

Se avete una vecchia versione di *Chime* Potete ricostruire sul vostro PC l'immagine del DNA che vedete sul sito [www.bayes.it](http://www.bayes.it) con questi due semplici passi:

- 1) copiate e salvate in un file di testo denominato "*dna.pdb*" le coordinate spaziali degli atomi che compongono la molecola (copiare da HEADER a END tutte le righe riportate qui sotto senza apportare modifiche);
- 2) copiate e salvate in un file di testo denominato "*DNA.htm*" il codice html che consente di avviare la presentazione della molecola in Explorer (copiare da <html> a </html> tutte le righe riportate qui sotto senza apportare modifiche).

A questo punto facendo doppio click sul file "*DNA.htm*" in Explorer comparirà la molecola in 3d. Facendo click su questa con il tasto destro del mouse potete accedere al menù di *Chime* che consente di modificare le modalità di rappresentazione della molecola.

Sui siti di proteomica potete trovare i file pdb che contengono le ricostruzioni 3d di molecole organiche (emoglobina, immunoglobuline, ormoni, enzimi, eccetera). Ovviamente per ogni file pdb dovete realizzare il corrispondente file html: per questo è sufficiente ricopiare il codice html che vi ho fornito e nella riga

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<p><embed src="dna.pdb" align="left" border="0" hspace="15"
sostituire "dna.pdb" con il nome del file pdb appropriato.
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Ora che *Chime* non è più supportato sul web potete trovare molti programmi che leggono direttamente i file .pdb e add-on che consentono di gestirli via browser con script html (per i dettagli si rimanda alle specifiche documentazioni).

```
HEADER      DEOXYRIBONUCLEIC ACID                      26-JAN-81   1BNA
TITLE       STRUCTURE OF A B-DNA DODECAMER. CONFORMATION AND DYNAMICS
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: DNA
COMPND      3 (5'-D(*CP*GP*CP*GP*AP*AP*TP*TP*CP*GP*CP*G)-3');
COMPND      4 CHAIN: A, B;
COMPND      5 ENGINEERED: YES
SOURCE      MOL_ID: 1;
SOURCE      2 SYNTHETIC: YES
KEYWDS      B-DNA, DOUBLE HELIX, DEOXYRIBONUCLEIC ACID
EXPDTA      X-RAY DIFFRACTION
AUTHOR      H.R.DREW,R.M.WING,T.TAKANO,C.BROKA,S.TANAKA,K.ITAKURA,
AUTHOR      2 R.E.DICKERSON
REVDAT      1   21-MAY-81 1BNA   0
JRNL        AUTH   H.R.DREW,R.M.WING,T.TAKANO,C.BROKA,S.TANAKA,
JRNL        AUTH 2 K.ITAKURA,R.E.DICKERSON
JRNL        TITL   STRUCTURE OF A B-DNA DODECAMER. CONFORMATION AND
JRNL        TITL 2 DYNAMICS
JRNL        REF    PROC.NAT.ACAD.SCI.USA                V.   78   2179 1981
JRNL        REFN   ASTM PNASA6   US ISSN 0027-8424                0040
REMARK      1
REMARK      1 REFERENCE 1
REMARK      1 AUTH   R.E.DICKERSON,H.R.DREW
REMARK      1 TITL   KINEMATIC MODEL FOR B-DNA
REMARK      1 REF    PROC.NAT.ACAD.SCI.USA                V.   78   7318 1981
REMARK      1 REFN   ASTM PNASA6   US ISSN 0027-8424                0040
REMARK      1 REFERENCE 2
REMARK      1 AUTH   R.E.DICKERSON,H.R.DREW
REMARK      1 TITL   STRUCTURE OF A B-DNA DODECAMER. II. INFLUENCE OF
REMARK      1 TITL 2 BASE SEQUENCE ON HELIX STRUCTURE
REMARK      1 REF    J.MOL.BIOL.                          V.  149   761 1981
REMARK      1 REFN   ASTM JMOBAK   UK ISSN 0022-2836                0070
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REMARK 1 REFERENCE 3  
 REMARK 1 AUTH H.R.DREW,R.E.DICKERSON  
 REMARK 1 TITL STRUCTURE OF A B-DNA DODECAMER. III. GEOMETRY OF  
 REMARK 1 TITL 2 HYDRATION  
 REMARK 1 REF J.MOL.BIOL. V. 151 535 1981  
 REMARK 1 REFN ASTM JMOBAK UK ISSN 0022-2836 0070  
 REMARK 1 REFERENCE 4  
 REMARK 1 AUTH R.WING,H.R.DREW,T.TAKANO,C.BROKA,S.TANAKA,  
 REMARK 1 AUTH 2 K.ITAKURA,R.E.DICKERSON  
 REMARK 1 TITL CRYSTAL STRUCTURE ANALYSIS OF A COMPLETE TURN OF  
 REMARK 1 TITL 2 B-DNA  
 REMARK 1 REF NATURE V. 287 755 1980  
 REMARK 1 REFN ASTM NATUAS UK ISSN 0028-0836 0006  
 REMARK 2  
 REMARK 2 RESOLUTION. 1.90 ANGSTROMS.  
 REMARK 3  
 REMARK 3 REFINEMENT.  
 REMARK 3 PROGRAM : JACK-LEVITT  
 REMARK 3 AUTHORS : JACK,LEVITT  
 REMARK 3  
 REMARK 3 DATA USED IN REFINEMENT.  
 REMARK 3 RESOLUTION RANGE HIGH (ANGSTROMS) : 1.9  
 REMARK 3 RESOLUTION RANGE LOW (ANGSTROMS) : 8.0  
 REMARK 3 DATA CUTOFF (SIGMA(F)) : NULL  
 REMARK 3 DATA CUTOFF HIGH (ABS(F)) : NULL  
 REMARK 3 DATA CUTOFF LOW (ABS(F)) : NULL  
 REMARK 3 COMPLETENESS (WORKING+TEST) (%) : NULL  
 REMARK 3 NUMBER OF REFLECTIONS : 2725  
 REMARK 3  
 REMARK 3  
 REMARK 3 FIT TO DATA USED IN REFINEMENT.  
 REMARK 3 CROSS-VALIDATION METHOD : NULL  
 REMARK 3 FREE R VALUE TEST SET SELECTION : NULL  
 REMARK 3 R VALUE (WORKING SET) : 0.178  
 REMARK 3 FREE R VALUE : NULL  
 REMARK 3 FREE R VALUE TEST SET SIZE (%) : NULL  
 REMARK 3 FREE R VALUE TEST SET COUNT : NULL  
 REMARK 3 ESTIMATED ERROR OF FREE R VALUE : NULL  
 REMARK 3  
 REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.  
 REMARK 3 TOTAL NUMBER OF BINS USED : NULL  
 REMARK 3 BIN RESOLUTION RANGE HIGH (A) : NULL  
 REMARK 3 BIN RESOLUTION RANGE LOW (A) : NULL  
 REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : NULL  
 REMARK 3 REFLECTIONS IN BIN (WORKING SET) : NULL  
 REMARK 3 BIN R VALUE (WORKING SET) : NULL  
 REMARK 3 BIN FREE R VALUE : NULL  
 REMARK 3 BIN FREE R VALUE TEST SET SIZE (%) : NULL  
 REMARK 3 BIN FREE R VALUE TEST SET COUNT : NULL  
 REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : NULL  
 REMARK 3  
 REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.  
 REMARK 3 PROTEIN ATOMS : 0  
 REMARK 3 NUCLEIC ACID ATOMS : 486  
 REMARK 3 HETEROGEN ATOMS : 0  
 REMARK 3 SOLVENT ATOMS : 80  
 REMARK 3  
 REMARK 3 B VALUES.  
 REMARK 3 FROM WILSON PLOT (A\*\*2) : NULL  
 REMARK 3 MEAN B VALUE (OVERALL, A\*\*2) : NULL  
 REMARK 3 OVERALL ANISOTROPIC B VALUE.  
 REMARK 3 B11 (A\*\*2) : NULL

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REMARK 3      B22 (A**2) : NULL
REMARK 3      B33 (A**2) : NULL
REMARK 3      B12 (A**2) : NULL
REMARK 3      B13 (A**2) : NULL
REMARK 3      B23 (A**2) : NULL
REMARK 3
REMARK 3      ESTIMATED COORDINATE ERROR.
REMARK 3      ESD FROM LUZZATI PLOT          (A) : NULL
REMARK 3      ESD FROM SIGMAA                (A) : NULL
REMARK 3      LOW RESOLUTION CUTOFF          (A) : NULL
REMARK 3
REMARK 3      CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3      ESD FROM C-V LUZZATI PLOT      (A) : NULL
REMARK 3      ESD FROM C-V SIGMAA            (A) : NULL
REMARK 3
REMARK 3      RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3      BOND LENGTHS                    (A) : NULL
REMARK 3      BOND ANGLES                     (DEGREES) : NULL
REMARK 3      DIHEDRAL ANGLES                 (DEGREES) : NULL
REMARK 3      IMPROPER ANGLES                 (DEGREES) : NULL
REMARK 3
REMARK 3      ISOTROPIC THERMAL MODEL : NULL
REMARK 3
REMARK 3      ISOTROPIC THERMAL FACTOR RESTRAINTS.      RMS      SIGMA
REMARK 3      MAIN-CHAIN BOND                        (A**2) : NULL ; NULL
REMARK 3      MAIN-CHAIN ANGLE                       (A**2) : NULL ; NULL
REMARK 3      SIDE-CHAIN BOND                        (A**2) : NULL ; NULL
REMARK 3      SIDE-CHAIN ANGLE                       (A**2) : NULL ; NULL
REMARK 3
REMARK 3
REMARK 3      NCS MODEL : NULL
REMARK 3
REMARK 3      NCS RESTRAINTS.                          RMS      SIGMA/WEIGHT
REMARK 3      GROUP 1 POSITIONAL                        (A) : NULL ; NULL
REMARK 3      GROUP 1 B-FACTOR                          (A**2) : NULL ; NULL
REMARK 3
REMARK 3      PARAMETER FILE 1 : NULL
REMARK 3      TOPOLOGY FILE 1 : NULL
REMARK 3
REMARK 3      OTHER REFINEMENT REMARKS: NULL
REMARK 105
REMARK 105 THE PROTEIN DATA BANK HAS ADOPTED THE SACCHARIDE CHEMISTS
REMARK 105 NOMENCLATURE FOR ATOMS OF THE DEOXYRIBOSE/RIBOSE MOIETY
REMARK 105 RATHER THAN THAT OF THE NUCLEOSIDE CHEMISTS. THE RING
REMARK 105 OXYGEN ATOM IS LABELLED O4* INSTEAD OF O1*.
REMARK 106
REMARK 106 THE HYDROGEN BONDS BETWEEN BASE PAIRS IN THIS ENTRY FOLLOW
REMARK 106 THE CONVENTIONAL WATSON-CRICK HYDROGEN BONDING PATTERN.
REMARK 106 THEY HAVE NOT BEEN PRESENTED ON *CONECT* RECORDS IN THIS
REMARK 106 ENTRY.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : NULL
REMARK 200 TEMPERATURE (KELVIN) : NULL
REMARK 200 PH : NULL
REMARK 200 NUMBER OF CRYSTALS USED : NULL
REMARK 200
REMARK 200 SYNCHROTRON (Y/N) : N
REMARK 200 RADIATION SOURCE : NULL
REMARK 200 BEAMLINE : NULL
REMARK 200 X-RAY GENERATOR MODEL : NULL

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REMARK 200 MONOCHROMATIC OR LAUE (M/L) : NULL  
 REMARK 200 WAVELENGTH OR RANGE (A) : NULL  
 REMARK 200 MONOCHROMATOR : NULL  
 REMARK 200 OPTICS : NULL  
 REMARK 200  
 REMARK 200 DETECTOR TYPE : DIFFRACTOMETER  
 REMARK 200 DETECTOR MANUFACTURER : NULL  
 REMARK 200 INTENSITY-INTEGRATION SOFTWARE : NULL  
 REMARK 200 DATA SCALING SOFTWARE : NULL  
 REMARK 200  
 REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 5691  
 REMARK 200 RESOLUTION RANGE HIGH (A) : 1.9  
 REMARK 200 RESOLUTION RANGE LOW (A) : NULL  
 REMARK 200 REJECTION CRITERIA (SIGMA(I)) : NULL  
 REMARK 200  
 REMARK 200 OVERALL.  
 REMARK 200 COMPLETENESS FOR RANGE (%) : NULL  
 REMARK 200 DATA REDUNDANCY : NULL  
 REMARK 200 R MERGE (I) : NULL  
 REMARK 200 R SYM (I) : NULL  
 REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : NULL  
 REMARK 200  
 REMARK 200 IN THE HIGHEST RESOLUTION SHELL.  
 REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : NULL  
 REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : NULL  
 REMARK 200 COMPLETENESS FOR SHELL (%) : NULL  
 REMARK 200 DATA REDUNDANCY IN SHELL : NULL  
 REMARK 200 R MERGE FOR SHELL (I) : NULL  
 REMARK 200 R SYM FOR SHELL (I) : NULL  
 REMARK 200 <I/SIGMA(I)> FOR SHELL : NULL  
 REMARK 200  
 REMARK 200 DIFFRACTION PROTOCOL: NULL  
 REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: NULL  
 REMARK 200 SOFTWARE USED: NULL  
 REMARK 200 STARTING MODEL: NULL  
 REMARK 200  
 REMARK 200 REMARK: NULL  
 REMARK 280  
 REMARK 280 CRYSTAL  
 REMARK 280 SOLVENT CONTENT, VS (%): NULL  
 REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS\*\*3/DA): NULL  
 REMARK 280  
 REMARK 280 CRYSTALLIZATION CONDITIONS:  
 REMARK 280 CRYSTALS WERE OBTAINED FROM A SOLUTION THAT CONTAINED  
 REMARK 280 MG ACETATE, SPERMINE\_HCL.  
 REMARK 290  
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY  
 REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 21 21 21  
 REMARK 290  

| SYMP   | SYMMETRY         |
|--------|------------------|
| NNNMMM | OPERATOR         |
| 1555   | X, Y, Z          |
| 2555   | 1/2-X, -Y, 1/2+Z |
| 3555   | -X, 1/2+Y, 1/2-Z |
| 4555   | 1/2+X, 1/2-Y, -Z |

 REMARK 290  
 REMARK 290 WHERE NNN -> OPERATOR NUMBER  
 REMARK 290 MMM -> TRANSLATION VECTOR  
 REMARK 290  
 REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS  
 REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM  
 REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY

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REMARK 290 RELATED MOLECULES.
REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 0.000000
REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.000000
REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.000000
REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 12.43500
REMARK 290 SMTRY2 2 0.000000 -1.000000 0.000000 0.000000
REMARK 290 SMTRY3 2 0.000000 0.000000 1.000000 33.10000
REMARK 290 SMTRY1 3 -1.000000 0.000000 0.000000 0.000000
REMARK 290 SMTRY2 3 0.000000 1.000000 0.000000 20.19500
REMARK 290 SMTRY3 3 0.000000 0.000000 -1.000000 33.10000
REMARK 290 SMTRY1 4 1.000000 0.000000 0.000000 12.43500
REMARK 290 SMTRY2 4 0.000000 -1.000000 0.000000 20.19500
REMARK 290 SMTRY3 4 0.000000 0.000000 -1.000000 0.000000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 500
REMARK 500
REMARK 500 GEOMETRY AND STEREOCHEMISTRY
REMARK 500 SUBTOPIC: CLOSE CONTACTS IN SAME ASYMMETRIC UNIT
REMARK 500
REMARK 500 THE FOLLOWING ATOMS ARE IN CLOSE CONTACT.
REMARK 500
REMARK 500 ATM1 RES C SSEQI ATM2 RES C SSEQI
REMARK 500 0 HOH 62 0 HOH 77 1.61
REMARK 500 02P A A 6 0 HOH 65 1.89
REMARK 500 0 HOH 70 02P G A 10 2.02
REMARK 500 0 HOH 54 0 HOH 86 2.07
REMARK 500 0 HOH 77 0 HOH 63 2.09
REMARK 500 0 HOH 31 0 HOH 99 2.12
REMARK 525
REMARK 525 SOLVENT
REMARK 525 THE FOLLOWING SOLVENT MOLECULES LIE FARTHER THAN EXPECTED
REMARK 525 FROM THE PROTEIN OR NUCLEIC ACID MOLECULE AND MAY BE
REMARK 525 ASSOCIATED WITH A SYMMETRY RELATED MOLECULE (M=MODEL
REMARK 525 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE
REMARK 525 NUMBER; I=INSERTION CODE):
REMARK 525
REMARK 525 M RES CSSEQI
REMARK 525 0 HOH 55 DISTANCE = 5.33 ANGSTROMS
REMARK 525 0 HOH 57 DISTANCE = 5.20 ANGSTROMS
REMARK 525 0 HOH 64 DISTANCE = 5.35 ANGSTROMS
REMARK 525 0 HOH 69 DISTANCE = 5.38 ANGSTROMS
REMARK 525 0 HOH 74 DISTANCE = 5.05 ANGSTROMS
REMARK 525 0 HOH 75 DISTANCE = 5.18 ANGSTROMS
REMARK 525 0 HOH 78 DISTANCE = 5.12 ANGSTROMS
REMARK 525 0 HOH 82 DISTANCE = 5.85 ANGSTROMS
REMARK 525 0 HOH 84 DISTANCE = 5.47 ANGSTROMS
REMARK 525 0 HOH 87 DISTANCE = 5.78 ANGSTROMS
REMARK 525 0 HOH 88 DISTANCE = 5.20 ANGSTROMS
REMARK 525 0 HOH 89 DISTANCE = 6.29 ANGSTROMS
REMARK 525 0 HOH 93 DISTANCE = 5.11 ANGSTROMS
REMARK 525 0 HOH 94 DISTANCE = 5.58 ANGSTROMS
REMARK 525 0 HOH 95 DISTANCE = 5.10 ANGSTROMS
REMARK 525 0 HOH 99 DISTANCE = 5.17 ANGSTROMS
REMARK 525 0 HOH 100 DISTANCE = 5.48 ANGSTROMS
REMARK 525 0 HOH 104 DISTANCE = 5.08 ANGSTROMS
DBREF 1BNA A 1 12 NDB BDL001 BDL001 1 12
DBREF 1BNA B 13 24 NDB BDL001 BDL001 13 24
SEQRES 1 A 12 C G C G A A T T C G C G
SEQRES 1 B 12 C G C G A A T T C G C G
FORMUL 3 HOH *80(H2 O1)
CRYST1 24.870 40.390 66.200 90.00 90.00 90.00 P 21 21 21 8

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|        |          |          |          |          |        |        |        |      |       |   |
|--------|----------|----------|----------|----------|--------|--------|--------|------|-------|---|
| ORIGX1 | 1.000000 | 0.000000 | 0.000000 | 0.000000 |        |        |        |      |       |   |
| ORIGX2 | 0.000000 | 1.000000 | 0.000000 | 0.000000 |        |        |        |      |       |   |
| ORIGX3 | 0.000000 | 0.000000 | 1.000000 | 0.000000 |        |        |        |      |       |   |
| SCALE1 | 0.040209 | 0.000000 | 0.000000 | 0.000000 |        |        |        |      |       |   |
| SCALE2 | 0.000000 | 0.024759 | 0.000000 | 0.000000 |        |        |        |      |       |   |
| SCALE3 | 0.000000 | 0.000000 | 0.015106 | 0.000000 |        |        |        |      |       |   |
| ATOM   | 1        | O5*      | C A      | 1        | 18.935 | 34.195 | 25.617 | 1.00 | 64.35 | O |
| ATOM   | 2        | C5*      | C A      | 1        | 19.130 | 33.921 | 24.219 | 1.00 | 44.69 | C |
| ATOM   | 3        | C4*      | C A      | 1        | 19.961 | 32.668 | 24.100 | 1.00 | 31.28 | C |
| ATOM   | 4        | O4*      | C A      | 1        | 19.360 | 31.583 | 24.852 | 1.00 | 37.45 | O |
| ATOM   | 5        | C3*      | C A      | 1        | 20.172 | 32.122 | 22.694 | 1.00 | 46.72 | C |
| ATOM   | 6        | O3*      | C A      | 1        | 21.350 | 31.325 | 22.681 | 1.00 | 48.89 | O |
| ATOM   | 7        | C2*      | C A      | 1        | 18.948 | 31.223 | 22.647 | 1.00 | 30.88 | C |
| ATOM   | 8        | C1*      | C A      | 1        | 19.231 | 30.482 | 23.944 | 1.00 | 36.58 | C |
| ATOM   | 9        | N1       | C A      | 1        | 18.070 | 29.661 | 24.380 | 1.00 | 40.51 | N |
| ATOM   | 10       | C2       | C A      | 1        | 18.224 | 28.454 | 25.015 | 1.00 | 16.62 | C |
| ATOM   | 11       | O2       | C A      | 1        | 19.360 | 28.014 | 25.214 | 1.00 | 27.75 | O |
| ATOM   | 12       | N3       | C A      | 1        | 17.143 | 27.761 | 25.377 | 1.00 | 20.55 | N |
| ATOM   | 13       | C4       | C A      | 1        | 15.917 | 28.226 | 25.120 | 1.00 | 34.72 | C |
| ATOM   | 14       | N4       | C A      | 1        | 14.828 | 27.477 | 25.444 | 1.00 | 40.31 | N |
| ATOM   | 15       | C5       | C A      | 1        | 15.719 | 29.442 | 24.471 | 1.00 | 30.78 | C |
| ATOM   | 16       | C6       | C A      | 1        | 16.843 | 30.171 | 24.101 | 1.00 | 25.90 | C |
| ATOM   | 17       | P        | G A      | 2        | 22.409 | 31.286 | 21.483 | 1.00 | 58.85 | P |
| ATOM   | 18       | O1P      | G A      | 2        | 23.536 | 32.157 | 21.851 | 1.00 | 57.82 | O |
| ATOM   | 19       | O2P      | G A      | 2        | 21.822 | 31.459 | 20.139 | 1.00 | 78.33 | O |
| ATOM   | 20       | O5*      | G A      | 2        | 22.840 | 29.751 | 21.498 | 1.00 | 40.36 | O |
| ATOM   | 21       | C5*      | G A      | 2        | 23.543 | 29.175 | 22.594 | 1.00 | 47.19 | C |
| ATOM   | 22       | C4*      | G A      | 2        | 23.494 | 27.709 | 22.279 | 1.00 | 47.81 | C |
| ATOM   | 23       | O4*      | G A      | 2        | 22.193 | 27.252 | 22.674 | 1.00 | 38.76 | O |
| ATOM   | 24       | C3*      | G A      | 2        | 23.693 | 27.325 | 20.807 | 1.00 | 28.58 | C |
| ATOM   | 25       | O3*      | G A      | 2        | 24.723 | 26.320 | 20.653 | 1.00 | 40.44 | O |
| ATOM   | 26       | C2*      | G A      | 2        | 22.273 | 26.885 | 20.416 | 1.00 | 21.14 | C |
| ATOM   | 27       | C1*      | G A      | 2        | 21.721 | 26.304 | 21.716 | 1.00 | 33.95 | C |
| ATOM   | 28       | N9       | G A      | 2        | 20.237 | 26.470 | 21.780 | 1.00 | 34.00 | N |
| ATOM   | 29       | C8       | G A      | 2        | 19.526 | 27.584 | 21.429 | 1.00 | 36.47 | C |
| ATOM   | 30       | N7       | G A      | 2        | 18.207 | 27.455 | 21.636 | 1.00 | 32.37 | N |
| ATOM   | 31       | C5       | G A      | 2        | 18.083 | 26.212 | 22.142 | 1.00 | 15.06 | C |
| ATOM   | 32       | C6       | G A      | 2        | 16.904 | 25.525 | 22.545 | 1.00 | 11.88 | C |
| ATOM   | 33       | O6       | G A      | 2        | 15.739 | 25.916 | 22.518 | 1.00 | 21.30 | O |
| ATOM   | 34       | N1       | G A      | 2        | 17.197 | 24.279 | 23.037 | 1.00 | 15.44 | N |
| ATOM   | 35       | C2       | G A      | 2        | 18.434 | 23.717 | 23.155 | 1.00 | 9.63  | C |
| ATOM   | 36       | N2       | G A      | 2        | 18.508 | 22.456 | 23.668 | 1.00 | 16.69 | N |
| ATOM   | 37       | N3       | G A      | 2        | 19.537 | 24.360 | 22.770 | 1.00 | 30.98 | N |
| ATOM   | 38       | C4       | G A      | 2        | 19.290 | 25.594 | 22.274 | 1.00 | 18.56 | C |
| ATOM   | 39       | P        | C A      | 3        | 25.064 | 25.621 | 19.252 | 1.00 | 44.67 | P |
| ATOM   | 40       | O1P      | C A      | 3        | 26.506 | 25.316 | 19.220 | 1.00 | 53.89 | O |
| ATOM   | 41       | O2P      | C A      | 3        | 24.559 | 26.412 | 18.115 | 1.00 | 57.79 | O |
| ATOM   | 42       | O5*      | C A      | 3        | 24.260 | 24.246 | 19.327 | 1.00 | 35.42 | O |
| ATOM   | 43       | C5*      | C A      | 3        | 24.584 | 23.285 | 20.335 | 1.00 | 45.75 | C |
| ATOM   | 44       | C4*      | C A      | 3        | 23.523 | 22.233 | 20.245 | 1.00 | 43.02 | C |
| ATOM   | 45       | O4*      | C A      | 3        | 22.256 | 22.844 | 20.453 | 1.00 | 36.85 | O |
| ATOM   | 46       | C3*      | C A      | 3        | 23.424 | 21.557 | 18.903 | 1.00 | 40.14 | C |
| ATOM   | 47       | O3*      | C A      | 3        | 24.121 | 20.309 | 18.928 | 1.00 | 49.62 | O |
| ATOM   | 48       | C2*      | C A      | 3        | 21.930 | 21.406 | 18.661 | 1.00 | 53.79 | C |
| ATOM   | 49       | C1*      | C A      | 3        | 21.278 | 21.966 | 19.909 | 1.00 | 22.18 | C |
| ATOM   | 50       | N1       | C A      | 3        | 20.196 | 22.889 | 19.521 | 1.00 | 25.44 | N |
| ATOM   | 51       | C2       | C A      | 3        | 18.909 | 22.584 | 19.816 | 1.00 | 19.81 | C |
| ATOM   | 52       | O2       | C A      | 3        | 18.685 | 21.512 | 20.382 | 1.00 | 29.92 | O |
| ATOM   | 53       | N3       | C A      | 3        | 17.935 | 23.447 | 19.502 | 1.00 | 21.59 | N |
| ATOM   | 54       | C4       | C A      | 3        | 18.217 | 24.603 | 18.897 | 1.00 | 14.01 | C |
| ATOM   | 55       | N4       | C A      | 3        | 17.221 | 25.499 | 18.629 | 1.00 | 26.88 | N |
| ATOM   | 56       | C5       | C A      | 3        | 19.526 | 24.945 | 18.571 | 1.00 | 27.59 | C |

|      |     |     |     |   |        |        |        |      |       |   |
|------|-----|-----|-----|---|--------|--------|--------|------|-------|---|
| ATOM | 57  | C6  | C A | 3 | 20.537 | 24.048 | 18.899 | 1.00 | 27.05 | C |
| ATOM | 58  | P   | G A | 4 | 24.249 | 19.412 | 17.617 | 1.00 | 44.54 | P |
| ATOM | 59  | 01P | G A | 4 | 25.420 | 18.535 | 17.765 | 1.00 | 61.90 | O |
| ATOM | 60  | 02P | G A | 4 | 24.208 | 20.296 | 16.440 | 1.00 | 37.36 | O |
| ATOM | 61  | 05* | G A | 4 | 22.931 | 18.537 | 17.670 | 1.00 | 32.01 | O |
| ATOM | 62  | C5* | G A | 4 | 22.714 | 17.625 | 18.753 | 1.00 | 37.89 | C |
| ATOM | 63  | C4* | G A | 4 | 21.393 | 16.960 | 18.505 | 1.00 | 53.00 | C |
| ATOM | 64  | 04* | G A | 4 | 20.353 | 17.952 | 18.496 | 1.00 | 38.79 | O |
| ATOM | 65  | C3* | G A | 4 | 21.264 | 16.229 | 17.176 | 1.00 | 56.72 | C |
| ATOM | 66  | 03* | G A | 4 | 20.284 | 15.214 | 17.238 | 1.00 | 64.12 | O |
| ATOM | 67  | C2* | G A | 4 | 20.793 | 17.368 | 16.288 | 1.00 | 40.81 | C |
| ATOM | 68  | C1* | G A | 4 | 19.716 | 17.901 | 17.218 | 1.00 | 30.52 | C |
| ATOM | 69  | N9  | G A | 4 | 19.305 | 19.281 | 16.869 | 1.00 | 28.53 | N |
| ATOM | 70  | C8  | G A | 4 | 20.017 | 20.263 | 16.232 | 1.00 | 27.82 | C |
| ATOM | 71  | N7  | G A | 4 | 19.313 | 21.394 | 16.077 | 1.00 | 28.01 | N |
| ATOM | 72  | C5  | G A | 4 | 18.121 | 21.100 | 16.635 | 1.00 | 23.22 | C |
| ATOM | 73  | C6  | G A | 4 | 16.952 | 21.904 | 16.749 | 1.00 | 29.21 | C |
| ATOM | 74  | O6  | G A | 4 | 16.769 | 23.057 | 16.368 | 1.00 | 38.58 | O |
| ATOM | 75  | N1  | G A | 4 | 15.933 | 21.214 | 17.352 | 1.00 | 27.94 | N |
| ATOM | 76  | C2  | G A | 4 | 15.972 | 19.930 | 17.816 | 1.00 | 23.44 | C |
| ATOM | 77  | N2  | G A | 4 | 14.831 | 19.416 | 18.353 | 1.00 | 42.64 | N |
| ATOM | 78  | N3  | G A | 4 | 17.068 | 19.179 | 17.717 | 1.00 | 21.56 | N |
| ATOM | 79  | C4  | G A | 4 | 18.084 | 19.825 | 17.121 | 1.00 | 23.44 | C |
| ATOM | 80  | P   | A A | 5 | 20.356 | 13.969 | 16.245 | 1.00 | 57.01 | P |
| ATOM | 81  | 01P | A A | 5 | 21.116 | 12.891 | 16.892 | 1.00 | 58.59 | O |
| ATOM | 82  | 02P | A A | 5 | 20.837 | 14.423 | 14.910 | 1.00 | 51.96 | O |
| ATOM | 83  | 05* | A A | 5 | 18.810 | 13.581 | 16.161 | 1.00 | 47.12 | O |
| ATOM | 84  | C5* | A A | 5 | 18.015 | 13.569 | 17.362 | 1.00 | 47.67 | C |
| ATOM | 85  | C4* | A A | 5 | 16.672 | 14.088 | 16.957 | 1.00 | 64.79 | C |
| ATOM | 86  | 04* | A A | 5 | 16.842 | 15.447 | 16.561 | 1.00 | 47.60 | O |
| ATOM | 87  | C3* | A A | 5 | 16.019 | 13.393 | 15.764 | 1.00 | 51.50 | C |
| ATOM | 88  | 03* | A A | 5 | 14.762 | 12.796 | 16.120 | 1.00 | 52.18 | O |
| ATOM | 89  | C2* | A A | 5 | 15.952 | 14.498 | 14.696 | 1.00 | 45.00 | C |
| ATOM | 90  | C1* | A A | 5 | 15.851 | 15.732 | 15.569 | 1.00 | 26.88 | C |
| ATOM | 91  | N9  | A A | 5 | 16.391 | 16.916 | 14.867 | 1.00 | 16.69 | N |
| ATOM | 92  | C8  | A A | 5 | 17.658 | 17.103 | 14.382 | 1.00 | 28.14 | C |
| ATOM | 93  | N7  | A A | 5 | 17.863 | 18.346 | 13.913 | 1.00 | 34.85 | N |
| ATOM | 94  | C5  | A A | 5 | 16.673 | 18.953 | 14.098 | 1.00 | 22.49 | C |
| ATOM | 95  | C6  | A A | 5 | 16.230 | 20.279 | 13.819 | 1.00 | 18.12 | C |
| ATOM | 96  | N6  | A A | 5 | 17.045 | 21.222 | 13.268 | 1.00 | 29.30 | N |
| ATOM | 97  | N1  | A A | 5 | 14.966 | 20.578 | 14.118 | 1.00 | 27.61 | N |
| ATOM | 98  | C2  | A A | 5 | 14.178 | 19.652 | 14.669 | 1.00 | 18.53 | C |
| ATOM | 99  | N3  | A A | 5 | 14.463 | 18.392 | 14.984 | 1.00 | 29.16 | N |
| ATOM | 100 | C4  | A A | 5 | 15.750 | 18.110 | 14.661 | 1.00 | 15.08 | C |
| ATOM | 101 | P   | A A | 6 | 13.866 | 12.006 | 15.063 | 1.00 | 43.68 | P |
| ATOM | 102 | 01P | A A | 6 | 13.028 | 11.039 | 15.800 | 1.00 | 42.55 | O |
| ATOM | 103 | 02P | A A | 6 | 14.715 | 11.499 | 13.968 | 1.00 | 54.20 | O |
| ATOM | 104 | 05* | A A | 6 | 12.879 | 13.111 | 14.480 | 1.00 | 28.20 | O |
| ATOM | 105 | C5* | A A | 6 | 11.802 | 13.597 | 15.290 | 1.00 | 42.29 | C |
| ATOM | 106 | C4* | A A | 6 | 11.111 | 14.603 | 14.435 | 1.00 | 33.23 | C |
| ATOM | 107 | 04* | A A | 6 | 12.152 | 15.460 | 13.962 | 1.00 | 41.48 | O |
| ATOM | 108 | C3* | A A | 6 | 10.417 | 14.070 | 13.187 | 1.00 | 18.16 | C |
| ATOM | 109 | 03* | A A | 6 | 9.007  | 14.369 | 13.181 | 1.00 | 30.42 | O |
| ATOM | 110 | C2* | A A | 6 | 11.240 | 14.692 | 12.061 | 1.00 | 52.97 | C |
| ATOM | 111 | C1* | A A | 6 | 11.699 | 15.974 | 12.719 | 1.00 | 38.93 | C |
| ATOM | 112 | N9  | A A | 6 | 12.918 | 16.526 | 12.078 | 1.00 | 19.06 | N |
| ATOM | 113 | C8  | A A | 6 | 14.115 | 15.899 | 11.868 | 1.00 | 17.83 | C |
| ATOM | 114 | N7  | A A | 6 | 15.049 | 16.714 | 11.356 | 1.00 | 29.55 | N |
| ATOM | 115 | C5  | A A | 6 | 14.416 | 17.901 | 11.246 | 1.00 | 19.88 | C |
| ATOM | 116 | C6  | A A | 6 | 14.873 | 19.187 | 10.815 | 1.00 | 17.26 | C |
| ATOM | 117 | N6  | A A | 6 | 16.161 | 19.418 | 10.427 | 1.00 | 19.85 | N |
| ATOM | 118 | N1  | A A | 6 | 13.999 | 20.191 | 10.852 | 1.00 | 17.93 | N |

|      |     |     |     |   |        |        |        |      |       |   |
|------|-----|-----|-----|---|--------|--------|--------|------|-------|---|
| ATOM | 119 | C2  | A A | 6 | 12.753 | 19.962 | 11.272 | 1.00 | 23.00 | C |
| ATOM | 120 | N3  | A A | 6 | 12.210 | 18.824 | 11.698 | 1.00 | 21.37 | N |
| ATOM | 121 | C4  | A A | 6 | 13.116 | 17.823 | 11.657 | 1.00 | 15.93 | C |
| ATOM | 122 | P   | T A | 7 | 8.081  | 14.050 | 11.915 | 1.00 | 40.72 | P |
| ATOM | 123 | 01P | T A | 7 | 6.668  | 13.960 | 12.342 | 1.00 | 46.75 | O |
| ATOM | 124 | 02P | T A | 7 | 8.600  | 12.894 | 11.137 | 1.00 | 42.53 | O |
| ATOM | 125 | 05* | T A | 7 | 8.239  | 15.387 | 11.076 | 1.00 | 35.21 | O |
| ATOM | 126 | C5* | T A | 7 | 7.907  | 16.635 | 11.686 | 1.00 | 34.88 | C |
| ATOM | 127 | C4* | T A | 7 | 8.162  | 17.628 | 10.598 | 1.00 | 31.45 | C |
| ATOM | 128 | 04* | T A | 7 | 9.543  | 17.580 | 10.279 | 1.00 | 46.82 | O |
| ATOM | 129 | C3* | T A | 7 | 7.461  | 17.284 | 9.296  | 1.00 | 23.76 | C |
| ATOM | 130 | 03* | T A | 7 | 6.251  | 18.034 | 9.162  | 1.00 | 44.27 | O |
| ATOM | 131 | C2* | T A | 7 | 8.532  | 17.527 | 8.223  | 1.00 | 26.30 | C |
| ATOM | 132 | C1* | T A | 7 | 9.644  | 18.209 | 9.019  | 1.00 | 28.96 | C |
| ATOM | 133 | N1  | T A | 7 | 11.021 | 17.903 | 8.565  | 1.00 | 20.47 | N |
| ATOM | 134 | C2  | T A | 7 | 11.822 | 18.923 | 8.176  | 1.00 | 28.01 | C |
| ATOM | 135 | 02  | T A | 7 | 11.383 | 20.077 | 8.143  | 1.00 | 40.01 | O |
| ATOM | 136 | N3  | T A | 7 | 13.119 | 18.641 | 7.852  | 1.00 | 27.94 | N |
| ATOM | 137 | C4  | T A | 7 | 13.633 | 17.372 | 7.882  | 1.00 | 15.14 | C |
| ATOM | 138 | 04  | T A | 7 | 14.830 | 17.222 | 7.619  | 1.00 | 32.54 | O |
| ATOM | 139 | C5  | T A | 7 | 12.781 | 16.325 | 8.235  | 1.00 | 10.83 | C |
| ATOM | 140 | C5M | T A | 7 | 13.269 | 14.902 | 8.236  | 1.00 | 36.33 | C |
| ATOM | 141 | C6  | T A | 7 | 11.465 | 16.616 | 8.594  | 1.00 | 12.19 | C |
| ATOM | 142 | P   | T A | 8 | 5.384  | 17.990 | 7.824  | 1.00 | 49.10 | P |
| ATOM | 143 | 01P | T A | 8 | 4.025  | 18.444 | 8.180  | 1.00 | 41.11 | O |
| ATOM | 144 | 02P | T A | 8 | 5.458  | 16.668 | 7.160  | 1.00 | 39.21 | O |
| ATOM | 145 | 05* | T A | 8 | 6.086  | 19.118 | 6.927  | 1.00 | 48.80 | O |
| ATOM | 146 | C5* | T A | 8 | 6.146  | 20.478 | 7.418  | 1.00 | 34.73 | C |
| ATOM | 147 | C4* | T A | 8 | 6.995  | 21.229 | 6.438  | 1.00 | 28.73 | C |
| ATOM | 148 | 04* | T A | 8 | 8.188  | 20.458 | 6.284  | 1.00 | 39.07 | O |
| ATOM | 149 | C3* | T A | 8 | 6.418  | 21.332 | 5.029  | 1.00 | 37.88 | C |
| ATOM | 150 | 03* | T A | 8 | 5.967  | 22.667 | 4.696  | 1.00 | 52.04 | O |
| ATOM | 151 | C2* | T A | 8 | 7.513  | 20.718 | 4.139  | 1.00 | 32.80 | C |
| ATOM | 152 | C1* | T A | 8 | 8.736  | 20.855 | 5.034  | 1.00 | 36.58 | C |
| ATOM | 153 | N1  | T A | 8 | 9.823  | 19.876 | 4.759  | 1.00 | 24.57 | N |
| ATOM | 154 | C2  | T A | 8 | 11.086 | 20.316 | 4.494  | 1.00 | 19.41 | C |
| ATOM | 155 | 02  | T A | 8 | 11.324 | 21.516 | 4.389  | 1.00 | 32.74 | O |
| ATOM | 156 | N3  | T A | 8 | 12.094 | 19.403 | 4.412  | 1.00 | 25.12 | N |
| ATOM | 157 | C4  | T A | 8 | 11.876 | 18.060 | 4.551  | 1.00 | 31.35 | C |
| ATOM | 158 | 04  | T A | 8 | 12.858 | 17.317 | 4.503  | 1.00 | 28.53 | O |
| ATOM | 159 | C5  | T A | 8 | 10.569 | 17.611 | 4.765  | 1.00 | 22.80 | C |
| ATOM | 160 | C5M | T A | 8 | 10.261 | 16.140 | 4.896  | 1.00 | 24.98 | C |
| ATOM | 161 | C6  | T A | 8 | 9.545  | 18.548 | 4.904  | 1.00 | 20.28 | C |
| ATOM | 162 | P   | C A | 9 | 5.531  | 23.071 | 3.209  | 1.00 | 48.97 | P |
| ATOM | 163 | 01P | C A | 9 | 4.648  | 24.244 | 3.269  | 1.00 | 62.33 | O |
| ATOM | 164 | 02P | C A | 9 | 5.010  | 21.905 | 2.470  | 1.00 | 51.53 | O |
| ATOM | 165 | 05* | C A | 9 | 6.926  | 23.547 | 2.611  | 1.00 | 43.99 | O |
| ATOM | 166 | C5* | C A | 9 | 7.636  | 24.627 | 3.249  | 1.00 | 50.86 | C |
| ATOM | 167 | C4* | C A | 9 | 8.897  | 24.853 | 2.457  | 1.00 | 46.66 | C |
| ATOM | 168 | 04* | C A | 9 | 9.638  | 23.627 | 2.448  | 1.00 | 42.69 | O |
| ATOM | 169 | C3* | C A | 9 | 8.717  | 25.240 | 0.998  | 1.00 | 56.96 | C |
| ATOM | 170 | 03* | C A | 9 | 9.470  | 26.414 | 0.667  | 1.00 | 63.54 | O |
| ATOM | 171 | C2* | C A | 9 | 9.126  | 23.965 | 0.253  | 1.00 | 50.41 | C |
| ATOM | 172 | C1* | C A | 9 | 10.241 | 23.483 | 1.157  | 1.00 | 41.08 | C |
| ATOM | 173 | N1  | C A | 9 | 10.524 | 22.022 | 1.015  | 1.00 | 37.23 | N |
| ATOM | 174 | C2  | C A | 9 | 11.814 | 21.603 | 0.840  | 1.00 | 40.54 | C |
| ATOM | 175 | 02  | C A | 9 | 12.691 | 22.447 | 0.670  | 1.00 | 43.89 | O |
| ATOM | 176 | N3  | C A | 9 | 12.106 | 20.297 | 0.873  | 1.00 | 32.57 | N |
| ATOM | 177 | C4  | C A | 9 | 11.141 | 19.395 | 1.046  | 1.00 | 24.65 | C |
| ATOM | 178 | N4  | C A | 9 | 11.461 | 18.075 | 1.089  | 1.00 | 27.84 | N |
| ATOM | 179 | C5  | C A | 9 | 9.803  | 19.775 | 1.177  | 1.00 | 17.61 | C |
| ATOM | 180 | C6  | C A | 9 | 9.499  | 21.133 | 1.167  | 1.00 | 30.63 | C |

|      |     |     |     |    |        |        |         |      |       |   |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|---|
| ATOM | 181 | P   | G A | 10 | 9.055  | 27.333 | -0.581  | 1.00 | 65.48 | P |
| ATOM | 182 | 01P | G A | 10 | 9.496  | 28.717 | -0.258  | 1.00 | 59.09 | O |
| ATOM | 183 | 02P | G A | 10 | 7.632  | 27.106 | -0.947  | 1.00 | 45.71 | O |
| ATOM | 184 | 05* | G A | 10 | 9.954  | 26.765 | -1.771  | 1.00 | 70.30 | O |
| ATOM | 185 | C5* | G A | 10 | 11.382 | 26.940 | -1.720  | 1.00 | 71.73 | C |
| ATOM | 186 | C4* | G A | 10 | 11.972 | 26.090 | -2.802  | 1.00 | 58.69 | C |
| ATOM | 187 | 04* | G A | 10 | 11.802 | 24.724 | -2.404  | 1.00 | 41.03 | O |
| ATOM | 188 | C3* | G A | 10 | 11.327 | 26.178 | -4.188  | 1.00 | 45.61 | C |
| ATOM | 189 | 03* | G A | 10 | 12.311 | 26.096 | -5.214  | 1.00 | 52.70 | O |
| ATOM | 190 | C2* | G A | 10 | 10.414 | 24.962 | -4.186  | 1.00 | 36.02 | C |
| ATOM | 191 | C1* | G A | 10 | 11.429 | 24.028 | -3.587  | 1.00 | 50.90 | C |
| ATOM | 192 | N9  | G A | 10 | 10.890 | 22.713 | -3.200  | 1.00 | 45.86 | N |
| ATOM | 193 | C8  | G A | 10 | 9.616  | 22.315 | -2.910  | 1.00 | 44.49 | C |
| ATOM | 194 | N7  | G A | 10 | 9.541  | 21.009 | -2.613  | 1.00 | 39.96 | N |
| ATOM | 195 | C5  | G A | 10 | 10.818 | 20.588 | -2.718  | 1.00 | 38.99 | C |
| ATOM | 196 | C6  | G A | 10 | 11.376 | 19.292 | -2.511  | 1.00 | 35.78 | C |
| ATOM | 197 | O6  | G A | 10 | 10.813 | 18.252 | -2.179  | 1.00 | 34.90 | O |
| ATOM | 198 | N1  | G A | 10 | 12.729 | 19.299 | -2.720  | 1.00 | 23.54 | N |
| ATOM | 199 | C2  | G A | 10 | 13.498 | 20.365 | -3.082  | 1.00 | 8.73  | C |
| ATOM | 200 | N2  | G A | 10 | 14.834 | 20.169 | -3.237  | 1.00 | 23.15 | N |
| ATOM | 201 | N3  | G A | 10 | 12.982 | 21.573 | -3.267  | 1.00 | 24.68 | N |
| ATOM | 202 | C4  | G A | 10 | 11.656 | 21.601 | -3.061  | 1.00 | 31.53 | C |
| ATOM | 203 | P   | C A | 11 | 12.763 | 27.421 | -5.980  | 1.00 | 60.62 | P |
| ATOM | 204 | 01P | C A | 11 | 12.796 | 28.572 | -5.049  | 1.00 | 63.74 | O |
| ATOM | 205 | 02P | C A | 11 | 11.886 | 27.542 | -7.164  | 1.00 | 52.44 | O |
| ATOM | 206 | 05* | C A | 11 | 14.272 | 27.086 | -6.366  | 1.00 | 57.57 | O |
| ATOM | 207 | C5* | C A | 11 | 15.275 | 27.108 | -5.318  | 1.00 | 54.70 | C |
| ATOM | 208 | C4* | C A | 11 | 16.222 | 25.946 | -5.510  | 1.00 | 72.51 | C |
| ATOM | 209 | 04* | C A | 11 | 15.443 | 24.754 | -5.397  | 1.00 | 47.18 | O |
| ATOM | 210 | C3* | C A | 11 | 16.942 | 25.827 | -6.848  | 1.00 | 29.82 | C |
| ATOM | 211 | 03* | C A | 11 | 18.340 | 25.511 | -6.701  | 1.00 | 43.53 | O |
| ATOM | 212 | C2* | C A | 11 | 16.118 | 24.767 | -7.578  | 1.00 | 51.34 | C |
| ATOM | 213 | C1* | C A | 11 | 15.856 | 23.836 | -6.414  | 1.00 | 30.07 | C |
| ATOM | 214 | N1  | C A | 11 | 14.672 | 22.975 | -6.637  | 1.00 | 23.25 | N |
| ATOM | 215 | C2  | C A | 11 | 14.802 | 21.628 | -6.529  | 1.00 | 20.38 | C |
| ATOM | 216 | O2  | C A | 11 | 15.924 | 21.178 | -6.314  | 1.00 | 38.77 | O |
| ATOM | 217 | N3  | C A | 11 | 13.723 | 20.842 | -6.627  | 1.00 | 15.92 | N |
| ATOM | 218 | C4  | C A | 11 | 12.515 | 21.373 | -6.836  | 1.00 | 15.82 | C |
| ATOM | 219 | N4  | C A | 11 | 11.410 | 20.574 | -6.872  | 1.00 | 28.04 | N |
| ATOM | 220 | C5  | C A | 11 | 12.348 | 22.744 | -6.978  | 1.00 | 26.17 | C |
| ATOM | 221 | C6  | C A | 11 | 13.470 | 23.558 | -6.869  | 1.00 | 35.50 | C |
| ATOM | 222 | P   | G A | 12 | 19.331 | 25.774 | -7.925  | 1.00 | 55.98 | P |
| ATOM | 223 | 01P | G A | 12 | 20.704 | 25.976 | -7.408  | 1.00 | 45.83 | O |
| ATOM | 224 | 02P | G A | 12 | 18.763 | 26.851 | -8.758  | 1.00 | 44.26 | O |
| ATOM | 225 | 05* | G A | 12 | 19.302 | 24.412 | -8.763  | 1.00 | 62.63 | O |
| ATOM | 226 | C5* | G A | 12 | 20.109 | 23.284 | -8.359  | 1.00 | 69.50 | C |
| ATOM | 227 | C4* | G A | 12 | 19.748 | 22.167 | -9.299  | 1.00 | 39.92 | C |
| ATOM | 228 | 04* | G A | 12 | 18.350 | 21.969 | -9.139  | 1.00 | 32.00 | O |
| ATOM | 229 | C3* | G A | 12 | 19.921 | 22.404 | -10.815 | 1.00 | 50.39 | C |
| ATOM | 230 | 03* | G A | 12 | 20.985 | 21.635 | -11.401 | 1.00 | 64.13 | O |
| ATOM | 231 | C2* | G A | 12 | 18.535 | 22.062 | -11.381 | 1.00 | 36.18 | C |
| ATOM | 232 | C1* | G A | 12 | 17.965 | 21.200 | -10.269 | 1.00 | 24.79 | C |
| ATOM | 233 | N9  | G A | 12 | 16.493 | 21.220 | -10.265 | 1.00 | 28.44 | N |
| ATOM | 234 | C8  | G A | 12 | 15.663 | 22.289 | -10.478 | 1.00 | 31.85 | C |
| ATOM | 235 | N7  | G A | 12 | 14.368 | 21.958 | -10.390 | 1.00 | 38.26 | N |
| ATOM | 236 | C5  | G A | 12 | 14.388 | 20.640 | -10.102 | 1.00 | 28.99 | C |
| ATOM | 237 | C6  | G A | 12 | 13.301 | 19.742 | -9.856  | 1.00 | 42.63 | C |
| ATOM | 238 | O6  | G A | 12 | 12.091 | 19.967 | -9.857  | 1.00 | 49.17 | O |
| ATOM | 239 | N1  | G A | 12 | 13.750 | 18.466 | -9.625  | 1.00 | 40.15 | N |
| ATOM | 240 | C2  | G A | 12 | 15.042 | 18.043 | -9.605  | 1.00 | 33.42 | C |
| ATOM | 241 | N2  | G A | 12 | 15.259 | 16.717 | -9.406  | 1.00 | 40.53 | N |
| ATOM | 242 | N3  | G A | 12 | 16.061 | 18.885 | -9.792  | 1.00 | 37.34 | N |

|      |     |     |     |    |        |        |         |      |       |   |
|------|-----|-----|-----|----|--------|--------|---------|------|-------|---|
| ATOM | 243 | C4  | G A | 12 | 15.660 | 20.156 | -10.027 | 1.00 | 31.14 | C |
| TER  | 244 |     | G A | 12 |        |        |         |      |       |   |
| ATOM | 245 | O5* | C B | 13 | 7.458  | 11.884 | -9.070  | 1.00 | 66.23 | O |
| ATOM | 246 | C5* | C B | 13 | 8.252  | 10.968 | -9.854  | 1.00 | 71.49 | C |
| ATOM | 247 | C4* | C B | 13 | 9.714  | 11.141 | -9.512  | 1.00 | 56.82 | C |
| ATOM | 248 | O4* | C B | 13 | 10.144 | 12.455 | -9.908  | 1.00 | 57.92 | O |
| ATOM | 249 | C3* | C B | 13 | 10.103 | 10.989 | -8.055  | 1.00 | 34.34 | C |
| ATOM | 250 | O3* | C B | 13 | 11.293 | 10.221 | -7.904  | 1.00 | 42.11 | O |
| ATOM | 251 | C2* | C B | 13 | 10.254 | 12.437 | -7.607  | 1.00 | 29.08 | C |
| ATOM | 252 | C1* | C B | 13 | 10.896 | 13.044 | -8.837  | 1.00 | 38.40 | C |
| ATOM | 253 | N1  | C B | 13 | 10.575 | 14.487 | -8.944  | 1.00 | 34.33 | N |
| ATOM | 254 | C2  | C B | 13 | 11.559 | 15.430 | -9.006  | 1.00 | 22.98 | C |
| ATOM | 255 | O2  | C B | 13 | 12.725 | 15.066 | -8.932  | 1.00 | 50.83 | O |
| ATOM | 256 | N3  | C B | 13 | 11.246 | 16.714 | -9.193  | 1.00 | 37.14 | N |
| ATOM | 257 | C4  | C B | 13 | 9.980  | 17.088 | -9.334  | 1.00 | 42.60 | C |
| ATOM | 258 | N4  | C B | 13 | 9.698  | 18.395 | -9.589  | 1.00 | 54.91 | N |
| ATOM | 259 | C5  | C B | 13 | 8.939  | 16.162 | -9.274  | 1.00 | 56.67 | C |
| ATOM | 260 | C6  | C B | 13 | 9.265  | 14.824 | -9.080  | 1.00 | 49.21 | C |
| ATOM | 261 | P   | G B | 14 | 11.602 | 9.510  | -6.502  | 1.00 | 60.42 | P |
| ATOM | 262 | O1P | G B | 14 | 11.666 | 8.032  | -6.664  | 1.00 | 57.44 | O |
| ATOM | 263 | O2P | G B | 14 | 10.644 | 10.010 | -5.494  | 1.00 | 46.07 | O |
| ATOM | 264 | O5* | G B | 14 | 13.051 | 10.094 | -6.177  | 1.00 | 50.94 | O |
| ATOM | 265 | C5* | G B | 14 | 14.100 | 10.021 | -7.156  | 1.00 | 34.84 | C |
| ATOM | 266 | C4* | G B | 14 | 15.113 | 10.992 | -6.657  | 1.00 | 48.06 | C |
| ATOM | 267 | O4* | G B | 14 | 14.556 | 12.300 | -6.755  | 1.00 | 37.01 | O |
| ATOM | 268 | C3* | G B | 14 | 15.445 | 10.806 | -5.189  | 1.00 | 50.58 | C |
| ATOM | 269 | O3* | G B | 14 | 16.836 | 10.560 | -5.013  | 1.00 | 51.98 | O |
| ATOM | 270 | C2* | G B | 14 | 14.937 | 12.100 | -4.529  | 1.00 | 40.32 | C |
| ATOM | 271 | C1* | G B | 14 | 15.058 | 13.086 | -5.671  | 1.00 | 46.69 | C |
| ATOM | 272 | N9  | G B | 14 | 14.036 | 14.140 | -5.536  | 1.00 | 29.17 | N |
| ATOM | 273 | C8  | G B | 14 | 12.710 | 13.957 | -5.259  | 1.00 | 23.48 | C |
| ATOM | 274 | N7  | G B | 14 | 12.016 | 15.103 | -5.269  | 1.00 | 37.54 | N |
| ATOM | 275 | C5  | G B | 14 | 12.937 | 16.041 | -5.558  | 1.00 | 26.27 | C |
| ATOM | 276 | C6  | G B | 14 | 12.761 | 17.451 | -5.710  | 1.00 | 40.82 | C |
| ATOM | 277 | O6  | G B | 14 | 11.723 | 18.111 | -5.630  | 1.00 | 44.39 | O |
| ATOM | 278 | N1  | G B | 14 | 13.952 | 18.079 | -5.973  | 1.00 | 19.52 | N |
| ATOM | 279 | C2  | G B | 14 | 15.171 | 17.485 | -6.107  | 1.00 | 18.48 | C |
| ATOM | 280 | N2  | G B | 14 | 16.244 | 18.292 | -6.325  | 1.00 | 36.58 | N |
| ATOM | 281 | N3  | G B | 14 | 15.329 | 16.161 | -5.986  | 1.00 | 46.96 | N |
| ATOM | 282 | C4  | G B | 14 | 14.179 | 15.499 | -5.721  | 1.00 | 35.70 | C |
| ATOM | 283 | P   | C B | 15 | 17.478 | 10.380 | -3.569  | 1.00 | 46.26 | P |
| ATOM | 284 | O1P | C B | 15 | 18.665 | 9.516  | -3.729  | 1.00 | 46.07 | O |
| ATOM | 285 | O2P | C B | 15 | 16.427 | 9.940  | -2.633  | 1.00 | 40.43 | O |
| ATOM | 286 | O5* | C B | 15 | 17.957 | 11.865 | -3.208  | 1.00 | 40.97 | O |
| ATOM | 287 | C5* | C B | 15 | 18.963 | 12.531 | -3.996  | 1.00 | 28.78 | C |
| ATOM | 288 | C4* | C B | 15 | 18.936 | 13.958 | -3.536  | 1.00 | 32.84 | C |
| ATOM | 289 | O4* | C B | 15 | 17.592 | 14.409 | -3.622  | 1.00 | 37.24 | O |
| ATOM | 290 | C3* | C B | 15 | 19.253 | 14.139 | -2.066  | 1.00 | 43.98 | C |
| ATOM | 291 | O3* | C B | 15 | 20.659 | 14.219 | -1.858  | 1.00 | 40.90 | O |
| ATOM | 292 | C2* | C B | 15 | 18.520 | 15.417 | -1.728  | 1.00 | 36.26 | C |
| ATOM | 293 | C1* | C B | 15 | 17.545 | 15.602 | -2.872  | 1.00 | 20.54 | C |
| ATOM | 294 | N1  | C B | 15 | 16.145 | 15.696 | -2.428  | 1.00 | 23.10 | N |
| ATOM | 295 | C2  | C B | 15 | 15.507 | 16.886 | -2.558  | 1.00 | 32.12 | C |
| ATOM | 296 | O2  | C B | 15 | 16.162 | 17.846 | -2.957  | 1.00 | 30.04 | O |
| ATOM | 297 | N3  | C B | 15 | 14.209 | 16.983 | -2.264  | 1.00 | 32.94 | N |
| ATOM | 298 | C4  | C B | 15 | 13.536 | 15.919 | -1.825  | 1.00 | 16.43 | C |
| ATOM | 299 | N4  | C B | 15 | 12.205 | 16.017 | -1.553  | 1.00 | 34.91 | N |
| ATOM | 300 | C5  | C B | 15 | 14.164 | 14.689 | -1.652  | 1.00 | 22.75 | C |
| ATOM | 301 | C6  | C B | 15 | 15.509 | 14.584 | -1.979  | 1.00 | 26.42 | C |
| ATOM | 302 | P   | G B | 16 | 21.304 | 14.529 | -0.436  | 1.00 | 42.39 | P |
| ATOM | 303 | O1P | G B | 16 | 22.696 | 14.087 | -0.524  | 1.00 | 60.41 | O |
| ATOM | 304 | O2P | G B | 16 | 20.488 | 13.954 | 0.650   | 1.00 | 51.09 | O |

|      |     |     |     |    |        |        |        |      |       |   |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|---|
| ATOM | 305 | 05* | G B | 16 | 21.306 | 16.117 | -0.363 | 1.00 | 45.08 | O |
| ATOM | 306 | C5* | G B | 16 | 22.177 | 16.876 | -1.212 | 1.00 | 33.20 | C |
| ATOM | 307 | C4* | G B | 16 | 21.739 | 18.292 | -1.021 | 1.00 | 24.95 | C |
| ATOM | 308 | 04* | G B | 16 | 20.305 | 18.225 | -1.048 | 1.00 | 32.83 | O |
| ATOM | 309 | C3* | G B | 16 | 22.101 | 18.959 | 0.293  | 1.00 | 41.12 | C |
| ATOM | 310 | 03* | G B | 16 | 22.592 | 20.293 | 0.097  | 1.00 | 53.45 | O |
| ATOM | 311 | C2* | G B | 16 | 20.820 | 18.829 | 1.121  | 1.00 | 28.93 | C |
| ATOM | 312 | C1* | G B | 16 | 19.765 | 18.985 | 0.046  | 1.00 | 37.44 | C |
| ATOM | 313 | N9  | G B | 16 | 18.513 | 18.299 | 0.468  | 1.00 | 17.75 | N |
| ATOM | 314 | C8  | G B | 16 | 18.363 | 17.062 | 1.039  | 1.00 | 17.96 | C |
| ATOM | 315 | N7  | G B | 16 | 17.080 | 16.744 | 1.281  | 1.00 | 24.14 | N |
| ATOM | 316 | C5  | G B | 16 | 16.400 | 17.832 | 0.868  | 1.00 | 9.96  | C |
| ATOM | 317 | C6  | G B | 16 | 14.996 | 18.090 | 0.882  | 1.00 | 18.10 | C |
| ATOM | 318 | 06  | G B | 16 | 14.082 | 17.378 | 1.280  | 1.00 | 31.13 | O |
| ATOM | 319 | N1  | G B | 16 | 14.712 | 19.349 | 0.418  | 1.00 | 17.72 | N |
| ATOM | 320 | C2  | G B | 16 | 15.606 | 20.268 | -0.027 | 1.00 | 16.23 | C |
| ATOM | 321 | N2  | G B | 16 | 15.134 | 21.493 | -0.382 | 1.00 | 33.42 | N |
| ATOM | 322 | N3  | G B | 16 | 16.912 | 20.017 | -0.072 | 1.00 | 26.37 | N |
| ATOM | 323 | C4  | G B | 16 | 17.236 | 18.794 | 0.384  | 1.00 | 31.72 | C |
| ATOM | 324 | P   | A B | 17 | 22.904 | 21.238 | 1.339  | 1.00 | 46.87 | P |
| ATOM | 325 | 01P | A B | 17 | 23.994 | 22.183 | 1.025  | 1.00 | 47.75 | O |
| ATOM | 326 | 02P | A B | 17 | 23.104 | 20.390 | 2.538  | 1.00 | 46.81 | O |
| ATOM | 327 | 05* | A B | 17 | 21.577 | 22.107 | 1.390  | 1.00 | 39.51 | O |
| ATOM | 328 | C5* | A B | 17 | 21.216 | 22.833 | 0.200  | 1.00 | 30.37 | C |
| ATOM | 329 | C4* | A B | 17 | 20.101 | 23.788 | 0.484  | 1.00 | 35.43 | C |
| ATOM | 330 | 04* | A B | 17 | 18.913 | 23.054 | 0.816  | 1.00 | 43.05 | O |
| ATOM | 331 | C3* | A B | 17 | 20.347 | 24.743 | 1.633  | 1.00 | 44.50 | C |
| ATOM | 332 | 03* | A B | 17 | 19.732 | 26.010 | 1.411  | 1.00 | 78.59 | O |
| ATOM | 333 | C2* | A B | 17 | 19.752 | 23.945 | 2.791  | 1.00 | 44.42 | C |
| ATOM | 334 | C1* | A B | 17 | 18.497 | 23.393 | 2.145  | 1.00 | 42.55 | C |
| ATOM | 335 | N9  | A B | 17 | 18.079 | 22.095 | 2.758  | 1.00 | 34.56 | N |
| ATOM | 336 | C8  | A B | 17 | 18.847 | 21.020 | 3.133  | 1.00 | 20.07 | C |
| ATOM | 337 | N7  | A B | 17 | 18.114 | 19.984 | 3.584  | 1.00 | 27.60 | N |
| ATOM | 338 | C5  | A B | 17 | 16.842 | 20.424 | 3.488  | 1.00 | 18.80 | C |
| ATOM | 339 | C6  | A B | 17 | 15.577 | 19.817 | 3.786  | 1.00 | 32.58 | C |
| ATOM | 340 | N6  | A B | 17 | 15.448 | 18.537 | 4.242  | 1.00 | 29.54 | N |
| ATOM | 341 | N1  | A B | 17 | 14.482 | 20.557 | 3.593  | 1.00 | 35.01 | N |
| ATOM | 342 | C2  | A B | 17 | 14.597 | 21.801 | 3.118  | 1.00 | 36.47 | C |
| ATOM | 343 | N3  | A B | 17 | 15.700 | 22.472 | 2.783  | 1.00 | 38.96 | N |
| ATOM | 344 | C4  | A B | 17 | 16.791 | 21.706 | 3.002  | 1.00 | 28.24 | C |
| ATOM | 345 | P   | A B | 18 | 19.803 | 27.141 | 2.526  | 1.00 | 46.11 | P |
| ATOM | 346 | 01P | A B | 18 | 19.796 | 28.478 | 1.888  | 1.00 | 49.20 | O |
| ATOM | 347 | 02P | A B | 18 | 20.953 | 26.858 | 3.426  | 1.00 | 43.48 | O |
| ATOM | 348 | 05* | A B | 18 | 18.396 | 26.939 | 3.241  | 1.00 | 40.83 | O |
| ATOM | 349 | C5* | A B | 18 | 17.203 | 27.028 | 2.452  | 1.00 | 40.72 | C |
| ATOM | 350 | C4* | A B | 18 | 16.035 | 26.958 | 3.388  | 1.00 | 66.52 | C |
| ATOM | 351 | 04* | A B | 18 | 15.856 | 25.612 | 3.850  | 1.00 | 44.25 | O |
| ATOM | 352 | C3* | A B | 18 | 16.101 | 27.861 | 4.615  | 1.00 | 63.34 | C |
| ATOM | 353 | 03* | A B | 18 | 14.890 | 28.608 | 4.757  | 1.00 | 55.65 | O |
| ATOM | 354 | C2* | A B | 18 | 16.368 | 26.844 | 5.724  | 1.00 | 34.49 | C |
| ATOM | 355 | C1* | A B | 18 | 15.561 | 25.655 | 5.243  | 1.00 | 29.45 | C |
| ATOM | 356 | N9  | A B | 18 | 16.104 | 24.373 | 5.755  | 1.00 | 20.03 | N |
| ATOM | 357 | C8  | A B | 18 | 17.411 | 23.967 | 5.830  | 1.00 | 16.51 | C |
| ATOM | 358 | N7  | A B | 18 | 17.539 | 22.706 | 6.276  | 1.00 | 20.58 | N |
| ATOM | 359 | C5  | A B | 18 | 16.266 | 22.309 | 6.480  | 1.00 | 21.66 | C |
| ATOM | 360 | C6  | A B | 18 | 15.715 | 21.073 | 6.933  | 1.00 | 17.93 | C |
| ATOM | 361 | N6  | A B | 18 | 16.483 | 19.994 | 7.243  | 1.00 | 20.37 | N |
| ATOM | 362 | N1  | A B | 18 | 14.389 | 20.994 | 7.036  | 1.00 | 20.81 | N |
| ATOM | 363 | C2  | A B | 18 | 13.636 | 22.041 | 6.708  | 1.00 | 26.77 | C |
| ATOM | 364 | N3  | A B | 18 | 14.019 | 23.234 | 6.265  | 1.00 | 26.83 | N |
| ATOM | 365 | C4  | A B | 18 | 15.367 | 23.291 | 6.174  | 1.00 | 27.48 | C |
| ATOM | 366 | P   | T B | 19 | 14.604 | 29.545 | 6.020  | 1.00 | 48.40 | P |

|      |     |     |     |    |        |        |        |      |       |   |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|---|
| ATOM | 367 | 01P | T B | 19 | 13.792 | 30.696 | 5.582  | 1.00 | 50.18 | O |
| ATOM | 368 | 02P | T B | 19 | 15.852 | 29.836 | 6.749  | 1.00 | 44.42 | O |
| ATOM | 369 | 05* | T B | 19 | 13.633 | 28.628 | 6.885  | 1.00 | 53.86 | O |
| ATOM | 370 | C5* | T B | 19 | 12.398 | 28.171 | 6.303  | 1.00 | 55.04 | C |
| ATOM | 371 | C4* | T B | 19 | 11.809 | 27.217 | 7.302  | 1.00 | 44.86 | C |
| ATOM | 372 | 04* | T B | 19 | 12.767 | 26.184 | 7.534  | 1.00 | 48.52 | O |
| ATOM | 373 | C3* | T B | 19 | 11.515 | 27.822 | 8.669  | 1.00 | 41.77 | C |
| ATOM | 374 | 03* | T B | 19 | 10.103 | 27.952 | 8.891  | 1.00 | 57.02 | O |
| ATOM | 375 | C2* | T B | 19 | 12.267 | 26.906 | 9.630  | 1.00 | 39.28 | C |
| ATOM | 376 | C1* | T B | 19 | 12.426 | 25.645 | 8.799  | 1.00 | 27.68 | C |
| ATOM | 377 | N1  | T B | 19 | 13.609 | 24.850 | 9.205  | 1.00 | 21.67 | N |
| ATOM | 378 | C2  | T B | 19 | 13.442 | 23.575 | 9.656  | 1.00 | 31.71 | C |
| ATOM | 379 | 02  | T B | 19 | 12.311 | 23.101 | 9.802  | 1.00 | 36.00 | O |
| ATOM | 380 | N3  | T B | 19 | 14.551 | 22.825 | 9.913  | 1.00 | 24.66 | N |
| ATOM | 381 | C4  | T B | 19 | 15.815 | 23.321 | 9.777  | 1.00 | 40.64 | C |
| ATOM | 382 | 04  | T B | 19 | 16.755 | 22.570 | 10.029 | 1.00 | 31.47 | O |
| ATOM | 383 | C5  | T B | 19 | 15.972 | 24.647 | 9.362  | 1.00 | 31.79 | C |
| ATOM | 384 | C5M | T B | 19 | 17.345 | 25.239 | 9.234  | 1.00 | 30.05 | C |
| ATOM | 385 | C6  | T B | 19 | 14.844 | 25.405 | 9.048  | 1.00 | 14.35 | C |
| ATOM | 386 | P   | T B | 20 | 9.513  | 28.533 | 10.260 | 1.00 | 48.24 | P |
| ATOM | 387 | 01P | T B | 20 | 8.145  | 29.007 | 9.998  | 1.00 | 41.28 | O |
| ATOM | 388 | 02P | T B | 20 | 10.455 | 29.513 | 10.841 | 1.00 | 53.39 | O |
| ATOM | 389 | 05* | T B | 20 | 9.395  | 27.223 | 11.153 | 1.00 | 36.57 | O |
| ATOM | 390 | C5* | T B | 20 | 8.576  | 26.148 | 10.664 | 1.00 | 50.41 | C |
| ATOM | 391 | C4* | T B | 20 | 8.655  | 25.060 | 11.678 | 1.00 | 32.08 | C |
| ATOM | 392 | 04* | T B | 20 | 10.003 | 24.615 | 11.764 | 1.00 | 48.38 | O |
| ATOM | 393 | C3* | T B | 20 | 8.272  | 25.471 | 13.087 | 1.00 | 29.99 | C |
| ATOM | 394 | 03* | T B | 20 | 7.199  | 24.657 | 13.553 | 1.00 | 45.14 | O |
| ATOM | 395 | C2* | T B | 20 | 9.586  | 25.307 | 13.860 | 1.00 | 32.42 | C |
| ATOM | 396 | C1* | T B | 20 | 10.190 | 24.148 | 13.089 | 1.00 | 39.56 | C |
| ATOM | 397 | N1  | T B | 20 | 11.660 | 24.070 | 13.205 | 1.00 | 20.36 | N |
| ATOM | 398 | C2  | T B | 20 | 12.257 | 22.880 | 13.486 | 1.00 | 27.55 | C |
| ATOM | 399 | 02  | T B | 20 | 11.583 | 21.866 | 13.691 | 1.00 | 38.33 | O |
| ATOM | 400 | N3  | T B | 20 | 13.620 | 22.829 | 13.497 | 1.00 | 29.60 | N |
| ATOM | 401 | C4  | T B | 20 | 14.402 | 23.914 | 13.225 | 1.00 | 30.11 | C |
| ATOM | 402 | 04  | T B | 20 | 15.625 | 23.764 | 13.252 | 1.00 | 32.92 | O |
| ATOM | 403 | C5  | T B | 20 | 13.774 | 25.126 | 12.933 | 1.00 | 24.11 | C |
| ATOM | 404 | C5M | T B | 20 | 14.563 | 26.358 | 12.612 | 1.00 | 23.96 | C |
| ATOM | 405 | C6  | T B | 20 | 12.385 | 25.187 | 12.926 | 1.00 | 19.78 | C |
| ATOM | 406 | P   | C B | 21 | 6.594  | 24.823 | 15.016 | 1.00 | 54.73 | P |
| ATOM | 407 | 01P | C B | 21 | 5.169  | 24.424 | 14.987 | 1.00 | 53.98 | O |
| ATOM | 408 | 02P | C B | 21 | 6.870  | 26.189 | 15.511 | 1.00 | 65.53 | O |
| ATOM | 409 | 05* | C B | 21 | 7.409  | 23.731 | 15.839 | 1.00 | 50.67 | O |
| ATOM | 410 | C5* | C B | 21 | 7.331  | 22.352 | 15.433 | 1.00 | 60.86 | C |
| ATOM | 411 | C4* | C B | 21 | 8.100  | 21.598 | 16.461 | 1.00 | 40.86 | C |
| ATOM | 412 | 04* | C B | 21 | 9.478  | 21.902 | 16.263 | 1.00 | 36.88 | O |
| ATOM | 413 | C3* | C B | 21 | 7.766  | 22.045 | 17.879 | 1.00 | 53.80 | C |
| ATOM | 414 | 03* | C B | 21 | 7.036  | 21.041 | 18.611 | 1.00 | 79.04 | O |
| ATOM | 415 | C2* | C B | 21 | 9.123  | 22.414 | 18.469 | 1.00 | 48.43 | C |
| ATOM | 416 | C1* | C B | 21 | 10.107 | 21.743 | 17.523 | 1.00 | 36.51 | C |
| ATOM | 417 | N1  | C B | 21 | 11.328 | 22.556 | 17.331 | 1.00 | 24.72 | N |
| ATOM | 418 | C2  | C B | 21 | 12.534 | 21.939 | 17.329 | 1.00 | 30.96 | C |
| ATOM | 419 | 02  | C B | 21 | 12.560 | 20.731 | 17.579 | 1.00 | 34.53 | O |
| ATOM | 420 | N3  | C B | 21 | 13.639 | 22.639 | 17.035 | 1.00 | 31.69 | N |
| ATOM | 421 | C4  | C B | 21 | 13.560 | 23.938 | 16.739 | 1.00 | 21.53 | C |
| ATOM | 422 | N4  | C B | 21 | 14.685 | 24.628 | 16.404 | 1.00 | 23.72 | N |
| ATOM | 423 | C5  | C B | 21 | 12.338 | 24.609 | 16.736 | 1.00 | 30.74 | C |
| ATOM | 424 | C6  | C B | 21 | 11.193 | 23.878 | 17.035 | 1.00 | 27.58 | C |
| ATOM | 425 | P   | G B | 22 | 6.509  | 21.324 | 20.099 | 1.00 | 56.50 | P |
| ATOM | 426 | 01P | G B | 22 | 5.387  | 20.397 | 20.396 | 1.00 | 50.81 | O |
| ATOM | 427 | 02P | G B | 22 | 6.235  | 22.774 | 20.306 | 1.00 | 53.84 | O |
| ATOM | 428 | 05* | G B | 22 | 7.767  | 20.924 | 20.993 | 1.00 | 66.30 | O |

|        |     |     |     |    |        |        |        |      |       |   |
|--------|-----|-----|-----|----|--------|--------|--------|------|-------|---|
| ATOM   | 429 | C5* | G B | 22 | 8.216  | 19.559 | 21.073 | 1.00 | 73.42 | C |
| ATOM   | 430 | C4* | G B | 22 | 9.422  | 19.557 | 21.977 | 1.00 | 42.96 | C |
| ATOM   | 431 | O4* | G B | 22 | 10.493 | 20.260 | 21.319 | 1.00 | 52.87 | O |
| ATOM   | 432 | C3* | G B | 22 | 9.267  | 20.267 | 23.325 | 1.00 | 38.51 | C |
| ATOM   | 433 | O3* | G B | 22 | 10.088 | 19.657 | 24.293 | 1.00 | 60.28 | O |
| ATOM   | 434 | C2* | G B | 22 | 9.751  | 21.670 | 22.990 | 1.00 | 22.00 | C |
| ATOM   | 435 | C1* | G B | 22 | 10.988 | 21.226 | 22.256 | 1.00 | 24.85 | C |
| ATOM   | 436 | N9  | G B | 22 | 11.599 | 22.357 | 21.543 | 1.00 | 25.91 | N |
| ATOM   | 437 | C8  | G B | 22 | 11.037 | 23.545 | 21.159 | 1.00 | 23.91 | C |
| ATOM   | 438 | N7  | G B | 22 | 11.921 | 24.362 | 20.566 | 1.00 | 39.18 | N |
| ATOM   | 439 | C5  | G B | 22 | 13.072 | 23.653 | 20.580 | 1.00 | 25.66 | C |
| ATOM   | 440 | C6  | G B | 22 | 14.370 | 24.003 | 20.102 | 1.00 | 28.34 | C |
| ATOM   | 441 | O6  | G B | 22 | 14.747 | 25.057 | 19.585 | 1.00 | 31.85 | O |
| ATOM   | 442 | N1  | G B | 22 | 15.268 | 22.983 | 20.308 | 1.00 | 25.22 | N |
| ATOM   | 443 | C2  | G B | 22 | 15.023 | 21.776 | 20.891 | 1.00 | 11.07 | C |
| ATOM   | 444 | N2  | G B | 22 | 16.066 | 20.914 | 21.038 | 1.00 | 25.92 | N |
| ATOM   | 445 | N3  | G B | 22 | 13.815 | 21.452 | 21.350 | 1.00 | 19.05 | N |
| ATOM   | 446 | C4  | G B | 22 | 12.902 | 22.429 | 21.151 | 1.00 | 23.69 | C |
| ATOM   | 447 | P   | C B | 23 | 9.477  | 18.627 | 25.340 | 1.00 | 55.93 | P |
| ATOM   | 448 | O1P | C B | 23 | 8.767  | 17.534 | 24.627 | 1.00 | 45.14 | O |
| ATOM   | 449 | O2P | C B | 23 | 8.670  | 19.409 | 26.312 | 1.00 | 41.61 | O |
| ATOM   | 450 | O5* | C B | 23 | 10.807 | 18.067 | 26.034 | 1.00 | 59.70 | O |
| ATOM   | 451 | C5* | C B | 23 | 11.688 | 17.170 | 25.310 | 1.00 | 63.13 | C |
| ATOM   | 452 | C4* | C B | 23 | 13.115 | 17.573 | 25.593 | 1.00 | 27.86 | C |
| ATOM   | 453 | O4* | C B | 23 | 13.284 | 18.804 | 24.893 | 1.00 | 50.51 | O |
| ATOM   | 454 | C3* | C B | 23 | 13.441 | 17.879 | 27.059 | 1.00 | 46.45 | C |
| ATOM   | 455 | O3* | C B | 23 | 14.341 | 16.938 | 27.677 | 1.00 | 57.21 | O |
| ATOM   | 456 | C2* | C B | 23 | 13.928 | 19.322 | 27.025 | 1.00 | 68.01 | C |
| ATOM   | 457 | C1* | C B | 23 | 14.312 | 19.508 | 25.568 | 1.00 | 32.05 | C |
| ATOM   | 458 | N1  | C B | 23 | 14.144 | 20.932 | 25.170 | 1.00 | 23.28 | N |
| ATOM   | 459 | C2  | C B | 23 | 15.199 | 21.595 | 24.630 | 1.00 | 20.62 | C |
| ATOM   | 460 | O2  | C B | 23 | 16.257 | 20.984 | 24.504 | 1.00 | 29.62 | O |
| ATOM   | 461 | N3  | C B | 23 | 15.067 | 22.877 | 24.257 | 1.00 | 39.00 | N |
| ATOM   | 462 | C4  | C B | 23 | 13.898 | 23.510 | 24.404 | 1.00 | 30.44 | C |
| ATOM   | 463 | N4  | C B | 23 | 13.771 | 24.813 | 24.018 | 1.00 | 34.66 | N |
| ATOM   | 464 | C5  | C B | 23 | 12.795 | 22.866 | 24.967 | 1.00 | 27.74 | C |
| ATOM   | 465 | C6  | C B | 23 | 12.935 | 21.540 | 25.359 | 1.00 | 24.58 | C |
| ATOM   | 466 | P   | G B | 24 | 14.658 | 17.064 | 29.247 | 1.00 | 53.70 | P |
| ATOM   | 467 | O1P | G B | 24 | 14.863 | 15.717 | 29.825 | 1.00 | 61.79 | O |
| ATOM   | 468 | O2P | G B | 24 | 13.633 | 17.912 | 29.920 | 1.00 | 36.06 | O |
| ATOM   | 469 | O5* | G B | 24 | 16.033 | 17.880 | 29.284 | 1.00 | 34.06 | O |
| ATOM   | 470 | C5* | G B | 24 | 17.243 | 17.320 | 28.742 | 1.00 | 46.57 | C |
| ATOM   | 471 | C4* | G B | 24 | 18.208 | 18.464 | 28.758 | 1.00 | 50.89 | C |
| ATOM   | 472 | O4* | G B | 24 | 17.716 | 19.428 | 27.829 | 1.00 | 32.02 | O |
| ATOM   | 473 | C3* | G B | 24 | 18.230 | 19.236 | 30.058 | 1.00 | 30.38 | C |
| ATOM   | 474 | O3* | G B | 24 | 18.978 | 18.583 | 31.084 | 1.00 | 61.06 | O |
| ATOM   | 475 | C2* | G B | 24 | 18.885 | 20.519 | 29.578 | 1.00 | 53.33 | C |
| ATOM   | 476 | C1* | G B | 24 | 18.276 | 20.693 | 28.188 | 1.00 | 35.03 | C |
| ATOM   | 477 | N9  | G B | 24 | 17.164 | 21.659 | 28.139 | 1.00 | 30.25 | N |
| ATOM   | 478 | C8  | G B | 24 | 15.874 | 21.536 | 28.580 | 1.00 | 30.86 | C |
| ATOM   | 479 | N7  | G B | 24 | 15.129 | 22.614 | 28.308 | 1.00 | 44.08 | N |
| ATOM   | 480 | C5  | G B | 24 | 15.990 | 23.436 | 27.673 | 1.00 | 16.87 | C |
| ATOM   | 481 | C6  | G B | 24 | 15.765 | 24.729 | 27.117 | 1.00 | 19.36 | C |
| ATOM   | 482 | O6  | G B | 24 | 14.719 | 25.373 | 27.067 | 1.00 | 33.30 | O |
| ATOM   | 483 | N1  | G B | 24 | 16.926 | 25.257 | 26.604 | 1.00 | 15.78 | N |
| ATOM   | 484 | C2  | G B | 24 | 18.157 | 24.666 | 26.579 | 1.00 | 11.92 | C |
| ATOM   | 485 | N2  | G B | 24 | 19.208 | 25.386 | 26.096 | 1.00 | 29.76 | N |
| ATOM   | 486 | N3  | G B | 24 | 18.350 | 23.438 | 27.053 | 1.00 | 21.95 | N |
| ATOM   | 487 | C4  | G B | 24 | 17.231 | 22.893 | 27.570 | 1.00 | 13.89 | C |
| TER    | 488 |     | G B | 24 |        |        |        |      |       |   |
| HETATM | 489 | O   | HOH | 25 | 19.736 | 30.706 | 18.656 | 1.00 | 51.86 | O |
| HETATM | 490 | O   | HOH | 26 | 14.354 | 27.683 | 16.369 | 1.00 | 40.92 | O |

|        |     |   |     |    |        |        |         |      |       |   |
|--------|-----|---|-----|----|--------|--------|---------|------|-------|---|
| HETATM | 491 | 0 | HOH | 27 | 9.864  | 22.509 | 9.123   | 1.00 | 39.67 | 0 |
| HETATM | 492 | 0 | HOH | 28 | 19.526 | 19.144 | 7.481   | 1.00 | 51.15 | 0 |
| HETATM | 493 | 0 | HOH | 29 | 25.754 | 12.744 | -1.835  | 1.00 | 51.80 | 0 |
| HETATM | 494 | 0 | HOH | 30 | 7.478  | 20.604 | -9.000  | 1.00 | 44.82 | 0 |
| HETATM | 495 | 0 | HOH | 31 | 10.879 | 26.039 | -8.906  | 1.00 | 47.07 | 0 |
| HETATM | 496 | 0 | HOH | 32 | 18.320 | 24.816 | 14.948  | 1.00 | 47.72 | 0 |
| HETATM | 497 | 0 | HOH | 33 | 9.012  | 24.586 | 7.009   | 1.00 | 43.42 | 0 |
| HETATM | 498 | 0 | HOH | 34 | 10.152 | 19.917 | 13.381  | 1.00 | 48.04 | 0 |
| HETATM | 499 | 0 | HOH | 35 | 7.764  | 21.397 | 11.075  | 1.00 | 41.41 | 0 |
| HETATM | 500 | 0 | HOH | 36 | 9.821  | 13.442 | 8.572   | 1.00 | 45.76 | 0 |
| HETATM | 501 | 0 | HOH | 37 | 13.239 | 14.428 | 2.049   | 1.00 | 55.54 | 0 |
| HETATM | 502 | 0 | HOH | 38 | 8.915  | 15.602 | -3.388  | 1.00 | 50.97 | 0 |
| HETATM | 503 | 0 | HOH | 39 | 17.505 | 26.340 | -10.581 | 1.00 | 51.90 | 0 |
| HETATM | 504 | 0 | HOH | 40 | 28.496 | 23.515 | 18.349  | 1.00 | 45.37 | 0 |
| HETATM | 505 | 0 | HOH | 41 | 11.346 | 24.175 | 4.920   | 1.00 | 45.03 | 0 |
| HETATM | 506 | 0 | HOH | 42 | 12.601 | 23.000 | 29.167  | 1.00 | 51.36 | 0 |
| HETATM | 507 | 0 | HOH | 43 | 10.440 | 25.542 | 24.443  | 1.00 | 56.79 | 0 |
| HETATM | 508 | 0 | HOH | 44 | 16.979 | 28.689 | 16.284  | 1.00 | 50.41 | 0 |
| HETATM | 509 | 0 | HOH | 45 | 4.794  | 22.966 | 13.368  | 1.00 | 45.95 | 0 |
| HETATM | 510 | 0 | HOH | 46 | 4.208  | 25.591 | 10.828  | 1.00 | 51.06 | 0 |
| HETATM | 511 | 0 | HOH | 47 | 6.362  | 24.374 | 9.188   | 1.00 | 51.85 | 0 |
| HETATM | 512 | 0 | HOH | 48 | 7.688  | 28.411 | 7.883   | 1.00 | 49.33 | 0 |
| HETATM | 513 | 0 | HOH | 49 | 18.379 | 17.074 | 4.809   | 1.00 | 50.72 | 0 |
| HETATM | 514 | 0 | HOH | 50 | 9.098  | 16.119 | 1.277   | 1.00 | 51.80 | 0 |
| HETATM | 515 | 0 | HOH | 51 | 26.464 | 23.826 | 1.396   | 1.00 | 53.21 | 0 |
| HETATM | 516 | 0 | HOH | 52 | 11.014 | 11.318 | -2.909  | 1.00 | 51.36 | 0 |
| HETATM | 517 | 0 | HOH | 53 | 9.476  | 27.782 | 26.498  | 1.00 | 60.04 | 0 |
| HETATM | 518 | 0 | HOH | 54 | 16.488 | 29.195 | 19.861  | 1.00 | 54.92 | 0 |
| HETATM | 519 | 0 | HOH | 55 | 22.078 | 25.894 | 15.396  | 1.00 | 62.20 | 0 |
| HETATM | 520 | 0 | HOH | 56 | 5.522  | 27.411 | 9.017   | 1.00 | 62.36 | 0 |
| HETATM | 521 | 0 | HOH | 57 | 18.456 | 28.409 | 8.821   | 1.00 | 59.63 | 0 |
| HETATM | 522 | 0 | HOH | 58 | 7.133  | 14.448 | 4.647   | 1.00 | 57.15 | 0 |
| HETATM | 523 | 0 | HOH | 59 | 22.610 | 15.544 | 3.846   | 1.00 | 57.52 | 0 |
| HETATM | 524 | 0 | HOH | 60 | 24.407 | 13.162 | 2.229   | 1.00 | 52.30 | 0 |
| HETATM | 525 | 0 | HOH | 61 | 7.988  | 11.556 | -2.976  | 1.00 | 59.14 | 0 |
| HETATM | 526 | 0 | HOH | 62 | 14.095 | 28.151 | 21.614  | 1.00 | 53.85 | 0 |
| HETATM | 527 | 0 | HOH | 63 | 14.213 | 27.722 | 18.905  | 1.00 | 57.29 | 0 |
| HETATM | 528 | 0 | HOH | 64 | 27.164 | 31.710 | 20.331  | 1.00 | 56.84 | 0 |
| HETATM | 529 | 0 | HOH | 65 | 15.295 | 11.873 | 12.209  | 1.00 | 57.34 | 0 |
| HETATM | 530 | 0 | HOH | 66 | 18.180 | 16.604 | 9.966   | 1.00 | 61.52 | 0 |
| HETATM | 531 | 0 | HOH | 67 | 6.216  | 17.035 | 1.672   | 1.00 | 62.91 | 0 |
| HETATM | 532 | 0 | HOH | 68 | 19.101 | 11.433 | 1.080   | 1.00 | 59.79 | 0 |
| HETATM | 533 | 0 | HOH | 69 | 12.607 | 10.967 | 0.261   | 1.00 | 60.87 | 0 |
| HETATM | 534 | 0 | HOH | 70 | 7.055  | 25.519 | -2.053  | 1.00 | 55.96 | 0 |
| HETATM | 535 | 0 | HOH | 71 | 15.062 | 26.024 | -0.766  | 1.00 | 56.35 | 0 |
| HETATM | 536 | 0 | HOH | 72 | 16.380 | 6.413  | -4.784  | 1.00 | 59.07 | 0 |
| HETATM | 537 | 0 | HOH | 73 | 14.059 | 5.751  | -6.198  | 1.00 | 56.68 | 0 |
| HETATM | 538 | 0 | HOH | 74 | 12.416 | 31.549 | 23.685  | 1.00 | 68.40 | 0 |
| HETATM | 539 | 0 | HOH | 75 | 9.613  | 17.039 | 29.793  | 1.00 | 63.48 | 0 |
| HETATM | 540 | 0 | HOH | 76 | 11.492 | 29.103 | 20.090  | 1.00 | 67.46 | 0 |
| HETATM | 541 | 0 | HOH | 77 | 14.220 | 29.189 | 20.392  | 1.00 | 48.22 | 0 |
| HETATM | 542 | 0 | HOH | 78 | 6.138  | 19.149 | 13.844  | 1.00 | 62.26 | 0 |
| HETATM | 543 | 0 | HOH | 79 | 17.315 | 9.638  | 13.392  | 1.00 | 65.70 | 0 |
| HETATM | 544 | 0 | HOH | 80 | 18.951 | 25.757 | 12.989  | 1.00 | 66.47 | 0 |
| HETATM | 545 | 0 | HOH | 81 | 20.460 | 18.861 | 12.664  | 1.00 | 63.00 | 0 |
| HETATM | 546 | 0 | HOH | 82 | 3.529  | 19.338 | 12.599  | 1.00 | 65.32 | 0 |
| HETATM | 547 | 0 | HOH | 83 | 25.276 | 15.890 | -1.301  | 1.00 | 64.53 | 0 |
| HETATM | 548 | 0 | HOH | 84 | 3.788  | 7.844  | -9.406  | 1.00 | 63.59 | 0 |
| HETATM | 549 | 0 | HOH | 85 | 12.989 | 29.901 | -9.282  | 1.00 | 64.97 | 0 |
| HETATM | 550 | 0 | HOH | 86 | 17.510 | 30.569 | 18.702  | 1.00 | 61.79 | 0 |
| HETATM | 551 | 0 | HOH | 87 | 25.377 | 12.891 | 19.011  | 1.00 | 73.80 | 0 |
| HETATM | 552 | 0 | HOH | 88 | 13.610 | 15.742 | 18.593  | 1.00 | 69.48 | 0 |

|        |     |     |     |     |        |        |         |      |       |   |   |   |
|--------|-----|-----|-----|-----|--------|--------|---------|------|-------|---|---|---|
| HETATM | 553 | 0   | HOH | 89  | 18.012 | 32.598 | 15.262  | 1.00 | 67.52 |   | 0 |   |
| HETATM | 554 | 0   | HOH | 90  | 2.622  | 23.030 | 10.332  | 1.00 | 68.01 |   | 0 |   |
| HETATM | 555 | 0   | HOH | 91  | 19.701 | 22.518 | 9.511   | 1.00 | 70.25 |   | 0 |   |
| HETATM | 556 | 0   | HOH | 92  | 8.723  | 13.216 | 6.359   | 1.00 | 70.66 |   | 0 |   |
| HETATM | 557 | 0   | HOH | 93  | 19.727 | 29.488 | 6.155   | 1.00 | 69.43 |   | 0 |   |
| HETATM | 558 | 0   | HOH | 94  | 17.241 | 11.563 | 4.511   | 1.00 | 72.18 |   | 0 |   |
| HETATM | 559 | 0   | HOH | 95  | 26.545 | 19.404 | -1.091  | 1.00 | 70.14 |   | 0 |   |
| HETATM | 560 | 0   | HOH | 96  | 9.697  | 18.315 | 14.885  | 1.00 | 69.10 |   | 0 |   |
| HETATM | 561 | 0   | HOH | 97  | 18.779 | 13.814 | 11.704  | 1.00 | 71.14 |   | 0 |   |
| HETATM | 562 | 0   | HOH | 98  | 14.292 | 25.159 | 2.287   | 1.00 | 68.44 |   | 0 |   |
| HETATM | 563 | 0   | HOH | 99  | 12.227 | 25.192 | -10.299 | 1.00 | 70.46 |   | 0 |   |
| HETATM | 564 | 0   | HOH | 100 | 12.292 | 30.291 | 27.102  | 1.00 | 73.04 |   | 0 |   |
| HETATM | 565 | 0   | HOH | 101 | 9.396  | 27.092 | 16.993  | 1.00 | 72.98 |   | 0 |   |
| HETATM | 566 | 0   | HOH | 102 | 20.170 | 23.000 | 12.999  | 1.00 | 73.63 |   | 0 |   |
| HETATM | 567 | 0   | HOH | 103 | 19.987 | 21.691 | 6.802   | 1.00 | 72.66 |   | 0 |   |
| HETATM | 568 | 0   | HOH | 104 | 18.692 | 31.584 | 4.596   | 1.00 | 72.98 |   | 0 |   |
| MASTER |     | 254 | 0   | 0   | 0      | 0      | 0       | 6    | 566   | 2 | 0 | 2 |
| END    |     |     |     |     |        |        |         |      |       |   |   |   |

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color green
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color cyan
select pyrimidine and t and not backbone

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