-C2-O2	-5.17	118.28	121.90
44	5	3393	U	N3-C2-O2	-5.17	118.58	122.20
44	5	503	С	C5-C6-N1	5.17	123.58	121.00
44	5	1349	G	N3-C2-N2	5.17	123.52	119.90
44	5	1574	C	C5-C6-N1	5.17	123.58	121.00
44	5	1867	A	C4-C5-N7	5.17	113.28	110.70
46	7	24	A	N7-C8-N9	5.17	116.38	113.80
44	5	515	С	N3-C2-O2	-5.17	118.28	121.90
44	5	1279	С	C5-C6-N1	5.17	123.58	121.00
44	5	2183	A	C8-N9-C4	5.17	107.87	105.80
44	5	915	A	C4-N9-C1'	5.17	135.60	126.30
44	5	1039	U	C5-C6-N1	5.17	125.28	122.70
44	5	399	A	C4-C5-N7	5.16	113.28	110.70
44	5	1226	G	C8-N9-C4	-5.16	104.33	106.40
44	5	1766	G	C5-N7-C8	-5.16	101.72	104.30
44	5	2568	C	C5-C6-N1	-5.16	118.42	121.00
45	8	25	G	C5-N7-C8	-5.16	101.72	104.30
46	7	105	C	C6-N1-C2	-5.16	118.23	120.30
44	5	2816	G	O4'-C1'-N9	-5.16	104.07	108.20
44	5	92	G	O4'-C1'-N9	5.16	112.33	108.20
44	5	552	G	N3-C2-N2	-5.16	116.29	119.90
44	5	2965	U	N3-C2-O2	-5.16	118.59	122.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	3257	С	C2-N1-C1'	-5.16	113.12	118.80
44	5	212	G	N1-C6-O6	-5.16	116.81	119.90
44	5	379	С	N1-C2-O2	5.16	122.00	118.90
44	5	2106	А	N1-C2-N3	-5.16	126.72	129.30
44	5	2192	С	C2-N3-C4	5.16	122.48	119.90
44	5	3324	С	C6-N1-C2	-5.16	118.24	120.30
44	5	937	G	C4-N9-C1'	5.16	133.20	126.50
44	5	2432	А	C5-C6-N6	-5.16	119.58	123.70
44	5	3318	G	C8-N9-C4	5.16	108.46	106.40
44	5	3333	G	N3-C4-N9	-5.16	122.91	126.00
44	5	564	G	C4-C5-N7	5.15	112.86	110.80
44	5	2995	А	N9-C4-C5	-5.15	103.74	105.80
44	5	787	G	C4-C5-N7	5.15	112.86	110.80
45	8	120	С	C2-N3-C4	5.15	122.47	119.90
44	5	870	G	N7-C8-N9	5.15	115.67	113.10
44	5	2526	С	C6-N1-C2	-5.15	118.24	120.30
44	5	2505	U	N1-C2-O2	-5.15	119.20	122.80
44	5	2687	G	N3-C2-N2	5.15	123.50	119.90
44	5	124	U	N1-C2-O2	5.15	126.40	122.80
44	5	411	U	N3-C2-O2	-5.15	118.60	122.20
44	5	1056	U	N3-C2-O2	-5.14	118.60	122.20
44	5	2838	А	C5-C6-N1	5.14	120.27	117.70
45	8	18	U	N3-C2-O2	-5.14	118.60	122.20
44	5	2873	U	N3-C2-O2	-5.14	118.60	122.20
44	5	349	A	N1-C6-N6	-5.14	115.52	118.60
44	5	1396	С	C2-N1-C1'	5.14	124.45	118.80
44	5	1217	A	C5-N7-C8	-5.14	101.33	103.90
44	5	681	U	C6-N1-C1'	-5.13	114.01	121.20
44	5	1759	С	C4-C5-C6	-5.13	114.83	117.40
44	5	2769	A	C4-C5-N7	5.13	113.27	110.70
44	5	775	A	C8-N9-C4	5.13	107.85	105.80
44	5	3212	С	C6-N1-C2	-5.13	118.25	120.30
45	8	61	A	C2-N3-C4	-5.13	108.03	110.60
44	5	726	G	C5-C6-O6	-5.13	125.52	128.60
44	5	113	С	C5-C6-N1	5.13	123.56	121.00
44	5	1756	C	C2-N1-C1'	5.13	124.44	118.80
44	5	3211	C	C5-C6-N1	5.13	123.56	121.00
29	b	88	LYS	C-N-CA	5.12	134.51	121.70
44	5	607	A	N3-C4-N9	5.12	131.50	127.40
44	5	1735	G	C4-C5-N7	5.12	112.85	110.80
45	8	12	A	N9-C4-C5	-5.12	103.75	105.80
45	8	88	A	N9-C1'-C2'	5.12	120.66	114.00



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	1890	U	C5-C6-N1	5.12	125.26	122.70
44	5	2782	U	C5-C6-N1	5.12	125.26	122.70
44	5	850	U	C5-C6-N1	5.12	125.26	122.70
44	5	1084	А	C4-C5-C6	-5.12	114.44	117.00
44	5	1482	А	C2-N3-C4	5.12	113.16	110.60
44	5	2468	А	C6-N1-C2	5.12	121.67	118.60
44	5	55	G	O4'-C1'-N9	5.12	112.30	108.20
44	5	1813	А	C2-N3-C4	5.12	113.16	110.60
44	5	2193	U	C5-C6-N1	5.12	125.26	122.70
44	5	527	А	N7-C8-N9	5.12	116.36	113.80
44	5	1690	С	C6-N1-C2	-5.12	118.25	120.30
44	5	344	A	N9-C4-C5	-5.11	103.75	105.80
44	5	2137	U	C2-N1-C1'	5.11	123.84	117.70
44	5	2298	U	N3-C2-O2	-5.11	118.62	122.20
44	5	2794	G	C8-N9-C4	5.11	108.44	106.40
44	5	239	G	C2-N3-C4	-5.11	109.34	111.90
44	5	2349	U	N3-C2-O2	-5.11	118.62	122.20
44	5	923	C	N3-C4-C5	5.11	123.94	121.90
44	5	2922	G	C6-C5-N7	-5.11	127.33	130.40
44	5	1927	G	N3-C4-N9	5.11	129.06	126.00
44	5	2788	С	C2-N1-C1'	5.11	124.42	118.80
44	5	67	A	N3-C4-C5	5.11	130.37	126.80
44	5	1254	С	N3-C2-O2	-5.11	118.33	121.90
44	5	770	G	N3-C4-N9	-5.10	122.94	126.00
44	5	2722	U	N1-C2-O2	5.10	126.37	122.80
44	5	2989	U	C5-C6-N1	-5.10	120.15	122.70
44	5	3266	G	C4-N9-C1'	-5.10	119.87	126.50
45	8	3	A	N7-C8-N9	5.10	116.35	113.80
44	5	3288	G	C6-C5-N7	5.10	133.46	130.40
44	5	1150	A	C2-N3-C4	5.10	113.15	110.60
44	5	1328	С	C6-N1-C2	-5.10	118.26	120.30
44	5	2671	A	N9-C4-C5	-5.10	103.76	105.80
44	5	3064	U	N1-C2-O2	5.10	126.37	122.80
44	5	3122	A	N1-C6-N6	5.10	121.66	118.60
44	5	3368	U	C6-N1-C2	5.10	124.06	121.00
45	8	132	G	C8-N9-C4	5.10	108.44	106.40
46	7	100	C	C6-N1-C2	-5.10	118.26	120.30
44	5	443	G	N3-C4-C5	5.09	131.15	128.60
44	5	659	G	C4-C5-N7	5.09	112.84	110.80
44	5	2829	U	C6-N1-C2	-5.09	117.94	121.00
44	5	2296	A	C2-N3-C4	-5.09	108.05	110.60
44	5	3166	C	C6-N1-C2	-5.09	118.26	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	2519	А	C8-N9-C4	5.09	107.84	105.80
44	5	711	А	C5-N7-C8	-5.09	101.36	103.90
44	5	2901	G	N1-C2-N3	5.09	126.95	123.90
44	5	3060	С	N1-C2-O2	5.09	121.95	118.90
44	5	733	G	C4-C5-N7	5.09	112.83	110.80
46	7	13	А	C8-N9-C4	5.09	107.83	105.80
44	5	622	А	N1-C6-N6	5.09	121.65	118.60
44	5	1236	G	C8-N9-C1'	-5.09	120.39	127.00
44	5	2375	G	C4-N9-C1'	-5.09	119.89	126.50
44	5	209	А	N1-C6-N6	5.08	121.65	118.60
44	5	1011	А	N9-C4-C5	-5.08	103.77	105.80
44	5	1113	G	N3-C4-C5	5.08	131.14	128.60
44	5	2223	А	N7-C8-N9	5.08	116.34	113.80
44	5	3325	G	C6-C5-N7	-5.08	127.35	130.40
46	7	29	С	N3-C4-N4	-5.08	114.44	118.00
46	7	38	U	N3-C2-O2	-5.08	118.64	122.20
44	5	518	G	N9-C4-C5	-5.08	103.37	105.40
44	5	1093	А	N1-C6-N6	-5.08	115.55	118.60
44	5	2146	С	N1-C2-O2	5.08	121.95	118.90
44	5	3118	С	N3-C4-C5	5.08	123.93	121.90
44	5	335	G	O4'-C1'-N9	-5.08	104.14	108.20
44	5	537	А	C5-C6-N6	-5.08	119.64	123.70
44	5	2199	G	N7-C8-N9	5.08	115.64	113.10
44	5	2721	А	C8-N9-C4	5.08	107.83	105.80
44	5	882	А	C2-N3-C4	5.08	113.14	110.60
44	5	2576	G	C6-C5-N7	-5.08	127.35	130.40
44	5	3368	U	N3-C4-C5	5.08	117.64	114.60
44	5	2449	А	N7-C8-N9	5.07	116.34	113.80
44	5	2683	U	O4'-C1'-N1	5.07	112.26	108.20
44	5	433	А	N1-C2-N3	5.07	131.84	129.30
44	5	949	С	C6-N1-C2	-5.07	118.27	120.30
44	5	3370	А	C8-N9-C4	5.07	107.83	105.80
44	5	123	А	C4-N9-C1'	5.07	135.43	126.30
44	5	641	С	C6-N1-C2	-5.07	118.27	120.30
44	5	938	C	N1-C2-O2	5.07	121.94	118.90
44	5	656	A	C5-N7-C8	-5.07	101.37	103.90
44	5	1363	A	C5-N7-C8	-5.07	101.37	103.90
44	5	2240	G	C5-N7-C8	-5.07	101.77	104.30
44	5	2858	U	C2-N1-C1'	-5.07	111.62	117.70
44	5	2704	A	O4'-C1'-N9	5.07	112.25	108.20
44	5	3344	A	N9-C4-C5	-5.07	103.77	105.80
45	8	146	U	C6-N1-C1'	5.06	128.29	121.20



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	122	А	C8-N9-C4	5.06	107.83	105.80
44	5	1229	G	N3-C2-N2	5.06	123.44	119.90
44	5	2233	А	C5-N7-C8	-5.06	101.37	103.90
44	5	2623	G	N3-C2-N2	-5.06	116.36	119.90
44	5	30	G	N9-C4-C5	-5.06	103.38	105.40
44	5	386	А	N1-C6-N6	5.06	121.64	118.60
44	5	1251	А	C5-C6-N6	5.06	127.75	123.70
44	5	1263	А	C5-C6-N1	5.06	120.23	117.70
44	5	3110	С	N3-C4-C5	-5.06	119.88	121.90
45	8	93	U	N1-C2-O2	5.06	126.34	122.80
44	5	1124	U	N1-C2-O2	5.06	126.34	122.80
44	5	911	С	C4-C5-C6	-5.05	114.87	117.40
44	5	207	U	N1-C2-N3	-5.05	111.87	114.90
44	5	2834	G	N3-C4-N9	5.05	129.03	126.00
44	5	139	G	N1-C2-N2	5.05	120.75	116.20
44	5	228	U	O4'-C1'-N1	5.05	112.24	108.20
44	5	2190	U	N3-C2-O2	-5.05	118.66	122.20
44	5	3211	С	C6-N1-C2	-5.05	118.28	120.30
44	5	3237	U	N1-C2-O2	5.05	126.34	122.80
45	8	155	А	C5-C6-N1	5.05	120.23	117.70
46	7	6	С	C4-C5-C6	-5.05	114.87	117.40
44	5	3173	G	C5-C6-O6	-5.05	125.57	128.60
44	5	663	С	C6-N1-C2	-5.05	118.28	120.30
44	5	2237	С	C6-N1-C2	-5.05	118.28	120.30
44	5	3372	А	C5-N7-C8	-5.05	101.38	103.90
45	8	28	С	C4-C5-C6	-5.05	114.88	117.40
46	7	56	А	C4-C5-N7	5.05	113.22	110.70
44	5	64	G	C4-C5-N7	5.04	112.82	110.80
44	5	1450	G	C5-C6-O6	5.04	131.63	128.60
44	5	2224	А	N7-C8-N9	5.04	116.32	113.80
44	5	2858	U	C6-N1-C1'	5.04	128.26	121.20
44	5	258	G	C6-C5-N7	-5.04	127.37	130.40
44	5	2084	С	C6-N1-C1'	5.04	126.85	120.80
44	5	2352	А	C4-C5-C6	-5.04	114.48	117.00
44	5	715	А	O4'-C1'-N9	5.04	112.23	108.20
44	5	1463	U	C5-C6-N1	5.04	125.22	122.70
45	8	33	Α	N3-C4-N9	-5.04	123.37	127.40
44	5	1749	A	C4-C5-N7	5.04	113.22	110.70
44	5	2562	A	N3-C4-N9	5.04	$131.4\overline{3}$	127.40
46	7	28	C	C2-N1-C1'	5.04	124.34	118.80
44	5	734	C	C2-N1-C1	5.04	124.34	118.80
44	5	2228	A	C5-N7-C8	-5.04	101.38	103.90



Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
44	5	12	А	P-O3'-C3'	5.03	125.74	119.70
44	5	1239	С	O4'-C1'-N1	5.03	112.23	108.20
44	5	1272	С	N3-C2-O2	-5.03	118.38	121.90
44	5	1824	U	C2-N1-C1'	5.03	123.74	117.70
44	5	2966	G	C2-N3-C4	-5.03	109.38	111.90
44	5	22	G	C8-N9-C4	-5.03	104.39	106.40
44	5	347	G	C8-N9-C4	-5.03	104.39	106.40
44	5	986	U	C2-N1-C1'	5.03	123.74	117.70
44	5	2184	U	N1-C2-O2	5.03	126.32	122.80
44	5	3201	С	C4-C5-C6	-5.03	114.88	117.40
45	8	26	U	C2-N1-C1'	-5.03	111.66	117.70
45	8	62	С	N1-C2-O2	-5.03	115.88	118.90
44	5	2921	U	N1-C2-O2	5.03	126.32	122.80
44	5	3030	G	N1-C2-N2	5.03	120.73	116.20
44	5	3197	G	C4-N9-C1'	-5.03	119.96	126.50
44	5	937	G	N3-C4-N9	5.03	129.02	126.00
44	5	55	G	N1-C2-N2	5.03	120.72	116.20
44	5	653	А	N9-C4-C5	-5.03	103.79	105.80
44	5	2928	С	C4-C5-C6	-5.03	114.89	117.40
44	5	3041	U	N1-C2-O2	5.03	126.32	122.80
44	5	289	А	C5-N7-C8	-5.02	101.39	103.90
44	5	2714	G	C4-N9-C1'	-5.02	119.97	126.50
44	5	1622	U	C5-C6-N1	5.02	125.21	122.70
44	5	1838	G	N3-C4-C5	5.02	131.11	128.60
44	5	1883	А	C8-N9-C4	5.02	107.81	105.80
44	5	2449	А	C2-N3-C4	-5.02	108.09	110.60
44	5	3023	U	N1-C2-O2	5.02	126.32	122.80
44	5	729	С	N1-C2-O2	5.02	121.91	118.90
44	5	2966	G	C8-N9-C1'	5.02	133.53	127.00
44	5	3372	А	N7-C8-N9	5.02	116.31	113.80
44	5	437	G	C8-N9-C4	-5.02	104.39	106.40
44	5	1331	U	C5-C4-O4	-5.02	122.89	125.90
44	5	1722	U	O4'-C1'-N1	5.02	112.22	108.20
44	5	2148	U	C2-N1-C1'	5.02	123.72	117.70
44	5	17	G	N1-C2-N2	5.02	120.72	116.20
44	5	2582	С	C2-N3-C4	5.02	122.41	119.90
44	5	489	U	C6-N1-C1'	-5.02	114.18	121.20
44	5	736	A	C4-C5-N7	5.02	113.21	110.70
44	5	1440	G	C4-C5-N7	5.02	112.81	110.80
44	5	2232	A	N7-C8-N9	5.02	116.31	113.80
44	5	2547	A	N9-C4-C5	-5.02	103.79	105.80
44	5	161	G	N7-C8-N9	5.01	$1\overline{15.61}$	113.10



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
44	5	322	U	N1-C2-O2	5.01	126.31	122.80
44	5	2493	U	C6-N1-C1'	5.01	128.22	121.20
44	5	2965	U	N1-C2-O2	5.01	126.31	122.80
44	5	3219	G	N7-C8-N9	-5.01	110.59	113.10
44	5	3294	А	C4-C5-N7	5.01	113.21	110.70
44	5	1292	С	N3-C2-O2	-5.01	118.39	121.90
44	5	24	G	N7-C8-N9	5.01	115.61	113.10
44	5	148	G	N9-C4-C5	-5.01	103.39	105.40
44	5	186	U	C6-N1-C2	-5.01	117.99	121.00
44	5	1775	G	C4-C5-N7	5.01	112.80	110.80
44	5	2451	G	N3-C2-N2	-5.01	116.39	119.90
44	5	1722	U	N1-C2-O2	5.01	126.31	122.80
45	8	33	А	N3-C4-C5	5.01	130.31	126.80
46	7	28	С	C6-N1-C2	-5.01	118.30	120.30
44	5	1325	U	N1-C2-O2	5.01	126.30	122.80
44	5	1333	С	N3-C2-O2	-5.01	118.39	121.90
44	5	2616	С	N1-C2-O2	5.01	121.90	118.90
44	5	3110	С	C6-N1-C2	-5.01	118.30	120.30
45	8	96	А	C2-N3-C4	-5.01	108.10	110.60
44	5	1227	С	C5-C4-N4	5.00	123.70	120.20
44	5	1232	С	C6-N1-C1'	5.00	126.81	120.80
44	5	1365	G	N7-C8-N9	5.00	115.60	113.10
44	5	1464	G	C2-N3-C4	-5.00	109.40	111.90
44	5	1686	U	C5-C6-N1	5.00	125.20	122.70
44	5	2509	U	C2-N1-C1'	5.00	123.70	117.70
44	5	307	A	N3-C4-N9	-5.00	123.40	127.40
44	5	1565	G	N7-C8-N9	5.00	115.60	113.10
44	5	2998	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (85) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	А	241	ARG	Peptide
2	А	247	ARG	Peptide
4	С	106	TRP	Peptide
4	С	107	ARG	Peptide
4	С	179	LEU	Peptide
4	С	182	LEU	Peptide
4	С	231	ALA	Peptide
4	С	233	LEU	Peptide
4	С	250	TRP	Peptide



Mol	Chain	Res	Type	Group
4	С	270	SER	Peptide
4	С	293	SER	Peptide
4	С	299	ILE	Peptide
4	С	360	LYS	Peptide
5	D	325	ILE	Peptide
5	D	446	GLU	Peptide
6	Е	227	ALA	Peptide
6	Е	231	PRO	Peptide
6	Е	283	GLU	Peptide
6	Е	384	SER	Peptide
7	F	302	ILE	Peptide
7	F	366	ILE	Peptide
7	F	368	LYS	Peptide
7	F	427	PRO	Peptide
8	G	240	ALA	Peptide
9	Н	203	TYR	Peptide
9	Н	222	SER	Peptide
10	Ι	375	VAL	Peptide
11	J	101	ARG	Peptide
11	J	192	ASN	Peptide
13	L	152	THR	Peptide
13	L	47	ALA	Peptide
13	L	62	THR	Peptide
14	М	214	LEU	Peptide
15	Ν	72	LYS	Peptide
17	Р	103	GLU	Peptide
17	Р	171	ARG	Peptide
18	Q	134	GLN	Peptide
18	Q	231	PHE	Peptide
19	R	264	GLY	Peptide
19	R	314	GLU	Peptide
19	R	319	LEU	Peptide
20	S	13	ARG	Peptide
20	S	163	PHE	Peptide
20	S	22	PRO	Peptide
21	Т	115	LYS	Peptide
21	Т	126	VAL	Peptide
21	Т	17	ARG	Peptide
21	Т	92	ARG	Peptide
24	W	171	SER	Peptide
24	W	189	LYS	Peptide
24	W	270	ALA	Peptide



Mol	Chain	Res	Type	Group
25	Х	179	GLN	Peptide
25	Х	208	GLN	Peptide
26	Y	10	SER	Peptide
26	Y	125	LYS	Peptide
26	Y	20	PHE	Peptide
26	Y	24	SER	Peptide
26	Y	75	ARG	Peptide
26	Y	81	GLN	Peptide
27	Ζ	32	SER	Peptide
28	a	120	HIS	Peptide
29	b	83	HIS	Peptide
29	b	85	ASN	Peptide
32	е	208	TYR	Peptide
32	е	272	ASN	Peptide
33	f	358	ASP	Peptide
34	g	4	ARG	Peptide
37	j	796	LYS	Peptide
37	j	810	ARG	Peptide
42	р	17	ARG	Peptide
43	q	32	ASN	Peptide
43	q	83	ASN	Peptide
43	q	91	GLU	Peptide
12	S	257	SER	Peptide
12	S	258	PHE	Peptide
12	S	275	SER	Peptide
12	S	276	VAL	Peptide
1	Z	345	ASP	Peptide
1	Z	347	ARG	Peptide
1	Z	355	LYS	Peptide
1	Z	361	ALA	Peptide
1	Z	367	VAL	Peptide
1	Z	378	ILE	Peptide
1	Z	391	LYS	Peptide
1	Z	401	VAL	Peptide

Continued from previous page...

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	ntiles
1	Z	199/204~(98%)	138~(69%)	61 (31%)	0	100	100
2	А	250/252~(99%)	204 (82%)	46 (18%)	0	100	100
3	В	384/386~(100%)	315 (82%)	67~(17%)	2 (0%)	29	66
4	С	359/361~(99%)	292 (81%)	65~(18%)	2 (1%)	25	62
5	D	294/296~(99%)	263 (90%)	31 (10%)	0	100	100
6	Ε	152/175~(87%)	133 (88%)	19~(12%)	0	100	100
7	F	220/222~(99%)	188 (86%)	31 (14%)	1 (0%)	29	66
8	G	231/233~(99%)	199 (86%)	32 (14%)	0	100	100
9	Н	189/191~(99%)	159 (84%)	30 (16%)	0	100	100
10	Ι	207/220~(94%)	173 (84%)	34 (16%)	0	100	100
11	J	167/169~(99%)	140 (84%)	27 (16%)	0	100	100
12	s	144/155~(93%)	93~(65%)	51 (35%)	0	100	100
13	L	191/193~(99%)	161 (84%)	27 (14%)	3 (2%)	9	44
14	М	134/136~(98%)	117 (87%)	17 (13%)	0	100	100
15	Ν	201/203~(99%)	171 (85%)	29 (14%)	1 (0%)	29	66
16	Ο	195/197~(99%)	171 (88%)	24 (12%)	0	100	100
17	Р	181/183~(99%)	156 (86%)	25~(14%)	0	100	100
18	Q	183/185~(99%)	157 (86%)	26 (14%)	0	100	100
19	R	186/188~(99%)	159 (86%)	26 (14%)	1 (0%)	29	66
20	S	170/172~(99%)	143 (84%)	27 (16%)	0	100	100
21	Т	157/159~(99%)	136 (87%)	21 (13%)	0	100	100
22	U	98/100~(98%)	86 (88%)	12 (12%)	0	100	100
23	V	134/136~(98%)	113 (84%)	21 (16%)	0	100	100
24	W	126/135~(93%)	101 (80%)	24 (19%)	1 (1%)	19	57
25	Х	119/121~(98%)	102 (86%)	17 (14%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
26	Y	124/126~(98%)	105 (85%)	19~(15%)	0	100	100
27	Z	133/135~(98%)	114 (86%)	18 (14%)	1 (1%)	19	57
28	a	146/148~(99%)	124 (85%)	21~(14%)	1 (1%)	22	60
29	b	56/58~(97%)	47 (84%)	8 (14%)	1 (2%)	8	42
30	с	95/97~(98%)	86 (90%)	9~(10%)	0	100	100
31	d	107/109~(98%)	88 (82%)	19~(18%)	0	100	100
32	е	125/127~(98%)	105 (84%)	20~(16%)	0	100	100
33	f	104/106~(98%)	86 (83%)	18 (17%)	0	100	100
34	g	110/112 (98%)	101 (92%)	9~(8%)	0	100	100
35	h	117/119~(98%)	103 (88%)	14 (12%)	0	100	100
36	i	97/99~(98%)	85 (88%)	12 (12%)	0	100	100
37	j	85/87~(98%)	70 (82%)	15~(18%)	0	100	100
38	k	75/77~(97%)	69 (92%)	6 (8%)	0	100	100
39	1	48/50~(96%)	41 (85%)	6 (12%)	1 (2%)	7	40
40	m	50/52~(96%)	37 (74%)	13 (26%)	0	100	100
41	О	103/105~(98%)	83 (81%)	20 (19%)	0	100	100
42	р	89/91~(98%)	75 (84%)	13 (15%)	1 (1%)	14	51
43	q	117/219~(53%)	91 (78%)	26 (22%)	0	100	100
All	All	6652/6889~(97%)	5580 (84%)	1056 (16%)	16 (0%)	50	79

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	F	369	GLN
13	L	62	THR
27	Ζ	33	LYS
13	L	61	PRO
15	Ν	146	ALA
28	a	121	HIS
42	р	18	TYR
3	В	4	ARG
4	С	339	LEU
19	R	266	ALA
4	С	232	SER
13	L	166	ALA
24	W	278	THR



Continued from previous page...

Mol	Chain	Res	Type
39	1	22	PRO
3	В	188	ILE
29	b	90	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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	179/185~(97%)	171 (96%)	8 (4%)	27 57	
2	А	194/194~(100%)	190 (98%)	4 (2%)	53 74	
3	В	322/322~(100%)	319~(99%)	3 (1%)	78 88	
4	С	288/288~(100%)	282~(98%)	6 (2%)	53 74	
5	D	244/244~(100%)	243 (100%)	1 (0%)	91 95	
6	Ε	134/152~(88%)	132 (98%)	2(2%)	65 81	
7	F	186/186~(100%)	184 (99%)	2 (1%)	73 85	
8	G	191/191 (100%)	187 (98%)	4 (2%)	53 74	
9	Н	171/171~(100%)	167 (98%)	4 (2%)	50 72	
10	Ι	180/186~(97%)	172 (96%)	8 (4%)	28 57	
11	J	147/147~(100%)	143 (97%)	4 (3%)	44 69	
13	L	154/154~(100%)	150 (97%)	4 (3%)	46 69	
14	М	107/107~(100%)	106 (99%)	1 (1%)	78 88	
15	Ν	175/175~(100%)	173~(99%)	2(1%)	73 85	
16	Ο	160/160~(100%)	158 (99%)	2(1%)	69 82	
17	Р	145/145~(100%)	142 (98%)	3~(2%)	53 74	
18	Q	150/150~(100%)	148 (99%)	2(1%)	69 82	
19	R	153/153~(100%)	148 (97%)	5(3%)	38 65	
20	S	$1\overline{56/156}~(100\%)$	154 (99%)	2 (1%)	69 82	
21	Т	$1\overline{36/136}\ (100\%)$	133 (98%)	3 (2%)	52 72	
22	U	87/87~(100%)	86 (99%)	1 (1%)	73 85	



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles	5
23	V	104/104~(100%)	102 (98%)	2 (2%)	57	76	
24	W	114/114 (100%)	111 (97%)	3 (3%)	46	69	
25	Х	105/105~(100%)	103 (98%)	2 (2%)	57	76	
26	Y	109/109~(100%)	106 (97%)	3 (3%)	43	68	
27	Z	115/115~(100%)	114 (99%)	1 (1%)	78	88	
28	a	118/118 (100%)	115 (98%)	3 (2%)	47	70	
29	b	46/46~(100%)	44 (96%)	2 (4%)	29	58	
30	с	81/81 (100%)	80 (99%)	1 (1%)	71	84	
31	d	96/96~(100%)	96 (100%)	0	100	100	
32	е	109/109~(100%)	108 (99%)	1 (1%)	78	88	
33	f	90/90~(100%)	86 (96%)	4 (4%)	28	57	
34	g	95/95~(100%)	93~(98%)	2 (2%)	53	74	
35	h	104/104~(100%)	102 (98%)	2 (2%)	57	76	
36	i	81/81 (100%)	78~(96%)	3 (4%)	34	62	
37	j	70/70~(100%)	66 (94%)	4 (6%)	20	52	
38	k	68/68~(100%)	67~(98%)	1 (2%)	65	81	
39	1	45/45~(100%)	43 (96%)	2 (4%)	28	57	
40	m	47/47~(100%)	47 (100%)	0	100	100	
41	0	90/90~(100%)	90 (100%)	0	100	100	
42	р	71/71 (100%)	70 (99%)	1 (1%)	67	81	-
43	q	105/165~(64%)	103 (98%)	2 (2%)	57	76	
All	All	5522/5612 (98%)	5412 (98%)	110 (2%)	57	75	_

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	209	LYS
1	Z	252	ASN
1	Z	303	ASN
1	Z	343	VAL
1	Z	344	THR
1	Z	356	LYS
1	Z	360	LEU
1	Z	410	ARG
2	А	70	ARG



Mol	Chain	Res	Type
2	А	193	ARG
2	А	241	ARG
2	А	242	ARG
3	В	70	ARG
3	В	332	ARG
3	В	345	ASN
4	С	93	MET
4	С	95	ARG
4	С	170	LYS
4	С	212	ASP
4	С	221	ASN
4	С	320	ASN
5	D	345	ARG
6	Е	255	ARG
6	Е	303	VAL
7	F	370	ARG
7	F	426	VAL
8	G	221	ARG
8	G	243	GLN
8	G	286	LYS
8	G	368	ARG
9	Н	262	ARG
9	Н	269	ARG
9	Н	316	ASN
9	Н	357	ASN
10	Ι	192	ARG
10	Ι	209	ARG
10	Ι	225	LYS
10	Ι	254	ARG
10	Ι	324	ARG
10	Ι	354	LYS
10	Ι	388	LYS
10	Ι	394	ASN
11	J	101	ARG
11	J	103	LEU
11	J	183	ARG
11	J	232	ARG
13	L	54	LEU
13	L	67	ARG
13	L	100	ARG
13	L	104	ARG
14	М	276	LYS



Mol	Chain	Res	Type
15	N	159	ARG
15	N	187	ARG
16	0	59	ARG
16	0	117	ARG
17	Р	30	ARG
17	Р	159	LYS
17	Р	171	ARG
18	Q	145	LYS
18	Q	276	ARG
19	R	174	ASN
19	R	177	ARG
19	R	220	ARG
19	R	239	ARG
19	R	301	ASN
20	S	12	ARG
20	S	13	ARG
21	Т	127	GLN
21	Т	128	LEU
21	Т	139	ARG
22	U	183	ARG
23	V	141	ARG
23	V	257	ARG
24	W	216	ARG
24	W	218	ARG
24	W	225	ARG
25	Х	136	LYS
25	Х	147	ARG
26	Y	12	ARG
26	Y	59	VAL
26	Y	114	ASP
27	Z	13	VAL
28	a	85	ARG
28	a	115	MET
28	a	125	ASN
29	b	116	THR
29	b	125	LYS
30	с	16	LEU
32	е	178	ARG
33	f	383	ARG
33	f	391	ARG
33	f	405	ASN
33	f	424	ASN



Mol	Chain	Res	Type
34	g	4	ARG
34	g	18	ASN
35	h	10	ARG
35	h	49	LYS
36	i	18	THR
36	i	36	ARG
36	i	57	LEU
37	j	831	ARG
37	j	842	ARG
37	j	851	ARG
37	j	871	LYS
38	k	46	ARG
39	1	5	LYS
39	1	43	ASN
42	р	17	ARG
43	q	52	LEU
43	q	76	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such side chains are listed below:

Mol	Chain	Res	Type
1	Z	252	ASN
1	Z	257	ASN
2	А	83	HIS
2	А	132	ASN
2	А	215	ASN
3	В	212	ASN
3	В	259	HIS
3	В	269	GLN
3	В	345	ASN
4	С	58	HIS
4	С	213	ASN
4	С	307	GLN
4	С	320	ASN
5	D	305	ASN
5	D	323	GLN
7	F	271	ASN
8	G	202	GLN
8	G	223	GLN
8	G	309	ASN
8	G	385	ASN
8	G	404	ASN



Mol	Chain	Res	Type
8	G	407	GLN
8	G	416	ASN
9	Н	208	GLN
9	Н	209	GLN
9	Н	250	ASN
9	Н	264	HIS
9	Н	277	ASN
9	Н	316	ASN
9	Н	362	GLN
10	Ι	208	ASN
10	Ι	240	ASN
11	J	111	ASN
11	J	186	ASN
13	L	12	ASN
13	L	37	ASN
14	М	190	GLN
15	Ν	57	GLN
15	Ν	86	ASN
16	0	14	HIS
16	0	31	GLN
16	0	182	ASN
17	Р	34	GLN
17	Р	96	GLN
18	Q	134	GLN
18	Q	270	ASN
18	Q	277	HIS
19	R	174	ASN
19	R	203	GLN
19	R	227	GLN
19	R	253	HIS
19	R	269	HIS
19	R	301	ASN
20	S	157	GLN
21	Т	54	HIS
21	Т	90	ASN
21	Т	127	GLN
21	Т	146	ASN
23	V	227	ASN
24	W	249	ASN
25	X	194	ASN
27	Ζ	56	HIS
27	Ζ	77	ASN



		-	
Mol	Chain	Res	Type
27	Z	121	HIS
28	a	106	HIS
28	a	125	ASN
28	a	143	HIS
28	a	145	GLN
28	a	201	ASN
29	b	72	ASN
29	b	111	HIS
31	d	115	GLN
31	d	145	ASN
32	е	171	HIS
32	е	177	HIS
32	е	182	ASN
33	f	360	GLN
33	f	405	ASN
33	f	406	ASN
33	f	424	ASN
34	g	18	ASN
35	h	59	ASN
35	h	104	GLN
35	h	108	GLN
35	h	113	GLN
36	i	63	ASN
36	i	91	ASN
36	i	92	ASN
36	i	100	HIS
37	j	798	HIS
$3\overline{7}$	j	814	HIS
$\overline{38}$	k	67	GLN
39	<u>l</u>	25	GLN
39	1	33	ASN
39	1	38	ASN
39	1	43	ASN
41	0	22	GLN
41	0	82	GLN
42	р	32	GLN
42	р	34	HIS
43	q	32	ASN
43	q	56	ASN
43	q	98	ASN



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	5	3231/3394~(95%)	1469~(45%)	32~(0%)
45	8	157/158~(99%)	85 (54%)	0
46	7	120/121~(99%)	41 (34%)	0
All	All	3508/3673~(95%)	1595~(45%)	32~(0%)

All (1595) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
44	5	4	U
44	5	5	G
44	5	6	А
44	5	7	С
44	5	8	С
44	5	11	А
44	5	12	А
44	5	13	А
44	5	14	U
44	5	15	С
44	5	18	G
44	5	19	U
44	5	21	G
44	5	26	А
44	5	30	G
44	5	31	С
44	5	37	U
44	5	38	U
44	5	40	А
44	5	42	С
44	5	43	А
44	5	46	U
44	5	47	С
44	5	49	А
44	5	50	U
44	5	53	G
44	5	54	С
44	5	55	G
44	5	57	А
44	5	58	G
44	5	59	G
44	5	60	А
44	5	63	А
44	5	66	А
44	5	67	А



Mol	Chain	Res	Type
44	5	71	А
44	5	72	С
44	5	74	G
44	5	77	А
44	5	79	U
44	5	82	С
44	5	83	U
44	5	87	U
44	5	92	G
44	5	96	G
44	5	102	С
44	5	104	G
44	5	109	A
44	5	110	G
44	5	111	C
44	5	112	U
44	5	113	С
44	5	114	А
44	5	115	А
44	5	116	А
44	5	117	U
44	5	118	U
44	5	120	G
44	5	121	А
44	5	122	А
44	5	129	U
44	5	130	А
44	5	131	С
44	5	132	С
44	5	134	U
44	5	135	C
44	5	136	G
44	5	138	U
44	5	139	G
44	5	144	A
44	5	145	G
44	5	146	U
44	5	148	G
44	5	150	A
44	5	151	A
44	5	153	U
44	5	154	U



Mol	Chain	Res	Type
44	5	155	G
44	5	156	G
44	5	157	А
44	5	158	G
44	5	159	А
44	5	160	G
44	5	161	G
44	5	162	G
44	5	163	С
44	5	164	А
44	5	166	С
44	5	168	U
44	5	169	U
44	5	170	G
44	5	172	G
44	5	173	G
44	5	174	С
44	5	175	С
44	5	176	G
44	5	177	U
44	5	178	U
44	5	182	U
44	5	183	G
44	5	185	С
44	5	187	А
44	5	188	U
44	5	189	G
44	5	190	U
44	5	191	U
44	5	192	C
44	5	193	С
44	5	194	U
44	5	196	G
44	5	199	A
44	5	200	C
44	5	203	G
44	5	204	A
44	5	206	G
44	5	209	A
44	5	210	U
44	5	211	A
44	5	212	G



Mol	Chain	Res	Type
44	5	213	А
44	5	215	G
44	5	216	G
44	5	217	U
44	5	218	G
44	5	219	А
44	5	220	G
44	5	221	А
44	5	222	А
44	5	224	С
44	5	227	G
44	5	228	U
44	5	229	G
44	5	230	U
44	5	234	G
44	5	236	G
44	5	237	G
44	5	238	А
44	5	240	U
44	5	241	G
44	5	242	C
44	5	243	G
44	5	244	G
44	5	247	С
44	5	248	U
44	5	249	U
44	5	251	G
44	5	252	U
44	5	256	G
44	5	257	U
44	5	258	G
44	5	259	C
44	5	260	С
44	5	261	U
44	5	263	С
44	5	264	G
44	5	265	A
44	5	266	A
44	5	267	G
44	5	268	A
44	5	269	G
44	5	273	A



Mol	Chain	Res	Type
44	5	274	G
44	5	283	G
44	5	284	A
44	5	286	U
44	5	295	А
44	5	305	U
44	5	306	А
44	5	307	А
44	5	309	U
44	5	311	С
44	5	316	U
44	5	319	А
44	5	322	U
44	5	324	A
44	5	325	A
44	5	329	U
44	5	330	G
44	5	331	G
44	5	332	С
44	5	333	G
44	5	334	A
44	5	335	G
44	5	336	А
44	5	337	G
44	5	338	А
44	5	339	С
44	5	341	G
44	5	342	А
44	5	348	А
44	5	349	A
44	5	350	C
44	5	351	А
44	5	352	A
44	5	354	U
44	5	361	A
44	5	362	U
44	5	368	G
44	5	369	A
44	5	370	U
44	5	374	A
44	5	375	A
44	5	376	G



Mol	Chain	Res	Type
44	5	380	U
44	5	387	А
44	5	388	G
44	5	390	G
44	5	397	А
44	5	398	А
44	5	401	U
44	5	402	А
44	5	403	С
44	5	404	G
44	5	407	А
44	5	408	А
44	5	411	U
44	5	412	G
44	5	413	U
44	5	415	G
44	5	420	G
44	5	421	G
44	5	422	А
44	5	426	G
44	5	430	U
44	5	439	С
44	5	440	А
44	5	441	U
44	5	442	G
44	5	446	U
44	5	447	U
44	5	489	U
44	5	490	С
44	5	492	С
44	5	493	U
44	5	494	G
44	5	495	G
44	5	497	C
44	5	498	A
44	5	503	C
44	5	504	А
44	5	510	G
44	5	515	C
44	5	516	A
44	5	517	G
44	5	518	G



Mol	Chain	Res	Type
44	5	519	А
44	5	520	U
44	5	521	А
44	5	523	А
44	5	533	А
44	5	534	U
44	5	535	G
44	5	536	U
44	5	537	А
44	5	540	U
44	5	542	G
44	5	543	С
44	5	545	U
44	5	546	С
44	5	547	G
44	5	549	U
44	5	550	А
44	5	551	А
44	5	552	G
44	5	554	А
44	5	555	U
44	5	556	U
44	5	557	А
44	5	558	U
44	5	559	А
44	5	565	U
44	5	569	А
44	5	578	A
44	5	579	G
44	5	581	U
44	5	582	G
44	5	585	A
44	5	586	С
44	5	588	G
44	5	589	A
44	5	594	U
44	5	595	G
44	5	597	G
44	5	607	A
44	5	608	A
44	5	609	G
44	5	610	G


Mol	Chain	Res	Type
44	5	611	А
44	5	612	U
44	5	614	С
44	5	616	G
44	5	620	U
44	5	621	А
44	5	623	U
44	5	625	G
44	5	632	G
44	5	636	C
44	5	637	С
44	5	638	С
44	5	643	U
44	5	645	A
44	5	646	A
44	5	649	А
44	5	651	G
44	5	653	А
44	5	656	А
44	5	657	А
44	5	661	G
44	5	665	А
44	5	666	А
44	5	674	G
44	5	675	С
44	5	677	А
44	5	679	U
44	5	681	U
44	5	682	U
44	5	690	A
44	5	691	A
44	5	692	A
44	5	696	С
44	5	699	A
44	5	700	С
44	5	705	А
44	5	712	G
44	5	715	A
44	5	716	A
44	5	719	U
44	5	720	A
44	5	721	G



Mol	Chain	Res	Type
44	5	724	U
44	5	725	G
44	5	726	G
44	5	730	С
44	5	731	U
44	5	737	G
44	5	738	А
44	5	739	G
44	5	740	G
44	5	742	G
44	5	743	С
44	5	747	А
44	5	750	G
44	5	751	A
44	5	752	С
44	5	753	С
44	5	761	А
44	5	762	U
44	5	763	G
44	5	765	С
44	5	766	U
44	5	767	U
44	5	770	G
44	5	771	А
44	5	774	G
44	5	776	U
44	5	777	U
44	5	779	G
44	5	780	А
44	5	781	G
44	5	785	G
44	5	786	A
44	5	790	U
44	5	793	C
44	5	795	G
44	5	799	G
44	5	801	A
44	5	806	A
44	5	811	U
44	5	812	G
44	5	813	G
44	5	816	A



Mol	Chain	Res	Type
44	5	817	А
44	5	818	С
44	5	826	G
44	5	830	А
44	5	832	G
44	5	835	G
44	5	836	А
44	5	837	А
44	5	838	G
44	5	839	С
44	5	844	G
44	5	849	С
44	5	850	U
44	5	851	С
44	5	852	U
44	5	854	G
44	5	856	G
44	5	857	G
44	5	860	G
44	5	861	С
44	5	866	А
44	5	868	С
44	5	874	U
44	5	875	G
44	5	876	А
44	5	879	U
44	5	880	G
44	5	884	А
44	5	896	А
44	5	897	U
44	5	901	G
44	5	904	А
44	5	907	G
44	5	908	G
44	5	910	G
44	5	913	A
44	5	914	А
44	5	916	G
44	5	917	А
44	5	920	А
44	5	921	А
44	5	923	С



Mol	Chain	Res	Type
44	5	924	G
44	5	925	A
44	5	926	А
44	5	932	U
44	5	935	U
44	5	937	G
44	5	938	С
44	5	939	U
44	5	943	U
44	5	944	С
44	5	955	U
44	5	956	U
44	5	959	С
44	5	960	U
44	5	962	A
44	5	963	G
44	5	964	G
44	5	969	С
44	5	974	G
44	5	979	U
44	5	981	U
44	5	984	G
44	5	985	U
44	5	990	U
44	5	991	G
44	5	993	G
44	5	995	U
44	5	999	G
44	5	1000	С
44	5	1001	G
44	5	1002	A
44	5	1003	A
44	5	1004	U
44	5	1010	G
44	5	1012	G
44	5	1013	G
44	5	1014	U
44	5	1015	U
44	5	1016	C
44	5	1017	C
44	5	1020	G
44	5	1024	G



Mol	Chain	Res	Type
44	5	1025	А
44	5	1027	A
44	5	1028	U
44	5	1029	G
44	5	1032	С
44	5	1034	U
44	5	1035	G
44	5	1036	А
44	5	1037	С
44	5	1041	U
44	5	1044	U
44	5	1045	С
44	5	1047	А
44	5	1049	С
44	5	1057	A
44	5	1058	U
44	5	1062	А
44	5	1063	G
44	5	1064	А
44	5	1065	A
44	5	1066	G
44	5	1069	С
44	5	1070	U
44	5	1071	U
44	5	1072	G
44	5	1074	U
44	5	1075	А
44	5	1081	U
44	5	1087	G
44	5	1088	U
44	5	1089	G
44	5	1094	U
44	5	1095	U
44	5	1096	U
44	5	1097	G
44	5	1098	A
44	5	1103	A
44	5	1104	G
44	5	1105	A
44	5	1109	U
44	5	1110	U
44	5	1113	G



Mol	Chain	Res	Type
44	5	1114	U
44	5	1115	G
44	5	1117	G
44	5	1118	С
44	5	1126	G
44	5	1128	U
44	5	1131	G
44	5	1135	А
44	5	1137	С
44	5	1140	G
44	5	1143	А
44	5	1144	U
44	5	1148	G
44	5	1151	U
44	5	1152	G
44	5	1154	A
44	5	1156	С
44	5	1159	А
44	5	1160	С
44	5	1161	G
44	5	1163	A
44	5	1165	А
44	5	1172	G
44	5	1173	U
44	5	1174	G
44	5	1175	С
44	5	1177	G
44	5	1178	G
44	5	1179	А
44	5	1180	A
44	5	1181	U
44	5	1182	A
44	5	1189	С
44	5	1190	A
44	5	1191	U
44	5	1195	A
44	5	1196	С
44	5	1197	A
44	5	1198	С
44	5	1199	С
44	5	1201	С
44	5	1206	G



Mol	Chain	Res	Type
44	5	1208	U
44	5	1210	U
44	5	1214	U
44	5	1218	U
44	5	1219	С
44	5	1220	U
44	5	1221	А
44	5	1222	G
44	5	1223	А
44	5	1225	А
44	5	1229	G
44	5	1230	G
44	5	1232	С
44	5	1233	G
44	5	1235	U
44	5	1236	G
44	5	1237	G
44	5	1238	С
44	5	1239	С
44	5	1241	U
44	5	1243	G
44	5	1244	А
44	5	1245	А
44	5	1246	G
44	5	1248	С
44	5	1252	А
44	5	1253	U
44	5	1256	G
44	5	1257	С
44	5	1258	U
44	5	1259	A
44	5	1260	A
44	5	1262	G
44	5	1263	А
44	5	1264	G
44	5	1265	U
44	5	1269	U
44	5	1271	A
44	5	1272	C
44	5	1280	С
44	5	1281	G
44	5	1282	G



Mol	Chain	Res	Type
44	5	1284	С
44	5	1285	G
44	5	1286	А
44	5	1288	U
44	5	1292	С
44	5	1293	U
44	5	1294	А
44	5	1295	G
44	5	1297	С
44	5	1301	А
44	5	1302	А
44	5	1303	А
44	5	1305	U
44	5	1308	А
44	5	1309	U
44	5	1312	С
44	5	1316	С
44	5	1317	А
44	5	1319	G
44	5	1324	U
44	5	1330	А
44	5	1334	U
44	5	1335	С
44	5	1341	U
44	5	1346	G
44	5	1348	U
44	5	1350	А
44	5	1351	U
44	5	1352	А
44	5	1354	G
44	5	1355	A
44	5	1357	G
44	5	1358	С
44	5	1359	C
44	5	1365	G
44	5	1366	A
44	5	1370	G
44	5	1383	G
44	5	1386	A
44	5	1387	G
44	5	1390	A
44	5	1391	С



Mol	Chain	Res	Type
44	5	1392	G
44	5	1393	А
44	5	1399	А
44	5	1400	G
44	5	1404	G
44	5	1405	U
44	5	1406	А
44	5	1407	А
44	5	1408	G
44	5	1411	С
44	5	1413	G
44	5	1417	G
44	5	1418	А
44	5	1419	A
44	5	1423	С
44	5	1425	U
44	5	1428	А
44	5	1429	G
44	5	1430	U
44	5	1431	G
44	5	1432	С
44	5	1434	G
44	5	1435	А
44	5	1436	U
44	5	1437	С
44	5	1440	G
44	5	1441	G
44	5	1446	А
44	5	1448	U
44	5	1450	G
44	5	1452	А
44	5	1455	U
44	5	1458	U
44	5	1460	A
44	5	1461	А
44	5	1463	U
44	5	1466	G
44	5	1467	A
44	5	1469	С
44	5	1470	U
44	5	1473	G
44	5	1476	G



Mol	Chain	Res	Type
44	5	1480	G
44	5	1481	А
44	5	1482	А
44	5	1485	G
44	5	1487	G
44	5	1489	А
44	5	1492	G
44	5	1497	С
44	5	1498	А
44	5	1499	С
44	5	1500	G
44	5	1501	U
44	5	1502	С
44	5	1504	А
44	5	1508	С
44	5	1511	U
44	5	1513	G
44	5	1514	G
44	5	1515	А
44	5	1516	С
44	5	1518	U
44	5	1523	U
44	5	1524	А
44	5	1527	С
44	5	1528	G
44	5	1536	G
44	5	1542	G
44	5	1543	G
44	5	1544	G
44	5	1549	U
44	5	1550	С
44	5	1551	C
44	5	1552	G
44	5	1553	U
44	5	1555	U
44	5	1556	С
44	5	1557	A
44	5	1558	А
44	5	1559	A
44	5	1561	G
44	5	$15\overline{62}$	C
44	5	1563	С



Mol	Chain	Res	Type
44	5	1567	U
44	5	1568	U
44	5	1569	U
44	5	1570	U
44	5	1572	U
44	5	1574	С
44	5	1578	С
44	5	1580	A
44	5	1581	С
44	5	1583	А
44	5	1585	С
44	5	1589	А
44	5	1592	G
44	5	1593	А
44	5	1594	А
44	5	1598	G
44	5	1601	U
44	5	1602	А
44	5	1604	G
44	5	1605	А
44	5	1606	U
44	5	1608	С
44	5	1618	G
44	5	1619	A
44	5	1621	А
44	5	1622	U
44	5	1623	G
44	5	1626	U
44	5	1627	U
44	5	1629	U
44	5	1630	U
44	5	1631	С
44	5	1632	A
44	5	1633	С
44	5	1634	G
44	5	1638	A
44	5	1639	С
44	5	1640	G
44	5	1641	U
44	5	1642	А
44	5	1643	A
44	5	1644	С



Mol	Chain	Res	Type
44	5	1645	U
44	5	1647	А
44	5	1648	А
44	5	1650	G
44	5	1651	U
44	5	1653	G
44	5	1657	С
44	5	1663	С
44	5	1666	G
44	5	1667	А
44	5	1675	G
44	5	1676	А
44	5	1677	G
44	5	1680	G
44	5	1683	A
44	5	1687	U
44	5	1688	U
44	5	1690	С
44	5	1692	U
44	5	1693	С
44	5	1694	U
44	5	1696	А
44	5	1697	А
44	5	1700	G
44	5	1701	С
44	5	1702	U
44	5	1705	U
44	5	1708	С
44	5	1709	С
44	5	1710	С
44	5	1711	C
44	5	1713	G
44	5	1714	A
44	5	1715	A
44	5	1717	U
44	5	1724	U
44	5	1725	C
44	5	1729	A
44	5	1730	G
44	5	1731	A
44	5	1734	G
44	5	1735	G



Mol	Chain	Res	Type
44	5	1736	G
44	5	1737	U
44	5	1741	A
44	5	1745	С
44	5	1746	U
44	5	1747	G
44	5	1749	А
44	5	1750	А
44	5	1751	G
44	5	1752	А
44	5	1753	G
44	5	1755	С
44	5	1756	С
44	5	1757	A
44	5	1759	С
44	5	1760	A
44	5	1761	С
44	5	1763	U
44	5	1764	U
44	5	1765	U
44	5	1768	U
44	5	1769	G
44	5	1770	G
44	5	1771	С
44	5	1773	С
44	5	1775	G
44	5	1777	U
44	5	1778	G
44	5	1780	G
44	5	1784	G
44	5	1787	A
44	5	1789	G
44	5	1791	С
44	5	1792	С
44	5	1793	С
44	5	1795	U
44	5	1797	A
44	5	1803	С
44	5	1804	A
44	5	1805	С
44	5	1806	A
44	5	1807	G



Mol	Chain	Res	Type
44	5	1808	G
44	5	1809	A
44	5	1812	G
44	5	1813	А
44	5	1814	А
44	5	1815	U
44	5	1816	А
44	5	1817	G
44	5	1819	U
44	5	1820	U
44	5	1821	U
44	5	1822	С
44	5	1824	U
44	5	1825	G
44	5	1826	С
44	5	1829	G
44	5	1830	G
44	5	1835	А
44	5	1839	А
44	5	1841	А
44	5	1842	А
44	5	1846	С
44	5	1847	А
44	5	1848	G
44	5	1849	С
44	5	1850	А
44	5	1851	G
44	5	1857	С
44	5	1858	А
44	5	1859	А
44	5	1866	С
44	5	1868	G
44	5	1869	С
44	5	1873	U
44	5	1874	A
44	5	1875	G
44	5	1877	U
44	5	1878	G
44	5	1879	A
44	5	1880	U
44	5	1881	A
44	5	1882	G



Mol	Chain	Res	Type
44	5	1884	А
44	5	1886	A
44	5	1890	U
44	5	1893	A
44	5	1894	U
44	5	1895	А
44	5	1896	А
44	5	1897	G
44	5	1899	G
44	5	1900	А
44	5	1901	А
44	5	1906	G
44	5	1912	U
44	5	1925	U
44	5	1926	С
44	5	1927	G
44	5	1930	А
44	5	1931	U
44	5	1932	А
44	5	1935	G
44	5	1939	G
44	5	1948	G
44	5	1950	U
44	5	1952	G
44	5	1953	G
44	5	1954	G
44	5	1955	U
44	5	1956	А
44	5	1957	G
44	5	1958	U
44	5	1959	G
44	5	1960	A
44	5	1961	G
44	5	1962	G
44	5	2077	U
44	5	$2\overline{079}$	G
44	5	2081	U
44	5	$2\overline{082}$	U
44	5	2083	G
44	5	2086	A
44	5	2088	A
44	5	2094	С



Mol	Chain	Res	Type
44	5	2095	G
44	5	2096	A
44	5	2098	С
44	5	2100	A
44	5	2101	С
44	5	2102	U
44	5	2105	G
44	5	2106	А
44	5	2107	A
44	5	2109	U
44	5	2110	G
44	5	2111	G
44	5	2112	U
44	5	2113	A
44	5	2114	С
44	5	2115	G
44	5	2116	G
44	5	2119	А
44	5	2121	G
44	5	2122	G
44	5	2131	А
44	5	2132	С
44	5	2134	G
44	5	2138	A
44	5	2139	А
44	5	2142	А
44	5	2144	A
44	5	2145	А
44	5	2153	U
44	5	2154	U
44	5	2158	A
44	5	2159	U
44	5	2160	G
44	5	2162	U
44	5	2164	A
44	5	2169	G
44	5	2175	U
44	5	2176	U
44	5	2177	G
44	5	2178	A
44	5	2184	U
44	5	2186	U



Mol	Chain	Res	Type
44	5	2187	G
44	5	2188	A
44	5	2198	A
44	5	2201	G
44	5	2202	С
44	5	2205	U
44	5	2206	G
44	5	2208	А
44	5	2209	U
44	5	2210	G
44	5	2222	А
44	5	2223	A
44	5	2232	А
44	5	2239	G
44	5	2243	A
44	5	2244	A
44	5	2245	С
44	5	2246	G
44	5	2255	A
44	5	2256	A
44	5	2260	U
44	5	2264	U
44	5	2273	G
44	5	2280	А
44	5	2281	А
44	5	2282	U
44	5	2284	С
44	5	2287	С
44	5	2288	G
44	5	2289	U
44	5	2290	С
44	5	2291	A
44	5	2292	U
44	5	2293	С
44	5	2297	U
44	5	2298	U
44	5	2301	U
44	5	2303	A
44	5	2304	С
44	5	2306	С
44	5	2307	G
44	5	2308	С



Mol	Chain	Res	Type
44	5	2310	U
44	5	2312	А
44	5	2313	А
44	5	2314	U
44	5	2315	G
44	5	2319	U
44	5	2325	G
44	5	2332	А
44	5	2335	G
44	5	2336	U
44	5	2339	С
44	5	2347	U
44	5	2352	A
44	5	2361	A
44	5	2365	С
44	5	2367	A
44	5	2372	А
44	5	2373	А
44	5	2374	С
44	5	2375	G
44	5	2376	G
44	5	2385	G
44	5	2386	А
44	5	2393	G
44	5	2394	G
44	5	2395	G
44	5	2396	G
44	5	2397	А
44	5	2398	А
44	5	2400	G
44	5	2401	A
44	5	2402	А
44	5	2403	G
44	5	2404	A
44	5	2406	С
44	5	2411	U
44	5	2418	G
44	5	2419	A
44	5	2420	С
44	5	2430	А
44	5	2432	A
44	5	2433	U



Mol	Chain	Res	Type
44	5	2434	U
44	5	2437	G
44	5	2440	G
44	5	2441	A
44	5	2443	А
44	5	2447	А
44	5	2452	G
44	5	2453	U
44	5	2454	G
44	5	2457	G
44	5	2458	А
44	5	2459	А
44	5	2460	U
44	5	2461	A
44	5	2462	A
44	5	2463	G
44	5	2464	U
44	5	2465	G
44	5	2468	А
44	5	2469	G
44	5	2470	С
44	5	2471	U
44	5	2473	С
44	5	2474	G
44	5	2475	G
44	5	2476	С
44	5	2477	G
44	5	2479	С
44	5	2480	A
44	5	2482	U
44	5	2485	A
44	5	2486	A
44	5	2487	U
44	5	$2\overline{488}$	A
44	5	2489	С
44	5	2490	С
44	5	2491	A
44	5	2492	С
44	5	$2\overline{493}$	U
44	5	2494	A
44	5	2496	С
44	5	2498	U



Mol	Chain	Res	Type
44	5	2499	U
44	5	2501	U
44	5	2503	G
44	5	2504	U
44	5	2506	U
44	5	2507	С
44	5	2508	U
44	5	2509	U
44	5	2510	U
44	5	2513	U
44	5	2516	U
44	5	2517	U
44	5	2518	С
44	5	2520	A
44	5	2521	U
44	5	2522	G
44	5	2523	А
44	5	2524	А
44	5	2526	С
44	5	2533	G
44	5	2534	G
44	5	2535	А
44	5	2537	U
44	5	2538	U
44	5	2539	С
44	5	2540	А
44	5	2541	U
44	5	2542	U
44	5	2543	U
44	5	2547	A
44	5	2549	G
44	5	2550	U
44	5	2552	C
44	5	$2\overline{553}$	U
44	5	2554	A
44	5	$25\overline{58}$	U
44	5	2561	A
44	5	2562	A
44	5	$25\overline{63}$	G
44	5	2566	C
44	5	$2\overline{568}$	C
44	5	2569	А



Mol	Chain	Res	Type
44	5	2571	U
44	5	2572	С
44	5	2573	G
44	5	2576	G
44	5	2581	U
44	5	2582	С
44	5	2583	С
44	5	2584	G
44	5	2585	G
44	5	2586	G
44	5	2590	А
44	5	2591	А
44	5	2593	А
44	5	2595	A
44	5	2596	U
44	5	2606	G
44	5	2607	G
44	5	2608	G
44	5	2610	G
44	5	2614	G
44	5	2616	С
44	5	2619	G
44	5	2621	G
44	5	2622	С
44	5	2623	G
44	5	2624	G
44	5	2626	А
44	5	2627	С
44	5	2628	А
44	5	2630	С
44	5	$2\overline{637}$	A
44	5	2640	A
44	5	2643	A
44	5	2645	G
44	5	2651	G
44	5	$2\overline{652}$	U
44	5	2656	A
44	5	$2\overline{662}$	G
44	5	2672	G
44	5	2674	A
44	5	2676	A
44	5	2677	G



Mol	Chain	Res	Type
44	5	2678	А
44	5	2679	A
44	5	2681	U
44	5	2682	С
44	5	2688	U
44	5	2689	А
44	5	2690	G
44	5	2694	А
44	5	2695	А
44	5	2696	А
44	5	2699	G
44	5	2700	G
44	5	2702	А
44	5	2704	A
44	5	2706	G
44	5	2711	С
44	5	2712	U
44	5	2713	U
44	5	2714	G
44	5	2727	А
44	5	2728	G
44	5	2729	U
44	5	2736	А
44	5	2737	С
44	5	2740	А
44	5	2741	C
44	5	2743	А
44	5	2744	U
44	5	2749	G
44	5	2752	U
44	5	2753	G
44	5	2755	C
44	5	$27\overline{60}$	C
44	5	2761	G
44	5	2762	А
44	5	2772	C
44	5	2773	С
44	5	2777	G
44	5	2778	G
44	5	2780	A
44	5	2781	U
44	5	2783	U



Mol	Chain	Res	Type
44	5	2786	G
44	5	2792	A
44	5	2794	G
44	5	2795	U
44	5	2796	G
44	5	2797	С
44	5	2799	А
44	5	2800	G
44	5	2801	А
44	5	2803	А
44	5	2804	А
44	5	2806	U
44	5	2810	С
44	5	2813	A
44	5	2817	A
44	5	2828	G
44	5	2834	G
44	5	2838	А
44	5	2840	С
44	5	2844	С
44	5	2845	А
44	5	2847	А
44	5	2849	С
44	5	2854	U
44	5	2859	U
44	5	2860	U
44	5	2861	U
44	5	2863	G
44	5	2864	А
44	5	2866	U
44	5	2867	С
44	5	2871	G
44	5	2872	A
44	5	2873	U
44	5	2874	G
44	5	2879	С
44	5	2880	U
44	5	2881	С
44	5	2885	С
44	5	2886	U
44	5	2887	A
44	5	2888	U



Mol	Chain	Res	Type
44	5	2895	G
44	5	2896	А
44	5	2899	С
44	5	2900	А
44	5	2906	С
44	5	2910	А
44	5	2913	С
44	5	2916	U
44	5	2922	G
44	5	2923	U
44	5	2927	С
44	5	2929	С
44	5	2932	U
44	5	2933	A
44	5	2934	A
44	5	2935	U
44	5	2936	А
44	5	2941	А
44	5	2942	С
44	5	2943	G
44	5	2945	G
44	5	2946	А
44	5	2952	G
44	5	2954	U
44	5	2955	U
44	5	2967	А
44	5	2971	А
44	5	2972	G
44	5	2973	G
44	5	2974	U
44	5	2977	G
44	5	2979	U
44	5	2980	U
44	5	2983	C
44	5	2984	C
44	5	2988	С
44	5	2992	U
44	5	2996	U
44	5	2997	G
44	5	3011	А
44	5	3012	A
44	5	3017	A



Mol	Chain	Res	Type
44	5	3020	U
44	5	3021	A
44	5	3022	G
44	5	3023	U
44	5	3026	G
44	5	3030	G
44	5	3033	А
44	5	3034	С
44	5	3036	G
44	5	3042	U
44	5	3049	А
44	5	3054	U
44	5	3055	U
44	5	3056	U
44	5	3059	G
44	5	3069	G
44	5	3074	G
44	5	3076	С
44	5	3078	U
44	5	3079	U
44	5	3080	G
44	5	3081	С
44	5	3085	G
44	5	3086	А
44	5	3091	А
44	5	3092	С
44	5	3093	С
44	5	3094	А
44	5	3096	С
44	5	3097	С
44	5	3099	С
44	5	3101	G
44	5	3109	G
44	5	3116	G
44	5	3118	С
44	5	3119	U
44	5	3122	A
44	5	3124	G
44	5	3125	U
44	5	3128	G
44	5	3130	A
44	5	3131	U



Mol	Chain	Res	Type	
44	5	3141	A	
44	5	3142	А	
44	5	3143	С	
44	5	3144	G	
44	5	3148	U	
44	5	3149	G	
44	5	3150	А	
44	5	3151	U	
44	5	3152	U	
44	5	3154	С	
44	5	3155	U	
44	5	3156	U	
44	5	3157	U	
44	5	3159	С	
44	5	3162	С	
44	5	3164	С	
44	5	3165	A	
44	5	3167	А	
44	5	3170	А	
44	5	3173	G	
44	5	3174	А	
44	5	3176	G	
44	5	3179	U	
44	5	3180	А	
44	5	3181	С	
44	5	3186	А	
44	5	3187	А	
44	5	3190	С	
44	5	3192	U	
44	5	3193	С	
44	5	3195	U	
44	5	3196	U	
44	5	3197	G	
44	5	3198	U	
44	5	3199	G	
44	5	3202	G	
44	5	3203	U	
44	5	3204	С	
44	5	3205	G	
44	5	3207	U	
44	5	3208	G	
44	5	3209	А	



Mol	Chain	Res	Type	
44	5	3210	А	
44	5	3214	U	
44	5	3215	A	
44	5	3216	G	
44	5	3217	С	
44	5	3218	А	
44	5	3219	G	
44	5	3220	G	
44	5	3221	С	
44	5	3222	U	
44	5	3223	А	
44	5	3224	G	
44	5	3227	A	
44	5	3228	С	
44	5	3229	G	
44	5	3230	G	
44	5	3233	С	
44	5	3243	А	
44	5	3244	А	
44	5	3247	G	
44	5	3250	U	
44	5	3258	U	
44	5	3259	U	
44	5	3260	G	
44	5	3263	G	
44	5	3265	С	
44	5	3266	G	
44	5	3267	А	
44	5	3268	А	
44	5	3269	U	
44	5	3271	G	
44	5	3272	С	
44	5	3273	A	
44	5	3274	A	
44	5	3275	U	
44	5	3276	G	
44	5	3277	U	
44	5	3278	С	
44	5	3279	A	
44	5	3281	U	
44	5	3286	G	
44	5	3287	U	



Mol	Chain	Res	Type
44	5	3288	G
44	5	3289	G
44	5	3293	U
44	5	3294	А
44	5	3299	А
44	5	3303	G
44	5	3304	U
44	5	3305	А
44	5	3307	А
44	5	3308	С
44	5	3315	G
44	5	3316	А
44	5	3317	U
44	5	3319	U
44	5	3320	A
44	5	3323	A
44	5	3324	С
44	5	3325	G
44	5	3326	G
44	5	3330	А
44	5	3331	U
44	5	3333	G
44	5	3334	U
44	5	3336	А
44	5	3342	А
44	5	3343	G
44	5	3347	А
44	5	3348	G
44	5	3351	U
44	5	3352	U
44	5	3354	U
44	5	3355	U
44	5	$3\overline{360}$	C
44	5	3366	G
44	5	$3\overline{368}$	U
44	5	$3\overline{369}$	G
44	5	3371	G
44	5	$3\overline{373}$	U
44	5	3375	A
44	5	3377	G
44	5	3378	С
44	5	3379	С



Mol	Chain	Res	Type	
44	5	3382	U	
44	5	3383	G	
44	5	3384	U	
44	5	3389	U	
44	5	3390	G	
44	5	3391	А	
45	8	7	U	
45	8	9	А	
45	8	11	С	
45	8	13	А	
45	8	14	С	
45	8	15	G	
45	8	16	G	
45	8	17	A	
45	8	19	C	
45	8	21	С	
45	8	22	U	
45	8	23	U	
45	8	24	G	
45	8	29	U	
45	8	30	С	
45	8	32	С	
45	8	34	U	
45	8	35	С	
45	8	37	А	
45	8	38	U	
45	8	40	А	
45	8	45	С	
45	8	49	G	
45	8	51	G	
45	8	52	A	
$\overline{45}$	8	53	A	
45	8	59	A	
$\overline{45}$	8	60	U	
45	8	61	А	
45	8	62	C	
45	8	63	G	
45	8	65	A	
45	8	66	A	
45	8	67	U	
45	8	69	U	
45	8	71	A	



Mol	Chain	Res	Type
45	8	73	U
45	8	75	G
45	8	79	А
45	8	80	А
45	8	81	U
45	8	82	U
45	8	83	С
45	8	84	С
45	8	85	G
45	8	86	U
45	8	87	G
45	8	88	А
45	8	90	U
45	8	91	С
45	8	93	U
45	8	95	G
45	8	96	А
45	8	100	U
45	8	101	U
45	8	104	А
45	8	105	А
45	8	106	С
45	8	107	G
45	8	109	А
45	8	111	А
45	8	112	U
45	8	113	U
45	8	114	G
45	8	116	G
45	8	117	С
45	8	119	С
45	8	120	C
45	8	121	U
45	8	$12\overline{4}$	G
45	8	125	U
45	8	126	A
45	8	127	U
45	8	136	G
45	8	138	A
45	8	142	C
45	8	$14\overline{3}$	U
45	8	144	G



Mol	Chain	Res	Type	
45	8	146	U	
45	8	148	G	
45	8	149	А	
45	8	150	G	
45	8	151	С	
45	8	152	G	
45	8	158	U	
46	7	2	G	
46	7	8	G	
46	7	11	А	
46	7	13	А	
46	7	14	U	
46	7	17	А	
46	7	18	С	
46	7	22	A	
46	7	31	U	
46	7	32	U	
46	7	33	U	
46	7	35	С	
46	7	38	U	
46	7	41	G	
46	7	42	А	
46	7	46	А	
46	7	47	С	
46	7	51	А	
46	7	52	G	
46	7	54	U	
46	7	55	А	
46	7	64	А	
46	7	65	G	
46	7	69	C	
46	7	74	С	
46	7	76	A	
46	7	78	U	
46	7	79	A	
46	7	82	G	
46	7	85	G	
46	7	86	U	
46	7	88	G	
46	7	93	C	
46	7	96	U	
46	7	99	G	



Continued from previous page...

Mol	Chain	\mathbf{Res}	Type
46	7	102	А
46	7	112	G
46	7	115	G
46	7	116	С
46	7	120	С
46	7	121	U

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
44	5	11	A
44	5	12	А
44	5	14	U
44	5	62	А
44	5	117	U
44	5	121	А
44	5	150	А
44	5	187	А
44	5	441	U
44	5	555	U
44	5	588	G
44	5	637	С
44	5	705	А
44	5	909	G
44	5	1154	А
44	5	1263	А
44	5	1307	G
44	5	1527	С
44	5	1625	А
44	5	1816	А
44	5	1958	U
44	5	2101	С
44	5	2209	U
44	5	2263	С
44	5	2279	А
44	5	2305	G
44	5	2392	С
44	5	2525	G
44	5	2541	U
44	5	3121	U
44	5	3228	С
44	5	3334	U



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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
44	5	9
24	W	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2083:G	O3'	2084:C	Р	19.95
1	W	217:SER	С	218:ARG	Ν	12.39
1	W	219:LYS	С	220:THR	Ν	9.79
1	W	229:GLY	С	230:ALA	Ν	9.10
1	5	2513:U	O3'	2514:U	Р	8.49
1	5	2501:U	O3'	2502:A	Р	7.73
1	5	2447:A	O3'	2448:G	Р	6.97
1	5	2445:A	O3'	2446:U	Р	6.77
1	W	228:THR	С	229:GLY	Ν	5.68
1	5	2435:G	O3'	2436:U	Р	4.30
1	5	2246:G	O3'	2247:G	Р	2.70
1	5	2279:A	O3'	2280:A	Р	1.96
1	5	2263:C	O3'	2264:U	P	0.61



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20077. 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: 192



Y Index: 192



Z Index: 192

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: 179

Y Index: 209

Z Index: 209

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

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

6.4.1 Primary map



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation (i)

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


7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 2037 $\rm nm^3;$ this corresponds to an approximate mass of 1840 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 0.263 $\mathrm{\AA^{-1}}$



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-20077 and PDB model 60IG. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.03 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 (0.03).



9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.9200	0.2310
5	0.9800	0.2690
7	0.9960	0.2860
8	0.9810	0.2620
А	0.8420	0.2020
В	0.8840	0.2050
С	0.8760	0.1820
D	0.8790	0.1900
E	0.8750	0.1800
F	0.8720	0.2000
G	0.8760	0.2030
Н	0.8720	0.1790
I	0.8260	0.1350
J	0.8600	0.1810
L	0.8950	0.1870
M	0.8800	0.1810
N	0.6720	0.0710
0	0.8790	0.2020
P	0.8680	0.1890
Q	0.8710	0.2090
R	0.7120	0.1660
S	0.8790	0.2100
T	0.9010	0.2100
U	0.8750	0.2240
V	0.7970	0.2140
W	0.3950	0.0920
X	0.8300	0.1850
Y	0.8830	0.1610
Z	0.8780	0.2180
a	0.8790	0.2060
b	0.8210	0.1460
С	0.8660	0.2460
d	0.8480	0.1830
e	0.8290	0.1620
f	0.8670	0.1840

Continued on next page...



Continued from previous page...

Chain	Atom inclusion	Q-score
g	0.8580	0.1910
h	0.8750	0.1740
i	0.8740	0.2150
j	0.8810	0.1430
k	0.8570	0.2030
1	0.8370	0.1750
m	0.8740	0.2340
0	0.8350	0.1790
р	0.8600	0.2020
q	0.7010	0.0560
S	0.9010	0.0890
X	0.4720	0.1690
У	0.2520	0.1190
Z	0.6650	0.0620

