

# Full wwPDB X-ray Structure Validation Report (i)

#### Jan 29, 2024 - 09:32 PM EST

PDB ID	:	1FFK
Title	:	CRYSTAL STRUCTURE OF THE LARGE RIBOSOMAL SUBUNIT FROM
		HALOARCULA MARISMORTUI AT 2.4 ANGSTROM RESOLUTION
Authors	:	Ban, N.; Nissen, P.; Hansen, J.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2000-07-25
Resolution	:	2.40  Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp 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:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
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:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.40 Å.

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



Metric Whole architemetric (#Entries)		${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	4398 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of	of chain	
1	0	2922	49%	34%	8% • 7%
2	9	122	43%	43%	11% •
3	А	239	98%		••
4	В	337	99%		·
5	С	246	100%	Ď	
6	D	176	80%		20%
7	Е	119	97%		•••
8	F	157	100%	, 0	
9	G	145	98%		
10	Н	132	99%		•



Mol	Chain	Length	Quality of chain	
11	Ι	194	100%	
12	J	164	87%	13%
13	К	186	100%	
14	L	115	100%	
15	М	148	97%	•
16	Ν	95	100%	
17	Ο	154	97%	•
18	Р	84	93%	7%
19	Q	119	100%	
20	R	66	80%	20%
21	$\mathbf{S}$	70	93%	7%
22	Т	154	100%	
23	U	91	92%	• 7%
24	V	143	99%	•
25	W	73	100%	
26	Х	56	100%	
27	Y	49	63% 37%	
28	Ζ	92	100%	
29	1	177	97%	·



## 2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 64281 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a RNA chain called 23S RRNA.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
1	0	2706	Total 58012	C 25885	N 10685	O 18737	Р 2705	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	С	U	conflict	GB 3377779

• Molecule 2 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	9	122	Total 2600	C 1160	N 472	O 847	Р 121	0	0	0

• Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	А	237	Total C 237 237	0	0	237

• Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	В	337	Total C 337 337	0	0	337

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	?	-	GLU	deletion	UNP P20279
В	311	PHE	-	insertion	UNP P20279



• Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	С	246	Total         C           246         246	0	0	246

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	73	LEU	GLN	conflict	UNP P12735

• Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	D	140	Total         C           140         140	0	0	140

• Molecule 7 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	Ε	118	Total C 118 118	0	0	118

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	108	LEU	-	insertion	UNP P12743
Е	109	GLU	-	insertion	UNP P12743
Е	110	GLU	-	insertion	UNP P12743

• Molecule 8 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	F	157	Total C 157 157	0	0	157

• Molecule 9 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	G	142	Total C 142 142	0	0	142

• Molecule 10 is a protein called RIBOSOMAL PROTEIN L14.



Mol	Chain	Residues	Ator	ms	ZeroOcc	AltConf	Trace
10	Н	132	Total 132	C 132	0	0	132

• Molecule 11 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atom	ıs	ZeroOcc	AltConf	Trace
11	Ι	194	Total 194	C 194	0	0	194

• Molecule 12 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	J	143	Total C 143 143	0	0	143

• Molecule 13 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	Κ	186	Total C 186 186	0	0	186

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	186	LEU	-	insertion	UNP P14123

• Molecule 14 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	L	115	Total C 115 115	0	0	115

• Molecule 15 is a protein called RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
15	М	143	Total C 143 143	0	0	143

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
М	71	LYS	TYR	conflict	UNP P14119



• Molecule 16 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	Ν	95	Total         C           95         95	0	0	95

• Molecule 17 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	О	150	Total C 150 150	0	0	150

• Molecule 18 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	Р	78	TotalC7878	0	0	78

• Molecule 19 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	Q	119	Total C 119 119	0	0	119

• Molecule 20 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	R	53	Total         C           53         53	0	0	53

• Molecule 21 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	S	65	$\begin{array}{cc} \text{Total} & \text{C} \\ 65 & 65 \end{array}$	0	0	65

• Molecule 22 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	Т	154	Total C 154 154	0	0	154

• Molecule 23 is a protein called RIBOSOMAL PROTEIN L31E.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	U	85	Total         C           85         85	0	0	85

• Molecule 24 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Ator	ns	ZeroOcc	AltConf	Trace
24	V	143	Total 143	C 143	0	0	143

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	109	ASN	ALA	conflict	UNP P12736

• Molecule 25 is a protein called RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	W	73	Total         C           73         73	0	0	73

• Molecule 26 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	Х	56	$\begin{array}{cc} {\rm Total} & {\rm C} \\ 56 & 56 \end{array}$	0	0	56

• Molecule 27 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	Y	31	TotalC3131	0	0	31

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	11	LYS	LEU	conflict	UNP P22452
Y	24	TYR	TRP	conflict	UNP P22452
Y	42	TRP	TYR	conflict	UNP P22452

• Molecule 28 is a protein called RIBOSOMAL PROTEIN L44E.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
28	Z	92	Total 92	C 92	0	0	92

• Molecule 29 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Ato	ms	ZeroOcc	AltConf	Trace
29	1	172	Total 172	C 172	0	0	172

• Molecule 30 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	0	1	Total K 1 1	0	0

• Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	0	2	Total Mg 2 2	0	0

• Molecule 32 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	R	1	Total Cd 1 1	0	0
32	W	1	Total Cd 1 1	0	0
32	Х	1	Total Cd 1 1	0	0
32	Ζ	1	Total Cd 1 1	0	0

• Molecule 33 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	6	Total O 6 6	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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Chain 0:		49%	34%	8% • 7%
	C 110 112 113 113 113 113 113 113 113 113 113	424 031 135 036 038 038 038 049 641	A45 A45 A60 A60 G61 C63 C64 A67 A70 A74 A74	0175 077 077 077 077 077 077 077 077 077 0
4102 6105 0107 0107 0108	A114 0115 0116 0116 A119 A120 0125 0 0 0 0	A129 A122 U133 U133 U137 U137 U137 U138 C140 C141 C141	C142 A148 A149 C149 C149 C150 A151 A155 A156 A166 A167 A168 A177	U178 01178 A186 A187 C188 A191 A191 A192 A192 A192 A192 A192 C195 C195 C195 C195
A199 U200 G201 A204 U205 G206	U207 C208 A212 Q213 Q219 G219 G219	02240 2240 4243 4248 6249 6249 6249 6251 6251	A255 A255 C256 C256 C256 A262 U263 U263 C271 A272 C271 A272 C275 C275 C275 C275	U277 U277 A778 C279 C280 U281 U281 U281 U288 U286 C284 C286 C286 C287 C287 C287 C287 C287 C287 C287 C287
6292 A293 C294 C295 G296 U297	C303 C304 C304 C306 C309 C309 C309 C322 C322	Ca255 Ca255 Ca255 Ca326 Ca320 Ca330 Ca330 Ca333 Ca335 Ca335 Ca335 Ca335 Ca335 Ca335 Ca335 Ca335 Ca335 Ca335 Ca355	0336 0337 0337 0338 0345 0345 0345 0345 0351 0351 0351 0351 0355 0355 0355 035	C356 C356 A357 A357 A350 C356 C361 C361 C361 C361 C365 C364 C365 C365 C365 C365 C365 C365 C365 C365
U371 A372 G373 U374 G375 G381	U382 A383 C384 C394 C393 C393 A395 A395 A395 V396 V396	C401 U402 A407 A411 C412 C413 C413 C414 C414 C414	0418 4419 14420 1425 0426 0433 0433 0433 0433 0438 0438 0438 0430 0438	4441 4441 4453 4453 4453 4453 6461 6461 6480 0482 0483 4484 4484
A486 G487 G496 A497 A498	6503 6504 6505 6505 6505 8507 8507 8508 8512 8512 6512	4015 6515 6515 6518 6519 4520 6523 6523 6523 1526 0526	U527 0528 0528 0528 0535 0535 0535 0536 0539 0539 0539 0539 0539 0539 0539 0539	A 449 (550 A 551 A 555 A 555 A 555 C555 C555 C555 C555 C
A566 U567 A569 A569 C574 C575	C578 C578 C581 C582 C583 C584 C586 C586 C586	U599 U595 C594 C594 C595 C598 C598 C598 C598 C598 C598 C598	A603 0604 0606 0606 0606 0612 0612 0613 0615 0615 0615 0615 0615 0615 0615 0615	0627 0627 0627 0627 0628 0633 0633 0633 0638 0638 0638 0638 0646 0646
C653 A654 G657 C658 A659	A660 6661 6667 6667 6667 6672 6672 6681	6685 6684 6684 6685 6685 6685 6685 6685	0000 0000 0000 0000 0000 0000 0000 0000 0000	C725 C725 C726 C736 A736 A736 A736 A736 A736 C745 C748 C748 C748
C764 G765 A766 A767 U777 C778	U779 A790 A791 A791 C795 C795 C803 C803 C803	A807 A808 A808 C810 C811 A812 A812 C816 C816 A819 A819	0820 1821 0834 0835 0834 0836 0846 0846 0848 0848 0848 0848 0848 084	00000000000000000000000000000000000000
G878 C881 U882 U883 C884 C885	A86 (3887 (3887 (3888 (3888 (3898 A894 A894 A894 A895 A895 A895 A895 A895 A895 A895 A895	U904 C905 C905 A907 A907 C920 C921 A922 A923	C934 6938 6938 6939 6940 0945 0945 0945 0947 0948 0953 0953	6956 8956 8956 8956 8956 8960 8966 8966 8966 8966 8966 8966 896
<b>ں ں ں ב ی ב ی</b>	U U ⊃ U U U ⊲ U ⊲ U α	96 0000004040 000004040	C1000 C1001 A1007 C1008 U1009 C1014 C1015 U1016 A1020 A1022 C1021 A1022	U1029 U1029 U1030 C1031 A1041 U1041 U1041 C1043 C1044 C1045 C1045 C1045 C1045 C1045 C1045 C1045

• Molecule 1: 23S RRNA















There are no outlier residues recorded for this chain.

Chain D:	80%	20%
SER SER SER GLU GLU SER GLY GLY ASP ASP	H29 GLY GLY GLY ARG ASP ASP ASP CIO THR ASP CIU THR CIU THR CIU THR CIU CIU CIU CIU CIU CIU CIU CIU CIU CIU	
• Molecule 7:	RIBOSOMAL PROTEIN L7AE	
Chain E:	97%	
PRO V2 P56 B119 B119		
• Molecule 8:	RIBOSOMAL PROTEIN L10E	
Chain F:	100%	
There are no c	outlier residues recorded for this chain.	
• Molecule 9:	RIBOSOMAL PROTEIN L13	
Chain G:	98%	•
MET SER VAL A4 W145		
• Molecule 10:	RIBOSOMAL PROTEIN L14	
Chain H:	99%	•
M1 G36 V132		
• Molecule 11:	RIBOSOMAL PROTEIN L15E	
Chain I:	100%	
There are no c	outlier residues recorded for this chain.	
• Molecule 12:	RIBOSOMAL PROTEIN L15	
Chain J:	87%	13%
T1 E83 VAL GLU GLY GLY PHE ARG VAT	ALA GLU GLU GLU GLU ASP ALA ALA ALA ALA ALA CLU GLU GLU	
• Molecule 13:	RIBOSOMAL PROTEIN L18	
Chain K:	100%	



There are no outlier residues recorded for this chain. • Molecule 14: RIBOSOMAL PROTEIN L18E	
Chain L: 100% There are no outlier residues recorded for this chain.	
• Molecule 15: RIBOSOMAL PROTEIN L19	
Chain M: 97%	
T1 A143 ASP ASP ALA ALA	
• Molecule 16: RIBOSOMAL PROTEIN L21E	
Chain N: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 17: RIBOSOMAL PROTEIN L22	
Chain O: 97%	·
AI PI 50 CLU CLU ASP ASP	
• Molecule 18: RIBOSOMAL PROTEIN L23	
Chain P: 93%	7%
SI ATG SER ARG CLY CLY PHE	
• Molecule 19: RIBOSOMAL PROTEIN L24	
Chain Q: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 20: RIBOSOMAL PROTEIN L24E	
Chain R: 80%	20%
PR0 ARG R4 R4 R4 CLY CLY CLY ALA ALA ALA ALA ALA	
• Molecule 21: RIBOSOMAL PROTEIN L29	
Chain S: 93%	7%





• Molecule 22: RIBOSOMAL PROTEIN L30	
Chain T: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 23: RIBOSOMAL PROTEIN L31E	
Chain U: 92%	• 7%
ALA SER SELA SELA SELA ALA ALA ALA GLU	
• Molecule 24: RIBOSOMAL PROTEIN L32E	
Chain V: 99%	
• Molecule 25: RIBOSOMAL PROTEIN L37AE	
Chain W: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 26: RIBOSOMAL PROTEIN L37E	
Chain X: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 27: RIBOSOMAL PROTEIN L39E	
Chain Y: 63% 37%	
C1 THR ASP ARC CLU VAL CLU CLU CLU CLU CLU CLU CLU CLU CLU CL	
• Molecule 28: RIBOSOMAL PROTEIN L44E	
Chain Z: 100%	
There are no outlier residues recorded for this chain.	
• Molecule 29: RIBOSOMAL PROTEIN L6	
Chain 1: 97%	•







## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	211.66Å 299.67Å 573.77Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
$\mathbf{Posolution} \left( \overset{\circ}{\mathbf{A}} \right)$	90.00 - 2.40	Depositor
Resolution (A)	89.24 - 2.40	EDS
% Data completeness	82.3 (90.00-2.40)	Depositor
(in resolution range)	95.5(89.24-2.40)	EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.28 (at 2.40 \text{\AA})$	Xtriage
Refinement program	CNS, TNT & CNS	Depositor
B B.	0.252 , $0.261$	Depositor
It, Itfree	0.345 , (Not available)	DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	42.3	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.04 , -7.2	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	64281	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CD, MG, K

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

Mal Chain		Bond	lengths	Bond angles		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	0	0.47	0/64945	0.72	73/101281~(0.1%)	
2	9	0.35	0/2905	0.75	4/4528~(0.1%)	
All	All	0.46	0/67850	0.72	77/105809~(0.1%)	

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	0	18	45
2	9	2	0
All	All	20	45

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	0	2749	U	C2'-C3'-O3'	11.07	133.85	109.50
1	0	904	U	C2'-C3'-O3'	10.39	132.35	109.50
1	0	1981	A	C2'-C3'-O3'	10.23	132.00	109.50
1	0	2692	G	N9-C1'-C2'	10.09	127.12	114.00
2	9	3	A	C2'-C3'-O3'	9.58	130.57	109.50
1	0	894	A	C2'-C3'-O3'	9.38	130.13	109.50
1	0	1059	G	C2'-C3'-O3'	8.85	128.97	109.50
1	0	713	U	C2'-C3'-O3'	8.71	128.66	109.50
1	0	1309	U	C2'-C3'-O3'	8.66	128.56	109.50
1	0	191	A	C2'-C3'-O3'	8.64	128.51	109.50
1	0	2616	G	C2'-C3'-O3'	8.34	127.84	109.50
1	0	480	C	C2'-C3'-O3'	8.34	127.84	109.50



Continued	from	previous	page

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
1	0	394	G	C2'-C3'-O3'	8.29	127.75	109.50
1	0	2482	G	C2'-C3'-O3'	8.25	127.66	109.50
1	0	282	С	C2'-C3'-O3'	8.13	127.39	109.50
1	0	1406	А	C2'-C3'-O3'	8.13	127.38	109.50
1	0	1835	U	C2'-C3'-O3'	8.11	127.34	109.50
1	0	1907	U	C2'-C3'-O3'	8.04	127.20	109.50
1	0	600	G	C2'-C3'-O3'	7.99	127.08	109.50
1	0	1853	С	C2'-C3'-O3'	7.97	127.05	109.50
1	0	2714	U	C2'-C3'-O3'	7.97	127.04	109.50
1	0	2321	А	C2'-C3'-O3'	7.91	126.89	109.50
1	0	2427	С	C2'-C3'-O3'	7.69	126.42	109.50
1	0	1699	С	C2'-C3'-O3'	7.68	126.39	109.50
1	0	2370	А	C2'-C3'-O3'	7.60	126.22	109.50
1	0	1506	U	C2'-C3'-O3'	7.48	125.96	109.50
1	0	554	G	C2'-C3'-O3'	7.44	125.87	109.50
2	9	28	U	C2'-C3'-O3'	7.31	125.58	109.50
1	0	2813	А	C2'-C3'-O3'	7.24	125.43	109.50
1	0	199	А	C2'-C3'-O3'	7.22	125.38	109.50
1	0	2283	G	C2'-C3'-O3'	7.17	125.26	109.50
1	0	452	G	N9-C1'-C2'	6.97	123.06	114.00
1	0	1214	G	C2'-C3'-O3'	6.96	124.84	113.70
1	0	1379	А	C2'-C3'-O3'	6.90	124.74	113.70
1	0	1690	С	C2'-C3'-O3'	6.86	124.67	113.70
1	0	196	G	C2'-C3'-O3'	6.83	124.63	113.70
1	0	1979	G	C2'-C3'-O3'	6.76	124.51	113.70
1	0	856	G	N9-C1'-C2'	6.74	122.76	114.00
1	0	548	U	C2'-C3'-O3'	6.55	124.19	113.70
1	0	1072	G	N9-C1'-C2'	6.46	122.39	114.00
1	0	1995	G	N9-C1'-C2'	6.44	122.37	114.00
1	0	2090	G	C2'-C3'-O3'	6.28	123.75	113.70
1	0	2692	G	O4'-C1'-N9	6.22	113.17	108.20
1	0	1682	A	N9-C1'-C2'	6.15	122.00	114.00
1	0	2083	A	C2'-C3'-O3'	6.14	123.52	113.70
1	0	1214	G	C4'-C3'-O3'	6.13	125.26	113.00
1	0	1126	С	C2'-C3'-O3'	6.12	123.50	113.70
1	0	$23\overline{95}$	A	C2'-C3'-O3'	6.11	123.48	113.70
1	0	2258	A	C2'-C3'-O3'	5.97	123.26	113.70
1	0	191	A	C4'-C3'-O3'	5.95	124.89	113.00
1	0	1120	U	$C5'-C4'-\overline{C3'}$	-5.85	106.64	116.00
1	0	1524	U	N1-C1'-C2	-5.74	105.69	112.00
1	0	1448	A	C2'-C3'-O3'	$5.6\overline{8}$	122.79	113.70
2	9	39	U	N1-C1'-C2'	5.67	121.38	114.00



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	0	1819	G	C5'-C4'-C3'	5.53	124.84	116.00
1	0	2506	A	N9-C1'-C2'	-5.51	105.94	112.00
1	0	1108	G	C2'-C3'-O3'	5.49	122.48	113.70
1	0	2914	А	C2'-C3'-O3'	5.36	122.27	113.70
1	0	1214	G	C4'-C3'-C2'	5.30	107.90	102.60
1	0	600	G	C4'-C3'-O3'	5.30	123.60	113.00
1	0	452	G	C2'-C3'-O3'	5.30	122.18	113.70
1	0	777	U	O4'-C1'-N1	5.29	112.43	108.20
1	0	1683	G	C2'-C3'-O3'	5.27	122.13	113.70
2	9	1	U	N1-C1'-C2'	5.26	120.84	114.00
1	0	1907	U	C4'-C3'-O3'	5.20	123.41	113.00
1	0	2316	G	N9-C1'-C2'	5.18	120.73	114.00
1	0	535	G	N9-C1'-C2'	5.15	120.70	114.00
1	0	2074	А	N9-C1'-C2'	5.14	120.68	114.00
1	0	1615	А	C5'-C4'-C3'	5.12	124.18	116.00
1	0	1369	А	N9-C1'-C2'	5.11	120.65	114.00
1	0	2427	С	C4'-C3'-O3'	5.10	123.19	113.00
1	0	2526	С	C2'-C3'-O3'	5.09	121.84	113.70
1	0	2506	A	O4'-C1'-N9	5.08	112.26	108.20
1	0	1835	U	C4'-C3'-O3'	5.07	123.13	113.00
1	0	1504	A	C1'-O4'-C4'	-5.05	105.86	109.90
1	0	857	A	C2'-C3'-O3'	5.05	121.78	113.70
1	0	894	A	C4'-C3'-O3'	5.01	123.01	113.00

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	191	А	C3'
1	0	282	С	C3'
1	0	600	G	C3'
1	0	894	А	C3'
1	0	904	U	C3'
1	0	1214	G	C3'
1	0	1309	U	C3'
1	0	1699	С	C3'
1	0	1835	U	C3'
1	0	1853	С	C3'
1	0	1907	U	C3'
1	0	1981	А	C3'
1	0	2083	А	C3'
1	0	2427	С	C3'
1	0	2482	G	C3'



Mol	Chain	Res	Type	Atom
1	0	2692	G	C1'
1	0	2714	U	C3'
1	0	2749	U	C3'
2	9	1	U	C1'
2	9	3	А	C3'

Continued from previous page...

All	(45)	planarity	outliers	are	listed	below:
-----	------	-----------	----------	-----	--------	--------

Mol	Chain	Res	Type	Group
1	0	1122	U	Sidechain
1	0	1342	С	Sidechain
1	0	138	U	Sidechain
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1524	U	Sidechain
1	0	1525	G	Sidechain
1	0	1555	G	Sidechain
1	0	1614	G	Sidechain
1	0	1682	А	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	А	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	189	А	Sidechain
1	0	1950	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	1995	G	Sidechain
1	0	2312	G	Sidechain
1	0	2313	С	Sidechain
1	0	2463	А	Sidechain
1	0	2493	С	Sidechain
1	0	2503	А	Sidechain
1	0	2506	A	Sidechain
1	0	2543	G	Sidechain
1	0	2564	G	Sidechain
1	0	2607	U	Sidechain
1	0	262	A	Sidechain



Mol	Chain	Res	Type	Group
1	0	2630	G	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	2866	U	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	469	G	Sidechain
1	0	482	G	Sidechain
1	0	485	А	Sidechain
1	0	518	G	Sidechain
1	0	529	G	Sidechain
1	0	791	А	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	58012	0	29282	976	0
2	9	2600	0	1326	62	0
3	А	237	0	0	1	0
4	В	337	0	0	2	0
5	С	246	0	0	0	0
6	D	140	0	0	0	0
7	Е	118	0	0	1	0
8	F	157	0	0	0	0
9	G	142	0	0	0	0
10	Н	132	0	0	1	0
11	Ι	194	0	0	0	0
12	J	143	0	0	0	0
13	Κ	186	0	0	0	0
14	L	115	0	0	0	0
15	М	143	0	0	0	0
16	Ν	95	0	0	0	0
17	0	150	0	0	0	0
18	Р	78	0	0	0	0
19	Q	119	0	0	0	0
20	R	53	0	0	0	0
21	S	65	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	Т	154	0	0	0	0
23	U	85	0	0	1	0
24	V	143	0	0	2	0
25	W	73	0	0	0	0
26	Х	56	0	0	0	0
27	Y	31	0	0	0	0
28	Ζ	92	0	0	0	0
29	1	172	0	0	0	0
30	0	1	0	0	0	0
31	0	2	0	0	0	0
32	R	1	0	0	0	0
32	W	1	0	0	0	0
32	Х	1	0	0	0	0
32	Ζ	1	0	0	0	0
33	0	6	0	0	0	0
All	All	64281	0	30608	1040	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1040) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	A +	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:9:76:G:H3'	2:9:77:A:H5"	1.29	1.10
1:0:1682:A:H2	1:0:1696:U:H3	1.05	1.01
1:0:795:G:H2'	1:0:817:G:H22	1.25	1.00
1:0:326:G:H1	1:0:330:C:H5	1.03	1.00
1:0:1355:A:O2'	1:0:1356:A:H3'	1.60	1.00
2:9:56:A:H2'	2:9:57:A:H5"	1.44	0.99
1:0:337:A:H2	1:0:1314:U:HO2'	1.00	0.95
1:0:1147:C:H2'	1:0:1148:C:H5"	1.47	0.95
1:0:2768:A:H2'	1:0:2769:C:O4'	1.66	0.94
1:0:289:G:H22	1:0:363:A:H2	1.08	0.93
1:0:282:C:H1'	1:0:368:C:N4	1.82	0.93
1:0:2717:C:C2'	1:0:2718:C:H5"	2.00	0.92
1:0:560:C:H42	1:0:597:A:H61	1.01	0.91
1:0:1751:G:H2'	1:0:1752:G:H5"	1.51	0.91
1:0:1116:U:HO2'	1:0:1118:A:H2	0.91	0.90
1:0:10:U:HO2'	1:0:11:A:H8	0.99	0.90
1:0:2890:A:H8	1:0:2890:A:H5"	1.37	0.90
1:0:1701:A:H4'	1:0:1702:U:H5"	1.54	0.90



	the second page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:1088:A:O2'	1:0:1089:G:H5"	1.71	0.90
1:0:45:A:H2	1:0:115:U:H3	0.94	0.89
1:0:199:A:O2'	1:0:200:U:H5"	1.72	0.88
1:0:2506:A:O2'	1:0:2507:G:H8	1.56	0.87
1:0:289:G:N2	1:0:363:A:H2	1.74	0.86
1:0:288:A:H61	1:0:364:C:H42	1.19	0.86
1:0:506:G:H22	1:0:509:A:H5'	1.43	0.84
1:0:2717:C:H2'	1:0:2718:C:H5"	1.57	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.77	0.82
1:0:283:U:H3'	1:0:284:C:C6	2.14	0.82
1:0:817:G:H4'	1:0:818:A:OP1	1.80	0.82
1:0:795:G:N2	1:0:817:G:H2'	1.94	0.81
1:0:795:G:H2'	1:0:817:G:N2	1.94	0.81
1:0:1147:C:C2'	1:0:1148:C:H5"	2.10	0.81
1:0:1106:A:H5'	1:0:1106:A:H8	1.46	0.81
1:0:371:U:H2'	1:0:372:A:C8	2.17	0.81
1:0:2812:A:H2	1:0:2814:A:H62	1.25	0.80
1:0:2090:G:H2'	1:0:2091:G:C8	2.17	0.79
1:0:2316:G:H4'	1:0:2316:G:OP1	1.81	0.79
2:9:29:C:H2'	2:9:30:C:H5'	1.65	0.79
2:9:56:A:C2'	2:9:57:A:H5"	2.13	0.78
1:0:2251:G:H2'	1:0:2252:A:C8	2.18	0.78
1:0:281:U:H2'	1:0:282:C:O4'	1.84	0.78
1:0:485:A:N3	1:0:487:G:H5"	1.98	0.78
1:0:1590:A:N6	1:0:1605:G:H1'	1.99	0.78
1:0:1148:C:H5'	1:0:1148:C:H6	1.49	0.77
1:0:2506:A:HO2'	1:0:2507:G:H8	0.79	0.77
1:0:45:A:H2	1:0:115:U:N3	1.77	0.77
1:0:506:G:H22	1:0:509:A:C5'	1.97	0.77
1:0:1088:A:H4'	1:0:1089:G:OP1	1.85	0.77
2:9:39:U:H1'	2:9:44:A:H61	1.50	0.76
1:0:1149:U:H5"	1:0:1151:G:O4'	1.84	0.76
1:0:2878:U:H2'	1:0:2879:A:O4'	1.86	0.76
1:0:796:A:N6	1:0:817:G:H1'	2.01	0.76
1:0:877:G:H5'	1:0:878:G:OP1	1.86	0.73
1:0:1438:G:N2	1:0:1685:A:H8	1.86	0.73
1:0:2103:A:H62	1:0:2538:A:H2	1.37	0.73
1:0:139:C:H4'	1:0:140:G:H5'	1.71	0.72
1:0:2866:U:H4'	1:0:2867:G:H5'	1.71	0.72
2:9:28:U:H2'	2:9:29:C:C6	2.24	0.72
1:0:1669:A:H2'	1:0:1670:G:C8	2.25	0.72



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:9:39:U:H1'	2:9:44:A:N6	2.05	0.72
1:0:2586:U:H3	1:0:2592:G:H22	1.37	0.71
1:0:2765:C:H4'	4:B:298:GLY:CA	2.20	0.71
1:0:544:G:H2'	1:0:545:G:H5"	1.72	0.71
2:9:76:G:C3'	2:9:77:A:H5"	2.16	0.71
1:0:1589:G:N2	1:0:1605:G:H2'	2.04	0.71
1:0:2851:G:O2'	1:0:2852:A:H5'	1.90	0.71
1:0:1972:U:H2'	1:0:1973:A:H5'	1.71	0.71
1:0:2903:C:H6	1:0:2903:C:H5'	1.54	0.71
1:0:2717:C:O2'	1:0:2718:C:H5"	1.89	0.71
1:0:2909:G:O2'	1:0:2910:A:H5'	1.91	0.71
1:0:138:U:H6	1:0:140:G:H1	1.39	0.71
1:0:371:U:H2'	1:0:372:A:H8	1.54	0.70
1:0:952:G:H4'	1:0:953:G:OP1	1.91	0.70
1:0:1441:G:O2'	1:0:1442:A:H5'	1.90	0.70
1:0:2866:U:H1'	1:0:2891:A:C4	2.25	0.70
1:0:67:A:OP2	1:0:108:U:H5'	1.91	0.70
1:0:2505:G:O2'	1:0:2506:A:H5'	1.91	0.70
1:0:1523:G:H2'	1:0:1524:U:C6	2.26	0.70
1:0:1119:G:N2	1:0:1246:A:C2	2.57	0.69
1:0:1751:G:C2'	1:0:1752:G:H5"	2.22	0.69
1:0:326:G:N1	1:0:330:C:H5	1.83	0.69
1:0:1681:G:H4'	1:0:1682:A:C8	2.27	0.69
1:0:2827:A:H2'	1:0:2828:G:O4'	1.92	0.69
1:0:362:G:H2'	1:0:363:A:H8	1.57	0.69
1:0:219:G:H3'	1:0:220:C:H5"	1.75	0.69
1:0:603:A:H4'	1:0:604:G:O5'	1.91	0.69
1:0:1209:C:H2'	1:0:1210:G:H8	1.57	0.69
1:0:1819:G:H2'	1:0:1820:G:H4'	1.74	0.69
1:0:2321:A:O2'	1:0:2322:U:H3'	1.93	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.75	0.69
1:0:2238:A:O2'	1:0:2239:C:H5'	1.93	0.68
2:9:14:G:H5'	2:9:14:G:H8	1.58	0.68
1:0:855:U:H4'	1:0:856:G:O5'	1.91	0.68
1:0:95:A:H5"	1:0:96:A:H3'	1.74	0.68
1:0:1380:U:H2'	1:0:1380:U:O2	1.92	0.68
1:0:2756:U:H3	1:0:2896:A:H2	1.41	0.68
1:0:12:U:H2'	1:0:13:G:H5'	1.75	0.68
1:0:1590:A:H61	1:0:1605:G:H1'	1.58	0.68
1:0:553:G:O2'	1:0:554:G:H5'	1.94	0.68
1:0:1666:C:H2'	1:0:1667:A:H8	1.59	0.68



	t i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:2890:A:H5"	1:0:2890:A:C8	2.26	0.68
1:0:74:A:H2'	1:0:75:U:C6	2.28	0.68
1:0:1313:A:H5"	24:V:113:GLY:CA	2.23	0.67
1:0:1730:G:H5'	1:0:1731:C:C5	2.30	0.67
1:0:162:C:H2'	1:0:163:U:H5'	1.76	0.67
1:0:2250:G:H2'	1:0:2251:G:C8	2.29	0.67
1:0:284:C:H1'	1:0:285:A:OP2	1.94	0.67
1:0:1116:U:O2'	1:0:1118:A:H2	1.70	0.67
1:0:1561:U:H2'	1:0:1562:C:H6	1.60	0.67
2:9:49:G:O2'	2:9:50:G:H5'	1.95	0.67
1:0:545:G:H5'	1:0:545:G:H8	1.60	0.67
1:0:1118:A:H3'	1:0:1118:A:H8	1.60	0.67
1:0:1158:G:O2'	1:0:1159:G:H5'	1.95	0.67
1:0:2251:G:H2'	1:0:2252:A:H8	1.58	0.66
1:0:1684:A:O2'	1:0:1685:A:H5"	1.94	0.66
1:0:681:G:H4'	1:0:682:A:O5'	1.95	0.66
1:0:337:A:H2	1:0:1314:U:O2'	1.76	0.66
1:0:544:G:C2'	1:0:545:G:H5"	2.26	0.66
1:0:285:A:N6	1:0:367:G:H1'	2.11	0.66
1:0:1667:A:H2'	1:0:1668:U:C6	2.31	0.66
1:0:960:G:N3	1:0:960:G:H2'	2.11	0.66
1:0:1701:A:H5"	1:0:1702:U:H3'	1.77	0.66
1:0:1130:U:H2'	1:0:1131:G:O4'	1.96	0.65
1:0:1106:A:H5'	1:0:1106:A:C8	2.29	0.65
1:0:1448:A:H5'	1:0:1507:C:OP1	1.96	0.65
1:0:289:G:O2'	1:0:290:C:H5'	1.96	0.65
1:0:2894:C:O2'	1:0:2895:C:H5'	1.97	0.65
1:0:95:A:C5'	1:0:96:A:H3'	2.27	0.65
1:0:1613:C:H2'	1:0:1614:G:O4'	1.96	0.65
1:0:285:A:H62	1:0:367:G:H1'	1.61	0.64
1:0:601:G:O2'	1:0:602:A:H5'	1.96	0.64
2:9:29:C:C2'	2:9:30:C:H5'	2.26	0.64
1:0:2670:G:O2'	1:0:2671:U:H5'	1.97	0.64
1:0:10:U:H1'	1:0:532:A:H62	1.63	0.64
1:0:1579:C:H2'	1:0:1580:A:C8	2.33	0.64
1:0:2598:U:H5"	10:H:36:GLY:CA	2.28	0.64
1:0:1217:G:H2'	1:0:1218:U:C6	2.33	0.64
1:0:1355:A:H4'	1:0:1355:A:OP1	1.98	0.64
1:0:1438:G:N2	1:0:1684:A:HO2'	1.95	0.64
1:0:2253:G:H2'	1:0:2254:G:H8	1.63	0.64
1:0:420:U:H2'	1:0:421:C:C6	2.33	0.64



	At and D	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:1766:U:O2	1:0:1778:A:H5'	1.98	0.64
1:0:1947:G:H2'	1:0:1948:G:H8	1.62	0.64
1:0:1778:A:H2'	1:0:1779:A:H5'	1.79	0.64
2:9:13:A:O2'	2:9:14:G:H5"	1.98	0.63
2:9:25:G:O2'	2:9:26:C:H5'	1.98	0.63
1:0:350:C:O2'	1:0:351:G:H5'	1.99	0.63
1:0:1118:A:H3'	1:0:1118:A:C8	2.32	0.63
1:0:349:U:O2'	1:0:350:C:H5'	1.98	0.63
1:0:362:G:H2'	1:0:363:A:C8	2.33	0.63
1:0:372:A:H2'	1:0:373:G:H8	1.64	0.63
1:0:582:C:H2'	1:0:583:G:H8	1.64	0.63
1:0:1947:G:H2'	1:0:1948:G:C8	2.34	0.63
1:0:2908:A:H2'	1:0:2909:G:O4'	1.98	0.63
1:0:795:G:H1'	1:0:818:A:N6	2.14	0.63
2:9:107:C:H2'	2:9:108:C:C6	2.34	0.63
1:0:646:G:H2'	1:0:647:U:C6	2.34	0.62
1:0:432:G:O2'	1:0:433:C:H5'	1.99	0.62
1:0:538:C:H5"	1:0:539:G:C8	2.34	0.62
1:0:1438:G:N2	1:0:1684:A:O2'	2.31	0.62
1:0:1525:G:H5'	1:0:1526:A:OP2	1.99	0.62
2:9:92:G:H2'	2:9:93:A:C8	2.33	0.62
1:0:2849:U:O2'	1:0:2850:C:OP2	2.17	0.62
2:9:55:U:H4'	2:9:56:A:O5'	1.99	0.62
1:0:613:C:H2'	1:0:614:U:H6	1.64	0.62
1:0:1211:G:O2'	1:0:1212:C:H5'	1.98	0.62
1:0:1450:C:O2'	1:0:1493:A:H2'	1.99	0.62
1:0:2266:A:H2'	1:0:2267:G:C8	2.35	0.62
1:0:2289:G:H21	1:0:2291:A:H2	1.47	0.62
1:0:2387:U:H2'	1:0:2388:C:C6	2.35	0.62
1:0:1474:C:H5'	1:0:1474:C:H6	1.65	0.62
1:0:702:G:O2'	1:0:703:G:H5'	2.00	0.62
1:0:2591:C:H2'	1:0:2592:G:O4'	1.99	0.62
2:9:20:G:O2'	2:9:21:G:H5'	1.99	0.62
1:0:999:C:H2'	1:0:1000:C:C6	2.35	0.61
1:0:2316:G:OP1	1:0:2316:G:C4'	2.47	0.61
1:0:671:A:O2'	1:0:672:G:H2'	2.00	0.61
1:0:625:U:H5"	1:0:1044:C:N4	2.15	0.61
1:0:2502:C:C2'	1:0:2503:A:H5'	2.30	0.61
1:0:1741:U:H5'	1:0:1742:A:OP1	2.01	0.61
2:9:22:G:O3'	2:9:23:U:H4'	2.01	0.61
1:0:968:G:O2'	1:0:969:G:H5'	2.00	0.61



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
1:0:2504:A:H2'	1:0:2505:G:O4'	2.01	0.61
1:0:283:U:C5	1:0:284:C:N4	2.68	0.61
1:0:2533:C:H6	1:0:2533:C:H5'	1.66	0.61
1:0:1120:U:H5'	1:0:1121:G:OP2	2.00	0.61
1:0:283:U:H3'	1:0:284:C:C5	2.35	0.60
1:0:1477:C:H5'	1:0:1868:G:C5'	2.31	0.60
1:0:1714:C:O2'	1:0:1715:C:H5'	2.00	0.60
1:0:255:A:H2'	1:0:256:C:C6	2.36	0.60
1:0:1149:U:O2'	1:0:1150:A:OP2	2.15	0.60
1:0:796:A:H62	1:0:817:G:H1'	1.64	0.60
1:0:2506:A:O2'	1:0:2507:G:C8	2.40	0.60
1:0:1528:A:H2'	1:0:1529:G:O4'	2.01	0.60
1:0:1377:C:H6	1:0:1377:C:H5'	1.66	0.60
1:0:1856:C:O2'	1:0:1857:A:OP2	2.19	0.60
1:0:2112:A:H2'	1:0:2113:G:C8	2.37	0.59
1:0:256:C:H2'	1:0:257:G:O4'	2.03	0.59
1:0:2240:U:O2'	1:0:2241:C:H5'	2.02	0.59
1:0:283:U:H5"	1:0:284:C:OP2	2.02	0.59
1:0:1557:G:O2'	1:0:1558:C:H5'	2.02	0.59
1:0:1636:G:O2'	1:0:1637:A:H5'	2.02	0.59
2:9:91:C:H2'	2:9:92:G:O4'	2.03	0.59
1:0:367:G:O2'	1:0:368:C:O5'	2.16	0.59
1:0:2488:A:H61	1:0:2534:C:H42	1.50	0.59
1:0:372:A:H2'	1:0:373:G:C8	2.38	0.59
1:0:599:G:O2'	1:0:600:G:H5'	2.03	0.59
1:0:795:G:C2'	1:0:817:G:N2	2.64	0.59
1:0:1506:U:H6	1:0:1506:U:H5'	1.67	0.59
1:0:2900:G:H2'	1:0:2901:C:O4'	2.02	0.59
1:0:1342:C:O2'	1:0:1343:C:H5'	2.03	0.59
1:0:1964:U:H2'	1:0:1965:C:C6	2.38	0.59
1:0:2507:G:H2'	1:0:2510:C:H42	1.67	0.59
1:0:1515:A:H2'	1:0:1516:C:C6	2.38	0.59
1:0:74:A:H2'	1:0:75:U:H6	1.67	0.59
1:0:290:C:O2'	1:0:291:C:H5'	2.03	0.59
1:0:820:G:H4'	1:0:856:G:H5'	1.84	0.59
1:0:2361:A:H2'	1:0:2362:A:C8	2.37	0.59
1:0:63:U:O2'	1:0:64:G:H5'	2.02	0.58
1:0:219:G:OP2	1:0:220:C:H5"	2.03	0.58
1:0:1280:A:H3'	1:0:1280:A:OP1	2.03	0.58
1:0:279:C:O2'	1:0:280:C:H5'	2.03	0.58
1:0:514:G:H3'	1:0:514:G:OP1	2.02	0.58



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:0:945:U:H2'	1:0:946:C:H6	1.69	0.58
1:0:2697:A:H2'	1:0:2698:G:O4'	2.03	0.58
1:0:1730:G:H5'	1:0:1731:C:C6	2.38	0.58
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.58
2:9:28:U:H5"	2:9:28:U:H6	1.68	0.58
1:0:1579:C:H2'	1:0:1580:A:H8	1.68	0.58
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.58
1:0:1804:A:H2'	1:0:1805:G:C8	2.39	0.58
1:0:1064:U:H2'	1:0:1065:G:C8	2.39	0.58
1:0:2907:C:H2'	1:0:2908:A:O4'	2.04	0.58
1:0:1497:G:H4'	1:0:1627:G:O2'	2.03	0.58
1:0:2866:U:H4'	1:0:2867:G:C5'	2.32	0.58
1:0:282:C:O2'	1:0:283:U:H4'	2.03	0.58
1:0:574:C:O2'	1:0:575:G:H5'	2.03	0.58
1:0:803:C:O2'	1:0:804:C:H5'	2.03	0.58
1:0:2679:G:H2'	1:0:2681:A:OP2	2.03	0.58
1:0:2819:C:H2'	1:0:2820:A:C8	2.38	0.58
1:0:945:U:H2'	1:0:946:C:C6	2.38	0.58
1:0:2780:C:H2'	1:0:2781:U:C6	2.38	0.58
2:9:22:G:O3'	2:9:23:U:C4'	2.52	0.58
1:0:795:G:C2'	1:0:817:G:H22	2.08	0.57
4:B:36:PRO:CA	4:B:167:GLY:CA	2.82	0.57
1:0:1477:C:O2'	1:0:1478:U:H5'	2.03	0.57
1:0:1522:A:O2'	1:0:1523:G:H5'	2.05	0.57
1:0:1805:G:H2'	1:0:1806:G:H8	1.68	0.57
1:0:195:C:H2'	1:0:196:G:H5'	1.84	0.57
1:0:703:G:O2'	1:0:704:C:H5'	2.04	0.57
1:0:2699:A:H2'	1:0:2700:G:O4'	2.05	0.57
1:0:1667:A:H2'	1:0:1668:U:H6	1.68	0.57
1:0:561:G:H2'	1:0:562:A:H8	1.67	0.57
1:0:807:A:H2'	1:0:808:A:O4'	2.03	0.57
1:0:1313:A:OP1	24:V:113:GLY:CA	2.53	0.57
1:0:2526:C:O2'	1:0:2527:U:H5'	2.05	0.57
1:0:2748:G:O2'	1:0:2749:U:OP2	2.20	0.57
2:9:14:G:H5'	2:9:14:G:C8	2.39	0.57
1:0:1147:C:H2'	1:0:1148:C:C5'	2.26	0.57
1:0:1562:C:H3'	1:0:1563:G:C8	2.40	0.57
2:9:26:C:O2'	2:9:27:C:H5'	2.05	0.57
1:0:1214:G:HO2'	1:0:1215:A:H8	1.52	0.57
1:0:1304:U:H2'	1:0:1305:C:C6	2.40	0.57
2:9:29:C:H2'	2:9:30:C:C5'	2.34	0.57



	r sjonn	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:396:U:O2'	1:0:418:C:H4'	2.05	0.56
1:0:660:A:H4'	1:0:661:G:O5'	2.04	0.56
1:0:1333:U:H2'	1:0:1334:C:C6	2.40	0.56
1:0:598:C:H2'	1:0:599:G:H8	1.70	0.56
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.56
1:0:566:A:H2'	1:0:567:U:O4'	2.06	0.56
1:0:1438:G:H21	1:0:1685:A:H8	1.52	0.56
1:0:1556:G:O2'	1:0:1557:G:H5'	2.05	0.56
1:0:1577:U:O2'	1:0:1578:C:H5'	2.05	0.56
1:0:1950:G:HO2'	1:0:1951:G:C5'	2.18	0.56
1:0:2414:A:H2'	1:0:2415:A:C8	2.40	0.56
1:0:2825:C:H4'	1:0:2826:G:O5'	2.05	0.56
1:0:1056:U:H2'	1:0:1057:A:O4'	2.05	0.56
1:0:1682:A:H2	1:0:1696:U:N3	1.89	0.56
1:0:281:U:O2'	1:0:282:C:H5'	2.05	0.56
1:0:326:G:O2'	1:0:327:A:H5'	2.05	0.56
1:0:1586:G:O2'	1:0:1587:U:H5'	2.06	0.56
1:0:1641:A:C2'	1:0:1642:A:H5'	2.35	0.56
1:0:1666:C:H2'	1:0:1667:A:C8	2.41	0.56
1:0:2814:A:OP2	1:0:2814:A:H3'	2.05	0.56
1:0:1214:G:H4'	1:0:1215:A:OP1	2.06	0.56
1:0:1555:G:O2'	1:0:1556:G:P	2.64	0.56
1:0:1735:C:O2'	1:0:1736:A:H5'	2.06	0.56
1:0:560:C:O2'	1:0:561:G:H5'	2.06	0.55
1:0:1250:C:O2'	1:0:1251:C:H5'	2.05	0.55
1:0:2468:A:H4'	1:0:2469:A:OP1	2.06	0.55
1:0:1072:G:O2'	1:0:1073:A:H8	1.89	0.55
1:0:37:A:H2'	1:0:38:G:H8	1.70	0.55
1:0:1210:G:O2'	1:0:1211:G:H5'	2.06	0.55
1:0:1523:G:C6	1:0:1524:U:O4	2.60	0.55
2:9:59:C:H2'	2:9:60:C:C6	2.40	0.55
1:0:1289:C:O2'	1:0:1290:G:H5'	2.07	0.55
1:0:303:C:O2'	1:0:304:G:H5'	2.06	0.55
1:0:684:G:H2'	1:0:685:C:C6	2.41	0.55
1:0:1438:G:N2	1:0:1685:A:C8	2.73	0.55
1:0:1515:A:H2'	1:0:1516:C:H6	1.69	0.55
1:0:1450:C:H4'	1:0:1451:C:OP2	2.06	0.55
1:0:1697:G:O2'	1:0:1698:U:H5'	2.05	0.55
1:0:137:U:H2'	1:0:139:C:C5	2.41	0.55
1:0:138:U:H6	1:0:140:G:N1	2.03	0.55
1:0:1909:A:H2'	1:0:1910:A:C8	2.42	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:1014:A:H2'	1:0:1015:C:H5'	1.88	0.55
1:0:1495:C:H2'	1:0:1496:G:C8	2.42	0.55
1:0:2072:G:C6	1:0:2533:C:H1'	2.42	0.55
1:0:370:G:O2'	1:0:371:U:H5'	2.07	0.54
1:0:817:G:O2'	1:0:818:A:H8	1.90	0.54
1:0:2692:G:H8	1:0:2693:U:C5	2.25	0.54
1:0:1450:C:O2'	1:0:1494:A:H5'	2.07	0.54
1:0:1761:U:H2'	1:0:1762:C:C6	2.42	0.54
1:0:2016:U:H2'	1:0:2017:U:C6	2.42	0.54
1:0:2237:G:H1'	1:0:2238:A:C8	2.42	0.54
1:0:2250:G:H2'	1:0:2251:G:H8	1.72	0.54
2:9:103:A:H2'	2:9:104:A:H8	1.71	0.54
1:0:1123:A:C2	1:0:1129:C:H4'	2.43	0.54
1:0:1367:A:H2'	1:0:1368:U:O4'	2.08	0.54
1:0:1804:A:H2'	1:0:1805:G:H8	1.71	0.54
1:0:2237:G:O2'	1:0:2238:A:C8	2.60	0.54
1:0:2769:C:H2'	1:0:2770:G:O4'	2.07	0.54
1:0:2795:C:O2'	1:0:2796:U:H5'	2.08	0.54
1:0:1088:A:H1'	1:0:1260:G:H21	1.72	0.54
1:0:2718:C:H5'	1:0:2718:C:H6	1.73	0.54
2:9:2:U:O5'	2:9:3:A:H5'	2.07	0.54
1:0:1730:G:C6	23:U:18:ARG:CA	2.90	0.54
1:0:2291:A:C8	1:0:2309:C:H5'	2.42	0.54
1:0:344:C:H2'	1:0:345:G:O4'	2.08	0.54
1:0:889:C:H2'	1:0:890:C:C6	2.43	0.54
1:0:1741:U:O2'	1:0:2723:G:H4'	2.08	0.54
1:0:2717:C:H2'	1:0:2718:C:C5'	2.32	0.54
1:0:37:A:H2'	1:0:38:G:C8	2.43	0.53
1:0:88:G:H2'	1:0:89:G:C8	2.43	0.53
1:0:1423:C:O2'	1:0:1424:A:H5'	2.08	0.53
1:0:1965:C:H6	1:0:1965:C:O5'	1.90	0.53
1:0:2681:A:N6	1:0:2714:U:H4'	2.22	0.53
1:0:597:A:O2'	1:0:598:C:H5'	2.09	0.53
1:0:1220:U:H2'	1:0:1221:G:H8	1.73	0.53
1:0:1327:G:N2	1:0:1329:A:H3'	2.23	0.53
1:0:1603:A:H5'	1:0:1605:G:O4'	2.07	0.53
1:0:1790:C:H2'	1:0:1791:U:H6	1.72	0.53
1:0:2463:A:O2'	1:0:2464:C:OP1	2.23	0.53
1:0:695:C:H2'	1:0:696:C:C6	2.43	0.53
1:0:1933:G:O2'	1:0:1934:A:H5'	2.08	0.53
1:0:1972:U:C2'	1:0:1973:A:H5'	2.37	0.53



Atom-1	Atom-2	Interatomic	Clash
1.0.0051.0.002		distance (A)	overlap (A)
1:0:2051:G:O2'	1:0:2052:0:H5 <sup>7</sup>	2.08	0.53
1:0:2912:C:H2 <sup>7</sup>	1:0:2913:A:04 <sup>7</sup>	2.09	0.53
1:0:367:G:H4	1:0:368:C:OP1	2.07	0.53
1:0:1925:G:O2'	1:0:1926:G:H5′	2.09	0.53
1:0:881:C:OP1	1:0:883:U:H5	1.90	0.53
1:0:1245:C:H6	1:0:1245:C:O5'	1.90	0.53
1:0:790:A:H2'	1:0:791:A:O4'	2.09	0.53
1:0:1118:A:C8	1:0:1118:A:C3'	2.92	0.53
1:0:1218:U:H2'	1:0:1219:U:C6	2.44	0.53
1:0:1477:C:H5'	1:0:1868:G:H5"	1.90	0.53
1:0:2250:G:N2	1:0:2251:G:H1'	2.22	0.53
1:0:187:A:H3'	1:0:188:C:C6	2.43	0.53
1:0:646:G:H2'	1:0:647:U:H6	1.73	0.53
1:0:1116:U:O2'	1:0:1118:A:C2	2.46	0.53
1:0:413:G:H2'	1:0:414:C:C6	2.44	0.53
1:0:820:G:H5'	1:0:821:U:H5'	1.90	0.53
1:0:204:A:C2'	1:0:205:U:H5'	2.39	0.52
1:0:873:G:H21	1:0:876:A:H62	1.56	0.52
1:0:2692:G:C8	1:0:2693:U:H5	2.26	0.52
1:0:2866:U:O2'	1:0:2867:G:P	2.67	0.52
1:0:282:C:H1'	1:0:368:C:H42	1.68	0.52
1:0:1098:A:H2'	1:0:1099:G:O4'	2.10	0.52
1:0:1471:A:H2'	1:0:1472:C:C6	2.43	0.52
1:0:2858:U:H2'	1:0:2859:C:C6	2.44	0.52
1:0:236:A:H4'	1:0:237:G:OP1	2.10	0.52
1:0:282:C:O2'	1:0:283:U:C4'	2.57	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.74	0.52
1:0:1588:G:C6	1:0:1589:G:N1	2.77	0.52
2:9:23:U:H3	2:9:54:A:H5"	1.74	0.52
1:0:503:G:H2'	1:0:504:G:H8	1.74	0.52
1:0:666:A:H2'	1:0:667:C:O4'	2.09	0.52
1:0:737:A:H2'	1:0:738:G:O4'	2.10	0.52
1:0:1117:A:N1	1:0:1244:U:H2'	2.23	0.52
1:0:280:C:O2'	1:0:281:U:H5'	2.10	0.52
1:0:484:A:N1	1:0:506:G:H4'	2.24	0.52
1:0:1398:G:H2'	1:0:1399:A:C8	2.44	0.52
1:0:1589:G:H22	1:0:1605:G:H2'	1.73	0.52
1:0:1950:G:O2'	1:0:1951:G:O5'	2.23	0.52
1:0:282:C:H2'	1:0:283:U:O4'	2.09	0.52
1:0:1309:U:H2'	1:0:1310:U:C5'	2.40	0.52
1:0:1835:U:C5	1:0:1840:A:N7	2.69	0.52



	<b>1 1 1</b>	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:2472:C:O2'	1:0:2634:G:H4'	2.10	0.52
1:0:2909:G:O2'	1:0:2910:A:C5'	2.56	0.52
1:0:1132:A:N6	1:0:1229:C:H2'	2.24	0.52
1:0:2768:A:C2'	1:0:2769:C:O4'	2.51	0.52
1:0:817:G:O2'	1:0:818:A:C8	2.62	0.52
1:0:1066:U:H2'	1:0:1067:A:C8	2.45	0.52
1:0:1591:A:H4'	1:0:1592:G:O5'	2.09	0.52
1:0:2345:A:OP1	1:0:2346:C:H5	1.92	0.52
1:0:2597:U:H2'	1:0:2598:U:H5'	1.91	0.52
2:9:107:C:H2'	2:9:108:C:H6	1.75	0.52
1:0:2727:A:H2'	1:0:2728:C:H5'	1.92	0.51
1:0:1060:C:H2'	1:0:1061:C:H6	1.75	0.51
1:0:1561:U:H2'	1:0:1562:C:C6	2.44	0.51
1:0:2906:A:H5'	1:0:2907:C:O4'	2.10	0.51
1:0:249:G:O2'	1:0:250:C:H5'	2.11	0.51
1:0:2791:U:H1'	1:0:2792:A:H5"	1.92	0.51
1:0:289:G:N2	1:0:363:A:C2	2.61	0.51
1:0:612:U:H2'	1:0:613:C:C6	2.45	0.51
1:0:1616:A:H2'	1:0:1618:G:C8	2.46	0.51
1:0:2667:G:O2'	1:0:2668:G:H5'	2.10	0.51
1:0:842:C:O2	1:0:1693:A:H2'	2.11	0.51
1:0:2445:U:H2'	1:0:2446:G:C8	2.46	0.51
1:0:2509:A:OP2	1:0:2510:C:H5	1.92	0.51
1:0:272:A:C2	1:0:369:G:H5"	2.46	0.51
1:0:1042:U:O2'	1:0:1043:C:H5'	2.10	0.51
2:9:106:C:O2'	2:9:107:C:H5'	2.11	0.51
1:0:289:G:N1	1:0:363:A:C2	2.77	0.51
1:0:581:G:O2'	1:0:582:C:H5'	2.11	0.51
1:0:1008:C:H2'	1:0:1009:U:C6	2.45	0.51
1:0:1099:G:OP1	2:9:87:U:H2'	2.11	0.51
1:0:1790:C:H2'	1:0:1791:U:C6	2.45	0.51
1:0:1804:A:O2'	1:0:1805:G:H5'	2.10	0.51
2:9:114:G:H2'	2:9:115:C:C6	2.46	0.51
1:0:255:A:H2'	1:0:256:C:H6	1.73	0.51
1:0:559:U:O2'	1:0:560:C:H5'	2.10	0.51
1:0:1217:G:H2'	1:0:1218:U:H6	1.75	0.51
2:9:64:C:C2'	2:9:65:A:H5'	2.41	0.51
1:0:1386:G:O2'	1:0:1387:G:H5'	2.11	0.51
1:0:1909:A:N1	1:0:2128:G:H1'	2.26	0.51
1:0:2242:U:O2'	1:0:2243:C:O5'	2.29	0.51
1:0:834:G:H3'	1:0:835:U:H4'	1.92	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:2564:G:OP2	1:0:2565:C:H5"	2.11	0.50
1:0:939:A:H4'	1:0:940:G:O5'	2.11	0.50
1:0:1132:A:H2'	1:0:1133:A:C8	2.46	0.50
1:0:941:G:O2'	1:0:942:U:H5'	2.12	0.50
1:0:1006:A:H2'	1:0:1007:A:C8	2.47	0.50
1:0:1072:G:O2'	1:0:1073:A:P	2.69	0.50
1:0:553:G:C2'	1:0:554:G:H5'	2.42	0.50
1:0:2348:C:O2'	1:0:2349:G:H5'	2.11	0.50
2:9:103:A:O2'	2:9:104:A:H5'	2.10	0.50
1:0:2064:U:H5'	1:0:2652:U:O3'	2.12	0.50
1:0:2578:G:H5'	1:0:2578:G:H8	1.76	0.50
1:0:2766:A:O2'	1:0:2767:C:H5'	2.11	0.50
1:0:291:C:H2'	1:0:292:G:O4'	2.12	0.50
1:0:555:U:OP2	1:0:555:U:H6	1.95	0.50
1:0:1730:G:H4'	1:0:1731:C:O5'	2.12	0.50
1:0:2300:A:H4'	1:0:2301:A:O5'	2.12	0.50
1:0:1072:G:H1'	1:0:1088:A:N6	2.27	0.50
1:0:485:A:O2'	1:0:487:G:H5'	2.11	0.50
1:0:848:C:H2'	1:0:849:C:C6	2.46	0.50
1:0:1342:C:C2'	1:0:1343:C:H5'	2.41	0.50
1:0:2133:U:H4'	1:0:2134:G:H5'	1.93	0.50
2:9:52:A:O2'	2:9:53:G:H5'	2.12	0.50
1:0:2515:C:C2'	1:0:2516:G:H5'	2.43	0.49
1:0:2756:U:N3	1:0:2896:A:H2	2.09	0.49
2:9:25:G:H3'	2:9:25:G:OP1	2.12	0.49
1:0:195:C:C2'	1:0:196:G:H5'	2.42	0.49
1:0:1380:U:O2	1:0:1380:U:C2'	2.60	0.49
1:0:2242:U:O2'	1:0:2243:C:P	2.69	0.49
1:0:2726:U:O2	1:0:2749:U:O5'	2.30	0.49
1:0:969:G:H2'	1:0:970:U:C6	2.48	0.49
1:0:2502:C:H2'	1:0:2503:A:H5'	1.93	0.49
1:0:2681:A:C6	1:0:2714:U:H4'	2.48	0.49
1:0:10:U:O2'	1:0:11:A:P	2.69	0.49
1:0:496:G:H4'	1:0:497:A:OP1	2.12	0.49
1:0:1887:U:H2'	1:0:1888:C:C6	2.48	0.49
1:0:2290:U:H4'	1:0:2291:A:OP1	2.12	0.49
1:0:2656:G:O2'	1:0:2657:G:H5'	2.12	0.49
2:9:42:C:H5'	2:9:43:G:OP2	2.12	0.49
1:0:284:C:H1'	1:0:285:A:P	2.52	0.49
1:0:604:G:H4'	1:0:605:C:O5'	2.11	0.49
1:0:2381:C:H2'	1:0:2382:A:C8	2.48	0.49



	At 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:2765:C:H2'	1:0:2766:A:C8	2.48	0.49
1:0:629:A:H2'	1:0:630:A:O4'	2.13	0.49
1:0:1461:U:H2'	1:0:1462:C:C6	2.48	0.49
1:0:2903:C:O2'	1:0:2904:U:H5'	2.12	0.49
1:0:44:G:H21	1:0:45:A:H62	1.60	0.49
1:0:639:A:H2'	1:0:640:G:C8	2.47	0.49
1:0:939:A:O2'	1:0:940:G:OP2	2.30	0.49
1:0:1309:U:C2'	1:0:1310:U:H5'	2.42	0.49
2:9:102:G:O2'	2:9:103:A:H5'	2.13	0.49
1:0:1477:C:C5'	1:0:1868:G:H5"	2.43	0.49
1:0:199:A:C2'	1:0:200:U:H5"	2.43	0.49
1:0:1511:U:O2'	1:0:1512:G:H5'	2.13	0.49
1:0:2011:A:H4'	1:0:2012:U:O5'	2.13	0.49
1:0:2242:U:O2'	1:0:2243:C:C6	2.63	0.49
1:0:2782:G:O6	1:0:2790:C:H5"	2.13	0.49
1:0:2842:G:H2'	1:0:2843:A:H5'	1.95	0.49
2:9:103:A:H2'	2:9:104:A:C8	2.48	0.49
1:0:1946:C:H2'	1:0:1971:G:C8	2.47	0.48
1:0:2883:A:H2'	1:0:2884:G:O4'	2.13	0.48
1:0:2912:C:O2'	1:0:2913:A:H5'	2.12	0.48
1:0:907:A:H2'	1:0:908:A:H8	1.77	0.48
1:0:1072:G:O2'	1:0:1073:A:C8	2.66	0.48
1:0:1669:A:H2'	1:0:1670:G:H8	1.72	0.48
1:0:2279:G:N2	1:0:2463:A:H1'	2.28	0.48
1:0:2329:C:O2'	1:0:2330:U:H5'	2.12	0.48
1:0:2804:C:H2'	1:0:2805:A:O4'	2.12	0.48
1:0:322:G:O2'	1:0:323:C:H5'	2.14	0.48
1:0:887:G:H2'	1:0:888:U:C6	2.48	0.48
1:0:1568:G:O2'	1:0:1569:U:H5'	2.12	0.48
1:0:2266:A:H2'	1:0:2267:G:H8	1.79	0.48
1:0:2473:U:O3'	1:0:2474:A:H3'	2.14	0.48
1:0:352:A:H2'	1:0:353:G:C8	2.49	0.48
1:0:1000:C:H2'	1:0:1001:U:O4'	2.13	0.48
1:0:1140:C:O2'	1:0:1141:U:H5'	2.14	0.48
1:0:1209:C:O2'	1:0:1210:G:H5'	2.12	0.48
1:0:1214:G:O2'	1:0:1215:A:H8	1.96	0.48
1:0:1257:C:H2'	1:0:1258:G:O4'	2.14	0.48
1:0:1425:G:O2'	1:0:1426:C:H5'	2.13	0.48
1:0:1624:A:O2'	1:0:1625:U:P	2.71	0.48
1:0:1657:A:H2'	1:0:1658:A:C8	2.49	0.48
1:0:2103:A:N7	1:0:2538:A:N1	2.62	0.48



	1 · · · · ·	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:9:108:C:O2'	2:9:109:G:H5'	2.14	0.48
1:0:197:C:OP2	1:0:198:A:H8	1.97	0.48
1:0:938:G:HO2'	1:0:939:A:H8	1.54	0.48
1:0:1329:A:H2'	1:0:1330:A:C8	2.48	0.48
1:0:1773:G:N2	1:0:1774:G:C8	2.82	0.48
1:0:1950:G:O2'	1:0:1951:G:P	2.71	0.48
1:0:2387:U:H2'	1:0:2388:C:H6	1.77	0.48
1:0:1120:U:C6	1:0:1120:U:H5"	2.48	0.48
1:0:1503:U:H2'	1:0:1504:A:O4'	2.13	0.48
1:0:1662:C:H2'	1:0:1663:G:O4'	2.14	0.48
1:0:2886:C:O2'	1:0:2887:G:H5'	2.13	0.48
1:0:162:C:C2'	1:0:163:U:H5'	2.43	0.48
1:0:353:G:O2'	1:0:354:A:H5'	2.14	0.48
1:0:440:C:H2'	1:0:441:A:C8	2.48	0.48
1:0:555:U:OP2	1:0:555:U:C6	2.67	0.48
1:0:598:C:O2'	1:0:599:G:H5'	2.13	0.48
1:0:1805:G:H2'	1:0:1806:G:C8	2.47	0.48
1:0:2074:A:H4'	1:0:2075:G:OP1	2.13	0.48
1:0:116:G:H5'	1:0:129:A:H2'	1.94	0.48
1:0:557:C:O2'	1:0:558:C:H5'	2.14	0.48
1:0:1153:C:O2'	1:0:1154:A:H5'	2.14	0.48
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.48
1:0:12:U:C2'	1:0:13:G:H5'	2.43	0.47
1:0:284:C:OP2	1:0:284:C:H6	1.95	0.47
1:0:1463:A:H2'	1:0:1464:U:C6	2.48	0.47
1:0:2252:A:H2'	1:0:2253:G:O4'	2.14	0.47
1:0:2353:A:H4'	1:0:2354:A:O5'	2.14	0.47
1:0:544:G:H2'	1:0:545:G:C5'	2.44	0.47
1:0:958:G:H2'	1:0:959:C:C6	2.49	0.47
1:0:2257:G:H4'	1:0:2259:C:C2	2.49	0.47
1:0:2264:A:H2'	1:0:2265:U:C6	2.48	0.47
1:0:2381:C:H2'	1:0:2382:A:H8	1.79	0.47
1:0:2836:G:H4'	1:0:2837:U:OP1	2.14	0.47
1:0:393:G:O2'	1:0:394:G:H5'	2.15	0.47
1:0:1119:G:N2	1:0:1246:A:N1	2.62	0.47
1:0:2692:G:H8	1:0:2693:U:H5	1.61	0.47
2:9:3:A:N7	2:9:25:G:N2	2.62	0.47
1:0:613:C:H2'	1:0:614:U:C6	2.48	0.47
1:0:2372:A:H2'	1:0:2373:U:C6	2.50	0.47
1:0:2748:G:H4'	1:0:2749:U:H5'	1.96	0.47
1:0:1791:U:O2'	1:0:1792:C:H5'	2.13	0.47



	i i i i i i i i i i i i i i i i i i i	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:2320:U:H4'	1:0:2321:A:O4'	2.15	0.47
1:0:2385:G:H2'	1:0:2386:U:C6	2.50	0.47
1:0:2842:G:C2'	1:0:2843:A:H5'	2.45	0.47
1:0:2885:A:H2'	1:0:2886:C:H6	1.78	0.47
1:0:425:U:O2'	1:0:426:G:H5'	2.15	0.47
1:0:795:G:H21	1:0:817:G:H2'	1.78	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.30	0.47
1:0:1865:A:H2'	1:0:1866:A:C8	2.50	0.47
1:0:2238:A:C2'	1:0:2239:C:H5'	2.45	0.47
1:0:2415:A:H2'	1:0:2416:G:H5'	1.95	0.47
1:0:2697:A:H2'	1:0:2698:G:C8	2.50	0.47
1:0:35:U:H2'	1:0:36:C:C6	2.49	0.47
1:0:101:C:O2'	1:0:102:A:H5'	2.13	0.47
1:0:136:C:H2'	1:0:137:U:O4'	2.14	0.47
1:0:506:G:H22	1:0:509:A:H5"	1.80	0.47
1:0:817:G:HO2'	1:0:818:A:H8	1.49	0.47
1:0:940:G:O2'	1:0:941:G:H5'	2.15	0.47
1:0:1160:G:H21	1:0:1207:A:H62	1.63	0.47
1:0:1948:G:O2'	1:0:1949:G:H5'	2.14	0.47
1:0:2326:U:H2'	1:0:2327:A:C8	2.49	0.47
1:0:2672:C:H2'	1:0:2673:U:H6	1.79	0.47
2:9:96:C:H2'	2:9:97:U:C6	2.50	0.47
1:0:637:C:H2'	1:0:638:C:C6	2.50	0.47
1:0:1127:C:OP1	1:0:1128:U:H5	1.96	0.47
1:0:1355:A:OP1	1:0:1355:A:C4'	2.63	0.47
1:0:1605:G:C8	1:0:1605:G:H5"	2.50	0.47
1:0:1730:G:C5'	1:0:1731:C:C6	2.97	0.47
1:0:2511:A:H5'	1:0:2511:A:H8	1.80	0.47
1:0:2897:C:O2'	1:0:2898:G:H5'	2.15	0.47
1:0:197:C:OP2	1:0:198:A:C8	2.68	0.47
1:0:1447:U:H3'	1:0:1506:U:O2	2.14	0.47
1:0:1544:U:O2'	1:0:1545:C:H5'	2.15	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
1:0:2350:G:O2'	1:0:2351:C:H5'	2.14	0.47
1:0:2398:A:H2'	1:0:2399:G:O4'	2.14	0.47
1:0:550:C:O2'	1:0:551:A:H5'	2.14	0.47
1:0:1015:C:H2'	1:0:1016:U:C6	2.50	0.47
1:0:1218:U:H2'	1:0:1219:U:H6	1.80	0.47
1:0:1878:G:O2'	1:0:1879:U:OP2	2.32	0.47
1:0:438:C:O2'	1:0:439:A:OP1	2.30	0.46
1:0:90:A:H2'	1:0:91:G:O4'	2.14	0.46



	A h a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:284:C:C1'	1:0:285:A:OP2	2.61	0.46
1:0:506:G:N2	1:0:509:A:H5'	2.21	0.46
1:0:508:A:H2'	1:0:509:A:H5"	1.96	0.46
1:0:946:C:H2'	1:0:947:U:C6	2.51	0.46
1:0:1109:U:OP1	1:0:1110:G:H5"	2.15	0.46
1:0:1309:U:H2'	1:0:1310:U:H5'	1.96	0.46
1:0:1321:A:H2'	1:0:1322:G:C8	2.50	0.46
1:0:1552:G:H2'	1:0:1553:C:C6	2.49	0.46
1:0:1603:A:H4'	1:0:1604:G:OP2	2.14	0.46
1:0:2005:G:OP2	1:0:2005:G:H3'	2.14	0.46
1:0:2129:U:H2'	1:0:2130:C:C6	2.50	0.46
1:0:2589:U:H2'	1:0:2590:U:C6	2.50	0.46
1:0:293:A:O2'	1:0:294:C:H5'	2.16	0.46
1:0:681:G:O2'	1:0:682:A:OP2	2.29	0.46
1:0:2754:G:O2'	1:0:2755:G:H5'	2.15	0.46
1:0:1527:A:C2	1:0:1528:A:C5	3.03	0.46
1:0:2064:U:H5'	1:0:2652:U:H4'	1.98	0.46
1:0:702:G:HO2'	1:0:703:G:H5'	1.81	0.46
1:0:1496:G:H5'	1:0:1572:A:H1'	1.98	0.46
1:0:2004:U:H6	1:0:2004:U:O5'	1.99	0.46
1:0:354:A:H2'	1:0:355:C:C6	2.51	0.46
1:0:657:G:H2'	1:0:658:C:C6	2.51	0.46
1:0:999:C:O2'	1:0:1000:C:H5'	2.15	0.46
1:0:1825:U:O2'	1:0:1826:C:H5'	2.16	0.46
1:0:2105:C:H2'	1:0:2106:C:C6	2.51	0.46
1:0:18:C:H2'	1:0:19:U:C6	2.51	0.46
1:0:939:A:O2'	1:0:940:G:P	2.74	0.46
1:0:1345:A:H2'	1:0:1346:U:C6	2.51	0.46
1:0:1730:G:H5'	1:0:1731:C:H5	1.80	0.46
1:0:1947:G:N2	1:0:1966:U:C2	2.84	0.46
1:0:2000:G:O2'	1:0:2001:G:H5'	2.16	0.46
1:0:2073:G:OP2	1:0:2490:A:H5'	2.16	0.46
1:0:2251:G:C6	1:0:2252:A:C6	3.04	0.46
1:0:2430:A:N6	1:0:2460:A:H2	2.14	0.46
2:9:76:G:H3'	2:9:77:A:C5'	2.21	0.46
1:0:295:C:O2'	1:0:296:G:H5'	2.15	0.46
1:0:2866:U:O2'	1:0:2867:G:OP2	2.29	0.46
1:0:2911:C:O2'	1:0:2912:C:H5'	2.15	0.46
1:0:337:A:H2	1:0:1314:U:C2'	2.29	0.46
1:0:945:U:O2'	1:0:946:C:H5'	2.16	0.46
1:0:1114:A:H2'	1:0:1115:U:C6	2.51	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	$(\dot{A})$
1:0:1450:C:C4'	1.0.1451.C.OP2	2.64	0.46
1:0:2575:C:H2'	1:0:2576:A:O4'	2.16	0.46
1:0:2772:G:O2'	1:0:2773:G:H5'	2.15	0.46
1:0:2871:G:H2'	1:0:2872:U:C6	2.51	0.46
1:0:168:C:O2'	1:0:169:A:H5'	2.16	0.46
1:0:1114:A:H2'	1:0:1115:U:H6	1.80	0.46
1:0:1422:U:H2'	1:0:1423:C:C6	2.50	0.46
1:0:1607:A:H2'	1:0:1608:G:O4'	2.15	0.46
1:0:2831:C:H2'	1:0:2832:C:H5'	1.96	0.46
1:0:141:C:C2'	1:0:141:C:O2	2.63	0.45
1:0:279:C:H2'	1:0:280:C:H6	1.80	0.45
1:0:1080:C:O2'	1:0:1081:A:OP1	2.26	0.45
1:0:1586:G:H2'	1:0:1587:U:O4'	2.16	0.45
1:0:2255:A:H2'	1:0:2256:G:O4'	2.16	0.45
1:0:2456:A:H2'	1:0:2457:U:C6	2.51	0.45
1:0:2819:C:H2'	1:0:2820:A:H8	1.81	0.45
1:0:204:A:O2'	1:0:205:U:H5'	2.16	0.45
1:0:296:G:O2'	1:0:297:U:H5'	2.16	0.45
1:0:693:A:H2'	1:0:694:A:C8	2.51	0.45
1:0:1965:C:H2'	1:0:1966:U:C6	2.52	0.45
1:0:2653:A:H2'	1:0:2654:C:C6	2.51	0.45
1:0:2781:U:O2'	1:0:2782:G:H5'	2.16	0.45
1:0:2831:C:C2'	1:0:2832:C:H5'	2.46	0.45
1:0:40:C:O2'	1:0:41:G:H5'	2.16	0.45
1:0:747:G:H2'	1:0:748:C:C6	2.51	0.45
1:0:947:U:O2'	1:0:948:G:H5'	2.16	0.45
1:0:1315:G:H4'	1:0:1316:G:OP2	2.17	0.45
1:0:1573:A:H2'	1:0:1574:C:O4'	2.16	0.45
1:0:2074:A:O2'	1:0:2075:G:P	2.75	0.45
1:0:2416:G:H2'	1:0:2417:C:C6	2.52	0.45
1:0:2776:A:H2'	1:0:2777:G:O4'	2.16	0.45
1:0:2871:G:H2'	1:0:2872:U:H6	1.81	0.45
1:0:549:A:O2'	1:0:550:C:H5'	2.16	0.45
1:0:582:C:H2'	1:0:583:G:C8	2.48	0.45
1:0:683:G:O2'	1:0:684:G:H5'	2.16	0.45
1:0:696:C:O2'	1:0:731:U:OP1	2.34	0.45
1:0:728:C:H2'	1:0:729:C:H6	1.81	0.45
1:0:2251:G:C2	1:0:2252:A:C4	3.05	0.45
1:0:2429:A:H2'	1:0:2430:A:C8	2.51	0.45
1:0:274:G:O2'	1:0:275:G:H5'	2.17	0.45
1:0:1965:C:O2'	1:0:1966:U:H5'	2.16	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:2115:U:H2'	1:0:2116:U:C6	2.52	0.45
1:0:2242:U:H4'	1:0:2243:C:OP1	2.17	0.45
1:0:2729:C:O2'	1:0:2730:G:H5'	2.17	0.45
1:0:219:G:O2'	1:0:220:C:P	2.75	0.45
1:0:631:A:N3	1:0:2073:G:O2'	2.49	0.45
1:0:1535:G:H2'	1:0:1536:C:C6	2.52	0.45
1:0:1815:A:H2'	1:0:1816:C:O4'	2.17	0.45
1:0:2133:U:N3	1:0:2259:C:OP2	2.45	0.45
1:0:2499:U:O2'	1:0:2500:C:H5'	2.16	0.45
1:0:2765:C:H2'	1:0:2766:A:H8	1.82	0.45
1:0:2890:A:C2'	1:0:2891:A:OP2	2.65	0.45
2:9:55:U:O2'	2:9:56:A:OP2	2.26	0.45
1:0:695:C:H2'	1:0:696:C:H6	1.82	0.45
1:0:1526:A:H1'	1:0:1527:A:N7	2.32	0.45
1:0:1730:G:C5'	1:0:1731:C:H6	2.29	0.45
1:0:1928:C:H2'	1:0:1929:G:O4'	2.17	0.45
1:0:1978:A:O2'	1:0:1979:G:OP1	2.24	0.45
2:9:18:U:O2'	2:9:19:G:H5'	2.16	0.45
1:0:248:A:H5'	1:0:249:G:OP2	2.17	0.45
1:0:816:G:C6	1:0:817:G:N1	2.85	0.45
1:0:2112:A:H2'	1:0:2113:G:H8	1.79	0.45
1:0:2506:A:O2'	1:0:2507:G:O5'	2.34	0.45
2:9:95:C:O2'	2:9:96:C:H5'	2.17	0.45
1:0:305:A:C5	1:0:329:A:C2	3.05	0.45
1:0:956:G:H2'	1:0:957:A:O4'	2.17	0.45
1:0:1120:U:H5"	1:0:1120:U:H6	1.82	0.45
1:0:1283:G:O2'	1:0:1284:G:H5'	2.16	0.45
1:0:1406:A:H4'	1:0:1407:A:O5'	2.17	0.45
1:0:2672:C:O2'	1:0:2673:U:H5'	2.17	0.45
2:9:94:G:O2'	2:9:95:C:H5'	2.17	0.45
1:0:282:C:H3'	1:0:283:U:H5'	1.99	0.44
1:0:820:G:O2'	1:0:856:G:H4'	2.17	0.44
1:0:1116:U:H3	1:0:1246:A:H62	1.66	0.44
1:0:1327:G:C2	1:0:1329:A:H3'	2.53	0.44
1:0:2419:U:H5"	1:0:2420:G:H5'	1.99	0.44
1:0:141:C:O2	1:0:141:C:H2'	2.17	0.44
1:0:219:G:HO2'	1:0:220:C:P	2.40	0.44
1:0:438:C:O2'	1:0:439:A:P	2.75	0.44
1:0:638:C:H2'	1:0:639:A:C8	2.52	0.44
1:0:1118:A:H8	1:0:1119:G:H5"	1.83	0.44
1:0:1148:C:H6	1:0:1148:C:C5'	2.25	0.44



Interatomic Cla			
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:1433:G:O2'	1:0:1434:A:H5'	2.18	0.44
1:0:1496:G:H2'	1:0:1497:G:C8	2.52	0.44
1:0:1882:C:O2'	1:0:2012:U:OP2	2.33	0.44
1:0:2106:C:H2'	1:0:2107:U:C6	2.52	0.44
2:9:71:C:O2'	2:9:72:C:H5'	2.17	0.44
1:0:419:A:H1'	1:0:1921:A:C2	2.53	0.44
1:0:790:A:H1'	1:0:1710:A:H2'	1.99	0.44
1:0:920:C:H5"	1:0:921:G:O5'	2.17	0.44
1:0:1006:A:N1	1:0:2311:A:H1'	2.31	0.44
1:0:1902:G:H2'	1:0:1903:U:C6	2.51	0.44
1:0:1930:A:H2'	1:0:1931:A:C8	2.52	0.44
1:0:2688:U:O2'	1:0:2689:A:H5'	2.17	0.44
1:0:383:A:H2'	1:0:384:G:O4'	2.18	0.44
1:0:907:A:H2'	1:0:908:A:C8	2.51	0.44
1:0:1149:U:H4'	1:0:1150:A:H5"	1.98	0.44
1:0:1380:U:H5	1:0:2043:U:O2'	2.00	0.44
1:0:2388:C:O2'	1:0:2389:U:H5'	2.17	0.44
1:0:2515:C:H2'	1:0:2516:G:H5'	1.98	0.44
1:0:140:G:H3'	1:0:140:G:H8	1.83	0.44
1:0:324:G:O2'	1:0:325:U:H5'	2.18	0.44
1:0:2563:U:H2'	1:0:2565:C:O5'	2.16	0.44
1:0:270:U:O2'	1:0:271:C:P	2.75	0.44
1:0:319:A:H4'	1:0:338:C:C4	2.53	0.44
1:0:2279:G:C2	1:0:2463:A:H1'	2.53	0.44
2:9:35:C:H5'	2:9:36:C:OP2	2.18	0.44
2:9:52:A:C2'	2:9:53:G:H5'	2.48	0.44
1:0:766:A:O2'	1:0:767:A:H5"	2.18	0.44
1:0:1587:U:C4	1:0:1588:G:C6	3.06	0.44
1:0:2247:C:O2'	1:0:2248:C:H5'	2.18	0.44
1:0:2256:G:O2'	1:0:2257:G:H5'	2.17	0.44
1:0:2885:A:H2'	1:0:2886:C:C6	2.52	0.44
1:0:45:A:C8	1:0:45:A:H5'	2.53	0.44
1:0:212:A:O4'	1:0:214:U:C6	2.70	0.44
1:0:294:C:H2'	1:0:295:C:O4'	2.18	0.44
1:0:615:G:H2'	1:0:616:U:C6	2.52	0.44
1:0:858:U:H2'	1:0:859:C:H6	1.82	0.44
1:0:1517:U:O2'	1:0:1518:A:H5'	2.18	0.44
1:0:2846:C:H2'	1:0:2847:G:H8	1.82	0.44
1:0:95:A:H5"	1:0:96:A:C3'	2.45	0.44
1:0:105:G:O2'	1:0:106:A:H5'	2.18	0.44
1:0:243:A:H61	1:0:269:G:H1'	1.83	0.44



	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:1589:G:N2	1:0:1605:G:C2'	2.80	0.44
1:0:1739:G:O2'	1:0:1740:U:H5'	2.18	0.44
2:9:61:C:H2'	2:9:62:A:H8	1.83	0.44
1:0:219:G:H3'	1:0:220:C:C5'	2.45	0.43
1:0:401:C:H2'	1:0:402:U:C6	2.52	0.43
1:0:1141:U:O2'	1:0:1142:C:H5'	2.18	0.43
1:0:2372:A:H2'	1:0:2373:U:H6	1.83	0.43
1:0:283:U:H5	1:0:284:C:H41	1.66	0.43
1:0:343:C:O2'	1:0:344:C:H5'	2.18	0.43
1:0:1524:U:O2'	1:0:1525:G:P	2.76	0.43
1:0:1609:C:H2'	1:0:1610:G:H8	1.83	0.43
1:0:1761:U:H2'	1:0:1762:C:H6	1.82	0.43
1:0:1878:G:O2'	1:0:1879:U:C6	2.66	0.43
1:0:2074:A:O2'	1:0:2076:U:OP2	2.24	0.43
1:0:2312:G:C2'	1:0:2313:C:H5'	2.48	0.43
1:0:2419:U:H5"	1:0:2420:G:C5'	2.48	0.43
1:0:2793:A:H2'	1:0:2794:G:H5'	1.99	0.43
1:0:737:A:O2'	1:0:738:G:H5'	2.18	0.43
1:0:1060:C:H2'	1:0:1061:C:C6	2.52	0.43
1:0:1399:A:H2'	1:0:1400:C:C6	2.54	0.43
1:0:1643:C:O2'	1:0:1644:C:H5'	2.18	0.43
1:0:1950:G:H4'	1:0:1951:G:OP1	2.17	0.43
1:0:2781:U:C2'	1:0:2782:G:H5'	2.48	0.43
1:0:2859:C:O2'	1:0:2860:G:H5'	2.18	0.43
1:0:45:A:H5'	1:0:45:A:H8	1.83	0.43
1:0:140:G:H3'	1:0:140:G:C8	2.53	0.43
1:0:735:C:C5	1:0:736:A:C5	3.06	0.43
1:0:875:A:H5'	1:0:876:A:C2	2.53	0.43
1:0:1246:A:O2'	1:0:1247:A:H3'	2.18	0.43
1:0:1968:A:H2'	1:0:1969:A:C8	2.53	0.43
1:0:2330:U:H4'	1:0:2331:C:OP1	2.19	0.43
1:0:2780:C:H2'	1:0:2781:U:H6	1.82	0.43
1:0:204:A:H2'	1:0:205:U:H5'	2.01	0.43
1:0:706:G:HO2'	1:0:707:C:H6	1.67	0.43
1:0:2460:A:O2'	1:0:2461:U:O4'	2.36	0.43
1:0:2756:U:N3	1:0:2896:A:C2	2.71	0.43
1:0:1850:U:H2'	1:0:1851:G:H8	1.82	0.43
1:0:1901:G:O2'	1:0:1902:G:H5'	2.18	0.43
1:0:2619:U:H2'	1:0:2620:U:C6	2.53	0.43
1:0:95:A:H5'	1:0:96:A:H3'	1.99	0.43
1:0:588:G:O2'	1:0:589:U:P	2.77	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:631:A:C6	1:0:2074:A:H5'	2.53	0.43
1:0:963:C:H2'	1:0:964:G:C8	2.54	0.43
1:0:1768:C:H2'	1:0:1769:C:O4'	2.18	0.43
1:0:1823:G:O2'	1:0:1824:C:H5'	2.18	0.43
1:0:2312:G:H2'	1:0:2313:C:H5'	2.01	0.43
1:0:2694:A:C2	1:0:2702:A:C4	3.07	0.43
2:9:59:C:H2'	2:9:60:C:H6	1.82	0.43
1:0:728:C:H2'	1:0:729:C:C6	2.54	0.43
1:0:858:U:H2'	1:0:859:C:C6	2.53	0.43
1:0:1379:A:O2'	1:0:1380:U:H5"	2.19	0.43
1:0:1641:A:H2'	1:0:1642:A:C5'	2.46	0.43
1:0:1869:A:H2'	1:0:1870:C:O4'	2.19	0.43
1:0:2133:U:H4'	1:0:2134:G:C5'	2.48	0.43
1:0:2407:G:O2'	1:0:2408:A:H5'	2.18	0.43
1:0:485:A:H1'	1:0:486:A:H5'	2.00	0.43
1:0:1496:G:H2'	1:0:1497:G:H8	1.83	0.43
1:0:1730:G:N3	1:0:1730:G:H2'	2.34	0.43
1:0:2078:U:O2'	1:0:2079:G:H5'	2.19	0.43
1:0:2692:G:C8	1:0:2693:U:C5	3.02	0.43
1:0:2838:A:H2'	1:0:2839:C:C6	2.54	0.43
2:9:52:A:H2'	2:9:53:G:O4'	2.19	0.43
2:9:117:G:H2'	2:9:118:C:C6	2.54	0.43
1:0:288:A:N1	1:0:364:C:N3	2.67	0.43
1:0:1053:G:O2'	1:0:1054:G:H5'	2.19	0.43
1:0:1521:C:O2'	1:0:1522:A:H5'	2.19	0.43
1:0:1666:C:O2'	1:0:1667:A:H5'	2.19	0.43
1:0:1902:G:H2'	1:0:1903:U:O4'	2.18	0.43
1:0:2291:A:H5"	1:0:2292:C:C5'	2.49	0.43
1:0:2406:U:O2'	1:0:2407:G:H5'	2.19	0.43
1:0:364:C:H2'	1:0:365:G:O4'	2.18	0.42
1:0:603:A:O2'	1:0:604:G:OP2	2.36	0.42
1:0:807:A:N1	1:0:808:A:C2	2.87	0.42
1:0:1363:G:H2'	1:0:1364:G:C8	2.54	0.42
1:0:1518:A:H2'	1:0:1519:U:C6	2.54	0.42
1:0:1791:U:H2'	1:0:1792:C:C6	2.54	0.42
1:0:1887:U:H2'	1:0:1888:C:H6	1.83	0.42
1:0:2511:A:H5'	1:0:2511:A:C8	2.53	0.42
1:0:2909:G:H2'	1:0:2910:A:H8	1.83	0.42
1:0:23:G:H1'	1:0:520:A:N6	2.35	0.42
1:0:653:C:H2'	1:0:654:A:C8	2.54	0.42
1:0:764:C:H2'	1:0:765:G:O4'	2.19	0.42



	At a set of the set of	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:0:846:A:O2'	1:0:847:C:H5'	2.19	0.42	
1:0:1021:G:O2'	1:0:1022:A:H5'	2.18	0.42	
1:0:1369:A:H8	1:0:1369:A:OP1	2.01	0.42	
1:0:1894:C:N4	1:0:1939:U:H2'	2.34	0.42	
1:0:2134:G:O6	1:0:2258:A:H5"	2.18	0.42	
1:0:2430:A:N6	1:0:2460:A:C2	2.87	0.42	
1:0:2626:C:H2'	1:0:2627:G:C8	2.54	0.42	
1:0:2899:A:O2'	1:0:2900:G:H5'	2.19	0.42	
2:9:72:C:O2'	2:9:73:G:H5'	2.18	0.42	
1:0:286:U:H2'	1:0:287:C:C6	2.54	0.42	
1:0:369:G:C2	1:0:370:G:C8	3.08	0.42	
1:0:947:U:H2'	1:0:948:G:C8	2.54	0.42	
1:0:1072:G:O2'	1:0:1073:A:OP2	2.34	0.42	
1:0:2301:A:H5"	1:0:2302:A:H5'	2.01	0.42	
1:0:2748:G:H4'	1:0:2749:U:C5'	2.50	0.42	
1:0:360:A:H2'	1:0:361:C:O4'	2.19	0.42	
1:0:598:C:C4	1:0:599:G:N7	2.87	0.42	
1:0:607:G:H2'	1:0:608:A:O4'	2.20	0.42	
1:0:1092:A:H2'	1:0:1093:G:C8	2.54	0.42	
1:0:1308:A:O2'	1:0:1309:U:H5'	2.20	0.42	
1:0:1594:C:O2'	1:0:1595:G:H5'	2.18	0.42	
1:0:2872:U:H2'	1:0:2873:C:H6	1.84	0.42	
7:E:55:GLN:CA	7:E:56:PRO:CA	2.97	0.42	
1:0:67:A:H5"	1:0:68:U:H3'	2.02	0.42	
1:0:119:A:H2'	1:0:120:A:H5"	2.02	0.42	
1:0:1088:A:O2'	1:0:1089:G:C5'	2.57	0.42	
1:0:1142:C:O2'	1:0:1143:G:H5'	2.19	0.42	
1:0:1462:C:H2'	1:0:1463:A:C8	2.55	0.42	
1:0:1495:C:H2'	1:0:1496:G:H8	1.83	0.42	
1:0:1526:A:O4'	1:0:1527:A:C5	2.72	0.42	
1:0:1545:C:H2'	1:0:1546:G:O4'	2.20	0.42	
1:0:1569:U:H3'	1:0:1570:C:H5'	2.00	0.42	
1:0:2276:U:H2'	1:0:2277:U:C6	2.55	0.42	
1:0:2335:C:H2'	1:0:2336:G:C8	2.55	0.42	
1:0:2724:U:H2'	1:0:2725:G:O4'	2.19	0.42	
1:0:2847:G:O2'	1:0:2848:G:H5'	2.19	0.42	
1:0:2885:A:O2'	1:0:2886:C:H5'	2.19	0.42	
1:0:60:A:O2'	1:0:61:G:H5'	2.19	0.42	
1:0:70:A:H4'	1:0:71:G:O5'	2.18	0.42	
1:0:2415:A:C2'	1:0:2416:G:H5'	2.49	0.42	
1:0:2563:U:O2'	1:0:2564:G:H3'	2.20	0.42	



	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:A:186:TRP:CA	3:A:187:PRO:CA	2.98	0.42
1:0:200:U:OP1	1:0:200:U:C6	2.73	0.42
1:0:1846:U:H2'	1:0:1847:A:C5	2.55	0.42
1:0:2253:G:O2'	1:0:2254:G:H5'	2.20	0.42
1:0:240:C:H5"	1:0:270:U:O4	2.20	0.42
1:0:333:G:O2'	1:0:334:G:H5'	2.20	0.42
1:0:850:U:H2'	1:0:851:C:O4'	2.19	0.42
1:0:1298:U:H2'	1:0:1299:G:C8	2.54	0.42
1:0:1516:C:H2'	1:0:1517:U:C6	2.54	0.42
1:0:1798:C:O2	1:0:1798:C:H2'	2.19	0.42
1:0:1850:U:H2'	1:0:1851:G:C8	2.54	0.42
1:0:2004:U:H2'	1:0:2005:G:OP1	2.20	0.42
2:9:3:A:H62	2:9:25:G:H1	1.66	0.42
1:0:345:G:H2'	1:0:346:U:H6	1.85	0.42
1:0:594:C:O2'	1:0:595:U:H5'	2.20	0.42
1:0:811:C:H2'	1:0:812:A:C8	2.54	0.42
1:0:1039:G:H2'	1:0:1040:A:O4'	2.20	0.42
1:0:1280:A:O5'	1:0:1280:A:H8	2.03	0.42
1:0:1457:U:O2'	1:0:1458:A:H5'	2.20	0.42
1:0:1626:A:H2'	1:0:1627:G:C5'	2.50	0.42
1:0:1805:G:O2'	1:0:1806:G:H5'	2.20	0.42
2:9:56:A:C3'	2:9:57:A:H5"	2.50	0.42
1:0:345:G:H2'	1:0:346:U:C6	2.55	0.42
1:0:375:G:C4	1:0:411:A:C6	3.08	0.42
1:0:778:C:H2'	1:0:779:U:O4'	2.20	0.42
1:0:1050:G:C6	1:0:1051:C:C4	3.08	0.42
1:0:1155:G:H2'	1:0:1156:C:C6	2.55	0.42
1:0:2025:G:O2'	1:0:2026:C:H5'	2.19	0.42
1:0:2325:C:H2'	1:0:2326:U:C6	2.55	0.42
1:0:2326:U:H4'	1:0:2412:G:C4'	2.50	0.42
1:0:2627:G:H2'	1:0:2628:U:C6	2.54	0.42
1:0:552:A:H3'	1:0:553:G:C5'	2.49	0.41
1:0:558:C:N3	1:0:600:G:C2	2.88	0.41
1:0:1735:C:H2'	1:0:1736:A:C8	2.54	0.41
1:0:1787:C:H4'	1:0:2883:A:O4'	2.20	0.41
1:0:1878:G:O2'	1:0:1879:U:P	2.76	0.41
1:0:2242:U:O2'	1:0:2243:C:H2'	2.19	0.41
1:0:2335:C:H2'	1:0:2336:G:H8	1.84	0.41
1:0:364:C:H2'	1:0:365:G:C8	2.54	0.41
1:0:433:C:O2'	1:0:434:U:H5'	2.20	0.41
1:0:1555:G:H4'	1:0:1630:A:H2	1.85	0.41



	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:2253:G:N3	1:0:2254:G:C8	2.88	0.41
1:0:2488:A:N6	1:0:2534:C:H42	2.16	0.41
1:0:2821:C:H2'	1:0:2822:C:C6	2.55	0.41
1:0:77:G:O2'	1:0:78:G:H5'	2.20	0.41
1:0:106:A:O2'	1:0:107:U:H5'	2.20	0.41
1:0:243:A:H61	1:0:269:G:C1'	2.33	0.41
1:0:281:U:O2	1:0:369:G:C2	2.73	0.41
1:0:659:A:N3	1:0:746:A:C2	2.89	0.41
1:0:694:A:H2'	1:0:695:C:H5'	2.03	0.41
1:0:810:G:O2'	1:0:811:C:H5'	2.21	0.41
1:0:1150:A:H4'	1:0:1151:G:OP2	2.19	0.41
1:0:1427:A:H61	1:0:1440:U:H1'	1.84	0.41
1:0:1706:G:H1'	1:0:1712:A:H61	1.85	0.41
1:0:2258:A:H1'	1:0:2259:C:OP2	2.19	0.41
2:9:97:U:H2'	2:9:98:C:C6	2.55	0.41
1:0:251:C:H2'	1:0:252:C:C6	2.56	0.41
1:0:281:U:C2'	1:0:282:C:O4'	2.60	0.41
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.41
1:0:578:C:O2	1:0:1112:G:H4'	2.20	0.41
1:0:1020:A:H2'	1:0:1021:G:C8	2.55	0.41
1:0:1706:G:C6	1:0:1707:G:C6	3.08	0.41
1:0:1993:C:C4	1:0:1994:A:C6	3.08	0.41
1:0:2120:U:H2'	1:0:2121:G:O4'	2.21	0.41
1:0:2124:G:H2'	1:0:2125:G:H8	1.84	0.41
1:0:2820:A:H2'	1:0:2821:C:C6	2.54	0.41
1:0:23:G:C6	1:0:24:G:N1	2.89	0.41
1:0:95:A:H4'	1:0:96:A:O5'	2.20	0.41
1:0:877:G:C5'	1:0:878:G:OP1	2.65	0.41
1:0:1627:G:O2'	1:0:1628:G:H5'	2.20	0.41
1:0:1914:C:C2	1:0:1926:G:C2	3.08	0.41
1:0:2249:G:C2	1:0:2253:G:C6	3.09	0.41
1:0:2515:C:H2'	1:0:2516:G:C5'	2.50	0.41
1:0:2836:G:O2'	1:0:2837:U:P	2.78	0.41
1:0:2893:C:O2'	1:0:2894:C:H5'	2.20	0.41
2:9:39:U:H3'	2:9:40:C:H5"	2.02	0.41
1:0:132:A:H2'	1:0:133:U:C6	2.55	0.41
1:0:569:A:H5"	1:0:587:A:N1	2.36	0.41
1:0:602:A:O2'	1:0:605:C:H4'	2.21	0.41
1:0:1029:U:H5'	1:0:1031:G:N7	2.36	0.41
1:0:1064:U:H2'	1:0:1065:G:H8	1.85	0.41
1:0:1269:G:H2'	1:0:1270:U:C6	2.56	0.41



Interatomic			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:0:1626:A:C2'	1:0:1627:G:H5'	2.50	0.41
1:0:2064:U:H2'	1:0:2065:C:C6	2.55	0.41
1:0:2640:U:H2'	1:0:2641:C:C6	2.56	0.41
1:0:2845:G:O2'	1:0:2846:C:H5'	2.20	0.41
2:9:76:G:C8	2:9:77:A:H2'	2.55	0.41
1:0:277:U:O2'	1:0:278:A:H5'	2.21	0.41
1:0:289:G:C2	1:0:363:A:H2	2.34	0.41
1:0:355:C:O2'	1:0:356:C:H5'	2.21	0.41
1:0:526:U:H2'	1:0:527:U:C6	2.56	0.41
1:0:1029:U:O2'	1:0:1273:C:OP1	2.30	0.41
1:0:1538:C:O2'	1:0:1539:U:H5'	2.21	0.41
1:0:1676:G:O2'	1:0:1677:U:H5'	2.20	0.41
1:0:2773:G:H22	1:0:2801:A:H2	1.69	0.41
1:0:255:A:O2'	1:0:256:C:H5'	2.20	0.41
1:0:512:G:O3'	1:0:513:A:H8	2.04	0.41
1:0:523:C:H2'	1:0:524:A:C8	2.56	0.41
1:0:934:C:H2'	1:0:935:G:C8	2.56	0.41
1:0:1391:G:H2'	1:0:1392:A:H5'	2.01	0.41
1:0:1665:G:O2'	1:0:1666:C:H5'	2.20	0.41
1:0:2004:U:C2'	1:0:2005:G:OP1	2.69	0.41
1:0:2238:A:C2	1:0:2239:C:C6	3.09	0.41
1:0:2757:A:H2'	1:0:2758:G:O4'	2.21	0.41
1:0:24:G:N2	1:0:518:G:H1'	2.35	0.41
1:0:431:G:O2'	1:0:432:G:H5'	2.20	0.41
1:0:585:C:H2'	1:0:586:C:C6	2.56	0.41
1:0:627:G:H2'	1:0:2071:C:C4	2.56	0.41
1:0:1088:A:HO2'	1:0:1089:G:H5"	1.79	0.41
1:0:1209:C:H2'	1:0:1210:G:C8	2.45	0.41
1:0:1555:G:O2'	1:0:1556:G:H8	2.03	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.21	0.41
1:0:1964:U:O2'	1:0:1965:C:H5'	2.21	0.41
1:0:2135:A:O2'	1:0:2136:G:H5'	2.20	0.41
1:0:2336:G:O2'	1:0:2337:G:H5'	2.20	0.41
1:0:2823:G:O2'	1:0:2824:C:H5'	2.21	0.41
1:0:2824:C:O3'	1:0:2825:C:H6	2.04	0.41
1:0:2880:A:H2'	1:0:2881:C:O4'	2.21	0.41
2:9:1:U:O2'	2:9:3:A:OP1	2.38	0.41
1:0:394:G:H2'	1:0:398:U:C6	2.56	0.41
1:0:1474:C:H5'	1:0:1474:C:C6	2.49	0.41
1:0:2239:C:O2'	1:0:2240:U:H5'	2.21	0.41
1:0:2334:C:O2'	1:0:2335:C:H5'	2.21	0.41



Atom-1	Atom-2	Interatomic	Clash	
7100HI-1	1100111-2	distance (Å)	overlap (Å)	
1:0:282:C:C2'	1:0:283:U:C5'	2.99	0.40	
1:0:1236:A:H2'	1:0:1237:U:O4'	2.20	0.40	
1:0:1782:G:O2'	1:0:1783:A:H5'	2.21	0.40	
1:0:2362:A:H2'	1:0:2363:G:C8	2.55	0.40	
1:0:2445:U:H2'	1:0:2446:G:H8	1.84	0.40	
1:0:2823:G:C5'	1:0:2827:A:H5'	2.51	0.40	
1:0:207:U:H2'	1:0:208:C:C6	2.56	0.40	
1:0:272:A:N1	1:0:369:G:C5'	2.84	0.40	
1:0:482:G:H4'	1:0:508:A:N1	2.36	0.40	
1:0:598:C:H2'	1:0:599:G:C8	2.52	0.40	
1:0:934:C:H2'	1:0:935:G:H8	1.87	0.40	
1:0:1453:G:H2'	1:0:1454:U:O4'	2.20	0.40	
1:0:1555:G:HO2'	1:0:1556:G:P	2.44	0.40	
1:0:2597:U:C2'	1:0:2598:U:H5'	2.51	0.40	
1:0:2825:C:C2	1:0:2826:G:C5	3.09	0.40	
1:0:10:U:C2'	1:0:11:A:OP2	2.69	0.40	
1:0:194:A:C2'	1:0:195:C:H5'	2.52	0.40	
1:0:735:C:C2'	1:0:736:A:H5'	2.50	0.40	
1:0:2704:C:H2'	1:0:2705:U:O4'	2.21	0.40	
1:0:148:A:O2'	1:0:149:G:H5'	2.22	0.40	
1:0:189:A:H2'	1:0:190:G:O4'	2.22	0.40	
1:0:270:U:O2'	1:0:271:C:OP2	2.33	0.40	
1:0:284:C:H4'	1:0:285:A:C8	2.57	0.40	
1:0:735:C:H2'	1:0:736:A:H5'	2.03	0.40	
1:0:907:A:H4'	1:0:1328:A:C2	2.56	0.40	
1:0:946:C:H2'	1:0:947:U:H6	1.85	0.40	
1:0:1796:A:H2'	1:0:1797:A:C8	2.57	0.40	
1:0:2265:U:H2'	1:0:2266:A:C8	2.56	0.40	
1:0:140:G:C8	1:0:140:G:C3'	3.04	0.40	
1:0:177:A:H2'	1:0:178:U:O4'	2.22	0.40	
1:0:196:G:H1'	1:0:197:C:OP2	2.21	0.40	
1:0:271:C:H4'	1:0:272:A:O5'	2.22	0.40	
1:0:807:A:N1	1:0:808:A:N3	2.69	0.40	
1:0:2252:A:H2'	1:0:2253:G:H5'	2.04	0.40	
1:0:2252:A:H2'	1:0:2253:G:C5'	2.51	0.40	
1:0:2750:G:O5'	1:0:2750:G:H8	2.05	0.40	
1:0:2797:C:O2'	1:0:2798:G:H5'	2.22	0.40	
2:9:64:C:O2'	2:9:65:A:H5'	2.22	0.40	

There are no symmetry-related clashes.



#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

#### 5.3.2 Protein sidechains (i)

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

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2697/2922~(92%)	334~(12%)	107 (3%)
2	9	122/122~(100%)	17 (13%)	5(4%)
All	All	2819/3044~(92%)	351 (12%)	112 (3%)

All (351) RNA backbone outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	0	11	А
1	0	31	С
1	0	60	А
1	0	67	А
1	0	70	А
1	0	71	G
1	0	87	С
1	0	95	А
1	0	96	А
1	0	114	А
1	0	115	U
1	0	116	G
1	0	120	А
1	0	139	С
1	0	141	С
1	0	142	G
1	0	151	А
1	0	166	А
1	0	169	А
1	0	186	А
1	0	192	А
1	0	196	G
1	0	197	С



Mol	Chain	Res	Type
1	0	198	A
1	0	200	U
1	0	201	G
1	0	204	A
1	0	219	G
1	0	220	С
1	0	236	А
1	0	237	G
1	0	262	А
1	0	263	U
1	0	271	С
1	0	272	A
1	0	273	G
1	0	282	С
1	0	283	U
1	0	284	С
1	0	285	A
1	0	308	U
1	0	309	С
1	0	336	G
1	0	337	А
1	0	345	G
1	0	358	G
1	0	368	С
1	0	381	G
1	0	395	А
1	0	397	А
1	0	398	U
1	0	407	А
1	0	417	G
1	0	439	A
1	0	453	A
1	0	461	С
1	0	481	U
1	0	485	A
1	0	486	A
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	512	G



Mol	Chain	Res	Type
1	0	514	G
1	0	515	С
1	0	537	G
1	0	538	С
1	0	539	G
1	0	545	G
1	0	548	U
1	0	549	А
1	0	553	G
1	0	554	G
1	0	555	U
1	0	588	G
1	0	600	G
1	0	601	G
1	0	604	G
1	0	620	A
1	0	632	А
1	0	660	А
1	0	682	А
1	0	688	А
1	0	699	С
1	0	700	А
1	0	701	U
1	0	714	U
1	0	759	С
1	0	777	U
1	0	809	G
1	0	817	G
1	0	818	А
1	0	821	U
1	0	835	U
1	0	840	U
1	0	856	G
1	0	857	А
1	0	858	U
1	0	868	G
1	0	869	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	895	А



Mol	Chain	Res	Type
1	0	898	G
1	0	905	С
1	0	920	С
1	0	921	G
1	0	923	А
1	0	940	G
1	0	953	G
1	0	960	G
1	0	961	А
1	0	965	А
1	0	1006	А
1	0	1008	С
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	С
1	0	1072	G
1	0	1073	А
1	0	1081	А
1	0	1089	G
1	0	1106	А
1	0	1107	А
1	0	1108	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1124	А
1	0	1126	С
1	0	1127	С
1	0	1130	U
1	0	1137	G
1	0	1148	C
1	0	1149	U
1	0	1150	A
1	0	1160	G
1	0	1215	A
1	0	1216	G
1	0	1237	U
1	0	1238	С
1	0	1239	G
1	0	1245	C
1	0	1279	U



Mol	Chain	Res	Type
1	0	1287	A
1	0	1289	С
1	0	1309	U
1	0	1310	U
1	0	1330	А
1	0	1331	А
1	0	1341	А
1	0	1342	С
1	0	1353	С
1	0	1355	А
1	0	1360	С
1	0	1369	А
1	0	1370	G
1	0	1377	С
1	0	1380	U
1	0	1407	A
1	0	1409	G
1	0	1449	G
1	0	1451	С
1	0	1474	С
1	0	1485	А
1	0	1488	U
1	0	1492	А
1	0	1506	U
1	0	1507	С
1	0	1524	U
1	0	1525	G
1	0	1526	А
1	0	1527	А
1	0	1528	A
1	0	1535	G
1	0	1556	G
1	0	1563	G
1	0	1564	C
1	0	1592	G
1	0	1593	С
1	0	1604	G
1	0	1605	G
1	0	1606	A
1	0	1624	A
1	0	$16\overline{25}$	U
1	0	1626	A



Mol	Chain	Res	Type
1	0	1633	С
1	0	1634	G
1	0	1656	А
1	0	1682	А
1	0	1684	А
1	0	1685	А
1	0	1691	А
1	0	1692	С
1	0	1693	А
1	0	1699	С
1	0	1700	С
1	0	1701	А
1	0	1710	А
1	0	1722	U
1	0	1723	G
1	0	1725	С
1	0	1731	С
1	0	1732	А
1	0	1752	G
1	0	1774	G
1	0	1778	А
1	0	1798	С
1	0	1819	G
1	0	1820	G
1	0	1829	А
1	0	1835	U
1	0	1836	А
1	0	1853	С
1	0	1854	С
1	0	1857	А
1	0	1879	U
1	0	1907	U
1	0	1908	G
1	0	1919	A
1	0	1942	А
1	0	1951	G
1	0	1971	G
1	0	1973	А
1	0	1979	G
1	0	1980	U
1	0	1981	A
1	0	1982	С



Mol	Chain	Res	Type
1	0	1996	U
1	0	2005	G
1	0	2008	U
1	0	2011	А
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2075	G
1	0	2077	С
1	0	2083	A
1	0	2084	С
1	0	2091	G
1	0	2096	А
1	0	2101	А
1	0	2102	G
1	0	2110	G
1	0	2238	А
1	0	2243	С
1	0	2258	А
1	0	2259	С
1	0	2271	G
1	0	2272	G
1	0	2283	G
1	0	2284	G
1	0	2291	A
1	0	2316	G
1	0	2317	С
1	0	2322	U
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2370	A
1	0	2371	G
1	0	2379	G
1	0	2396	С
1	0	2422	U



Mol	Chain	Res	Type
1	0	2427	С
1	0	2428	G
1	0	2462	G
1	0	2464	С
1	0	2466	G
1	0	2467	А
1	0	2469	А
1	0	2476	С
1	0	2482	G
1	0	2483	А
1	0	2507	G
1	0	2509	А
1	0	2511	A
1	0	2527	U
1	0	2533	С
1	0	2537	G
1	0	2538	А
1	0	2541	U
1	0	2553	А
1	0	2564	G
1	0	2589	U
1	0	2601	А
1	0	2602	G
1	0	2608	С
1	0	2613	G
1	0	2617	G
1	0	2634	G
1	0	2637	А
1	0	2638	G
1	0	2649	А
1	0	2681	А
1	0	2682	С
1	0	2714	U
1	0	2715	G
1	0	2719	A
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A



Mol	Chain	Res	Type
1	0	2783	А
1	0	2786	G
1	0	2792	А
1	0	2800	А
1	0	2811	А
1	0	2814	А
1	0	2815	G
1	0	2826	G
1	0	2827	А
1	0	2837	U
1	0	2850	С
1	0	2867	G
1	0	2876	G
1	0	2890	А
1	0	2891	А
1	0	2903	С
1	0	2914	А
2	9	2	U
2	9	4	G
2	9	14	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	29	С
2	9	34	А
2	9	41	С
2	9	43	G
2	9	56	А
2	9	57	А
2	9	66	G
2	9	77	А
2	9	87	U
2	9	114	G
2	9	122	С

Continued from previous page...

All (112) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	95	А
1	0	115	U
1	0	191	А



Mol	Chain	Res	Type
1	0	196	G
1	0	199	А
1	0	270	U
1	0	282	С
1	0	283	U
1	0	284	С
1	0	338	С
1	0	367	G
1	0	394	G
1	0	438	С
1	0	452	G
1	0	480	С
1	0	485	A
1	0	496	G
1	0	514	G
1	0	548	U
1	0	554	G
1	0	600	G
1	0	603	A
1	0	681	G
1	0	699	С
1	0	713	U
1	0	817	G
1	0	855	U
1	0	857	А
1	0	877	G
1	0	894	А
1	0	904	U
1	0	939	A
1	0	952	G
1	0	1044	С
1	0	1059	G
1	0	1072	G
1	0	1080	C
1	0	1088	A
1	0	1106	A
1	0	1108	G
1	0	1126	С
1	0	1137	G
1	0	1149	U
1	0	1214	G
1	0	1237	U



Mol	Chain	Res	Type
1	0	1309	U
1	0	1329	A
1	0	1352	А
1	0	1369	А
1	0	1379	А
1	0	1406	А
1	0	1408	U
1	0	1448	А
1	0	1450	С
1	0	1506	U
1	0	1534	С
1	0	1591	А
1	0	1603	A
1	0	1605	G
1	0	1624	A
1	0	1683	G
1	0	1690	С
1	0	1699	С
1	0	1835	U
1	0	1853	С
1	0	1856	С
1	0	1907	U
1	0	1950	G
1	0	1978	А
1	0	1979	G
1	0	1981	А
1	0	2011	A
1	0	2074	А
1	0	2076	U
1	0	2083	A
1	0	2090	G
1	0	2242	U
1	0	2258	A
1	0	2282	U
1	0	2283	G
1	0	2290	U
1	0	2316	G
1	0	2321	A
1	0	2370	A
1	0	2395	A
1	0	2421	G
1	0	2427	C



Mol	Chain	Res	Type
1	0	2463	А
1	0	2465	А
1	0	2467	А
1	0	2468	А
1	0	2482	G
1	0	2526	С
1	0	2616	G
1	0	2692	G
1	0	2714	U
1	0	2718	С
1	0	2748	G
1	0	2749	U
1	0	2791	U
1	0	2813	А
1	0	2814	А
1	0	2836	G
1	0	2849	U
1	0	2866	U
1	0	2890	А
2	9	1	U
2	9	3	А
2	9	28	U
2	9	55	U
2	9	65	А

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

#### 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

