Electronic Supplementary Information (ESI)

Investigating Coordination Flexibility of Glycerophosphodiesterase (GpdQ) Through Interactions with Mono-, Di-, and Triphosphoester (NPP, BNPP, GPE, and Paraoxon) Substrates

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Fax: 305-284-4571.

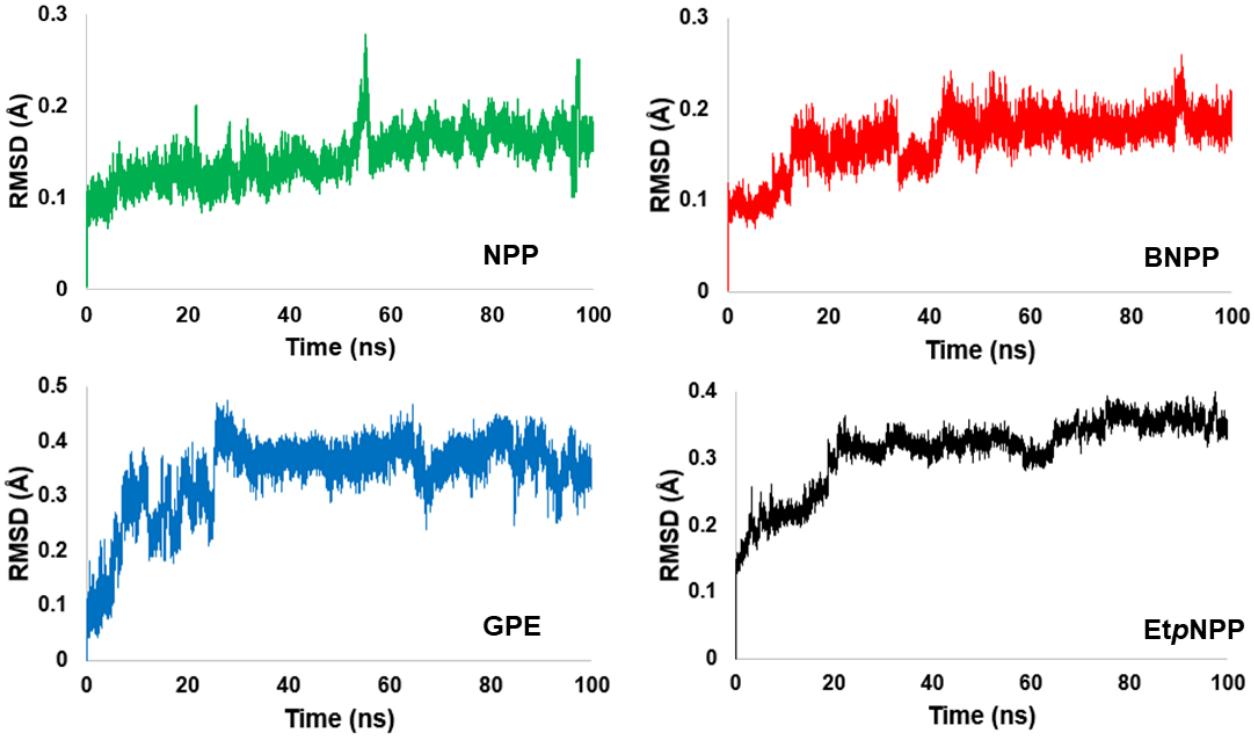

Figure S1: Per-residue root mean square deviation (RMSD) of GpdQ-NPP, GpdQ-BNPP, GpdQ-GPE, and GpdQ-Et*p*NPP complex trajectories calculated along the 100ns MD simulation.

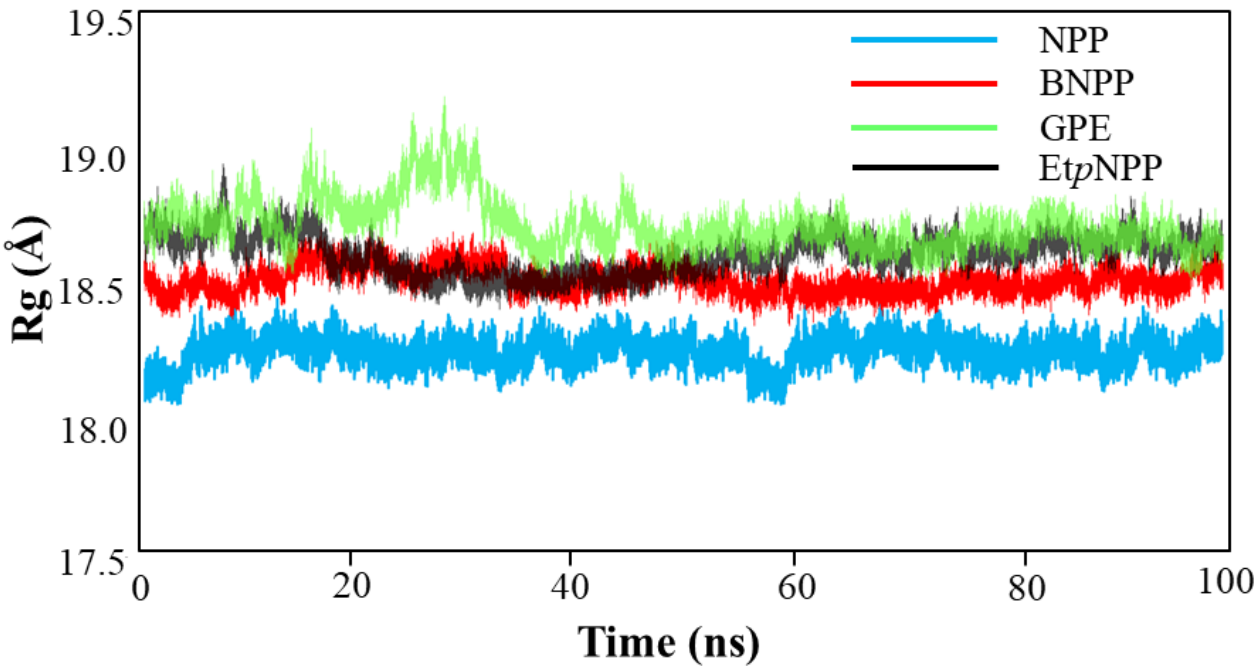

Figure S2: Radius of gyration (Rg) of (a) GpdQ-NPP, (b) GpdQ-BNPP, (c) GpdQ-GPE, and (d) GpdQ-Et*p*NPP complex trajectories calculated along the 100ns MD simulation.

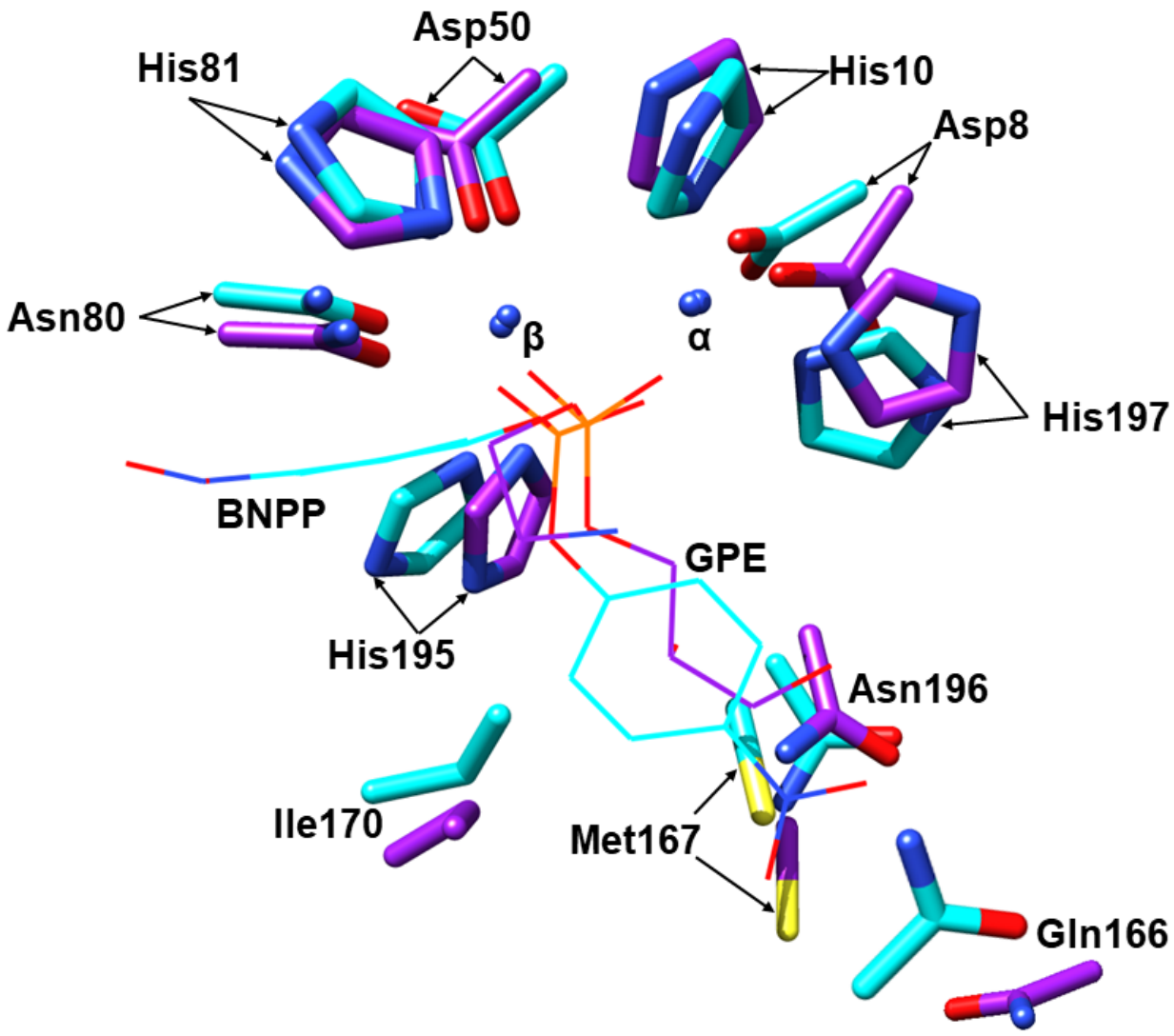

Figure S3: Superposition of equilibrated **GpdQ-BNPP** (cyan) and **GpdQ-GPE** (purple) structure.

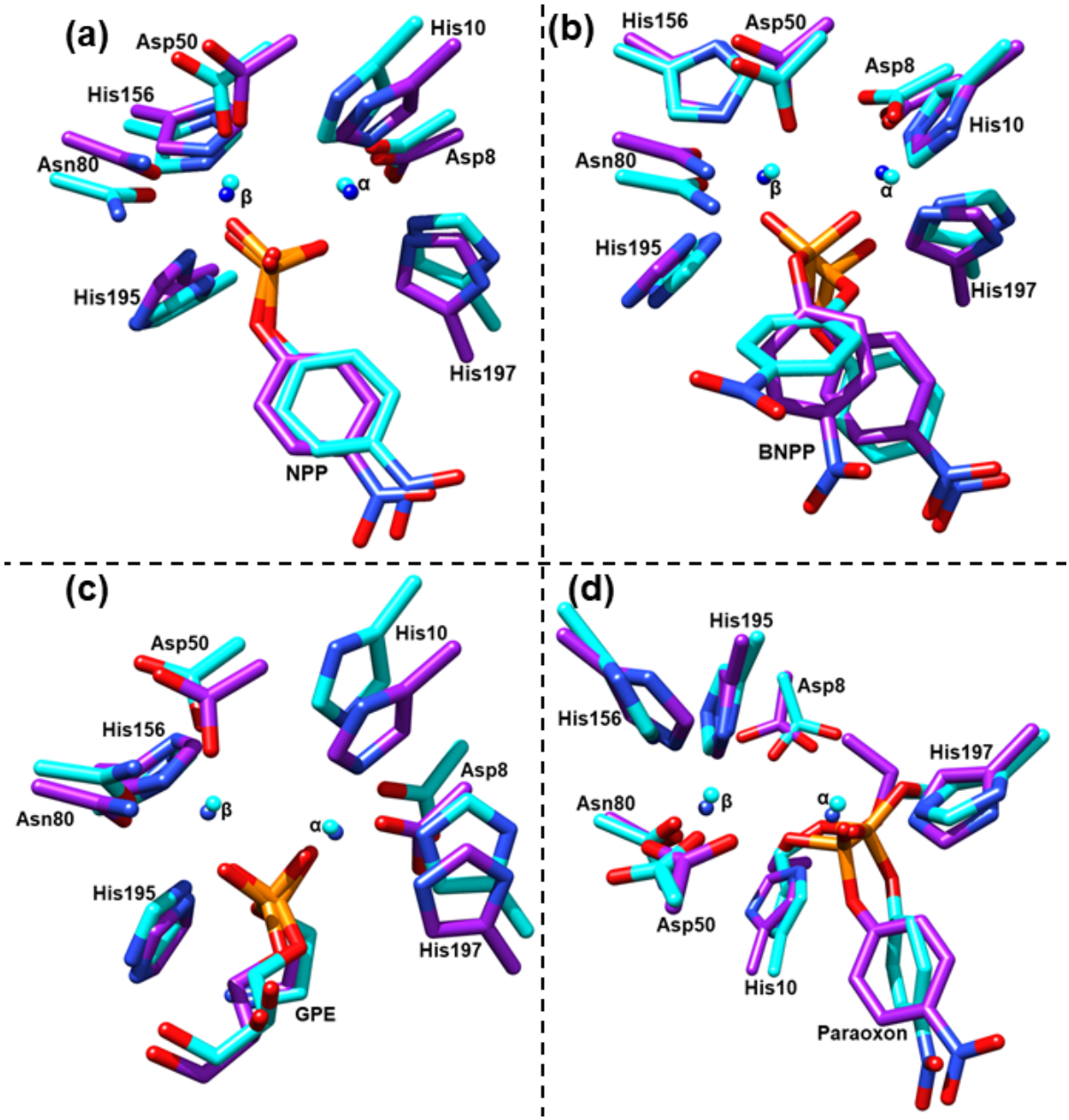

Figure S4: Superposition of the conformation of the GpdQ derived from the most representative structure of the GpdQ using AMOEBA force field (purple carbons) with (a) NPP, (b) BNPP, (c) Paraoxon, and (d) GPE with the corresponding GpdQ structure using AMBER force field (cyan carbons).

AMOEBA	E-NPP	E-BNPP	E-GPE	E-Et*p*NPP
Coordination number	5(α), 6(β)	5(α), 6(β)	5(α), 6(β)	5(α), 6(β)
Substrate	2.06 (α), 1.87 (β)	2.06 (α), 1.87 (β)	1.71(α), 1.83(β)	2.08 (α)
Asp8	1.83 (α)	1.85 (α)	1.74 (α)	1.84(α), 1.93(β)
His10	1.89 (α)	2.03 (α)	1.98 (α)	1.97 (α)
His197	2.04 (α)	1.99 (α)	2.54 (α)	2.15 (α)
Asp50	1.81 (β)	1.77 (β)	1.72 (β)	1.95 (β)
Asn80	2.08 (β)	1.93 (β)	2.08 (β)	1.98 (β)
His156	2.12 (β)	2.01 (β)	2.24 (β)	1.87 (β)
His195	2.63 (β)	2.55 (β)	2.49 (β)	3.02 (β)

Table S1: Metal coordination number, metal-substrate and metal-ligand distances (Å) of first coordination shell residues. Metal coordination sites (α and β) are shown in parentheses. AMOEBA force field are used in the MD simulations.

Table S2: Parameters of NPP, BNPP, GPE, and Paraoxon.

NPP PARAMETERS

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[ atomtypes ]
;name   bond_type     mass     charge   ptype   sigma         epsilon       Amb
 p3       p3         0.00000  0.00000   A     3.74177e-01   8.36800e-01 ; 2.10  0.2000
 o        o          0.00000  0.00000   A     2.95992e-01   8.78640e-01 ; 1.66  0.2100
 ca       ca         0.00000  0.00000   A     3.39967e-01   3.59824e-01 ; 1.91  0.0860
 ha       ha         0.00000  0.00000   A     2.59964e-01   6.27600e-02 ; 1.46  0.0150
 no       no         0.00000  0.00000   A     3.25000e-01   7.11280e-01 ; 1.82  0.1700
 os       os         0.00000  0.00000   A     3.00001e-01   7.11280e-01 ; 1.68  0.1700
 ho       ho         0.00000  0.00000   A     2.59964e-01   6.27600e-02 ; 0.00  0.0000

[ moleculetype ]
;name            nrexcl
 MOL               3

[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       ; qtot   bond_type
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    2    o     1   MOL    O1    2   -0.902865     16.00000 ; qtot 0.673
    3    o     1   MOL    O2    3   -0.902865     16.00000 ; qtot -0.230
    4    o     1   MOL    O3    4   -0.902865     16.00000 ; qtot -1.133
    5    o     1   MOL    O4    5   -0.738870     16.00000 ; qtot -1.872
    6   ca     1   MOL    C1    6    0.805525     12.01000 ; qtot -1.066
    7   ca     1   MOL    C2    7   -0.450121     12.01000 ; qtot -1.517
    8   ca     1   MOL    C3    8   -0.450121     12.01000 ; qtot -1.967
    9   ca     1   MOL    C4    9   -0.080261     12.01000 ; qtot -2.047
   10   ha     1   MOL    H1   10    0.201557      1.00800 ; qtot -1.845
   11   ca     1   MOL    C5   11   -0.080261     12.01000 ; qtot -1.926
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   13   ca     1   MOL    C6   13   -0.105761     12.01000 ; qtot -1.830
   14   ha     1   MOL    H3   14    0.102653      1.00800 ; qtot -1.727
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   16   no     1   MOL    N1   16    0.669247     14.01000 ; qtot -0.955
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   18    o     1   MOL    O6   18   -0.522334     16.00000 ; qtot -2.000

[ bonds ]
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    1     3   1    1.5150e-01    3.6853e+05 ;    P1 - O2
    1     4   1    1.5150e-01    3.6853e+05 ;    P1 - O3
    5     6   1    1.2358e-01    5.0049e+05 ;    O4 - C1
    6     7   1    1.3984e-01    3.8585e+05 ;    C1 - C2
    6     8   1    1.3984e-01    3.8585e+05 ;    C1 - C3
    7     9   1    1.3984e-01    3.8585e+05 ;    C2 - C4
    7    10   1    1.0860e-01    2.8937e+05 ;    C2 - H1
    8    11   1    1.3984e-01    3.8585e+05 ;    C3 - C5
    8    12   1    1.0860e-01    2.8937e+05 ;    C3 - H2
    9    13   1    1.3984e-01    3.8585e+05 ;    C4 - C6
    9    14   1    1.0860e-01    2.8937e+05 ;    C4 - H3
   11    13   1    1.3984e-01    3.8585e+05 ;    C5 - C6
   11    15   1    1.0860e-01    2.8937e+05 ;    C5 - H4
   13    16   1    1.4689e-01    2.6920e+05 ;    C6 - N1
   16    17   1    1.2260e-01    6.2074e+05 ;    N1 - O5
   16    18   1    1.2260e-01    6.2074e+05 ;    N1 - O6

[ pairs ]
;   ai    aj    funct
    5     9     1 ;    O4 - C4
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    5    11     1 ;    O4 - C5
    5    12     1 ;    O4 - H2
    6    13     1 ;    C1 - C6
    6    14     1 ;    C1 - H3
    6    15     1 ;    C1 - H4
    7    11     1 ;    C2 - C5
    7    12     1 ;    C2 - H2
    7    16     1 ;    C2 - N1
    8     9     1 ;    C3 - C4
    8    10     1 ;    C3 - H1
    8    16     1 ;    C3 - N1
    9    15     1 ;    C4 - H4
    9    17     1 ;    C4 - O5
    9    18     1 ;    C4 - O6
   10    13     1 ;    H1 - C6
   10    14     1 ;    H1 - H3
   11    14     1 ;    C5 - H3
   11    17     1 ;    C5 - O5
   11    18     1 ;    C5 - O6
   12    13     1 ;    H2 - C6
   12    15     1 ;    H2 - H4
   14    16     1 ;    H3 - N1
   15    16     1 ;    H4 - N1

[ angles ]
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    2     1     4     1    1.2218e+02    3.6635e+02 ;    O1 - P1    - O3
    3     1     4     1    1.2218e+02    3.6635e+02 ;    O2 - P1    - O3
    5     6     7     1    1.2326e+02    5.9722e+02 ;    O4 - C1    - C2
    5     6     8     1    1.2326e+02    5.9722e+02 ;    O4 - C1    - C3
    6     7     9     1    1.2002e+02    5.5748e+02 ;    C1 - C2    - C4
    6     7    10     1    1.1988e+02    4.0317e+02 ;    C1 - C2    - H1
    6     8    11     1    1.2002e+02    5.5748e+02 ;    C1 - C3    - C5
    6     8    12     1    1.1988e+02    4.0317e+02 ;    C1 - C3    - H2
    7     6     8     1    1.2002e+02    5.5748e+02 ;    C2 - C1    - C3
    7     9    13     1    1.2002e+02    5.5748e+02 ;    C2 - C4    - C6
    7     9    14     1    1.1988e+02    4.0317e+02 ;    C2 - C4    - H3
    8    11    13     1    1.2002e+02    5.5748e+02 ;    C3 - C5    - C6
    8    11    15     1    1.1988e+02    4.0317e+02 ;    C3 - C5    - H4
    9     7    10     1    1.1988e+02    4.0317e+02 ;    C4 - C2    - H1
    9    13    11     1    1.2002e+02    5.5748e+02 ;    C4 - C6    - C5
    9    13    16     1    1.1901e+02    5.5873e+02 ;    C4 - C6    - N1
   11     8    12     1    1.1988e+02    4.0317e+02 ;    C5 - C3    - H2
   11    13    16     1    1.1901e+02    5.5873e+02 ;    C5 - C6    - N1
   13     9    14     1    1.1988e+02    4.0317e+02 ;    C6 - C4    - H3
   13    11    15     1    1.1988e+02    4.0317e+02 ;    C6 - C5    - H4
   13    16    17     1    1.1776e+02    5.7488e+02 ;    C6 - N1    - O5
   13    16    18     1    1.1776e+02    5.7488e+02 ;    C6 - N1    - O6
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[ dihedrals ] ; propers
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    5     6     8    12     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    O4-   C1-   C3-   H2
    6     7     9    13     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C2-   C4-   C6
    6     7     9    14     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C2-   C4-   H3
    6     8    11    13     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C3-   C5-   C6
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   7     6     8    12     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C1-   C3-   H2
   7     9    13    11     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C4-   C6-   C5
   7     9    13    16     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C4-   C6-   N1
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   8    11    13     9     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C3-   C5-   C6-   C4
   8    11    13    16     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C3-   C5-   C6-   N1
   9    13    11    15     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C4-   C6-   C5-   H4
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  11    13     9    14     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C5-   C6-   C4-   H3
  11    13    16    17     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;    C5-   C6-   N1-   O5
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[ dihedrals ] ; impropers
; treated as propers in GROMACS to use correct AMBER analytical function
;   i     j     k     l   func   phase     kd      pn
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   7     8     6     5     1   180.00   4.60240   2 ;    C2-   C3-   C1-   O4
   7    13     9    14     1   180.00   4.60240   2 ;    C2-   C6-   C4-   H3
   8    13    11    15     1   180.00   4.60240   2 ;    C3-   C6-   C5-   H4
   9    11    13    16     1   180.00   4.60240   2 ;    C4-   C5-   C6-   N1
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BNPP PARAMETERS

```
[ atomtypes ]
;name   bond_type     mass     charge   ptype   sigma         epsilon       Amb
 p5       p5         0.00000  0.00000   A     3.74177e-01   8.36800e-01 ; 2.10  0.2000
 o        o          0.00000  0.00000   A     2.95992e-01   8.78640e-01 ; 1.66  0.2100
 os       os         0.00000  0.00000   A     3.00001e-01   7.11280e-01 ; 1.68  0.1700
 ca       ca         0.00000  0.00000   A     3.39967e-01   3.59824e-01 ; 1.91  0.0860
 ha       ha         0.00000  0.00000   A     2.59964e-01   6.27600e-02 ; 1.46  0.0150
 no       no         0.00000  0.00000   A     3.25000e-01   7.11280e-01 ; 1.82  0.1700

[ moleculetype ]
;name            nrexcl
 bpNPP           3

[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       ; qtot   bond_type
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     2   o      1   bpN    O1    2    -0.660333     16.00000 ; qtot 0.478
     3   os     1   bpN    O2    3    -0.473039     16.00000 ; qtot 0.005
     4   o      1   bpN    O3    4    -0.660333     16.00000 ; qtot -0.656
     5   os     1   bpN    O4    5    -0.473039     16.00000 ; qtot -1.129
     6   ca     1   bpN    C1    6     0.494727     12.01000 ; qtot -0.634
     7   ca     1   bpN    C2    7    -0.271273     12.01000 ; qtot -0.905
     8   ca     1   bpN    C3    8    -0.271273     12.01000 ; qtot -1.177
     9   ca     1   bpN    C4    9    -0.151061     12.01000 ; qtot -1.328
    10   ha     1   bpN    H1   10     0.168200      1.00800 ; qtot -1.159
    11   ca     1   bpN    C5   11    -0.151061     12.01000 ; qtot -1.311
    12   ha     1   bpN    H2   12     0.168200      1.00800 ; qtot -1.142
    13   ca     1   bpN    C6   13    -0.064296     12.01000 ; qtot -1.207
    14   ha     1   bpN    H3   14     0.159301      1.00800 ; qtot -1.047
    15   ha     1   bpN    H4   15     0.159301      1.00800 ; qtot -0.888
    16   ca     1   bpN    C7   16     0.494727     12.01000 ; qtot -0.393
    17   ca     1   bpN    C8   17    -0.271273     12.01000 ; qtot -0.665
    18   ca     1   bpN    C9   18    -0.271273     12.01000 ; qtot -0.936
    19   ca     1   bpN   C10   19    -0.151061     12.01000 ; qtot -1.087
    20   ha     1   bpN    H5   20     0.168200      1.00800 ; qtot -0.919
    21   ca     1   bpN   C11   21    -0.151061     12.01000 ; qtot -1.070
    22   ha     1   bpN    H6   22     0.168200      1.00800 ; qtot -0.902
    23   ca     1   bpN   C12   23    -0.064296     12.01000 ; qtot -0.966
    24   ha     1   bpN    H7   24     0.159301      1.00800 ; qtot -0.807
    25   ha     1   bpN    H8   25     0.159301      1.00800 ; qtot -0.647
    26   no     1   bpN    N1   26     0.752210     14.01000 ; qtot 0.105
    27   no     1   bpN    N2   27     0.752210     14.01000 ; qtot 0.857
    28   o      1   bpN    O5   28    -0.464297     16.00000 ; qtot 0.393
    29   o      1   bpN    O6   29    -0.464297     16.00000 ; qtot -0.071
    30   o      1   bpN    O7   30    -0.464297     16.00000 ; qtot -0.536
    31   o      1   bpN    O8   31    -0.464297     16.00000 ; qtot -1.000

[ bonds ]
;   ai    aj funct   r             k
     1     2   1    1.4810e-01    4.0811e+05 ;    P1 - O1
     1     3   1    1.6020e-01    2.8660e+05 ;    P1 - O2
     1     4   1    1.4810e-01    4.0811e+05 ;    P1 - O3
     1     5   1    1.6020e-01    2.8660e+05 ;    P1 - O4
     3    16   1    1.3730e-01    3.1162e+05 ;    O2 - C7
     5     6   1    1.3730e-01    3.1162e+05 ;    O4 - C1
     6     7   1    1.3870e-01    4.0033e+05 ;    C1 - C2
     6     8   1    1.3870e-01    4.0033e+05 ;    C1 - C3
     7     9   1    1.3870e-01    4.0033e+05 ;    C2 - C4
     7    10   1    1.0870e-01    2.8811e+05 ;    C2 - H1
     8    11   1    1.3870e-01    4.0033e+05 ;    C3 - C5
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    8    12   1    1.0870e-01    2.8811e+05 ;     C3 - H2
    9    13   1    1.3870e-01    4.0033e+05 ;     C4 - C6
    9    14   1    1.0870e-01    2.8811e+05 ;     C4 - H3
   11    13   1    1.3870e-01    4.0033e+05 ;     C5 - C6
   11    15   1    1.0870e-01    2.8811e+05 ;     C5 - H4
   13    26   1    1.4680e-01    2.6995e+05 ;     C6 - N1
   16    17   1    1.3870e-01    4.0033e+05 ;     C7 - C8
   16    18   1    1.3870e-01    4.0033e+05 ;     C7 - C9
   17    19   1    1.3870e-01    4.0033e+05 ;     C8 - C10
   17    20   1    1.0870e-01    2.8811e+05 ;     C8 - H5
   18    21   1    1.3870e-01    4.0033e+05 ;     C9 - C11
   18    22   1    1.0870e-01    2.8811e+05 ;     C9 - H6
   19    23   1    1.3870e-01    4.0033e+05 ;    C10 - C12
   19    24   1    1.0870e-01    2.8811e+05 ;    C10 - H7
   21    23   1    1.3870e-01    4.0033e+05 ;    C11 - C12
   21    25   1    1.0870e-01    2.8811e+05 ;    C11 - H8
   23    27   1    1.4680e-01    2.6995e+05 ;    C12 - N2
   26    30   1    1.2190e-01    6.3697e+05 ;     N1 - O7
   26    31   1    1.2190e-01    6.3697e+05 ;     N1 - O8
   27    28   1    1.2190e-01    6.3697e+05 ;     N2 - O5
   27    29   1    1.2190e-01    6.3697e+05 ;     N2 - O6

[ pairs ]
;   ai    aj    funct
    1     7     1 ;     P1 - C2
    1     8     1 ;     P1 - C3
    1    17     1 ;     P1 - C8
    1    18     1 ;     P1 - C9
    2     6     1 ;     O1 - C1
    2    16     1 ;     O1 - C7
    3     6     1 ;     O2 - C1
    3    19     1 ;     O2 - C10
    3    20     1 ;     O2 - H5
    3    21     1 ;     O2 - C11
    3    22     1 ;     O2 - H6
    4     6     1 ;     O3 - C1
    4    16     1 ;     O3 - C7
    5     9     1 ;     O4 - C4
    5    10     1 ;     O4 - H1
    5    11     1 ;     O4 - C5
    5    12     1 ;     O4 - H2
    5    16     1 ;     O4 - C7
    6    13     1 ;     C1 - C6
    6    14     1 ;     C1 - H3
    6    15     1 ;     C1 - H4
    7    11     1 ;     C2 - C5
    7    12     1 ;     C2 - H2
    7    26     1 ;     C2 - N1
    8     9     1 ;     C3 - C4
    8    10     1 ;     C3 - H1
    8    26     1 ;     C3 - N1
    9    15     1 ;     C4 - H4
    9    30     1 ;     C4 - O7
    9    31     1 ;     C4 - O8
   10    13     1 ;     H1 - C6
   10    14     1 ;     H1 - H3
   11    14     1 ;     C5 - H3
   11    30     1 ;     C5 - O7
   11    31     1 ;     C5 - O8
   12    13     1 ;     H2 - C6
   12    15     1 ;     H2 - H4
   14    26     1 ;     H3 - N1
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    15    26     1 ;    H4 - N1
    16    23     1 ;    C7 - C12
    16    24     1 ;    C7 - H7
    16    25     1 ;    C7 - H8
    17    21     1 ;    C8 - C11
    17    22     1 ;    C8 - H6
    17    27     1 ;    C8 - N2
    18    19     1 ;    C9 - C10
    18    20     1 ;    C9 - H5
    18    27     1 ;    C9 - N2
    19    25     1 ;   C10 - H8
    19    28     1 ;   C10 - O5
    19    29     1 ;   C10 - O6
    20    23     1 ;    H5 - C12
    20    24     1 ;    H5 - H7
    21    24     1 ;   C11 - H7
    21    28     1 ;   C11 - O5
    21    29     1 ;   C11 - O6
    22    23     1 ;    H6 - C12
    22    25     1 ;    H6 - H8
    24    27     1 ;    H7 - N2
    25    27     1 ;    H8 - N2

[ angles ]
;  ai    aj    ak    funct   theta         cth
    1     3    16     1    1.2342e+02    6.5237e+02 ;    P1 - O2    - C7
    1     5     6     1    1.2342e+02    6.5237e+02 ;    P1 - O4    - C1
    2     1     3     1    1.1609e+02    3.6828e+02 ;    O1 - P1    - O2
    2     1     4     1    1.1580e+02    3.8501e+02 ;    O1 - P1    - O3
    2     1     5     1    1.1609e+02    3.6828e+02 ;    O1 - P1    - O4
    3     1     4     1    1.1609e+02    3.6828e+02 ;    O2 - P1    - O3
    3     1     5     1    1.0177e+02    3.7966e+02 ;    O2 - P1    - O4
    3    16    17     1    1.1920e+02    5.8400e+02 ;    O2 - C7    - C8
    3    16    18     1    1.1920e+02    5.8400e+02 ;    O2 - C7    - C9
    4     1     5     1    1.1609e+02    3.6828e+02 ;    O3 - P1    - O4
    5     6     7     1    1.1920e+02    5.8400e+02 ;    O4 - C1    - C2
    5     6     8     1    1.1920e+02    5.8400e+02 ;    O4 - C1    - C3
    6     7     9     1    1.1997e+02    5.6216e+02 ;    C1 - C2    - C4
    6     7    10     1    1.2001e+02    4.0551e+02 ;    C1 - C2    - H1
    6     8    11     1    1.1997e+02    5.6216e+02 ;    C1 - C3    - C5
    6     8    12     1    1.2001e+02    4.0551e+02 ;    C1 - C3    - H2
    7     6     8     1    1.1997e+02    5.6216e+02 ;    C2 - C1    - C3
    7     9    13     1    1.1997e+02    5.6216e+02 ;    C2 - C4    - C6
    7     9    14     1    1.2001e+02    4.0551e+02 ;    C2 - C4    - H3
    8    11    13     1    1.1997e+02    5.6216e+02 ;    C3 - C5    - C6
    8    11    15     1    1.2001e+02    4.0551e+02 ;    C3 - C5    - H4
    9     7    10     1    1.2001e+02    4.0551e+02 ;    C4 - C2    - H1
    9    13    11     1    1.1997e+02    5.6216e+02 ;    C4 - C6    - C5
    9    13    26     1    1.1954e+02    5.5965e+02 ;    C4 - C6    - N1
   11     8    12     1    1.2001e+02    4.0551e+02 ;    C5 - C3    - H2
   11    13    26     1    1.1954e+02    5.5965e+02 ;    C5 - C6    - N1
   13     9    14     1    1.2001e+02    4.0551e+02 ;    C6 - C4    - H3
   13    11    15     1    1.2001e+02    4.0551e+02 ;    C6 - C5    - H4
   13    26    30     1    1.1810e+02    5.7522e+02 ;    C6 - N1    - O7
   13    26    31     1    1.1810e+02    5.7522e+02 ;    C6 - N1    - O8
   16    17    19     1    1.1997e+02    5.6216e+02 ;    C7 - C8    - C10
   16    17    20     1    1.2001e+02    4.0551e+02 ;    C7 - C8    - H5
   16    18    21     1    1.1997e+02    5.6216e+02 ;    C7 - C9    - C11
   16    18    22     1    1.2001e+02    4.0551e+02 ;    C7 - C9    - H6
   17    16    18     1    1.1997e+02    5.6216e+02 ;    C8 - C7    - C9
   17    19    23     1    1.1997e+02    5.6216e+02 ;    C8 - C10   - C12
   17    19    24     1    1.2001e+02    4.0551e+02 ;    C8 - C10   - H7
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   18    21    23     1    1.1997e+02    5.6216e+02 ;     C9 - C11    - C12
   18    21    25     1    1.2001e+02    4.0551e+02 ;     C9 - C11    - H8
   19    17    20     1    1.2001e+02    4.0551e+02 ;    C10 - C8     - H5
   19    23    21     1    1.1997e+02    5.6216e+02 ;    C10 - C12    - C11
   19    23    27     1    1.1954e+02    5.5965e+02 ;    C10 - C12    - N2
   21    18    22     1    1.2001e+02    4.0551e+02 ;    C11 - C9     - H6
   21    23    27     1    1.1954e+02    5.5965e+02 ;    C11 - C12    - N2
   23    19    24     1    1.2001e+02    4.0551e+02 ;    C12 - C10    - H7
   23    21    25     1    1.2001e+02    4.0551e+02 ;    C12 - C11    - H8
   23    27    28     1    1.1810e+02    5.7522e+02 ;    C12 - N2     - O5
   23    27    29     1    1.1810e+02    5.7522e+02 ;    C12 - N2     - O6
   28    27    29     1    1.2513e+02    6.4559e+02 ;     O5 - N2     - O6
   30    26    31     1    1.2513e+02    6.4559e+02 ;     O7 - N1     - O8

[ dihedrals ] ; propers
; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet
;    i     j     k     l   func    C0         C1         C2         C3         C4         C5
     1     3    16    17     3    7.53120    0.00000   -7.53120    0.00000    0.00000    0.00000 ;    P1-   O2-   C7-   C8
     1     3    16    18     3    7.53120    0.00000   -7.53120    0.00000    0.00000    0.00000 ;    P1-   O2-   C7-   C9
     1     5     6     7     3    7.53120    0.00000   -7.53120    0.00000    0.00000    0.00000 ;    P1-   O4-   C1-   C2
     1     5     6     8     3    7.53120    0.00000   -7.53120    0.00000    0.00000    0.00000 ;    P1-   O4-   C1-   C3
     2     1     3    16     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    O1-   P1-   O2-   C7
     2     1     5     6     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    O1-   P1-   O4-   C1
     3     1     5     6     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    O2-   P1-   O4-   C1
     3    16    17    19     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    O2-   C7-   C8-   C10
     3    16    17    20     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    O2-   C7-   C8-   H5
     3    16    18    21     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    O2-   C7-   C9-   C11
     3    16    18    22     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    O2-   C7-   C9-   H6
     4     1     3    16     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    O3-   P1-   O2-   C7
     4     1     5     6     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    O3-   P1-   O4-   C1
     5     1     3    16     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    O4-   P1-   O2-   C7
     5     6     7     9     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    O4-   C1-   C2-   C4
     5     6     7    10     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    O4-   C1-   C2-   H1
     5     6     8    11     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    O4-   C1-   C3-   C5
     5     6     8    12     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    O4-   C1-   C3-   H2
     6     7     9    13     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C2-   C4-   C6
     6     7     9    14     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C2-   C4-   H3
     6     8    11    13     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C3-   C5-   C6
     6     8    11    15     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C3-   C5-   H4
     7     6     8    11     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C1-   C3-   C5
     7     6     8    12     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C1-   C3-   H2
     7     9    13    11     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C4-   C6-   C5
     7     9    13    26     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C4-   C6-   N1
     8     6     7     9     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C3-   C1-   C2-   C4
     8     6     7    10     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C3-   C1-   C2-   H1
     8    11    13     9     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C3-   C5-   C6-   C4
     8    11    13    26     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C3-   C5-   C6-   N1
     9    13    11    15     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C4-   C6-   C5-   H4
     9    13    26    30     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;    C4-   C6-   N1-   O7
     9    13    26    31     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;    C4-   C6-   N1-   O8
    10     7     9    13     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H1-   C2-   C4-   C6
    10     7     9    14     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H1-   C2-   C4-   H3
    11    13     9    14     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C5-   C6-   C4-   H3
    11    13    26    30     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;    C5-   C6-   N1-   O7
    11    13    26    31     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;    C5-   C6-   N1-   O8
    12     8    11    13     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H2-   C3-   C5-   C6
    12     8    11    15     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H2-   C3-   C5-   H4
    14     9    13    26     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H3-   C4-   C6-   N1
    15    11    13    26     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H4-   C5-   C6-   N1
    16    17    19    23     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C7-   C8-   C10-  C12
    16    17    19    24     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C7-   C8-   C10-  H7
    16    18    21    23     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C7-   C9-   C11-  C12
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   16    18    21    25     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C7-   C9-  C11-   H8
   17    16    18    21     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C8-   C7-   C9-  C11
   17    16    18    22     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C8-   C7-   C9-   H6
   17    19    23    21     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C8-  C10-  C12-  C11
   17    19    23    27     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C8-  C10-  C12-   N2
   18    16    17    19     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C9-   C7-   C8-  C10
   18    16    17    20     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C9-   C7-   C8-   H5
   18    21    23    19     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C9-  C11-  C12-  C10
   18    21    23    27     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C9-  C11-  C12-   N2
   19    23    21    25     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;   C10-  C12-  C11-   H8
   19    23    27    28     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;   C10-  C12-   N2-   O5
   19    23    27    29     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;   C10-  C12-   N2-   O6
   20    17    19    23     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H5-   C8-  C10-  C12
   20    17    19    24     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H5-   C8-  C10-   H7
   21    23    19    24     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;   C11-  C12-  C10-   H7
   21    23    27    28     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;   C11-  C12-   N2-   O5
   21    23    27    29     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;   C11-  C12-   N2-   O6
   22    18    21    23     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H6-   C9-  C11-  C12
   22    18    21    25     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H6-   C9-  C11-   H8
   24    19    23    27     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H7-  C10-  C12-   N2
   25    21    23    27     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    H8-  C11-  C12-   N2

[ dihedrals ] ; impropers
; treated as propers in GROMACS to use correct AMBER analytical function
;   i     j     k     l  func   phase     kd      pn
    6     9     7    10     1   180.00   4.60240   2 ;    C1-   C4-   C2-   H1
    6    11     8    12     1   180.00   4.60240   2 ;    C1-   C5-   C3-   H2
    7     8     6     5     1   180.00   4.60240   2 ;    C2-   C3-   C1-   O4
    7    13     9    14     1   180.00   4.60240   2 ;    C2-   C6-   C4-   H3
    8    13    11    15     1   180.00   4.60240   2 ;    C3-   C6-   C5-   H4
    9    11    13    26     1   180.00   4.60240   2 ;    C4-   C5-   C6-   N1
   16    19    17    20     1   180.00   4.60240   2 ;    C7-  C10-   C8-   H5
   16    21    18    22     1   180.00   4.60240   2 ;    C7-  C11-   C9-   H6
   17    18    16     3     1   180.00   4.60240   2 ;    C8-   C9-   C7-   O2
   17    23    19    24     1   180.00   4.60240   2 ;    C8-  C12-  C10-   H7
   18    23    21    25     1   180.00   4.60240   2 ;    C9-  C12-  C11-   H8
   19    21    23    27     1   180.00   4.60240   2 ;   C10-  C11-  C12-   N2
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GPE PARAMETERS

```
[ atomtypes ]
;name   bond  type     mass     charge   ptype   sigma         epsilon       Amb
 os       os         0.00000  0.00000   A     3.00001e-01   7.11280e-01 ; 1.68  0.1700
 p5       p5         0.00000  0.00000   A     3.74177e-01   8.36800e-01 ; 2.10  0.2000
 o        o          0.00000  0.00000   A     2.95992e-01   8.78640e-01 ; 1.66  0.2100
 c3       c3         0.00000  0.00000   A     3.39967e-01   4.57730e-01 ; 1.91  0.1094
 h1       h1         0.00000  0.00000   A     2.47135e-01   6.56888e-02 ; 1.39  0.0157
 n3       n3         0.00000  0.00000   A     3.25000e-01   7.11280e-01 ; 1.82  0.1700
 hn       hn         0.00000  0.00000   A     1.06908e-01   6.56888e-02 ; 0.60  0.0157
 oh       oh         0.00000  0.00000   A     3.06647e-01   8.80314e-01 ; 1.72  0.2104
 ho       ho         0.00000  0.00000   A     2.59996e-01   6.27600e-02 ; 1.46  0.0150

[ moleculetype ]
;name            nrexcl
 GPE              3

[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge       mass       ; qtot   bond_type
    1   os     1   MOL    O1    1    -0.597934     16.00000 ; qtot -0.598
    2   p5     1   MOL    P1    2     1.755015     30.97000 ; qtot 1.157
    3   os     1   MOL    O2    3    -0.762162     16.00000 ; qtot 0.395
    4    o     1   MOL    O3    4    -0.927473     16.00000 ; qtot -0.533
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     5   c3     1   MOL     C1    5     0.319386     12.01000 ; qtot -0.213
     6   h1     1   MOL     H1    6     0.010134      1.00800 ; qtot -0.203
     7   h1     1   MOL     H2    7     0.010134      1.00800 ; qtot -0.193
     8   c3     1   MOL     C2    8     0.339082     12.01000 ; qtot 0.146
     9   h1     1   MOL     H3    9    -0.017855      1.00800 ; qtot 0.128
    10   h1     1   MOL     H4   10    -0.017855      1.00800 ; qtot 0.110
    11   n3     1   MOL     N1   11    -1.140095     14.01000 ; qtot -1.030
    12   hn     1   MOL     H5   12     0.392948      1.00800 ; qtot -0.637
    13   hn     1   MOL     H6   13     0.392948      1.00800 ; qtot -0.244
    14   c3     1   MOL     C3   14     0.115066     12.01000 ; qtot -0.129
    15   h1     1   MOL     H7   15     0.040438      1.00800 ; qtot -0.088
    16   h1     1   MOL     H8   16     0.040438      1.00800 ; qtot -0.048
    17   c3     1   MOL     C4   17     0.329940     12.01000 ; qtot 0.282
    18   h1     1   MOL     H9   18     0.037393      1.00800 ; qtot 0.320
    19   c3     1   MOL     C5   19     0.228606     12.01000 ; qtot 0.548
    20   h1     1   MOL     H10  20    -0.023161      1.00800 ; qtot 0.525
    21   h1     1   MOL     H11  21    -0.023161      1.00800 ; qtot 0.502
    22   oh     1   MOL     O4   22    -0.764897     16.00000 ; qtot -0.263
    23   ho     1   MOL     H12  23     0.467101      1.00800 ; qtot 0.204
    24   oh     1   MOL     O5   24    -0.712150     16.00000 ; qtot -0.508
    25   ho     1   MOL     H13  25     0.435583      1.00800 ; qtot -0.073
    26   o      1   MOL     O6   26    -0.927473     16.00000 ; qtot -1.000

[ bonds ]
;   ai    aj funct   r             k
     1     2   1    1.6020e-01    2.8660e+05 ;    O1 - P1
     1    14   1    1.4390e-01    2.5230e+05 ;    O1 - C3
     2     3   1    1.6020e-01    2.8660e+05 ;    P1 - O2
     2     4   1    1.4810e-01    4.0811e+05 ;    P1 - O3
     2    26   1    1.4810e-01    4.0811e+05 ;    P1 - O6
     3     5   1    1.4390e-01    2.5230e+05 ;    O2 - C1
     5     6   1    1.0930e-01    2.8108e+05 ;    C1 - H1
     5     7   1    1.0930e-01    2.8108e+05 ;    C1 - H2
     5     8   1    1.5350e-01    2.5363e+05 ;    C1 - C2
     8     9   1    1.0930e-01    2.8108e+05 ;    C2 - H3
     8    10   1    1.0930e-01    2.8108e+05 ;    C2 - H4
     8    11   1    1.4700e-01    2.6828e+05 ;    C2 - N1
    11    12   1    1.0180e-01    3.2978e+05 ;    N1 - H5
    11    13   1    1.0180e-01    3.2978e+05 ;    N1 - H6
    14    15   1    1.0930e-01    2.8108e+05 ;    C3 - H7
    14    16   1    1.0930e-01    2.8108e+05 ;    C3 - H8
    14    17   1    1.5350e-01    2.5363e+05 ;    C3 - C4
    17    18   1    1.0930e-01    2.8108e+05 ;    C4 - H9
    17    19   1    1.5350e-01    2.5363e+05 ;    C4 - C5
    17    24   1    1.4260e-01    2.6284e+05 ;    C4 - O5
    19    20   1    1.0930e-01    2.8108e+05 ;    C5 - H10
    19    21   1    1.0930e-01    2.8108e+05 ;    C5 - H11
    19    22   1    1.4260e-01    2.6284e+05 ;    C5 - O4
    22    23   1    9.7400e-02    3.0928e+05 ;    O4 - H12
    24    25   1    9.7400e-02    3.0928e+05 ;    O5 - H13

[ pairs ]
;   ai    aj    funct
     1     5     1 ;    O1 - C1
     1    18     1 ;    O1 - H9
     1    19     1 ;    O1 - C5
     1    24     1 ;    O1 - O5
     2     6     1 ;    P1 - H1
     2     7     1 ;    P1 - H2
     2     8     1 ;    P1 - C2
     2    15     1 ;    P1 - H7
     2    16     1 ;    P1 - H8
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    2    17     1 ;    P1 - C4
    3     9     1 ;    O2 - H3
    3    10     1 ;    O2 - H4
    3    11     1 ;    O2 - N1
    4     5     1 ;    O3 - C1
    5    12     1 ;    C1 - H5
    5    13     1 ;    C1 - H6
    5    26     1 ;    C1 - O6
    6     9     1 ;    H1 - H3
    6    10     1 ;    H1 - H4
    6    11     1 ;    H1 - N1
    7     9     1 ;    H2 - H3
    7    10     1 ;    H2 - H4
    7    11     1 ;    H2 - N1
    9    12     1 ;    H3 - H5
    9    13     1 ;    H3 - H6
   10    12     1 ;    H4 - H5
   10    13     1 ;    H4 - H6
   14     3     1 ;    C3 - O2
   14     4     1 ;    C3 - O3
   14    20     1 ;    C3 - H10
   14    21     1 ;    C3 - H11
   14    22     1 ;    C3 - O4
   14    25     1 ;    C3 - H13
   14    26     1 ;    C3 - O6
   15    18     1 ;    H7 - H9
   15    19     1 ;    H7 - C5
   15    24     1 ;    H7 - O5
   16    18     1 ;    H8 - H9
   16    19     1 ;    H8 - C5
   16    24     1 ;    H8 - O5
   17    23     1 ;    C4 - H12
   18    20     1 ;    H9 - H10
   18    21     1 ;    H9 - H11
   18    22     1 ;    H9 - O4
   18    25     1 ;    H9 - H13
   19    25     1 ;    C5 - H13
   20    23     1 ;   H10 - H12
   20    24     1 ;   H10 - O5
   21    23     1 ;   H11 - H12
   21    24     1 ;   H11 - O5
   22    24     1 ;    O4 - O5

[ angles ]
;  ai    aj    ak    funct   theta         cth
    1     2     3     1    1.0177e+02    3.7966e+02 ;    O1 - P1    - O2
    1     2     4     1    1.1609e+02    3.6828e+02 ;    O1 - P1    - O3
    1     2    26     1    1.1609e+02    3.6828e+02 ;    O1 - P1    - O6
    1    14    15     1    1.0882e+02    4.2543e+02 ;    O1 - C3    - H7
    1    14    16     1    1.0882e+02    4.2543e+02 ;    O1 - C3    - H8
    1    14    17     1    1.0842e+02    5.6718e+02 ;    O1 - C3    - C4
    2     1    14     1    1.1800e+02    6.5672e+02 ;    P1 - O1    - C3
    2     3     5     1    1.1800e+02    6.5672e+02 ;    P1 - O2    - C1
    3     2     4     1    1.1609e+02    3.6828e+02 ;    O2 - P1    - O3
    3     2    26     1    1.1609e+02    3.6828e+02 ;    O2 - P1    - O6
    3     5     6     1    1.0882e+02    4.2543e+02 ;    O2 - C1    - H1
    3     5     7     1    1.0882e+02    4.2543e+02 ;    O2 - C1    - H2
    3     5     8     1    1.0842e+02    5.6718e+02 ;    O2 - C1    - C2
    4     2    26     1    1.1580e+02    3.8501e+02 ;    O3 - P1    - O6
    5     8     9     1    1.1007e+02    3.8794e+02 ;    C1 - C2    - H3
    5     8    10     1    1.1007e+02    3.8794e+02 ;    C1 - C2    - H4
    5     8    11     1    1.1038e+02    5.5379e+02 ;    C1 - C2    - N1
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  6     5     7     1    1.0955e+02    3.2786e+02 ;    H1 - C1    - H2
  6     5     8     1    1.1007e+02    3.8794e+02 ;    H1 - C1    - C2
  7     5     8     1    1.1007e+02    3.8794e+02 ;    H2 - C1    - C2
  8    11    12     1    1.0992e+02    3.9438e+02 ;    C2 - N1    - H5
  8    11    13     1    1.0992e+02    3.9438e+02 ;    C2 - N1    - H6
  9     8    10     1    1.0955e+02    3.2786e+02 ;    H3 - C2    - H4
  9     8    11     1    1.0992e+02    4.1330e+02 ;    H3 - C2    - N1
 10     8    11     1    1.0992e+02    4.1330e+02 ;    H4 - C2    - N1
 12    11    13     1    1.0713e+02    3.4560e+02 ;    H5 - N1    - H6
 14    17    18     1    1.1007e+02    3.8794e+02 ;    C3 - C4    - H9
 14    17    19     1    1.1063e+02    5.2894e+02 ;    C3 - C4    - C5
 14    17    24     1    1.0943e+02    5.6668e+02 ;    C3 - C4    - O5
 15    14    16     1    1.0955e+02    3.2786e+02 ;    H7 - C3    - H8
 15    14    17     1    1.1007e+02    3.8794e+02 ;    H7 - C3    - C4
 16    14    17     1    1.1007e+02    3.8794e+02 ;    H8 - C3    - C4
 17    19    20     1    1.1007e+02    3.8794e+02 ;    C4 - C5    - H10
 17    19    21     1    1.1007e+02    3.8794e+02 ;    C4 - C5    - H11
 17    19    22     1    1.0943e+02    5.6668e+02 ;    C4 - C5    - O4
 17    24    25     1    1.0816e+02    3.9405e+02 ;    C4 - O5    - H13
 18    17    19     1    1.1007e+02    3.8794e+02 ;    H9 - C4    - C5
 18    17    24     1    1.0988e+02    4.2652e+02 ;    H9 - C4    - O5
 19    17    24     1    1.0943e+02    5.6668e+02 ;    C5 - C4    - O5
 19    22    23     1    1.0816e+02    3.9405e+02 ;    C5 - O4    - H12
 20    19    21     1    1.0955e+02    3.2786e+02 ;    H10 - C5    - H11
 20    19    22     1    1.0988e+02    4.2652e+02 ;    H10 - C5    - O4
 21    19    22     1    1.0988e+02    4.2652e+02 ;    H11 - C5    - O4

[ dihedrals ] ; propers
; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet
;   i     j     k     l   func    C0         C1         C2         C3         C4         C5
    1     2     3     5     3    1.04600    3.13800   10.04160   -4.18400    0.00000    0.00000 ;    O1-   P1-   O2-   C1
    1    14    17    18     3    1.04600   -1.04600    0.00000    0.00000    0.00000    0.00000 ;    O1-   C3-   C4-   H9
    1    14    17    19     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    O1-   C3-   C4-   C5
    1    14    17    24     3    0.60250    1.80749    9.83240   -2.40998    0.00000    0.00000 ;    O1-   C3-   C4-   O5
    2     1    14    15     3    1.60387    4.81160    0.00000   -6.41547    0.00000    0.00000 ;    P1-   O1-   C3-   H7
    2     1    14    16     3    1.60387    4.81160    0.00000   -6.41547    0.00000    0.00000 ;    P1-   O1-   C3-   H8
    2     1    14    17     3    1.60387    4.81160    0.00000   -6.41547    0.00000    0.00000 ;    P1-   O1-   C3-   C4
    2     3     5     6     3    1.60387    4.81160    0.00000   -6.41547    0.00000    0.00000 ;    P1-   O2-   C1-   H1
    2     3     5     7     3    1.60387    4.81160    0.00000   -6.41547    0.00000    0.00000 ;    P1-   O2-   C1-   H2
    2     3     5     8     3    1.60387    4.81160    0.00000   -6.41547    0.00000    0.00000 ;    P1-   O2-   C1-   C2
    3     5     8     9     3    1.04600   -1.04600    0.00000    0.00000    0.00000    0.00000 ;    O2-   C1-   C2-   H3
    3     5     8    10     3    1.04600   -1.04600    0.00000    0.00000    0.00000    0.00000 ;    O2-   C1-   C2-   H4
    3     5     8    11     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    O2-   C1-   C2-   N1
    4     2     3     5     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    O3-   P1-   O2-   C1
    5     3     2    26     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    C1-   O2-   P1-   O6
    5     8    11    12     3    1.25520    3.76560    0.00000   -5.02080    0.00000    0.00000 ;    C1-   C2-   N1-   H5
    5     8    11    13     3    1.25520    3.76560    0.00000   -5.02080    0.00000    0.00000 ;    C1-   C2-   N1-   H6
    6     5     8     9     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    H1-   C1-   C2-   H3
    6     5     8    10     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    H1-   C1-   C2-   H4
    6     5     8    11     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    H1-   C1-   C2-   N1
    7     5     8     9     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    H2-   C1-   C2-   H3
    7     5     8    10     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    H2-   C1-   C2-   H4
    7     5     8    11     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    H2-   C1-   C2-   N1
    9     8    11    12     3    1.25520    3.76560    0.00000   -5.02080    0.00000    0.00000 ;    H3-   C2-   N1-   H5
    9     8    11    13     3    1.25520    3.76560    0.00000   -5.02080    0.00000    0.00000 ;    H3-   C2-   N1-   H6
   10     8    11    12     3    1.25520    3.76560    0.00000   -5.02080    0.00000    0.00000 ;    H4-   C2-   N1-   H5
   10     8    11    13     3    1.25520    3.76560    0.00000   -5.02080    0.00000    0.00000 ;    H4-   C2-   N1-   H6
   14     1     2     3     3    1.04600    3.13800   10.04160   -4.18400    0.00000    0.00000 ;    C3-   O1-   P1-   O2
   14     1     2     4     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    C3-   O1-   P1-   O3
   14     1     2    26     3    0.00000    0.00000    6.69440    0.00000    0.00000    0.00000 ;    C3-   O1-   P1-   O6
   14    17    19    20     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    C3-   C4-   C5-   H10
   14    17    19    21     3    0.65084    1.95253    0.00000   -2.60338    0.00000    0.00000 ;    C3-   C4-   C5-   H11
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   14    17    19    22     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   C3-   C4-   C5-   O4
   14    17    24    25     3   1.71544   0.96232   0.00000  -2.67776   0.00000   0.00000 ;   C3-   C4-   O5-  H13
   15    14    17    18     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H7-   C3-   C4-   H9
   15    14    17    19     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H7-   C3-   C4-   C5
   15    14    17    24     3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;   H7-   C3-   C4-   O5
   16    14    17    18     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H8-   C3-   C4-   H9
   16    14    17    19     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H8-   C3-   C4-   C5
   16    14    17    24     3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;   H8-   C3-   C4-   O5
   17    19    22    23     3   1.71544   0.96232   0.00000  -2.67776   0.00000   0.00000 ;   C4-   C5-   O4-  H12
   18    17    19    20     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H9-   C4-   C5-  H10
   18    17    19    21     3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H9-   C4-   C5-  H11
   18    17    19    22     3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;   H9-   C4-   C5-   O4
   18    17    24    25     3   0.69733   2.09200   0.00000  -2.78933   0.00000   0.00000 ;   H9-   C4-   O5-  H13
   19    17    24    25     3   1.71544   0.96232   0.00000  -2.67776   0.00000   0.00000 ;   C5-   C4-   O5-  H13
   20    19    17    24     3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;  H10-   C5-   C4-   O5
   20    19    22    23     3   0.69733   2.09200   0.00000  -2.78933   0.00000   0.00000 ;  H10-   C5-   O4-  H12
   21    19    17    24     3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;  H11-   C5-   C4-   O5
   21    19    22    23     3   0.69733   2.09200   0.00000  -2.78933   0.00000   0.00000 ;  H11-   C5-   O4-  H12
   22    19    17    24     3   0.60250   1.80749   9.83240  -2.40998   0.00000   0.00000 ;   O4-   C5-   C4-   O5
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PARAOXON PARAMETERS

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[ atomtypes ]
;name   bond_type     mass     charge   ptype   sigma         epsilon       Amb
 ca       ca          0.00000  0.00000   A     3.39967e-01   3.59824e-01 ; 1.91  0.0860
 no       no          0.00000  0.00000   A     3.25000e-01   7.11280e-01 ; 1.82  0.1700
 o        o           0.00000  0.00000   A     2.95992e-01   8.78640e-01 ; 1.66  0.2100
 os       os          0.00000  0.00000   A     3.00001e-01   7.11280e-01 ; 1.68  0.1700
 p5       p5          0.00000  0.00000   A     3.74177e-01   8.36800e-01 ; 2.10  0.2000
 c3       c3          0.00000  0.00000   A     3.39967e-01   4.57730e-01 ; 1.91  0.1094
 ha       ha          0.00000  0.00000   A     2.59964e-01   6.27600e-02 ; 1.46  0.0150
 h1       h1          0.00000  0.00000   A     2.47135e-01   6.56888e-02 ; 1.39  0.0157
 hc       hc          0.00000  0.00000   A     2.64953e-01   6.56888e-02 ; 1.49  0.0157

[ moleculetype ]
;name            nrexcl
 para             3
[ atoms ]
;   nr  type  resi  res  atom  cgnr     charge      mass       ; qtot   bond_type
    1    ca     1   MOL    C1     1    -0.003142    12.01000 ; qtot -0.003
    2    ca     1   MOL    C2     2    -0.082173    12.01000 ; qtot -0.085
    3    ca     1   MOL    C3     3    -0.003142    12.01000 ; qtot -0.088
    4    ca     1   MOL    C4     4    -0.312863    12.01000 ; qtot -0.401
    5    ca     1   MOL    C5     5     0.356963    12.01000 ; qtot -0.044
    6    ca     1   MOL    C6     6    -0.312863    12.01000 ; qtot -0.357
    7    no     1   MOL    N1     7     0.631163    14.01000 ; qtot 0.274
    8    o      1   MOL    O1     8    -0.381203    16.00000 ; qtot -0.107
    9    o      1   MOL    O2     9    -0.381203    16.00000 ; qtot -0.488
   10    os     1   MOL    O3    10    -0.267191    16.00000 ; qtot -0.756
   11    p5     1   MOL    P1    11     1.103069    30.97000 ; qtot 0.347
   12    os     1   MOL    O4    12    -0.443057    16.00000 ; qtot -0.096
   13    o      1   MOL    O5    13    -0.576476    16.00000 ; qtot -0.672
   14    c3     1   MOL    C7    14     0.155740    12.01000 ; qtot -0.516
   15    c3     1   MOL    C8    15    -0.096059    12.01000 ; qtot -0.612
   16    os     1   MOL    O6    16    -0.443057    16.00000 ; qtot -1.055
   17    c3     1   MOL    C9    17     0.155740    12.01000 ; qtot -0.900
   18    c3     1   MOL   C10    18    -0.096059    12.01000 ; qtot -0.996
   19    ha     1   MOL    H1    19     0.121857     1.00800 ; qtot -0.874
   20    ha     1   MOL    H2    20     0.121857     1.00800 ; qtot -0.752
   21    ha     1   MOL    H3    21     0.179120     1.00800 ; qtot -0.573
   22    ha     1   MOL    H4    22     0.179120     1.00800 ; qtot -0.394
   23    h1     1   MOL    H5    23     0.049214     1.00800 ; qtot -0.345
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    24   h1    1   MOL    H6   24     0.049214      1.00800 ; qtot -0.295
    25   hc    1   MOL    H7   25     0.032834      1.00800 ; qtot -0.263
    26   hc    1   MOL    H8   26     0.032834      1.00800 ; qtot -0.230
    27   hc    1   MOL    H9   27     0.032834      1.00800 ; qtot -0.197
    28   h1    1   MOL   H10   28     0.049214      1.00800 ; qtot -0.148
    29   h1    1   MOL   H11   29     0.049214      1.00800 ; qtot -0.099
    30   hc    1   MOL   H12   30     0.032834      1.00800 ; qtot -0.066
    31   hc    1   MOL   H13   31     0.032834      1.00800 ; qtot -0.033
    32   hc    1   MOL   H14   32     0.032834      1.00800 ; qtot -0.000

[ bonds ]
;   ai     aj funct   r             k
     1      2   1    1.3984e-01    3.8585e+05 ;    C1 - C2
     1      6   1    1.3984e-01    3.8585e+05 ;    C1 - C6
     1     19   1    1.0860e-01    2.8937e+05 ;    C1 - H1
     2      3   1    1.3984e-01    3.8585e+05 ;    C2 - C3
     2      7   1    1.4689e-01    2.6920e+05 ;    C2 - N1
     3      4   1    1.3984e-01    3.8585e+05 ;    C3 - C4
     3     20   1    1.0860e-01    2.8937e+05 ;    C3 - H2
     4      5   1    1.3984e-01    3.8585e+05 ;    C4 - C5
     4     21   1    1.0860e-01    2.8937e+05 ;    C4 - H3
     5      6   1    1.3984e-01    3.8585e+05 ;    C5 - C6
     5     10   1    1.3696e-01    3.1514e+05 ;    C5 - O3
     6     22   1    1.0860e-01    2.8937e+05 ;    C6 - H4
     7      8   1    1.2260e-01    6.2074e+05 ;    N1 - O1
     7      9   1    1.2260e-01    6.2074e+05 ;    N1 - O2
    10     11   1    1.6147e-01    2.7665e+05 ;    O3 - P1
    11     12   1    1.6147e-01    2.7665e+05 ;    P1 - O4
    11     13   1    1.4866e-01    4.0125e+05 ;    P1 - O5
    11     16   1    1.6147e-01    2.7665e+05 ;    P1 - O6
    12     14   1    1.4316e-01    2.5824e+05 ;    O4 - C7
    14     15   1    1.5375e-01    2.5179e+05 ;    C7 - C8
    14     23   1    1.0969e-01    2.7665e+05 ;    C7 - H5
    14     24   1    1.0969e-01    2.7665e+05 ;    C7 - H6
    15     25   1    1.0969e-01    2.7665e+05 ;    C8 - H7
    15     26   1    1.0969e-01    2.7665e+05 ;    C8 - H8
    15     27   1    1.0969e-01    2.7665e+05 ;    C8 - H9
    16     17   1    1.4316e-01    2.5824e+05 ;    O6 - C9
    17     18   1    1.5375e-01    2.5179e+05 ;    C9 - C10
    17     28   1    1.0969e-01    2.7665e+05 ;    C9 - H10
    17     29   1    1.0969e-01    2.7665e+05 ;    C9 - H11
    18     30   1    1.0969e-01    2.7665e+05 ;   C10 - H12
    18     31   1    1.0969e-01    2.7665e+05 ;   C10 - H13
    18     32   1    1.0969e-01    2.7665e+05 ;   C10 - H14

[ pairs ]
;   ai     aj    funct
     1      4     1 ;    C1 - C4
     1      8     1 ;    C1 - O1
     1      9     1 ;    C1 - O2
     1     10     1 ;    C1 - O3
     1     20     1 ;    C1 - H2
     2      5     1 ;    C2 - C5
     2     21     1 ;    C2 - H3
     2     22     1 ;    C2 - H4
     3      8     1 ;    C3 - O1
     3      9     1 ;    C3 - O2
     3     10     1 ;    C3 - O3
     4      7     1 ;    C4 - N1
     4     11     1 ;    C4 - P1
     4     22     1 ;    C4 - H4
     5     12     1 ;    C5 - O4
```

```
    5    13     1 ;    C5 - O5
    5    16     1 ;    C5 - O6
    5    20     1 ;    C5 - H2
    6     3     1 ;    C6 - C3
    6     7     1 ;    C6 - N1
    6    11     1 ;    C6 - P1
    6    21     1 ;    C6 - H3
    7    20     1 ;    N1 - H2
   10    14     1 ;    O3 - C7
   10    17     1 ;    O3 - C9
   10    21     1 ;    O3 - H3
   10    22     1 ;    O3 - H4
   11    15     1 ;    P1 - C8
   11    18     1 ;    P1 - C10
   11    23     1 ;    P1 - H5
   11    24     1 ;    P1 - H6
   11    28     1 ;    P1 - H10
   11    29     1 ;    P1 - H11
   12    17     1 ;    O4 - C9
   12    25     1 ;    O4 - H7
   12    26     1 ;    O4 - H8
   12    27     1 ;    O4 - H9
   13    14     1 ;    O5 - C7
   13    17     1 ;    O5 - C9
   14    16     1 ;    C7 - O6
   16    30     1 ;    O6 - H12
   16    31     1 ;    O6 - H13
   16    32     1 ;    O6 - H14
   19     3     1 ;    H1 - C3
   19     5     1 ;    H1 - C5
   19     7     1 ;    H1 - N1
   19    22     1 ;    H1 - H4
   20    21     1 ;    H2 - H3
   23    25     1 ;    H5 - H7
   23    26     1 ;    H5 - H8
   23    27     1 ;    H5 - H9
   24    25     1 ;    H6 - H7
   24    26     1 ;    H6 - H8
   24    27     1 ;    H6 - H9
   28    30     1 ;   H10 - H12
   28    31     1 ;   H10 - H13
   28    32     1 ;   H10 - H14
   29    30     1 ;   H11 - H12
   29    31     1 ;   H11 - H13
   29    32     1 ;   H11 - H14

[ angles ]
;  ai    aj    ak    funct   theta         cth
    1     2     3     1    1.2002e+02    5.5748e+02 ;    C1 - C2    - C3
    1     2     7     1    1.1901e+02    5.5873e+02 ;    C1 - C2    - N1
    1     6     5     1    1.2002e+02    5.5748e+02 ;    C1 - C6    - C5
    1     6    22     1    1.1988e+02    4.0317e+02 ;    C1 - C6    - H4
    2     1     6     1    1.2002e+02    5.5748e+02 ;    C2 - C1    - C6
    2     1    19     1    1.1988e+02    4.0317e+02 ;    C2 - C1    - H1
    2     3     4     1    1.2002e+02    5.5748e+02 ;    C2 - C3    - C4
    2     3    20     1    1.1988e+02    4.0317e+02 ;    C2 - C3    - H2
    2     7     8     1    1.1776e+02    5.7488e+02 ;    C2 - N1    - O1
    2     7     9     1    1.1776e+02    5.7488e+02 ;    C2 - N1    - O2
    3     2     7     1    1.1901e+02    5.5873e+02 ;    C3 - C2    - N1
    3     4     5     1    1.2002e+02    5.5748e+02 ;    C3 - C4    - C5
    3     4    21     1    1.1988e+02    4.0317e+02 ;    C3 - C4    - H3
    4     3    20     1    1.1988e+02    4.0317e+02 ;    C4 - C3    - H2
```

```
  4     5     6     1    1.2002e+02    5.5748e+02 ;     C4 - C5     - C6
  4     5    10     1    1.1920e+02    5.8225e+02 ;     C4 - C5     - O3
  5     4    21     1    1.1988e+02    4.0317e+02 ;     C5 - C4     - H3
  5     6    22     1    1.1988e+02    4.0317e+02 ;     C5 - C6     - H4
  5    10    11     1    1.2318e+02    6.4986e+02 ;     C5 - O3     - P1
  6     1    19     1    1.1988e+02    4.0317e+02 ;     C6 - C1     - H1
  6     5    10     1    1.1920e+02    5.8225e+02 ;     C6 - C5     - O3
  8     7     9     1    1.2508e+02    6.4208e+02 ;     O1 - N1     - O2
 10    11    12     1    1.0184e+02    3.7656e+02 ;     O3 - P1     - O4
 10    11    13     1    1.1546e+02    3.6694e+02 ;     O3 - P1     - O5
 10    11    16     1    1.0184e+02    3.7656e+02 ;     O3 - P1     - O6
 11    12    14     1    1.1954e+02    6.5036e+02 ;     P1 - O4     - C7
 11    16    17     1    1.1954e+02    6.5036e+02 ;     P1 - O6     - C9
 12    11    13     1    1.1546e+02    3.6694e+02 ;     O4 - P1     - O5
 12    11    16     1    1.0184e+02    3.7656e+02 ;     O4 - P1     - O6
 12    14    15     1    1.0797e+02    5.6902e+02 ;     O4 - C7     - C8
 12    14    23     1    1.0978e+02    4.2509e+02 ;     O4 - C7     - H5
 12    14    24     1    1.0978e+02    4.2509e+02 ;     O4 - C7     - H6
 13    11    16     1    1.1546e+02    3.6694e+02 ;     O5 - P1     - O6
 14    15    25     1    1.0980e+02    3.8777e+02 ;     C7 - C8     - H7
 14    15    26     1    1.0980e+02    3.8777e+02 ;     C7 - C8     - H8
 14    15    27     1    1.0980e+02    3.8777e+02 ;     C7 - C8     - H9
 15    14    23     1    1.0956e+02    3.8819e+02 ;     C8 - C7     - H5
 15    14    24     1    1.0956e+02    3.8819e+02 ;     C8 - C7     - H6
 16    17    18     1    1.0797e+02    5.6902e+02 ;     O6 - C9     - C10
 16    17    28     1    1.0978e+02    4.2509e+02 ;     O6 - C9     - H10
 16    17    29     1    1.0978e+02    4.2509e+02 ;     O6 - C9     - H11
 17    18    30     1    1.0980e+02    3.8777e+02 ;     C9 - C10    - H12
 17    18    31     1    1.0980e+02    3.8777e+02 ;     C9 - C10    - H13
 17    18    32     1    1.0980e+02    3.8777e+02 ;     C9 - C10    - H14
 18    17    28     1    1.0956e+02    3.8819e+02 ;    C10 - C9     - H10
 18    17    29     1    1.0956e+02    3.8819e+02 ;    C10 - C9     - H11
 23    14    24     1    1.0846e+02    3.2836e+02 ;     H5 - C7     - H6
 25    15    26     1    1.0758e+02    3.2970e+02 ;     H7 - C8     - H8
 25    15    27     1    1.0758e+02    3.2970e+02 ;     H7 - C8     - H9
 26    15    27     1    1.0758e+02    3.2970e+02 ;     H8 - C8     - H9
 28    17    29     1    1.0846e+02    3.2836e+02 ;    H10 - C9     - H11
 30    18    31     1    1.0758e+02    3.2970e+02 ;    H12 - C10    - H13
 30    18    32     1    1.0758e+02    3.2970e+02 ;    H12 - C10    - H14
 31    18    32     1    1.0758e+02    3.2970e+02 ;    H13 - C10    - H14

[ dihedrals ] ; propers
; treated as RBs in GROMACS to use combine multiple AMBER torsions per quartet
;   i     j     k     l   func    C0        C1        C2        C3        C4        C5
    1     2     3     4     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C2-   C3-   C4
    1     2     3    20     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C2-   C3-   H2
    1     2     7     8     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;    C1-   C2-   N1-   O1
    1     2     7     9     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;    C1-   C2-   N1-   O2
    1     6     5     4     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C6-   C5-   C4
    1     6     5    10     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C1-   C6-   C5-   O3
    2     1     6     5     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C1-   C6-   C5
    2     1     6    22     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C1-   C6-   H4
    2     3     4     5     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C3-   C4-   C5
    2     3     4    21     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C2-   C3-   C4-   H3
    3     2     7     8     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;    C3-   C2-   N1-   O1
    3     2     7     9     3    5.02080    0.00000   -5.02080    0.00000    0.00000    0.00000 ;    C3-   C2-   N1-   O2
    3     4     5     6     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C3-   C4-   C5-   C6
    3     4     5    10     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C3-   C4-   C5-   O3
    4     3     2     7     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C4-   C3-   C2-   N1
    4     5     6    22     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C4-   C5-   C6-   H4
    4     5    10    11     3   14.64400    0.00000  -14.64400    0.00000    0.00000    0.00000 ;    C4-   C5-   O3-   P1
    5     4     3    20     3   30.33400    0.00000  -30.33400    0.00000    0.00000    0.00000 ;    C5-   C4-   C3-   H2
```

```
  5   10   11   12    3   0.00000   0.00000   6.69440   0.00000   0.00000   0.00000 ;   C5-  O3-  P1-  O4
  5   10   11   13    3   7.11280   1.25520  -6.69440  -1.67360   0.00000   0.00000 ;   C5-  O3-  P1-  O5
  5   10   11   16    3   0.00000   0.00000   6.69440   0.00000   0.00000   0.00000 ;   C5-  O3-  P1-  O6
  6    1    2    3    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   C6-  C1-  C2-  C3
  6    1    2    7    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   C6-  C1-  C2-  N1
  6    5    4   21    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   C6-  C5-  C4-  H3
  6    5   10   11    3  14.64400   0.00000 -14.64400   0.00000   0.00000   0.00000 ;   C6-  C5-  O3-  P1
  7    2    3   20    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   N1-  C2-  C3-  H2
 10    5    4   21    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   O3-  C5-  C4-  H3
 10    5    6   22    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   O3-  C5-  C6-  H4
 10   11   12   14    3   1.04600   3.13800  10.04160  -4.18400   0.00000   0.00000 ;   O3-  P1-  O4-  C7
 10   11   16   17    3   1.04600   3.13800  10.04160  -4.18400   0.00000   0.00000 ;   O3-  P1-  O6-  C9
 11   12   14   15    3  18.13067  21.33840   0.00000  -6.41547   0.00000   0.00000 ;   P1-  O4-  C7-  C8
 11   12   14   23    3   1.60387   4.81160   0.00000  -6.41547   0.00000   0.00000 ;   P1-  O4-  C7-  H5
 11   12   14   24    3   1.60387   4.81160   0.00000  -6.41547   0.00000   0.00000 ;   P1-  O4-  C7-  H6
 11   16   17   18    3  18.13067  21.33840   0.00000  -6.41547   0.00000   0.00000 ;   P1-  O6-  C9-  C10
 11   16   17   28    3   1.60387   4.81160   0.00000  -6.41547   0.00000   0.00000 ;   P1-  O6-  C9-  H10
 11   16   17   29    3   1.60387   4.81160   0.00000  -6.41547   0.00000   0.00000 ;   P1-  O6-  C9-  H11
 12   11   16   17    3   1.04600   3.13800  10.04160  -4.18400   0.00000   0.00000 ;   O4-  P1-  O6-  C9
 12   14   15   25    3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;   O4-  C7-  C8-  H7
 12   14   15   26    3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;   O4-  C7-  C8-  H8
 12   14   15   27    3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;   O4-  C7-  C8-  H9
 13   11   12   14    3   2.30120   6.90360   6.69440  -9.20480   0.00000   0.00000 ;   O5-  P1-  O4-  C7
 13   11   16   17    3   2.30120   6.90360   6.69440  -9.20480   0.00000   0.00000 ;   O5-  P1-  O6-  C9
 14   12   11   16    3   1.04600   3.13800  10.04160  -4.18400   0.00000   0.00000 ;   C7-  O4-  P1-  O6
 16   17   18   30    3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;   O6-  C9-  C10-  H12
 16   17   18   31    3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;   O6-  C9-  C10-  H13
 16   17   18   32    3   1.04600  -1.04600   0.00000   0.00000   0.00000   0.00000 ;   O6-  C9-  C10-  H14
 19    1    2    3    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   H1-  C1-  C2-  C3
 19    1    2    7    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   H1-  C1-  C2-  N1
 19    1    6    5    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   H1-  C1-  C6-  C5
 19    1    6   22    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   H1-  C1-  C6-  H4
 20    3    4   21    3  30.33400   0.00000 -30.33400   0.00000   0.00000   0.00000 ;   H2-  C3-  C4-  H3
 23   14   15   25    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H5-  C7-  C8-  H7
 23   14   15   26    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H5-  C7-  C8-  H8
 23   14   15   27    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H5-  C7-  C8-  H9
 24   14   15   25    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H6-  C7-  C8-  H7
 24   14   15   26    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H6-  C7-  C8-  H8
 24   14   15   27    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H6-  C7-  C8-  H9
 28   17   18   30    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H10-  C9-  C10-  H12
 28   17   18   31    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H10-  C9-  C10-  H13
 28   17   18   32    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H10-  C9-  C10-  H14
 29   17   18   30    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H11-  C9-  C10-  H12
 29   17   18   31    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H11-  C9-  C10-  H13
 29   17   18   32    3   0.65084   1.95253   0.00000  -2.60338   0.00000   0.00000 ;   H11-  C9-  C10-  H14

[ dihedrals ] ; impropers
; treated as propers in GROMACS to use correct AMBER analytical function
;   i    j    k    l  func   phase     kd      pn
    1    3    2    7     1  180.00   4.60240   2 ;    C1-   C3-   C2-   N1
    1    5    6   22     1  180.00   4.60240   2 ;    C1-   C5-   C6-   H4
    2    4    3   20     1  180.00   4.60240   2 ;    C2-   C4-   C3-   H2
    3    5    4   21     1  180.00   4.60240   2 ;    C3-   C5-   C4-   H3
    4    6    5   10     1  180.00   4.60240   2 ;    C4-   C6-   C5-   O3
   19    1    6    2     1  180.00   4.60240   2 ;    H1-   C1-   C6-   C2
```

Table S2: Structures of GpdQ-NPP, GpdQ-BNPP, GpdQ-GPE, and GpdQ-paraoxon.

GpdQ-NPP Structure

```
ATOM      1  N   ASP A   8      4.249   0.858   2.848  1.00  0.00           N
ATOM      2  H   ASP A   8      3.447   1.399   2.542  1.00  0.00           H
ATOM      3  CA  ASP A   8      4.507   0.815   4.277  1.00  0.00           C
ATOM      4  HA  ASP A   8      3.892   1.600   4.727  1.00  0.00           H
ATOM      5  CB  ASP A   8      4.013  -0.509   4.844  1.00  0.00           C
ATOM      6 1HB  ASP A   8      4.313  -1.382   4.257  1.00  0.00           H
ATOM      7 2HB  ASP A   8      4.401  -0.552   5.856  1.00  0.00           H
ATOM      8  CG  ASP A   8      2.495  -0.447   4.995  1.00  0.00           C
ATOM      9  OD1 ASP A   8      1.770  -1.128   4.239  1.00  0.00           O
ATOM     10  OD2 ASP A   8      2.133   0.178   6.011  1.00  0.00           O
ATOM     11  C   ASP A   8      5.962   1.135   4.554  1.00  0.00           C
ATOM     12  O   ASP A   8      6.619   0.384   5.265  1.00  0.00           O
ATOM     13  N   HIS A  10      6.719   3.749   6.626  1.00  0.00           N
ATOM     14  H   HIS A  10      5.878   3.931   6.107  1.00  0.00           H
ATOM     15  CA  HIS A  10      6.614   4.296   7.969  1.00  0.00           C
ATOM     16  HA  HIS A  10      5.827   5.044   7.926  1.00  0.00           H
ATOM     17  CB  HIS A  10      6.149   3.159   8.867  1.00  0.00           C
ATOM     18 1HB  HIS A  10      6.859   2.342   8.723  1.00  0.00           H
ATOM     19 2HB  HIS A  10      6.455   3.504   9.858  1.00  0.00           H
ATOM     20  CG  HIS A  10      4.732   2.676   8.877  1.00  0.00           C
ATOM     21  ND1 HIS A  10      3.744   2.973   9.797  1.00  0.00           N
ATOM     22  HD1 HIS A  10      3.835   3.534  10.632  1.00  0.00           H
ATOM     23  CE1 HIS A  10      2.632   2.346   9.371  1.00  0.00           C
ATOM     24  HE1 HIS A  10      1.748   2.370   9.993  1.00  0.00           H
ATOM     25  NE2 HIS A  10      2.817   1.566   8.300  1.00  0.00           N
ATOM     26  CD2 HIS A  10      4.145   1.821   7.962  1.00  0.00           C
ATOM     27  HD2 HIS A  10      4.625   1.479   7.054  1.00  0.00           H
ATOM     28  C   HIS A  10      7.907   4.949   8.438  1.00  0.00           C
ATOM     29  O   HIS A  10      8.603   4.596   9.392  1.00  0.00           O
ATOM     30  N   ASP A  50      1.007   5.100   4.416  1.00  0.00           N
ATOM     31  H   ASP A  50      0.645   5.994   4.115  1.00  0.00           H
ATOM     32  CA  ASP A  50      1.862   5.370   5.552  1.00  0.00           C
ATOM     33  HA  ASP A  50      1.435   6.261   6.014  1.00  0.00           H
ATOM     34  CB  ASP A  50      1.745   4.290   6.634  1.00  0.00           C
ATOM     35 1HB  ASP A  50      1.864   3.309   6.175  1.00  0.00           H
ATOM     36 2HB  ASP A  50      2.545   4.433   7.350  1.00  0.00           H
ATOM     37  CG  ASP A  50      0.491   4.310   7.484  1.00  0.00           C
ATOM     38  OD1 ASP A  50      0.208   5.435   7.952  1.00  0.00           O
ATOM     39  OD2 ASP A  50     -0.127   3.248   7.699  1.00  0.00           O
ATOM     40  C   ASP A  50      3.274   5.639   5.069  1.00  0.00           C
ATOM     41  O   ASP A  50      4.148   4.783   5.227  1.00  0.00           O
ATOM     42  N   ASN A  53      5.664   7.894   9.753  1.00  0.00           N
ATOM     43  H   ASN A  53      6.557   8.362   9.657  1.00  0.00           H
ATOM     44  CA  ASN A  53      5.148   7.152  10.888  1.00  0.00           C
ATOM     45  HA  ASN A  53      4.559   6.298  10.564  1.00  0.00           H
ATOM     46  CB  ASN A  53      6.294   6.406  11.556  1.00  0.00           C
ATOM     47 1HB  ASN A  53      6.934   5.956  10.799  1.00  0.00           H
ATOM     48 2HB  ASN A  53      6.840   7.134  12.161  1.00  0.00           H
ATOM     49  CG  ASN A  53      5.800   5.337  12.516  1.00  0.00           C
ATOM     50  OD1 ASN A  53      5.264   4.295  12.137  1.00  0.00           O
ATOM     51  ND2 ASN A  53      5.972   5.603  13.813  1.00  0.00           N
ATOM     52 1HD2 ASN A  53      5.612   4.932  14.472  1.00  0.00           H
ATOM     53 2HD2 ASN A  53      6.538   6.407  14.018  1.00  0.00           H
ATOM     54  C   ASN A  53      4.202   7.819  11.872  1.00  0.00           C
ATOM     55  O   ASN A  53      3.317   7.223  12.496  1.00  0.00           O
ATOM     56  N   ASN A  80     -2.759   5.928   7.136  1.00  0.00           N
ATOM     57  H   ASN A  80     -2.339   5.020   7.174  1.00  0.00           H
ATOM     58  CA  ASN A  80     -3.518   6.309   8.317  1.00  0.00           C
ATOM     59  HA  ASN A  80     -4.464   6.813   8.118  1.00  0.00           H
ATOM     60  CB  ASN A  80     -3.923   5.084   9.131  1.00  0.00           C
ATOM     61 1HB  ASN A  80     -4.247   5.390  10.131  1.00  0.00           H
ATOM     62 2HB  ASN A  80     -4.810   4.613   8.706  1.00  0.00           H
ATOM     63  CG  ASN A  80     -2.843   4.014   9.257  1.00  0.00           C
ATOM     64  OD1 ASN A  80     -2.632   3.111   8.454  1.00  0.00           O
ATOM     65  ND2 ASN A  80     -2.034   4.073  10.321  1.00  0.00           N
ATOM     66 1HD2 ASN A  80     -1.342   3.360  10.520  1.00  0.00           H
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ATOM     67 2HD2 ASN A  80      -2.236   4.797  10.991  1.00  0.00           H
ATOM     68  C   ASN A  80      -2.941   7.414   9.186  1.00  0.00           C
ATOM     69  O   ASN A  80      -3.670   8.214   9.761  1.00  0.00           O
ATOM     70  N   HIS A  81      -1.613   7.461   9.345  1.00  0.00           N
ATOM     71  H   HIS A  81      -1.046   6.826   8.820  1.00  0.00           H
ATOM     72  CA  HIS A  81      -0.894   8.432  10.145  1.00  0.00           C
ATOM     73  HA  HIS A  81      -1.629   9.022  10.688  1.00  0.00           H
ATOM     74  CB  HIS A  81       0.033   7.814  11.175  1.00  0.00           C
ATOM     75 1HB  HIS A  81       0.864   7.347  10.640  1.00  0.00           H
ATOM     76 2HB  HIS A  81       0.458   8.609  11.797  1.00  0.00           H
ATOM     77  CG  HIS A  81      -0.637   6.752  12.003  1.00  0.00           C
ATOM     78  ND1 HIS A  81       0.014   5.672  12.580  1.00  0.00           N
ATOM     79  HD1 HIS A  81       0.929   5.272  12.402  1.00  0.00           H
ATOM     80  CE1 HIS A  81      -0.851   5.044  13.383  1.00  0.00           C
ATOM     81  HE1 HIS A  81      -0.633   4.339  14.164  1.00  0.00           H
ATOM     82  NE2 HIS A  81      -2.076   5.560  13.236  1.00  0.00           N
ATOM     83  CD2 HIS A  81      -1.958   6.657  12.384  1.00  0.00           C
ATOM     84  HD2 HIS A  81      -2.805   7.313  12.272  1.00  0.00           H
ATOM     85  C   HIS A  81      -0.173   9.516   9.355  1.00  0.00           C
ATOM     86  O   HIS A  81       0.025  10.553   9.990  1.00  0.00           O
ATOM     87  N   HIS A 156      -5.124   2.377   0.842  1.00  0.00           N
ATOM     88  H   HIS A 156      -5.900   3.022   0.946  1.00  0.00           H
ATOM     89  CA  HIS A 156      -4.455   1.999   2.077  1.00  0.00           C
ATOM     90  HA  HIS A 156      -3.562   1.470   1.748  1.00  0.00           H
ATOM     91  CB  HIS A 156      -4.184   3.133   3.060  1.00  0.00           C
ATOM     92 1HB  HIS A 156      -3.917   4.010   2.479  1.00  0.00           H
ATOM     93 2HB  HIS A 156      -5.048   3.228   3.713  1.00  0.00           H
ATOM     94  CG  HIS A 156      -3.078   2.862   4.047  1.00  0.00           C
ATOM     95  ND1 HIS A 156      -1.765   2.616   3.682  1.00  0.00           N
ATOM     96  HD1 HIS A 156      -1.471   2.679   2.718  1.00  0.00           H
ATOM     97  CE1 HIS A 156      -1.121   2.249   4.808  1.00  0.00           C
ATOM     98  HE1 HIS A 156      -0.060   2.030   4.866  1.00  0.00           H
ATOM     99  NE2 HIS A 156      -1.953   2.189   5.848  1.00  0.00           N
ATOM    100  CD2 HIS A 156      -3.199   2.638   5.401  1.00  0.00           C
ATOM    101  HD2 HIS A 156      -4.121   2.803   5.927  1.00  0.00           H
ATOM    102  C   HIS A 156      -5.274   0.855   2.661  1.00  0.00           C
ATOM    103  O   HIS A 156      -4.923  -0.316   2.759  1.00  0.00           O
ATOM    104  N   GLN A 166      -5.012 -11.664  13.677  1.00  0.00           N
ATOM    105  H   GLN A 166      -4.521 -12.291  13.056  1.00  0.00           H
ATOM    106  CA  GLN A 166      -4.334 -10.490  14.182  1.00  0.00           C
ATOM    107  HA  GLN A 166      -4.669 -10.425  15.219  1.00  0.00           H
ATOM    108  CB  GLN A 166      -2.834 -10.765  14.158  1.00  0.00           C
ATOM    109 1HB  GLN A 166      -2.648 -11.620  14.809  1.00  0.00           H
ATOM    110 2HB  GLN A 166      -2.449 -11.080  13.185  1.00  0.00           H
ATOM    111  CG  GLN A 166      -2.088  -9.529  14.660  1.00  0.00           C
ATOM    112 1HG  GLN A 166      -2.195  -8.702  13.965  1.00  0.00           H
ATOM    113 2HG  GLN A 166      -2.336  -9.111  15.629  1.00  0.00           H
ATOM    114  CD  GLN A 166      -0.579  -9.734  14.658  1.00  0.00           C
ATOM    115  OE1 GLN A 166      -0.152 -10.892  14.683  1.00  0.00           O
ATOM    116  NE2 GLN A 166       0.284  -8.726  14.510  1.00  0.00           N
ATOM    117 1HE2 GLN A 166       1.252  -9.016  14.462  1.00  0.00           H
ATOM    118 2HE2 GLN A 166       0.052  -7.751  14.464  1.00  0.00           H
ATOM    119  C   GLN A 166      -4.656  -9.160  13.523  1.00  0.00           C
ATOM    120  O   GLN A 166      -4.575  -8.137  14.214  1.00  0.00           O
ATOM    121  N   MET A 167      -4.935  -9.199  12.224  1.00  0.00           N
ATOM    122  H   MET A 167      -4.826 -10.110  11.807  1.00  0.00           H
ATOM    123  CA  MET A 167      -5.132  -8.101  11.287  1.00  0.00           C
ATOM    124  HA  MET A 167      -4.882  -7.211  11.868  1.00  0.00           H
ATOM    125  CB  MET A 167      -4.208  -8.036  10.083  1.00  0.00           C
ATOM    126 1HB  MET A 167      -4.500  -8.774   9.336  1.00  0.00           H
ATOM    127 2HB  MET A 167      -4.258  -7.021   9.678  1.00  0.00           H
ATOM    128  CG  MET A 167      -2.768  -8.269  10.524  1.00  0.00           C
ATOM    129 1HG  MET A 167      -2.628  -9.262  10.945  1.00  0.00           H
ATOM    130 2HG  MET A 167      -2.177  -8.348   9.604  1.00  0.00           H
ATOM    131  SD  MET A 167      -1.815  -7.125  11.546  1.00  0.00           S
ATOM    132  CE  MET A 167      -1.966  -5.594  10.592  1.00  0.00           C
ATOM    133 1HE  MET A 167      -1.856  -5.866   9.542  1.00  0.00           H
ATOM    134 2HE  MET A 167      -2.897  -5.044  10.752  1.00  0.00           H
ATOM    135 3HE  MET A 167      -1.151  -4.934  10.893  1.00  0.00           H
ATOM    136  C   MET A 167      -6.597  -7.969  10.886  1.00  0.00           C
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ATOM    137  O   MET A 167      -6.890  -7.651   9.733  1.00  0.00           O
ATOM    138  N   HIS A 195      -1.570  -1.621   4.458  1.00  0.00           N
ATOM    139  H   HIS A 195      -0.780  -0.987   4.420  1.00  0.00           H
ATOM    140  CA  HIS A 195      -2.240  -1.670   5.740  1.00  0.00           C
ATOM    141  HA  HIS A 195      -1.594  -1.130   6.428  1.00  0.00           H
ATOM    142  CB  HIS A 195      -3.635  -1.050   5.663  1.00  0.00           C
ATOM    143 1HB  HIS A 195      -3.643  -0.200   4.974  1.00  0.00           H
ATOM    144 2HB  HIS A 195      -4.358  -1.788   5.337  1.00  0.00           H
ATOM    145  CG  HIS A 195      -4.000  -0.501   7.019  1.00  0.00           C
ATOM    146  ND1 HIS A 195      -3.200   0.363   7.774  1.00  0.00           N
ATOM    147  CE1 HIS A 195      -3.838   0.397   8.945  1.00  0.00           C
ATOM    148  HE1 HIS A 195      -3.510   1.045   9.750  1.00  0.00           H
ATOM    149  NE2 HIS A 195      -4.934  -0.377   8.986  1.00  0.00           N
ATOM    150  HE2 HIS A 195      -5.653  -0.369   9.691  1.00  0.00           H
ATOM    151  CD2 HIS A 195      -5.129  -0.845   7.708  1.00  0.00           C
ATOM    152  HD2 HIS A 195      -5.987  -1.426   7.400  1.00  0.00           H
ATOM    153  C   HIS A 195      -2.307  -3.023   6.436  1.00  0.00           C
ATOM    154  O   HIS A 195      -2.462  -2.965   7.656  1.00  0.00           O
ATOM    155  N   HIS A 197       0.341  -5.204   6.374  1.00  0.00           N
ATOM    156  H   HIS A 197       0.158  -4.450   5.732  1.00  0.00           H
ATOM    157  CA  HIS A 197       1.710  -5.674   6.425  1.00  0.00           C
ATOM    158  HA  HIS A 197       2.280  -5.175   5.644  1.00  0.00           H
ATOM    159  CB  HIS A 197       2.222  -5.268   7.798  1.00  0.00           C
ATOM    160 1HB  HIS A 197       1.536  -5.531   8.607  1.00  0.00           H
ATOM    161 2HB  HIS A 197       3.140  -5.814   8.018  1.00  0.00           H
ATOM    162  CG  HIS A 197       2.457  -3.793   8.007  1.00  0.00           C
ATOM    163  ND1 HIS A 197       3.717  -3.299   8.295  1.00  0.00           N
ATOM    164  HD1 HIS A 197       4.534  -3.868   8.479  1.00  0.00           H
ATOM    165  CE1 HIS A 197       3.683  -1.959   8.244  1.00  0.00           C
ATOM    166  HE1 HIS A 197       4.516  -1.327   8.484  1.00  0.00           H
ATOM    167  NE2 HIS A 197       2.437  -1.552   7.977  1.00  0.00           N
ATOM    168  CD2 HIS A 197       1.636  -2.695   7.879  1.00  0.00           C
ATOM    169  HD2 HIS A 197       0.574  -2.644   7.689  1.00  0.00           H
ATOM    170  C   HIS A 197       1.919  -7.143   6.075  1.00  0.00           C
ATOM    171  O   HIS A 197       2.844  -7.754   6.615  1.00  0.00           O
ATOM    172  N   HIS A 217       8.224  -3.489   7.952  1.00  0.00           N
ATOM    173  H   HIS A 217       7.400  -3.236   7.423  1.00  0.00           H
ATOM    174  CA  HIS A 217       8.249  -4.827   8.484  1.00  0.00           C
ATOM    175  HA  HIS A 217       9.132  -5.376   8.155  1.00  0.00           H
ATOM    176  CB  HIS A 217       8.320  -4.817  10.013  1.00  0.00           C
ATOM    177 1HB  HIS A 217       8.615  -5.823  10.326  1.00  0.00           H
ATOM    178 2HB  HIS A 217       9.087  -4.149  10.386  1.00  0.00           H
ATOM    179  CG  HIS A 217       7.064  -4.526  10.776  1.00  0.00           C
ATOM    180  ND1 HIS A 217       6.193  -5.499  11.234  1.00  0.00           N
ATOM    181  HD1 HIS A 217       6.076  -6.438  10.897  1.00  0.00           H
ATOM    182  CE1 HIS A 217       5.277  -4.867  11.986  1.00  0.00           C
ATOM    183  HE1 HIS A 217       4.322  -5.300  12.275  1.00  0.00           H
ATOM    184  NE2 HIS A 217       5.533  -3.570  12.101  1.00  0.00           N
ATOM    185  CD2 HIS A 217       6.662  -3.325  11.321  1.00  0.00           C
ATOM    186  HD2 HIS A 217       7.041  -2.350  11.076  1.00  0.00           H
ATOM    187  C   HIS A 217       6.988  -5.559   8.023  1.00  0.00           C
ATOM    188  O   HIS A 217       5.987  -4.885   7.818  1.00  0.00           O
HETATM  190  ZN  ZN A1001       1.569   0.256   7.751  1.00  0.00           N
HETATM  191  ZN  ZN A1002      -1.180   1.784   7.779  1.00  0.00           N
HETATM  193  P1  MOL B1003      -0.309   0.389  10.533  1.00  0.00           P
HETATM  194  O1  MOL B1003      -1.023   1.332   9.587  1.00  0.00           O
HETATM  195  O2  MOL B1003       0.301   0.990  11.784  1.00  0.00           O
HETATM  196  O3  MOL B1003       0.695  -0.187   9.558  1.00  0.00           O
HETATM  197  O4  MOL B1003      -1.224  -0.808  11.191  1.00  0.00           O
HETATM  198  C1  MOL B1003      -0.793  -1.756  11.859  1.00  0.00           C
HETATM  199  C2  MOL B1003       0.386  -2.446  11.555  1.00  0.00           C
HETATM  200  C3  MOL B1003      -1.540  -2.174  12.969  1.00  0.00           C
HETATM  201  C4  MOL B1003       0.812  -3.604  12.210  1.00  0.00           C
HETATM  202  H1  MOL B1003       0.979  -2.176  10.690  1.00  0.00           H
HETATM  203  C5  MOL B1003      -1.052  -3.231  13.734  1.00  0.00           C
HETATM  204  H2  MOL B1003      -2.410  -1.656  13.357  1.00  0.00           H
HETATM  205  C6  MOL B1003       0.003  -4.024  13.274  1.00  0.00           C
HETATM  206  H3  MOL B1003       1.605  -4.235  11.825  1.00  0.00           H
HETATM  207  H4  MOL B1003      -1.542  -3.480  14.674  1.00  0.00           H
HETATM  208  N1  MOL B1003       0.437  -5.143  14.120  1.00  0.00           N
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HETATM  209  O5  MOL B1003      -0.431  -5.886  14.561  1.00  0.00           O
HETATM  210  O6  MOL B1003       1.591  -5.579  14.110  1.00  0.00           O
HETATM  212  O1  MOL  1004       0.011   0.716   7.279  1.00  0.00           O
HETATM  213  H1  MOL  1004      -0.262   0.431   6.376  1.00  0.00           H
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GpdQ-BNPP Structure

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ATOM      1  N   ASP A   8      4.082   0.372   2.757  1.00  0.00           N
ATOM      2  H   ASP A   8      3.298   0.831   2.329  1.00  0.00           H
ATOM      3  CA  ASP A   8      4.299   0.558   4.178  1.00  0.00           C
ATOM      4  HA  ASP A   8      3.809   1.464   4.535  1.00  0.00           H
ATOM      5  CB  ASP A   8      3.613  -0.635   4.842  1.00  0.00           C
ATOM      6 1HB  ASP A   8      3.607  -1.511   4.206  1.00  0.00           H
ATOM      7 2HB  ASP A   8      4.185  -0.948   5.713  1.00  0.00           H
ATOM      8  CG  ASP A   8      2.176  -0.333   5.239  1.00  0.00           C
ATOM      9  OD1 ASP A   8      1.251  -0.652   4.463  1.00  0.00           O
ATOM     10  OD2 ASP A   8      2.061   0.214   6.364  1.00  0.00           O
ATOM     11  C   ASP A   8      5.761   0.843   4.485  1.00  0.00           C
ATOM     12  O   ASP A   8      6.505  -0.016   4.943  1.00  0.00           O
ATOM     13  N   HIS A  10      6.373   3.740   6.385  1.00  0.00           N
ATOM     14  H   HIS A  10      5.562   3.783   5.785  1.00  0.00           H
ATOM     15  CA  HIS A  10      6.289   4.382   7.680  1.00  0.00           C
ATOM     16  HA  HIS A  10      5.543   5.179   7.608  1.00  0.00           H
ATOM     17  CB  HIS A  10      5.944   3.284   8.676  1.00  0.00           C
ATOM     18 1HB  HIS A  10      6.617   2.474   8.419  1.00  0.00           H
ATOM     19 2HB  HIS A  10      6.252   3.747   9.615  1.00  0.00           H
ATOM     20  CG  HIS A  10      4.542   2.754   8.816  1.00  0.00           C
ATOM     21  ND1 HIS A  10      3.845   2.643  10.007  1.00  0.00           N
ATOM     22  HD1 HIS A  10      4.242   2.866  10.909  1.00  0.00           H
ATOM     23  CE1 HIS A  10      2.665   2.030   9.785  1.00  0.00           C
ATOM     24  HE1 HIS A  10      1.851   2.077  10.498  1.00  0.00           H
ATOM     25  NE2 HIS A  10      2.635   1.597   8.529  1.00  0.00           N
ATOM     26  CD2 HIS A  10      3.831   1.988   7.933  1.00  0.00           C
ATOM     27  HD2 HIS A  10      4.246   1.782   6.955  1.00  0.00           H
ATOM     28  C   HIS A  10      7.559   5.153   8.037  1.00  0.00           C
ATOM     29  O   HIS A  10      8.238   4.856   9.014  1.00  0.00           O
ATOM     30  N   TYR A  19      8.442  -0.287  18.612  1.00  0.00           N
ATOM     31  H   TYR A  19      7.720   0.279  18.201  1.00  0.00           H
ATOM     32  CA  TYR A  19      8.245  -0.911  19.900  1.00  0.00           C
ATOM     33  HA  TYR A  19      7.222  -0.714  20.207  1.00  0.00           H
ATOM     34  CB  TYR A  19      8.303  -2.423  19.785  1.00  0.00           C
ATOM     35 1HB  TYR A  19      9.350  -2.679  19.588  1.00  0.00           H
ATOM     36 2HB  TYR A  19      7.987  -2.872  20.726  1.00  0.00           H
ATOM     37  CG  TYR A  19      7.408  -3.084  18.758  1.00  0.00           C
ATOM     38  CD1 TYR A  19      7.867  -4.310  18.269  1.00  0.00           C
ATOM     39  HD1 TYR A  19      8.750  -4.787  18.665  1.00  0.00           H
ATOM     40  CE1 TYR A  19      7.122  -4.838  17.205  1.00  0.00           C
ATOM     41  HE1 TYR A  19      7.483  -5.721  16.699  1.00  0.00           H
ATOM     42  CZ  TYR A  19      5.888  -4.304  16.785  1.00  0.00           C
ATOM     43  OH  TYR A  19      5.230  -4.933  15.777  1.00  0.00           O
ATOM     44  HH  TYR A  19      4.684  -4.250  15.377  1.00  0.00           H
ATOM     45  CE2 TYR A  19      5.482  -3.043  17.274  1.00  0.00           C
ATOM     46  HE2 TYR A  19      4.493  -2.659  17.027  1.00  0.00           H
ATOM     47  CD2 TYR A  19      6.218  -2.497  18.323  1.00  0.00           C
ATOM     48  HD2 TYR A  19      5.904  -1.536  18.705  1.00  0.00           H
ATOM     49  C   TYR A  19      9.135  -0.487  21.071  1.00  0.00           C
ATOM     50  O   TYR A  19      9.061  -1.047  22.166  1.00  0.00           O
ATOM     51  N   ASP A  50      0.702   4.986   4.331  1.00  0.00           N
ATOM     52  H   ASP A  50     -0.082   5.625   4.288  1.00  0.00           H
ATOM     53  CA  ASP A  50      1.677   5.179   5.380  1.00  0.00           C
ATOM     54  HA  ASP A  50      1.437   6.130   5.869  1.00  0.00           H
ATOM     55  CB  ASP A  50      1.621   4.160   6.506  1.00  0.00           C
ATOM     56 1HB  ASP A  50      1.767   3.131   6.165  1.00  0.00           H
ATOM     57 2HB  ASP A  50      2.504   4.367   7.104  1.00  0.00           H
ATOM     58  CG  ASP A  50      0.319   4.230   7.306  1.00  0.00           C
ATOM     59  OD1 ASP A  50     -0.317   5.304   7.304  1.00  0.00           O
ATOM     60  OD2 ASP A  50      0.002   3.156   7.866  1.00  0.00           O
ATOM     61  C   ASP A  50      3.069   5.431   4.813  1.00  0.00           C
ATOM     62  O   ASP A  50      3.992   4.632   4.975  1.00  0.00           O
ATOM     63  N   ASN A  53      5.077   7.772   9.731  1.00  0.00           N
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ATOM     64  H   ASN A  53       5.689   8.548   9.934  1.00  0.00           H
ATOM     65  CA  ASN A  53       4.766   6.957  10.887  1.00  0.00           C
ATOM     66  HA  ASN A  53       4.145   6.121  10.531  1.00  0.00           H
ATOM     67  CB  ASN A  53       6.112   6.556  11.472  1.00  0.00           C
ATOM     68 1HB  ASN A  53       6.453   5.640  10.990  1.00  0.00           H
ATOM     69 2HB  ASN A  53       6.862   7.291  11.187  1.00  0.00           H
ATOM     70  CG  ASN A  53       6.252   6.314  12.975  1.00  0.00           C
ATOM     71  OD1 ASN A  53       5.753   5.268  13.398  1.00  0.00           O
ATOM     72  ND2 ASN A  53       6.807   7.232  13.770  1.00  0.00           N
ATOM     73 1HD2 ASN A  53       6.953   7.127  14.767  1.00  0.00           H
ATOM     74 2HD2 ASN A  53       7.021   8.152  13.414  1.00  0.00           H
ATOM     75  C   ASN A  53       3.924   7.576  11.989  1.00  0.00           C
ATOM     76  O   ASN A  53       3.247   6.910  12.777  1.00  0.00           O
ATOM     77  N   ASN A  80      -3.037   5.982   7.100  1.00  0.00           N
ATOM     78  H   ASN A  80      -2.575   5.094   6.952  1.00  0.00           H
ATOM     79  CA  ASN A  80      -3.631   6.470   8.331  1.00  0.00           C
ATOM     80  HA  ASN A  80      -4.562   6.975   8.108  1.00  0.00           H
ATOM     81  CB  ASN A  80      -3.998   5.153   8.999  1.00  0.00           C
ATOM     82 1HB  ASN A  80      -4.494   5.280   9.961  1.00  0.00           H
ATOM     83 2HB  ASN A  80      -4.674   4.598   8.344  1.00  0.00           H
ATOM     84  CG  ASN A  80      -2.847   4.199   9.292  1.00  0.00           C
ATOM     85  OD1 ASN A  80      -2.641   3.249   8.548  1.00  0.00           O
ATOM     86  ND2 ASN A  80      -2.151   4.301  10.432  1.00  0.00           N
ATOM     87 1HD2 ASN A  80      -1.265   3.828  10.506  1.00  0.00           H
ATOM     88 2HD2 ASN A  80      -2.350   4.976  11.154  1.00  0.00           H
ATOM     89  C   ASN A  80      -2.791   7.377   9.223  1.00  0.00           C
ATOM     90  O   ASN A  80      -3.317   8.209   9.964  1.00  0.00           O
ATOM     91  N   HIS A  81      -1.468   7.293   9.092  1.00  0.00           N
ATOM     92  H   HIS A  81      -1.104   6.589   8.474  1.00  0.00           H
ATOM     93  CA  HIS A  81      -0.522   8.172   9.748  1.00  0.00           C
ATOM     94  HA  HIS A  81      -0.886   8.416  10.736  1.00  0.00           H
ATOM     95  CB  HIS A  81       0.798   7.420   9.950  1.00  0.00           C
ATOM     96 1HB  HIS A  81       1.079   7.051   8.966  1.00  0.00           H
ATOM     97 2HB  HIS A  81       1.547   8.117  10.305  1.00  0.00           H
ATOM     98  CG  HIS A  81       0.704   6.319  10.964  1.00  0.00           C
ATOM     99  ND1 HIS A  81       0.314   6.400  12.295  1.00  0.00           N
ATOM    100  HD1 HIS A  81       0.166   7.256  12.798  1.00  0.00           H
ATOM    101  CE1 HIS A  81       0.331   5.143  12.749  1.00  0.00           C
ATOM    102  HE1 HIS A  81      -0.006   4.895  13.746  1.00  0.00           H
ATOM    103  NE2 HIS A  81       0.597   4.229  11.821  1.00  0.00           N
ATOM    104  CD2 HIS A  81       0.934   4.989  10.701  1.00  0.00           C
ATOM    105  HD2 HIS A  81       1.192   4.466   9.790  1.00  0.00           H
ATOM    106  C   HIS A  81      -0.275   9.457   8.975  1.00  0.00           C
ATOM    107  O   HIS A  81       0.074  10.468   9.583  1.00  0.00           O
ATOM    108  N   HIS A 156      -4.729   2.838   0.585  1.00  0.00           N
ATOM    109  H   HIS A 156      -5.126   3.773   0.557  1.00  0.00           H
ATOM    110  CA  HIS A 156      -4.302   2.297   1.856  1.00  0.00           C
ATOM    111  HA  HIS A 156      -3.365   1.814   1.588  1.00  0.00           H
ATOM    112  CB  HIS A 156      -3.940   3.343   2.914  1.00  0.00           C
ATOM    113 1HB  HIS A 156      -3.558   4.245   2.433  1.00  0.00           H
ATOM    114 2HB  HIS A 156      -4.826   3.708   3.433  1.00  0.00           H
ATOM    115  CG  HIS A 156      -2.886   2.823   3.852  1.00  0.00           C
ATOM    116  ND1 HIS A 156      -1.527   2.652   3.643  1.00  0.00           N
ATOM    117  HD1 HIS A 156      -1.012   2.840   2.800  1.00  0.00           H
ATOM    118  CE1 HIS A 156      -0.957   2.385   4.834  1.00  0.00           C
ATOM    119  HE1 HIS A 156       0.096   2.184   4.988  1.00  0.00           H
ATOM    120  NE2 HIS A 156      -1.852   2.370   5.819  1.00  0.00           N
ATOM    121  CD2 HIS A 156      -3.075   2.595   5.199  1.00  0.00           C
ATOM    122  HD2 HIS A 156      -4.058   2.709   5.634  1.00  0.00           H
ATOM    123  C   HIS A 156      -5.176   1.206   2.459  1.00  0.00           C
ATOM    124  O   HIS A 156      -4.678   0.115   2.734  1.00  0.00           O
ATOM    125  N   GLN A 166      -5.068 -11.347  12.895  1.00  0.00           N
ATOM    126  H   GLN A 166      -4.470 -11.913  12.314  1.00  0.00           H
ATOM    127  CA  GLN A 166      -4.504 -10.203  13.589  1.00  0.00           C
ATOM    128  HA  GLN A 166      -4.889 -10.080  14.601  1.00  0.00           H
ATOM    129  CB  GLN A 166      -2.993 -10.323  13.557  1.00  0.00           C
ATOM    130 1HB  GLN A 166      -2.733 -11.323  13.900  1.00  0.00           H
ATOM    131 2HB  GLN A 166      -2.687 -10.362  12.505  1.00  0.00           H
ATOM    132  CG  GLN A 166      -2.161  -9.328  14.357  1.00  0.00           C
ATOM    133 1HG  GLN A 166      -2.367  -8.402  13.832  1.00  0.00           H
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ATOM    134 2HG  GLN A 166      -2.528  -9.398  15.382  1.00  0.00           H
ATOM    135  CD  GLN A 166      -0.666  -9.520  14.121  1.00  0.00           C
ATOM    136  OE1 GLN A 166      -0.171 -10.645  14.040  1.00  0.00           O
ATOM    137  NE2 GLN A 166       0.130  -8.442  14.058  1.00  0.00           N
ATOM    138 1HE2 GLN A 166       1.058  -8.715  13.784  1.00  0.00           H
ATOM    139 2HE2 GLN A 166      -0.085  -7.460  14.016  1.00  0.00           H
ATOM    140  C   GLN A 166      -4.927  -8.919  12.890  1.00  0.00           C
ATOM    141  O   GLN A 166      -5.216  -7.969  13.611  1.00  0.00           O
ATOM    142  N   MET A 167      -4.766  -8.870  11.569  1.00  0.00           N
ATOM    143  H   MET A 167      -4.433  -9.711  11.132  1.00  0.00           H
ATOM    144  CA  MET A 167      -4.965  -7.639  10.812  1.00  0.00           C
ATOM    145  HA  MET A 167      -4.845  -6.821  11.521  1.00  0.00           H
ATOM    146  CB  MET A 167      -3.866  -7.639   9.759  1.00  0.00           C
ATOM    147 1HB  MET A 167      -4.047  -8.549   9.186  1.00  0.00           H
ATOM    148 2HB  MET A 167      -4.033  -6.825   9.047  1.00  0.00           H
ATOM    149  CG  MET A 167      -2.464  -7.608  10.381  1.00  0.00           C
ATOM    150 1HG  MET A 167      -2.305  -8.488  11.003  1.00  0.00           H
ATOM    151 2HG  MET A 167      -1.705  -7.619   9.599  1.00  0.00           H
ATOM    152  SD  MET A 167      -2.166  -6.180  11.449  1.00  0.00           S
ATOM    153  CE  MET A 167      -1.892  -4.996  10.112  1.00  0.00           C
ATOM    154 1HE  MET A 167      -1.854  -4.009  10.585  1.00  0.00           H
ATOM    155 2HE  MET A 167      -0.944  -5.155   9.599  1.00  0.00           H
ATOM    156 3HE  MET A 167      -2.719  -5.002   9.407  1.00  0.00           H
ATOM    157  C   MET A 167      -6.347  -7.428  10.212  1.00  0.00           C
ATOM    158  O   MET A 167      -6.591  -6.310   9.774  1.00  0.00           O
ATOM    159  N   ILE A 170      -9.040  -3.989  10.783  1.00  0.00           N
ATOM    160  H   ILE A 170      -8.313  -4.684  10.830  1.00  0.00           H
ATOM    161  CA  ILE A 170      -8.719  -2.618  10.428  1.00  0.00           C
ATOM    162  HA  ILE A 170      -9.369  -1.848  10.842  1.00  0.00           H
ATOM    163  CB  ILE A 170      -7.312  -2.272  10.930  1.00  0.00           C
ATOM    164  HB  ILE A 170      -7.088  -1.232  10.704  1.00  0.00           H
ATOM    165  CG2 ILE A 170      -7.243  -2.431  12.445  1.00  0.00           C
ATOM    166 1HG2 ILE A 170      -8.119  -1.944  12.856  1.00  0.00           H
ATOM    167 2HG2 ILE A 170      -7.146  -3.455  12.799  1.00  0.00           H
ATOM    168 3HG2 ILE A 170      -6.419  -1.885  12.897  1.00  0.00           H
ATOM    169  CG1 ILE A 170      -6.212  -3.123  10.291  1.00  0.00           C
ATOM    170 1HG1 ILE A 170      -6.384  -4.139  10.654  1.00  0.00           H
ATOM    171 2HG1 ILE A 170      -6.412  -3.124   9.215  1.00  0.00           H
ATOM    172  CD1 ILE A 170      -4.828  -2.584  10.634  1.00  0.00           C
ATOM    173 1HD1 ILE A 170      -4.638  -3.099  11.573  1.00  0.00           H
ATOM    174 2HD1 ILE A 170      -4.127  -2.990   9.909  1.00  0.00           H
ATOM    175 3HD1 ILE A 170      -4.819  -1.504  10.770  1.00  0.00           H
ATOM    176  C   ILE A 170      -8.953  -2.260   8.967  1.00  0.00           C
ATOM    177  O   ILE A 170      -8.395  -1.296   8.448  1.00  0.00           O
ATOM    178  N   HIS A 195      -1.871  -1.508   4.401  1.00  0.00           N
ATOM    179  H   HIS A 195      -1.095  -0.859   4.356  1.00  0.00           H
ATOM    180  CA  HIS A 195      -2.487  -1.622   5.698  1.00  0.00           C
ATOM    181  HA  HIS A 195      -1.903  -1.006   6.377  1.00  0.00           H
ATOM    182  CB  HIS A 195      -3.825  -0.870   5.752  1.00  0.00           C
ATOM    183 1HB  HIS A 195      -3.732  -0.001   5.089  1.00  0.00           H
ATOM    184 2HB  HIS A 195      -4.570  -1.601   5.467  1.00  0.00           H
ATOM    185  CG  HIS A 195      -4.282  -0.440   7.109  1.00  0.00           C
ATOM    186  ND1 HIS A 195      -3.501   0.427   7.887  1.00  0.00           N
ATOM    187  CE1 HIS A 195      -4.330   0.806   8.868  1.00  0.00           C
ATOM    188  HE1 HIS A 195      -4.011   1.465   9.672  1.00  0.00           H
ATOM    189  NE2 HIS A 195      -5.533   0.216   8.813  1.00  0.00           N
ATOM    190  HE2 HIS A 195      -6.325   0.595   9.312  1.00  0.00           H
ATOM    191  CD2 HIS A 195      -5.555  -0.473   7.615  1.00  0.00           C
ATOM    192  HD2 HIS A 195      -6.440  -0.950   7.232  1.00  0.00           H
ATOM    193  C   HIS A 195      -2.453  -2.985   6.375  1.00  0.00           C
ATOM    194  O   HIS A 195      -2.311  -3.104   7.593  1.00  0.00           O
ATOM    195  N   HIS A 197       0.142  -5.319   6.012  1.00  0.00           N
ATOM    196  H   HIS A 197       0.076  -4.553   5.358  1.00  0.00           H
ATOM    197  CA  HIS A 197       1.512  -5.673   6.352  1.00  0.00           C
ATOM    198  HA  HIS A 197       2.186  -5.174   5.663  1.00  0.00           H
ATOM    199  CB  HIS A 197       1.777  -5.229   7.786  1.00  0.00           C
ATOM    200 1HB  HIS A 197       0.896  -5.380   8.409  1.00  0.00           H
ATOM    201 2HB  HIS A 197       2.590  -5.845   8.160  1.00  0.00           H
ATOM    202  CG  HIS A 197       2.167  -3.783   7.963  1.00  0.00           C
ATOM    203  ND1 HIS A 197       3.489  -3.403   8.123  1.00  0.00           N
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ATOM    204  HD1 HIS A 197       4.223  -4.081   8.271  1.00  0.00           H
ATOM    205  CE1 HIS A 197       3.476  -2.072   8.315  1.00  0.00           C
ATOM    206  HE1 HIS A 197       4.369  -1.503   8.524  1.00  0.00           H
ATOM    207  NE2 HIS A 197       2.232  -1.566   8.303  1.00  0.00           N
ATOM    208  CD2 HIS A 197       1.393  -2.651   8.082  1.00  0.00           C
ATOM    209  HD2 HIS A 197       0.323  -2.649   8.238  1.00  0.00           H
ATOM    210  C   HIS A 197      1.766  -7.158   6.137  1.00  0.00           C
ATOM    211  O   HIS A 197      2.851  -7.606   6.496  1.00  0.00           O
ATOM    212  N   HIS A 217      7.981  -3.177   8.721  1.00  0.00           N
ATOM    213  H   HIS A 217      7.203  -2.917   8.130  1.00  0.00           H
ATOM    214  CA  HIS A 217      7.904  -4.555   9.146  1.00  0.00           C
ATOM    215  HA  HIS A 217      8.899  -4.983   8.989  1.00  0.00           H
ATOM    216  CB  HIS A 217      7.550  -4.550  10.633  1.00  0.00           C
ATOM    217 1HB  HIS A 217      7.877  -5.492  11.066  1.00  0.00           H
ATOM    218 2HB  HIS A 217      8.258  -3.872  11.111  1.00  0.00           H
ATOM    219  CG  HIS A 217      6.105  -4.406  11.043  1.00  0.00           C
ATOM    220  ND1 HIS A 217      5.203  -5.423  11.263  1.00  0.00           N
ATOM    221  HD1 HIS A 217      5.304  -6.428  11.199  1.00  0.00           H
ATOM    222  CE1 HIS A 217      4.029  -4.883  11.637  1.00  0.00           C
ATOM    223  HE1 HIS A 217      3.100  -5.380  11.873  1.00  0.00           H
ATOM    224  NE2 HIS A 217      4.077  -3.556  11.508  1.00  0.00           N
ATOM    225  CD2 HIS A 217      5.404  -3.236  11.227  1.00  0.00           C
ATOM    226  HD2 HIS A 217      5.759  -2.228  11.081  1.00  0.00           H
ATOM    227  C   HIS A 217      6.862  -5.435   8.466  1.00  0.00           C
ATOM    228  O   HIS A 217      5.954  -4.813   7.921  1.00  0.00           O
ATOM    229  N   PRO A 228     -1.098  -9.027  18.626  1.00  0.00           N
ATOM    230  CD  PRO A 228     -1.511  -7.785  19.252  1.00  0.00           C
ATOM    231 1HD  PRO A 228     -1.242  -7.638  20.296  1.00  0.00           H
ATOM    232 2HD  PRO A 228     -2.596  -7.781  19.178  1.00  0.00           H
ATOM    233  CG  PRO A 228     -1.031  -6.672  18.315  1.00  0.00           C
ATOM    234 1HG  PRO A 228     -1.024  -5.709  18.829  1.00  0.00           H
ATOM    235 2HG  PRO A 228     -1.637  -6.592  17.407  1.00  0.00           H
ATOM    236  CB  PRO A 228      0.361  -7.208  18.035  1.00  0.00           C
ATOM    237 1HB  PRO A 228      1.079  -7.081  18.842  1.00  0.00           H
ATOM    238 2HB  PRO A 228      0.845  -6.783  17.157  1.00  0.00           H
ATOM    239  CA  PRO A 228      0.040  -8.677  17.791  1.00  0.00           C
ATOM    240  HA  PRO A 228     -0.463  -8.823  16.835  1.00  0.00           H
ATOM    241  C   PRO A 228      1.294  -9.531  17.716  1.00  0.00           C
ATOM    242  O   PRO A 228      1.760  -9.998  18.759  1.00  0.00           O
HETATM  244  ZN  ZN A1001       1.344   0.230   8.042  1.00  0.00           N
HETATM  245  ZN  ZN A1002      -1.349   1.839   7.928  1.00  0.00           N
HETATM  247  P1  bpN B1003     -0.665   0.451  10.687  1.00  0.00           P
HETATM  248  O1  bpN B1003     -1.293   1.414   9.748  1.00  0.00           O
HETATM  249  O2  bpN B1003     -0.070   1.075  12.039  1.00  0.00           O
HETATM  250  O3  bpN B1003      0.369  -0.155   9.820  1.00  0.00           O
HETATM  251  O4  bpN B1003     -1.659  -0.631  11.322  1.00  0.00           O
HETATM  252  C1  bpN B1003     -1.249  -1.692  12.104  1.00  0.00           C
HETATM  253  C2  bpN B1003     -0.080  -2.385  11.825  1.00  0.00           C
HETATM  254  C3  bpN B1003     -2.077  -2.034  13.160  1.00  0.00           C
HETATM  255  C4  bpN B1003      0.260  -3.540  12.524  1.00  0.00           C
HETATM  256  H1  bpN B1003      0.549  -2.134  10.976  1.00  0.00           H
HETATM  257  C5  bpN B1003     -1.640  -3.092  13.946  1.00  0.00           C
HETATM  258  H2  bpN B1003     -2.945  -1.472  13.483  1.00  0.00           H
HETATM  259  C6  bpN B1003     -0.594  -3.916  13.542  1.00  0.00           C
HETATM  260  H3  bpN B1003      1.057  -4.189  12.178  1.00  0.00           H
HETATM  261  H4  bpN B1003     -2.187  -3.310  14.863  1.00  0.00           H
HETATM  262  C7  bpN B1003     -0.763   1.670  13.065  1.00  0.00           C
HETATM  263  C8  bpN B1003     -0.108   1.912  14.262  1.00  0.00           C
HETATM  264  C9  bpN B1003     -2.028   2.225  12.874  1.00  0.00           C
HETATM  265  C10 bpN B1003     -0.702   2.598  15.314  1.00  0.00           C
HETATM  266  H5  bpN B1003      0.952   1.673  14.342  1.00  0.00           H
HETATM  267  C11 bpN B1003     -2.577   2.976  13.898  1.00  0.00           C
HETATM  268  H6  bpN B1003     -2.586   2.014  11.975  1.00  0.00           H
HETATM  269  C12 bpN B1003     -1.929   3.198  15.108  1.00  0.00           C
HETATM  270  H7  bpN B1003     -0.156   2.657  16.254  1.00  0.00           H
HETATM  271  H8  bpN B1003     -3.526   3.458  13.678  1.00  0.00           H
HETATM  272  N1  bpN B1003     -0.238  -5.041  14.424  1.00  0.00           N
HETATM  273  N2  bpN B1003     -2.456   4.063  16.173  1.00  0.00           N
HETATM  274  O5  bpN B1003     -3.308   4.868  15.844  1.00  0.00           O
HETATM  275  O6  bpN B1003     -1.786   4.147  17.189  1.00  0.00           O
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HETATM  276  O7  bpN B1003      -1.144  -5.742  14.832  1.00  0.00           O
HETATM  277  O8  bpN B1003       0.886  -5.498  14.479  1.00  0.00           O
HETATM  279  O1  MOL  1004      -0.172   0.730   7.493  1.00  0.00           O
HETATM  280  H1  MOL  1004      -0.410   0.444   6.587  1.00  0.00           H
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GpdQ-GPE Structure

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ATOM      1  N   ASP A   8       3.180   1.414   3.047  1.00  0.00           N
ATOM      2  H   ASP A   8       3.211   0.770   3.821  1.00  0.00           H
ATOM      3  CA  ASP A   8       3.534   2.779   3.406  1.00  0.00           C
ATOM      4  HA  ASP A   8       2.615   3.362   3.398  1.00  0.00           H
ATOM      5  CB  ASP A   8       4.114   2.813   4.814  1.00  0.00           C
ATOM      6 1HB  ASP A   8       4.915   2.102   4.996  1.00  0.00           H
ATOM      7 2HB  ASP A   8       4.532   3.807   4.933  1.00  0.00           H
ATOM      8  CG  ASP A   8       2.978   2.658   5.814  1.00  0.00           C
ATOM      9  OD1 ASP A   8       2.854   1.507   6.281  1.00  0.00           O
ATOM     10  OD2 ASP A   8       2.117   3.557   5.964  1.00  0.00           O
ATOM     11  C   ASP A   8       4.516   3.345   2.391  1.00  0.00           C
ATOM     12  O   ASP A   8       5.604   2.788   2.270  1.00  0.00           O
ATOM     13  N   HIS A  10       4.131   7.253   1.620  1.00  0.00           N
ATOM     14  H   HIS A  10       3.266   6.872   1.271  1.00  0.00           H
ATOM     15  CA  HIS A  10       4.042   8.537   2.295  1.00  0.00           C
ATOM     16  HA  HIS A  10       3.015   8.836   2.081  1.00  0.00           H
ATOM     17  CB  HIS A  10       4.268   8.298   3.784  1.00  0.00           C
ATOM     18 1HB  HIS A  10       5.116   7.630   3.913  1.00  0.00           H
ATOM     19 2HB  HIS A  10       4.464   9.207   4.349  1.00  0.00           H
ATOM     20  CG  HIS A  10       3.070   7.745   4.506  1.00  0.00           C
ATOM     21  ND1 HIS A  10       2.125   8.430   5.242  1.00  0.00           N
ATOM     22  HD1 HIS A  10       2.298   9.390   5.488  1.00  0.00           H
ATOM     23  CE1 HIS A  10       1.395   7.556   5.968  1.00  0.00           C
ATOM     24  HE1 HIS A  10       0.720   7.915   6.732  1.00  0.00           H
ATOM     25  NE2 HIS A  10       1.778   6.307   5.714  1.00  0.00           N
ATOM     26  CD2 HIS A  10       2.886   6.440   4.887  1.00  0.00           C
ATOM     27  HD2 HIS A  10       3.549   5.612   4.660  1.00  0.00           H
ATOM     28  C   HIS A  10       4.845   9.745   1.816  1.00  0.00           C
ATOM     29  O   HIS A  10       5.500  10.399   2.627  1.00  0.00           O
ATOM     30  N   TYR A  19      12.802  10.915  11.079  1.00  0.00           N
ATOM     31  H   TYR A  19      11.933  11.311  11.401  1.00  0.00           H
ATOM     32  CA  TYR A  19      13.676  10.537  12.169  1.00  0.00           C
ATOM     33  HA  TYR A  19      13.136  10.930  13.034  1.00  0.00           H
ATOM     34  CB  TYR A  19      13.827   9.018  12.235  1.00  0.00           C
ATOM     35 1HB  TYR A  19      14.035   8.737  11.206  1.00  0.00           H
ATOM     36 2HB  TYR A  19      14.639   8.707  12.884  1.00  0.00           H
ATOM     37  CG  TYR A  19      12.657   8.247  12.780  1.00  0.00           C
ATOM     38  CD1 TYR A  19      12.326   8.233  14.149  1.00  0.00           C
ATOM     39  HD1 TYR A  19      12.986   8.715  14.846  1.00  0.00           H
ATOM     40  CE1 TYR A  19      11.121   7.712  14.634  1.00  0.00           C
ATOM     41  HE1 TYR A  19      10.885   7.880  15.676  1.00  0.00           H
ATOM     42  CZ  TYR A  19      10.233   7.130  13.709  1.00  0.00           C
ATOM     43  OH  TYR A  19       9.045   6.583  14.125  1.00  0.00           O
ATOM     44  HH  TYR A  19       9.030   6.407  15.069  1.00  0.00           H
ATOM     45  CE2 TYR A  19      10.623   7.040  12.363  1.00  0.00           C
ATOM     46  HE2 TYR A  19       9.946   6.633  11.625  1.00  0.00           H
ATOM     47  CD2 TYR A  19      11.814   7.588  11.879  1.00  0.00           C
ATOM     48  HD2 TYR A  19      12.015   7.568  10.824  1.00  0.00           H
ATOM     49  C   TYR A  19      15.032  11.210  12.029  1.00  0.00           C
ATOM     50  O   TYR A  19      16.045  10.658  12.438  1.00  0.00           O
ATOM     51  N   ASP A  50      -1.559   5.752   1.169  1.00  0.00           N
ATOM     52  H   ASP A  50      -2.307   6.050   0.567  1.00  0.00           H
ATOM     53  CA  ASP A  50      -0.761   6.837   1.698  1.00  0.00           C
ATOM     54  HA  ASP A  50      -1.316   7.761   1.544  1.00  0.00           H
ATOM     55  CB  ASP A  50      -0.474   6.906   3.192  1.00  0.00           C
ATOM     56 1HB  ASP A  50       0.152   6.073   3.491  1.00  0.00           H
ATOM     57 2HB  ASP A  50       0.170   7.781   3.280  1.00  0.00           H
ATOM     58  CG  ASP A  50      -1.706   7.119   4.048  1.00  0.00           C
ATOM     59  OD1 ASP A  50      -2.770   7.610   3.611  1.00  0.00           O
ATOM     60  OD2 ASP A  50      -1.687   6.729   5.238  1.00  0.00           O
ATOM     61  C   ASP A  50       0.395   7.088   0.741  1.00  0.00           C
ATOM     62  O   ASP A  50       1.554   6.916   1.103  1.00  0.00           O
ATOM     63  N   ASN A  53       2.305  12.247   1.797  1.00  0.00           N
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ATOM     64  H   ASN A  53       2.929  12.745   1.185  1.00  0.00           H
ATOM     65  CA  ASN A  53       2.561  12.389   3.220  1.00  0.00           C
ATOM     66  HA  ASN A  53       2.761  11.381   3.559  1.00  0.00           H
ATOM     67  CB  ASN A  53       3.812  13.247   3.389  1.00  0.00           C
ATOM     68 1HB  ASN A  53       4.741  12.724   3.155  1.00  0.00           H
ATOM     69 2HB  ASN A  53       3.799  14.135   2.770  1.00  0.00           H
ATOM     70  CG  ASN A  53       3.903  13.700   4.844  1.00  0.00           C
ATOM     71  OD1 ASN A  53       4.159  12.904   5.748  1.00  0.00           O
ATOM     72  ND2 ASN A  53       3.688  14.975   5.150  1.00  0.00           N
ATOM     73 1HD2 ASN A  53       3.778  15.363   6.085  1.00  0.00           H
ATOM     74 2HD2 ASN A  53       3.510  15.551   4.338  1.00  0.00           H
ATOM     75  C   ASN A  53       1.405  12.952   4.035  1.00  0.00           C
ATOM     76  O   ASN A  53       1.068  12.315   5.036  1.00  0.00           O
ATOM     77  N   ASN A  80      -5.383   7.124   4.154  1.00  0.00           N
ATOM     78  H   ASN A  80      -4.667   6.572   4.598  1.00  0.00           H
ATOM     79  CA  ASN A  80      -5.934   8.153   5.015  1.00  0.00           C
ATOM     80  HA  ASN A  80      -7.023   8.120   5.021  1.00  0.00           H
ATOM     81  CB  ASN A  80      -5.621   7.716   6.439  1.00  0.00           C
ATOM     82 1HB  ASN A  80      -5.969   8.481   7.127  1.00  0.00           H
ATOM     83 2HB  ASN A  80      -6.208   6.837   6.688  1.00  0.00           H
ATOM     84  CG  ASN A  80      -4.182   7.378   6.812  1.00  0.00           C
ATOM     85  OD1 ASN A  80      -3.870   6.197   6.690  1.00  0.00           O
ATOM     86  ND2 ASN A  80      -3.350   8.241   7.411  1.00  0.00           N
ATOM     87 1HD2 ASN A  80      -2.353   8.108   7.535  1.00  0.00           H
ATOM     88 2HD2 ASN A  80      -3.758   9.141   7.615  1.00  0.00           H
ATOM     89  C   ASN A  80      -5.505   9.574   4.694  1.00  0.00           C
ATOM     90  O   ASN A  80      -6.286  10.465   5.021  1.00  0.00           O
ATOM     91  N   HIS A 156      -6.007  -0.677   2.537  1.00  0.00           N
ATOM     92  H   HIS A 156      -6.900  -0.288   2.286  1.00  0.00           H
ATOM     93  CA  HIS A 156      -5.085   0.147   3.301  1.00  0.00           C
ATOM     94  HA  HIS A 156      -4.093  -0.119   2.926  1.00  0.00           H
ATOM     95  CB  HIS A 156      -5.311   1.641   3.084  1.00  0.00           C
ATOM     96 1HB  HIS A 156      -5.271   1.733   2.004  1.00  0.00           H
ATOM     97 2HB  HIS A 156      -6.316   1.906   3.429  1.00  0.00           H
ATOM     98  CG  HIS A 156      -4.301   2.601   3.655  1.00  0.00           C
ATOM     99  ND1 HIS A 156      -3.130   2.906   2.994  1.00  0.00           N
ATOM    100  HD1 HIS A 156      -2.842   2.464   2.131  1.00  0.00           H
ATOM    101  CE1 HIS A 156      -2.528   3.879   3.697  1.00  0.00           C
ATOM    102  HE1 HIS A 156      -1.573   4.347   3.527  1.00  0.00           H
ATOM    103  NE2 HIS A 156      -3.233   4.272   4.767  1.00  0.00           N
ATOM    104  CD2 HIS A 156      -4.429   3.574   4.625  1.00  0.00           C
ATOM    105  HD2 HIS A 156      -5.276   3.591   5.291  1.00  0.00           H
ATOM    106  C   HIS A 156      -5.183  -0.215   4.773  1.00  0.00           C
ATOM    107  O   HIS A 156      -4.241  -0.777   5.315  1.00  0.00           O
ATOM    108  N   HIS A 195      -0.622   0.421   5.230  1.00  0.00           N
ATOM    109  H   HIS A 195      -0.470   0.727   4.286  1.00  0.00           H
ATOM    110  CA  HIS A 195      -0.963   1.319   6.326  1.00  0.00           C
ATOM    111  HA  HIS A 195      -0.804   2.289   5.855  1.00  0.00           H
ATOM    112  CB  HIS A 195      -2.452   1.152   6.606  1.00  0.00           C
ATOM    113 1HB  HIS A 195      -2.986   1.332   5.672  1.00  0.00           H
ATOM    114 2HB  HIS A 195      -2.565   0.128   6.968  1.00  0.00           H
ATOM    115  CG  HIS A 195      -3.044   2.065   7.652  1.00  0.00           C
ATOM    116  ND1 HIS A 195      -2.758   3.432   7.667  1.00  0.00           N
ATOM    117  CE1 HIS A 195      -3.460   3.935   8.686  1.00  0.00           C
ATOM    118  HE1 HIS A 195      -3.484   4.999   8.875  1.00  0.00           H
ATOM    119  NE2 HIS A 195      -4.059   2.972   9.401  1.00  0.00           N
ATOM    120  HE2 HIS A 195      -4.529   3.110  10.285  1.00  0.00           H
ATOM    121  CD2 HIS A 195      -3.851   1.786   8.722  1.00  0.00           C
ATOM    122  HD2 HIS A 195      -4.356   0.880   9.019  1.00  0.00           H
ATOM    123  C   HIS A 195      -0.053   1.268   7.542  1.00  0.00           C
ATOM    124  O   HIS A 195       0.347   2.367   7.909  1.00  0.00
ATOM    125  N   ASN A 196       0.329   0.132   8.133  1.00  0.00           N
ATOM    126  H   ASN A 196       0.162  -0.754   7.673  1.00  0.00           H
ATOM    127  CA  ASN A 196       0.895   0.180   9.472  1.00  0.00           C
ATOM    128  HA  ASN A 196       0.496   1.098   9.900  1.00  0.00           H
ATOM    129  CB  ASN A 196       0.276  -0.992  10.217  1.00  0.00           C
ATOM    130 1HB  ASN A 196      -0.795  -0.913  10.022  1.00  0.00           H
ATOM    131 2HB  ASN A 196       0.733  -1.894   9.801  1.00  0.00           H
ATOM    132  CG  ASN A 196       0.394  -1.023  11.737  1.00  0.00           C
ATOM    133  OD1 ASN A 196       1.040  -1.900  12.320  1.00  0.00           O
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ATOM    134  ND2 ASN A 196      -0.137  -0.077  12.508  1.00  0.00           N
ATOM    135 1HD2 ASN A 196      -0.176  -0.173  13.512  1.00  0.00           H
ATOM    136 2HD2 ASN A 196      -0.597   0.722  12.097  1.00  0.00           H
ATOM    137  C   ASN A 196       2.402   0.217   9.672  1.00  0.00           C
ATOM    138  O   ASN A 196       3.002   0.272  10.742  1.00  0.00           O
ATOM    139  N   HIS A 197       3.185   0.364   8.599  1.00  0.00           N
ATOM    140  H   HIS A 197       2.763   0.524   7.694  1.00  0.00           H
ATOM    141  CA  HIS A 197       4.622   0.501   8.581  1.00  0.00           C
ATOM    142  HA  HIS A 197       4.853   0.635   7.528  1.00  0.00           H
ATOM    143  CB  HIS A 197       5.096   1.804   9.231  1.00  0.00           C
ATOM    144 1HB  HIS A 197       5.016   1.713  10.320  1.00  0.00           H
ATOM    145 2HB  HIS A 197       6.143   1.998   9.029  1.00  0.00           H
ATOM    146  CG  HIS A 197       4.515   3.057   8.633  1.00  0.00           C
ATOM    147  ND1 HIS A 197       5.097   3.944   7.755  1.00  0.00           N
ATOM    148  HD1 HIS A 197       6.089   4.014   7.532  1.00  0.00           H
ATOM    149  CE1 HIS A 197       4.236   4.939   7.482  1.00  0.00           C
ATOM    150  HE1 HIS A 197       4.344   5.863   6.941  1.00  0.00           H
ATOM    151  NE2 HIS A 197       3.126   4.803   8.210  1.00  0.00           N
ATOM    152  CD2 HIS A 197       3.287   3.608   8.911  1.00  0.00           C
ATOM    153  HD2 HIS A 197       2.620   3.111   9.599  1.00  0.00           H
ATOM    154  C   HIS A 197       5.427  -0.667   9.124  1.00  0.00           C
ATOM    155  O   HIS A 197       6.560  -0.487   9.546  1.00  0.00           O
ATOM    156  N   HIS A 217       9.989   4.013   5.582  1.00  0.00           N
ATOM    157  H   HIS A 217       9.201   3.966   4.953  1.00  0.00           H
ATOM    158  CA  HIS A 217       9.622   4.124   6.981  1.00  0.00           C
ATOM    159  HA  HIS A 217      10.460   4.449   7.596  1.00  0.00           H
ATOM    160  CB  HIS A 217       8.685   5.316   7.163  1.00  0.00           C
ATOM    161 1HB  HIS A 217       9.327   6.144   6.880  1.00  0.00           H
ATOM    162 2HB  HIS A 217       7.934   5.155   6.387  1.00  0.00           H
ATOM    163  CG  HIS A 217       8.091   5.528   8.535  1.00  0.00           C
ATOM    164  ND1 HIS A 217       8.644   5.142   9.747  1.00  0.00           N
ATOM    165  HD1 HIS A 217       9.501   4.629   9.872  1.00  0.00           H
ATOM    166  CE1 HIS A 217       7.758   5.490  10.699  1.00  0.00           C
ATOM    167  HE1 HIS A 217       7.965   5.357  11.753  1.00  0.00           H
ATOM    168  NE2 HIS A 217       6.741   6.186  10.192  1.00  0.00           N
ATOM    169  CD2 HIS A 217       6.925   6.201   8.811  1.00  0.00           C
ATOM    170  HD2 HIS A 217       6.331   6.679   8.038  1.00  0.00           H
ATOM    171  C   HIS A 217       9.005   2.812   7.419  1.00  0.00           C
ATOM    172  O   HIS A 217       7.863   2.466   7.118  1.00  0.00           O
HETATM  174  ZN   ZN A1001       1.061   4.711   6.661  1.00  0.00           N
HETATM  175  ZN   ZN A1002      -1.967   5.259   6.185  1.00  0.00           N
HETATM  176  O1  MOL B1003      -1.080   5.185  10.159  1.00  0.00           O
HETATM  177  P1  MOL B1003      -0.529   6.064   8.934  1.00  0.00           P
HETATM  178  O2  MOL B1003      -0.126   7.545   9.364  1.00  0.00           O
HETATM  179  O3  MOL B1003       0.514   5.382   8.130  1.00  0.00           O
HETATM  180  C1  MOL B1003      -1.179   8.296  10.005  1.00  0.00           C
HETATM  181  H1  MOL B1003      -2.180   7.959   9.734  1.00  0.00           H
HETATM  182  H2  MOL B1003      -1.052   9.342   9.719  1.00  0.00           H
HETATM  183  C2  MOL B1003      -0.953   8.089  11.513  1.00  0.00           C
HETATM  184  H3  MOL B1003      -1.330   8.959  12.059  1.00  0.00           H
HETATM  185  H4  MOL B1003      -1.418   7.176  11.905  1.00  0.00           H
HETATM  186  N1  MOL B1003       0.482   7.983  11.760  1.00  0.00           N
HETATM  187  H5  MOL B1003       0.974   7.347  11.139  1.00  0.00           H
HETATM  188  H6  MOL B1003       0.984   8.843  11.551  1.00  0.00           H
HETATM  189  C3  MOL B1003      -0.012   4.492  10.832  1.00  0.00           C
HETATM  190  H7  MOL B1003       0.579   5.201  11.409  1.00  0.00           H
HETATM  191  H8  MOL B1003       0.526   3.932  10.065  1.00  0.00           H
HETATM  192  C4  MOL B1003      -0.609   3.552  11.893  1.00  0.00           C
HETATM  193  H9  MOL B1003      -1.437   4.065  12.400  1.00  0.00           H
HETATM  194  C5  MOL B1003       0.495   3.244  12.922  1.00  0.00           C
HETATM  195  H10 MOL B1003       0.808   4.138  13.457  1.00  0.00           H
HETATM  196  H11 MOL B1003       0.098   2.620  13.718  1.00  0.00           H
HETATM  197  O4  MOL B1003       1.658   2.644  12.356  1.00  0.00           O
HETATM  198  H12 MOL B1003       1.435   1.695  12.295  1.00  0.00           H
HETATM  199  O5  MOL B1003      -0.924   2.360  11.190  1.00  0.00           O
HETATM  200  H13 MOL B1003      -1.555   2.661  10.504  1.00  0.00           H
HETATM  201  O6  MOL B1003      -1.391   6.055   7.734  1.00  0.00           O
HETATM  202  O1  MOL  1004      -0.431   4.498   5.886  1.00  0.00           O
HETATM  203  H1  MOL  1004      -0.199   4.122   5.017  1.00  0.00           H
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GpdQ-paraoxon Structure

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ATOM      1  N   ASP A   8      13.147   4.703   4.862  1.00  0.00           N
ATOM      2  H   ASP A   8      13.068   4.057   5.622  1.00  0.00           H
ATOM      3  CA  ASP A   8      13.501   6.068   5.221  1.00  0.00           C
ATOM      4  HA  ASP A   8      12.656   6.603   5.197  1.00  0.00           H
ATOM      5  CB  ASP A   8      14.081   6.102   6.629  1.00  0.00           C
ATOM      6 1HB  ASP A   8      14.733   5.353   6.743  1.00  0.00           H
ATOM      7 2HB  ASP A   8      14.546   6.974   6.781  1.00  0.00           H
ATOM      8  CG  ASP A   8      12.945   5.947   7.629  1.00  0.00           C
ATOM      9  OD1 ASP A   8      12.821   4.796   8.096  1.00  0.00           O
ATOM     10  OD2 ASP A   8      12.084   6.846   7.779  1.00  0.00           O
ATOM     11  C   ASP A   8      14.483   6.634   4.206  1.00  0.00           C
ATOM     12  O   ASP A   8      15.571   6.077   4.085  1.00  0.00           O
ATOM     13  N   HIS A  10      14.098  10.542   3.435  1.00  0.00           N
ATOM     14  H   HIS A  10      13.240  10.182   3.069  1.00  0.00           H
ATOM     15  CA  HIS A  10      14.009  11.826   4.110  1.00  0.00           C
ATOM     16  HA  HIS A  10      13.084  12.087   3.833  1.00  0.00           H
ATOM     17  CB  HIS A  10      14.235  11.587   5.599  1.00  0.00           C
ATOM     18 1HB  HIS A  10      14.988  10.938   5.707  1.00  0.00           H
ATOM     19 2HB  HIS A  10      14.480  12.456   6.028  1.00  0.00           H
ATOM     20  CG  HIS A  10      13.037  11.034   6.321  1.00  0.00           C
ATOM     21  ND1 HIS A  10      12.092  11.719   7.057  1.00  0.00           N
ATOM     22  HD1 HIS A  10      11.967  12.711   7.053  1.00  0.00           H
ATOM     23  CE1 HIS A  10      11.362  10.845   7.783  1.00  0.00           C
ATOM     24  HE1 HIS A  10      10.636  11.100   8.421  1.00  0.00           H
ATOM     25  NE2 HIS A  10      11.745   9.596   7.529  1.00  0.00           N
ATOM     26  CD2 HIS A  10      12.853   9.729   6.702  1.00  0.00           C
ATOM     27  HD2 HIS A  10      13.441   8.971   6.420  1.00  0.00           H
ATOM     28  C   HIS A  10      14.812  13.034   3.631  1.00  0.00           C
ATOM     29  O   HIS A  10      15.467  13.688   4.442  1.00  0.00           O
ATOM     30  N   ARG A  12      17.074  16.127   2.500  1.00  0.00           N
ATOM     31  H   ARG A  12      17.839  15.493   2.385  1.00  0.00           H
ATOM     32  CA  ARG A  12      17.369  17.489   2.896  1.00  0.00           C
ATOM     33  HA  ARG A  12      16.560  17.914   3.303  1.00  0.00           H
ATOM     34  CB  ARG A  12      18.443  17.484   3.975  1.00  0.00           C
ATOM     35 1HB  ARG A  12      19.228  16.966   3.636  1.00  0.00           H
ATOM     36 2HB  ARG A  12      18.718  18.429   4.151  1.00  0.00           H
ATOM     37  CG  ARG A  12      17.978  16.859   5.291  1.00  0.00           C
ATOM     38 1HG  ARG A  12      17.063  17.204   5.500  1.00  0.00           H
ATOM     39 2HG  ARG A  12      17.941  15.866   5.175  1.00  0.00           H
ATOM     40  CD  ARG A  12      18.898  17.176   6.473  1.00  0.00           C
ATOM     41 1HD  ARG A  12      19.842  16.935   6.245  1.00  0.00           H
ATOM     42 2HD  ARG A  12      18.846  18.150   6.694  1.00  0.00           H
ATOM     43  NE  ARG A  12      18.509  16.417   7.664  1.00  0.00           N
ATOM     44  HE  ARG A  12      18.125  15.505   7.519  1.00  0.00           H
ATOM     45  CZ  ARG A  12      18.623  16.838   8.927  1.00  0.00           C
ATOM     46  NH1 ARG A  12      19.606  17.706   9.186  1.00  0.00           N
ATOM     47 1HH1 ARG A  12      20.212  18.009   8.451  1.00  0.00           H
ATOM     48 2HH1 ARG A  12      19.735  18.053  10.115  1.00  0.00           H
ATOM     49  NH2 ARG A  12      17.765  16.591   9.927  1.00  0.00           N
ATOM     50 1HH2 ARG A  12      16.946  16.043   9.759  1.00  0.00           H
ATOM     51 2HH2 ARG A  12      17.944  16.955  10.841  1.00  0.00           H
ATOM     52  C   ARG A  12      17.750  18.247   1.630  1.00  0.00           C
ATOM     53  O   ARG A  12      18.369  17.695   0.729  1.00  0.00           O
ATOM     54  N   ASP A  50       8.408   9.041   2.984  1.00  0.00           N
ATOM     55  H   ASP A  50       7.437   9.195   2.799  1.00  0.00           H
ATOM     56  CA  ASP A  50       9.206  10.126   3.513  1.00  0.00           C
ATOM     57  HA  ASP A  50       8.561  10.890   3.505  1.00  0.00           H
ATOM     58  CB  ASP A  50       9.493  10.195   5.007  1.00  0.00           C
ATOM     59 1HB  ASP A  50       9.923   9.336   5.286  1.00  0.00           H
ATOM     60 2HB  ASP A  50      10.124  10.953   5.173  1.00  0.00           H
ATOM     61  CG  ASP A  50       8.261  10.408   5.863  1.00  0.00           C
ATOM     62  OD1 ASP A  50       7.197  10.899   5.426  1.00  0.00           O
ATOM     63  OD2 ASP A  50       8.280  10.018   7.053  1.00  0.00           O
ATOM     64  C   ASP A  50      10.362  10.377   2.556  1.00  0.00           C
ATOM     65  O   ASP A  50      11.521  10.205   2.918  1.00  0.00           O
ATOM     66  N   ASN A  80       4.584  10.413   5.969  1.00  0.00           N
ATOM     67  H   ASN A  80       5.317   9.850   6.351  1.00  0.00           H
ATOM     68  CA  ASN A  80       4.033  11.442   6.830  1.00  0.00           C
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ATOM     69  HA  ASN A  80       3.051  11.476   6.646  1.00  0.00           H
ATOM     70  CB  ASN A  80       4.346  11.005   8.254  1.00  0.00           C
ATOM     71 1HB  ASN A  80       4.053  11.746   8.858  1.00  0.00           H
ATOM     72 2HB  ASN A  80       3.797  10.190   8.436  1.00  0.00           H
ATOM     73  CG  ASN A  80       5.785  10.667   8.627  1.00  0.00           C
ATOM     74  OD1 ASN A  80       6.097   9.486   8.505  1.00  0.00           O
ATOM     75  ND2 ASN A  80       6.617  11.530   9.226  1.00  0.00           N
ATOM     76 1HD2 ASN A  80       7.552  11.252   9.447  1.00  0.00           H
ATOM     77 2HD2 ASN A  80       6.303  12.452   9.452  1.00  0.00           H
ATOM     78  C   ASN A  80       4.462  12.863   6.509  1.00  0.00           C
ATOM     79  O   ASN A  80       3.681  13.754   6.836  1.00  0.00           O
ATOM     80  N   HIS A 156       3.960   2.612   4.352  1.00  0.00           N
ATOM     81  H   HIS A 156       3.099   2.991   4.012  1.00  0.00           H
ATOM     82  CA  HIS A 156       4.882   3.436   5.116  1.00  0.00           C
ATOM     83  HA  HIS A 156       5.789   3.212   4.759  1.00  0.00           H
ATOM     84  CB  HIS A 156       4.656   4.930   4.899  1.00  0.00           C
ATOM     85 1HB  HIS A 156       4.626   5.091   3.913  1.00  0.00           H
ATOM     86 2HB  HIS A 156       3.771   5.164   5.302  1.00  0.00           H
ATOM     87  CG  HIS A 156       5.666   5.890   5.470  1.00  0.00           C
ATOM     88  ND1 HIS A 156       6.837   6.195   4.809  1.00  0.00           N
ATOM     89  HD1 HIS A 156       7.174   5.773   3.967  1.00  0.00           H
ATOM     90  CE1 HIS A 156       7.439   7.168   5.512  1.00  0.00           C
ATOM     91  HE1 HIS A 156       8.324   7.560   5.262  1.00  0.00           H
ATOM     92  NE2 HIS A 156       6.734   7.561   6.582  1.00  0.00           N
ATOM     93  CD2 HIS A 156       5.538   6.863   6.440  1.00  0.00           C
ATOM     94  HD2 HIS A 156       4.706   7.041   6.965  1.00  0.00           H
ATOM     95  C   HIS A 156       4.784   3.074   6.588  1.00  0.00           C
ATOM     96  O   HIS A 156       5.726   2.512   7.130  1.00  0.00           O
ATOM     97  N   HIS A 195       9.345   3.710   7.045  1.00  0.00           N
ATOM     98  H   HIS A 195       9.774   4.073   6.218  1.00  0.00           H
ATOM     99  CA  HIS A 195       9.004   4.608   8.141  1.00  0.00           C
ATOM    100  HA  HIS A 195       9.201   5.531   7.810  1.00  0.00           H
ATOM    101  CB  HIS A 195       7.515   4.441   8.421  1.00  0.00           C
ATOM    102 1HB  HIS A 195       7.021   4.602   7.567  1.00  0.00           H
ATOM    103 2HB  HIS A 195       7.362   3.500   8.722  1.00  0.00           H
ATOM    104  CG  HIS A 195       6.923   5.354   9.467  1.00  0.00           C
ATOM    105  ND1 HIS A 195       7.209   6.721   9.482  1.00  0.00           N
ATOM    106  CE1 HIS A 195       6.507   7.224  10.501  1.00  0.00           C
ATOM    107  HE1 HIS A 195       6.437   8.200  10.706  1.00  0.00           H
ATOM    108  NE2 HIS A 195       5.908   6.261  11.216  1.00  0.00           N
ATOM    109  HE2 HIS A 195       5.408   6.378  12.074  1.00  0.00           H
ATOM    110  CD2 HIS A 195       6.116   5.075  10.537  1.00  0.00           C
ATOM    111  HD2 HIS A 195       5.746   4.179  10.782  1.00  0.00           H
ATOM    112  C   HIS A 195       9.914   4.557   9.357  1.00  0.00           C
ATOM    113  O   HIS A 195      10.314   5.656   9.724  1.00  0.00           O
ATOM    114  N   HIS A 197      13.152   3.653  10.414  1.00  0.00           N
ATOM    115  H   HIS A 197      12.692   3.670   9.526  1.00  0.00           H
ATOM    116  CA  HIS A 197      14.589   3.790  10.396  1.00  0.00           C
ATOM    117  HA  HIS A 197      14.718   3.792   9.404  1.00  0.00           H
ATOM    118  CB  HIS A 197      15.063   5.093  11.046  1.00  0.00           C
ATOM    119 1HB  HIS A 197      14.813   5.074  12.014  1.00  0.00           H
ATOM    120 2HB  HIS A 197      16.058   5.147  10.959  1.00  0.00           H
ATOM    121  CG  HIS A 197      14.482   6.346  10.448  1.00  0.00           C
ATOM    122  ND1 HIS A 197      15.064   7.233   9.570  1.00  0.00           N
ATOM    123  HD1 HIS A 197      15.986   7.149   9.193  1.00  0.00           H
ATOM    124  CE1 HIS A 197      14.203   8.228   9.297  1.00  0.00           C
ATOM    125  HE1 HIS A 197      14.370   8.965   8.642  1.00  0.00           H
ATOM    126  NE2 HIS A 197      13.093   8.092  10.025  1.00  0.00           N
ATOM    127  CD2 HIS A 197      13.254   6.897  10.726  1.00  0.00           C
ATOM    128  HD2 HIS A 197      12.574   6.499  11.342  1.00  0.00           H
ATOM    129  C   HIS A 197      15.394   2.622  10.939  1.00  0.00           C
ATOM    130  O   HIS A 197      16.527   2.802  11.361  1.00  0.00           O
ATOM    131  N   HIS A 217      19.956   7.302   7.397  1.00  0.00           N
ATOM    132  H   HIS A 217      19.211   7.155   6.746  1.00  0.00           H
ATOM    133  CA  HIS A 217      19.589   7.413   8.796  1.00  0.00           C
ATOM    134  HA  HIS A 217      20.414   7.574   9.338  1.00  0.00           H
ATOM    135  CB  HIS A 217      18.652   8.605   8.978  1.00  0.00           C
ATOM    136 1HB  HIS A 217      19.163   9.433   8.746  1.00  0.00           H
ATOM    137 2HB  HIS A 217      17.890   8.494   8.340  1.00  0.00           H
ATOM    138  CG  HIS A 217      18.058   8.817  10.350  1.00  0.00           C
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ATOM    139  ND1 HIS A 217      18.611   8.431  11.562  1.00  0.00           N
ATOM    140  HD1 HIS A 217      19.494   7.983  11.701  1.00  0.00           H
ATOM    141  CE1 HIS A 217      17.725   8.779  12.514  1.00  0.00           C
ATOM    142  HE1 HIS A 217      17.818   8.544  13.482  1.00  0.00           H
ATOM    143  NE2 HIS A 217      16.708   9.475  12.007  1.00  0.00           N
ATOM    144  CD2 HIS A 217      16.892   9.490  10.626  1.00  0.00           C
ATOM    145  HD2 HIS A 217      16.284   9.915   9.955  1.00  0.00           H
ATOM    146  C   HIS A 217     18.972   6.101   9.234  1.00  0.00           C
ATOM    147  O   HIS A 217     17.830   5.755   8.933  1.00  0.00           O
ATOM    148  N   THR A 226      12.634   8.647  22.833  1.00  0.00           N
ATOM    149  H   THR A 226      12.757   8.473  23.810  1.00  0.00           H
ATOM    150  CA  THR A 226      12.142   9.953  22.447  1.00  0.00           C
ATOM    151  HA  THR A 226      11.652   9.792  21.590  1.00  0.00           H
ATOM    152  CB  THR A 226      11.145  10.524  23.459  1.00  0.00           C
ATOM    153  HB  THR A 226      11.071  11.497  23.239  1.00  0.00           H
ATOM    154  CG2 THR A 226       9.784   9.850  23.455  1.00  0.00           C
ATOM    155 1HG2 THR A 226       9.197  10.280  24.141  1.00  0.00           H
ATOM    156 2HG2 THR A 226       9.367   9.946  22.551  1.00  0.00           H
ATOM    157 3HG2 THR A 226       9.892   8.879  23.670  1.00  0.00           H
ATOM    158  OG1 THR A 226      11.613  10.404  24.784  1.00  0.00           O
ATOM    159  HG1 THR A 226      10.936  10.787  25.413  1.00  0.00           H
ATOM    160  C   THR A 226     13.296  10.901  22.185  1.00  0.00           C
ATOM    161  O   THR A 226     13.150  12.089  21.909  1.00  0.00           O
HETATM  163 ZN    ZN A1001      11.028   8.000   8.476  1.00  0.00          ZN
HETATM  164 ZN    ZN A1002       8.000   8.548   8.000  1.00  0.00          ZN
HETATM  166  C1  MOL B1003      11.273  12.379  13.953  0.00  0.00           C
HETATM  167  C2  MOL B1003      11.399  13.608  13.316  0.00  0.00           C
HETATM  168  C3  MOL B1003      11.427  13.677  11.929  0.00  0.00           C
HETATM  169  C4  MOL B1003      11.316  12.516  11.180  0.00  0.00           C
HETATM  170  C5  MOL B1003      11.164  11.295  11.813  0.00  0.00           C
HETATM  171  C6  MOL B1003      11.158  11.222  13.197  0.00  0.00           C
HETATM  172  H1  MOL B1003      11.267  12.323  15.040  0.00  0.00           H
HETATM  173  H2  MOL B1003      11.534  14.636  11.425  0.00  0.00           H
HETATM  174  H3  MOL B1003      11.338  12.569  10.098  0.00  0.00           H
HETATM  175  H4  MOL B1003      11.069  10.258  13.688  0.00  0.00           H
HETATM  176  N1  MOL B1003      11.510  14.842  14.114  0.00  0.00           N
HETATM  177  O1  MOL B1003      11.613  15.891  13.502  0.00  0.00           O
HETATM  178  O2  MOL B1003      11.480  14.724  15.327  0.00  0.00           O
HETATM  179  O3  MOL B1003      11.038  10.156  11.085  0.00  0.00           O
HETATM  180  P1  MOL B1003       9.626   9.605  10.638  0.00  0.00           P
HETATM  181  O4  MOL B1003       8.668  10.824  11.036  0.00  0.00           O
HETATM  182  O5  MOL B1003       9.520   9.129   9.233  0.00  0.00           O
HETATM  183  C7  MOL B1003       7.971  10.786  12.302  0.00  0.00           C
HETATM  184  C8  MOL B1003       7.325  12.157  12.539  0.00  0.00           C
HETATM  185  O6  MOL B1003       9.300   8.529  11.778  0.00  0.00           O
HETATM  186  C9  MOL B1003      10.335   7.614  12.167  0.00  0.00           C
HETATM  187  H5  MOL B1003      11.171   8.166  12.607  0.00  0.00           H
HETATM  188  C10 MOL B1003       9.741   6.653  13.204  0.00  0.00           C
HETATM  189  H6  MOL B1003      10.685   7.067  11.293  0.00  0.00           H
HETATM  190  H7  MOL B1003      10.503   5.952  13.547  0.00  0.00           H
HETATM  191  H8  MOL B1003       8.916   6.089  12.765  0.00  0.00           H
HETATM  192  H9  MOL B1003       9.366   7.209  14.066  0.00  0.00           H
HETATM  193  H10 MOL B1003       8.679  10.576  13.108  0.00  0.00           H
HETATM  194  H11 MOL B1003       7.205  10.005  12.275  0.00  0.00           H
HETATM  195  H12 MOL B1003       6.815  12.172  13.504  0.00  0.00           H
HETATM  196  H13 MOL B1003       6.595  12.376  11.758  0.00  0.00           H
HETATM  197  H14 MOL B1003       8.088  12.939  12.536  0.00  0.00           H
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