Recognition of O^6-Benzyl-2'-deoxyguanosine by a Perimidinone-Derived Synthetic Nucleoside: A DNA Interstrand Stacking Interaction

Supplementary Data

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Table of Contents

Complete listings of references (30), (31), (45), (59) 4

Table S1, CIF File for Diffraction Data of the Second Crystal of the DDD-XY Duplex 6

Table S2, Crystal and Data Collection Statistics for the First Crystal Used to Obtain Phases for the DDD-XY Duplex 48

Table S3, Crystal Data, Data Collection, and Refinement Statistics for the Second Crystal Used to Obtain the Final Structure of the DDD-XY Duplex 49

Table S4, NMR Restraints Used for the DDD-GY Structure Calculations and Refinement Statistics 50

Table S5, Structural Statistics for the DDD-GY Duplex 51

Figure S1, Structure of the DDD-XY duplex with water molecules and Sr^{2+} ion and spermine molecule 52

Figure S2, Interbase pair parameters, helical rise, roll, and twist for the DDD-XY, DDD (PDB entry 355D) duplexes 53

Figure S3, Comparison of backbone torsion angles α and β in the crystal structures of the DDD-XY, DDD (PDB entry 355D) duplexes 54

Figure S4, Comparison of γ, δ, and ε angles in the crystal structures of the DDD-XY, DDD (PDB entry 355D) duplexes 55

Figure S5, Comparison of χ and ζ angles in the crystal structures of the DDD-XY, DDD (PDB entry 355D) duplexes 56

Figure S6, NOESY spectrum of the DDD-XY duplex showing sequential NOEs between the aromatic and anomeric protons from C^{1} to G^{12} 57

Figure S7, Interstrand NOE cross peaks between complementary bases for the DDD-XY

duplex and NOE connectivity of DDD-XY duplex, for the imino protons 58

Figure S8, NMR spectra, showing the imino proton resonances for the DDD-XY duplex as a function of temperature 59

Figure S9, The average structure obtained from a series of rMD calculations for the DDD-GY duplex 60

Figure S10, The superimposed nine structures obtained from a series of rMD calculations for the DDD-GY duplex 61

Figure S11, Interbase pair parameters helical rise, roll, and twist for the DDD-GY, DDD (PDB entry 355D) duplexes 62

Figure S12, Comparison of backbone torsion angles α and β in the structures of the DDD-GY, DDD (PDB entry 355D) duplexes 63

Figure S13, Comparison of γ, δ, and ε angles in the structures of the DDD-GY, DDD (PDB entry 355D) duplexes 64

Figure S14, Comparison of χ and ζ angles in the crystal structures of the DDD-GY, DDD (PDB entry 355D) duplexes. 65

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Table S1. CIF File for Diffraction Data of the Second Crystal of the DDD-XY duplex.

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_audit_author.pdbx_ordinal
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'Lad, R.'      2
'Pallan, P.S.' 3
'Muffly, E.'   4
'Wawrzak, Z.'  5
'Egli, M.'     6
'Sturla, S.J.' 7
'Stone, M.P.'  8
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_pdbx_database_status.process_site     RCSB
_pdbx_database_status.status_code_sf   HPUB
_pdbx_database_status.status_code_mr   ?
_pdbx_database_status.SG_entry         ?
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_struct_ref_seq.seq_align_end
_struct_ref_seq.pdbx_seq_align_end_ins_code
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2 1 4HQI B 1 ? 12 ? 4HQI 13 24 13 24
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Dodecamer, DNA
;
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1 'ABSA (A^2)' 1890 ?
1 'SSA (A^2)'  4860 ?
1 MORE         -24  ?
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_exptl_crystal_grow.pH
_exptl_crystal_grow.pdbx_details
_exptl_crystal_grow.pdbx_pH_range
1 'VAPOR DIFFUSION, HANGING DROP' 291 ? 7.0
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Methyl-2,4-pentanediol (MPD), VAPOR DIFFUSION, HANGING DROP, temperature 291K
;
?
2 'VAPOR DIFFUSION, HANGING DROP' 291 ? 7.0
;20 mM sodium cacodylate (pH 7.0), 6 mM spermine tetra-HCl, 40 mM KCl, 10 mM BaCl2 and  5% v/v 2-
Methyl-2,4-pentanediol (MPD), VAPOR DIFFUSION, HANGING DROP, temperature 291K
;
?
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_exptl_crystal.preparation
1 ? 2.46 50.02 ? ? ?
2 ? ?    ?     ? ? ?
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_symmetry.cell_setting                      ?
_symmetry.Int_Tables_number                 ?
_symmetry.space_group_name_Hall             ?
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1 SYNCHROTRON 'APS BEAMLINE 21-ID-D' APS 21-ID-D ? 1.60499
2 SYNCHROTRON 'APS BEAMLINE 21-ID-G' APS 21-ID-G ? 0.97857
#
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_diffrn_detector.type
_diffrn_detector.pdbx_collection_date
_diffrn_detector.details
1 CCD 'MARMOSAIC 300 mm CCD' 2009-07-17 Si(111)
2 CCD 'MARMOSAIC 300 mm CCD' 2008-07-18 C(111)
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loop_
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_diffrn.ambient_temp
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1 100 ? 1
2 100 ? 2
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_diffrn_radiation.monochromator
_diffrn_radiation.pdbx_diffrn_protocol
1 1 M Si(111) 'SINGLE WAVELENGTH'
2 1 M C(111)  'SINGLE WAVELENGTH'
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_reflns_shell.number_measured_obs    ?
_reflns_shell.number_unique_obs      ?
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r_angle_refined_deg  1.652 1.578 ? 833 ? 'X-RAY DIFFRACTION'
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r_gen_planes_refined 0.023 0.020 ? 260 ? 'X-RAY DIFFRACTION'
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_refine_ls_shell.R_factor_all                     ?
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4HQI 'mismatched base pair'
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_ndb_struct_na_base_pair.opening
_ndb_struct_na_base_pair.pair_number
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_ndb_struct_na_base_pair.i_auth_asym_id
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1 A DC 3  1_555 B DG 10 1_555 0.199  -0.225 -0.317 2.151   -1.099 2 A_DC3:DG22_B  A 3  ? B 22 ? 19 1
1 A DA 5  1_555 B DT 8  1_555 -0.236 -0.008 -0.460 -12.406 1.251  3 A_DA5:DT20_B  A 5  ? B 20 ? 20 1
1 A DA 6  1_555 B DT 7  1_555 -0.009 -0.142 -0.125 -5.111  0.172  4 A_DA6:DT19_B  A 6  ? B 19 ? 20 1
1 A DT 7  1_555 B DA 6  1_555 0.132  -0.121 -0.126 2.516   1.351  5 A_DT7:DA18_B  A 7  ? B 18 ? 20 1
1 A DT 8  1_555 B DA 5  1_555 0.024  -0.181 -0.510 8.065   4.832  6 A_DT8:DA17_B  A 8  ? B 17 ? 20 1
1 A DG 10 1_555 B DC 3  1_555 -0.259 -0.158 -0.143 -0.234  0.472  7 A_DG10:DC15_B A 10 ? B 15 ? 19 1
1 A DC 11 1_555 B DG 2  1_555 0.194  -0.224 -0.063 10.713  -1.590 8 A_DC11:DG14_B A 11 ? B 14 ? 19 1
#
loop_
_ndb_struct_na_base_pair_step.model_number
_ndb_struct_na_base_pair_step.i_label_asym_id_1
_ndb_struct_na_base_pair_step.i_label_comp_id_1
_ndb_struct_na_base_pair_step.i_label_seq_id_1
_ndb_struct_na_base_pair_step.i_symmetry_1
_ndb_struct_na_base_pair_step.j_label_asym_id_1
_ndb_struct_na_base_pair_step.j_label_comp_id_1
_ndb_struct_na_base_pair_step.j_label_seq_id_1
_ndb_struct_na_base_pair_step.j_symmetry_1
_ndb_struct_na_base_pair_step.i_label_asym_id_2
_ndb_struct_na_base_pair_step.i_label_comp_id_2
_ndb_struct_na_base_pair_step.i_label_seq_id_2
_ndb_struct_na_base_pair_step.i_symmetry_2
_ndb_struct_na_base_pair_step.j_label_asym_id_2
_ndb_struct_na_base_pair_step.j_label_comp_id_2
_ndb_struct_na_base_pair_step.j_label_seq_id_2
_ndb_struct_na_base_pair_step.j_symmetry_2
_ndb_struct_na_base_pair_step.shift
_ndb_struct_na_base_pair_step.slide
_ndb_struct_na_base_pair_step.rise
```

```
_ndb_struct_na_base_pair_step.tilt
_ndb_struct_na_base_pair_step.roll
_ndb_struct_na_base_pair_step.twist
_ndb_struct_na_base_pair_step.x_displacement
_ndb_struct_na_base_pair_step.y_displacement
_ndb_struct_na_base_pair_step.helical_rise
_ndb_struct_na_base_pair_step.inclination
_ndb_struct_na_base_pair_step.tip
_ndb_struct_na_base_pair_step.helical_twist
_ndb_struct_na_base_pair_step.step_number
_ndb_struct_na_base_pair_step.step_name
_ndb_struct_na_base_pair_step.i_auth_asym_id_1
_ndb_struct_na_base_pair_step.i_auth_seq_id_1
_ndb_struct_na_base_pair_step.i_PDB_ins_code_1
_ndb_struct_na_base_pair_step.j_auth_asym_id_1
_ndb_struct_na_base_pair_step.j_auth_seq_id_1
_ndb_struct_na_base_pair_step.j_PDB_ins_code_1
_ndb_struct_na_base_pair_step.i_auth_asym_id_2
_ndb_struct_na_base_pair_step.i_auth_seq_id_2
_ndb_struct_na_base_pair_step.i_PDB_ins_code_2
_ndb_struct_na_base_pair_step.j_auth_asym_id_2
_ndb_struct_na_base_pair_step.j_auth_seq_id_2
_ndb_struct_na_base_pair_step.j_PDB_ins_code_2
1 A DG 2  1_555 B DC 11 1_555 A DC 3  1_555 B DG 10 1_555 0.825  -0.036 3.016 -1.267 -2.600 30.408
0.405  -1.796 2.973 -4.943 2.408   30.542 1
AA_DG2DC3:DG22DC23_BB   A 2  ? B 23 ? A 3  ? B 22 ?
1 A DA 5  1_555 B DT 8  1_555 A DA 6  1_555 B DT 7  1_555 -0.057 -0.095 3.259 -2.570 8.650  26.842 -
2.189 -0.476 3.072 18.000 5.348   28.292 2
AA_DA5DA6:DT19DT20_BB   A 5  ? B 20 ? A 6  ? B 19 ?
1 A DA 6  1_555 B DT 7  1_555 A DT 7  1_555 B DA 6  1_555 -0.148 -0.601 3.135 0.082  6.206  27.711 -
2.567 0.320  2.933 12.755 -0.169  28.384 3
AA_DA6DT7:DA18DT19_BB   A 6  ? B 19 ? A 7  ? B 18 ?
1 A DT 7  1_555 B DA 6  1_555 A DT 8  1_555 B DA 5  1_555 1.209  0.289  3.235 6.047  7.993  32.969 -
0.800 -1.070 3.374 13.696 -10.360 34.418 4
AA_DT7DT8:DA17DA18_BB   A 7  ? B 18 ? A 8  ? B 17 ?
1 A DG 10 1_555 B DC 3  1_555 A DC 11 1_555 B DG 2  1_555 -0.894 0.014  3.141 0.568  -2.918 30.844
0.565  1.778  3.110 -5.470 -1.064  30.984 5
```

```
AA_DG10DC11:DG14DC15_BB A 10 ? B 15 ? A 11 ? B 14 ?
#
loop_
_software.name
_software.classification
_software.version
_software.citation_id
_software.pdbx_ordinal
MD-2   'data collection' 'diffractometer software from EMBL (with LS-CAT developed extensions)' ? 1
PHENIX 'model building'  .                                                                       ? 2
REFMAC refinement        5.7.0029                                                                ? 3
#
_entry.id   4HQI
#
_pdbx_unobs_or_zero_occ_residues.id               1
_pdbx_unobs_or_zero_occ_residues.polymer_flag     Y
_pdbx_unobs_or_zero_occ_residues.occupancy_flag   1
_pdbx_unobs_or_zero_occ_residues.PDB_model_num    1
_pdbx_unobs_or_zero_occ_residues.auth_asym_id     A
_pdbx_unobs_or_zero_occ_residues.auth_comp_id     DC
_pdbx_unobs_or_zero_occ_residues.auth_seq_id      1
_pdbx_unobs_or_zero_occ_residues.PDB_ins_code     ?
#
loop_
_pdbx_unobs_or_zero_occ_atoms.id
_pdbx_unobs_or_zero_occ_atoms.polymer_flag
_pdbx_unobs_or_zero_occ_atoms.occupancy_flag
_pdbx_unobs_or_zero_occ_atoms.PDB_model_num
_pdbx_unobs_or_zero_occ_atoms.auth_asym_id
_pdbx_unobs_or_zero_occ_atoms.auth_comp_id
_pdbx_unobs_or_zero_occ_atoms.auth_seq_id
_pdbx_unobs_or_zero_occ_atoms.PDB_ins_code
_pdbx_unobs_or_zero_occ_atoms.auth_atom_id
_pdbx_unobs_or_zero_occ_atoms.label_alt_id
1  Y 1 1 B DC 13 ? 'O5'' ?
2  Y 1 1 B DC 13 ? 'C5'' ?
3  Y 1 1 B DC 13 ? 'C4'' ?
```

```
4  Y 1 1 B DC 13 ? 'O4'' ?
5  Y 1 1 B DC 13 ? 'C3'' ?
6  Y 1 1 B DC 13 ? 'C2'' ?
7  Y 1 1 B DC 13 ? 'C1'' ?
8  Y 1 1 B DC 13 ? N1    ?
9  Y 1 1 B DC 13 ? C2    ?
10 Y 1 1 B DC 13 ? O2    ?
11 Y 1 1 B DC 13 ? N3    ?
12 Y 1 1 B DC 13 ? C4    ?
13 Y 1 1 B DC 13 ? N4    ?
14 Y 1 1 B DC 13 ? C5    ?
15 Y 1 1 B DC 13 ? C6    ?
#
loop_
_struct_site.id
_struct_site.details
_struct_site.pdbx_evidence_code
AC1 'BINDING SITE FOR RESIDUE SPM A 101' SOFTWARE
AC2 'BINDING SITE FOR RESIDUE SR A 102'  SOFTWARE
#
_atom_sites.entry_id                    4HQI
_atom_sites.Cartn_transform_axes        ?
_atom_sites.fract_transf_matrix[1][1]   0.037902
_atom_sites.fract_transf_matrix[1][2]   0.000000
_atom_sites.fract_transf_matrix[1][3]   0.000000
_atom_sites.fract_transf_matrix[2][1]   -0.000000
_atom_sites.fract_transf_matrix[2][2]   0.027193
_atom_sites.fract_transf_matrix[2][3]   0.000000
_atom_sites.fract_transf_matrix[3][1]   0.000000
_atom_sites.fract_transf_matrix[3][2]   -0.000000
_atom_sites.fract_transf_matrix[3][3]   0.012878
_atom_sites.fract_transf_vector[1]      0.00000
_atom_sites.fract_transf_vector[2]      0.00000
_atom_sites.fract_transf_vector[3]      0.00000
#
_citation.id                        primary
_citation.title
```

```
;Recognition of O6-Benzyl-2'-deoxyguanosine by a Perimidinone-Derived Synthetic Nucleoside: A Unique
Interstrand Stacking Interaction
;
_citation.journal_abbrev            'To be Published'
_citation.journal_volume            ?
_citation.page_first                ?
_citation.page_last                 ?
_citation.year                      ?
_citation.journal_id_ASTM           ?
_citation.country                   ?
_citation.journal_id_ISSN           ?
_citation.journal_id_CSD            0353
_citation.book_publisher            ?
_citation.pdbx_database_id_PubMed   ?
_citation.pdbx_database_id_DOI      ?
#
loop_
_citation_author.citation_id
_citation_author.name
_citation_author.ordinal
primary 'Kowal, E.A.'  1
primary 'Lad, R.'      2
primary 'Pallan, P.S.' 3
primary 'Muffly, E.'   4
primary 'Wawrzak, Z.'  5
primary 'Egli, M.'     6
primary 'Sturla, S.J.' 7
primary 'Stone, M.P.'  8
#
_computing.entry_id                             4HQI
_computing.pdbx_data_reduction_ii               HKL2000
_computing.pdbx_data_reduction_ds               HKL2000
_computing.data_collection                      'MD-2 diffractometer software from EMBL (with LS-CAT
developed extensions)'
_computing.structure_solution                   PHENIX
_computing.structure_refinement                 'REFMAC 5.7.0029'
_computing.pdbx_structure_refinement_method     ?
```

```
#
_database.entry_id   4HQI
_database.code_CSD   ?
#
loop_
_database_2.database_id
_database_2.database_code
PDB  4HQI
NDB  NA2104
RCSB RCSB075793
#
loop_
_entity.id
_entity.type
_entity.src_method
_entity.pdbx_description
_entity.formula_weight
_entity.pdbx_number_of_molecules
_entity.details
1 polymer     syn 'Short modified nucleic acids' 3826.640 2  ?
2 non-polymer syn SPERMINE                       202.342  1  ?
3 non-polymer syn 'STRONTIUM ION'                87.620   1  ?
4 water       nat water                          18.015   49 ?
#
loop_
_entity_poly_seq.entity_id
_entity_poly_seq.num
_entity_poly_seq.mon_id
_entity_poly_seq.hetero
1 1  DC  n
1 2  DG  n
1 3  DC  n
1 4  BZG n
1 5  DA  n
1 6  DA  n
1 7  DT  n
1 8  DT  n
```

```
1 9  D3N n
1 10 DG  n
1 11 DC  n
1 12 DG  n
#
_entity_poly.entity_id                      1
_entity_poly.type                           polydeoxyribonucleotide
_entity_poly.nstd_linkage                   no
_entity_poly.nstd_monomer                   yes
_entity_poly.pdbx_seq_one_letter_code       (DC)(DG)(DC)(BZG)(DA)(DA)(DT)(DT)(D3N)(DG)(DC)(DG)
_entity_poly.pdbx_seq_one_letter_code_can   CGCNAATTXGCG
#
loop_
_pdbx_poly_seq_scheme.asym_id
_pdbx_poly_seq_scheme.entity_id
_pdbx_poly_seq_scheme.seq_id
_pdbx_poly_seq_scheme.mon_id
_pdbx_poly_seq_scheme.ndb_seq_num
_pdbx_poly_seq_scheme.pdb_seq_num
_pdbx_poly_seq_scheme.auth_seq_num
_pdbx_poly_seq_scheme.pdb_mon_id
_pdbx_poly_seq_scheme.auth_mon_id
_pdbx_poly_seq_scheme.pdb_strand_id
_pdbx_poly_seq_scheme.pdb_ins_code
_pdbx_poly_seq_scheme.hetero
A 1 1  DC  1  1  ?  ?   ?   A . n
A 1 2  DG  2  2  2  DG  DG  A . n
A 1 3  DC  3  3  3  DC  DC  A . n
A 1 4  BZG 4  4  4  BZG BZG A . n
A 1 5  DA  5  5  5  DA  DA  A . n
A 1 6  DA  6  6  6  DA  DA  A . n
A 1 7  DT  7  7  7  DT  DT  A . n
A 1 8  DT  8  8  8  DT  DT  A . n
A 1 9  D3N 9  9  9  D3N D3N A . n
A 1 10 DG  10 10 10 DG  DG  A . n
A 1 11 DC  11 11 11 DC  DC  A . n
A 1 12 DG  12 12 12 DG  DG  A . n
```

```
B 1 1  DC  1  13 13 DC  DC  B . n
B 1 2  DG  2  14 14 DG  DG  B . n
B 1 3  DC  3  15 15 DC  DC  B . n
B 1 4  BZG 4  16 16 BZG BZG B . n
B 1 5  DA  5  17 17 DA  DA  B . n
B 1 6  DA  6  18 18 DA  DA  B . n
B 1 7  DT  7  19 19 DT  DT  B . n
B 1 8  DT  8  20 20 DT  DT  B . n
B 1 9  D3N 9  21 21 D3N D3N B . n
B 1 10 DG  10 22 22 DG  DG  B . n
B 1 11 DC  11 23 23 DC  DC  B . n
B 1 12 DG  12 24 24 DG  DG  B . n
#
loop_
_pdbx_nonpoly_scheme.asym_id
_pdbx_nonpoly_scheme.entity_id
_pdbx_nonpoly_scheme.mon_id
_pdbx_nonpoly_scheme.ndb_seq_num
_pdbx_nonpoly_scheme.pdb_seq_num
_pdbx_nonpoly_scheme.auth_seq_num
_pdbx_nonpoly_scheme.pdb_mon_id
_pdbx_nonpoly_scheme.auth_mon_id
_pdbx_nonpoly_scheme.pdb_strand_id
_pdbx_nonpoly_scheme.pdb_ins_code
C 2 SPM 1  101 330 SPM SPM A .
D 3 SR  1  102 1   SR  SR  A .
E 4 HOH 1  201 4   HOH HOH A .
E 4 HOH 2  202 7   HOH HOH A .
E 4 HOH 3  203 11  HOH HOH A .
E 4 HOH 4  204 12  HOH HOH A .
E 4 HOH 5  205 13  HOH HOH A .
E 4 HOH 6  206 19  HOH HOH A .
E 4 HOH 7  207 20  HOH HOH A .
E 4 HOH 8  208 21  HOH HOH A .
E 4 HOH 9  209 22  HOH HOH A .
E 4 HOH 10 210 23  HOH HOH A .
E 4 HOH 11 211 24  HOH HOH A .
```

```
E 4 HOH 12 212 25  HOH HOH A .
E 4 HOH 13 213 26  HOH HOH A .
E 4 HOH 14 214 28  HOH HOH A .
E 4 HOH 15 215 30  HOH HOH A .
E 4 HOH 16 216 31  HOH HOH A .
E 4 HOH 17 217 32  HOH HOH A .
E 4 HOH 18 218 33  HOH HOH A .
E 4 HOH 19 219 34  HOH HOH A .
E 4 HOH 20 220 35  HOH HOH A .
E 4 HOH 21 221 37  HOH HOH A .
E 4 HOH 22 222 38  HOH HOH A .
E 4 HOH 23 223 39  HOH HOH A .
E 4 HOH 24 224 41  HOH HOH A .
E 4 HOH 25 225 44  HOH HOH A .
E 4 HOH 26 226 48  HOH HOH A .
E 4 HOH 27 227 49  HOH HOH A .
E 4 HOH 28 228 50  HOH HOH A .
F 4 HOH 1  101 2   HOH HOH B .
F 4 HOH 2  102 3   HOH HOH B .
F 4 HOH 3  103 5   HOH HOH B .
F 4 HOH 4  104 6   HOH HOH B .
F 4 HOH 5  105 8   HOH HOH B .
F 4 HOH 6  106 9   HOH HOH B .
F 4 HOH 7  107 10  HOH HOH B .
F 4 HOH 8  108 14  HOH HOH B .
F 4 HOH 9  109 15  HOH HOH B .
F 4 HOH 10 110 16  HOH HOH B .
F 4 HOH 11 111 17  HOH HOH B .
F 4 HOH 12 112 18  HOH HOH B .
F 4 HOH 13 113 27  HOH HOH B .
F 4 HOH 14 114 29  HOH HOH B .
F 4 HOH 15 115 36  HOH HOH B .
F 4 HOH 16 116 40  HOH HOH B .
F 4 HOH 17 117 42  HOH HOH B .
F 4 HOH 18 118 43  HOH HOH B .
F 4 HOH 19 119 45  HOH HOH B .
F 4 HOH 20 120 46  HOH HOH B .
```

```
F 4 HOH 21 121 47  HOH HOH B .
#
_pdbx_entity_src_syn.entity_id              1
_pdbx_entity_src_syn.organism_scientific    'SYNTHETIC CONSTRUCT'
_pdbx_entity_src_syn.organism_common_name   ?
_pdbx_entity_src_syn.ncbi_taxonomy_id       32630
_pdbx_entity_src_syn.details                'Chemically synthesized modified oligonucleotides'
#
_refine_hist.pdbx_refine_id                   'X-RAY DIFFRACTION'
_refine_hist.cycle_id                         LAST
_refine_hist.pdbx_number_atoms_protein        0
_refine_hist.pdbx_number_atoms_nucleic_acid   481
_refine_hist.pdbx_number_atoms_ligand         15
_refine_hist.number_atoms_solvent             49
_refine_hist.number_atoms_total               545
_refine_hist.d_res_high                       1.70
_refine_hist.d_res_low                        20.67
#
_struct.entry_id                  4HQI
_struct.title
;Structure of O6-Benzyl-2'-deoxyguanosine opposite perimidinone-derived synthetic nucleoside in DNA
duplex
;
_struct.pdbx_descriptor           '5'-D(*CP*GP*CP*(BZG)P*AP*AP*TP*TP*(D3N)P*GP*CP*G)-3''
_struct.pdbx_model_details        ?
_struct.pdbx_CASP_flag            ?
_struct.pdbx_model_type_details   ?
#
loop_
_struct_asym.id
_struct_asym.pdbx_blank_PDB_chainid_flag
_struct_asym.pdbx_modified
_struct_asym.entity_id
_struct_asym.details
A N N 1 ?
B N N 1 ?
C N N 2 ?
```

```
D N N 3 ?
E N N 4 ?
F N N 4 ?
#
loop_
_struct_conn.id
_struct_conn.conn_type_id
_struct_conn.pdbx_PDB_id
_struct_conn.ptnr1_label_asym_id
_struct_conn.ptnr1_label_comp_id
_struct_conn.ptnr1_label_seq_id
_struct_conn.ptnr1_label_atom_id
_struct_conn.pdbx_ptnr1_label_alt_id
_struct_conn.pdbx_ptnr1_PDB_ins_code
_struct_conn.pdbx_ptnr1_standard_comp_id
_struct_conn.ptnr1_symmetry
_struct_conn.ptnr2_label_asym_id
_struct_conn.ptnr2_label_comp_id
_struct_conn.ptnr2_label_seq_id
_struct_conn.ptnr2_label_atom_id
_struct_conn.pdbx_ptnr2_label_alt_id
_struct_conn.pdbx_ptnr2_PDB_ins_code
_struct_conn.ptnr1_auth_asym_id
_struct_conn.ptnr1_auth_comp_id
_struct_conn.ptnr1_auth_seq_id
_struct_conn.ptnr2_auth_asym_id
_struct_conn.ptnr2_auth_comp_id
_struct_conn.ptnr2_auth_seq_id
_struct_conn.ptnr2_symmetry
_struct_conn.pdbx_ptnr3_label_atom_id
_struct_conn.pdbx_ptnr3_label_seq_id
_struct_conn.pdbx_ptnr3_label_comp_id
_struct_conn.pdbx_ptnr3_label_asym_id
_struct_conn.pdbx_ptnr3_label_alt_id
_struct_conn.pdbx_ptnr3_PDB_ins_code
_struct_conn.details
_struct_conn.pdbx_dist_value
```

```
_struct_conn.pdbx_value_order
metalc1  metalc ? A DG 12 O6    ? ? ? 1_555 D SR  .  SR ? ? A DG 12 A SR  102 1_555 ? ? ? ? ? ? ?
2.690 ?
covale1  covale ? A DT 8  'O3'' ? ? ? 1_555 A D3N 9  P  ? ? A DT 8  A D3N 9   1_555 ? ? ? ? ? ? ?
1.578 ?
covale2  covale ? B DT 8  'O3'' ? ? ? 1_555 B D3N 9  P  ? ? B DT 20 B D3N 21  1_555 ? ? ? ? ? ? ?
1.591 ?
covale3  covale ? A DC 3  'O3'' ? ? ? 1_555 A BZG 4  P  ? ? A DC 3  A BZG 4   1_555 ? ? ? ? ? ? ?
1.586 ?
covale4  covale ? B DC 3  'O3'' ? ? ? 1_555 B BZG 4  P  ? ? B DC 15 B BZG 16  1_555 ? ? ? ? ? ? ?
1.595 ?
hydrog1  hydrog ? A DG 2  N1    ? ? ? 1_555 B DC  11 N3 ? ? A DG 2  B DC  23  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog2  hydrog ? A DG 2  N2    ? ? ? 1_555 B DC  11 O2 ? ? A DG 2  B DC  23  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog3  hydrog ? A DG 2  O6    ? ? ? 1_555 B DC  11 N4 ? ? A DG 2  B DC  23  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog4  hydrog ? A DC 3  N3    ? ? ? 1_555 B DG  10 N1 ? ? A DC 3  B DG  22  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog5  hydrog ? A DC 3  N4    ? ? ? 1_555 B DG  10 O6 ? ? A DC 3  B DG  22  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog6  hydrog ? A DC 3  O2    ? ? ? 1_555 B DG  10 N2 ? ? A DC 3  B DG  22  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog7  hydrog ? A DA 5  N1    ? ? ? 1_555 B DT  8  N3 ? ? A DA 5  B DT  20  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog8  hydrog ? A DA 5  N6    ? ? ? 1_555 B DT  8  O4 ? ? A DA 5  B DT  20  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog9  hydrog ? A DA 6  N1    ? ? ? 1_555 B DT  7  N3 ? ? A DA 6  B DT  19  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog10 hydrog ? A DA 6  N6    ? ? ? 1_555 B DT  7  O4 ? ? A DA 6  B DT  19  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog11 hydrog ? A DT 7  N3    ? ? ? 1_555 B DA  6  N1 ? ? A DT 7  B DA  18  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog12 hydrog ? A DT 7  O4    ? ? ? 1_555 B DA  6  N6 ? ? A DT 7  B DA  18  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog13 hydrog ? A DT 8  N3    ? ? ? 1_555 B DA  5  N1 ? ? A DT 8  B DA  17  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
```

```
hydrog14 hydrog ? A DT 8  O4    ? ? ? 1_555 B DA  5  N6 ? ? A DT 8  B DA  17  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog15 hydrog ? A DG 10 N1    ? ? ? 1_555 B DC  3  N3 ? ? A DG 10 B DC  15  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog16 hydrog ? A DG 10 N2    ? ? ? 1_555 B DC  3  O2 ? ? A DG 10 B DC  15  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog17 hydrog ? A DG 10 O6    ? ? ? 1_555 B DC  3  N4 ? ? A DG 10 B DC  15  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog18 hydrog ? A DC 11 N3    ? ? ? 1_555 B DG  2  N1 ? ? A DC 11 B DG  14  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog19 hydrog ? A DC 11 N4    ? ? ? 1_555 B DG  2  O6 ? ? A DC 11 B DG  14  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
hydrog20 hydrog ? A DC 11 O2    ? ? ? 1_555 B DG  2  N2 ? ? A DC 11 B DG  14  1_555 ? ? ? ? ? ?
WATSON-CRICK ?     ?
#
loop_
_struct_conn_type.id
_struct_conn_type.criteria
_struct_conn_type.reference
covale ?
?
metalc ?
?
hydrog 'For hydrogen bonding between nucleic acid bases, donor to acceptor distance of 2.2 -3.5
Angstroms was used.' ?
#
loop_
_struct_site_gen.id
_struct_site_gen.site_id
_struct_site_gen.pdbx_num_res
_struct_site_gen.label_comp_id
_struct_site_gen.label_asym_id
_struct_site_gen.label_seq_id
_struct_site_gen.pdbx_auth_ins_code
_struct_site_gen.auth_comp_id
_struct_site_gen.auth_asym_id
_struct_site_gen.auth_seq_id
```

```
_struct_site_gen.label_atom_id
_struct_site_gen.label_alt_id
_struct_site_gen.symmetry
_struct_site_gen.details
1 AC1 6 DG  A 2  ? DG  A 2  . . 1_555 ?
2 AC1 6 D3N A 9  ? D3N A 9  . . 2_555 ?
3 AC1 6 D3N A 9  ? D3N A 9  . . 3_645 ?
4 AC1 6 DG  A 10 ? DG  A 10 . . 2_555 ?
5 AC1 6 DG  B 2  ? DG  B 14 . . 2_555 ?
6 AC1 6 DG  B 10 ? DG  B 22 . . 1_555 ?
7 AC2 1 DG  A 12 ? DG  A 12 . . 1_555 ?
#
loop_
_diffrn_radiation_wavelength.id
_diffrn_radiation_wavelength.wavelength
_diffrn_radiation_wavelength.wt
1 1.60499 1.0
2 0.97857 1.0
#
loop_
_atom_type.symbol
P
O
C
N
SR
#
loop_
_chem_comp.id
_chem_comp.type
_chem_comp.mon_nstd_flag
_chem_comp.name
_chem_comp.pdbx_synonyms
_chem_comp.formula
_chem_comp.formula_weight
DG  'DNA linking' y '2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE'
?
```

```
'C10 H14 N5 O7 P' 347.224
DC  'DNA linking' y '2'-DEOXYCYTIDINE-5'-MONOPHOSPHATE'
?
'C9 H14 N3 O7 P'  307.199
BZG 'DNA linking' . 6-(BENZYLOXY)-9-(2-DEOXY-5-O-PHOSPHONO-BETA-D-ERYTHRO-PENTOFURANOSYL)-9H-PURIN-2-
AMINE 'O6-BENZYL-2'-DEOXYGUANOSINE-5'-MONOPHOSPHATE'
'C17 H20 N5 O7 P' 437.348
DA  'DNA linking' y '2'-DEOXYADENOSINE-5'-MONOPHOSPHATE'
?
'C10 H14 N5 O6 P' 331.224
DT  'DNA linking' y 'THYMIDINE-5'-MONOPHOSPHATE'
?
'C10 H15 N2 O8 P' 322.211
D3N 'DNA linking' . 1-(2-DEOXY-5-O-PHOSPHONO-BETA-D-ERYTHRO-PENTOFURANOSYL)-1H-PERIMIDIN-2(3H)-ONE
?
'C16 H17 N2 O7 P' 380.293
SPM NON-POLYMER   . SPERMINE
?
'C10 H26 N4'      202.342
SR  NON-POLYMER   . 'STRONTIUM ION'
?
'SR 2'            87.620
HOH NON-POLYMER   . WATER
?
'H2 O'            18.015
#
loop_
_pdbx_validate_close_contact.id
_pdbx_validate_close_contact.PDB_model_num
_pdbx_validate_close_contact.auth_atom_id_1
_pdbx_validate_close_contact.auth_asym_id_1
_pdbx_validate_close_contact.auth_comp_id_1
_pdbx_validate_close_contact.auth_seq_id_1
_pdbx_validate_close_contact.PDB_ins_code_1
_pdbx_validate_close_contact.label_alt_id_1
_pdbx_validate_close_contact.auth_atom_id_2
_pdbx_validate_close_contact.auth_asym_id_2
```

```
_pdbx_validate_close_contact.auth_comp_id_2
_pdbx_validate_close_contact.auth_seq_id_2
_pdbx_validate_close_contact.PDB_ins_code_2
_pdbx_validate_close_contact.label_alt_id_2
_pdbx_validate_close_contact.dist
1 1 O A HOH 225 ? ? O A HOH 226 ? ? 2.09
2 1 O B HOH 103 ? ? O B HOH 104 ? ? 2.19
#
_pdbx_validate_rmsd_angle.id                 1
_pdbx_validate_rmsd_angle.PDB_model_num      1
_pdbx_validate_rmsd_angle.auth_atom_id_1     'C1''
_pdbx_validate_rmsd_angle.auth_asym_id_1     A
_pdbx_validate_rmsd_angle.auth_comp_id_1     DC
_pdbx_validate_rmsd_angle.auth_seq_id_1      3
_pdbx_validate_rmsd_angle.PDB_ins_code_1     ?
_pdbx_validate_rmsd_angle.label_alt_id_1     ?
_pdbx_validate_rmsd_angle.auth_atom_id_2     'O4''
_pdbx_validate_rmsd_angle.auth_asym_id_2     A
_pdbx_validate_rmsd_angle.auth_comp_id_2     DC
_pdbx_validate_rmsd_angle.auth_seq_id_2      3
_pdbx_validate_rmsd_angle.PDB_ins_code_2     ?
_pdbx_validate_rmsd_angle.label_alt_id_2     ?
_pdbx_validate_rmsd_angle.auth_atom_id_3     'C4''
_pdbx_validate_rmsd_angle.auth_asym_id_3     A
_pdbx_validate_rmsd_angle.auth_comp_id_3     DC
_pdbx_validate_rmsd_angle.auth_seq_id_3      3
_pdbx_validate_rmsd_angle.PDB_ins_code_3     ?
_pdbx_validate_rmsd_angle.label_alt_id_3     ?
_pdbx_validate_rmsd_angle.angle_deviation    -6.2
#
loop_
_pdbx_entity_nonpoly.entity_id
_pdbx_entity_nonpoly.name
_pdbx_entity_nonpoly.comp_id
2 SPERMINE        SPM
3 'STRONTIUM ION' SR
4 water           HOH
```

```
#
loop_
_atom_site.group_PDB
_atom_site.id
_atom_site.type_symbol
_atom_site.label_atom_id
_atom_site.label_alt_id
_atom_site.label_comp_id
_atom_site.label_asym_id
_atom_site.label_entity_id
_atom_site.label_seq_id
_atom_site.pdbx_PDB_ins_code
_atom_site.Cartn_x
_atom_site.Cartn_y
_atom_site.Cartn_z
_atom_site.occupancy
_atom_site.B_iso_or_equiv
_atom_site.Cartn_x_esd
_atom_site.Cartn_y_esd
_atom_site.Cartn_z_esd
_atom_site.occupancy_esd
_atom_site.B_iso_or_equiv_esd
_atom_site.pdbx_formal_charge
_atom_site.auth_seq_id
_atom_site.auth_comp_id
_atom_site.auth_asym_id
_atom_site.auth_atom_id
_atom_site.pdbx_PDB_model_num
ATOM   1   P  P     . DG  A 1 2  ? 9.239  -10.993 30.734  0.60 64.21  ? ? ? ? ? ? 2   DG  A P     1
ATOM   2   O  OP1   . DG  A 1 2  ? 9.072  -10.756 32.190  0.60 60.29  ? ? ? ? ? ? 2   DG  A OP1   1
ATOM   3   O  OP2   . DG  A 1 2  ? 9.385  -12.395 30.228  0.60 53.30  ? ? ? ? ? ? 2   DG  A OP2   1
ATOM   4   O  'O5'' . DG  A 1 2  ? 8.014  -10.291 29.981  1.00 66.68  ? ? ? ? ? ? 2   DG  A 'O5'' 1
ATOM   5   C  'C5'' . DG  A 1 2  ? 6.825  -9.899  30.702  1.00 55.81  ? ? ? ? ? ? 2   DG  A 'C5'' 1
ATOM   6   C  'C4'' . DG  A 1 2  ? 5.949  -8.961  29.894  1.00 52.59  ? ? ? ? ? ? 2   DG  A 'C4'' 1
ATOM   7   O  'O4'' . DG  A 1 2  ? 6.194  -7.574  30.229  1.00 47.03  ? ? ? ? ? ? 2   DG  A 'O4'' 1
ATOM   8   C  'C3'' . DG  A 1 2  ? 6.021  -9.044  28.371  1.00 47.01  ? ? ? ? ? ? 2   DG  A 'C3'' 1
ATOM   9   O  'O3'' . DG  A 1 2  ? 4.664  -8.805  27.971  1.00 43.95  ? ? ? ? ? ? 2   DG  A 'O3'' 1
```

```
ATOM   10  C  'C2'' . DG  A 1 2  ? 6.953  -7.905  28.004  1.00 43.36  ? ? ? ? ? ? 2  DG  A 'C2'' 1
ATOM   11  C  'C1'' . DG  A 1 2  ? 6.723  -6.873  29.101  1.00 38.71  ? ? ? ? ? ? 2  DG  A 'C1'' 1
ATOM   12  N  N9    . DG  A 1 2  ? 7.941  -6.215  29.539  1.00 38.13  ? ? ? ? ? ? 2  DG  A N9    1
ATOM   13  C  C8    . DG  A 1 2  ? 9.159  -6.806  29.783  1.00 40.71  ? ? ? ? ? ? 2  DG  A C8    1
ATOM   14  N  N7    . DG  A 1 2  ? 10.037 -5.980  30.285  1.00 37.92  ? ? ? ? ? ? 2  DG  A N7    1
ATOM   15  C  C5    . DG  A 1 2  ? 9.326  -4.799  30.471  1.00 34.44  ? ? ? ? ? ? 2  DG  A C5    1
ATOM   16  C  C6    . DG  A 1 2  ? 9.751  -3.550  30.963  1.00 33.16  ? ? ? ? ? ? 2  DG  A C6    1
ATOM   17  O  O6    . DG  A 1 2  ? 10.873 -3.233  31.386  1.00 39.27  ? ? ? ? ? ? 2  DG  A O6    1
ATOM   18  N  N1    . DG  A 1 2  ? 8.717  -2.611  30.947  1.00 31.66  ? ? ? ? ? ? 2  DG  A N1    1
ATOM   19  C  C2    . DG  A 1 2  ? 7.432  -2.858  30.522  1.00 26.82  ? ? ? ? ? ? 2  DG  A C2    1
ATOM   20  N  N2    . DG  A 1 2  ? 6.580  -1.803  30.529  1.00 29.37  ? ? ? ? ? ? 2  DG  A N2    1
ATOM   21  N  N3    . DG  A 1 2  ? 7.035  -4.016  30.020  1.00 32.27  ? ? ? ? ? ? 2  DG  A N3    1
ATOM   22  C  C4    . DG  A 1 2  ? 8.029  -4.933  30.021  1.00 32.15  ? ? ? ? ? ? 2  DG  A C4    1
ATOM   23  P  P     . DC  A 1 3  ? 4.239  -8.657  26.447  1.00 46.97  ? ? ? ? ? ? 3  DC  A P     1
ATOM   24  O  OP1   . DC  A 1 3  ? 2.751  -8.762  26.393  1.00 49.89  ? ? ? ? ? ? 3  DC  A OP1   1
ATOM   25  O  OP2   . DC  A 1 3  ? 5.133  -9.515  25.605  1.00 53.26  ? ? ? ? ? ? 3  DC  A OP2   1
ATOM   26  O  'O5'' . DC  A 1 3  ? 4.520  -7.119  26.124  1.00 43.44  ? ? ? ? ? ? 3  DC  A 'O5'' 1
ATOM   27  C  'C5'' . DC  A 1 3  ? 3.632  -6.106  26.576  1.00 38.31  ? ? ? ? ? ? 3  DC  A 'C5'' 1
ATOM   28  C  'C4'' . DC  A 1 3  ? 4.287  -4.774  26.306  1.00 36.86  ? ? ? ? ? ? 3  DC  A 'C4'' 1
ATOM   29  O  'O4'' . DC  A 1 3  ? 5.592  -4.779  26.930  1.00 42.11  ? ? ? ? ? ? 3  DC  A 'O4'' 1
ATOM   30  C  'C3'' . DC  A 1 3  ? 4.561  -4.493  24.826  1.00 34.95  ? ? ? ? ? ? 3  DC  A 'C3'' 1
ATOM   31  O  'O3'' . DC  A 1 3  ? 3.753  -3.403  24.382  1.00 46.76  ? ? ? ? ? ? 3  DC  A 'O3'' 1
ATOM   32  C  'C2'' . DC  A 1 3  ? 6.019  -4.016  24.799  1.00 40.64  ? ? ? ? ? ? 3  DC  A 'C2'' 1
ATOM   33  C  'C1'' . DC  A 1 3  ? 6.290  -3.756  26.261  1.00 38.02  ? ? ? ? ? ? 3  DC  A 'C1'' 1
ATOM   34  N  N1    . DC  A 1 3  ? 7.686  -3.832  26.664  1.00 41.53  ? ? ? ? ? ? 3  DC  A N1    1
ATOM   35  C  C2    . DC  A 1 3  ? 8.245  -2.738  27.324  1.00 33.63  ? ? ? ? ? ? 3  DC  A C2    1
ATOM   36  O  O2    . DC  A 1 3  ? 7.552  -1.720  27.493  1.00 33.20  ? ? ? ? ? ? 3  DC  A O2    1
ATOM   37  N  N3    . DC  A 1 3  ? 9.537  -2.790  27.708  1.00 34.36  ? ? ? ? ? ? 3  DC  A N3    1
ATOM   38  C  C4    . DC  A 1 3  ? 10.247 -3.901  27.511  1.00 35.83  ? ? ? ? ? ? 3  DC  A C4    1
ATOM   39  N  N4    . DC  A 1 3  ? 11.529 -3.895  27.888  1.00 38.69  ? ? ? ? ? ? 3  DC  A N4    1
ATOM   40  C  C5    . DC  A 1 3  ? 9.691  -5.046  26.867  1.00 36.91  ? ? ? ? ? ? 3  DC  A C5    1
ATOM   41  C  C6    . DC  A 1 3  ? 8.397  -4.990  26.524  1.00 35.23  ? ? ? ? ? ? 3  DC  A C6    1
ATOM   42  P  P     . BZG A 1 4  ? 2.649  -3.637  23.267  1.00 46.63  ? ? ? ? ? ? 4  BZG A P     1
ATOM   43  O  O1P   . BZG A 1 4  ? 3.306  -3.955  21.993  1.00 44.93  ? ? ? ? ? ? 4  BZG A O1P   1
ATOM   44  O  O2P   . BZG A 1 4  ? 1.836  -4.638  23.969  1.00 55.23  ? ? ? ? ? ? 4  BZG A O2P   1
ATOM   45  O  'O5'' . BZG A 1 4  ? 1.933  -2.246  23.191  1.00 39.01  ? ? ? ? ? ? 4  BZG A 'O5'' 1
ATOM   46  C  CZ1   . BZG A 1 4  ? 11.175 0.290   21.777  1.00 37.59  ? ? ? ? ? ? 4  BZG A CZ1   1
```

```
ATOM   47  C  CT1   . BZG A 1 4  ? 12.294 -0.517  21.686  1.00 39.06  ? ? ? ? ? ? 4   BZG A CT1   1
ATOM   48  C  CI    . BZG A 1 4  ? 13.507 0.035   22.067  1.00 33.85  ? ? ? ? ? ? 4   BZG A CI    1
ATOM   49  C  CT2   . BZG A 1 4  ? 13.624 1.374   22.446  1.00 36.75  ? ? ? ? ? ? 4   BZG A CT2   1
ATOM   50  C  CZ2   . BZG A 1 4  ? 12.497 2.161   22.581  1.00 36.31  ? ? ? ? ? ? 4   BZG A CZ2   1
ATOM   51  C  CE    . BZG A 1 4  ? 11.293 1.609   22.203  1.00 36.33  ? ? ? ? ? ? 4   BZG A CE    1
ATOM   52  C  CW    . BZG A 1 4  ? 10.069 2.471   22.307  1.00 34.89  ? ? ? ? ? ? 4   BZG A CW    1
ATOM   53  O  OL    . BZG A 1 4  ? 8.937  1.590   22.071  1.00 37.78  ? ? ? ? ? ? 4   BZG A OL    1
ATOM   54  C  CK    . BZG A 1 4  ? 7.707  2.091   22.327  1.00 35.01  ? ? ? ? ? ? 4   BZG A CK    1
ATOM   55  N  NJ    . BZG A 1 4  ? 7.570  3.379   22.668  1.00 36.53  ? ? ? ? ? ? 4   BZG A NJ    1
ATOM   56  C  CH    . BZG A 1 4  ? 6.358  3.899   22.966  1.00 39.60  ? ? ? ? ? ? 4   BZG A CH    1
ATOM   57  N  NI    . BZG A 1 4  ? 6.258  5.215   23.214  1.00 42.29  ? ? ? ? ? ? 4   BZG A NI    1
ATOM   58  N  NG    . BZG A 1 4  ? 5.249  3.116   22.978  1.00 37.80  ? ? ? ? ? ? 4   BZG A NG    1
ATOM   59  C  CF    . BZG A 1 4  ? 5.361  1.799   22.674  1.00 35.38  ? ? ? ? ? ? 4   BZG A CF    1
ATOM   60  C  CM    . BZG A 1 4  ? 6.607  1.239   22.361  1.00 37.85  ? ? ? ? ? ? 4   BZG A CM    1
ATOM   61  N  NN    . BZG A 1 4  ? 6.455  -0.083  22.118  1.00 39.19  ? ? ? ? ? ? 4   BZG A NN    1
ATOM   62  C  CO    . BZG A 1 4  ? 5.137  -0.349  22.296  1.00 39.06  ? ? ? ? ? ? 4   BZG A CO    1
ATOM   63  N  NE    . BZG A 1 4  ? 4.484  0.814   22.580  1.00 38.14  ? ? ? ? ? ? 4   BZG A NE    1
ATOM   64  C  'CT'' . BZG A 1 4  ? 3.049  1.004   22.890  1.00 40.97  ? ? ? ? ? ? 4   BZG A 'CT'' 1
ATOM   65  O  'OS'' . BZG A 1 4  ? 2.752  0.367   24.126  1.00 41.96  ? ? ? ? ? ? 4   BZG A 'OS'' 1
ATOM   66  C  'CP'' . BZG A 1 4  ? 2.139  0.420   21.818  1.00 42.75  ? ? ? ? ? ? 4   BZG A 'CP'' 1
ATOM   67  C  'C5'' . BZG A 1 4  ? 1.432  -1.656  24.357  1.00 40.60  ? ? ? ? ? ? 4   BZG A 'C5'' 1
ATOM   68  C  'C4'' . BZG A 1 4  ? 1.409  -0.173  24.040  1.00 46.89  ? ? ? ? ? ? 4   BZG A 'C4'' 1
ATOM   69  C  'C3'' . BZG A 1 4  ? 0.883  0.134   22.623  1.00 46.88  ? ? ? ? ? ? 4   BZG A 'C3'' 1
ATOM   70  O  'O3'' . BZG A 1 4  ? 0.164  1.363   22.838  1.00 55.09  ? ? ? ? ? ? 4   BZG A 'O3'' 1
ATOM   71  P  P     . DA  A 1 5  ? -0.648 2.070   21.637  1.00 58.27  ? ? ? ? ? ? 5   DA  A P     1
ATOM   72  O  OP1   . DA  A 1 5  ? -1.834 2.738   22.239  1.00 59.14  ? ? ? ? ? ? 5   DA  A OP1   1
ATOM   73  O  OP2   . DA  A 1 5  ? -0.808 1.074   20.536  1.00 59.17  ? ? ? ? ? ? 5   DA  A OP2   1
ATOM   74  O  'O5'' . DA  A 1 5  ? 0.307  3.265   21.217  1.00 49.03  ? ? ? ? ? ? 5   DA  A 'O5'' 1
ATOM   75  C  'C5'' . DA  A 1 5  ? 0.681  4.240   22.198  1.00 48.58  ? ? ? ? ? ? 5   DA  A 'C5'' 1
ATOM   76  C  'C4'' . DA  A 1 5  ? 1.593  5.267   21.581  1.00 56.65  ? ? ? ? ? ? 5   DA  A 'C4'' 1
ATOM   77  O  'O4'' . DA  A 1 5  ? 2.908  4.711   21.358  1.00 53.36  ? ? ? ? ? ? 5   DA  A 'O4'' 1
ATOM   78  C  'C3'' . DA  A 1 5  ? 1.123  5.797   20.227  1.00 59.46  ? ? ? ? ? ? 5   DA  A 'C3'' 1
ATOM   79  O  'O3'' . DA  A 1 5  ? 1.300  7.208   20.242  1.00 60.34  ? ? ? ? ? ? 5   DA  A 'O3'' 1
ATOM   80  C  'C2'' . DA  A 1 5  ? 2.038  5.114   19.223  1.00 55.75  ? ? ? ? ? ? 5   DA  A 'C2'' 1
ATOM   81  C  'C1'' . DA  A 1 5  ? 3.316  4.936   20.017  1.00 51.87  ? ? ? ? ? ? 5   DA  A 'C1'' 1
ATOM   82  N  N9    . DA  A 1 5  ? 4.126  3.793   19.610  1.00 46.83  ? ? ? ? ? ? 5   DA  A N9    1
ATOM   83  C  C8    . DA  A 1 5  ? 3.701  2.511   19.368  1.00 43.90  ? ? ? ? ? ? 5   DA  A C8    1
```

```
ATOM   84  N  N7    . DA  A 1 5  ? 4.669  1.681   19.062  1.00 44.68  ? ? ? ? ? ? 5  DA  A N7    1
ATOM   85  C  C5    . DA  A 1 5  ? 5.813  2.463   19.135  1.00 42.49  ? ? ? ? ? ? 5  DA  A C5    1
ATOM   86  C  C6    . DA  A 1 5  ? 7.172  2.158   18.979  1.00 36.19  ? ? ? ? ? ? 5  DA  A C6    1
ATOM   87  N  N6    . DA  A 1 5  ? 7.619  0.949   18.637  1.00 36.49  ? ? ? ? ? ? 5  DA  A N6    1
ATOM   88  N  N1    . DA  A 1 5  ? 8.060  3.168   19.099  1.00 36.14  ? ? ? ? ? ? 5  DA  A N1    1
ATOM   89  C  C2    . DA  A 1 5  ? 7.610  4.377   19.460  1.00 36.19  ? ? ? ? ? ? 5  DA  A C2    1
ATOM   90  N  N3    . DA  A 1 5  ? 6.358  4.781   19.670  1.00 42.40  ? ? ? ? ? ? 5  DA  A N3    1
ATOM   91  C  C4    . DA  A 1 5  ? 5.498  3.760   19.499  1.00 35.08  ? ? ? ? ? ? 5  DA  A C4    1
ATOM   92  P  P     . DA  A 1 6  ? 0.679  8.066   19.071  1.00 66.25  ? ? ? ? ? ? 6  DA  A P     1
ATOM   93  O  OP1   . DA  A 1 6  ? -0.038 9.214   19.677  1.00 73.87  ? ? ? ? ? ? 6  DA  A OP1   1
ATOM   94  O  OP2   . DA  A 1 6  ? -0.026 7.124   18.154  1.00 62.28  ? ? ? ? ? ? 6  DA  A OP2   1
ATOM   95  O  'O5'' . DA  A 1 6  ? 1.965  8.619   18.327  1.00 55.29  ? ? ? ? ? ? 6  DA  A 'O5'' 1
ATOM   96  C  'C5'' . DA  A 1 6  ? 3.074  9.156   19.054  1.00 56.56  ? ? ? ? ? ? 6  DA  A 'C5'' 1
ATOM   97  C  'C4'' . DA  A 1 6  ? 4.288  9.061   18.166  1.00 53.18  ? ? ? ? ? ? 6  DA  A 'C4'' 1
ATOM   98  O  'O4'' . DA  A 1 6  ? 4.605  7.667   17.970  1.00 48.57  ? ? ? ? ? ? 6  DA  A 'O4'' 1
ATOM   99  C  'C3'' . DA  A 1 6  ? 4.033  9.623   16.761  1.00 59.75  ? ? ? ? ? ? 6  DA  A 'C3'' 1
ATOM   100 O  'O3'' . DA  A 1 6  ? 4.671  10.904  16.635  1.00 59.83  ? ? ? ? ? ? 6  DA  A 'O3'' 1
ATOM   101 C  'C2'' . DA  A 1 6  ? 4.466  8.501   15.815  1.00 57.57  ? ? ? ? ? ? 6  DA  A 'C2'' 1
ATOM   102 C  'C1'' . DA  A 1 6  ? 5.241  7.571   16.732  1.00 43.65  ? ? ? ? ? ? 6  DA  A 'C1'' 1
ATOM   103 N  N9    . DA  A 1 6  ? 5.326  6.159   16.375  1.00 38.41  ? ? ? ? ? ? 6  DA  A N9    1
ATOM   104 C  C8    . DA  A 1 6  ? 4.358  5.195   16.240  1.00 32.72  ? ? ? ? ? ? 6  DA  A C8    1
ATOM   105 N  N7    . DA  A 1 6  ? 4.833  4.013   15.917  1.00 34.57  ? ? ? ? ? ? 6  DA  A N7    1
ATOM   106 C  C5    . DA  A 1 6  ? 6.209  4.200   15.909  1.00 39.39  ? ? ? ? ? ? 6  DA  A C5    1
ATOM   107 C  C6    . DA  A 1 6  ? 7.281  3.323   15.681  1.00 36.78  ? ? ? ? ? ? 6  DA  A C6    1
ATOM   108 N  N6    . DA  A 1 6  ? 7.130  2.029   15.402  1.00 36.24  ? ? ? ? ? ? 6  DA  A N6    1
ATOM   109 N  N1    . DA  A 1 6  ? 8.529  3.843   15.685  1.00 40.20  ? ? ? ? ? ? 6  DA  A N1    1
ATOM   110 C  C2    . DA  A 1 6  ? 8.683  5.138   15.979  1.00 42.40  ? ? ? ? ? ? 6  DA  A C2    1
ATOM   111 N  N3    . DA  A 1 6  ? 7.757  6.057   16.242  1.00 44.66  ? ? ? ? ? ? 6  DA  A N3    1
ATOM   112 C  C4    . DA  A 1 6  ? 6.526  5.514   16.198  1.00 39.31  ? ? ? ? ? ? 6  DA  A C4    1
ATOM   113 P  P     . DT  A 1 7  ? 4.489  11.764  15.293  1.00 63.69  ? ? ? ? ? ? 7  DT  A P     1
ATOM   114 O  OP1   . DT  A 1 7  ? 4.824  13.180  15.604  1.00 69.37  ? ? ? ? ? ? 7  DT  A OP1   1
ATOM   115 O  OP2   . DT  A 1 7  ? 3.191  11.401  14.662  1.00 58.46  ? ? ? ? ? ? 7  DT  A OP2   1
ATOM   116 O  'O5'' . DT  A 1 7  ? 5.636  11.175  14.367  1.00 46.43  ? ? ? ? ? ? 7  DT  A 'O5'' 1
ATOM   117 C  'C5'' . DT  A 1 7  ? 7.007  11.417  14.718  1.00 51.47  ? ? ? ? ? ? 7  DT  A 'C5'' 1
ATOM   118 C  'C4'' . DT  A 1 7  ? 7.866  10.655  13.748  1.00 46.90  ? ? ? ? ? ? 7  DT  A 'C4'' 1
ATOM   119 O  'O4'' . DT  A 1 7  ? 7.578  9.255   13.892  1.00 48.09  ? ? ? ? ? ? 7  DT  A 'O4'' 1
ATOM   120 C  'C3'' . DT  A 1 7  ? 7.495  10.983  12.306  1.00 43.45  ? ? ? ? ? ? 7  DT  A 'C3'' 1
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ATOM   121 O  'O3'' . DT  A 1 7  ? 8.490  11.822  11.752  1.00 52.70  ? ? ? ? ? ? 7   DT  A 'O3'' 1
ATOM   122 C  'C2'' . DT  A 1 7  ? 7.380  9.628   11.617  1.00 50.70  ? ? ? ? ? ? 7   DT  A 'C2'' 1
ATOM   123 C  'C1'' . DT  A 1 7  ? 7.913  8.677   12.663  1.00 47.48  ? ? ? ? ? ? 7   DT  A 'C1'' 1
ATOM   124 N  N1    . DT  A 1 7  ? 7.376  7.317   12.639  1.00 41.31  ? ? ? ? ? ? 7   DT  A N1    1
ATOM   125 C  C2    . DT  A 1 7  ? 8.289  6.297   12.506  1.00 41.88  ? ? ? ? ? ? 7   DT  A C2    1
ATOM   126 O  O2    . DT  A 1 7  ? 9.493  6.487   12.429  1.00 42.96  ? ? ? ? ? ? 7   DT  A O2    1
ATOM   127 N  N3    . DT  A 1 7  ? 7.745  5.043   12.494  1.00 38.18  ? ? ? ? ? ? 7   DT  A N3    1
ATOM   128 C  C4    . DT  A 1 7  ? 6.413  4.714   12.593  1.00 39.17  ? ? ? ? ? ? 7   DT  A C4    1
ATOM   129 O  O4    . DT  A 1 7  ? 6.074  3.542   12.534  1.00 42.62  ? ? ? ? ? ? 7   DT  A O4    1
ATOM   130 C  C5    . DT  A 1 7  ? 5.502  5.840   12.688  1.00 39.25  ? ? ? ? ? ? 7   DT  A C5    1
ATOM   131 C  C7    . DT  A 1 7  ? 4.033  5.582   12.805  1.00 37.23  ? ? ? ? ? ? 7   DT  A C7    1
ATOM   132 C  C6    . DT  A 1 7  ? 6.024  7.068   12.690  1.00 36.63  ? ? ? ? ? ? 7   DT  A C6    1
ATOM   133 P  P     . DT  A 1 8  ? 8.228  12.450  10.338  1.00 52.32  ? ? ? ? ? ? 8   DT  A P     1
ATOM   134 O  OP1   . DT  A 1 8  ? 8.908  13.746  10.289  1.00 52.05  ? ? ? ? ? ? 8   DT  A OP1   1
ATOM   135 O  OP2   . DT  A 1 8  ? 6.757  12.374  10.063  1.00 55.19  ? ? ? ? ? ? 8   DT  A OP2   1
ATOM   136 O  'O5'' . DT  A 1 8  ? 8.910  11.384  9.375   1.00 46.41  ? ? ? ? ? ? 8   DT  A 'O5'' 1
ATOM   137 C  'C5'' . DT  A 1 8  ? 10.246 10.929  9.583   1.00 44.52  ? ? ? ? ? ? 8   DT  A 'C5'' 1
ATOM   138 C  'C4'' . DT  A 1 8  ? 10.482 9.804   8.610   1.00 43.89  ? ? ? ? ? ? 8   DT  A 'C4'' 1
ATOM   139 O  'O4'' . DT  A 1 8  ? 9.790  8.651   9.114   1.00 42.41  ? ? ? ? ? ? 8   DT  A 'O4'' 1
ATOM   140 C  'C3'' . DT  A 1 8  ? 9.850  10.104  7.249   1.00 48.97  ? ? ? ? ? ? 8   DT  A 'C3'' 1
ATOM   141 O  'O3'' . DT  A 1 8  ? 10.867 10.316  6.277   1.00 53.05  ? ? ? ? ? ? 8   DT  A 'O3'' 1
ATOM   142 C  'C2'' . DT  A 1 8  ? 8.964  8.904   6.950   1.00 40.46  ? ? ? ? ? ? 8   DT  A 'C2'' 1
ATOM   143 C  'C1'' . DT  A 1 8  ? 9.334  7.892   8.018   1.00 41.47  ? ? ? ? ? ? 8   DT  A 'C1'' 1
ATOM   144 N  N1    . DT  A 1 8  ? 8.211  7.065   8.474   1.00 38.36  ? ? ? ? ? ? 8   DT  A N1    1
ATOM   145 C  C2    . DT  A 1 8  ? 8.433  5.721   8.676   1.00 39.71  ? ? ? ? ? ? 8   DT  A C2    1
ATOM   146 O  O2    . DT  A 1 8  ? 9.530  5.206   8.573   1.00 42.69  ? ? ? ? ? ? 8   DT  A O2    1
ATOM   147 N  N3    . DT  A 1 8  ? 7.323  5.008   9.045   1.00 37.19  ? ? ? ? ? ? 8   DT  A N3    1
ATOM   148 C  C4    . DT  A 1 8  ? 6.055  5.502   9.280   1.00 42.23  ? ? ? ? ? ? 8   DT  A C4    1
ATOM   149 O  O4    . DT  A 1 8  ? 5.156  4.739   9.627   1.00 44.03  ? ? ? ? ? ? 8   DT  A O4    1
ATOM   150 C  C5    . DT  A 1 8  ? 5.887  6.917   9.020   1.00 38.33  ? ? ? ? ? ? 8   DT  A C5    1
ATOM   151 C  C7    . DT  A 1 8  ? 4.544  7.541   9.235   1.00 43.91  ? ? ? ? ? ? 8   DT  A C7    1
ATOM   152 C  C6    . DT  A 1 8  ? 6.956  7.612   8.618   1.00 36.11  ? ? ? ? ? ? 8   DT  A C6    1
ATOM   153 O  O1P   . D3N A 1 9  ? 9.151  11.502  5.034   1.00 57.06  ? ? ? ? ? ? 9   D3N A O1P   1
ATOM   154 P  P     . D3N A 1 9  ? 10.467 10.803  4.830   1.00 59.57  ? ? ? ? ? ? 9   D3N A P     1
ATOM   155 O  O2P   . D3N A 1 9  ? 11.529 11.563  4.178   1.00 57.35  ? ? ? ? ? ? 9   D3N A O2P   1
ATOM   156 O  'O5'' . D3N A 1 9  ? 10.132 9.407   4.099   1.00 45.73  ? ? ? ? ? ? 9   D3N A 'O5'' 1
ATOM   157 C  'C5'' . D3N A 1 9  ? 9.339  9.445   2.962   1.00 56.53  ? ? ? ? ? ? 9   D3N A 'C5'' 1
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ATOM   158 C  'C4''' . D3N A 1 9  ? 9.661  8.312  2.011   1.00 49.95  ? ? ? ? ? ? 9  D3N A 'C4''' 1
ATOM   159 O  'O4''' . D3N A 1 9  ? 8.863  7.224  2.387   1.00 46.67  ? ? ? ? ? ? 9  D3N A 'O4''' 1
ATOM   160 C  'C3''' . D3N A 1 9  ? 9.320  8.677  0.601   1.00 47.42  ? ? ? ? ? ? 9  D3N A 'C3''' 1
ATOM   161 O  'O3''' . D3N A 1 9  ? 10.640 8.976  -0.003  1.00 54.09  ? ? ? ? ? ? 9  D3N A 'O3''' 1
ATOM   162 C  'C2''' . D3N A 1 9  ? 8.658  7.422  0.042   1.00 44.59  ? ? ? ? ? ? 9  D3N A 'C2''' 1
ATOM   163 C  'C1''' . D3N A 1 9  ? 8.417  6.534  1.230   1.00 46.91  ? ? ? ? ? ? 9  D3N A 'C1''' 1
ATOM   164 N  N1     . D3N A 1 9  ? 7.078  6.124  1.580   1.00 36.46  ? ? ? ? ? ? 9  D3N A N1     1
ATOM   165 C  C2     . D3N A 1 9  ? 6.110  7.057  1.685   1.00 38.72  ? ? ? ? ? ? 9  D3N A C2     1
ATOM   166 O  O2     . D3N A 1 9  ? 6.297  8.251  1.417   1.00 48.10  ? ? ? ? ? ? 9  D3N A O2     1
ATOM   167 N  N3     . D3N A 1 9  ? 4.887  6.635  2.099   1.00 41.54  ? ? ? ? ? ? 9  D3N A N3     1
ATOM   168 C  C4     . D3N A 1 9  ? 4.594  5.301  2.451   1.00 36.92  ? ? ? ? ? ? 9  D3N A C4     1
ATOM   169 C  C5     . D3N A 1 9  ? 5.607  4.371  2.331   1.00 36.17  ? ? ? ? ? ? 9  D3N A C5     1
ATOM   170 C  C6     . D3N A 1 9  ? 6.891  4.763  1.888   1.00 36.76  ? ? ? ? ? ? 9  D3N A C6     1
ATOM   171 C  C7     . D3N A 1 9  ? 7.850  3.823  1.781   1.00 37.28  ? ? ? ? ? ? 9  D3N A C7     1
ATOM   172 C  C8     . D3N A 1 9  ? 7.548  2.482  2.091   1.00 38.67  ? ? ? ? ? ? 9  D3N A C8     1
ATOM   173 C  C9     . D3N A 1 9  ? 6.313  2.075  2.503   1.00 34.82  ? ? ? ? ? ? 9  D3N A C9     1
ATOM   174 C  C10    . D3N A 1 9  ? 5.329  3.022  2.649   1.00 36.15  ? ? ? ? ? ? 9  D3N A C10    1
ATOM   175 C  C11    . D3N A 1 9  ? 4.040  2.682  3.115   1.00 39.57  ? ? ? ? ? ? 9  D3N A C11    1
ATOM   176 C  C12    . D3N A 1 9  ? 3.039  3.617  3.226   1.00 43.64  ? ? ? ? ? ? 9  D3N A C12    1
ATOM   177 C  C13    . D3N A 1 9  ? 3.306  4.953  2.885   1.00 37.78  ? ? ? ? ? ? 9  D3N A C13    1
ATOM   178 P  P      . DG  A 1 10 ? 10.766 9.455  -1.541  1.00 52.40  ? ? ? ? ? ? 10 DG  A P      1
ATOM   179 O  OP1    . DG  A 1 10 ? 11.926 10.387 -1.619  1.00 52.96  ? ? ? ? ? ? 10 DG  A OP1    1
ATOM   180 O  OP2    . DG  A 1 10 ? 9.429  9.942  -2.020  1.00 49.83  ? ? ? ? ? ? 10 DG  A OP2    1
ATOM   181 O  'O5''' . DG  A 1 10 ? 11.122 8.085  -2.299  1.00 46.54  ? ? ? ? ? ? 10 DG  A 'O5''' 1
ATOM   182 C  'C5''' . DG  A 1 10 ? 12.098 7.130  -1.833  1.00 40.41  ? ? ? ? ? ? 10 DG  A 'C5''' 1
ATOM   183 C  'C4''' . DG  A 1 10 ? 11.817 5.781  -2.467  1.00 46.19  ? ? ? ? ? ? 10 DG  A 'C4''' 1
ATOM   184 O  'O4''' . DG  A 1 10 ? 10.495 5.337  -2.050  1.00 41.89  ? ? ? ? ? ? 10 DG  A 'O4''' 1
ATOM   185 C  'C3''' . DG  A 1 10 ? 11.772 5.751  -3.999  1.00 42.11  ? ? ? ? ? ? 10 DG  A 'C3''' 1
ATOM   186 O  'O3''' . DG  A 1 10 ? 11.986 4.386  -4.405  1.00 43.10  ? ? ? ? ? ? 10 DG  A 'O3''' 1
ATOM   187 C  'C2''' . DG  A 1 10 ? 10.312 6.041  -4.278  1.00 37.56  ? ? ? ? ? ? 10 DG  A 'C2''' 1
ATOM   188 C  'C1''' . DG  A 1 10 ? 9.649  5.223  -3.182  1.00 39.74  ? ? ? ? ? ? 10 DG  A 'C1''' 1
ATOM   189 N  N9     . DG  A 1 10 ? 8.318  5.670  -2.791  1.00 36.64  ? ? ? ? ? ? 10 DG  A N9     1
ATOM   190 C  C8     . DG  A 1 10 ? 7.813  6.946  -2.904  1.00 38.12  ? ? ? ? ? ? 10 DG  A C8     1
ATOM   191 N  N7     . DG  A 1 10 ? 6.596  7.058  -2.443  1.00 33.59  ? ? ? ? ? ? 10 DG  A N7     1
ATOM   192 C  C5     . DG  A 1 10 ? 6.277  5.778  -1.999  1.00 32.82  ? ? ? ? ? ? 10 DG  A C5     1
ATOM   193 C  C6     . DG  A 1 10 ? 5.098  5.289  -1.387  1.00 33.36  ? ? ? ? ? ? 10 DG  A C6     1
ATOM   194 O  O6     . DG  A 1 10 ? 4.056  5.900  -1.124  1.00 33.85  ? ? ? ? ? ? 10 DG  A O6     1
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ATOM   195 N  N1    . DG  A 1 10 ? 5.178  3.921   -1.139  1.00 32.10  ? ? ? ? ? ? 10  DG  A N1    1
ATOM   196 C  C2    . DG  A 1 10 ? 6.298  3.154   -1.316  1.00 32.80  ? ? ? ? ? ? 10  DG  A C2    1
ATOM   197 N  N2    . DG  A 1 10 ? 6.170  1.847   -1.011  1.00 30.07  ? ? ? ? ? ? 10  DG  A N2    1
ATOM   198 N  N3    . DG  A 1 10 ? 7.410  3.596   -1.892  1.00 30.93  ? ? ? ? ? ? 10  DG  A N3    1
ATOM   199 C  C4    . DG  A 1 10 ? 7.337  4.916   -2.184  1.00 36.17  ? ? ? ? ? ? 10  DG  A C4    1
ATOM   200 P  P     . DC  A 1 11 ? 12.576 3.993   -5.867  1.00 45.72  ? ? ? ? ? ? 11  DC  A P     1
ATOM   201 O  OP1   . DC  A 1 11 ? 14.013 3.708   -5.707  1.00 55.46  ? ? ? ? ? ? 11  DC  A OP1   1
ATOM   202 O  OP2   . DC  A 1 11 ? 12.140 4.979   -6.893  1.00 40.18  ? ? ? ? ? ? 11  DC  A OP2   1
ATOM   203 O  'O5'' . DC  A 1 11 ? 11.897 2.569   -6.086  1.00 42.94  ? ? ? ? ? ? 11  DC  A 'O5'' 1
ATOM   204 C  'C5'' . DC  A 1 11 ? 12.323 1.462   -5.304  1.00 35.76  ? ? ? ? ? ? 11  DC  A 'C5'' 1
ATOM   205 C  'C4'' . DC  A 1 11 ? 11.244 0.407   -5.260  1.00 38.62  ? ? ? ? ? ? 11  DC  A 'C4'' 1
ATOM   206 O  'O4'' . DC  A 1 11 ? 10.071 0.969   -4.638  1.00 38.55  ? ? ? ? ? ? 11  DC  A 'O4'' 1
ATOM   207 C  'C3'' . DC  A 1 11 ? 10.785 -0.117  -6.624  1.00 41.61  ? ? ? ? ? ? 11  DC  A 'C3'' 1
ATOM   208 O  'O3'' . DC  A 1 11 ? 10.597 -1.537  -6.580  1.00 36.55  ? ? ? ? ? ? 11  DC  A 'O3'' 1
ATOM   209 C  'C2'' . DC  A 1 11 ? 9.399  0.483   -6.801  1.00 35.59  ? ? ? ? ? ? 11  DC  A 'C2'' 1
ATOM   210 C  'C1'' . DC  A 1 11 ? 8.928  0.621   -5.361  1.00 32.15  ? ? ? ? ? ? 11  DC  A 'C1'' 1
ATOM   211 N  N1    . DC  A 1 11 ? 7.930  1.697   -5.184  1.00 32.78  ? ? ? ? ? ? 11  DC  A N1    1
ATOM   212 C  C2    . DC  A 1 11 ? 6.724  1.419   -4.517  1.00 33.71  ? ? ? ? ? ? 11  DC  A C2    1
ATOM   213 O  O2    . DC  A 1 11 ? 6.588  0.324   -3.936  1.00 35.86  ? ? ? ? ? ? 11  DC  A O2    1
ATOM   214 N  N3    . DC  A 1 11 ? 5.767  2.369   -4.474  1.00 30.73  ? ? ? ? ? ? 11  DC  A N3    1
ATOM   215 C  C4    . DC  A 1 11 ? 5.992  3.574   -5.013  1.00 31.53  ? ? ? ? ? ? 11  DC  A C4    1
ATOM   216 N  N4    . DC  A 1 11 ? 5.017  4.482   -4.943  1.00 29.21  ? ? ? ? ? ? 11  DC  A N4    1
ATOM   217 C  C5    . DC  A 1 11 ? 7.212  3.886   -5.677  1.00 29.13  ? ? ? ? ? ? 11  DC  A C5    1
ATOM   218 C  C6    . DC  A 1 11 ? 8.141  2.926   -5.747  1.00 34.19  ? ? ? ? ? ? 11  DC  A C6    1
ATOM   219 P  P     . DG  A 1 12 ? 11.039 -2.438  -7.862  1.00 43.78  ? ? ? ? ? ? 12  DG  A P     1
ATOM   220 O  OP1   . DG  A 1 12 ? 10.876 -3.861  -7.477  1.00 44.28  ? ? ? ? ? ? 12  DG  A OP1   1
ATOM   221 O  OP2   . DG  A 1 12 ? 12.357 -1.933  -8.370  1.00 40.00  ? ? ? ? ? ? 12  DG  A OP2   1
ATOM   222 O  'O5'' . DG  A 1 12 ? 9.983  -2.054  -8.975  1.00 40.27  ? ? ? ? ? ? 12  DG  A 'O5'' 1
ATOM   223 C  'C5'' . DG  A 1 12 ? 8.619  -2.501  -8.874  1.00 43.08  ? ? ? ? ? ? 12  DG  A 'C5'' 1
ATOM   224 C  'C4'' . DG  A 1 12 ? 7.882  -2.053  -10.106 1.00 39.93  ? ? ? ? ? ? 12  DG  A 'C4'' 1
ATOM   225 O  'O4'' . DG  A 1 12 ? 7.921  -0.607  -10.134 1.00 36.76  ? ? ? ? ? ? 12  DG  A 'O4'' 1
ATOM   226 C  'C3'' . DG  A 1 12 ? 8.562  -2.505  -11.397 1.00 40.02  ? ? ? ? ? ? 12  DG  A 'C3'' 1
ATOM   227 O  'O3'' . DG  A 1 12 ? 7.910  -3.662  -11.897 1.00 39.85  ? ? ? ? ? ? 12  DG  A 'O3'' 1
ATOM   228 C  'C2'' . DG  A 1 12 ? 8.360  -1.335  -12.320 1.00 38.74  ? ? ? ? ? ? 12  DG  A 'C2'' 1
ATOM   229 C  'C1'' . DG  A 1 12 ? 8.439  -0.157  -11.368 1.00 39.35  ? ? ? ? ? ? 12  DG  A 'C1'' 1
ATOM   230 N  N9    . DG  A 1 12 ? 9.781  0.359   -11.119 1.00 37.62  ? ? ? ? ? ? 12  DG  A N9    1
ATOM   231 C  C8    . DG  A 1 12 ? 10.976 -0.269  -11.381 1.00 44.00  ? ? ? ? ? ? 12  DG  A C8    1
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ATOM   232 N  N7    . DG  A 1 12 ? 12.012 0.429   -11.001 1.00 42.04  ? ? ? ? ? ? 12  DG  A N7    1
ATOM   233 C  C5    . DG  A 1 12 ? 11.465 1.537   -10.366 1.00 41.36  ? ? ? ? ? ? 12  DG  A C5    1
ATOM   234 C  C6    . DG  A 1 12 ? 12.096 2.635   -9.733  1.00 46.68  ? ? ? ? ? ? 12  DG  A C6    1
ATOM   235 O  O6    . DG  A 1 12 ? 13.304 2.848   -9.585  1.00 44.90  ? ? ? ? ? ? 12  DG  A O6    1
ATOM   236 N  N1    . DG  A 1 12 ? 11.166 3.555   -9.257  1.00 37.19  ? ? ? ? ? ? 12  DG  A N1    1
ATOM   237 C  C2    . DG  A 1 12 ? 9.805  3.432   -9.369  1.00 37.43  ? ? ? ? ? ? 12  DG  A C2    1
ATOM   238 N  N2    . DG  A 1 12 ? 9.081  4.437   -8.858  1.00 34.27  ? ? ? ? ? ? 12  DG  A N2    1
ATOM   239 N  N3    . DG  A 1 12 ? 9.202  2.383   -9.905  1.00 34.44  ? ? ? ? ? ? 12  DG  A N3    1
ATOM   240 C  C4    . DG  A 1 12 ? 10.088 1.495   -10.408 1.00 38.94  ? ? ? ? ? ? 12  DG  A C4    1
ATOM   241 O  'O3'' . DC  B 1 1  ? -6.095 1.968   -3.008  1.00 104.56 ? ? ? ? ? ? 13  DC  B 'O3'' 1
ATOM   242 P  P     . DG  B 1 2  ? -4.822 1.409   -3.812  1.00 105.65 ? ? ? ? ? ? 14  DG  B P     1
ATOM   243 O  OP1   . DG  B 1 2  ? -3.885 2.550   -4.035  1.00 96.18  ? ? ? ? ? ? 14  DG  B OP1   1
ATOM   244 O  OP2   . DG  B 1 2  ? -5.315 0.603   -4.976  1.00 78.96  ? ? ? ? ? ? 14  DG  B OP2   1
ATOM   245 O  'O5'' . DG  B 1 2  ? -4.185 0.364   -2.794  1.00 74.48  ? ? ? ? ? ? 14  DG  B 'O5'' 1
ATOM   246 C  'C5'' . DG  B 1 2  ? -3.928 -0.984  -3.220  1.00 57.72  ? ? ? ? ? ? 14  DG  B 'C5'' 1
ATOM   247 C  'C4'' . DG  B 1 2  ? -2.876 -1.621  -2.345  1.00 54.83  ? ? ? ? ? ? 14  DG  B 'C4'' 1
ATOM   248 O  'O4'' . DG  B 1 2  ? -1.555 -1.129  -2.675  1.00 52.37  ? ? ? ? ? ? 14  DG  B 'O4'' 1
ATOM   249 C  'C3'' . DG  B 1 2  ? -3.040 -1.398  -0.847  1.00 47.69  ? ? ? ? ? ? 14  DG  B 'C3'' 1
ATOM   250 O  'O3'' . DG  B 1 2  ? -2.610 -2.634  -0.294  1.00 47.75  ? ? ? ? ? ? 14  DG  B 'O3'' 1
ATOM   251 C  'C2'' . DG  B 1 2  ? -2.064 -0.272  -0.550  1.00 44.50  ? ? ? ? ? ? 14  DG  B 'C2'' 1
ATOM   252 C  'C1'' . DG  B 1 2  ? -0.942 -0.523  -1.550  1.00 46.21  ? ? ? ? ? ? 14  DG  B 'C1'' 1
ATOM   253 N  N9    . DG  B 1 2  ? -0.301 0.694   -2.022  1.00 32.96  ? ? ? ? ? ? 14  DG  B N9    1
ATOM   254 C  C8    . DG  B 1 2  ? -0.949 1.860   -2.348  1.00 38.11  ? ? ? ? ? ? 14  DG  B C8    1
ATOM   255 N  N7    . DG  B 1 2  ? -0.162 2.749   -2.890  1.00 34.89  ? ? ? ? ? ? 14  DG  B N7    1
ATOM   256 C  C5    . DG  B 1 2  ? 1.083  2.136   -2.918  1.00 35.32  ? ? ? ? ? ? 14  DG  B C5    1
ATOM   257 C  C6    . DG  B 1 2  ? 2.324  2.613   -3.403  1.00 32.74  ? ? ? ? ? ? 14  DG  B C6    1
ATOM   258 O  O6    . DG  B 1 2  ? 2.594  3.731   -3.859  1.00 38.67  ? ? ? ? ? ? 14  DG  B O6    1
ATOM   259 N  N1    . DG  B 1 2  ? 3.340  1.683   -3.204  1.00 33.06  ? ? ? ? ? ? 14  DG  B N1    1
ATOM   260 C  C2    . DG  B 1 2  ? 3.155  0.400   -2.738  1.00 30.22  ? ? ? ? ? ? 14  DG  B C2    1
ATOM   261 N  N2    . DG  B 1 2  ? 4.259  -0.379  -2.677  1.00 32.78  ? ? ? ? ? ? 14  DG  B N2    1
ATOM   262 N  N3    . DG  B 1 2  ? 1.989  -0.073  -2.324  1.00 33.84  ? ? ? ? ? ? 14  DG  B N3    1
ATOM   263 C  C4    . DG  B 1 2  ? 1.002  0.844   -2.441  1.00 34.05  ? ? ? ? ? ? 14  DG  B C4    1
ATOM   264 P  P     . DC  B 1 3  ? -2.707 -2.910  1.247   1.00 52.14  ? ? ? ? ? ? 15  DC  B P     1
ATOM   265 O  OP1   . DC  B 1 3  ? -2.794 -4.367  1.421   1.00 52.06  ? ? ? ? ? ? 15  DC  B OP1   1
ATOM   266 O  OP2   . DC  B 1 3  ? -3.707 -1.995  1.828   1.00 47.13  ? ? ? ? ? ? 15  DC  B OP2   1
ATOM   267 O  'O5'' . DC  B 1 3  ? -1.258 -2.522  1.759   1.00 45.23  ? ? ? ? ? ? 15  DC  B 'O5'' 1
ATOM   268 C  'C5'' . DC  B 1 3  ? -0.153 -3.310  1.307   1.00 46.29  ? ? ? ? ? ? 15  DC  B 'C5'' 1
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ATOM   269 C  'C4'' . DC  B 1 3  ? 1.130  -2.589  1.622   1.00 42.32  ? ? ? ? ? ? 15  DC  B 'C4'' 1
ATOM   270 O  'O4'' . DC  B 1 3  ? 1.192  -1.371  0.856   1.00 45.55  ? ? ? ? ? ? 15  DC  B 'O4'' 1
ATOM   271 C  'C3'' . DC  B 1 3  ? 1.296  -2.166  3.088   1.00 47.96  ? ? ? ? ? ? 15  DC  B 'C3'' 1
ATOM   272 O  'O3'' . DC  B 1 3  ? 2.440  -2.809  3.642   1.00 56.55  ? ? ? ? ? ? 15  DC  B 'O3'' 1
ATOM   273 C  'C2'' . DC  B 1 3  ? 1.637  -0.684  3.018   1.00 42.57  ? ? ? ? ? ? 15  DC  B 'C2'' 1
ATOM   274 C  'C1'' . DC  B 1 3  ? 2.050  -0.520  1.577   1.00 36.84  ? ? ? ? ? ? 15  DC  B 'C1'' 1
ATOM   275 N  N1    . DC  B 1 3  ? 1.874  0.836   1.061   1.00 37.49  ? ? ? ? ? ? 15  DC  B N1    1
ATOM   276 C  C2    . DC  B 1 3  ? 2.964  1.476   0.473   1.00 35.12  ? ? ? ? ? ? 15  DC  B C2    1
ATOM   277 O  O2    . DC  B 1 3  ? 4.049  0.859   0.377   1.00 30.92  ? ? ? ? ? ? 15  DC  B O2    1
ATOM   278 N  N3    . DC  B 1 3  ? 2.818  2.739   0.015   1.00 30.96  ? ? ? ? ? ? 15  DC  B N3    1
ATOM   279 C  C4    . DC  B 1 3  ? 1.651  3.370   0.160   1.00 35.63  ? ? ? ? ? ? 15  DC  B C4    1
ATOM   280 N  N4    . DC  B 1 3  ? 1.553  4.608   -0.306  1.00 31.76  ? ? ? ? ? ? 15  DC  B N4    1
ATOM   281 C  C5    . DC  B 1 3  ? 0.510  2.724   0.715   1.00 31.16  ? ? ? ? ? ? 15  DC  B C5    1
ATOM   282 C  C6    . DC  B 1 3  ? 0.664  1.466   1.147   1.00 30.61  ? ? ? ? ? ? 15  DC  B C6    1
ATOM   283 P  P     . BZG B 1 4  ? 2.251  -3.983  4.705   1.00 59.25  ? ? ? ? ? ? 16  BZG B P     1
ATOM   284 O  O1P   . BZG B 1 4  ? 1.758  -3.334  5.965   1.00 59.84  ? ? ? ? ? ? 16  BZG B O1P   1
ATOM   285 O  O2P   . BZG B 1 4  ? 1.431  -4.994  3.984   1.00 58.44  ? ? ? ? ? ? 16  BZG B O2P   1
ATOM   286 O  'O5'' . BZG B 1 4  ? 3.716  -4.525  4.868   1.00 53.19  ? ? ? ? ? ? 16  BZG B 'O5'' 1
ATOM   287 C  CZ1   . BZG B 1 4  ? 6.738  6.622   5.264   1.00 37.15  ? ? ? ? ? ? 16  BZG B CZ1   1
ATOM   288 C  CT1   . BZG B 1 4  ? 5.819  7.656   5.321   1.00 40.05  ? ? ? ? ? ? 16  BZG B CT1   1
ATOM   289 C  CI    . BZG B 1 4  ? 4.485  7.425   5.686   1.00 46.13  ? ? ? ? ? ? 16  BZG B CI    1
ATOM   290 C  CT2   . BZG B 1 4  ? 4.042  6.151   6.055   1.00 42.60  ? ? ? ? ? ? 16  BZG B CT2   1
ATOM   291 C  CZ2   . BZG B 1 4  ? 4.968  5.094   6.004   1.00 41.87  ? ? ? ? ? ? 16  BZG B CZ2   1
ATOM   292 C  CE    . BZG B 1 4  ? 6.295  5.331   5.627   1.00 36.41  ? ? ? ? ? ? 16  BZG B CE    1
ATOM   293 C  CW    . BZG B 1 4  ? 7.263  4.189   5.618   1.00 39.93  ? ? ? ? ? ? 16  BZG B CW    1
ATOM   294 O  OL    . BZG B 1 4  ? 6.564  2.941   5.856   1.00 43.12  ? ? ? ? ? ? 16  BZG B OL    1
ATOM   295 C  CK    . BZG B 1 4  ? 7.211  1.733   5.634   1.00 40.04  ? ? ? ? ? ? 16  BZG B CK    1
ATOM   296 N  NJ    . BZG B 1 4  ? 8.525  1.744   5.314   1.00 43.22  ? ? ? ? ? ? 16  BZG B NJ    1
ATOM   297 C  CH    . BZG B 1 4  ? 9.182  0.577   5.068   1.00 43.83  ? ? ? ? ? ? 16  BZG B CH    1
ATOM   298 N  NI    . BZG B 1 4  ? 10.491 0.578   4.779   1.00 45.60  ? ? ? ? ? ? 16  BZG B NI    1
ATOM   299 N  NG    . BZG B 1 4  ? 8.549  -0.623  5.114   1.00 42.53  ? ? ? ? ? ? 16  BZG B NG    1
ATOM   300 C  CF    . BZG B 1 4  ? 7.252  -0.663  5.426   1.00 39.41  ? ? ? ? ? ? 16  BZG B CF    1
ATOM   301 C  CM    . BZG B 1 4  ? 6.539  0.509   5.663   1.00 37.34  ? ? ? ? ? ? 16  BZG B CM    1
ATOM   302 N  NN    . BZG B 1 4  ? 5.264  0.119   5.947   1.00 45.16  ? ? ? ? ? ? 16  BZG B NN    1
ATOM   303 C  CO    . BZG B 1 4  ? 5.213  -1.240  5.844   1.00 37.18  ? ? ? ? ? ? 16  BZG B CO    1
ATOM   304 N  NE    . BZG B 1 4  ? 6.447  -1.687  5.551   1.00 41.81  ? ? ? ? ? ? 16  BZG B NE    1
ATOM   305 C  'CT'' . BZG B 1 4  ? 6.866  -3.092  5.296   1.00 48.18  ? ? ? ? ? ? 16  BZG B 'CT'' 1
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ATOM   306 O  'OS'' . BZG B 1 4  ? 6.296  -3.544  4.063   1.00 50.49  ? ? ? ? ? ? 16  BZG B 'OS'' 1
ATOM   307 C  'CP'' . BZG B 1 4  ? 6.358  -4.070  6.336   1.00 51.14  ? ? ? ? ? ? 16  BZG B 'CP'' 1
ATOM   308 C  'C5'' . BZG B 1 4  ? 4.448  -5.049  3.759   1.00 55.03  ? ? ? ? ? ? 16  BZG B 'C5'' 1
ATOM   309 C  'C4'' . BZG B 1 4  ? 5.918  -4.932  4.128   1.00 54.38  ? ? ? ? ? ? 16  BZG B 'C4'' 1
ATOM   310 C  'C3'' . BZG B 1 4  ? 6.225  -5.365  5.557   1.00 49.35  ? ? ? ? ? ? 16  BZG B 'C3'' 1
ATOM   311 O  'O3'' . BZG B 1 4  ? 7.520  -5.968  5.495   1.00 53.57  ? ? ? ? ? ? 16  BZG B 'O3'' 1
ATOM   312 P  P     . DA  B 1 5  ? 8.189  -6.628  6.814   1.00 57.46  ? ? ? ? ? ? 17  DA  B P     1
ATOM   313 O  OP1   . DA  B 1 5  ? 9.109  -7.704  6.368   1.00 58.86  ? ? ? ? ? ? 17  DA  B OP1   1
ATOM   314 O  OP2   . DA  B 1 5  ? 7.101  -6.947  7.780   1.00 55.69  ? ? ? ? ? ? 17  DA  B OP2   1
ATOM   315 O  'O5'' . DA  B 1 5  ? 9.148  -5.476  7.354   1.00 51.31  ? ? ? ? ? ? 17  DA  B 'O5'' 1
ATOM   316 C  'C5'' . DA  B 1 5  ? 10.239 -4.994  6.552   1.00 51.08  ? ? ? ? ? ? 17  DA  B 'C5'' 1
ATOM   317 C  'C4'' . DA  B 1 5  ? 10.920 -3.871  7.294   1.00 53.59  ? ? ? ? ? ? 17  DA  B 'C4'' 1
ATOM   318 O  'O4'' . DA  B 1 5  ? 10.038 -2.714  7.363   1.00 48.85  ? ? ? ? ? ? 17  DA  B 'O4'' 1
ATOM   319 C  'C3'' . DA  B 1 5  ? 11.227 -4.235  8.747   1.00 51.37  ? ? ? ? ? ? 17  DA  B 'C3'' 1
ATOM   320 O  'O3'' . DA  B 1 5  ? 12.439 -3.577  9.077   1.00 65.84  ? ? ? ? ? ? 17  DA  B 'O3'' 1
ATOM   321 C  'C2'' . DA  B 1 5  ? 10.084 -3.589  9.514   1.00 43.01  ? ? ? ? ? ? 17  DA  B 'C2'' 1
ATOM   322 C  'C1'' . DA  B 1 5  ? 9.935  -2.310  8.712   1.00 45.18  ? ? ? ? ? ? 17  DA  B 'C1'' 1
ATOM   323 N  N9    . DA  B 1 5  ? 8.669  -1.606  8.891   1.00 38.03  ? ? ? ? ? ? 17  DA  B N9    1
ATOM   324 C  C8    . DA  B 1 5  ? 7.432  -2.107  9.213   1.00 42.14  ? ? ? ? ? ? 17  DA  B C8    1
ATOM   325 N  N7    . DA  B 1 5  ? 6.518  -1.183  9.394   1.00 44.19  ? ? ? ? ? ? 17  DA  B N7    1
ATOM   326 C  C5    . DA  B 1 5  ? 7.198  0.006   9.158   1.00 37.91  ? ? ? ? ? ? 17  DA  B C5    1
ATOM   327 C  C6    . DA  B 1 5  ? 6.787  1.346   9.175   1.00 34.62  ? ? ? ? ? ? 17  DA  B C6    1
ATOM   328 N  N6    . DA  B 1 5  ? 5.538  1.734   9.450   1.00 40.59  ? ? ? ? ? ? 17  DA  B N6    1
ATOM   329 N  N1    . DA  B 1 5  ? 7.719  2.290   8.930   1.00 38.79  ? ? ? ? ? ? 17  DA  B N1    1
ATOM   330 C  C2    . DA  B 1 5  ? 8.969  1.901   8.648   1.00 40.00  ? ? ? ? ? ? 17  DA  B C2    1
ATOM   331 N  N3    . DA  B 1 5  ? 9.474  0.671   8.592   1.00 45.23  ? ? ? ? ? ? 17  DA  B N3    1
ATOM   332 C  C4    . DA  B 1 5  ? 8.526  -0.240  8.865   1.00 35.76  ? ? ? ? ? ? 17  DA  B C4    1
ATOM   333 P  P     . DA  B 1 6  ? 13.626 -4.397  9.688   1.00 60.35  ? ? ? ? ? ? 18  DA  B P     1
ATOM   334 O  OP1   . DA  B 1 6  ? 14.221 -5.214  8.602   1.00 63.82  ? ? ? ? ? ? 18  DA  B OP1   1
ATOM   335 O  OP2   . DA  B 1 6  ? 13.144 -5.035  10.931  1.00 49.85  ? ? ? ? ? ? 18  DA  B OP2   1
ATOM   336 O  'O5'' . DA  B 1 6  ? 14.622 -3.248  10.144  1.00 59.82  ? ? ? ? ? ? 18  DA  B 'O5'' 1
ATOM   337 C  'C5'' . DA  B 1 6  ? 15.222 -2.375  9.182   1.00 53.72  ? ? ? ? ? ? 18  DA  B 'C5'' 1
ATOM   338 C  'C4'' . DA  B 1 6  ? 15.373 -1.007  9.798   1.00 52.59  ? ? ? ? ? ? 18  DA  B 'C4'' 1
ATOM   339 O  'O4'' . DA  B 1 6  ? 14.075 -0.384  9.913   1.00 55.38  ? ? ? ? ? ? 18  DA  B 'O4'' 1
ATOM   340 C  'C3'' . DA  B 1 6  ? 15.965 -1.026  11.205  1.00 44.97  ? ? ? ? ? ? 18  DA  B 'C3'' 1
ATOM   341 O  'O3'' . DA  B 1 6  ? 17.114 -0.188  11.173  1.00 59.93  ? ? ? ? ? ? 18  DA  B 'O3'' 1
ATOM   342 C  'C2'' . DA  B 1 6  ? 14.828 -0.567  12.111  1.00 50.88  ? ? ? ? ? ? 18  DA  B 'C2'' 1
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ATOM   343 C  'C1'' . DA  B 1 6  ? 13.928 0.218   11.180  1.00 45.59  ? ? ? ? ? ? 18  DA  B 'C1'' 1
ATOM   344 N  N9    . DA  B 1 6  ? 12.502 0.193   11.505  1.00 41.89  ? ? ? ? ? ? 18  DA  B N9    1
ATOM   345 C  C8    . DA  B 1 6  ? 11.681 -0.902  11.603  1.00 35.00  ? ? ? ? ? ? 18  DA  B C8    1
ATOM   346 N  N7    . DA  B 1 6  ? 10.436 -0.601  11.890  1.00 40.93  ? ? ? ? ? ? 18  DA  B N7    1
ATOM   347 C  C5    . DA  B 1 6  ? 10.425 0.789   11.911  1.00 39.79  ? ? ? ? ? ? 18  DA  B C5    1
ATOM   348 C  C6    . DA  B 1 6  ? 9.393  1.726   12.103  1.00 41.31  ? ? ? ? ? ? 18  DA  B C6    1
ATOM   349 N  N6    . DA  B 1 6  ? 8.115  1.390   12.303  1.00 35.05  ? ? ? ? ? ? 18  DA  B N6    1
ATOM   350 N  N1    . DA  B 1 6  ? 9.715  3.037   12.035  1.00 37.78  ? ? ? ? ? ? 18  DA  B N1    1
ATOM   351 C  C2    . DA  B 1 6  ? 10.985 3.371   11.805  1.00 39.76  ? ? ? ? ? ? 18  DA  B C2    1
ATOM   352 N  N3    . DA  B 1 6  ? 12.041 2.585   11.605  1.00 44.05  ? ? ? ? ? ? 18  DA  B N3    1
ATOM   353 C  C4    . DA  B 1 6  ? 11.682 1.290   11.641  1.00 39.60  ? ? ? ? ? ? 18  DA  B C4    1
ATOM   354 P  P     . DT  B 1 7  ? 18.150 -0.225  12.366  1.00 66.24  ? ? ? ? ? ? 19  DT  B P     1
ATOM   355 O  OP1   . DT  B 1 7  ? 19.404 0.414   11.889  1.00 73.70  ? ? ? ? ? ? 19  DT  B OP1   1
ATOM   356 O  OP2   . DT  B 1 7  ? 18.168 -1.604  12.915  1.00 73.00  ? ? ? ? ? ? 19  DT  B OP2   1
ATOM   357 O  'O5'' . DT  B 1 7  ? 17.480 0.772   13.403  1.00 63.34  ? ? ? ? ? ? 19  DT  B 'O5'' 1
ATOM   358 C  'C5'' . DT  B 1 7  ? 17.286 2.131   12.994  1.00 59.35  ? ? ? ? ? ? 19  DT  B 'C5'' 1
ATOM   359 C  'C4'' . DT  B 1 7  ? 16.414 2.851   13.989  1.00 52.77  ? ? ? ? ? ? 19  DT  B 'C4'' 1
ATOM   360 O  'O4'' . DT  B 1 7  ? 15.043 2.464   13.823  1.00 43.01  ? ? ? ? ? ? 19  DT  B 'O4'' 1
ATOM   361 C  'C3'' . DT  B 1 7  ? 16.741 2.544   15.448  1.00 50.15  ? ? ? ? ? ? 19  DT  B 'C3'' 1
ATOM   362 O  'O3'' . DT  B 1 7  ? 17.589 3.588   15.904  1.00 57.13  ? ? ? ? ? ? 19  DT  B 'O3'' 1
ATOM   363 C  'C2'' . DT  B 1 7  ? 15.385 2.585   16.142  1.00 47.40  ? ? ? ? ? ? 19  DT  B 'C2'' 1
ATOM   364 C  'C1'' . DT  B 1 7  ? 14.405 2.874   15.005  1.00 44.86  ? ? ? ? ? ? 19  DT  B 'C1'' 1
ATOM   365 N  N1    . DT  B 1 7  ? 13.128 2.183   15.087  1.00 41.99  ? ? ? ? ? ? 19  DT  B N1    1
ATOM   366 C  C2    . DT  B 1 7  ? 11.999 2.961   15.192  1.00 40.74  ? ? ? ? ? ? 19  DT  B C2    1
ATOM   367 O  O2    . DT  B 1 7  ? 12.029 4.180   15.200  1.00 45.09  ? ? ? ? ? ? 19  DT  B O2    1
ATOM   368 N  N3    . DT  B 1 7  ? 10.821 2.257   15.242  1.00 38.44  ? ? ? ? ? ? 19  DT  B N3    1
ATOM   369 C  C4    . DT  B 1 7  ? 10.670 0.889   15.267  1.00 39.65  ? ? ? ? ? ? 19  DT  B C4    1
ATOM   370 O  O4    . DT  B 1 7  ? 9.546  0.403   15.355  1.00 40.87  ? ? ? ? ? ? 19  DT  B O4    1
ATOM   371 C  C5    . DT  B 1 7  ? 11.901 0.129   15.196  1.00 37.60  ? ? ? ? ? ? 19  DT  B C5    1
ATOM   372 C  C7    . DT  B 1 7  ? 11.834 -1.365  15.237  1.00 38.18  ? ? ? ? ? ? 19  DT  B C7    1
ATOM   373 C  C6    . DT  B 1 7  ? 13.055 0.806   15.109  1.00 40.86  ? ? ? ? ? ? 19  DT  B C6    1
ATOM   374 P  P     . DT  B 1 8  ? 18.294 3.480   17.302  1.00 61.96  ? ? ? ? ? ? 20  DT  B P     1
ATOM   375 O  OP1   . DT  B 1 8  ? 19.496 4.353   17.267  1.00 72.95  ? ? ? ? ? ? 20  DT  B OP1   1
ATOM   376 O  OP2   . DT  B 1 8  ? 18.438 2.030   17.625  1.00 58.29  ? ? ? ? ? ? 20  DT  B OP2   1
ATOM   377 O  'O5'' . DT  B 1 8  ? 17.227 4.175   18.257  1.00 52.32  ? ? ? ? ? ? 20  DT  B 'O5'' 1
ATOM   378 C  'C5'' . DT  B 1 8  ? 16.699 5.464   17.926  1.00 47.16  ? ? ? ? ? ? 20  DT  B 'C5'' 1
ATOM   379 C  'C4'' . DT  B 1 8  ? 15.636 5.844   18.927  1.00 54.14  ? ? ? ? ? ? 20  DT  B 'C4'' 1
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ATOM   380 O  'O4'' . DT  B 1 8  ? 14.406 5.175   18.571  1.00 51.72  ? ? ? ? ? ? 20  DT  B 'O4'' 1
ATOM   381 C  'C3'' . DT  B 1 8  ? 15.945 5.420   20.366  1.00 55.66  ? ? ? ? ? ? 20  DT  B 'C3'' 1
ATOM   382 O  'O3'' . DT  B 1 8  ? 15.647 6.479   21.276  1.00 62.72  ? ? ? ? ? ? 20  DT  B 'O3'' 1
ATOM   383 C  'C2'' . DT  B 1 8  ? 15.020 4.243   20.607  1.00 48.82  ? ? ? ? ? ? 20  DT  B 'C2'' 1
ATOM   384 C  'C1'' . DT  B 1 8  ? 13.848 4.604   19.724  1.00 48.53  ? ? ? ? ? ? 20  DT  B 'C1'' 1
ATOM   385 N  N1    . DT  B 1 8  ? 13.035 3.471   19.303  1.00 41.47  ? ? ? ? ? ? 20  DT  B N1    1
ATOM   386 C  C2    . DT  B 1 8  ? 11.693 3.702   19.147  1.00 42.38  ? ? ? ? ? ? 20  DT  B C2    1
ATOM   387 O  O2    . DT  B 1 8  ? 11.182 4.786   19.358  1.00 40.94  ? ? ? ? ? ? 20  DT  B O2    1
ATOM   388 N  N3    . DT  B 1 8  ? 10.961 2.597   18.790  1.00 39.48  ? ? ? ? ? ? 20  DT  B N3    1
ATOM   389 C  C4    . DT  B 1 8  ? 11.440 1.329   18.529  1.00 43.13  ? ? ? ? ? ? 20  DT  B C4    1
ATOM   390 O  O4    . DT  B 1 8  ? 10.665 0.442   18.187  1.00 43.85  ? ? ? ? ? ? 20  DT  B O4    1
ATOM   391 C  C5    . DT  B 1 8  ? 12.874 1.170   18.676  1.00 36.61  ? ? ? ? ? ? 20  DT  B C5    1
ATOM   392 C  C7    . DT  B 1 8  ? 13.491 -0.170  18.421  1.00 41.24  ? ? ? ? ? ? 20  DT  B C7    1
ATOM   393 C  C6    . DT  B 1 8  ? 13.588 2.240   19.037  1.00 31.95  ? ? ? ? ? ? 20  DT  B C6    1
ATOM   394 O  O1P   . D3N B 1 9  ? 17.527 5.577   22.677  1.00 57.63  ? ? ? ? ? ? 21  D3N B O1P   1
ATOM   395 P  P     . D3N B 1 9  ? 16.324 6.477   22.716  1.00 73.10  ? ? ? ? ? ? 21  D3N B P     1
ATOM   396 O  O2P   . D3N B 1 9  ? 16.449 7.907   23.055  1.00 71.06  ? ? ? ? ? ? 21  D3N B O2P   1
ATOM   397 O  'O5'' . D3N B 1 9  ? 15.191 5.843   23.617  1.00 65.54  ? ? ? ? ? ? 21  D3N B 'O5'' 1
ATOM   398 C  'C5'' . D3N B 1 9  ? 15.589 5.167   24.785  1.00 68.44  ? ? ? ? ? ? 21  D3N B 'C5'' 1
ATOM   399 C  'C4'' . D3N B 1 9  ? 14.459 5.106   25.773  1.00 63.43  ? ? ? ? ? ? 21  D3N B 'C4'' 1
ATOM   400 O  'O4'' . D3N B 1 9  ? 13.681 4.031   25.359  1.00 56.75  ? ? ? ? ? ? 21  D3N B 'O4'' 1
ATOM   401 C  'C3'' . D3N B 1 9  ? 14.935 4.721   27.123  1.00 63.88  ? ? ? ? ? ? 21  D3N B 'C3'' 1
ATOM   402 O  'O3'' . D3N B 1 9  ? 15.133 5.944   27.827  1.00 67.07  ? ? ? ? ? ? 21  D3N B 'O3'' 1
ATOM   403 C  'C2'' . D3N B 1 9  ? 13.814 3.859   27.696  1.00 56.92  ? ? ? ? ? ? 21  D3N B 'C2'' 1
ATOM   404 C  'C1'' . D3N B 1 9  ? 12.920 3.605   26.492  1.00 52.83  ? ? ? ? ? ? 21  D3N B 'C1'' 1
ATOM   405 N  N1    . D3N B 1 9  ? 12.484 2.276   26.132  1.00 47.27  ? ? ? ? ? ? 21  D3N B N1    1
ATOM   406 C  C2    . D3N B 1 9  ? 13.435 1.323   25.912  1.00 47.67  ? ? ? ? ? ? 21  D3N B C2    1
ATOM   407 O  O2    . D3N B 1 9  ? 14.627 1.553   26.095  1.00 53.65  ? ? ? ? ? ? 21  D3N B O2    1
ATOM   408 N  N3    . D3N B 1 9  ? 13.009 0.096   25.555  1.00 43.83  ? ? ? ? ? ? 21  D3N B N3    1
ATOM   409 C  C4    . D3N B 1 9  ? 11.663 -0.223  25.295  1.00 39.23  ? ? ? ? ? ? 21  D3N B C4    1
ATOM   410 C  C5    . D3N B 1 9  ? 10.696 0.762   25.488  1.00 44.29  ? ? ? ? ? ? 21  D3N B C5    1
ATOM   411 C  C6    . D3N B 1 9  ? 11.081 2.040   25.924  1.00 42.62  ? ? ? ? ? ? 21  D3N B C6    1
ATOM   412 C  C7    . D3N B 1 9  ? 10.111 2.990   26.145  1.00 52.13  ? ? ? ? ? ? 21  D3N B C7    1
ATOM   413 C  C8    . D3N B 1 9  ? 8.771  2.646   25.913  1.00 39.74  ? ? ? ? ? ? 21  D3N B C8    1
ATOM   414 C  C9    . D3N B 1 9  ? 8.378  1.426   25.500  1.00 47.35  ? ? ? ? ? ? 21  D3N B C9    1
ATOM   415 C  C10   . D3N B 1 9  ? 9.330  0.451   25.258  1.00 41.01  ? ? ? ? ? ? 21  D3N B C10   1
ATOM   416 C  C11   . D3N B 1 9  ? 8.992  -0.837  24.848  1.00 43.98  ? ? ? ? ? ? 21  D3N B C11   1
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ATOM   417 C  C12   . D3N B 1 9  ? 9.952  -1.768  24.635  1.00 45.05  ? ? ? ? ? ? 21  D3N B C12   1
ATOM   418 C  C13   . D3N B 1 9  ? 11.312 -1.482  24.872  1.00 47.17  ? ? ? ? ? ? 21  D3N B C13   1
ATOM   419 P  P     . DG  B 1 10 ? 15.736 5.916   29.307  1.00 60.70  ? ? ? ? ? ? 22  DG  B P     1
ATOM   420 O  OP1   . DG  B 1 10 ? 16.433 7.208   29.532  1.00 63.59  ? ? ? ? ? ? 22  DG  B OP1   1
ATOM   421 O  OP2   . DG  B 1 10 ? 16.495 4.640   29.465  1.00 51.49  ? ? ? ? ? ? 22  DG  B OP2   1
ATOM   422 O  'O5'' . DG  B 1 10 ? 14.420 5.963   30.208  1.00 56.71  ? ? ? ? ? ? 22  DG  B 'O5'' 1
ATOM   423 C  'C5'' . DG  B 1 10 ? 13.283 6.789   29.854  1.00 44.99  ? ? ? ? ? ? 22  DG  B 'C5'' 1
ATOM   424 C  'C4'' . DG  B 1 10 ? 12.025 6.262   30.509  1.00 50.00  ? ? ? ? ? ? 22  DG  B 'C4'' 1
ATOM   425 O  'O4'' . DG  B 1 10 ? 11.708 4.952   29.984  1.00 42.89  ? ? ? ? ? ? 22  DG  B 'O4'' 1
ATOM   426 C  'C3'' . DG  B 1 10 ? 12.105 6.068   32.024  1.00 48.07  ? ? ? ? ? ? 22  DG  B 'C3'' 1
ATOM   427 O  'O3'' . DG  B 1 10 ? 10.760 6.110   32.488  1.00 50.84  ? ? ? ? ? ? 22  DG  B 'O3'' 1
ATOM   428 C  'C2'' . DG  B 1 10 ? 12.570 4.634   32.149  1.00 41.22  ? ? ? ? ? ? 22  DG  B 'C2'' 1
ATOM   429 C  'C1'' . DG  B 1 10 ? 11.752 3.990   31.034  1.00 41.10  ? ? ? ? ? ? 22  DG  B 'C1'' 1
ATOM   430 N  N9    . DG  B 1 10 ? 12.282 2.747   30.485  1.00 35.88  ? ? ? ? ? ? 22  DG  B N9    1
ATOM   431 C  C8    . DG  B 1 10 ? 13.594 2.339   30.459  1.00 41.27  ? ? ? ? ? ? 22  DG  B C8    1
ATOM   432 N  N7    . DG  B 1 10 ? 13.753 1.160   29.926  1.00 35.66  ? ? ? ? ? ? 22  DG  B N7    1
ATOM   433 C  C5    . DG  B 1 10 ? 12.468 0.765   29.576  1.00 38.68  ? ? ? ? ? ? 22  DG  B C5    1
ATOM   434 C  C6    . DG  B 1 10 ? 12.009 -0.426  28.970  1.00 36.57  ? ? ? ? ? ? 22  DG  B C6    1
ATOM   435 O  O6    . DG  B 1 10 ? 12.660 -1.408  28.615  1.00 38.62  ? ? ? ? ? ? 22  DG  B O6    1
ATOM   436 N  N1    . DG  B 1 10 ? 10.636 -0.396  28.759  1.00 32.06  ? ? ? ? ? ? 22  DG  B N1    1
ATOM   437 C  C2    . DG  B 1 10 ? 9.801  0.614   29.146  1.00 37.35  ? ? ? ? ? ? 22  DG  B C2    1
ATOM   438 N  N2    . DG  B 1 10 ? 8.497  0.408   28.941  1.00 33.23  ? ? ? ? ? ? 22  DG  B N2    1
ATOM   439 N  N3    . DG  B 1 10 ? 10.210 1.716   29.751  1.00 37.31  ? ? ? ? ? ? 22  DG  B N3    1
ATOM   440 C  C4    . DG  B 1 10 ? 11.553 1.741   29.897  1.00 35.81  ? ? ? ? ? ? 22  DG  B C4    1
ATOM   441 P  P     . DC  B 1 11 ? 10.442 6.622   33.947  1.00 54.63  ? ? ? ? ? ? 23  DC  B P     1
ATOM   442 O  OP1   . DC  B 1 11 ? 10.081 8.062   33.835  1.00 72.54  ? ? ? ? ? ? 23  DC  B OP1   1
ATOM   443 O  OP2   . DC  B 1 11 ? 11.572 6.234   34.816  1.00 46.04  ? ? ? ? ? ? 23  DC  B OP2   1
ATOM   444 O  'O5'' . DC  B 1 11 ? 9.071  5.874   34.286  1.00 50.89  ? ? ? ? ? ? 23  DC  B 'O5'' 1
ATOM   445 C  'C5'' . DC  B 1 11 ? 7.872  6.214   33.569  1.00 44.12  ? ? ? ? ? ? 23  DC  B 'C5'' 1
ATOM   446 C  'C4'' . DC  B 1 11 ? 6.937  5.029   33.482  1.00 43.81  ? ? ? ? ? ? 23  DC  B 'C4'' 1
ATOM   447 O  'O4'' . DC  B 1 11 ? 7.576  3.958   32.740  1.00 42.06  ? ? ? ? ? ? 23  DC  B 'O4'' 1
ATOM   448 C  'C3'' . DC  B 1 11 ? 6.528  4.432   34.832  1.00 38.81  ? ? ? ? ? ? 23  DC  B 'C3'' 1
ATOM   449 O  'O3'' . DC  B 1 11 ? 5.132  4.149   34.847  1.00 45.37  ? ? ? ? ? ? 23  DC  B 'O3'' 1
ATOM   450 C  'C2'' . DC  B 1 11 ? 7.300  3.124   34.901  1.00 40.79  ? ? ? ? ? ? 23  DC  B 'C2'' 1
ATOM   451 C  'C1'' . DC  B 1 11 ? 7.379  2.736   33.434  1.00 33.88  ? ? ? ? ? ? 23  DC  B 'C1'' 1
ATOM   452 N  N1    . DC  B 1 11 ? 8.504  1.846   33.120  1.00 36.40  ? ? ? ? ? ? 23  DC  B N1    1
ATOM   453 C  C2    . DC  B 1 11 ? 8.272  0.685   32.369  1.00 32.79  ? ? ? ? ? ? 23  DC  B C2    1
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ATOM   454 O  O2    . DC  B 1 11 ? 7.131  0.479   31.908  1.00 36.07  ? ? ? ? ? ? 23  DC  B O2    1
ATOM   455 N  N3    . DC  B 1 11 ? 9.293  -0.184  32.167  1.00 30.32  ? ? ? ? ? ? 23  DC  B N3    1
ATOM   456 C  C4    . DC  B 1 11 ? 10.503 0.081   32.671  1.00 32.96  ? ? ? ? ? ? 23  DC  B C4    1
ATOM   457 N  N4    . DC  B 1 11 ? 11.472 -0.815  32.470  1.00 32.29  ? ? ? ? ? ? 23  DC  B N4    1
ATOM   458 C  C5    . DC  B 1 11 ? 10.777 1.286   33.385  1.00 32.52  ? ? ? ? ? ? 23  DC  B C5    1
ATOM   459 C  C6    . DC  B 1 11 ? 9.753  2.117   33.606  1.00 37.44  ? ? ? ? ? ? 23  DC  B C6    1
ATOM   460 P  P     . DG  B 1 12 ? 4.277  4.492   36.173  1.00 52.39  ? ? ? ? ? ? 24  DG  B P     1
ATOM   461 O  OP1   . DG  B 1 12 ? 2.829  4.210   35.898  1.00 51.58  ? ? ? ? ? ? 24  DG  B OP1   1
ATOM   462 O  OP2   . DG  B 1 12 ? 4.739  5.811   36.678  1.00 48.36  ? ? ? ? ? ? 24  DG  B OP2   1
ATOM   463 O  'O5'' . DG  B 1 12 ? 4.756  3.384   37.209  1.00 46.27  ? ? ? ? ? ? 24  DG  B 'O5'' 1
ATOM   464 C  'C5'' . DG  B 1 12 ? 4.451  2.002   36.974  1.00 44.58  ? ? ? ? ? ? 24  DG  B 'C5'' 1
ATOM   465 C  'C4'' . DG  B 1 12 ? 5.053  1.193   38.090  1.00 39.93  ? ? ? ? ? ? 24  DG  B 'C4'' 1
ATOM   466 O  'O4'' . DG  B 1 12 ? 6.494  1.319   38.004  1.00 36.23  ? ? ? ? ? ? 24  DG  B 'O4'' 1
ATOM   467 C  'C3'' . DG  B 1 12 ? 4.673  1.705   39.476  1.00 41.18  ? ? ? ? ? ? 24  DG  B 'C3'' 1
ATOM   468 O  'O3'' . DG  B 1 12 ? 3.540  0.965   39.948  1.00 45.43  ? ? ? ? ? ? 24  DG  B 'O3'' 1
ATOM   469 C  'C2'' . DG  B 1 12 ? 5.937  1.493   40.281  1.00 44.61  ? ? ? ? ? ? 24  DG  B 'C2'' 1
ATOM   470 C  'C1'' . DG  B 1 12 ? 7.030  1.711   39.250  1.00 39.64  ? ? ? ? ? ? 24  DG  B 'C1'' 1
ATOM   471 N  N9    . DG  B 1 12 ? 7.442  3.094   39.113  1.00 44.84  ? ? ? ? ? ? 24  DG  B N9    1
ATOM   472 C  C8    . DG  B 1 12 ? 6.712  4.200   39.471  1.00 50.34  ? ? ? ? ? ? 24  DG  B C8    1
ATOM   473 N  N7    . DG  B 1 12 ? 7.292  5.323   39.143  1.00 46.30  ? ? ? ? ? ? 24  DG  B N7    1
ATOM   474 C  C5    . DG  B 1 12 ? 8.422  4.933   38.443  1.00 46.08  ? ? ? ? ? ? 24  DG  B C5    1
ATOM   475 C  C6    . DG  B 1 12 ? 9.446  5.712   37.846  1.00 53.78  ? ? ? ? ? ? 24  DG  B C6    1
ATOM   476 O  O6    . DG  B 1 12 ? 9.530  6.948   37.769  1.00 50.57  ? ? ? ? ? ? 24  DG  B O6    1
ATOM   477 N  N1    . DG  B 1 12 ? 10.419 4.908   37.254  1.00 42.62  ? ? ? ? ? ? 24  DG  B N1    1
ATOM   478 C  C2    . DG  B 1 12 ? 10.434 3.531   37.278  1.00 42.89  ? ? ? ? ? ? 24  DG  B C2    1
ATOM   479 N  N2    . DG  B 1 12 ? 11.496 2.933   36.700  1.00 37.64  ? ? ? ? ? ? 24  DG  B N2    1
ATOM   480 N  N3    . DG  B 1 12 ? 9.495  2.796   37.851  1.00 42.44  ? ? ? ? ? ? 24  DG  B N3    1
ATOM   481 C  C4    . DG  B 1 12 ? 8.524  3.556   38.405  1.00 45.36  ? ? ? ? ? ? 24  DG  B C4    1
HETATM 482 N  N1    . SPM C 2 .  ? 15.307 -2.224  30.707  0.50 45.16  ? ? ? ? ? ? 101 SPM A N1    1
HETATM 483 C  C2    . SPM C 2 .  ? 14.648 -3.505  30.906  1.00 50.52  ? ? ? ? ? ? 101 SPM A C2    1
HETATM 484 C  C3    . SPM C 2 .  ? 14.177 -3.681  32.355  1.00 49.96  ? ? ? ? ? ? 101 SPM A C3    1
HETATM 485 C  C4    . SPM C 2 .  ? 13.198 -4.830  32.413  1.00 46.18  ? ? ? ? ? ? 101 SPM A C4    1
HETATM 486 N  N5    . SPM C 2 .  ? 12.876 -5.334  33.745  1.00 49.66  ? ? ? ? ? ? 101 SPM A N5    1
HETATM 487 C  C6    . SPM C 2 .  ? 11.836 -6.363  33.800  1.00 40.82  ? ? ? ? ? ? 101 SPM A C6    1
HETATM 488 C  C7    . SPM C 2 .  ? 11.700 -6.958  35.173  1.00 44.69  ? ? ? ? ? ? 101 SPM A C7    1
HETATM 489 C  C8    . SPM C 2 .  ? 10.292 -7.489  35.304  1.00 45.41  ? ? ? ? ? ? 101 SPM A C8    1
HETATM 490 C  C9    . SPM C 2 .  ? 10.370 -8.593  36.328  1.00 39.65  ? ? ? ? ? ? 101 SPM A C9    1
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HETATM 491 N  N10   . SPM C 2 .  ? 9.328  -8.480  37.308  1.00 48.73  ? ? ? ? ? ? 101 SPM A N10   1
HETATM 492 C  C11   . SPM C 2 .  ? 8.275  -9.514  37.339  1.00 42.36  ? ? ? ? ? ? 101 SPM A C11   1
HETATM 493 C  C12   . SPM C 2 .  ? 8.417  -10.350 38.617  1.00 40.48  ? ? ? ? ? ? 101 SPM A C12   1
HETATM 494 C  C13   . SPM C 2 .  ? 7.395  -11.529 38.711  1.00 36.10  ? ? ? ? ? ? 101 SPM A C13   1
HETATM 495 N  N14   . SPM C 2 .  ? 7.319  -12.113 37.413  1.00 26.41  ? ? ? ? ? ? 101 SPM A N14   1
HETATM 496 SR SR    . SR  D 3 .  ? 15.511 4.253   -10.211 1.00 80.43  ? ? ? ? ? ? 102 SR  A SR    1
HETATM 497 O  O     . HOH E 4 .  ? 5.745  10.707  7.973   1.00 50.57  ? ? ? ? ? ? 201 HOH A O     1
HETATM 498 O  O     . HOH E 4 .  ? 3.981  2.092   12.526  1.00 55.74  ? ? ? ? ? ? 202 HOH A O     1
HETATM 499 O  O     . HOH E 4 .  ? 5.535  7.189   -5.997  1.00 37.30  ? ? ? ? ? ? 203 HOH A O     1
HETATM 500 O  O     . HOH E 4 .  ? 5.857  10.607  2.957   1.00 39.96  ? ? ? ? ? ? 204 HOH A O     1
HETATM 501 O  O     . HOH E 4 .  ? 16.122 -0.073  -7.306  1.00 76.18  ? ? ? ? ? ? 205 HOH A O     1
HETATM 502 O  O     . HOH E 4 .  ? 12.456 -9.842  29.587  0.50 39.91  ? ? ? ? ? ? 206 HOH A O     1
HETATM 503 O  O     . HOH E 4 .  ? 15.126 0.991   -11.310 1.00 64.27  ? ? ? ? ? ? 207 HOH A O     1
HETATM 504 O  O     . HOH E 4 .  ? 11.936 -2.931  -12.948 1.00 43.14  ? ? ? ? ? ? 208 HOH A O     1
HETATM 505 O  O     . HOH E 4 .  ? 16.727 -3.172  -8.920  1.00 68.21  ? ? ? ? ? ? 209 HOH A O     1
HETATM 506 O  O     . HOH E 4 .  ? 13.771 10.608  -3.551  0.50 32.95  ? ? ? ? ? ? 210 HOH A O     1
HETATM 507 O  O     . HOH E 4 .  ? 9.441  1.770   -2.007  1.00 36.92  ? ? ? ? ? ? 211 HOH A O     1
HETATM 508 O  O     . HOH E 4 .  ? 9.916  -4.279  -14.180 1.00 39.00  ? ? ? ? ? ? 212 HOH A O     1
HETATM 509 O  O     . HOH E 4 .  ? 5.425  -5.959  -10.092 1.00 56.75  ? ? ? ? ? ? 213 HOH A O     1
HETATM 510 O  O     . HOH E 4 .  ? 6.736  11.394  5.248   0.50 34.77  ? ? ? ? ? ? 214 HOH A O     1
HETATM 511 O  O     . HOH E 4 .  ? 11.867 -15.768 30.801  1.00 47.55  ? ? ? ? ? ? 215 HOH A O     1
HETATM 512 O  O     . HOH E 4 .  ? 14.392 -5.303  36.717  0.50 36.19  ? ? ? ? ? ? 216 HOH A O     1
HETATM 513 O  O     . HOH E 4 .  ? 3.012  -10.254 22.862  1.00 67.16  ? ? ? ? ? ? 217 HOH A O     1
HETATM 514 O  O     . HOH E 4 .  ? 13.213 9.047   -5.011  0.50 43.01  ? ? ? ? ? ? 218 HOH A O     1
HETATM 515 O  O     . HOH E 4 .  ? -2.568 -2.294  17.282  0.50 44.49  ? ? ? ? ? ? 219 HOH A O     1
HETATM 516 O  O     . HOH E 4 .  ? 10.725 -14.748 28.779  0.50 39.46  ? ? ? ? ? ? 220 HOH A O     1
HETATM 517 O  O     . HOH E 4 .  ? 15.703 9.836   -2.496  0.50 31.11  ? ? ? ? ? ? 221 HOH A O     1
HETATM 518 O  O     . HOH E 4 .  ? 9.346  8.423   16.634  1.00 52.47  ? ? ? ? ? ? 222 HOH A O     1
HETATM 519 O  O     . HOH E 4 .  ? 11.510 1.193   -0.164  0.50 40.92  ? ? ? ? ? ? 223 HOH A O     1
HETATM 520 O  O     . HOH E 4 .  ? 12.332 12.804  -0.232  1.00 59.02  ? ? ? ? ? ? 224 HOH A O     1
HETATM 521 O  O     . HOH E 4 .  ? 14.811 -18.153 31.387  1.00 54.50  ? ? ? ? ? ? 225 HOH A O     1
HETATM 522 O  O     . HOH E 4 .  ? 12.781 -17.856 31.806  1.00 47.82  ? ? ? ? ? ? 226 HOH A O     1
HETATM 523 O  O     . HOH E 4 .  ? 1.224  6.114   15.685  1.00 60.25  ? ? ? ? ? ? 227 HOH A O     1
HETATM 524 O  O     . HOH E 4 .  ? 10.603 6.919   -7.970  1.00 37.70  ? ? ? ? ? ? 228 HOH A O     1
HETATM 525 O  O     . HOH F 4 .  ? -0.922 0.065   -5.369  1.00 42.62  ? ? ? ? ? ? 101 HOH B O     1
HETATM 526 O  O     . HOH F 4 .  ? 8.026  9.832   35.707  1.00 68.74  ? ? ? ? ? ? 102 HOH B O     1
HETATM 527 O  O     . HOH F 4 .  ? 15.975 -1.008  15.507  1.00 52.27  ? ? ? ? ? ? 103 HOH B O     1
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HETATM 528 O  O     . HOH F 4 .  ? 14.793 -2.822  15.169  1.00 58.11  ? ? ? ? ? ? 104 HOH B O     1
HETATM 529 O  O     . HOH F 4 .  ? -0.287 5.138   4.841   1.00 62.89  ? ? ? ? ? ? 105 HOH B O     1
HETATM 530 O  O     . HOH F 4 .  ? 2.869  1.485   6.566   1.00 45.01  ? ? ? ? ? ? 106 HOH B O     1
HETATM 531 O  O     . HOH F 4 .  ? 2.751  0.192   9.510   0.50 39.34  ? ? ? ? ? ? 107 HOH B O     1
HETATM 532 O  O     . HOH F 4 .  ? 17.774 2.975   22.558  1.00 57.77  ? ? ? ? ? ? 108 HOH B O     1
HETATM 533 O  O     . HOH F 4 .  ? 16.850 0.536   28.081  1.00 66.55  ? ? ? ? ? ? 109 HOH B O     1
HETATM 534 O  O     . HOH F 4 .  ? 8.401  -1.858  12.571  0.50 37.14  ? ? ? ? ? ? 110 HOH B O     1
HETATM 535 O  O     . HOH F 4 .  ? 5.873  -5.073  9.869   1.00 47.64  ? ? ? ? ? ? 111 HOH B O     1
HETATM 536 O  O     . HOH F 4 .  ? 6.830  8.002   40.323  1.00 55.54  ? ? ? ? ? ? 112 HOH B O     1
HETATM 537 O  O     . HOH F 4 .  ? 12.523 -2.219  4.994   1.00 56.73  ? ? ? ? ? ? 113 HOH B O     1
HETATM 538 O  O     . HOH F 4 .  ? 8.144  3.642   30.083  1.00 38.91  ? ? ? ? ? ? 114 HOH B O     1
HETATM 539 O  O     . HOH F 4 .  ? 10.239 -1.894  19.211  1.00 41.32  ? ? ? ? ? ? 115 HOH B O     1
HETATM 540 O  O     . HOH F 4 .  ? 11.394 6.208   23.097  1.00 61.62  ? ? ? ? ? ? 116 HOH B O     1
HETATM 541 O  O     . HOH F 4 .  ? -8.777 1.487   -2.112  1.00 70.13  ? ? ? ? ? ? 117 HOH B O     1
HETATM 542 O  O     . HOH F 4 .  ? -1.820 0.663   3.075   1.00 52.05  ? ? ? ? ? ? 118 HOH B O     1
HETATM 543 O  O     . HOH F 4 .  ? 21.214 2.225   19.730  1.00 65.35  ? ? ? ? ? ? 119 HOH B O     1
HETATM 544 O  O     . HOH F 4 .  ? 16.869 1.303   20.043  1.00 54.01  ? ? ? ? ? ? 120 HOH B O     1
HETATM 545 O  O     . HOH F 4 .  ? -2.810 -4.632  7.767   1.00 63.68  ? ? ? ? ? ? 121 HOH B O     1
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Table S2. Crystal and Data Collection Statistics for the First Crystal. It was used to obtain phases for the DDD-XY duplex.

Space group	Orthorhombic $P2_12_12_1$
Cell parameters (Å)	a=26.4, b=37.3, c=77.6
Temperature of data collection (° C)	-170
Wavelength (Å)	1.605
Min resolution (Å)	26.9
Max resolution (Å)	1.95
Unique reflections (observed)	5861
Completeness all(%)/1.98-1.95 Å	99.0/98.0
I/σ (I) all/1.98-1.95 Å	20.3/4.34
R_{merge} all/1.98-1.95 Å	0.08/0.63
R_{work}	0.36
R_{free}	0.39
Number of DNA atoms	427
Number of water molecules	14
Number of ions	4 Ba^{2+}

Table S3. Crystal Data, Data Collection, and Refinement Statistics for the Second Crystal. It was used to obtain the final structure of the DDD-XY duplex.

Space group	Orthorhombic $P2_12_12_1$
Cell parameters (Å)	a=26.38, b=36.77, c=77.65
Temperature of data collection (° C)	-170
Wavelength (Å)	0.97857
Min resolution (Å)	30.0
Max resolution (Å)	1.7
Unique reflections (all)	8811
Unique reflections (observed)	8236
Completeness all/1.76-1.70 Å (%)	93.4/61.1
Redundancy all/1.76-1.70 Å	6.4/4.0
I/σ (I) all/1.76-1.70 Å	52.3/5.65
R_{merge} all/1.76-1.70 Å	0.04/0.23
R_{work}	0.26
R_{free}	0.30
Number of DNA atoms	481
Number of water molecules	49
Number of ions	1 Sr^{2+}
r.m.s. distances (Å)	0.01
r.m.s. angles (°)	1.6

Table S4. NMR Restraints Used for the DDD-GY Structure Calculations and Refinement Statistics.

NMR restraints	
NOE restraints	
Internucleotide	75
Intranucleotide	78
Total	153
Backbone torsion angle restraints	100
H-bonding restraints	50
Deoxyribose restraints	18
Total number of restraints	321
Refinement Statistics	
Number of distance restraint violations	25
Number of torsion restraint violations	14
Total distance penalty/Maximum penalty [kcal mol^{-1}]	2.60/0.46
Total torsion penalty/Maximum penalty [kcal mol^{-1}]	1.24/0.36
r.m.s. distances (Å)	0.012
r.m.s. angles (°)	2.4
Distance restraint force field [kcal mol^{-1} $Å^{-2}$]	32
Torsion restraint force field [kcal mol^{-1} deg^{-2}]	32

Table S5. Structural Statistics for the DDD-GY Duplex.

Average structure (obtained from 9 structures)			
RMS pairwise difference between structures		0.71	
RMS difference from average structure		0.47	
CORMA analysis for average structure[a]			
	Intranucleotide	Internucleotide	Total
Rx[b]	0.10	0.10	0.10
Average error[c]			0.02

[a] The mixing time was 250 ms. [b] Rx is 6th root R factor: $\Sigma[((Io)_i^{1/6})-((Ic)_i^{1/6})/\Sigma((Io)_i^{1/6})]$. [c] Average error: $\Sigma(Ic-Io)/n$, where Ic are NOE intensities calculated from refined structure, Io are experimental NOE intensities.

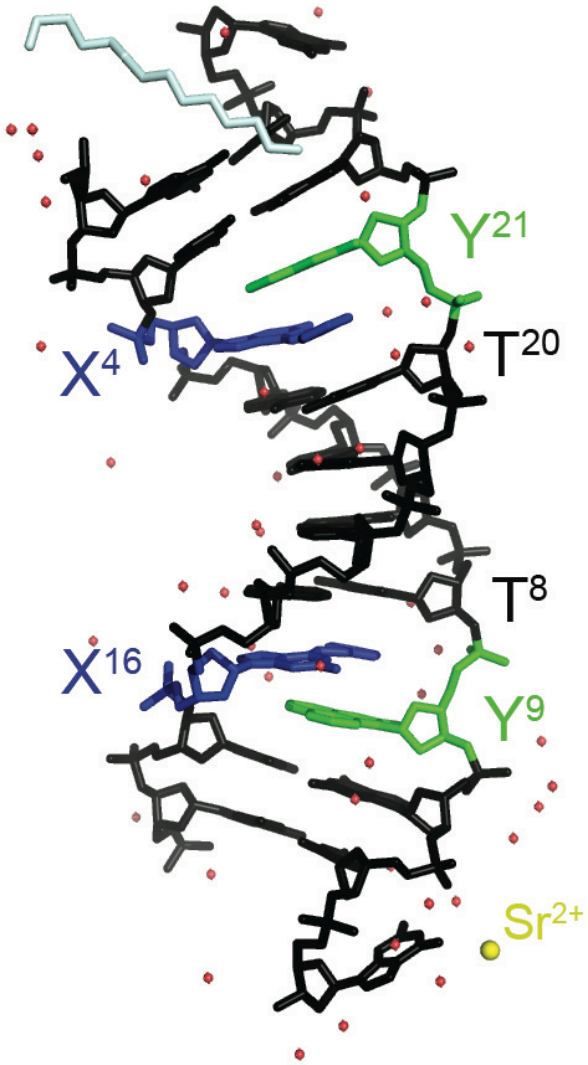

Figure S1. Structure of the DDD-XY duplex with water molecules (red spheres) and Sr^{2+} ion (yellow sphere) and spermine molecule (light blue). The benzyl groups of O^6-Bn-dG (shown in blue) intercalate between the thymine and dPer bases (shown in green) from the opposite strand. The dPer bases are in the *syn* conformation about the glycosyl bond. Electron density for bases C^1 and C^{13} was not visible. Bases G^{12} and G^{24} flipped out from the duplex. The intercalated structures unwind the duplex as compared to the unmodified DDD.

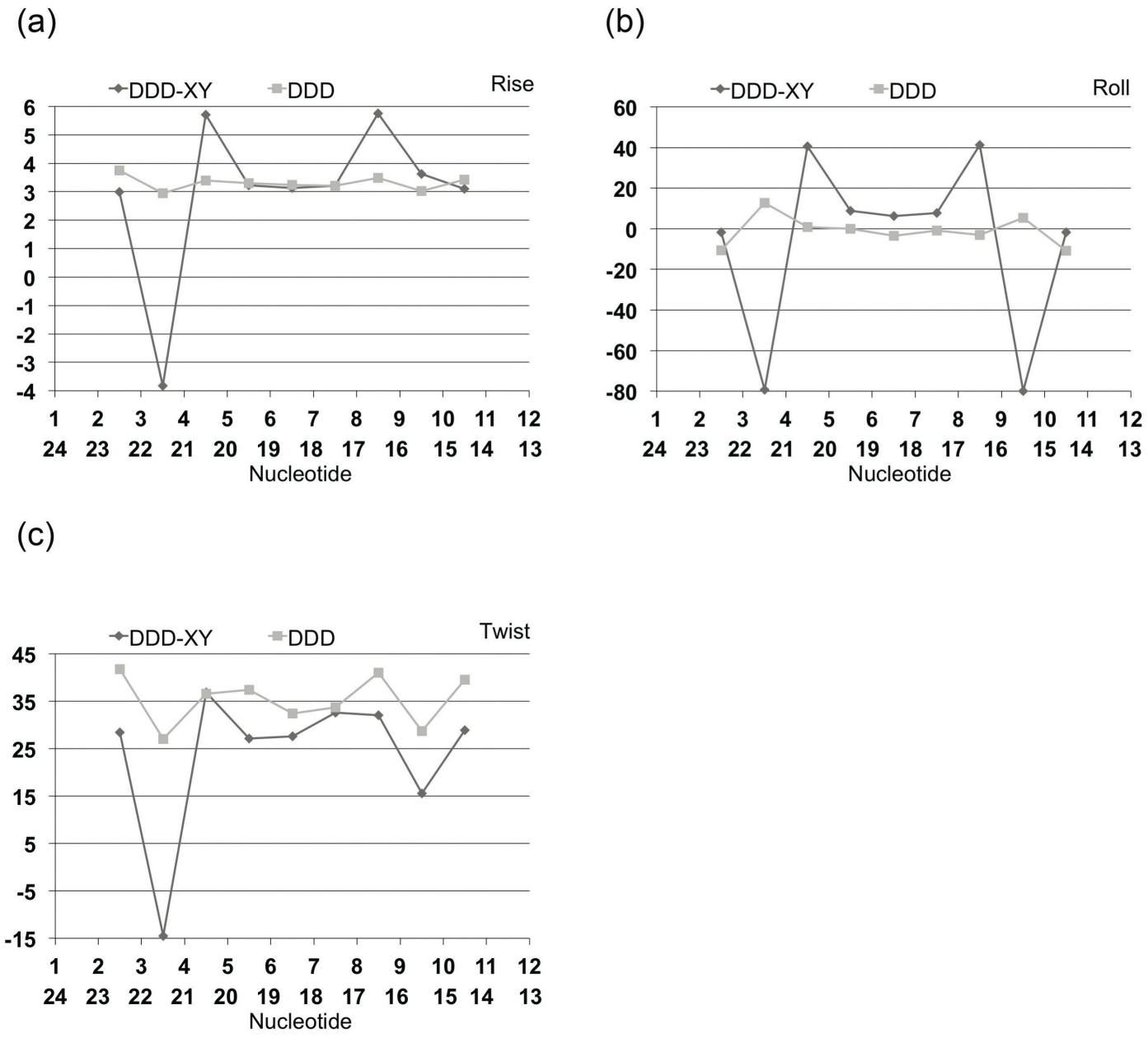

Figure S2. Interbase pair parameters: (a) helical rise, (b) roll and (c) twist for the DDD-XY, DDD (PDB entry 355D) duplexes.

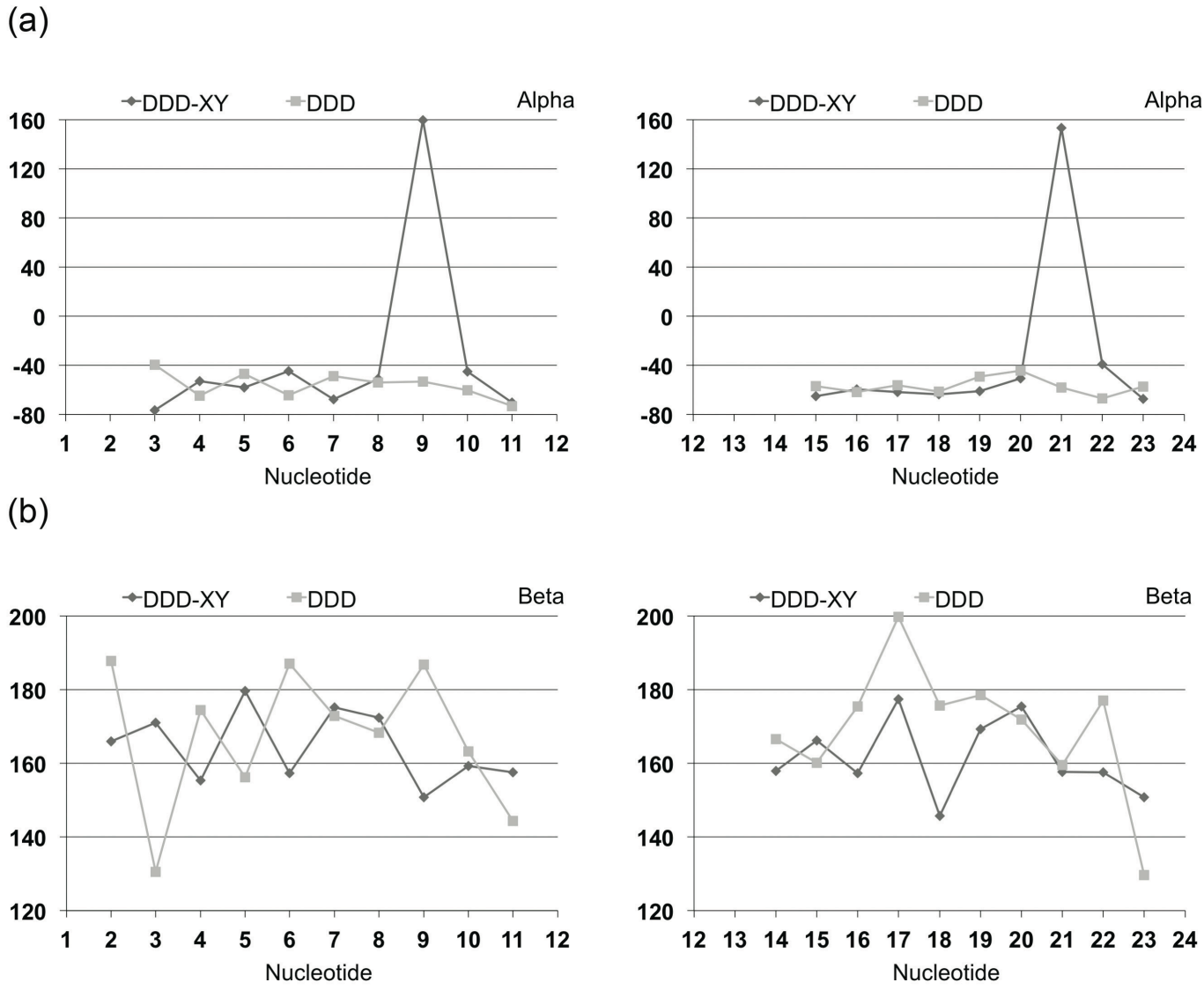

Figure S3. Comparison of backbone torsion angles (a) α and (b) β in the crystal structures of the DDD-XY, DDD (PDB entry 355D) duplexes.

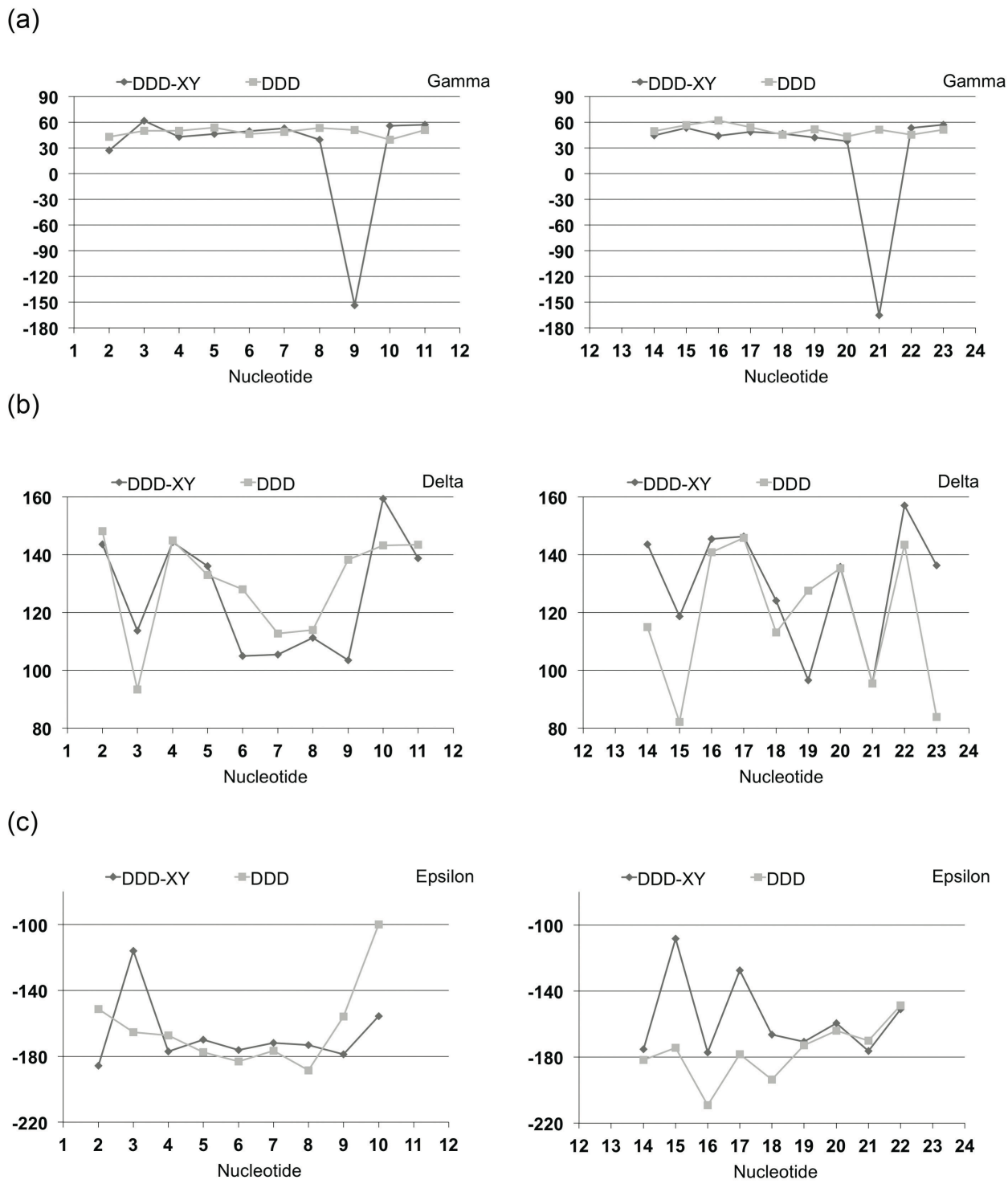

Figure S4. Comparison of (a) γ, (b) δ, (c) ε angles in the crystal structures of the DDD-XY, DDD (PDB entry 355D) duplexes.

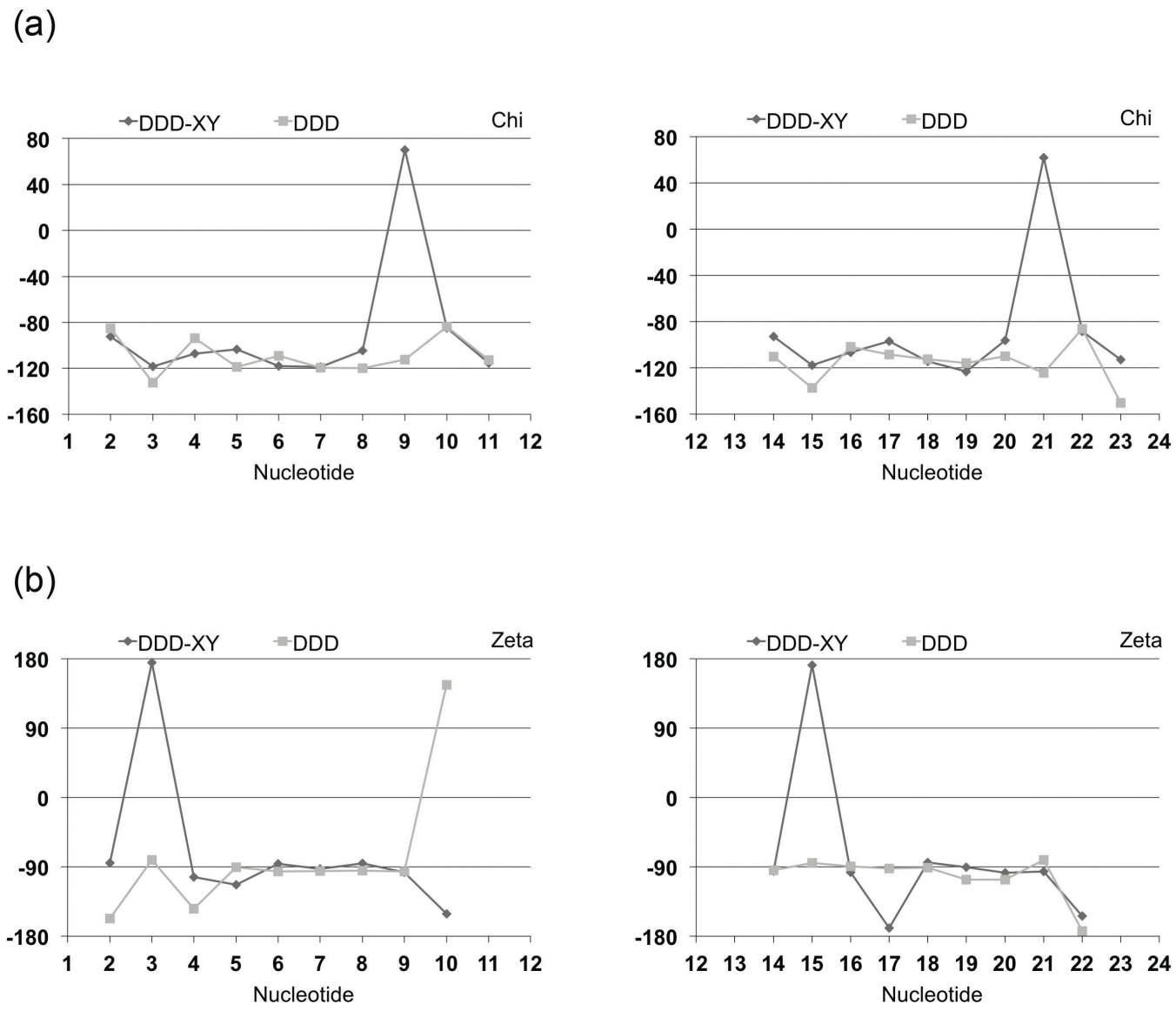

Figure S5. Comparison of (a) χ and (b) ζ angles in the crystal structures of the DDD-XY, DDD (PDB entry 355D) duplexes.

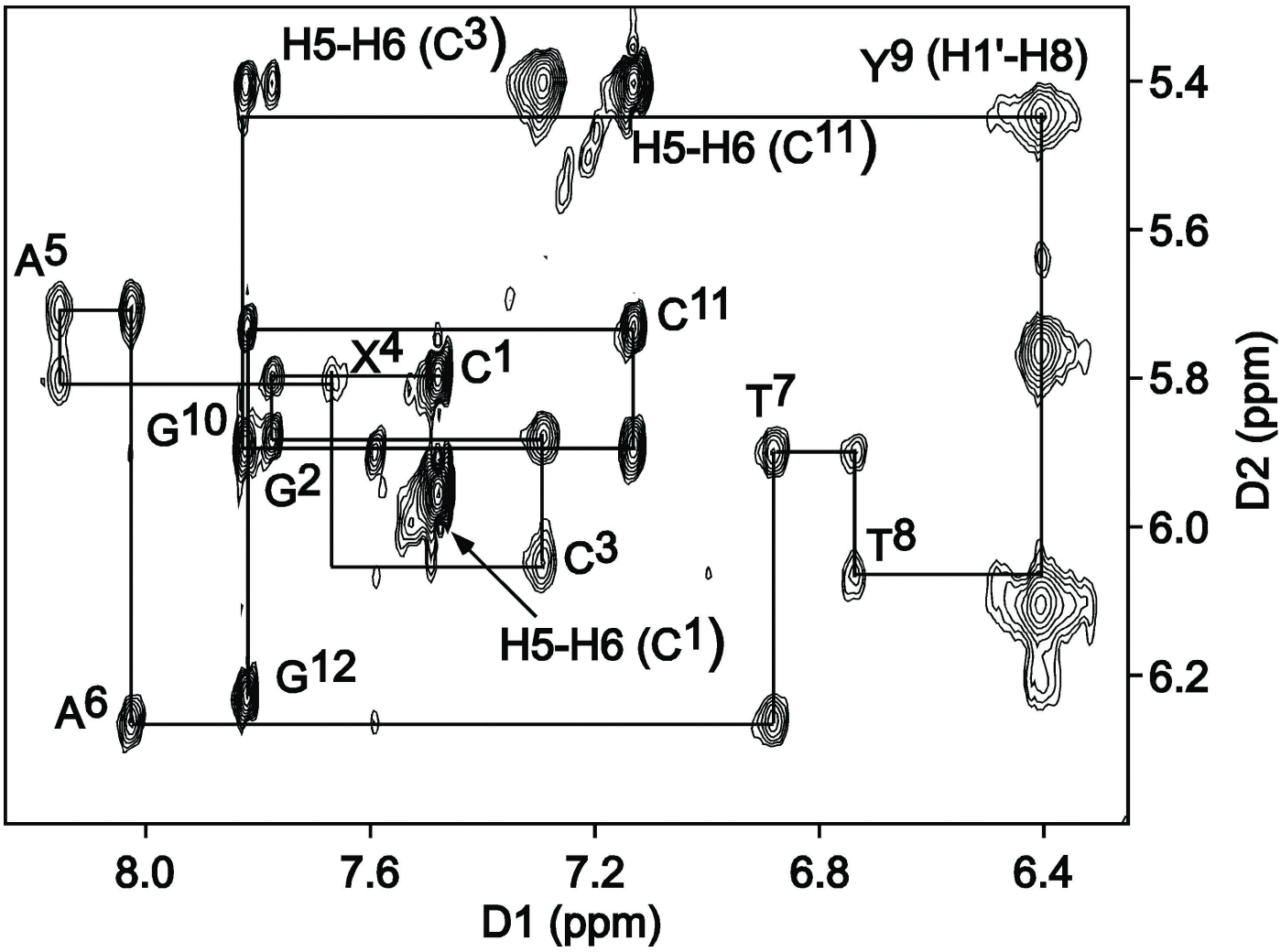

Figure S6. NOESY spectrum of the DDD-XY duplex showing sequential NOEs between the aromatic and anomeric protons from C^{1} to G^{12}. The spectrum was collected at 10 °C at 900 MHz with 250 ms mixing time.

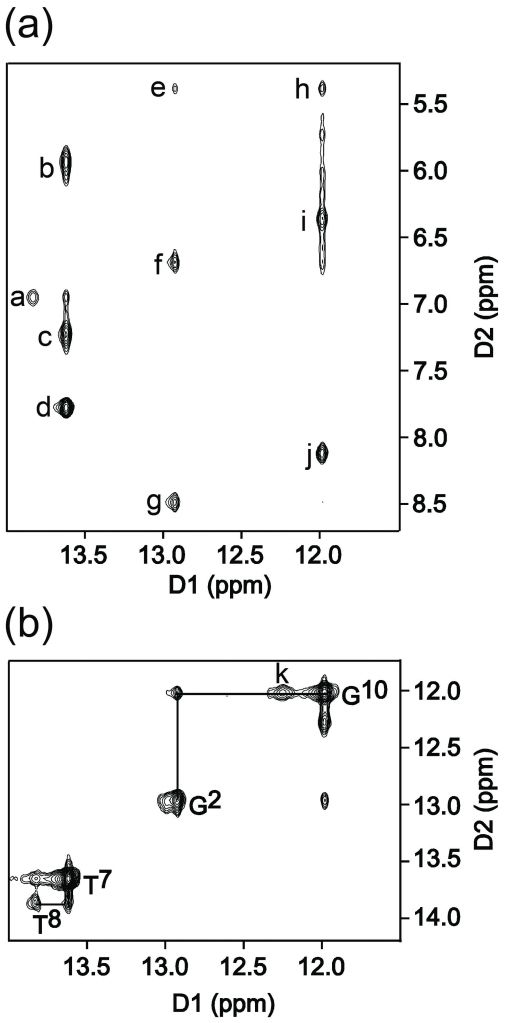

Figure S7. (a) Interstrand NOE cross peaks between complementary bases for the DDD-XY duplex: a, A^5 H2→T^8 N3H; b, A^5 N^6H2→T7 N3H; c, A^6 N^2H2→T^7 N3H; d, A^6 H2→T^7 N3H; e, C^{11} H5→G^2 N1H; f, C^{11} N^2H1→G^2 N1H; g, C^{11} N^2H2→G^2 N1H; h, C^3 H5→G^{10} N1H; i, C^3 N^2H1→G^{10} N1H; j, C^3 N^2H2→G^{10} N1H. (b) NOE connectivity of DDD-XY duplex, for the imino protons for the base pairs G^2:C^{11}, C^3:G^{10}, X^4:Y^9, A^5:T^8, A^5:T^7. Cross peaks between T^8 N3H→T^7 N3H and G^2 N1H→G^{10} N1H were present. There is no cross-peak between T^8→Y^9 and Y^9→G^{10}. G^{10} N1H has a cross peak with peak which is not visible on the diagonal and could not be assigned (k). The experiment was carried out at 500 MHz using a mixing time of 250 ms and at 7 °C.

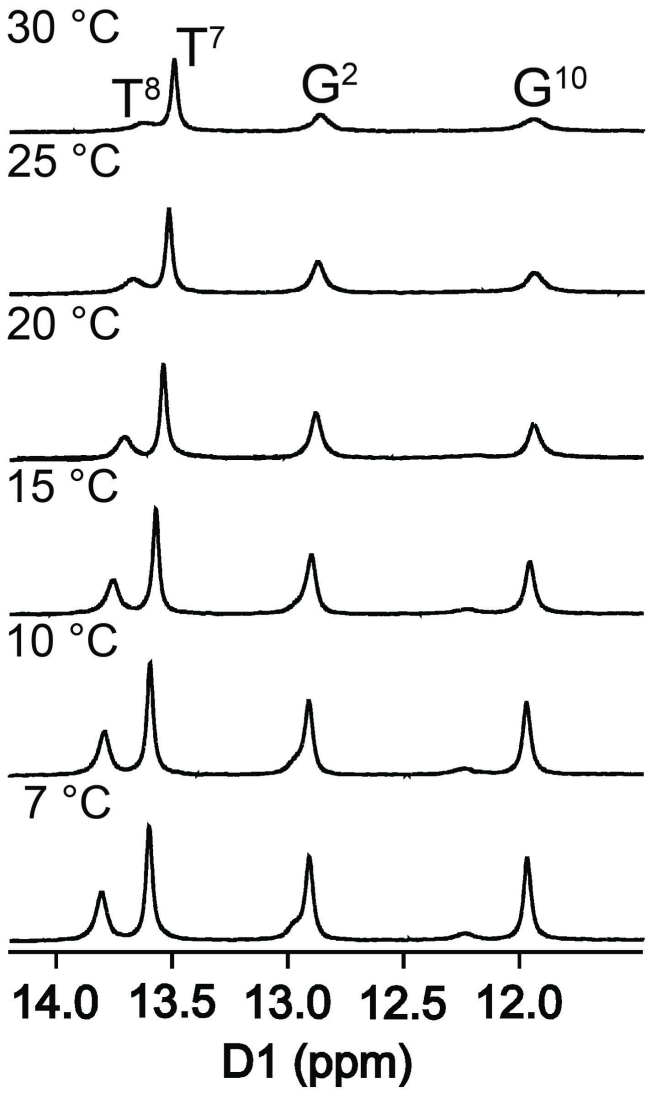

Figure S8. One-dimentional NMR spectra, showing the imino proton resonances for the DDD-XY duplex as a function of temperature. Note that the imine nitrogen of the O^6-Bn-dG nucleotide X^4 is not protonated at neutral pH. The individual nucleotides are identified as superscripts. The experiments were carried out at 500 MHz.

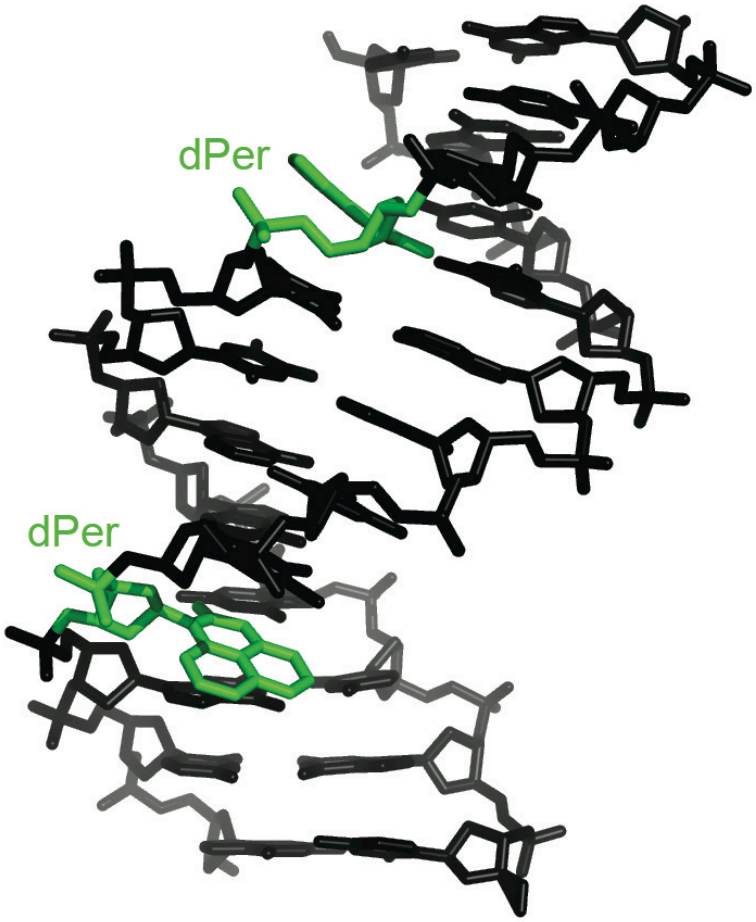

Figure S9. The average structure obtained from a series of rMD calculations for the DDD-GY duplex. dPer bases are shown in green. The dPer base is in the *anti* conformation about the glycosyl bond and it forms wobble pair with the complementary dG. The dPer ring is oriented in the major groove. Hydrogens are omitted on the picture for clarity.

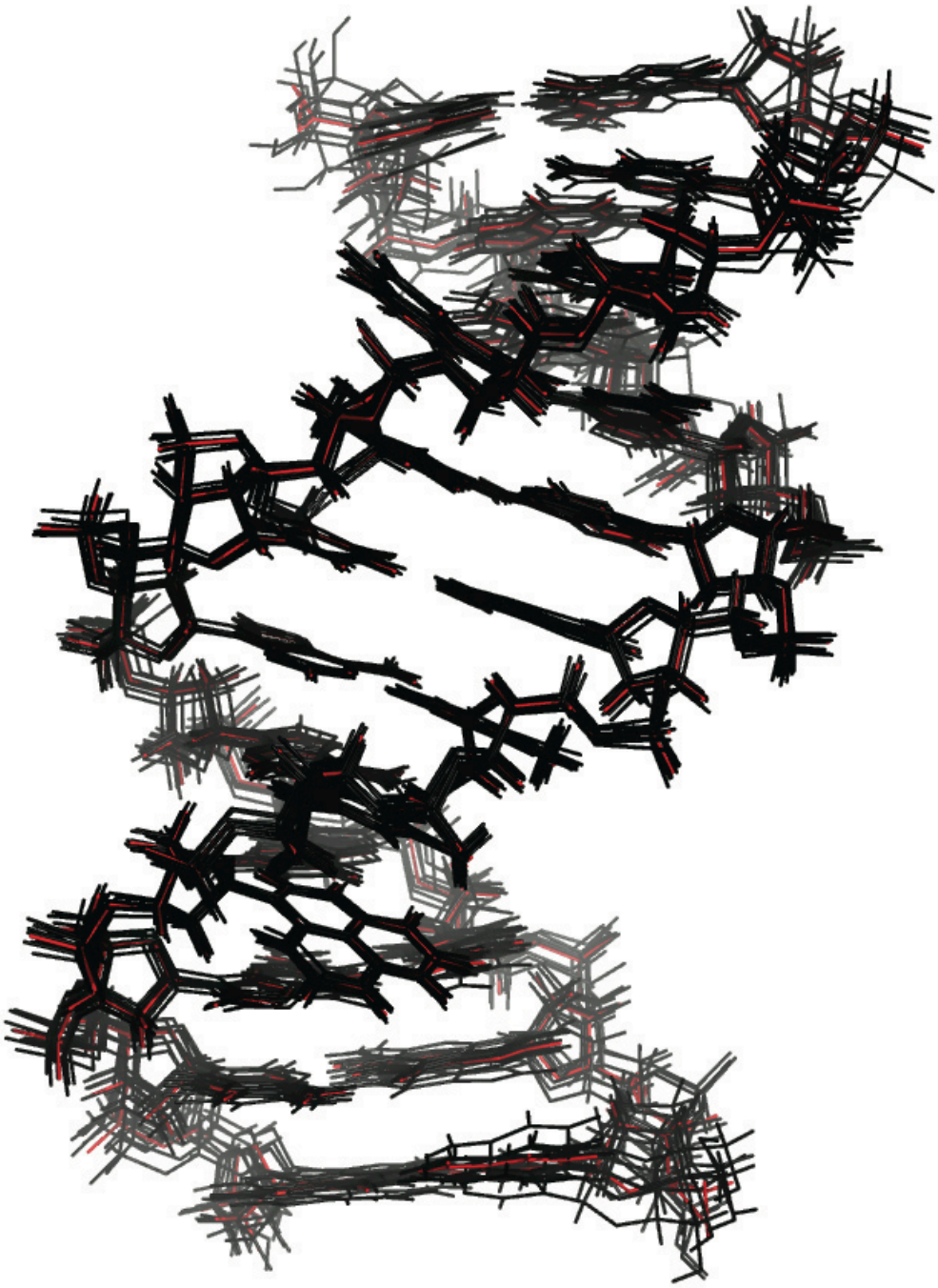

Figure S10. The superimposed nine structures obtained from a series of rMD calculations for the DDD-GY duplex. The average structure obtained from nine structures is shown in red.

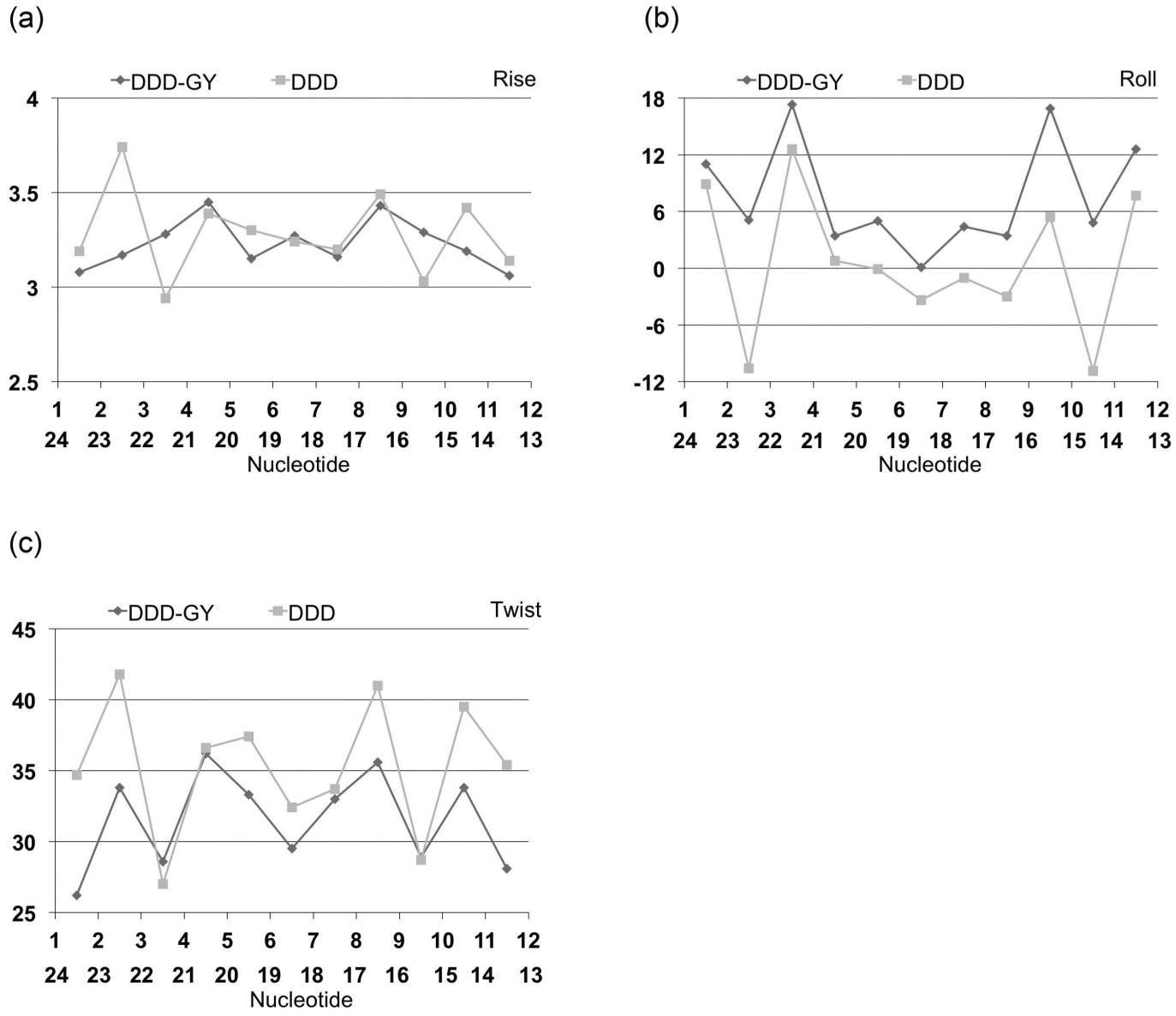

Figure S11. Interbase pair parameters: (a) helical rise, (b) roll and (c) twist for the DDD-GY, DDD (PDB entry 355D) duplexes.

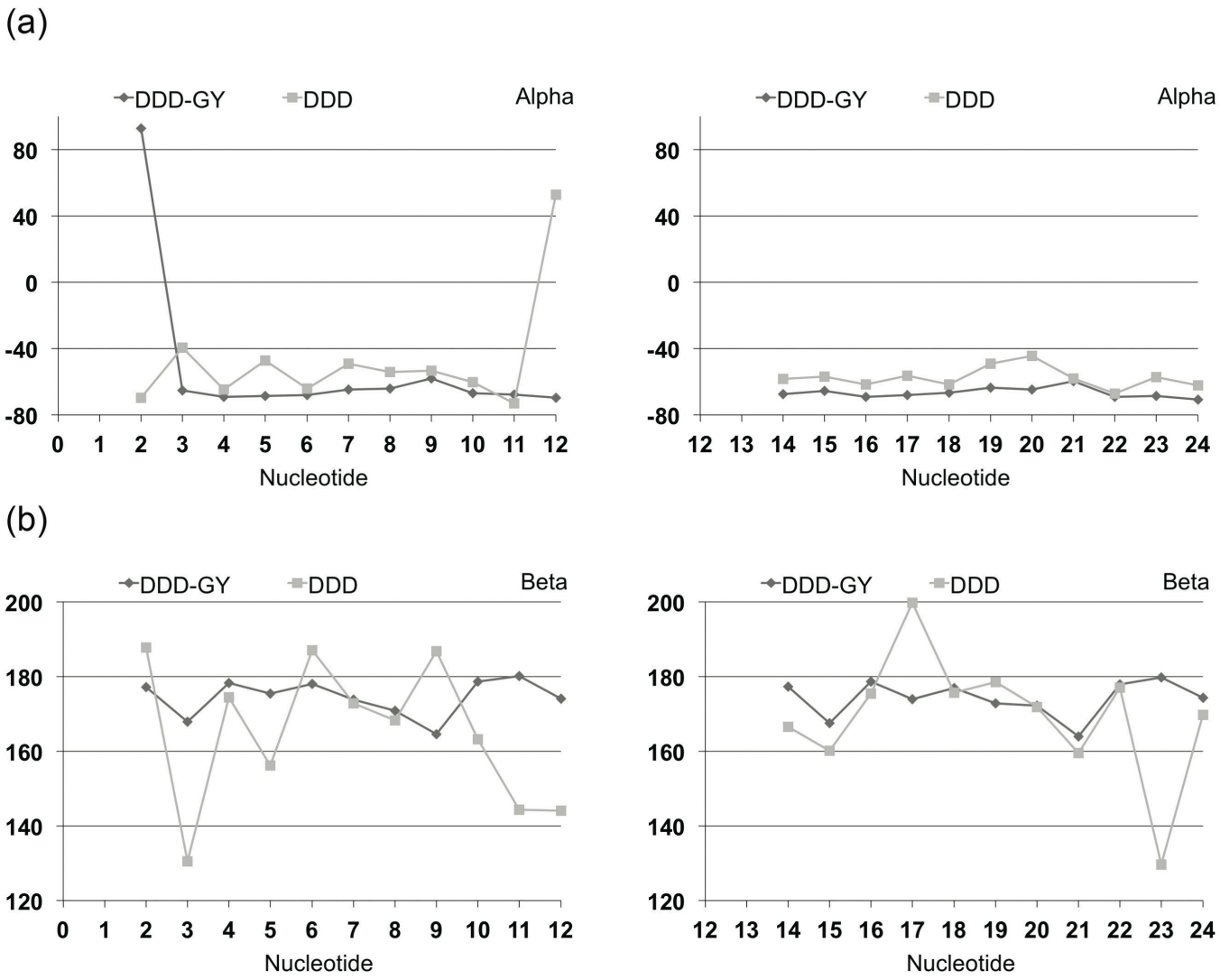

Figure S12. Comparison of backbone torsion angles (a) α and (b) β in the structures of the DDD-GY, DDD (PDB entry 355D) duplexes.

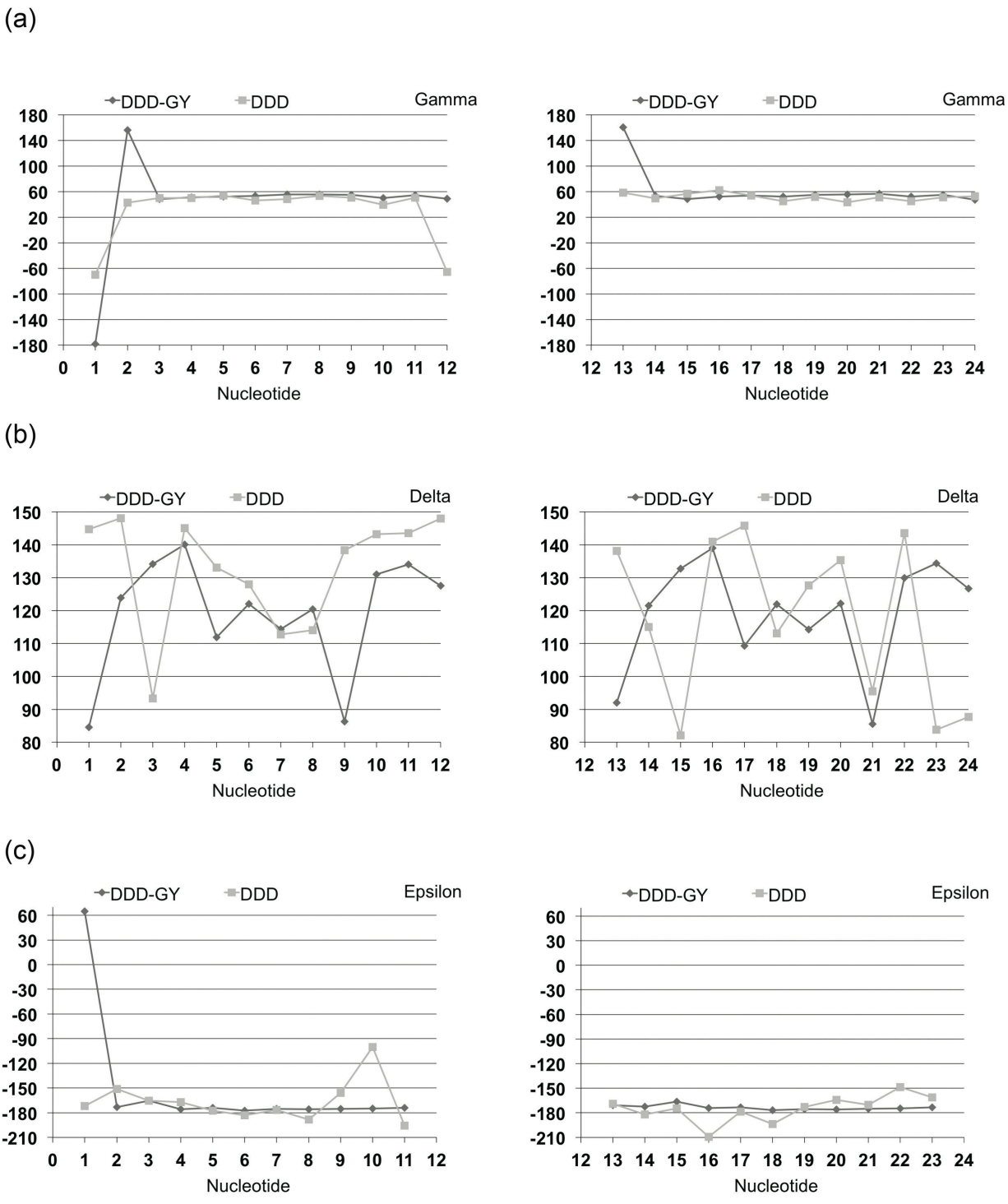

Figure S13. Comparison of (a) γ, (b) δ, (c) ε angles in the structures of the DDD-GY, DDD (PDB entry 355D) duplexes.

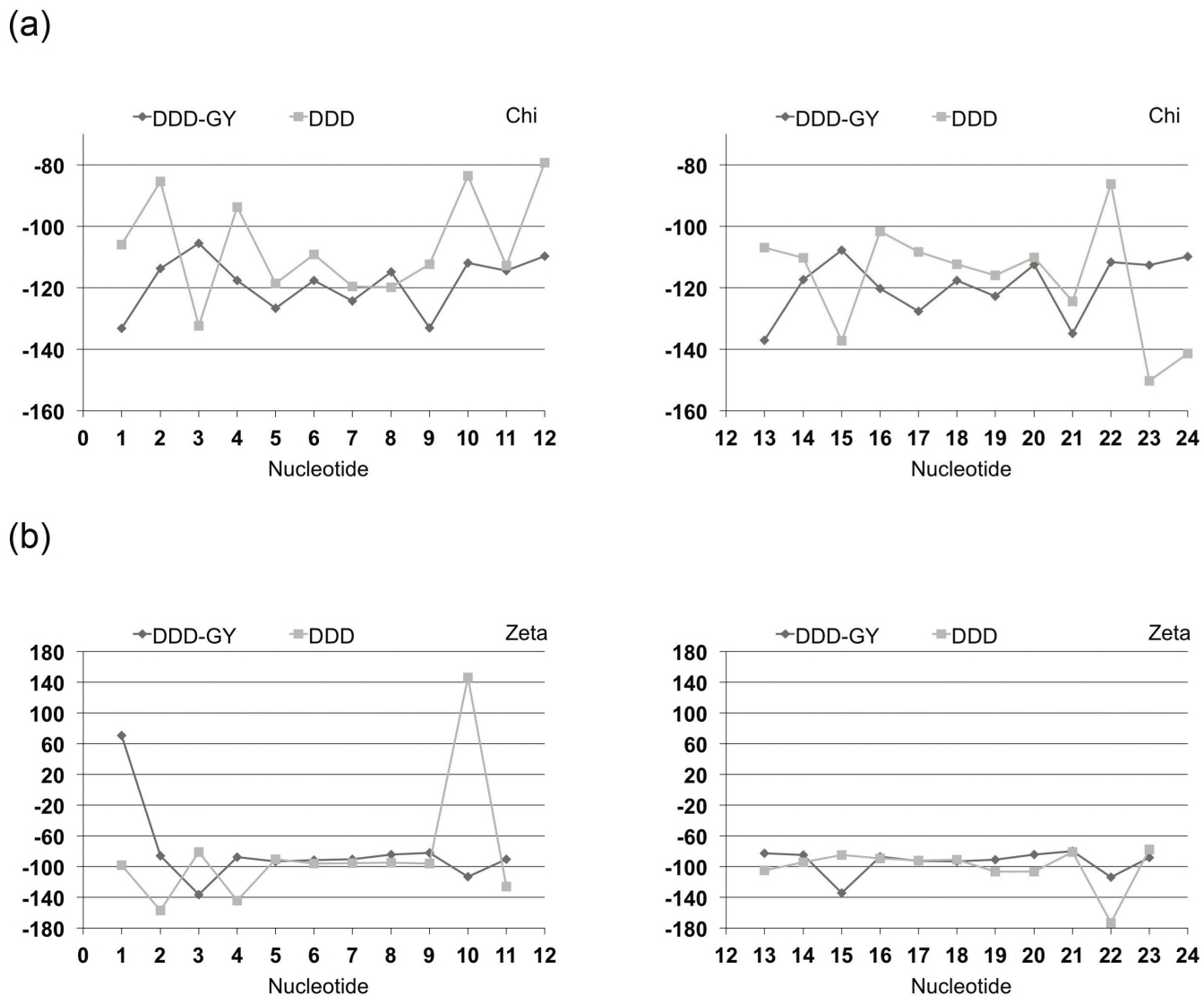

Figure S14. Comparison of (a) χ and (b) ζ angles in the crystal structures of the DDD-GY, DDD (PDB entry 355D) duplexes.