

Electronic Supplementary Information

From Groove Binding to Intercalation: Unraveling the Weak Interactions and Other Factors Modulating the Modes of Interaction between Methylated Phenanthroline Based Drugs and Duplex DNA

Ángel Sánchez-Gonzalez^a, Tarsila G. Castro^b, Manuel Melle-Franco^c, Adrià Gil^{ad*}

^a Centro de Química e Bioquímica and BioISI – Biosystems and Integrative Sciences Institute, Faculdade de Ciências, Universidade de Lisboa, Campo Grande 1749-016

Lisboa, Portugal

^b Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710-057,

Braga, Portugal

^c CICECO-Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro (Portugal).

^d CIC nanoGUNE BRTA, Tolosa Hiribidea 76, E-20018 Donostia – San Sebastian, Euskadi, Spain.

Index

Table S1. AutoDock4 binding energies between the Pt complex and DNA hexanucleotide d(GTCGAC)₂, indicating the number of conformations in the major clusters out of 300 runs.....S4

Figure S1. Lowest energy docking poses of Pt complexes on the hexanucleotide d(GTCGAC)₂. a) [Pt(en)(phen)]²⁺, b) [Pt(en)(4-Mephen)]²⁺, c) [Pt(en)(5-Mephen)]²⁺, d) [Pt(en)(4,7-Me₂phen)]²⁺, e) [Pt(en)(5,6-Me₂phen)]²⁺ and f) [Pt(en)(3,4,7,8-Me₄phen)]²⁺. Grey lines for nucleotides, dashed yellow lines for hydrogen bonds, green spheres for C, blue for N, white for H, grey for Pt and cyan highlighting the methyl groups.....S5

Observations in the docking screening.....S5

Considered [Pt(en)(phen)]²⁺ systems from the Docking studies: Optimized geometries, EDA's, Solvent Effects and Cartesian coordinates of the optimized systems.....S6

Considered [Pt(en)(4-Mephen)]²⁺ systems from the Docking studies: Optimized geometries, EDA's, Solvent Effects and Cartesian coordinates of the optimized systems.....S36

Considered [Pt(en)(5-Mephen)]²⁺ systems from the Docking studies: Optimized geometries, EDA's, Solvent Effects and Cartesian coordinates of the optimized systems.....S117

Considered $[\text{Pt}(\text{en})(4,7\text{-Me}_2\text{phen})]^{2+}$ systems from the Docking studies: Optimized geometries, EDA's, Solvent Effects and Cartesian coordinates of the optimized systems.....	S156
Considered $[\text{Pt}(\text{en})(5,6\text{-Me}_2\text{phen})]^{2+}$ systems from the Docking studies: Optimized geometries, EDA's, Solvent Effects and Cartesian coordinates of the optimized systems.....	S186
Considered $[\text{Pt}(\text{en})(3,4,7,8\text{-Me}_4\text{phen})]^{2+}$ systems from the Docking studies: Optimized geometries, EDA's, Solvent Effects and Cartesian coordinates of the optimized systems.....	S206

Table S1. AutoDock4 binding energies between the Pt complex and DNA hexanucleotide d(GTCGAC)₂, indicating the number of conformations in the major clusters out of 300 runs.

Pt complexes	Cluster number	Number of conformations in Cluster	Binding Energy (kcal mol⁻¹)^a
[Pt(en)(phen)] ²⁺	1	140	-7.68
	3	103	-7.66
[Pt(en)(4-Mephen)] ²⁺	1	121	-7.62
	2	111	-7.59
[Pt(en)(5-Mephen)] ²⁺	1	145	-7.85
	2	126	-7.81
[Pt(en)(4,7-Me ₂ phen)] ²⁺	1	156	-7.68
	2	108	-7.64
[Pt(en)(5,6-Me ₂ phen)] ²⁺	1	176	-8.09
	2	122	-8.04

	1	280	-7.71
$[\text{Pt}(\text{en})(3,4,7,8\text{-Me}_4\text{phen})]^{2+}$	5	9	-7.55

a) In terms of Gibbs Free Energies.

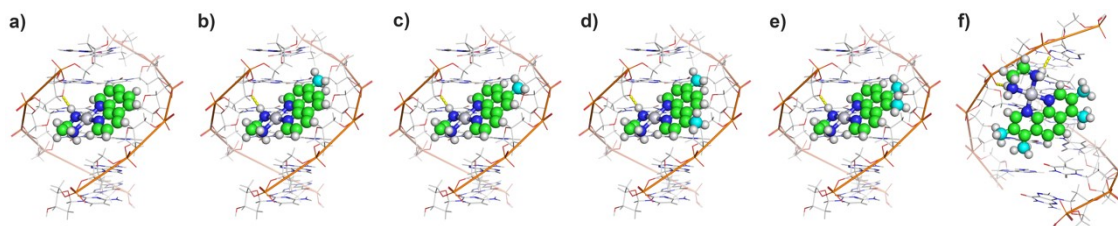


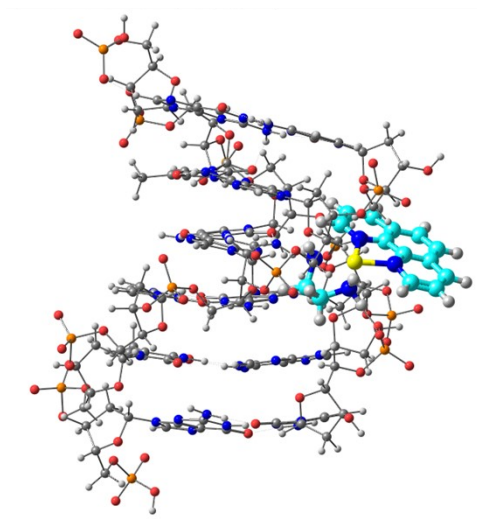
Figure S1. Lowest energy docking poses of Pt complexes on the hexanucleotide d(GTCGAC)₂. a) $[\text{Pt}(\text{en})(\text{phen})]^{2+}$, b) $[\text{Pt}(\text{en})(4\text{-Mephen})]^{2+}$, c) $[\text{Pt}(\text{en})(5\text{-Mephen})]^{2+}$, d) $[\text{Pt}(\text{en})(4,7\text{-Me}_2\text{phen})]^{2+}$, e) $[\text{Pt}(\text{en})(5,6\text{-Me}_2\text{phen})]^{2+}$ and f) $[\text{Pt}(\text{en})(3,4,7,8\text{-Me}_4\text{phen})]^{2+}$. Grey lines for nucleotides, dashed yellow lines for hydrogen bonds, green spheres for C, blue for N, white for H, grey for Pt and cyan highlighting the methyl groups.

Observations in the docking screening:

- All Pt complexes interact via minor groove, showing a hydrogen bond with adenine, except $[\text{Pt}(\text{en})(3,4,7,8\text{-Me}_4\text{phen})]^{2+}$, which for its most representative interacting conformations, are placed at the major groove. For the most populated cluster, two hydrogen bonds are seen, with the phosphate groups of thymine and cytosine.
- The binding energies are very similar among the series, revealing that all these planar platinum compounds are equally able to bind the hexanucleotide double helix under study.

[Pt(en)(phen)]²⁺ systems

[Pt(en)(phen)]²⁺ minor groove
Dock_ID: 299-cl1_phen



EDA for 299-cl1_phen in kcal mol⁻¹.

Electrostatic interaction	-802.9
Orbital interaction	-101.5
Dispersion energy	-64.9
Pauli repulsion	128.7
Total Bonding Energy	-840.6

Contributions of the solvation energies for 299-cl1_phen in kcal mol⁻¹.

E _{solv} (total system)	-1744.1
E _{solv} (intercalator)	-164.4
E _{solv} (duplex DNA)	-2360.6
ΔE _{solv}	781.0

$\Delta E_{\text{int}}(\text{EDA})$	-840.6
ΔE_{aq}	-59.7

$$\Delta E_{\text{solv}} = E_{\text{solv}}(\text{total system}) - E_{\text{solv}}(\text{intercalator}) - E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 299-cl1_phen system.
([Pt(en)(phen)]²⁺ minor groove)

P	-2.131000000	6.206000000	2.615000000
C	0.348000000	5.246000000	2.618000000
O	-0.485000000	6.395000000	2.861000000
C	1.243000000	5.487000000	1.390000000
O	1.382000000	4.201000000	0.722000000
C	0.681000000	6.459000000	0.321000000
O	1.799000000	7.234000000	-0.135000000
C	-0.017000000	5.549000000	-0.694000000
C	0.582000000	4.157000000	-0.485000000
N	-0.203000000	-0.996000000	-0.501000000
C	0.909000000	-0.247000000	-0.961000000
N	1.994000000	-0.948000000	-1.432000000
N	0.984000000	1.119000000	-0.885000000
C	-0.158000000	1.718000000	-0.403000000
C	-1.338000000	1.039000000	0.031000000
C	-1.402000000	-0.390000000	-0.010000000
O	-2.315000000	-1.145000000	0.330000000
N	-2.312000000	1.981000000	0.420000000
C	-1.757000000	3.182000000	0.248000000
N	-0.424000000	3.090000000	-0.282000000
O	-2.732000000	7.355000000	3.384000000
O	-2.456000000	5.958000000	1.165000000
H	-0.198000000	-2.062000000	-0.637000000
H	-2.217000000	4.158000000	0.456000000
H	1.304000000	3.827000000	-1.283000000
H	-1.118000000	5.584000000	-0.506000000
H	2.620000000	-0.470000000	-2.102000000
H	0.011000000	7.239000000	0.748000000
H	1.932000000	-1.983000000	-1.533000000
H	2.283000000	5.749000000	1.682000000
H	-0.233000000	4.306000000	2.508000000
H	0.084000000	5.891000000	-1.757000000
H	0.958000000	5.164000000	3.541000000
P	2.472000000	7.122000000	-1.662000000
C	3.881000000	4.970000000	-1.018000000
O	2.860000000	5.519000000	-1.877000000
C	4.970000000	4.326000000	-1.876000000
O	4.523000000	3.014000000	-2.320000000
C	5.376000000	5.105000000	-3.153000000
O	6.813000000	5.124000000	-3.047000000
C	4.821000000	4.286000000	-4.327000000
C	4.240000000	3.003000000	-3.729000000
N	2.758000000	2.866000000	-3.912000000
C	2.213000000	1.548000000	-3.779000000
O	2.945000000	0.569000000	-3.685000000
N	0.812000000	1.427000000	-3.850000000

C	-0.076000000	2.538000000	-3.763000000
O	-1.262000000	2.315000000	-3.547000000
C	0.548000000	3.852000000	-3.915000000
C	1.902000000	3.984000000	-3.921000000
C	-0.350000000	5.032000000	-4.045000000
O	3.712000000	7.968000000	-1.518000000
O	1.436000000	7.378000000	-2.723000000
H	0.410000000	0.443000000	-3.815000000
H	2.392000000	4.974000000	-3.961000000
H	4.723000000	2.056000000	-4.108000000
H	4.088000000	4.890000000	-4.902000000
H	5.039000000	6.164000000	-3.157000000
H	5.865000000	4.088000000	-1.248000000
H	3.354000000	4.196000000	-0.412000000
H	-0.357000000	5.433000000	-5.068000000
H	-1.390000000	4.790000000	-3.782000000
H	-0.031000000	5.863000000	-3.381000000
H	5.611000000	4.015000000	-5.069000000
H	4.321000000	5.721000000	-0.335000000
P	7.800000000	5.420000000	-4.361000000
C	7.918000000	2.791000000	-4.400000000
O	7.723000000	3.980000000	-5.203000000
C	7.681000000	1.598000000	-5.323000000
O	6.249000000	1.396000000	-5.477000000
C	8.279000000	1.760000000	-6.750000000
O	9.056000000	0.557000000	-6.896000000
C	7.065000000	1.921000000	-7.667000000
C	5.913000000	1.277000000	-6.893000000
N	4.587000000	1.911000000	-7.044000000
C	3.414000000	1.031000000	-6.983000000
O	3.603000000	-0.174000000	-6.905000000
N	2.165000000	1.615000000	-7.006000000
C	2.014000000	2.975000000	-7.121000000
N	0.741000000	3.459000000	-7.124000000
C	3.166000000	3.832000000	-7.270000000
C	4.416000000	3.279000000	-7.237000000
O	9.148000000	5.598000000	-3.708000000
O	7.233000000	6.443000000	-5.306000000
H	3.034000000	4.902000000	-7.427000000
H	5.330000000	3.887000000	-7.351000000
H	5.802000000	0.165000000	-7.090000000
H	6.904000000	3.003000000	-7.869000000
H	9.003000000	2.600000000	-6.833000000
H	8.050000000	0.659000000	-4.840000000
H	0.567000000	4.453000000	-7.056000000
H	7.200000000	2.781000000	-3.552000000
H	-0.058000000	2.834000000	-6.897000000
H	7.189000000	1.473000000	-8.674000000
H	8.956000000	2.777000000	-4.009000000
P	9.165000000	-0.312000000	-8.314000000

C	7.102000000	-1.844000000	-7.640000000
O	7.615000000	-0.854000000	-8.563000000
C	6.521000000	-3.016000000	-8.440000000
O	5.129000000	-2.724000000	-8.718000000
C	7.189000000	-3.262000000	-9.820000000
O	7.319000000	-4.681000000	-9.975000000
C	6.289000000	-2.521000000	-10.816000000
C	4.954000000	-2.315000000	-10.086000000
N	0.779000000	0.767000000	-10.159000000
C	0.881000000	-0.639000000	-10.046000000
N	-0.278000000	-1.371000000	-10.063000000
N	2.069000000	-1.315000000	-9.992000000
C	3.173000000	-0.506000000	-10.088000000
C	3.165000000	0.923000000	-10.201000000
C	1.919000000	1.631000000	-10.191000000
O	1.698000000	2.843000000	-10.214000000
N	4.491000000	1.394000000	-10.259000000
C	5.274000000	0.312000000	-10.176000000
N	4.513000000	-0.899000000	-10.081000000
O	10.090000000	-1.434000000	-7.913000000
O	9.439000000	0.582000000	-9.495000000
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H	-1.208000000	-0.926000000	-9.943000000
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H	6.265000000	-1.314000000	-7.109000000
H	6.154000000	-3.055000000	-11.780000000
H	7.859000000	-2.190000000	-6.916000000
P	6.381000000	-5.604000000	-11.011000000
C	4.130000000	-5.597000000	-9.586000000
O	4.814000000	-5.151000000	-10.781000000
C	2.751000000	-6.100000000	-10.002000000
O	1.943000000	-5.037000000	-10.588000000
C	2.775000000	-7.220000000	-11.076000000
O	1.603000000	-7.974000000	-10.708000000
C	2.643000000	-6.456000000	-12.403000000
C	1.847000000	-5.204000000	-12.016000000
N	0.359000000	-0.406000000	-13.256000000
C	-0.368000000	-1.532000000	-12.961000000
N	0.116000000	-2.779000000	-12.738000000
C	1.489000000	-2.847000000	-12.838000000
C	2.346000000	-1.760000000	-13.213000000
C	1.735000000	-0.482000000	-13.392000000
N	2.419000000	0.653000000	-13.717000000
N	3.684000000	-2.202000000	-13.245000000
C	3.657000000	-3.491000000	-12.881000000

N	2.326000000	-3.956000000	-12.644000000
O	6.703000000	-7.010000000	-10.590000000
O	6.612000000	-5.147000000	-12.440000000
H	-1.462000000	-1.378000000	-12.881000000
H	4.520000000	-4.156000000	-12.777000000
H	0.739000000	-5.285000000	-12.225000000
H	3.652000000	-6.219000000	-12.798000000
H	3.645000000	-7.901000000	-11.022000000
H	2.138000000	-6.407000000	-9.101000000
H	4.046000000	-4.690000000	-8.940000000
H	1.948000000	1.573000000	-13.674000000
H	3.431000000	0.655000000	-13.689000000
H	2.154000000	-7.025000000	-13.213000000
H	4.687000000	-6.393000000	-9.047000000
P	0.751000000	-8.957000000	-11.710000000
C	-0.948000000	-7.062000000	-12.496000000
O	0.152000000	-7.892000000	-12.872000000
C	-2.108000000	-7.284000000	-13.479000000
O	-2.457000000	-5.967000000	-13.999000000
C	-1.790000000	-8.170000000	-14.705000000
O	-2.808000000	-9.185000000	-14.692000000
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C	-2.118000000	-5.838000000	-15.388000000
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O	-2.145000000	-3.076000000	-15.640000000
N	0.104000000	-2.815000000	-15.963000000
C	1.357000000	-3.395000000	-15.998000000
N	2.398000000	-2.611000000	-16.373000000
C	1.515000000	-4.787000000	-15.647000000
C	0.409000000	-5.550000000	-15.401000000
O	-0.364000000	-9.387000000	-10.774000000
O	1.548000000	-9.915000000	-12.547000000
H	-2.668000000	-9.825000000	-15.431000000
H	2.514000000	-5.219000000	-15.587000000
H	0.491000000	-6.614000000	-15.118000000
H	-2.967000000	-5.254000000	-15.827000000
H	-1.115000000	-7.367000000	-16.657000000
H	-0.797000000	-8.670000000	-14.662000000
H	-3.038000000	-7.624000000	-12.968000000
H	3.356000000	-2.944000000	-16.326000000
H	-0.566000000	-6.008000000	-12.582000000
H	2.274000000	-1.597000000	-16.549000000
H	-2.837000000	-7.552000000	-16.526000000
H	-1.292000000	-7.240000000	-11.449000000
P	0.983000000	6.558000000	-19.735000000
C	-1.596000000	6.434000000	-19.109000000
O	-0.272000000	6.822000000	-18.677000000
C	-2.457000000	6.425000000	-17.840000000
O	-2.434000000	5.090000000	-17.265000000

C	-1.929000000	7.376000000	-16.732000000
O	-3.077000000	8.011000000	-16.155000000
C	-1.087000000	6.471000000	-15.828000000
C	-1.560000000	5.042000000	-16.114000000
N	-0.129000000	0.030000000	-16.287000000
C	-1.360000000	0.611000000	-15.887000000
N	-2.316000000	-0.230000000	-15.395000000
N	-1.616000000	1.960000000	-15.951000000
C	-0.536000000	2.715000000	-16.344000000
C	0.748000000	2.209000000	-16.721000000
C	1.000000000	0.801000000	-16.697000000
O	2.025000000	0.178000000	-16.988000000
N	1.603000000	3.281000000	-17.049000000
C	0.882000000	4.393000000	-16.891000000
N	-0.452000000	4.111000000	-16.432000000
O	0.849000000	7.445000000	-20.952000000
O	2.198000000	6.583000000	-18.846000000
H	-0.010000000	-1.031000000	-16.199000000
H	1.214000000	5.416000000	-17.074000000
H	-2.203000000	4.578000000	-15.313000000
H	-0.014000000	6.628000000	-16.079000000
H	-3.179000000	0.156000000	-15.015000000
H	-1.350000000	8.233000000	-17.147000000
H	-2.246000000	-1.258000000	-15.511000000
H	-3.531000000	6.592000000	-18.080000000
H	-1.582000000	5.423000000	-19.568000000
H	-1.155000000	6.726000000	-14.739000000
H	-1.965000000	7.178000000	-19.841000000
P	-3.609000000	7.742000000	-14.592000000
C	-4.892000000	5.499000000	-15.218000000
O	-3.827000000	6.103000000	-14.456000000
C	-5.673000000	4.567000000	-14.288000000
O	-4.867000000	3.402000000	-13.967000000
C	-6.071000000	5.192000000	-12.924000000
O	-7.387000000	4.660000000	-12.693000000
C	-4.972000000	4.725000000	-11.964000000
C	-4.377000000	3.468000000	-12.609000000
N	-2.884000000	3.449000000	-12.660000000
C	-2.261000000	2.165000000	-12.827000000
O	-2.916000000	1.136000000	-12.809000000
N	-0.858000000	2.164000000	-12.936000000
C	-0.060000000	3.329000000	-13.068000000
O	1.129000000	3.181000000	-13.346000000
C	-0.763000000	4.595000000	-12.861000000
C	-2.117000000	4.624000000	-12.729000000
C	0.055000000	5.838000000	-12.809000000
O	-4.917000000	8.490000000	-14.583000000
O	-2.512000000	8.008000000	-13.592000000
H	-0.404000000	1.199000000	-13.075000000
H	-2.677000000	5.576000000	-12.637000000

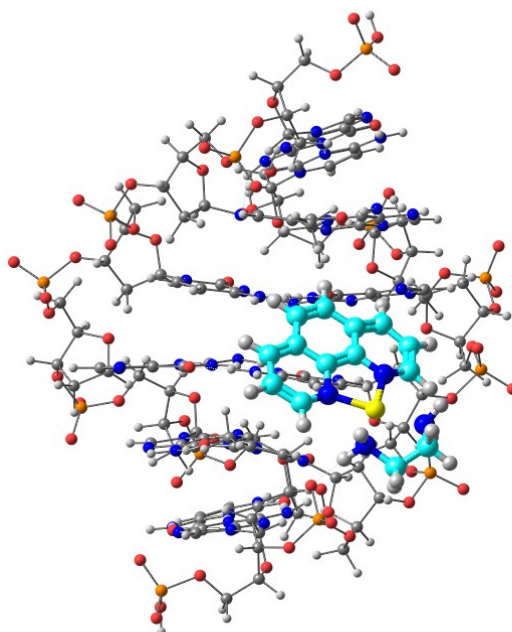
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H	-4.228000000	5.546000000	-11.847000000
H	-6.194000000	6.296000000	-12.955000000
H	-6.553000000	4.136000000	-14.820000000
H	-4.383000000	4.918000000	-16.021000000
H	0.386000000	6.060000000	-11.783000000
H	0.953000000	5.763000000	-13.439000000
H	-0.515000000	6.718000000	-13.167000000
H	-5.327000000	4.530000000	-10.932000000
H	-5.566000000	6.243000000	-15.682000000
P	-7.940000000	4.206000000	-11.183000000
C	-7.188000000	1.719000000	-11.639000000
O	-7.015000000	2.879000000	-10.792000000
C	-7.075000000	0.470000000	-10.760000000
O	-5.673000000	0.198000000	-10.524000000
C	-7.724000000	0.591000000	-9.355000000
O	-8.377000000	-0.667000000	-9.114000000
C	-6.565000000	0.972000000	-8.427000000
C	-5.302000000	0.509000000	-9.159000000
N	-4.200000000	1.508000000	-9.244000000
C	-2.873000000	0.961000000	-9.531000000
O	-2.768000000	-0.259000000	-9.602000000
N	-1.820000000	1.836000000	-9.688000000
C	-2.005000000	3.192000000	-9.555000000
N	-0.914000000	3.982000000	-9.748000000
C	-3.312000000	3.732000000	-9.276000000
C	-4.379000000	2.879000000	-9.161000000
O	-9.364000000	3.814000000	-11.489000000
O	-7.592000000	5.223000000	-10.131000000
H	-3.446000000	4.807000000	-9.176000000
H	-5.410000000	3.243000000	-8.988000000
H	-4.856000000	-0.452000000	-8.761000000
H	-6.596000000	2.072000000	-8.259000000
H	-8.568000000	1.314000000	-9.322000000
H	-7.434000000	-0.430000000	-11.313000000
H	-0.970000000	4.988000000	-9.678000000
H	-6.343000000	1.746000000	-12.368000000
H	0.027000000	3.571000000	-9.912000000
H	-6.644000000	0.534000000	-7.409000000
H	-8.150000000	1.732000000	-12.185000000
P	-7.826000000	-1.832000000	-8.053000000
C	-5.733000000	-2.833000000	-9.418000000
O	-6.199000000	-2.024000000	-8.325000000
C	-5.167000000	-4.164000000	-8.910000000
O	-3.785000000	-3.990000000	-8.485000000
C	-5.904000000	-4.772000000	-7.689000000
O	-5.958000000	-6.170000000	-8.044000000
C	-5.007000000	-4.463000000	-6.479000000
C	-3.696000000	-3.903000000	-7.047000000
N	-0.108000000	-0.104000000	-6.796000000

C	0.076000000	-1.486000000	-7.001000000
N	1.373000000	-1.955000000	-7.037000000
N	-0.959000000	-2.387000000	-7.075000000
C	-2.199000000	-1.836000000	-6.815000000
C	-2.453000000	-0.462000000	-6.518000000
C	-1.394000000	0.499000000	-6.578000000
O	-1.429000000	1.722000000	-6.474000000
N	-3.822000000	-0.267000000	-6.251000000
C	-4.393000000	-1.468000000	-6.369000000
N	-3.436000000	-2.491000000	-6.698000000
O	-8.610000000	-3.053000000	-8.465000000
O	-7.842000000	-1.300000000	-6.641000000
H	0.744000000	0.549000000	-6.818000000
H	-5.451000000	-1.695000000	-6.252000000
H	-2.795000000	-4.513000000	-6.781000000
H	-5.518000000	-3.778000000	-5.777000000
H	1.586000000	-2.818000000	-7.529000000
H	-6.951000000	-4.421000000	-7.563000000
H	2.172000000	-1.282000000	-7.019000000
H	-5.077000000	-4.900000000	-9.745000000
H	-4.912000000	-2.207000000	-9.851000000
H	-4.787000000	-5.369000000	-5.868000000
H	-6.511000000	-3.002000000	-10.184000000
P	-6.552000000	-7.285000000	-6.956000000
C	-3.989000000	-7.797000000	-6.771000000
O	-5.192000000	-7.545000000	-6.013000000
C	-2.833000000	-7.808000000	-5.773000000
O	-2.413000000	-6.436000000	-5.530000000
C	-3.188000000	-8.434000000	-4.395000000
O	-2.376000000	-9.609000000	-4.307000000
C	-2.970000000	-7.315000000	-3.372000000
C	-2.149000000	-6.249000000	-4.102000000
N	-0.447000000	-1.308000000	-3.722000000
C	0.204000000	-2.469000000	-4.060000000
N	-0.332000000	-3.712000000	-4.171000000
C	-1.669000000	-3.761000000	-3.860000000
C	-2.463000000	-2.623000000	-3.501000000
C	-1.805000000	-1.355000000	-3.431000000
N	-2.431000000	-0.213000000	-3.032000000
N	-3.792000000	-3.017000000	-3.259000000
C	-3.827000000	-4.339000000	-3.454000000
N	-2.543000000	-4.864000000	-3.819000000
O	-6.840000000	-8.482000000	-7.827000000
O	-7.576000000	-6.714000000	-6.016000000
H	1.286000000	-2.369000000	-4.285000000
H	-4.693000000	-4.984000000	-3.351000000
H	-1.033000000	-6.355000000	-3.970000000
H	-3.952000000	-6.946000000	-3.010000000
H	-4.226000000	-8.842000000	-4.358000000
H	-1.938000000	-8.312000000	-6.217000000

H	-3.831000000	-6.995000000	-7.537000000
H	-1.971000000	0.703000000	-3.156000000
H	-3.443000000	-0.193000000	-2.964000000
H	-2.475000000	-7.657000000	-2.438000000
H	-4.074000000	-8.787000000	-7.267000000
P	-1.063000000	-9.771000000	-3.283000000
C	0.776000000	-8.245000000	-4.493000000
O	-0.229000000	-8.346000000	-3.460000000
C	2.148000000	-8.043000000	-3.847000000
O	2.270000000	-6.639000000	-3.473000000
C	2.457000000	-8.863000000	-2.576000000
O	3.647000000	-9.605000000	-2.907000000
C	2.743000000	-7.838000000	-1.464000000
C	2.427000000	-6.468000000	-2.072000000
N	1.152000000	-5.863000000	-1.530000000
C	1.093000000	-4.423000000	-1.361000000
O	2.115000000	-3.761000000	-1.571000000
N	-0.073000000	-3.832000000	-0.917000000
C	-1.191000000	-4.599000000	-0.660000000
N	-2.330000000	-3.952000000	-0.295000000
C	-1.143000000	-6.025000000	-0.837000000
C	0.012000000	-6.617000000	-1.278000000
O	-0.324000000	-10.939000000	-3.883000000
O	-1.522000000	-9.743000000	-1.851000000
H	3.885000000	-10.217000000	-2.172000000
H	-2.018000000	-6.631000000	-0.607000000
H	0.072000000	-7.708000000	-1.447000000
H	3.232000000	-5.696000000	-1.965000000
H	2.190000000	-8.061000000	-0.535000000
H	1.676000000	-9.592000000	-2.288000000
H	2.960000000	-8.175000000	-4.615000000
H	-3.148000000	-4.468000000	0.010000000
H	0.488000000	-7.320000000	-5.064000000
H	-2.337000000	-2.932000000	-0.114000000
H	3.810000000	-7.890000000	-1.160000000
H	0.783000000	-9.116000000	-5.178000000
O	0.738000000	4.984000000	-20.234000000
O	-2.426000000	4.752000000	3.376000000
H	0.369000000	4.876000000	-21.155000000
H	-2.413000000	4.764000000	4.372000000
N	2.065000000	-8.669000000	-7.545000000
N	-0.275000000	-5.378000000	-7.258000000
N	-0.696000000	-7.750000000	-8.498000000
N	2.505000000	-6.230000000	-6.534000000
C	5.094000000	-5.326000000	-5.841000000
C	4.972000000	-6.577000000	-6.386000000
C	3.641000000	-7.066000000	-6.724000000
C	3.423000000	-8.299000000	-7.278000000
C	4.528000000	-9.174000000	-7.656000000
C	4.255000000	-10.319000000	-8.341000000

C	2.888000000	-10.622000000	-8.708000000
C	1.869000000	-9.774000000	-8.360000000
C	5.864000000	-8.689000000	-7.294000000
C	-0.842000000	-5.264000000	-8.648000000
C	-1.546000000	-6.590000000	-8.969000000
C	2.675000000	-5.010000000	-5.937000000
C	6.067000000	-7.486000000	-6.711000000
C	3.930000000	-4.533000000	-5.599000000
Pt	0.911000000	-7.024000000	-7.432000000
H	0.193000000	-4.505000000	-6.974000000
H	-1.024000000	-5.543000000	-6.562000000
H	-0.370000000	-8.307000000	-9.339000000
H	-1.256000000	-8.390000000	-7.921000000
H	6.068000000	-4.913000000	-5.591000000
H	5.032000000	-11.006000000	-8.652000000
H	2.697000000	-11.516000000	-9.280000000
H	0.833000000	-9.961000000	-8.663000000
H	6.696000000	-9.343000000	-7.540000000
H	-1.556000000	-4.408000000	-8.750000000
H	0.014000000	-5.087000000	-9.360000000
H	-2.560000000	-6.622000000	-8.493000000
H	-1.724000000	-6.679000000	-10.071000000
H	1.761000000	-4.435000000	-5.734000000
H	7.074000000	-7.148000000	-6.470000000
H	4.037000000	-3.546000000	-5.171000000

[Pt(en)(phen)]²⁺ major groove
Dock_ID: 52-cl3_phen



EDA for 52-cl3_phen in kcal mol⁻¹.

Electrostatic interaction	-776.3
Orbital interaction	-92.5
Dispersion energy	-53.0
Pauli repulsion	121.2
Total Bonding Energy	-800.7

Contributions of the solvation energies for 52-cl3_phen in kcal mol⁻¹.

E _{solv} (total system)	-1753.9
E _{solv} (intercalator)	-163.7
E _{solv} (duplex DNA)	-2331.2
ΔE _{solv}	741.0
ΔE _{int} (EDA)	-800.7
ΔE _{aq}	-59.7

$$\Delta E_{\text{solv}} = E_{\text{solv}}(\text{total system}) - E_{\text{solv}}(\text{intercalator}) - E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 52-cl3_phen system.
([Pt(en)(phen)]²⁺ major groove)

P	-2.31900000	6.92800000	2.30000000
C	0.29200000	6.54000000	2.18700000
O	-0.88700000	6.92300000	1.44200000
C	1.44500000	6.50000000	1.18200000
O	1.59200000	5.14600000	0.66900000
C	1.25200000	7.39800000	-0.06800000
O	2.52700000	8.02800000	-0.26200000
C	0.75700000	6.45400000	-1.16300000
C	1.05800000	5.03800000	-0.67000000
N	-0.51600000	0.09400000	-0.91700000
C	0.73400000	0.66700000	-1.24500000
N	1.73700000	-0.16700000	-1.67900000
N	1.01500000	2.00100000	-1.08900000
C	-0.06700000	2.76200000	-0.71300000
C	-1.37900000	2.27300000	-0.43400000
C	-1.64500000	0.86700000	-0.48700000
O	-2.67100000	0.24200000	-0.21900000
N	-2.23900000	3.35800000	-0.15900000
C	-1.48900000	4.45800000	-0.24200000
N	-0.12900000	4.15800000	-0.60800000
O	-2.26900000	7.91600000	3.44000000
O	-3.36400000	6.98100000	1.21800000
H	-0.64400000	-0.96400000	-1.02800000
H	-1.81000000	5.48800000	-0.07800000
H	1.87600000	4.49600000	-1.23900000
H	-0.32700000	6.62700000	-1.34000000
H	2.48800000	0.25300000	-2.24300000
H	0.56400000	8.25600000	0.11600000
H	1.52000000	-1.16100000	-1.90200000
H	2.41900000	6.68900000	1.69500000
H	0.14600000	5.53500000	2.63900000
H	1.22900000	6.65300000	-2.15500000
H	0.48700000	7.28800000	2.98000000
P	3.52100000	8.05200000	-1.58800000
C	4.55900000	5.78000000	-0.56100000
O	4.79600000	7.07900000	-1.12300000
C	4.87800000	4.66100000	-1.55300000
O	3.62100000	4.03400000	-1.94900000
C	5.59800000	5.08000000	-2.86500000
O	6.75800000	4.23200000	-2.87900000
C	4.55100000	4.88400000	-3.96400000
C	3.65800000	3.78600000	-3.39000000
N	2.25400000	3.76500000	-3.84900000
C	1.63800000	2.46800000	-3.92600000
O	2.32400000	1.45500000	-3.95600000
N	0.23800000	2.44200000	-4.04200000

C	-0.57800000	3.60900000	-3.97000000
O	-1.78700000	3.45100000	-3.84400000
C	0.13300000	4.88300000	-4.07800000
C	1.48800000	4.93900000	-3.97400000
C	-0.70300000	6.09900000	-4.27500000
O	4.11300000	9.43700000	-1.52600000
O	2.95000000	7.54300000	-2.89100000
H	-0.22700000	1.46800000	-4.07900000
H	2.06200000	5.89400000	-3.99100000
H	4.08000000	2.74400000	-3.50500000
H	3.97900000	5.83900000	-4.11800000
H	6.01200000	6.12100000	-2.82700000
H	5.44800000	3.84700000	-1.03900000
H	3.53300000	5.66800000	-0.15400000
H	-1.02200000	6.19700000	-5.32600000
H	-1.60900000	6.07400000	-3.65100000
H	-0.16500000	7.02500000	-4.02700000
H	4.95800000	4.67500000	-4.98300000
H	5.26900000	5.75100000	0.29500000
P	7.36000000	3.43600000	-4.21200000
C	5.49600000	1.77800000	-5.13600000
O	6.52000000	1.99100000	-4.15100000
C	5.82800000	0.46800000	-5.86000000
O	4.58600000	-0.28600000	-5.95700000
C	6.34400000	0.65000000	-7.31100000
O	7.49800000	-0.20000000	-7.35600000
C	5.20500000	0.15100000	-8.21500000
C	4.05100000	-0.24700000	-7.29700000
N	2.91700000	0.73200000	-7.32000000
C	1.54400000	0.25000000	-7.25000000
O	1.35000000	-0.96700000	-7.26300000
N	0.51100000	1.16500000	-7.20100000
C	0.77100000	2.51300000	-7.10800000
N	-0.28000000	3.38400000	-7.10500000
C	2.12500000	2.98200000	-7.02300000
C	3.15400000	2.10300000	-7.18000000
O	8.76000000	3.09100000	-3.77800000
O	7.05600000	4.19100000	-5.48000000
H	2.32600000	4.05000000	-6.88800000
H	4.20000000	2.45100000	-7.20900000
H	3.63300000	-1.27200000	-7.46200000
H	4.92900000	0.92600000	-8.96600000
H	6.65000000	1.69800000	-7.54400000
H	6.50400000	-0.17700000	-5.25500000
H	-0.11500000	4.38100000	-6.98400000
H	5.38700000	2.64000000	-5.83500000
H	-1.25800000	3.05100000	-7.04900000
H	5.52700000	-0.72100000	-8.82500000
H	4.54700000	1.64700000	-4.54400000
P	8.48300000	-0.13700000	-8.71200000

C	7.68600000	-2.61900000	-8.78200000
O	7.89800000	-1.43000000	-9.58700000
C	7.24600000	-3.74100000	-9.72200000
O	5.83500000	-3.59500000	-10.02900000
C	7.98400000	-3.78400000	-11.08700000
O	8.34400000	-5.15900000	-11.28300000
C	7.00800000	-3.16000000	-12.08900000
C	5.64400000	-3.14300000	-11.38900000
N	1.27900000	-0.45700000	-10.47800000
C	1.50700000	-1.84500000	-10.44700000
N	0.43600000	-2.67100000	-10.13000000
N	2.73500000	-2.41500000	-10.64100000
C	3.72300000	-1.51600000	-10.97200000
C	3.57700000	-0.09400000	-11.03800000
C	2.31300000	0.51200000	-10.74300000
O	1.98800000	1.68900000	-10.67100000
N	4.80000000	0.49400000	-11.41100000
C	5.66600000	-0.51400000	-11.55200000
N	5.04900000	-1.79000000	-11.32300000
O	9.84800000	-0.46800000	-8.14700000
O	8.26500000	1.10100000	-9.53400000
H	0.27900000	-0.09600000	-10.32400000
H	6.72400000	-0.43600000	-11.78700000
H	4.88200000	-3.85700000	-11.80100000
H	7.37100000	-2.14800000	-12.37400000
H	0.51100000	-3.64800000	-10.41400000
H	8.96800000	-3.26300000	-11.06400000
H	-0.52600000	-2.27200000	-10.20100000
H	7.29700000	-4.72500000	-9.19500000
H	6.88500000	-2.41100000	-8.03700000
H	6.95900000	-3.68800000	-13.06400000
H	8.62500000	-2.90000000	-8.26500000
P	7.70800000	-6.15100000	-12.46700000
C	5.38000000	-6.57900000	-11.25900000
O	6.05800000	-5.98300000	-12.38600000
C	4.18500000	-7.38000000	-11.78300000
O	3.10400000	-6.47100000	-12.12400000
C	4.46600000	-8.20100000	-13.07200000
O	3.82600000	-9.46900000	-12.86200000
C	3.93100000	-7.32800000	-14.21300000
C	2.98600000	-6.31600000	-13.55200000
N	1.30900000	-1.33500000	-13.68000000
C	0.66300000	-2.49600000	-13.33600000
N	1.17200000	-3.75100000	-13.32800000
C	2.48400000	-3.80900000	-13.74500000
C	3.25800000	-2.67100000	-14.15400000
C	2.62900000	-1.38900000	-14.10300000
N	3.24800000	-0.23600000	-14.47600000
N	4.55600000	-3.07300000	-14.51900000
C	4.58900000	-4.39900000	-14.34000000

N	3.33300000	-4.91700000	-13.89100000
O	8.15400000	-7.51300000	-11.99600000
O	8.04300000	-5.61300000	-13.83500000
H	-0.39200000	-2.37500000	-13.01800000
H	5.44700000	-5.05200000	-14.49500000
H	1.89200000	-6.47400000	-13.74700000
H	4.78800000	-6.85600000	-14.73900000
H	5.53500000	-8.47100000	-13.20600000
H	3.74500000	-8.01600000	-10.97800000
H	5.02800000	-5.71400000	-10.64500000
H	2.80900000	0.68000000	-14.28400000
H	4.24100000	-0.23700000	-14.67700000
H	3.43100000	-7.89200000	-15.02700000
H	6.04200000	-7.22800000	-10.65400000
P	2.60900000	-10.07100000	-13.83500000
C	0.69100000	-8.68200000	-12.65000000
O	1.44300000	-8.88100000	-13.86800000
C	-0.78200000	-8.49900000	-13.02000000
O	-1.00300000	-7.09500000	-13.34300000
C	-1.28100000	-9.31800000	-14.23400000
O	-2.29300000	-10.18700000	-13.70000000
C	-1.89800000	-8.29500000	-15.20500000
C	-1.49400000	-6.91900000	-14.68000000
N	-0.40200000	-6.27900000	-15.49100000
C	-0.45000000	-4.84200000	-15.71300000
O	-1.44900000	-4.22800000	-15.32500000
N	0.58400000	-4.22200000	-16.37900000
C	1.67300000	-4.95100000	-16.81500000
N	2.68900000	-4.27200000	-17.40100000
C	1.71700000	-6.37900000	-16.61700000
C	0.70000000	-7.00100000	-15.94600000
O	2.14600000	-11.26600000	-13.04100000
O	3.05700000	-10.17700000	-15.26800000
H	-2.57700000	-10.84300000	-14.38200000
H	2.55800000	-6.95300000	-17.00300000
H	0.72500000	-8.08600000	-15.73300000
H	-2.33100000	-6.17900000	-14.58400000
H	-1.60500000	-8.48200000	-16.25400000
H	-0.50000000	-9.94100000	-14.71300000
H	-1.43300000	-8.67100000	-12.12500000
H	3.51100000	-4.74900000	-17.75600000
H	1.09700000	-7.74600000	-12.19400000
H	2.66800000	-3.24100000	-17.50700000
H	-3.00400000	-8.40300000	-15.22700000
H	0.80400000	-9.52600000	-11.94000000
P	2.10000000	5.58600000	-20.75700000
C	-0.31300000	4.96900000	-19.89900000
O	1.04100000	5.30400000	-19.50600000
C	-1.18600000	5.14800000	-18.65300000
O	-1.36000000	3.85100000	-18.01300000

C	-0.57300000	6.07700000	-17.57000000
O	-1.64300000	6.89500000	-17.08500000
C	0.08300000	5.12000000	-16.56900000
C	-0.52200000	3.74000000	-16.84200000
N	0.55200000	-1.37000000	-16.75600000
C	-0.55900000	-0.67000000	-16.22700000
N	-1.57300000	-1.40700000	-15.65500000
N	-0.71100000	0.68900000	-16.32200000
C	0.33300000	1.33100000	-16.94400000
C	1.49000000	0.70200000	-17.49900000
C	1.64400000	-0.71900000	-17.41600000
O	2.55400000	-1.43900000	-17.83000000
N	2.34600000	1.67900000	-18.04900000
C	1.74200000	2.85200000	-17.85300000
N	0.50200000	2.70900000	-17.13600000
O	1.44600000	6.37000000	-21.87000000
O	3.37400000	6.03300000	-20.09200000
H	0.59900000	-2.43500000	-16.64100000
H	2.08900000	3.83300000	-18.17200000
H	-1.21600000	3.35200000	-16.04300000
H	1.18500000	5.14600000	-16.70400000
H	-2.16100000	-0.93300000	-14.94900000
H	0.14100000	6.81800000	-17.99700000
H	-1.44000000	-2.42700000	-15.50900000
H	-2.22300000	5.44000000	-18.93300000
H	-0.33000000	3.91100000	-20.23500000
H	-0.06000000	5.42800000	-15.50600000
H	-0.65800000	5.62600000	-20.72200000
P	-2.30900000	6.80000000	-15.54900000
C	-3.76600000	4.65500000	-16.12000000
O	-2.70600000	5.20700000	-15.30900000
C	-4.57800000	3.71500000	-15.22800000
O	-3.75900000	2.58100000	-14.84100000
C	-5.09000000	4.35400000	-13.90800000
O	-6.43400000	3.85500000	-13.80100000
C	-4.09100000	3.88600000	-12.84500000
C	-3.44800000	2.62400000	-13.43000000
N	-1.96000000	2.58100000	-13.30000000
C	-1.34700000	1.28500000	-13.40900000
O	-2.03000000	0.27100000	-13.38200000
N	0.05800000	1.26200000	-13.45200000
C	0.87100000	2.42200000	-13.59400000
O	2.05700000	2.26500000	-13.86400000
C	0.17900000	3.70000000	-13.42900000
C	-1.17800000	3.74700000	-13.35700000
C	1.01700000	4.93000000	-13.38200000
O	-3.52900000	7.67200000	-15.70400000
O	-1.26400000	7.04600000	-14.49300000
H	0.51600000	0.29400000	-13.51500000
H	-1.73000000	4.70600000	-13.31500000

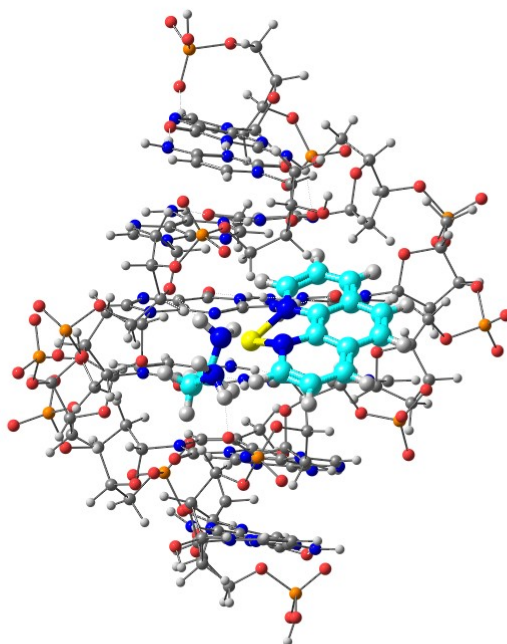
H	-3.86200000	1.65700000	-13.02200000
H	-3.35400000	4.70300000	-12.66500000
H	-5.19300000	5.46000000	-13.95700000
H	-5.41300000	3.25600000	-15.81000000
H	-3.26500000	4.08500000	-16.93500000
H	1.48900000	5.05400000	-12.39500000
H	1.83000000	4.89600000	-14.12200000
H	0.42700000	5.84200000	-13.58700000
H	-4.53500000	3.69700000	-11.84500000
H	-4.41500000	5.43400000	-16.56200000
P	-7.08100000	3.26900000	-12.38100000
C	-6.30800000	0.77000000	-12.86800000
O	-6.14400000	1.93100000	-12.03000000
C	-6.63500000	-0.44300000	-11.98900000
O	-5.39000000	-1.17600000	-11.77300000
C	-7.21000000	-0.13100000	-10.58400000
O	-8.44000000	-0.87400000	-10.53700000
C	-6.17600000	-0.67600000	-9.58800000
C	-4.95200000	-1.07500000	-10.40800000
N	-3.84100000	-0.06900000	-10.33700000
C	-2.46200000	-0.53800000	-10.41100000
O	-2.25900000	-1.74600000	-10.54700000
N	-1.44400000	0.38200000	-10.28600000
C	-1.71000000	1.72600000	-10.16200000
N	-0.65200000	2.57600000	-10.14700000
C	-3.07000000	2.19400000	-10.08500000
C	-4.09400000	1.29600000	-10.19900000
O	-8.47000000	2.87800000	-12.81300000
O	-6.81100000	4.19700000	-11.22900000
H	-3.27500000	3.25400000	-9.95100000
H	-5.15000000	1.62300000	-10.18500000
H	-4.52300000	-2.08300000	-10.17500000
H	-5.96900000	0.05900000	-8.79100000
H	-7.42500000	0.95100000	-10.42300000
H	-7.27500000	-1.17500000	-12.53600000
H	-0.76600000	3.56200000	-9.95900000
H	-5.30800000	0.63200000	-13.34900000
H	0.32300000	2.23100000	-10.24100000
H	-6.56800000	-1.56400000	-9.03200000
H	-7.08000000	0.90900000	-13.64800000
P	-9.51800000	-0.48800000	-9.31300000
C	-8.87800000	-2.94300000	-8.62900000
O	-9.16500000	-1.61400000	-8.13600000
C	-8.02400000	-3.64200000	-7.56900000
O	-6.71700000	-3.01400000	-7.50900000
C	-8.61300000	-3.60100000	-6.13200000
O	-8.60800000	-4.95300000	-5.65400000
C	-7.75400000	-2.58200000	-5.37800000
C	-6.46200000	-2.46900000	-6.18800000
N	-2.21500000	0.33100000	-7.11300000

C	-2.41500000	-1.06900000	-7.16200000
N	-1.35100000	-1.85600000	-7.52400000
N	-3.62600000	-1.66800000	-6.92900000
C	-4.63900000	-0.78500000	-6.66100000
C	-4.54100000	0.64200000	-6.65600000
C	-3.27000000	1.26700000	-6.86500000
O	-2.97300000	2.46100000	-6.86300000
N	-5.81000000	1.20400000	-6.40300000
C	-6.65100000	0.17600000	-6.25400000
N	-5.97700000	-1.08700000	-6.36800000
O	-10.85800000	-0.81100000	-9.93900000
O	-9.24300000	0.85600000	-8.70100000
H	-1.20900000	0.70300000	-7.22400000
H	-7.72200000	0.22900000	-6.07600000
H	-5.60100000	-3.08400000	-5.79400000
H	-8.31000000	-1.62200000	-5.30800000
H	-1.43800000	-2.86200000	-7.41200000
H	-9.69600000	-3.34500000	-6.11500000
H	-0.38400000	-1.47500000	-7.52500000
H	-7.81200000	-4.69000000	-7.89400000
H	-8.33100000	-2.90800000	-9.59800000
H	-7.56500000	-2.85400000	-4.31700000
H	-9.84000000	-3.47500000	-8.76700000
P	-7.49800000	-5.57200000	-4.56700000
C	-5.40900000	-5.67700000	-6.24300000
O	-6.00500000	-5.05500000	-5.08600000
C	-4.11500000	-6.38600000	-5.83500000
O	-3.03500000	-5.41400000	-5.71500000
C	-4.17500000	-7.12400000	-4.47300000
O	-3.45700000	-8.34400000	-4.73600000
C	-3.50700000	-6.15900000	-3.48500000
C	-2.71900000	-5.15200000	-4.33500000
N	-1.03900000	-0.15800000	-4.07300000
C	-0.38800000	-1.30300000	-4.44200000
N	-0.90000000	-2.56300000	-4.49600000
C	-2.22300000	-2.63900000	-4.11900000
C	-3.00800000	-1.50700000	-3.71000000
C	-2.38400000	-0.22200000	-3.71800000
N	-3.03800000	0.93100000	-3.43400000
N	-4.31400000	-1.91600000	-3.38400000
C	-4.34400000	-3.23600000	-3.59200000
N	-3.07800000	-3.74800000	-4.03200000
O	-7.66300000	-7.05800000	-4.75100000
O	-7.63000000	-4.88400000	-3.23400000
H	0.67100000	-1.17800000	-4.74600000
H	-5.20400000	-3.89400000	-3.45900000
H	-1.60100000	-5.25500000	-4.28100000
H	-4.28400000	-5.68500000	-2.84900000
H	-5.19800000	-7.42900000	-4.16600000
H	-3.75600000	-7.05700000	-6.65200000

H	-5.17700000	-4.81500000	-6.91400000
H	-2.57200000	1.84900000	-3.51200000
H	-4.01000000	0.91700000	-3.14700000
H	-2.85000000	-6.66500000	-2.74900000
H	-6.09400000	-6.37600000	-6.75700000
P	-2.65500000	-9.17000000	-3.52500000
C	-0.52000000	-7.95300000	-4.44100000
O	-1.33100000	-8.18100000	-3.26200000
C	0.86900000	-7.53600000	-3.96400000
O	0.88300000	-6.08100000	-3.84900000
C	1.30800000	-8.10200000	-2.59400000
O	2.41200000	-8.97000000	-2.89600000
C	1.77600000	-6.89200000	-1.77200000
C	1.35500000	-5.65200000	-2.56000000
N	0.22400000	-4.90400000	-1.91700000
C	0.34100000	-3.46400000	-1.76200000
O	1.40100000	-2.93200000	-2.10600000
N	-0.71000000	-2.75200000	-1.22700000
C	-1.86800000	-3.39700000	-0.84100000
N	-2.87200000	-2.63400000	-0.34200000
C	-1.97000000	-4.83200000	-0.95100000
C	-0.93500000	-5.54600000	-1.48900000
O	-2.25300000	-10.44700000	-4.21700000
O	-3.39900000	-9.15800000	-2.21800000
H	2.66800000	-9.49200000	-2.09700000
H	-2.86700000	-5.33600000	-0.59200000
H	-0.98500000	-6.64400000	-1.62700000
H	2.17900000	-4.92200000	-2.77400000
H	1.38500000	-6.91500000	-0.73700000
H	0.52000000	-8.69400000	-2.08200000
H	1.63300000	-7.75300000	-4.75200000
H	-3.77500000	-3.03700000	-0.11200000
H	-0.99700000	-7.13900000	-5.03100000
H	-2.82300000	-1.59900000	-0.35600000
H	2.88000000	-6.91800000	-1.63400000
H	-0.44600000	-8.87100000	-5.06000000
O	2.36900000	4.02700000	-21.30300000
O	-2.33600000	5.39100000	2.95300000
H	1.90200000	3.77000000	-22.14100000
H	-2.15100000	5.33300000	3.93100000
N	2.97500000	6.82100000	-6.64800000
N	6.99400000	6.86900000	-6.08600000
N	4.87900000	8.26900000	-4.86500000
N	4.97500000	5.52000000	-7.83800000
C	4.43800000	3.58000000	-9.83700000
C	3.44600000	4.46800000	-9.51700000
C	3.68500000	5.41600000	-8.43400000
C	2.67300000	6.14200000	-7.86700000
C	1.32400000	6.16200000	-8.42800000
C	0.38600000	6.95200000	-7.83700000

C	0.75100000	7.74700000	-6.68400000
C	2.01400000	7.68700000	-6.15100000
C	1.12600000	5.30600000	-9.59900000
C	7.33100000	8.05200000	-5.21800000
C	6.22100000	8.26400000	-4.18100000
C	5.90300000	4.56100000	-8.13900000
C	2.10800000	4.51300000	-10.09000000
C	5.67800000	3.61300000	-9.12500000
Pt	4.94100000	6.86200000	-6.36800000
H	7.51100000	6.93600000	-6.97300000
H	7.28200000	5.96000000	-5.64800000
H	4.67500000	9.20500000	-5.23500000
H	4.11100000	8.02600000	-4.17100000
H	4.28900000	2.81700000	-10.60500000
H	-0.63800000	7.01200000	-8.19300000
H	-0.00500000	8.37500000	-6.23300000
H	2.28900000	8.24900000	-5.25200000
H	0.13700000	5.33400000	-10.05500000
H	7.44700000	8.95900000	-5.85900000
H	8.31100000	7.91500000	-4.70400000
H	6.39800000	9.21200000	-3.62300000
H	6.24400000	7.44400000	-3.40800000
H	6.84400000	4.58600000	-7.57000000
H	1.93300000	3.84900000	-10.94700000
H	6.44100000	2.87600000	-9.36100000

[Pt(en)(phen)]²⁺ minor groove
Dock_ID: 113-cl2_phen



EDA for 113-cl2_phen in kcal mol⁻¹.

Electrostatic interaction	-807.7
Orbital interaction	-98.1
Dispersion energy	-66.6
Pauli repulsion	129.2
Total Bonding Energy	-843.2

Contributions of the solvation energies for 113-cl2_phen in kcal mol⁻¹.

E _{solv} (total system)	-1732.2
E _{solv} (intercalator)	-164.4
E _{solv} (duplex DNA)	-2351.5
ΔE _{solv}	783.7
ΔE _{int} (EDA)	-843.2
ΔE _{aq}	-59.5

$$\Delta E_{\text{solv}} = E_{\text{solv}}(\text{total system}) - E_{\text{solv}}(\text{intercalator}) - E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 113-cl2_phen system.
([Pt(en)(phen)]²⁺ minor groove)

P	-1.131000000	7.373000000	2.492000000
C	1.435000000	6.959000000	2.002000000
O	0.136000000	7.229000000	1.425000000
C	2.419000000	6.926000000	0.828000000
O	2.571000000	5.550000000	0.373000000
C	1.952000000	7.736000000	-0.412000000
O	3.112000000	8.454000000	-0.851000000
C	1.360000000	6.688000000	-1.362000000
C	1.831000000	5.323000000	-0.842000000
N	0.222000000	0.351000000	-0.657000000
C	1.489000000	0.880000000	-1.002000000
N	2.466000000	-0.006000000	-1.378000000
N	1.795000000	2.218000000	-0.947000000
C	0.740000000	3.019000000	-0.574000000
C	-0.566000000	2.563000000	-0.211000000
C	-0.875000000	1.165000000	-0.236000000
O	-1.926000000	0.586000000	0.047000000
N	-1.390000000	3.669000000	0.081000000
C	-0.632000000	4.753000000	-0.093000000
N	0.700000000	4.417000000	-0.524000000
O	-0.846000000	8.403000000	3.559000000
O	-2.340000000	7.442000000	1.598000000
H	0.062000000	-0.706000000	-0.752000000
H	-0.926000000	5.793000000	0.056000000
H	2.563000000	4.775000000	-1.502000000
H	0.253000000	6.794000000	-1.365000000
H	3.245000000	0.342000000	-1.948000000
H	1.223000000	8.538000000	-0.147000000
H	2.253000000	-1.021000000	-1.456000000
H	3.446000000	7.203000000	1.157000000
H	1.416000000	5.975000000	2.516000000
H	1.643000000	6.835000000	-2.428000000
H	1.703000000	7.757000000	2.721000000
P	3.752000000	8.350000000	-2.393000000
C	5.066000000	6.155000000	-1.730000000
O	4.083000000	6.738000000	-2.617000000
C	5.698000000	4.991000000	-2.492000000
O	4.719000000	3.920000000	-2.607000000
C	6.140000000	5.347000000	-3.939000000
O	7.379000000	4.632000000	-4.085000000
C	4.982000000	4.849000000	-4.809000000
C	4.369000000	3.703000000	-3.999000000
N	2.887000000	3.618000000	-4.066000000
C	2.312000000	2.312000000	-3.911000000
O	3.016000000	1.315000000	-3.871000000
N	0.908000000	2.252000000	-3.882000000

C	0.058000000	3.387000000	-3.819000000
O	-1.130000000	3.196000000	-3.578000000
C	0.716000000	4.677000000	-4.048000000
C	2.072000000	4.764000000	-4.101000000
C	-0.170000000	5.862000000	-4.212000000
O	5.006000000	9.176000000	-2.249000000
O	2.712000000	8.637000000	-3.441000000
H	0.478000000	1.268000000	-3.798000000
H	2.609000000	5.728000000	-4.203000000
H	4.796000000	2.685000000	-4.252000000
H	4.269000000	5.692000000	-4.963000000
H	6.371000000	6.425000000	-4.081000000
H	6.531000000	4.539000000	-1.904000000
H	4.522000000	5.789000000	-0.831000000
H	-0.896000000	5.706000000	-5.027000000
H	-0.755000000	6.058000000	-3.300000000
H	0.386000000	6.782000000	-4.443000000
H	5.279000000	4.530000000	-5.827000000
H	5.835000000	6.888000000	-1.420000000
P	7.923000000	4.063000000	-5.558000000
C	6.976000000	1.663000000	-4.990000000
O	6.896000000	2.794000000	-5.889000000
C	6.959000000	0.371000000	-5.812000000
O	5.580000000	-0.018000000	-6.030000000
C	7.592000000	0.468000000	-7.226000000
O	8.286000000	-0.780000000	-7.405000000
C	6.404000000	0.757000000	-8.151000000
C	5.169000000	0.264000000	-7.387000000
N	4.047000000	1.243000000	-7.308000000
C	2.710000000	0.689000000	-7.100000000
O	2.601000000	-0.528000000	-6.997000000
N	1.642000000	1.560000000	-7.040000000
C	1.826000000	2.916000000	-7.147000000
N	0.720000000	3.705000000	-7.039000000
C	3.146000000	3.465000000	-7.323000000
C	4.221000000	2.616000000	-7.373000000
O	9.306000000	3.574000000	-5.208000000
O	7.671000000	5.041000000	-6.673000000
H	3.282000000	4.541000000	-7.401000000
H	5.260000000	2.988000000	-7.477000000
H	4.745000000	-0.714000000	-7.760000000
H	6.384000000	1.849000000	-8.366000000
H	8.401000000	1.226000000	-7.300000000
H	7.381000000	-0.477000000	-5.222000000
H	0.787000000	4.713000000	-7.073000000
H	6.045000000	1.724000000	-4.368000000
H	-0.227000000	3.299000000	-6.899000000
H	6.484000000	0.288000000	-9.154000000
H	7.864000000	1.702000000	-4.331000000
P	7.901000000	-1.903000000	-8.575000000

C	5.773000000	-3.072000000	-7.433000000
O	6.267000000	-2.183000000	-8.450000000
C	5.219000000	-4.355000000	-8.064000000
O	3.843000000	-4.136000000	-8.485000000
C	5.969000000	-4.857000000	-9.324000000
O	6.038000000	-6.277000000	-9.082000000
C	5.077000000	-4.460000000	-10.511000000
C	3.756000000	-3.961000000	-9.914000000
N	0.049000000	-0.275000000	-10.172000000
C	-0.093000000	-1.674000000	-10.046000000
N	-1.372000000	-2.171000000	-10.090000000
N	0.970000000	-2.551000000	-9.990000000
C	2.197000000	-1.937000000	-10.115000000
C	2.419000000	-0.535000000	-10.290000000
C	1.322000000	0.382000000	-10.234000000
O	1.315000000	1.612000000	-10.251000000
N	3.798000000	-0.275000000	-10.426000000
C	4.405000000	-1.459000000	-10.347000000
N	3.467000000	-2.538000000	-10.175000000
O	8.706000000	-3.106000000	-8.156000000
O	8.014000000	-1.287000000	-9.948000000
H	-0.829000000	0.341000000	-10.123000000
H	5.474000000	-1.648000000	-10.399000000
H	2.868000000	-4.573000000	-10.225000000
H	5.586000000	-3.715000000	-11.152000000
H	-1.568000000	-3.114000000	-9.772000000
H	7.011000000	-4.485000000	-9.414000000
H	-2.195000000	-1.533000000	-10.054000000
H	5.120000000	-5.162000000	-7.297000000
H	4.941000000	-2.484000000	-6.970000000
H	4.872000000	-5.317000000	-11.195000000
H	6.530000000	-3.305000000	-6.664000000
P	6.584000000	-7.315000000	-10.269000000
C	4.029000000	-7.847000000	-10.424000000
O	5.200000000	-7.504000000	-11.194000000
C	2.828000000	-7.737000000	-11.359000000
O	2.507000000	-6.329000000	-11.546000000
C	3.057000000	-8.347000000	-12.772000000
O	2.103000000	-9.419000000	-12.803000000
C	2.882000000	-7.179000000	-13.747000000
C	2.148000000	-6.100000000	-12.948000000
N	0.472000000	-1.168000000	-13.303000000
C	-0.202000000	-2.343000000	-13.093000000
N	0.329000000	-3.592000000	-13.018000000
C	1.687000000	-3.619000000	-13.214000000
C	2.506000000	-2.468000000	-13.450000000
C	1.850000000	-1.196000000	-13.489000000
N	2.498000000	-0.027000000	-13.735000000
N	3.848000000	-2.860000000	-13.618000000
C	3.866000000	-4.190000000	-13.481000000

N	2.560000000	-4.722000000	-13.225000000
O	6.888000000	-8.573000000	-9.495000000
O	7.584000000	-6.682000000	-11.196000000
H	-1.298000000	-2.255000000	-12.952000000
H	4.736000000	-4.835000000	-13.554000000
H	1.020000000	-6.174000000	-13.002000000
H	3.877000000	-6.848000000	-14.113000000
H	4.045000000	-8.847000000	-12.883000000
H	1.912000000	-8.182000000	-10.889000000
H	3.911000000	-7.149000000	-9.556000000
H	2.013000000	0.877000000	-13.607000000
H	3.510000000	0.001000000	-13.749000000
H	2.343000000	-7.442000000	-14.680000000
H	4.130000000	-8.891000000	-10.056000000
P	0.975000000	-9.637000000	-14.013000000
C	-0.773000000	-7.878000000	-12.995000000
O	0.159000000	-8.188000000	-14.054000000
C	-2.183000000	-7.734000000	-13.576000000
O	-2.386000000	-6.339000000	-13.945000000
C	-2.486000000	-8.560000000	-14.844000000
O	-3.730000000	-9.226000000	-14.553000000
C	-2.666000000	-7.539000000	-15.984000000
C	-2.433000000	-6.161000000	-15.355000000
N	-1.144000000	-5.509000000	-15.792000000
C	-1.106000000	-4.059000000	-15.870000000
O	-2.155000000	-3.435000000	-15.680000000
N	0.071000000	-3.421000000	-16.200000000
C	1.221000000	-4.151000000	-16.426000000
N	2.364000000	-3.459000000	-16.673000000
C	1.195000000	-5.586000000	-16.336000000
C	0.028000000	-6.225000000	-16.010000000
O	0.111000000	-10.741000000	-13.462000000
O	1.644000000	-9.723000000	-15.356000000
H	-3.974000000	-9.834000000	-15.290000000
H	2.098000000	-6.158000000	-16.540000000
H	-0.021000000	-7.326000000	-15.910000000
H	-3.255000000	-5.417000000	-15.520000000
H	-2.011000000	-7.760000000	-16.845000000
H	-1.735000000	-9.337000000	-15.084000000
H	-2.959000000	-7.890000000	-12.780000000
H	3.216000000	-3.937000000	-16.944000000
H	-0.415000000	-6.879000000	-12.623000000
H	2.361000000	-2.429000000	-16.783000000
H	-3.688000000	-7.606000000	-16.410000000
H	-0.752000000	-8.612000000	-12.163000000
P	1.713000000	6.575000000	-19.155000000
C	-0.913000000	6.048000000	-19.174000000
O	0.111000000	7.055000000	-19.226000000
C	-1.610000000	6.015000000	-17.807000000
O	-1.537000000	4.645000000	-17.324000000

C	-1.005000000	6.911000000	-16.696000000
O	-2.104000000	7.613000000	-16.100000000
C	-0.209000000	5.953000000	-15.804000000
C	-0.744000000	4.555000000	-16.113000000
N	0.180000000	-0.557000000	-16.408000000
C	-0.993000000	0.134000000	-16.019000000
N	-2.103000000	-0.621000000	-15.706000000
N	-1.098000000	1.499000000	-16.008000000
C	0.062000000	2.154000000	-16.357000000
C	1.292000000	1.533000000	-16.737000000
C	1.392000000	0.105000000	-16.783000000
O	2.344000000	-0.611000000	-17.096000000
N	2.263000000	2.523000000	-16.995000000
C	1.660000000	3.696000000	-16.791000000
N	0.296000000	3.536000000	-16.370000000
O	2.404000000	7.486000000	-20.140000000
O	2.176000000	6.469000000	-17.725000000
H	0.184000000	-1.629000000	-16.359000000
H	2.101000000	4.696000000	-16.910000000
H	-1.459000000	4.144000000	-15.341000000
H	0.877000000	6.064000000	-16.043000000
H	-2.788000000	-0.205000000	-15.058000000
H	-0.389000000	7.747000000	-17.102000000
H	-2.010000000	-1.657000000	-15.642000000
H	-2.704000000	6.194000000	-17.928000000
H	-0.534000000	5.038000000	-19.441000000
H	-0.276000000	6.192000000	-14.713000000
H	-1.616000000	6.371000000	-19.971000000
P	-2.774000000	7.254000000	-14.609000000
C	-4.058000000	5.110000000	-15.515000000
O	-3.056000000	5.615000000	-14.609000000
C	-5.120000000	4.341000000	-14.728000000
O	-4.621000000	3.011000000	-14.412000000
C	-5.562000000	4.976000000	-13.385000000
O	-6.997000000	4.951000000	-13.509000000
C	-4.984000000	4.065000000	-12.293000000
C	-4.340000000	2.875000000	-13.009000000
N	-2.852000000	2.791000000	-12.834000000
C	-2.252000000	1.510000000	-13.052000000
O	-2.945000000	0.510000000	-13.216000000
N	-0.849000000	1.442000000	-12.998000000
C	-0.006000000	2.589000000	-12.984000000
O	1.192000000	2.431000000	-13.188000000
C	-0.684000000	3.864000000	-12.746000000
C	-2.043000000	3.938000000	-12.728000000
C	0.169000000	5.064000000	-12.524000000
O	-4.069000000	8.026000000	-14.646000000
O	-1.753000000	7.435000000	-13.520000000
H	-0.403000000	0.473000000	-13.097000000
H	-2.573000000	4.899000000	-12.607000000

H	-4.779000000	1.876000000	-12.727000000
H	-4.286000000	4.636000000	-11.646000000
H	-5.267000000	6.041000000	-13.273000000
H	-6.002000000	4.131000000	-15.384000000
H	-3.499000000	4.417000000	-16.188000000
H	0.224000000	5.332000000	-11.460000000
H	1.200000000	4.906000000	-12.873000000
H	-0.224000000	5.952000000	-13.061000000
H	-5.774000000	3.685000000	-11.600000000
H	-4.529000000	5.903000000	-16.124000000
P	-8.011000000	5.099000000	-12.191000000
C	-8.054000000	2.483000000	-12.398000000
O	-7.889000000	3.594000000	-11.482000000
C	-7.819000000	1.213000000	-11.582000000
O	-6.386000000	1.012000000	-11.421000000
C	-8.443000000	1.248000000	-10.159000000
O	-9.173000000	0.008000000	-10.122000000
C	-7.247000000	1.366000000	-9.211000000
C	-6.065000000	0.815000000	-10.011000000
N	-4.763000000	1.485000000	-9.804000000
C	-3.557000000	0.666000000	-9.950000000
O	-3.697000000	-0.536000000	-10.137000000
N	-2.331000000	1.290000000	-9.878000000
C	-2.233000000	2.641000000	-9.636000000
N	-0.986000000	3.176000000	-9.640000000
C	-3.418000000	3.431000000	-9.388000000
C	-4.644000000	2.836000000	-9.476000000
O	-9.356000000	5.287000000	-12.849000000
O	-7.496000000	6.060000000	-11.155000000
H	-3.325000000	4.484000000	-9.127000000
H	-5.583000000	3.390000000	-9.297000000
H	-5.922000000	-0.302000000	-9.882000000
H	-7.119000000	2.432000000	-8.918000000
H	-9.190000000	2.061000000	-10.023000000
H	-8.166000000	0.316000000	-12.153000000
H	-0.831000000	4.156000000	-9.455000000
H	-7.318000000	2.561000000	-13.227000000
H	-0.150000000	2.599000000	-9.878000000
H	-7.376000000	0.830000000	-8.248000000
H	-9.082000000	2.491000000	-12.811000000
P	-9.428000000	-0.861000000	-8.723000000
C	-7.300000000	-2.330000000	-9.277000000
O	-7.905000000	-1.407000000	-8.340000000
C	-6.589000000	-3.425000000	-8.474000000
O	-5.247000000	-2.966000000	-8.185000000
C	-7.237000000	-3.739000000	-7.098000000
O	-7.160000000	-5.156000000	-6.905000000
C	-6.467000000	-2.848000000	-6.113000000
C	-5.131000000	-2.563000000	-6.805000000
N	-1.006000000	0.521000000	-6.799000000

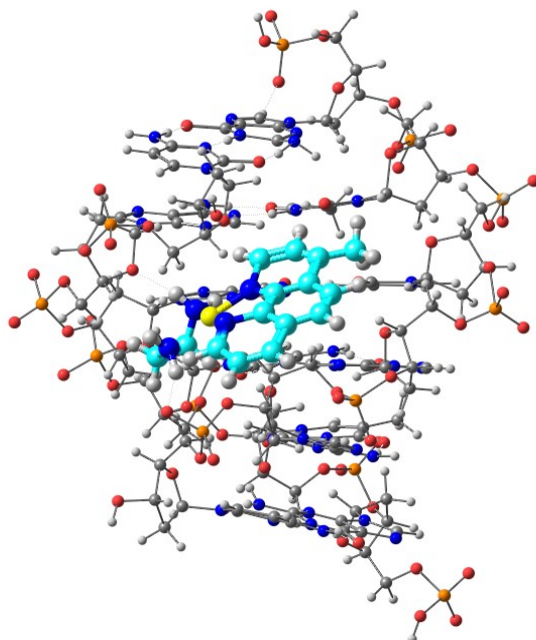
C	-1.117000000	-0.878000000	-6.974000000
N	0.029000000	-1.604000000	-7.209000000
N	-2.305000000	-1.545000000	-6.978000000
C	-3.400000000	-0.734000000	-6.826000000
C	-3.390000000	0.689000000	-6.665000000
C	-2.138000000	1.391000000	-6.682000000
O	-1.904000000	2.596000000	-6.601000000
N	-4.714000000	1.151000000	-6.546000000
C	-5.498000000	0.067000000	-6.627000000
N	-4.738000000	-1.134000000	-6.790000000
O	-10.307000000	-1.985000000	-9.213000000
O	-9.819000000	0.026000000	-7.571000000
H	-0.032000000	0.968000000	-6.831000000
H	-6.584000000	0.045000000	-6.600000000
H	-4.253000000	-3.165000000	-6.424000000
H	-7.061000000	-1.929000000	-5.925000000
H	-0.025000000	-2.615000000	-7.109000000
H	-8.333000000	-3.553000000	-7.077000000
H	0.964000000	-1.185000000	-7.037000000
H	-6.425000000	-4.344000000	-9.083000000
H	-6.535000000	-1.725000000	-9.831000000
H	-6.332000000	-3.304000000	-5.111000000
H	-8.033000000	-2.765000000	-9.979000000
P	-6.084000000	-5.914000000	-5.867000000
C	-3.871000000	-5.665000000	-7.350000000
O	-4.587000000	-5.277000000	-6.153000000
C	-2.495000000	-6.184000000	-6.946000000
O	-1.651000000	-5.128000000	-6.395000000
C	-2.535000000	-7.272000000	-5.841000000
O	-1.383000000	-8.067000000	-6.188000000
C	-2.364000000	-6.479000000	-4.535000000
C	-1.580000000	-5.232000000	-4.962000000
N	-0.228000000	-0.363000000	-3.740000000
C	0.526000000	-1.452000000	-4.097000000
N	0.079000000	-2.708000000	-4.343000000
C	-1.286000000	-2.839000000	-4.191000000
C	-2.170000000	-1.788000000	-3.775000000
C	-1.600000000	-0.492000000	-3.577000000
N	-2.321000000	0.609000000	-3.236000000
N	-3.490000000	-2.275000000	-3.718000000
C	-3.427000000	-3.558000000	-4.098000000
N	-2.086000000	-3.973000000	-4.375000000
O	-6.230000000	-7.364000000	-6.219000000
O	-6.334000000	-5.430000000	-4.449000000
H	1.609000000	-1.257000000	-4.217000000
H	-4.268000000	-4.250000000	-4.190000000
H	-0.472000000	-5.288000000	-4.739000000
H	-3.359000000	-6.240000000	-4.109000000
H	-3.426000000	-7.930000000	-5.869000000
H	-1.901000000	-6.524000000	-7.851000000

H	-3.785000000	-4.722000000	-7.942000000
H	-1.889000000	1.548000000	-3.252000000
H	-3.333000000	0.560000000	-3.186000000
H	-1.849000000	-7.033000000	-3.729000000
H	-4.416000000	-6.433000000	-7.940000000
P	-0.646000000	-9.119000000	-5.163000000
C	1.099000000	-7.248000000	-4.409000000
O	0.023000000	-8.100000000	-4.003000000
C	2.137000000	-7.221000000	-3.280000000
O	2.293000000	-5.819000000	-2.908000000
C	1.756000000	-7.986000000	-1.994000000
O	2.769000000	-8.995000000	-1.860000000
C	1.854000000	-6.958000000	-0.854000000
C	2.021000000	-5.592000000	-1.515000000
N	0.801000000	-4.725000000	-1.418000000
C	0.982000000	-3.290000000	-1.287000000
O	2.121000000	-2.828000000	-1.408000000
N	-0.105000000	-2.490000000	-1.010000000
C	-1.370000000	-3.036000000	-0.905000000
N	-2.379000000	-2.212000000	-0.534000000
C	-1.574000000	-4.439000000	-1.186000000
C	-0.498000000	-5.241000000	-1.440000000
O	0.436000000	-9.670000000	-6.072000000
O	-1.539000000	-9.991000000	-4.327000000
H	2.557000000	-9.601000000	-1.110000000
H	-2.586000000	-4.844000000	-1.199000000
H	-0.614000000	-6.316000000	-1.656000000
H	2.896000000	-4.992000000	-1.150000000
H	1.003000000	-7.025000000	-0.151000000
H	0.762000000	-8.488000000	-2.042000000
H	3.151000000	-7.522000000	-3.635000000
H	-3.343000000	-2.531000000	-0.507000000
H	0.664000000	-6.221000000	-4.546000000
H	-2.227000000	-1.199000000	-0.382000000
H	2.728000000	-7.188000000	-0.205000000
H	1.576000000	-7.586000000	-5.359000000
O	1.679000000	5.018000000	-19.744000000
O	-1.136000000	5.871000000	3.225000000
H	1.644000000	4.926000000	-20.738000000
H	-0.768000000	5.836000000	4.149000000
N	-2.001000000	-6.322000000	-10.526000000
N	0.926000000	-8.079000000	-8.336000000
N	0.667000000	-5.567000000	-9.432000000
N	-1.851000000	-8.768000000	-9.468000000
C	-4.231000000	-9.987000000	-8.420000000
C	-4.364000000	-8.878000000	-9.198000000
C	-3.162000000	-8.220000000	-9.700000000
C	-3.232000000	-6.992000000	-10.303000000
C	-4.491000000	-6.341000000	-10.642000000
C	-4.448000000	-5.124000000	-11.275000000

C	-3.192000000	-4.523000000	-11.586000000
C	-2.010000000	-5.128000000	-11.194000000
C	-5.690000000	-7.048000000	-10.206000000
C	1.865000000	-7.004000000	-7.840000000
C	1.221000000	-5.625000000	-8.035000000
C	-1.792000000	-9.812000000	-8.538000000
C	-5.631000000	-8.219000000	-9.532000000
C	-2.903000000	-10.462000000	-8.082000000
P	-0.568000000	-7.211000000	-9.463000000
H	1.439000000	-8.771000000	-8.894000000
H	0.532000000	-8.603000000	-7.503000000
H	1.424000000	-5.624000000	-10.141000000
H	0.195000000	-4.661000000	-9.589000000
H	-5.084000000	-10.505000000	-8.001000000
H	-5.361000000	-4.592000000	-11.535000000
H	-3.167000000	-3.593000000	-12.137000000
H	-1.028000000	-4.685000000	-11.418000000
H	-6.648000000	-6.580000000	-10.431000000
H	2.097000000	-7.175000000	-6.756000000
H	2.849000000	-7.060000000	-8.371000000
H	0.364000000	-5.481000000	-7.318000000
H	1.972000000	-4.816000000	-7.843000000
H	-0.782000000	-10.124000000	-8.249000000
H	-6.535000000	-8.707000000	-9.173000000
H	-2.821000000	-11.321000000	-7.433000000

[Pt(en)(4-Mephen)]²⁺ systems

[Pt(en)(4-Mephen)]²⁺ minor groove
Dock_ID: 69-cl1_4-Mephen



EDA for 69-cl1_4-Mephen in kcal mol⁻¹.

Electrostatic interaction	-778.2
Orbital interaction	-108.9
Dispersion energy	-69.0
Pauli repulsion	133.9
Total Bonding Energy	-822.2

Contributions of the solvation energies for 69-cl1_4-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1841.8
E _{solv} (intercalator)	-162.7
E _{solv} (duplex DNA)	-2426.2
ΔE _{solv}	747.0
ΔE _{int} (EDA)	-822.2
ΔE _{aq}	-75.1

$$\Delta E_{\text{solv}} = E_{\text{solv}}(\text{total system}) - E_{\text{solv}}(\text{intercalator}) - E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 69-cl1_4-Mephen system.
([Pt(en)(phen)]²⁺ minor groove)

P	-2.38400000	5.28800000	2.68900000
C	0.26200000	5.04900000	2.82600000
O	-0.85600000	5.94300000	2.88600000
C	0.99100000	5.14100000	1.48400000
O	0.93800000	3.80600000	0.88900000
C	0.39900000	6.11600000	0.44300000
O	1.47400000	6.91200000	-0.02400000
C	-0.33400000	5.23400000	-0.57700000
C	0.21900000	3.82400000	-0.37100000
N	-0.54100000	-1.31400000	-0.42100000
C	0.74000000	-0.64900000	-0.77800000
N	1.85200000	-1.17000000	-0.83200000
N	0.69900000	0.82100000	-0.61300000
C	-0.45500000	1.40800000	-0.34300000
C	-1.76600000	0.65800000	-0.10100000
C	-1.63600000	-0.61700000	-0.14600000
O	-2.78300000	-1.59400000	0.12100000
N	-2.77700000	1.65200000	0.07600000
C	-2.21400000	2.81200000	-0.02000000
N	-0.81100000	2.75100000	-0.29600000
O	-3.21900000	5.94100000	3.82100000
O	-2.84800000	5.42900000	1.22700000
H	-0.42800000	-2.39900000	-0.52900000
H	-2.70800000	3.80300000	0.08200000
H	0.99100000	3.51000000	-1.12600000
H	-1.43400000	5.30200000	-0.37300000
H	2.52900000	-0.78400000	-1.50600000
H	-0.27100000	6.88200000	0.90900000
H	1.78700000	-2.28800000	-1.21200000
H	2.09200000	5.30800000	1.63600000
H	0.01500000	4.01200000	3.09300000
H	-0.21900000	5.57700000	-1.62000000
H	0.94200000	5.43800000	3.67400000
P	2.19600000	6.72900000	-1.54300000
C	3.52400000	4.51300000	-0.75800000
O	2.57700000	5.09300000	-1.67500000
C	4.53200000	3.71900000	-1.53600000
O	3.96200000	2.39300000	-1.77100000
C	4.98600000	4.30600000	-2.91200000
O	6.40900000	4.38000000	-2.75900000
C	4.55700000	3.29000000	-3.99000000
C	3.75500000	2.10500000	-3.33200000
N	2.29100000	2.24100000	-3.55100000
C	1.70400000	0.85100000	-3.55800000
O	2.18200000	0.04500000	-3.44100000
N	0.18500000	1.01800000	-3.67100000

C	-0.73900000	2.17900000	-3.66800000
O	-1.66400000	2.12600000	-3.57500000
C	0.20000000	3.44200000	-3.73500000
C	1.54100000	3.44700000	-3.63300000
C	-0.57600000	4.71800000	-3.92200000
O	3.52200000	7.56000000	-1.30100000
O	1.29400000	6.98600000	-2.60400000
H	-0.30400000	0.04800000	-3.69600000
H	2.14100000	4.35800000	-3.60800000
H	4.08900000	1.19200000	-3.43200000
H	3.97100000	3.79200000	-4.77700000
H	4.59400000	5.31100000	-3.08400000
H	5.40800000	3.43400000	-0.90700000
H	2.91900000	3.85400000	-0.10100000
H	-0.49400000	5.07700000	-4.97600000
H	-1.62800000	4.58700000	-3.69900000
H	-0.19100000	5.51400000	-3.29400000
H	5.39600000	2.80000000	-4.48400000
H	4.04200000	5.27600000	-0.14000000
P	7.35500000	4.87200000	-4.04300000
C	7.94300000	2.32800000	-4.19500000
O	7.48000000	3.46000000	-4.96700000
C	7.88400000	1.10100000	-5.11100000
O	6.51100000	0.72000000	-5.30300000
C	8.50400000	1.29400000	-6.48000000
O	9.40600000	0.20200000	-6.44000000
C	7.35700000	1.24100000	-7.47100000
C	6.15800000	0.64300000	-6.72000000
N	4.93100000	1.43300000	-6.87100000
C	3.66900000	0.49200000	-6.70300000
O	3.74600000	-0.53300000	-6.60900000
N	2.46000000	1.36000000	-6.78200000
C	2.41100000	2.59100000	-6.93200000
N	1.17300000	3.26700000	-6.98400000
C	3.60800000	3.44800000	-7.10500000
C	4.84400000	2.74200000	-7.05000000
O	8.62400000	5.25300000	-3.42100000
O	6.60600000	5.84200000	-4.97700000
H	3.57300000	4.48400000	-7.28300000
H	5.77300000	3.31300000	-7.14300000
H	5.96700000	-0.43500000	-6.93500000
H	7.19200000	2.22800000	-7.90000000
H	9.13900000	2.19200000	-6.58100000
H	8.32000000	0.21500000	-4.55400000
H	1.08100000	4.23900000	-6.94000000
H	7.29400000	2.19500000	-3.30100000
H	0.31600000	2.68000000	-6.78900000
H	7.59300000	0.57600000	-8.40300000
H	8.99400000	2.51600000	-3.86100000
P	9.92100000	-0.47900000	-8.05200000

C	8.12200000	-2.22800000	-7.66600000
O	8.74500000	-1.27100000	-8.52000000
C	7.07700000	-3.02100000	-8.51400000
O	5.85800000	-2.25700000	-8.58800000
C	7.58300000	-3.25900000	-9.96400000
O	7.47400000	-4.67200000	-10.20000000
C	6.76000000	-2.32600000	-10.84300000
C	5.50800000	-1.98100000	-9.97100000
N	1.25600000	0.97900000	-9.90900000
C	1.29500000	-0.64400000	-9.75600000
N	0.41100000	-1.18500000	-9.47600000
N	2.78600000	-1.02000000	-9.79200000
C	3.55000000	-0.31400000	-9.93700000
C	3.50200000	1.17600000	-10.08600000
C	2.44800000	1.70400000	-10.05300000
O	1.98600000	3.08000000	-10.11600000
N	4.85600000	1.64800000	-10.28900000
C	5.72600000	0.61600000	-10.25500000
N	5.05600000	-0.63700000	-10.02100000
O	11.06100000	-1.59600000	-7.38100000
O	10.47100000	0.53400000	-8.92900000
H	0.24000000	1.22900000	-9.84300000
H	6.80900000	0.67100000	-10.36000000
H	4.59500000	-2.67800000	-10.20900000
H	7.36500000	-1.41800000	-11.04800000
H	0.33900000	-2.38800000	-9.69900000
H	8.67800000	-3.10300000	-10.07800000
H	-0.66600000	-0.97700000	-9.74700000
H	6.78300000	-4.01500000	-8.00000000
H	7.58700000	-1.69000000	-6.81700000
H	6.47900000	-2.73100000	-11.80200000
H	8.84000000	-2.91400000	-7.20400000
P	6.17700000	-5.38900000	-11.00300000
C	4.14000000	-5.16300000	-9.46400000
O	4.90700000	-4.70900000	-10.67200000
C	2.73200000	-5.73700000	-9.86300000
O	1.90100000	-4.81200000	-10.44200000
C	2.89500000	-6.85800000	-10.95100000
O	1.77500000	-7.78800000	-10.62600000
C	2.69600000	-6.11500000	-12.30300000
C	1.80600000	-4.84400000	-11.77500000
N	0.69500000	0.06300000	-13.05800000
C	-0.20000000	-1.01400000	-12.54200000
N	0.06100000	-2.10200000	-12.49500000
C	1.46000000	-2.37700000	-12.56500000
C	2.38800000	-1.37600000	-13.02800000
C	1.73900000	-0.12400000	-13.18500000
N	2.58600000	1.01000000	-13.61900000
N	3.70600000	-1.85600000	-13.14600000
C	3.62800000	-3.23200000	-12.72300000

N	2.32200000	-3.46900000	-12.47800000
O	6.36600000	-6.90500000	-10.76400000
O	6.33500000	-4.87100000	-12.65800000
H	-1.31200000	-0.76200000	-12.48500000
H	4.50400000	-3.88200000	-12.68600000
H	0.70000000	-4.92900000	-12.06900000
H	3.62500000	-5.83000000	-12.71500000
H	3.81000000	-7.44300000	-10.93500000
H	2.20600000	-6.14100000	-8.95200000
H	3.94700000	-4.17500000	-8.88800000
H	2.19600000	1.92000000	-13.57200000
H	3.61900000	0.97900000	-13.66900000
H	2.13400000	-6.66700000	-13.04400000
H	4.69900000	-5.84100000	-8.86800000
P	1.03300000	-8.60200000	-11.63200000
C	-0.88700000	-6.94300000	-12.04500000
O	0.26500000	-7.76500000	-12.70400000
C	-2.13300000	-7.02100000	-12.90200000
O	-2.45900000	-5.70800000	-13.35900000
C	-1.99400000	-7.86900000	-14.21600000
O	-3.06300000	-8.87100000	-14.11300000
C	-2.30300000	-6.90200000	-15.38200000
C	-2.30400000	-5.47900000	-14.68600000
N	-1.02100000	-4.70300000	-14.99300000
C	-1.18900000	-3.29000000	-15.15300000
O	-2.13300000	-2.76900000	-15.04800000
N	0.01900000	-2.61800000	-15.65300000
C	1.23600000	-3.27500000	-15.73300000
N	2.25400000	-2.58500000	-16.22400000
C	1.36700000	-4.64400000	-15.40000000
C	0.16400000	-5.37100000	-14.97400000
O	0.05300000	-9.49900000	-10.69000000
O	1.98500000	-9.51600000	-12.70800000
H	-3.05700000	-9.44600000	-14.88800000
H	2.29400000	-5.15100000	-15.39200000
H	0.26200000	-6.41600000	-14.69000000
H	-3.16200000	-4.84900000	-15.01100000
H	-1.57600000	-6.99600000	-16.20000000
H	-1.04300000	-8.40500000	-14.33100000
H	-2.97400000	-7.35800000	-12.30900000
H	3.19600000	-2.95800000	-16.27100000
H	-0.48300000	-5.83300000	-12.05900000
H	2.18900000	-1.55800000	-16.43700000
H	-3.27200000	-7.11100000	-15.82700000
H	-1.04600000	-7.24200000	-11.04800000
P	1.48100000	6.82400000	-19.67100000
C	-1.08900000	6.70600000	-18.99400000
O	0.27100000	6.89400000	-18.53000000
C	-1.96300000	6.79300000	-17.73500000
O	-2.10900000	5.46900000	-17.16100000

C	-1.36700000	7.68400000	-16.61100000
O	-2.45400000	8.44700000	-16.07600000
C	-0.66400000	6.69300000	-15.67700000
C	-1.25800000	5.31200000	-16.00000000
N	-0.11000000	0.23200000	-16.09000000
C	-1.30400000	0.88200000	-15.63300000
N	-2.36200000	0.11700000	-15.15900000
N	-1.46600000	2.25300000	-15.74900000
C	-0.43200000	2.91800000	-16.19500000
C	0.84600000	2.29800000	-16.65800000
C	0.84600000	1.04800000	-16.52000000
O	2.09100000	0.10700000	-16.95200000
N	1.74900000	3.34000000	-17.06000000
C	1.08600000	4.48600000	-16.87900000
N	-0.23700000	4.29700000	-16.32500000
O	1.25700000	7.82600000	-20.75100000
O	2.74800000	6.77200000	-18.84900000
H	-0.07000000	-0.85800000	-15.94200000
H	1.46700000	5.48800000	-17.10400000
H	-1.95300000	4.89100000	-15.21600000
H	0.42700000	6.74600000	-15.86000000
H	-2.99200000	0.54400000	-14.49900000
H	-0.67300000	8.46400000	-17.00900000
H	-2.21600000	-0.91800000	-15.05300000
H	-3.01300000	7.08300000	-18.00000000
H	-1.19500000	5.71500000	-19.47200000
H	-0.76800000	6.94500000	-14.58800000
H	-1.35000000	7.50500000	-19.71800000
P	-3.02200000	8.29400000	-14.50500000
C	-4.54400000	6.20100000	-15.09000000
O	-3.43200000	6.70600000	-14.31500000
C	-5.30600000	5.20900000	-14.19500000
O	-4.47000000	4.05400000	-13.93800000
C	-5.73500000	5.75800000	-12.81000000
O	-7.03200000	5.20600000	-12.58900000
C	-4.61300000	5.28200000	-11.86700000
C	-4.01300000	4.04400000	-12.55300000
N	-2.54800000	4.02100000	-12.56100000
C	-1.91900000	2.69200000	-12.76800000
O	-2.66200000	1.67500000	-12.78700000
N	-0.55900000	2.70000000	-12.86000000
C	0.25600000	3.76900000	-12.94100000
O	1.48100000	3.61200000	-13.25400000
C	-0.37300000	5.09500000	-12.68500000
C	-1.74200000	5.13900000	-12.56900000
C	0.48500000	6.28800000	-12.54900000
O	-4.24300000	9.19700000	-14.54000000
O	-1.91300000	8.47600000	-13.50200000
H	-0.11400000	1.68100000	-12.98100000
H	-2.26100000	6.10300000	-12.44600000

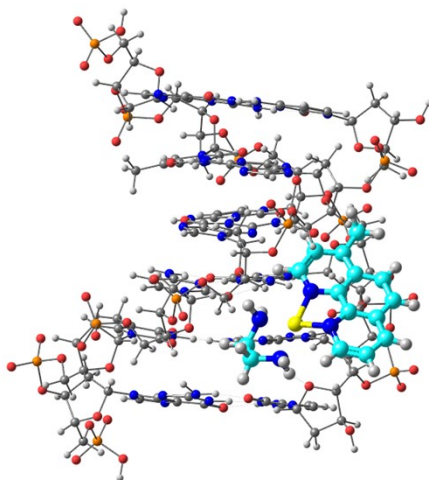
H	-4.39800000	3.05900000	-12.15500000
H	-3.86200000	6.10600000	-11.75200000
H	-5.86900000	6.85800000	-12.79200000
H	-6.17700000	4.78700000	-14.75100000
H	-4.09600000	5.67500000	-15.95800000
H	0.83100000	6.41200000	-11.51100000
H	1.37900000	6.22600000	-13.18800000
H	-0.05500000	7.21100000	-12.83000000
H	-4.93700000	5.06400000	-10.83200000
H	-5.21100000	7.00000000	-15.44400000
P	-7.54000000	4.31400000	-11.31600000
C	-6.69600000	2.00900000	-12.07800000
O	-6.50500000	3.05900000	-11.11500000
C	-6.69100000	0.65700000	-11.34700000
O	-5.33000000	0.24100000	-11.10300000
C	-7.39400000	0.63800000	-9.96700000
O	-8.09200000	-0.62000000	-9.98900000
C	-6.25900000	0.78500000	-8.95500000
C	-4.94500000	0.39100000	-9.69100000
N	-3.89800000	1.35400000	-9.61000000
C	-2.49400000	0.95800000	-9.74200000
O	-2.31100000	-0.28000000	-9.92500000
N	-1.54700000	1.80900000	-9.71500000
C	-1.78700000	3.06100000	-9.56500000
N	-0.63900000	3.94000000	-9.52100000
C	-2.96800000	3.60500000	-9.36900000
C	-4.07000000	2.67400000	-9.45500000
O	-8.85400000	4.00200000	-11.52600000
O	-7.11700000	5.26400000	-9.85300000
H	-3.23500000	4.65700000	-9.22000000
H	-5.12300000	3.03800000	-9.36800000
H	-4.57800000	-0.64100000	-9.42300000
H	-6.23300000	1.84900000	-8.60700000
H	-8.19300000	1.40400000	-9.85300000
H	-7.09600000	-0.13400000	-12.02400000
H	-0.71600000	4.95200000	-9.46900000
H	-5.78500000	2.07900000	-12.75600000
H	0.34000000	3.61300000	-9.69900000
H	-6.38100000	0.20800000	-8.01600000
H	-7.60500000	2.13300000	-12.65200000
P	-8.02800000	-1.68700000	-8.72200000
C	-5.81600000	-2.91500000	-9.34500000
O	-6.55900000	-2.03100000	-8.39900000
C	-5.30900000	-4.21900000	-8.60800000
O	-3.98700000	-4.11900000	-8.25900000
C	-6.08600000	-4.50500000	-7.30000000
O	-6.45600000	-5.97400000	-7.43200000
C	-5.09800000	-4.24500000	-6.14500000
C	-3.76500000	-3.85700000	-6.93800000
N	-0.04600000	-0.18700000	-6.62400000

C	0.18400000	-1.70600000	-6.78800000
N	1.35100000	-2.16700000	-6.67400000
N	-0.96500000	-2.39900000	-6.76400000
C	-2.10100000	-1.89000000	-6.77100000
C	-2.30700000	-0.35000000	-6.63400000
C	-1.20000000	0.30600000	-6.63800000
O	-1.17600000	1.78600000	-6.58800000
N	-3.73400000	-0.14800000	-6.59400000
C	-4.33900000	-1.31600000	-6.64300000
N	-3.44100000	-2.29000000	-6.69200000
O	-8.85700000	-2.91800000	-9.30900000
O	-8.55400000	-0.96800000	-7.35900000
H	0.90900000	0.34300000	-6.64200000
H	-5.41500000	-1.44200000	-6.65600000
H	-2.89100000	-4.43900000	-6.58600000
H	-5.46100000	-3.48900000	-5.48200000
H	1.56800000	-3.13300000	-6.94500000
H	-7.04600000	-3.97300000	-7.15300000
H	2.26800000	-1.61400000	-6.64200000
H	-5.38500000	-5.06800000	-9.31400000
H	-4.89900000	-2.31800000	-9.61800000
H	-4.88700000	-5.12800000	-5.55900000
H	-6.40300000	-3.14100000	-10.22100000
P	-6.94500000	-6.87200000	-6.22900000
C	-4.54800000	-7.74300000	-6.30400000
O	-5.57000000	-7.22200000	-5.38900000
C	-3.28600000	-7.97400000	-5.45000000
O	-2.67300000	-6.72100000	-5.15100000
C	-3.57200000	-8.68200000	-4.09400000
O	-2.72900000	-9.85900000	-4.09000000
C	-3.32800000	-7.63600000	-3.02100000
C	-2.50400000	-6.52600000	-3.72900000
N	-1.04800000	-1.52900000	-3.57600000
C	-0.31500000	-2.68400000	-3.78700000
N	-0.84200000	-3.97100000	-3.80900000
C	-2.11900000	-4.01600000	-3.56200000
C	-3.01400000	-2.86500000	-3.30600000
C	-2.39900000	-1.65200000	-3.36100000
N	-3.12300000	-0.39900000	-3.13800000
N	-4.33400000	-3.35500000	-3.04800000
C	-4.29400000	-4.69300000	-3.14800000
N	-2.99200000	-5.18300000	-3.43500000
O	-7.58400000	-7.98200000	-6.81700000
O	-7.79400000	-5.95000000	-5.09100000
H	0.75400000	-2.54300000	-3.95700000
H	-5.12000000	-5.35700000	-3.01800000
H	-1.39600000	-6.58700000	-3.53700000
H	-4.29600000	-7.26500000	-2.64300000
H	-4.58900000	-9.12400000	-4.04400000
H	-2.52300000	-8.54300000	-6.05500000

H	-4.34300000	-6.96600000	-7.08600000
H	-2.61300000	0.48800000	-3.29600000
H	-4.08500000	-0.43500000	-3.05900000
H	-2.82200000	-8.01000000	-2.12800000
H	-4.89500000	-8.67700000	-6.75600000
P	-1.35500000	-9.97300000	-3.13000000
C	0.47700000	-8.52900000	-4.46300000
O	-0.51200000	-8.60900000	-3.37900000
C	1.85600000	-8.23800000	-3.87000000
O	1.90000000	-6.87400000	-3.45900000
C	2.27700000	-9.08800000	-2.64700000
O	3.47000000	-9.79700000	-3.08300000
C	2.62200000	-8.09600000	-1.52100000
C	2.19100000	-6.69400000	-2.09200000
N	0.92200000	-6.19700000	-1.39100000
C	0.83600000	-4.82600000	-1.20800000
O	1.95800000	-4.01000000	-1.39500000
N	-0.37300000	-4.15500000	-0.68200000
C	-1.39200000	-4.97900000	-0.46600000
N	-2.53200000	-4.36000000	-0.09400000
C	-1.31700000	-6.38900000	-0.62600000
C	-0.12400000	-6.93200000	-1.13500000
O	-0.64300000	-11.21500000	-3.82200000
O	-1.69000000	-9.97000000	-1.72300000
H	3.75900000	-10.42000000	-2.38700000
H	-2.14600000	-7.02100000	-0.37500000
H	-0.07300000	-8.03800000	-1.31600000
H	2.97900000	-5.91500000	-2.02000000
H	2.16800000	-8.35000000	-0.57500000
H	1.54100000	-9.85200000	-2.32600000
H	2.63900000	-8.31400000	-4.68800000
H	-3.37500000	-4.85900000	0.12100000
H	0.14500000	-7.62800000	-5.06600000
H	-2.60200000	-3.31600000	-0.01600000
H	3.70900000	-8.10400000	-1.32700000
H	0.48700000	-9.42400000	-5.09300000
O	1.24700000	5.30700000	-20.32900000
O	-2.18500000	3.70600000	2.96500000
H	0.77800000	5.27500000	-21.20900000
H	-2.19700000	3.41600000	3.94100000
N	2.37400000	-6.21300000	-6.28600000
N	-0.39200000	-8.19800000	-8.25000000
N	-0.56100000	-5.75600000	-6.95500000
N	2.50100000	-8.48100000	-7.39000000
C	5.03700000	-9.22700000	-8.63400000
C	5.00700000	-8.01200000	-7.66800000
C	3.80300000	-7.63300000	-7.15800000
C	3.64400000	-6.48200000	-6.50200000
C	2.10500000	-4.86200000	-5.18600000
C	3.39300000	-4.26000000	-4.98500000

C	4.43200000	-4.30500000	-5.33400000
C	5.61100000	-3.43700000	-5.18500000
C	-1.57100000	-7.26900000	-8.60200000
C	-1.14000000	-5.81600000	-8.32800000
C	4.82300000	-5.76400000	-6.22300000
C	6.02500000	-6.15900000	-6.70100000
C	2.62200000	-9.34700000	-8.33000000
C	6.17300000	-7.23600000	-7.37300000
C	3.80000000	-9.83800000	-8.92200000
Pt	0.98600000	-7.13000000	-7.18800000
H	-0.72300000	-8.97200000	-7.74400000
H	0.03300000	-8.54900000	-9.20400000
H	-1.22600000	-6.00400000	-6.25800000
H	-0.27800000	-4.77400000	-6.75500000
H	5.89400000	-9.49400000	-9.05100000
H	1.15900000	-4.80800000	-4.95600000
H	3.04700000	-3.29300000	-4.30700000
H	6.60000000	-3.72400000	-5.49300000
H	5.65700000	-3.12600000	-4.12200000
H	5.33400000	-2.51000000	-5.74200000
H	-2.42800000	-7.53700000	-8.04300000
H	-1.82300000	-7.37600000	-9.69400000
H	-2.08200000	-5.09200000	-8.48000000
H	-0.38000000	-5.43500000	-9.09200000
H	6.95900000	-5.50400000	-6.44900000
H	1.61100000	-9.84000000	-8.64700000
H	7.10400000	-7.57400000	-7.79100000
H	3.79600000	-10.62700000	-9.60100000

[Pt(en)(4-Mephen)]²⁺ minor groove
Dock_ID: 84-cl5_4-Mephen



EDA for 84-cl5_4-Mephen in kcal mol⁻¹.

Electrostatic interaction	-749.4
Orbital interaction	-78.6
Dispersion energy	-58.4
Pauli repulsion	80.8
Total Bonding Energy	-805.8

Contributions of the solvation energies for 84-cl5_4-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1763.6
E _{solv} (intercalator)	-161.1
E _{solv} (duplex DNA)	-2335.2
ΔE _{solv}	732.6
ΔE _{int} (EDA)	-805.8
ΔE _{aq}	-73.2

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 84-cl5_4-Mephen system.
([Pt(en)(4-Mephen)]²⁺ minor groove)

P	-2.131000000	6.907000000	1.965000000
C	0.494000000	6.660000000	1.748000000
O	-0.753000000	6.845000000	1.039000000
C	1.584000000	6.618000000	0.671000000
O	1.800000000	5.234000000	0.273000000
C	1.210000000	7.379000000	-0.628000000
O	2.392000000	8.079000000	-1.036000000
C	0.673000000	6.294000000	-1.567000000
C	1.164000000	4.960000000	-0.992000000
N	-0.110000000	-0.079000000	-0.501000000
C	1.136000000	0.515000000	-0.828000000
N	2.196000000	-0.321000000	-1.064000000
N	1.340000000	1.871000000	-0.854000000
C	0.198000000	2.614000000	-0.660000000
C	-1.103000000	2.092000000	-0.380000000
C	-1.304000000	0.678000000	-0.281000000
O	-2.331000000	0.048000000	-0.026000000
N	-2.028000000	3.152000000	-0.275000000
C	-1.330000000	4.273000000	-0.468000000
N	0.057000000	4.004000000	-0.742000000
O	-2.042000000	7.988000000	3.016000000
O	-3.242000000	6.849000000	0.951000000
H	-0.188000000	-1.146000000	-0.500000000
H	-1.708000000	5.295000000	-0.441000000
H	1.966000000	4.440000000	-1.587000000
H	-0.436000000	6.372000000	-1.599000000
H	2.994000000	0.043000000	-1.596000000
H	0.474000000	8.197000000	-0.444000000
H	2.066000000	-1.353000000	-1.073000000
H	2.570000000	6.927000000	1.085000000
H	0.469000000	5.700000000	2.306000000
H	0.984000000	6.425000000	-2.631000000
H	0.658000000	7.500000000	2.449000000
P	3.211000000	7.777000000	-2.465000000
C	4.522000000	5.716000000	-1.435000000
O	3.584000000	6.161000000	-2.439000000
C	5.386000000	4.629000000	-2.079000000
O	4.563000000	3.457000000	-2.326000000
C	5.999000000	5.024000000	-3.450000000
O	7.301000000	4.413000000	-3.410000000
C	5.022000000	4.436000000	-4.474000000
C	4.356000000	3.265000000	-3.745000000
N	2.885000000	3.160000000	-3.964000000
C	2.298000000	1.868000000	-3.767000000
O	2.995000000	0.879000000	-3.580000000
N	0.899000000	1.796000000	-3.878000000

C	0.044000000	2.925000000	-4.001000000
O	-1.161000000	2.749000000	-3.856000000
C	0.722000000	4.196000000	-4.268000000
C	2.075000000	4.290000000	-4.179000000
C	-0.130000000	5.360000000	-4.637000000
O	4.433000000	8.642000000	-2.296000000
O	2.291000000	7.889000000	-3.653000000
H	0.469000000	0.817000000	-3.758000000
H	2.613000000	5.253000000	-4.296000000
H	4.819000000	2.258000000	-3.965000000
H	4.296000000	5.232000000	-4.767000000
H	6.165000000	6.116000000	-3.570000000
H	6.163000000	4.268000000	-1.365000000
H	3.910000000	5.294000000	-0.606000000
H	-0.584000000	5.220000000	-5.631000000
H	-0.960000000	5.498000000	-3.928000000
H	0.437000000	6.305000000	-4.665000000
H	5.490000000	4.121000000	-5.428000000
H	5.152000000	6.538000000	-1.045000000
P	8.063000000	3.857000000	-4.786000000
C	7.212000000	1.410000000	-4.248000000
O	7.180000000	2.499000000	-5.195000000
C	7.498000000	0.103000000	-4.993000000
O	6.226000000	-0.558000000	-5.242000000
C	8.192000000	0.240000000	-6.374000000
O	9.224000000	-0.764000000	-6.299000000
C	7.101000000	-0.053000000	-7.411000000
C	5.857000000	-0.483000000	-6.628000000
N	4.707000000	0.465000000	-6.751000000
C	3.362000000	-0.093000000	-6.684000000
O	3.251000000	-1.307000000	-6.519000000
N	2.285000000	0.751000000	-6.835000000
C	2.465000000	2.105000000	-7.009000000
N	1.346000000	2.877000000	-7.066000000
C	3.792000000	2.663000000	-7.073000000
C	4.872000000	1.836000000	-6.923000000
O	9.427000000	3.483000000	-4.264000000
O	7.866000000	4.781000000	-5.957000000
H	3.927000000	3.732000000	-7.223000000
H	5.909000000	2.223000000	-6.932000000
H	5.487000000	-1.517000000	-6.879000000
H	6.947000000	0.822000000	-8.071000000
H	8.688000000	1.223000000	-6.527000000
H	8.039000000	-0.621000000	-4.336000000
H	1.405000000	3.870000000	-7.242000000
H	6.179000000	1.379000000	-3.812000000
H	0.396000000	2.459000000	-7.033000000
H	7.381000000	-0.877000000	-8.112000000
H	7.948000000	1.569000000	-3.437000000
P	10.046000000	-1.255000000	-7.667000000

C	8.368000000	-3.275000000	-7.512000000
O	8.966000000	-2.299000000	-8.400000000
C	7.206000000	-3.917000000	-8.267000000
O	6.088000000	-2.981000000	-8.305000000
C	7.513000000	-4.317000000	-9.740000000
O	7.083000000	-5.689000000	-9.792000000
C	6.721000000	-3.314000000	-10.582000000
C	5.560000000	-2.923000000	-9.666000000
N	1.163000000	-0.261000000	-9.858000000
C	1.391000000	-1.649000000	-9.709000000
N	0.293000000	-2.477000000	-9.593000000
N	2.639000000	-2.200000000	-9.617000000
C	3.655000000	-1.293000000	-9.789000000
C	3.521000000	0.112000000	-10.002000000
C	2.216000000	0.707000000	-9.977000000
O	1.891000000	1.888000000	-10.059000000
N	4.788000000	0.681000000	-10.229000000
C	5.670000000	-0.320000000	-10.147000000
N	5.028000000	-1.572000000	-9.858000000
O	11.210000000	-2.017000000	-7.080000000
O	10.244000000	-0.145000000	-8.663000000
H	0.153000000	0.104000000	-9.842000000
H	6.742000000	-0.258000000	-10.298000000
H	4.696000000	-3.650000000	-9.695000000
H	7.375000000	-2.453000000	-10.839000000
H	0.445000000	-3.478000000	-9.746000000
H	8.597000000	-4.335000000	-9.979000000
H	-0.643000000	-2.117000000	-9.878000000
H	6.822000000	-4.796000000	-7.691000000
H	8.000000000	-2.783000000	-6.584000000
H	6.383000000	-3.699000000	-11.564000000
H	9.129000000	-4.039000000	-7.254000000
P	6.154000000	-6.337000000	-11.018000000
C	3.687000000	-5.885000000	-10.091000000
O	4.742000000	-5.453000000	-10.980000000
C	2.518000000	-6.503000000	-10.870000000
O	1.536000000	-5.453000000	-11.108000000
C	2.869000000	-7.097000000	-12.260000000
O	2.127000000	-8.331000000	-12.301000000
C	2.415000000	-6.031000000	-13.266000000
C	1.538000000	-5.050000000	-12.479000000
N	0.363000000	0.019000000	-13.028000000
C	-0.445000000	-1.064000000	-12.783000000
N	-0.048000000	-2.350000000	-12.637000000
C	1.317000000	-2.513000000	-12.731000000
C	2.259000000	-1.447000000	-12.947000000
C	1.736000000	-0.130000000	-13.114000000
N	2.494000000	0.974000000	-13.373000000
N	3.572000000	-1.951000000	-12.903000000
C	3.452000000	-3.262000000	-12.667000000

N	2.083000000	-3.672000000	-12.575000000
O	5.935000000	-7.747000000	-10.534000000
O	6.755000000	-6.018000000	-12.361000000
H	-1.528000000	-0.843000000	-12.680000000
H	4.262000000	-3.977000000	-12.518000000
H	0.451000000	-5.027000000	-12.763000000
H	3.296000000	-5.564000000	-13.746000000
H	3.938000000	-7.366000000	-12.380000000
H	1.938000000	-7.234000000	-10.250000000
H	3.352000000	-4.921000000	-9.626000000
H	2.073000000	1.915000000	-13.315000000
H	3.504000000	0.924000000	-13.280000000
H	1.853000000	-6.446000000	-14.130000000
H	4.052000000	-6.574000000	-9.309000000
P	1.835000000	-9.042000000	-13.781000000
C	-0.546000000	-7.967000000	-13.603000000
O	0.641000000	-8.060000000	-14.426000000
C	-1.721000000	-7.634000000	-14.518000000
O	-2.002000000	-6.203000000	-14.374000000
C	-1.544000000	-7.901000000	-16.029000000
O	-2.503000000	-8.931000000	-16.321000000
C	-1.925000000	-6.585000000	-16.731000000
C	-1.979000000	-5.521000000	-15.636000000
N	-0.781000000	-4.618000000	-15.660000000
C	-0.985000000	-3.179000000	-15.585000000
O	-2.123000000	-2.764000000	-15.350000000
N	0.082000000	-2.337000000	-15.816000000
C	1.349000000	-2.847000000	-16.022000000
N	2.351000000	-1.965000000	-16.246000000
C	1.573000000	-4.273000000	-15.982000000
C	0.512000000	-5.118000000	-15.817000000
O	1.335000000	-10.426000000	-13.478000000
O	3.001000000	-8.842000000	-14.726000000
H	-2.447000000	-9.200000000	-17.269000000
H	2.582000000	-4.664000000	-16.108000000
H	0.637000000	-6.218000000	-15.785000000
H	-2.897000000	-4.876000000	-15.637000000
H	-1.241000000	-6.342000000	-17.565000000
H	-0.535000000	-8.272000000	-16.307000000
H	-2.654000000	-8.125000000	-14.148000000
H	3.308000000	-2.274000000	-16.387000000
H	-0.392000000	-7.154000000	-12.853000000
H	2.183000000	-0.944000000	-16.288000000
H	-2.913000000	-6.688000000	-17.229000000
H	-0.737000000	-8.925000000	-13.067000000
P	0.929000000	7.613000000	-18.973000000
C	-1.628000000	7.029000000	-18.630000000
O	-0.385000000	7.381000000	-17.980000000
C	-2.684000000	6.969000000	-17.521000000
O	-2.822000000	5.592000000	-17.067000000

C	-2.330000000	7.799000000	-16.257000000
O	-3.557000000	8.455000000	-15.906000000
C	-1.768000000	6.775000000	-15.263000000
C	-2.145000000	5.394000000	-15.811000000
N	-0.337000000	0.494000000	-16.025000000
C	-1.626000000	0.968000000	-15.696000000
N	-2.594000000	0.038000000	-15.382000000
N	-1.981000000	2.293000000	-15.735000000
C	-0.947000000	3.143000000	-16.052000000
C	0.389000000	2.747000000	-16.375000000
C	0.747000000	1.361000000	-16.380000000
O	1.825000000	0.829000000	-16.646000000
N	1.177000000	3.889000000	-16.622000000
C	0.372000000	4.938000000	-16.449000000
N	-0.956000000	4.542000000	-16.061000000
O	0.657000000	8.664000000	-20.022000000
O	2.081000000	7.705000000	-18.009000000
H	-0.138000000	-0.560000000	-15.953000000
H	0.629000000	5.991000000	-16.573000000
H	-2.891000000	4.807000000	-15.193000000
H	-0.670000000	6.923000000	-15.174000000
H	-3.375000000	0.354000000	-14.801000000
H	-1.617000000	8.629000000	-16.473000000
H	-2.333000000	-0.966000000	-15.275000000
H	-3.696000000	7.211000000	-17.919000000
H	-1.522000000	6.035000000	-19.115000000
H	-2.136000000	6.909000000	-14.222000000
H	-1.893000000	7.792000000	-19.386000000
P	-4.198000000	8.472000000	-14.361000000
C	-5.361000000	6.186000000	-14.948000000
O	-4.500000000	6.876000000	-14.012000000
C	-5.756000000	4.874000000	-14.272000000
O	-4.583000000	4.016000000	-14.183000000
C	-6.296000000	5.046000000	-12.823000000
O	-7.411000000	4.135000000	-12.781000000
C	-5.093000000	4.705000000	-11.940000000
C	-4.303000000	3.708000000	-12.789000000
N	-2.831000000	3.749000000	-12.623000000
C	-2.156000000	2.494000000	-12.809000000
O	-2.779000000	1.443000000	-12.864000000
N	-0.757000000	2.549000000	-12.837000000
C	0.014000000	3.741000000	-12.808000000
O	1.224000000	3.627000000	-12.974000000
C	-0.748000000	4.971000000	-12.569000000
C	-2.109000000	4.951000000	-12.538000000
C	0.036000000	6.223000000	-12.389000000
O	-5.471000000	9.253000000	-14.575000000
O	-3.173000000	8.872000000	-13.334000000
H	-0.254000000	1.590000000	-12.942000000
H	-2.719000000	5.867000000	-12.420000000

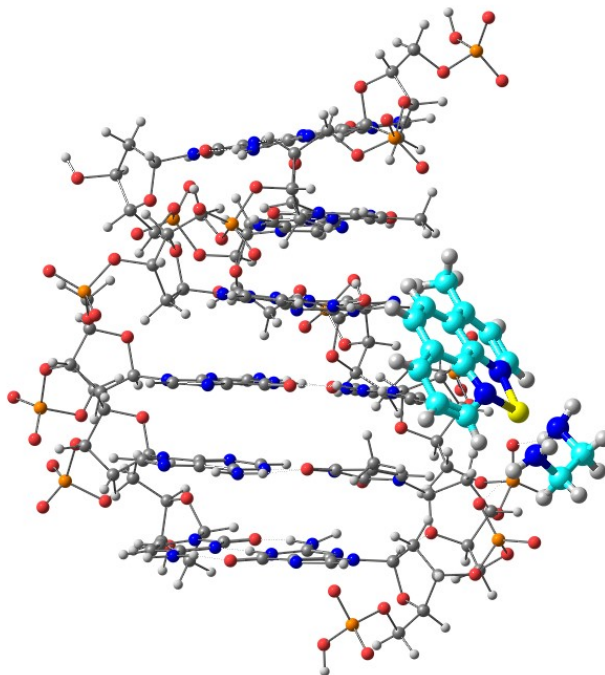
H	-4.627000000	2.634000000	-12.649000000
H	-4.523000000	5.643000000	-11.743000000
H	-6.723000000	6.053000000	-12.625000000
H	-6.469000000	4.303000000	-14.913000000
H	-4.787000000	5.991000000	-15.880000000
H	0.662000000	6.176000000	-11.483000000
H	0.714000000	6.400000000	-13.238000000
H	-0.598000000	7.116000000	-12.292000000
H	-5.352000000	4.306000000	-10.939000000
H	-6.258000000	6.791000000	-15.187000000
P	-7.734000000	3.146000000	-11.481000000
C	-6.372000000	1.067000000	-12.479000000
O	-6.453000000	2.076000000	-11.453000000
C	-6.591000000	-0.327000000	-11.886000000
O	-5.301000000	-0.915000000	-11.555000000
C	-7.413000000	-0.371000000	-10.574000000
O	-8.228000000	-1.543000000	-10.775000000
C	-6.367000000	-0.495000000	-9.454000000
C	-5.039000000	-0.835000000	-10.141000000
N	-3.949000000	0.166000000	-9.941000000
C	-2.566000000	-0.286000000	-10.005000000
O	-2.337000000	-1.483000000	-10.200000000
N	-1.555000000	0.634000000	-9.847000000
C	-1.834000000	1.975000000	-9.697000000
N	-0.776000000	2.829000000	-9.635000000
C	-3.197000000	2.433000000	-9.634000000
C	-4.212000000	1.526000000	-9.774000000
O	-9.007000000	2.456000000	-11.895000000
O	-7.599000000	3.880000000	-10.174000000
H	-3.412000000	3.490000000	-9.495000000
H	-5.274000000	1.836000000	-9.759000000
H	-4.632000000	-1.849000000	-9.864000000
H	-6.337000000	0.440000000	-8.860000000
H	-8.101000000	0.489000000	-10.439000000
H	-6.994000000	-1.031000000	-12.653000000
H	-0.911000000	3.822000000	-9.512000000
H	-5.312000000	1.163000000	-12.841000000
H	0.194000000	2.489000000	-9.774000000
H	-6.618000000	-1.289000000	-8.713000000
H	-7.065000000	1.257000000	-13.319000000
P	-9.095000000	-2.193000000	-9.508000000
C	-7.060000000	-3.860000000	-9.518000000
O	-7.897000000	-3.017000000	-8.688000000
C	-6.002000000	-4.447000000	-8.585000000
O	-4.907000000	-3.493000000	-8.454000000
C	-6.538000000	-4.733000000	-7.152000000
O	-6.247000000	-6.134000000	-7.002000000
C	-5.780000000	-3.762000000	-6.240000000
C	-4.542000000	-3.363000000	-7.041000000
N	-0.365000000	-0.321000000	-6.770000000

C	-0.464000000	-1.730000000	-6.793000000
N	0.680000000	-2.460000000	-6.620000000
N	-1.661000000	-2.399000000	-6.910000000
C	-2.756000000	-1.584000000	-6.846000000
C	-2.753000000	-0.159000000	-6.726000000
C	-1.504000000	0.550000000	-6.734000000
O	-1.276000000	1.757000000	-6.730000000
N	-4.075000000	0.309000000	-6.605000000
C	-4.863000000	-0.765000000	-6.684000000
N	-4.104000000	-1.976000000	-6.859000000
O	-10.039000000	-3.144000000	-10.200000000
O	-9.583000000	-1.151000000	-8.537000000
H	0.609000000	0.127000000	-6.726000000
H	-5.944000000	-0.787000000	-6.616000000
H	-3.664000000	-4.056000000	-6.879000000
H	-6.436000000	-2.900000000	-5.995000000
H	0.632000000	-3.477000000	-6.741000000
H	-7.642000000	-4.626000000	-7.065000000
H	1.616000000	-2.016000000	-6.672000000
H	-5.528000000	-5.358000000	-9.035000000
H	-6.594000000	-3.254000000	-10.324000000
H	-5.508000000	-4.181000000	-5.249000000
H	-7.675000000	-4.670000000	-9.961000000
P	-5.990000000	-6.829000000	-5.512000000
C	-3.400000000	-6.516000000	-5.995000000
O	-4.496000000	-6.212000000	-5.105000000
C	-2.324000000	-7.294000000	-5.226000000
O	-1.257000000	-6.374000000	-4.865000000
C	-2.791000000	-7.915000000	-3.881000000
O	-2.115000000	-9.185000000	-3.856000000
C	-2.375000000	-6.887000000	-2.815000000
C	-1.420000000	-5.912000000	-3.521000000
N	-0.211000000	-0.814000000	-3.581000000
C	0.584000000	-1.930000000	-3.645000000
N	0.177000000	-3.223000000	-3.639000000
C	-1.191000000	-3.363000000	-3.585000000
C	-2.125000000	-2.271000000	-3.541000000
C	-1.589000000	-0.946000000	-3.522000000
N	-2.347000000	0.181000000	-3.419000000
N	-3.440000000	-2.766000000	-3.505000000
C	-3.328000000	-4.099000000	-3.529000000
N	-1.963000000	-4.531000000	-3.555000000
O	-5.914000000	-8.299000000	-5.839000000
O	-6.914000000	-6.289000000	-4.454000000
H	1.671000000	-1.732000000	-3.714000000
H	-4.147000000	-4.818000000	-3.536000000
H	-0.367000000	-5.877000000	-3.122000000
H	-3.277000000	-6.402000000	-2.391000000
H	-3.873000000	-8.156000000	-3.837000000
H	-1.804000000	-8.035000000	-5.876000000

H	-3.001000000	-5.509000000	-6.291000000
H	-1.919000000	1.117000000	-3.539000000
H	-3.354000000	0.122000000	-3.515000000
H	-1.892000000	-7.335000000	-1.924000000
H	-3.720000000	-7.064000000	-6.902000000
P	-1.532000000	-9.868000000	-2.449000000
C	0.689000000	-8.622000000	-3.059000000
O	-0.297000000	-8.829000000	-2.020000000
C	1.908000000	-7.985000000	-2.397000000
O	1.734000000	-6.536000000	-2.445000000
C	2.135000000	-8.356000000	-0.913000000
O	3.292000000	-9.206000000	-0.924000000
C	2.435000000	-7.029000000	-0.200000000
C	2.071000000	-5.920000000	-1.185000000
N	0.863000000	-5.140000000	-0.765000000
C	0.935000000	-3.687000000	-0.751000000
O	2.030000000	-3.160000000	-0.968000000
N	-0.200000000	-2.958000000	-0.477000000
C	-1.398000000	-3.594000000	-0.221000000
N	-2.487000000	-2.815000000	-0.018000000
C	-1.462000000	-5.037000000	-0.181000000
C	-0.341000000	-5.770000000	-0.454000000
O	-0.991000000	-11.188000000	-2.943000000
O	-2.508000000	-9.779000000	-1.307000000
H	3.440000000	-9.596000000	-0.029000000
H	-2.398000000	-5.527000000	0.084000000
H	-0.349000000	-6.877000000	-0.465000000
H	2.897000000	-5.198000000	-1.410000000
H	1.913000000	-6.953000000	0.772000000
H	1.288000000	-8.911000000	-0.456000000
H	2.828000000	-8.178000000	-3.004000000
H	-3.402000000	-3.216000000	0.156000000
H	0.253000000	-7.942000000	-3.830000000
H	-2.440000000	-1.782000000	-0.093000000
H	3.508000000	-6.978000000	0.086000000
H	0.974000000	-9.588000000	-3.527000000
O	1.039000000	6.137000000	-19.750000000
O	-2.099000000	5.434000000	2.757000000
H	0.742000000	6.123000000	-20.701000000
H	-1.805000000	5.460000000	3.709000000
N	-1.970000000	-6.093000000	-9.498000000
N	-4.370000000	-5.762000000	-12.736000000
N	-3.240000000	-3.871000000	-11.020000000
N	-3.170000000	-7.944000000	-10.973000000
C	-1.826000000	-10.437000000	-11.503000000
C	-1.282000000	-9.587000000	-10.585000000
C	-1.930000000	-8.311000000	-10.334000000
C	-1.365000000	-7.376000000	-9.501000000
C	-1.562000000	-5.179000000	-8.580000000
C	-0.556000000	-5.476000000	-7.667000000

C	0.148000000	-6.710000000	-7.716000000
C	1.253000000	-6.923000000	-6.736000000
C	-4.844000000	-4.332000000	-12.833000000
C	-3.705000000	-3.413000000	-12.378000000
C	-0.225000000	-7.668000000	-8.651000000
C	0.405000000	-8.950000000	-8.894000000
C	-3.575000000	-8.796000000	-12.020000000
C	-0.069000000	-9.836000000	-9.806000000
C	-3.004000000	-10.012000000	-12.242000000
Pt	-3.204000000	-5.934000000	-11.062000000
H	-5.166000000	-6.408000000	-12.755000000
H	-3.763000000	-5.988000000	-13.552000000
H	-3.872000000	-3.524000000	-10.276000000
H	-2.315000000	-3.455000000	-10.821000000
H	-1.377000000	-11.385000000	-11.756000000
H	-2.062000000	-4.198000000	-8.575000000
H	-0.341000000	-4.775000000	-6.861000000
H	1.656000000	-7.942000000	-6.746000000
H	0.895000000	-6.723000000	-5.709000000
H	2.095000000	-6.241000000	-6.925000000
H	-5.751000000	-4.199000000	-12.199000000
H	-5.160000000	-4.079000000	-13.871000000
H	-4.048000000	-2.347000000	-12.360000000
H	-2.843000000	-3.456000000	-13.095000000
H	1.304000000	-9.175000000	-8.317000000
H	-4.445000000	-8.455000000	-12.584000000
H	0.453000000	-10.766000000	-10.010000000
H	-3.397000000	-10.690000000	-12.988000000

[Pt(en)(4-Mephen)]²⁺ major groove
Dock_ID: 164-cl7_4-Mephen



EDA for 164-cl7_4-Mephen in kcal mol⁻¹.

Electrostatic interaction	-762.0
Orbital interaction	-93.1
Dispersion energy	-54.0
Pauli repulsion	114.7
Total Bonding Energy	-794.3

Contributions of the solvation energies for 164-cl7_4-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1751.5
E _{solv} (intercalator)	-161.1
E _{solv} (duplex DNA)	-2323.0
ΔE _{solv}	732.6
ΔE _{int} (EDA)	-794.3
ΔE _{aq}	-61.7

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 164-cl7_4-Mephen system.
([Pt(en)(4-Mephen)]²⁺ major groove)

P	-1.62900000	6.87000000	2.56800000
C	0.98800000	6.48400000	2.40200000
O	-0.20500000	6.89500000	1.69900000
C	2.10500000	6.43300000	1.35600000
O	2.22700000	5.07500000	0.84400000
C	1.86600000	7.32600000	0.10900000
O	3.15200000	7.92200000	-0.13100000
C	1.32600000	6.37600000	-0.95900000
C	1.63400000	4.96100000	-0.46700000
N	-0.11300000	0.05900000	-0.62000000
C	1.15800000	0.58100000	-0.96700000
N	2.11500000	-0.29500000	-1.40500000
N	1.49100000	1.90700000	-0.82800000
C	0.44100000	2.71100000	-0.45400000
C	-0.89200000	2.27700000	-0.17900000
C	-1.21800000	0.88400000	-0.23000000
O	-2.28100000	0.31600000	0.02000000
N	-1.71000000	3.39400000	0.09400000
C	-0.92000000	4.46300000	0.00400000
N	0.43100000	4.10800000	-0.34900000
O	-1.60000000	7.88100000	3.68800000
O	-2.67800000	6.87600000	1.48900000
H	-0.29200000	-0.98700000	-0.74900000
H	-1.20500000	5.50500000	0.16200000
H	2.41500000	4.40100000	-1.06500000
H	0.23800000	6.56200000	-1.09200000
H	2.91200000	0.07800000	-1.92900000
H	1.19300000	8.19000000	0.31300000
H	1.89000000	-1.30000000	-1.55000000
H	3.09900000	6.62000000	1.82900000
H	0.84100000	5.48000000	2.85400000
H	1.76000000	6.56300000	-1.97300000
H	1.22200000	7.22300000	3.19200000
P	3.96100000	8.08600000	-1.56700000
C	5.12700000	5.81600000	-0.71800000
O	5.29600000	7.11400000	-1.31000000
C	5.38600000	4.70800000	-1.73900000
O	4.12200000	4.03500000	-2.01600000
C	5.96000000	5.14900000	-3.11500000
O	7.07000000	4.24500000	-3.24200000
C	4.81100000	4.93100000	-4.10800000
C	4.03800000	3.78200000	-3.45800000
N	2.59600000	3.67200000	-3.75800000
C	2.05500000	2.33800000	-3.76600000
O	2.79100000	1.36400000	-3.81400000
N	0.65400000	2.22800000	-3.79500000

C	-0.22900000	3.33300000	-3.64300000
O	-1.41900000	3.10100000	-3.46800000
C	0.39600000	4.65900000	-3.71300000
C	1.74700000	4.79800000	-3.73500000
C	-0.54100000	5.81400000	-3.73400000
O	4.52500000	9.48100000	-1.51100000
O	3.24800000	7.62000000	-2.81700000
H	0.24800000	1.23200000	-3.82100000
H	2.25400000	5.78900000	-3.74500000
H	4.51400000	2.78000000	-3.62900000
H	4.20100000	5.86500000	-4.19600000
H	6.36500000	6.19100000	-3.11800000
H	6.03300000	3.91400000	-1.28600000
H	4.13900000	5.68500000	-0.23000000
H	-1.06500000	5.88100000	-4.70200000
H	-1.31300000	5.72000000	-2.95500000
H	-0.03700000	6.77700000	-3.57600000
H	5.14000000	4.73600000	-5.15500000
H	5.90400000	5.79900000	0.07800000
P	7.90100000	3.94000000	-4.65500000
C	6.50400000	1.73100000	-5.03300000
O	7.77800000	2.27400000	-4.63000000
C	6.80300000	0.65200000	-6.08300000
O	5.53800000	0.01600000	-6.39400000
C	7.35500000	1.20200000	-7.42600000
O	8.45800000	0.35300000	-7.76000000
C	6.15400000	1.22500000	-8.37400000
C	5.01700000	0.48300000	-7.66200000
N	3.83300000	1.34200000	-7.36200000
C	2.51500000	0.72900000	-7.27700000
O	2.42800000	-0.49500000	-7.39800000
N	1.41200000	1.53400000	-7.08300000
C	1.55500000	2.89400000	-6.92100000
N	0.43300000	3.63800000	-6.73900000
C	2.86800000	3.48800000	-6.87600000
C	3.96100000	2.71000000	-7.11000000
O	9.35000000	4.20900000	-4.35100000
O	7.20200000	4.52900000	-5.85200000
H	2.97500000	4.55600000	-6.67100000
H	4.97800000	3.14000000	-7.12100000
H	4.66200000	-0.45300000	-8.17100000
H	5.89100000	2.26300000	-8.67600000
H	7.83900000	2.20300000	-7.32700000
H	7.44000000	-0.16100000	-5.67400000
H	0.48600000	4.65300000	-6.67300000
H	5.81400000	2.50200000	-5.43000000
H	-0.51200000	3.21400000	-6.77800000
H	6.36200000	0.76400000	-9.36600000
H	6.06300000	1.27600000	-4.12100000
P	8.50100000	-0.72900000	-9.03300000

C	6.82500000	-2.54900000	-8.04600000
O	7.05000000	-1.52500000	-9.03700000
C	6.31400000	-3.80500000	-8.76300000
O	4.92300000	-3.62100000	-9.13600000
C	7.05500000	-4.14800000	-10.08400000
O	7.14100000	-5.58600000	-10.05400000
C	6.18200000	-3.53000000	-11.18100000
C	4.79700000	-3.33400000	-10.55000000
N	0.60600000	-0.22500000	-10.30400000
C	0.68200000	-1.63500000	-10.28800000
N	-0.50500000	-2.32600000	-10.35600000
N	1.86200000	-2.33500000	-10.28700000
C	2.97100000	-1.54600000	-10.48600000
C	2.97200000	-0.12000000	-10.61900000
C	1.75700000	0.62100000	-10.45200000
O	1.56000000	1.83100000	-10.41700000
N	4.27300000	0.33600000	-10.89800000
C	5.04700000	-0.74800000	-10.91500000
N	4.29700000	-1.95300000	-10.67800000
O	9.64300000	-1.62800000	-8.62900000
O	8.48000000	0.01900000	-10.34100000
H	-0.35400000	0.24400000	-10.22100000
H	6.12300000	-0.78300000	-11.07400000
H	4.00700000	-4.05100000	-10.90100000
H	6.64500000	-2.57800000	-11.52300000
H	-0.49800000	-3.33500000	-10.25700000
H	8.10800000	-3.80000000	-10.11600000
H	-1.40800000	-1.84300000	-10.18800000
H	6.28300000	-4.67700000	-8.06800000
H	6.03600000	-2.13000000	-7.37800000
H	6.12600000	-4.13000000	-12.11000000
H	7.72900000	-2.78100000	-7.45400000
P	6.88100000	-6.54800000	-11.39000000
C	4.30500000	-6.74800000	-10.81300000
O	5.28100000	-6.29800000	-11.78000000
C	3.16600000	-7.44200000	-11.56500000
O	2.19000000	-6.44500000	-11.97300000
C	3.58900000	-8.17600000	-12.86700000
O	2.86500000	-9.41600000	-12.84200000
C	3.26000000	-7.18900000	-13.99300000
C	2.28900000	-6.16900000	-13.38300000
N	0.92100000	-1.08800000	-13.50400000
C	0.16600000	-2.22200000	-13.33300000
N	0.59900000	-3.50700000	-13.31400000
C	1.95800000	-3.62700000	-13.49500000
C	2.84800000	-2.52000000	-13.70500000
C	2.28800000	-1.20600000	-13.70300000
N	3.02500000	-0.08300000	-13.94600000
N	4.16700000	-2.98300000	-13.86200000
C	4.10200000	-4.31400000	-13.74200000

N	2.76300000	-4.77600000	-13.54000000
O	7.10100000	-7.92800000	-10.82200000
O	7.62400000	-6.04300000	-12.59900000
H	-0.91700000	-2.05000000	-13.18000000
H	4.93700000	-5.01300000	-13.77800000
H	1.22900000	-6.23400000	-13.74600000
H	4.20600000	-6.73700000	-14.36300000
H	4.65400000	-8.49200000	-12.87400000
H	2.58600000	-8.10800000	-10.88400000
H	3.92700000	-5.82200000	-10.31900000
H	2.59900000	0.85000000	-13.80900000
H	4.03300000	-0.12700000	-13.84200000
H	2.84300000	-7.65900000	-14.90700000
H	4.74000000	-7.42600000	-10.05300000
P	1.79800000	-9.89500000	-14.03300000
C	-0.22600000	-8.46100000	-13.09100000
O	0.71400000	-8.63300000	-14.17200000
C	-1.63600000	-8.34800000	-13.67700000
O	-1.91400000	-6.93900000	-13.93500000
C	-1.88200000	-9.09700000	-15.00700000
O	-2.96600000	-9.99600000	-14.71900000
C	-2.31300000	-8.02400000	-16.02200000
C	-2.10900000	-6.67600000	-15.33200000
N	-0.90500000	-5.92800000	-15.82900000
C	-0.97500000	-4.47700000	-15.93000000
O	-2.04800000	-3.92900000	-15.65800000
N	0.12800000	-3.77100000	-16.35200000
C	1.30900000	-4.42300000	-16.64600000
N	2.37100000	-3.66400000	-17.01000000
C	1.38500000	-5.85900000	-16.55400000
C	0.29100000	-6.57100000	-16.14200000
O	1.14900000	-11.10000000	-13.40300000
O	2.46900000	-9.94300000	-15.37800000
H	-3.14700000	-10.58000000	-15.49400000
H	2.30800000	-6.37100000	-16.82200000
H	0.32600000	-7.67200000	-16.02800000
H	-2.98900000	-5.98300000	-15.37200000
H	-1.78500000	-8.12300000	-16.98800000
H	-1.02000000	-9.69400000	-15.36500000
H	-2.40300000	-8.62600000	-12.91200000
H	3.27500000	-4.07900000	-17.21100000
H	0.06800000	-7.50100000	-12.60000000
H	2.32400000	-2.62800000	-17.01400000
H	-3.37800000	-8.16400000	-16.30800000
H	-0.18400000	-9.29000000	-12.35600000
P	2.11800000	5.99000000	-19.74300000
C	-0.42900000	5.41700000	-19.36400000
O	0.82200000	5.76100000	-18.72300000
C	-1.52600000	5.60500000	-18.31100000
O	-1.86500000	4.30900000	-17.74000000

C	-1.13200000	6.51000000	-17.11200000
O	-2.27300000	7.36700000	-16.95200000
C	-0.82500000	5.53800000	-15.96600000
C	-1.27300000	4.15000000	-16.43600000
N	0.03500000	-0.89600000	-16.47700000
C	-1.17100000	-0.27800000	-16.05900000
N	-2.15500000	-1.08400000	-15.56800000
N	-1.38400000	1.08000000	-16.11900000
C	-0.27900000	1.80000000	-16.50000000
C	0.99500000	1.26100000	-16.85800000
C	1.19800000	-0.15500000	-16.86900000
O	2.19100000	-0.81100000	-17.18200000
N	1.89100000	2.30900000	-17.15900000
C	1.20300000	3.43900000	-17.00300000
N	-0.14700000	3.19600000	-16.55800000
O	1.75700000	6.89100000	-20.89900000
O	3.27200000	6.27300000	-18.81800000
H	0.11400000	-1.95900000	-16.42800000
H	1.55700000	4.45600000	-17.16900000
H	-2.08900000	3.67300000	-15.81700000
H	0.25800000	5.58800000	-15.70200000
H	-3.00500000	-0.67200000	-15.18300000
H	-0.28300000	7.19200000	-17.34500000
H	-2.09600000	-2.11600000	-15.62300000
H	-2.48100000	5.93100000	-18.78600000
H	-0.38200000	4.35600000	-19.68800000
H	-1.33800000	5.79900000	-15.01200000
H	-0.61100000	6.06700000	-20.24200000
P	-2.91900000	7.80000000	-15.47200000
C	-4.30300000	5.56600000	-15.60700000
O	-3.39300000	6.35200000	-14.80100000
C	-4.87100000	4.48900000	-14.68300000
O	-3.88900000	3.42600000	-14.52300000
C	-5.23400000	5.00400000	-13.26400000
O	-6.58100000	4.52800000	-13.09800000
C	-4.17900000	4.39100000	-12.34000000
C	-3.61500000	3.19600000	-13.11300000
N	-2.14300000	3.02800000	-12.99400000
C	-1.61900000	1.68600000	-13.10300000
O	-2.36400000	0.72500000	-13.05400000
N	-0.21900000	1.57500000	-13.20200000
C	0.66500000	2.68000000	-13.32600000
O	1.84900000	2.46200000	-13.56100000
C	0.06000000	4.00800000	-13.17400000
C	-1.28700000	4.14300000	-13.06200000
C	0.98800000	5.17200000	-13.22400000
O	-4.10100000	8.63500000	-15.89200000
O	-1.87000000	8.31600000	-14.52400000
H	0.17200000	0.57800000	-13.30200000
H	-1.77900000	5.13100000	-13.00700000

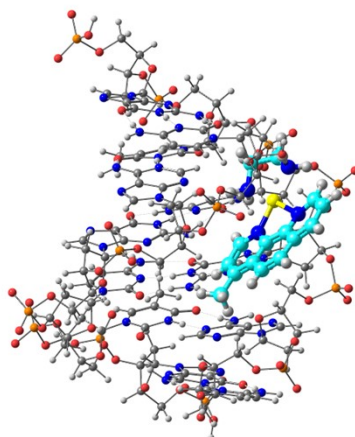
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H	2.00900000	4.89000000	-12.90300000
H	1.08600000	5.56300000	-14.25300000
H	0.65800000	6.00600000	-12.59000000
H	-4.56700000	4.08600000	-11.34500000
H	-5.12000000	6.19600000	-16.01200000
P	-7.21200000	4.13800000	-11.60600000
C	-6.61200000	1.61600000	-12.18300000
O	-6.42800000	2.70600000	-11.25800000
C	-7.09300000	0.37900000	-11.41700000
O	-5.93500000	-0.40400000	-11.01800000
C	-7.87100000	0.66100000	-10.10300000
O	-8.93200000	-0.31100000	-10.17000000
C	-6.84400000	0.44700000	-8.98100000
C	-5.60000000	-0.15800000	-9.64000000
N	-4.39900000	0.73600000	-9.63300000
C	-3.09900000	0.12200000	-9.88000000
O	-3.05200000	-1.10000000	-10.02000000
N	-1.98400000	0.92600000	-9.90900000
C	-2.08300000	2.28500000	-9.71000000
N	-0.92500000	2.99700000	-9.71300000
C	-3.36300000	2.89900000	-9.48400000
C	-4.48500000	2.11500000	-9.46200000
O	-8.66800000	3.90700000	-11.91600000
O	-6.75100000	5.06800000	-10.51800000
H	-3.43500000	3.97100000	-9.31400000
H	-5.49100000	2.54500000	-9.29600000
H	-5.29500000	-1.16600000	-9.23900000
H	-6.65900000	1.39900000	-8.44200000
H	-8.35400000	1.65900000	-10.06600000
H	-7.65200000	-0.31700000	-12.08700000
H	-0.91800000	4.00600000	-9.59700000
H	-5.59000000	1.43400000	-12.60500000
H	-0.01400000	2.54600000	-9.92200000
H	-7.21000000	-0.23400000	-8.17900000
H	-7.30600000	1.86400000	-13.00600000
P	-9.74500000	-0.85600000	-8.81700000
C	-7.95400000	-2.77400000	-8.92500000
O	-8.60500000	-1.81000000	-8.06200000
C	-7.00400000	-3.58000000	-8.03900000
O	-5.74100000	-2.86800000	-7.91900000
C	-7.52800000	-3.83400000	-6.59800000
O	-7.47700000	-5.26600000	-6.48500000
C	-6.61600000	-3.01100000	-5.68500000
C	-5.37400000	-2.69700000	-6.52200000
N	-1.21000000	0.41500000	-6.86800000

C	-1.30100000	-0.98700000	-7.00400000
N	-0.14800000	-1.67000000	-7.28700000
N	-2.47500000	-1.69300000	-6.87400000
C	-3.56200000	-0.90900000	-6.58800000
C	-3.55500000	0.51200000	-6.41400000
C	-2.33700000	1.25100000	-6.57600000
O	-2.14200000	2.46000000	-6.51100000
N	-4.85200000	0.96600000	-6.11300000
C	-5.63300000	-0.11600000	-6.10600000
N	-4.89100000	-1.31400000	-6.39200000
O	-10.83500000	-1.69700000	-9.43500000
O	-10.04700000	0.24600000	-7.83900000
H	-0.24900000	0.88500000	-6.99500000
H	-6.69700000	-0.14900000	-5.89900000
H	-4.51200000	-3.40700000	-6.35400000
H	-7.16100000	-2.10000000	-5.35400000
H	-0.14600000	-2.68300000	-7.26600000
H	-8.60400000	-3.57600000	-6.47100000
H	0.76800000	-1.18000000	-7.36700000
H	-6.73100000	-4.54100000	-8.54200000
H	-7.39400000	-2.24200000	-9.72600000
H	-6.35500000	-3.50700000	-4.72800000
H	-8.71000000	-3.44500000	-9.38000000
P	-6.84400000	-6.08500000	-5.18000000
C	-4.43100000	-5.97600000	-6.29000000
O	-5.24400000	-5.60600000	-5.15800000
C	-3.19900000	-6.74700000	-5.80500000
O	-2.09200000	-5.80800000	-5.65900000
C	-3.34400000	-7.44700000	-4.43000000
O	-2.70800000	-8.71900000	-4.65800000
C	-2.61100000	-6.53200000	-3.43700000
C	-1.85000000	-5.49900000	-4.27700000
N	-0.48000000	-0.43800000	-3.77400000
C	0.25700000	-1.53700000	-4.12300000
N	-0.18300000	-2.81600000	-4.26400000
C	-1.52700000	-2.96500000	-4.00100000
C	-2.40100000	-1.89100000	-3.61900000
C	-1.84200000	-0.57900000	-3.52500000
N	-2.56500000	0.52000000	-3.19800000
N	-3.70800000	-2.37600000	-3.43100000
C	-3.64800000	-3.68800000	-3.67900000
N	-2.32400000	-4.11800000	-4.02500000
O	-6.97900000	-7.52100000	-5.61600000
O	-7.38500000	-5.57100000	-3.87400000
H	1.33000000	-1.34900000	-4.32000000
H	-4.47700000	-4.39500000	-3.64300000
H	-0.73100000	-5.52700000	-4.17100000
H	-3.33500000	-6.08400000	-2.72800000
H	-4.39300000	-7.65000000	-4.13200000
H	-2.82700000	-7.45300000	-6.58700000

H	-4.11100000	-4.99800000	-6.73100000
H	-2.15000000	1.46400000	-3.24300000
H	-3.57200000	0.45800000	-3.08700000
H	-1.90700000	-7.08400000	-2.77500000
H	-4.98700000	-6.56100000	-7.04700000
P	-2.22200000	-9.68800000	-3.38600000
C	0.10700000	-8.58000000	-3.86900000
O	-0.86600000	-8.87300000	-2.83600000
C	1.28600000	-7.88700000	-3.19300000
O	1.02100000	-6.44900000	-3.18500000
C	1.55800000	-8.28300000	-1.72300000
O	2.70100000	-9.15000000	-1.78400000
C	1.90800000	-6.96900000	-1.00900000
C	1.51700000	-5.84300000	-1.96700000
N	0.39600000	-4.99900000	-1.45100000
C	0.58400000	-3.56000000	-1.34200000
O	1.69300000	-3.09700000	-1.62200000
N	-0.46700000	-2.77600000	-0.92200000
C	-1.68100000	-3.34500000	-0.58700000
N	-2.67400000	-2.51300000	-0.19500000
C	-1.85200000	-4.77800000	-0.64500000
C	-0.81500000	-5.56500000	-1.05900000
O	-1.82800000	-10.96300000	-4.08900000
O	-3.18200000	-9.66500000	-2.23000000
H	2.85900000	-9.57200000	-0.90500000
H	-2.79900000	-5.22000000	-0.33300000
H	-0.90300000	-6.66500000	-1.12700000
H	2.35900000	-5.16900000	-2.27400000
H	1.42500000	-6.89700000	-0.01600000
H	0.71600000	-8.82800000	-1.24600000
H	2.21100000	-8.00900000	-3.81200000
H	-3.60400000	-2.86000000	0.01500000
H	-0.35100000	-7.91800000	-4.63800000
H	-2.55800000	-1.48200000	-0.20500000
H	2.99400000	-6.93400000	-0.77000000
H	0.44700000	-9.52700000	-4.33900000
O	2.35300000	4.44700000	-20.34500000
O	-1.60900000	5.34700000	3.25100000
H	2.01200000	4.28200000	-21.26500000
H	-1.39000000	5.30900000	4.22300000
N	4.82100000	6.13300000	-8.14500000
N	4.94100000	8.54500000	-4.90500000
N	6.97000000	7.24400000	-6.35200000
N	2.96100000	7.59900000	-6.91300000
C	0.19600000	6.98800000	-7.33500000
C	1.11000000	6.49800000	-8.22100000
C	2.52700000	6.71300000	-7.95800000
C	3.49200000	6.00700000	-8.63400000
C	5.78900000	5.34500000	-8.67300000
C	5.53400000	4.50700000	-9.76000000

C	4.23000000	4.38500000	-10.30600000
C	3.99600000	3.49300000	-11.46500000
C	6.31700000	8.46400000	-4.29500000
C	7.37400000	8.33300000	-5.39700000
C	3.18400000	5.10800000	-9.72700000
C	1.78400000	4.98000000	-10.04400000
C	2.00300000	7.81600000	-5.89400000
C	0.81300000	5.66100000	-9.37700000
C	0.67500000	7.63500000	-6.12500000
Pt	4.89700000	7.33400000	-6.56900000
H	4.21500000	8.21600000	-4.20100000
H	4.71800000	9.52100000	-5.14100000
H	7.23300000	6.29000000	-6.00300000
H	7.46500000	7.37400000	-7.24400000
H	-0.87100000	6.87600000	-7.46600000
H	6.78500000	5.38100000	-8.21000000
H	6.35000000	3.93500000	-10.18800000
H	4.88500000	2.93900000	-11.78700000
H	3.57400000	4.01200000	-12.33800000
H	3.25900000	2.69300000	-11.20500000
H	6.53300000	9.35700000	-3.66400000
H	6.37000000	7.57800000	-3.60100000
H	7.48000000	9.29500000	-5.95600000
H	8.37300000	8.13500000	-4.94500000
H	1.52400000	4.27400000	-10.84100000
H	2.39000000	8.21100000	-4.95100000
H	-0.23600000	5.56100000	-9.65200000
H	-0.06000000	7.94200000	-5.39000000

[Pt(en)(4-Mephen)]²⁺ minor groove
Dock_ID: 131-cl2_4-Mephen



EDA for 131-cl2_4-Mephen in kcal mol⁻¹.

Electrostatic interaction	-784.3
Orbital interaction	-89.6
Dispersion energy	-74.5
Pauli repulsion	132.9
Total Bonding Energy	-815.5

Contributions of the solvation energies for 131-cl2_4-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1745.8
E _{solv} (intercalator)	-161.6
E _{solv} (duplex DNA)	-2338
ΔE _{solv}	753.8
ΔE _{int} (EDA)	-815.5
ΔE _{aq}	-61.7

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 131-cl2_4-Mephen system.
([Pt(en)(4-Mephen)]²⁺ minor groove)

P	-1.504000000	7.251000000	2.169000000
C	1.069000000	6.912000000	1.679000000
O	-0.222000000	7.235000000	1.110000000
C	2.046000000	6.860000000	0.499000000
O	2.089000000	5.500000000	-0.015000000
C	1.625000000	7.750000000	-0.703000000
O	2.825000000	8.349000000	-1.206000000
C	0.870000000	6.795000000	-1.633000000
C	1.309000000	5.386000000	-1.225000000
N	-0.179000000	0.408000000	-0.852000000
C	1.070000000	0.962000000	-1.215000000
N	2.101000000	0.095000000	-1.514000000
N	1.330000000	2.305000000	-1.219000000
C	0.240000000	3.089000000	-0.918000000
C	-1.065000000	2.614000000	-0.584000000
C	-1.329000000	1.208000000	-0.547000000
O	-2.372000000	0.605000000	-0.291000000
N	-1.924000000	3.710000000	-0.361000000
C	-1.186000000	4.805000000	-0.552000000
N	0.163000000	4.487000000	-0.939000000
O	-1.230000000	8.165000000	3.340000000
O	-2.706000000	7.412000000	1.277000000
H	-0.310000000	-0.656000000	-0.896000000
H	-1.509000000	5.841000000	-0.452000000
H	2.007000000	4.865000000	-1.940000000
H	-0.222000000	6.964000000	-1.498000000
H	2.830000000	0.445000000	-2.148000000
H	1.012000000	8.625000000	-0.389000000
H	1.919000000	-0.930000000	-1.543000000
H	3.091000000	7.049000000	0.832000000
H	1.027000000	5.923000000	2.182000000
H	1.040000000	6.994000000	-2.721000000
H	1.361000000	7.695000000	2.404000000
P	3.484000000	8.019000000	-2.710000000
C	4.706000000	5.814000000	-1.870000000
O	3.732000000	6.380000000	-2.773000000
C	5.385000000	4.656000000	-2.609000000
O	4.410000000	3.618000000	-2.881000000
C	5.997000000	5.032000000	-3.987000000
O	7.228000000	4.295000000	-4.057000000
C	4.904000000	4.662000000	-4.994000000
C	4.095000000	3.569000000	-4.293000000
N	2.615000000	3.688000000	-4.423000000
C	1.883000000	2.480000000	-4.165000000
O	2.455000000	1.406000000	-4.036000000

N	0.486000000	2.596000000	-4.176000000
C	-0.235000000	3.817000000	-4.260000000
O	-1.449000000	3.761000000	-4.083000000
C	0.585000000	4.995000000	-4.543000000
C	1.945000000	4.914000000	-4.550000000
C	-0.114000000	6.285000000	-4.797000000
O	4.780000000	8.788000000	-2.639000000
O	2.472000000	8.231000000	-3.805000000
H	-0.049000000	1.675000000	-4.019000000
H	2.588000000	5.807000000	-4.687000000
H	4.366000000	2.515000000	-4.602000000
H	4.297000000	5.572000000	-5.213000000
H	6.319000000	6.095000000	-4.054000000
H	6.131000000	4.158000000	-1.946000000
H	4.131000000	5.430000000	-0.996000000
H	-0.292000000	6.444000000	-5.870000000
H	-1.092000000	6.331000000	-4.295000000
H	0.477000000	7.147000000	-4.432000000
H	5.292000000	4.340000000	-5.983000000
H	5.452000000	6.556000000	-1.530000000
P	7.595000000	3.141000000	-5.208000000
C	6.332000000	1.103000000	-4.028000000
O	6.382000000	2.003000000	-5.155000000
C	6.346000000	-0.344000000	-4.525000000
O	5.017000000	-0.741000000	-4.959000000
C	7.281000000	-0.637000000	-5.727000000
O	7.828000000	-1.916000000	-5.342000000
C	6.355000000	-0.690000000	-6.952000000
C	4.934000000	-0.829000000	-6.399000000
N	3.965000000	0.217000000	-6.840000000
C	2.550000000	-0.127000000	-6.864000000
O	2.222000000	-1.302000000	-6.668000000
N	1.627000000	0.861000000	-7.114000000
C	2.019000000	2.164000000	-7.319000000
N	1.035000000	3.089000000	-7.512000000
C	3.419000000	2.505000000	-7.343000000
C	4.348000000	1.537000000	-7.076000000
O	8.893000000	2.584000000	-4.681000000
O	7.452000000	3.706000000	-6.596000000
H	3.725000000	3.526000000	-7.558000000
H	5.431000000	1.760000000	-7.045000000
H	4.468000000	-1.836000000	-6.607000000
H	6.504000000	0.212000000	-7.578000000
H	8.119000000	0.080000000	-5.838000000
H	6.548000000	-1.037000000	-3.671000000
H	1.254000000	4.076000000	-7.511000000
H	5.351000000	1.330000000	-3.541000000
H	0.041000000	2.837000000	-7.344000000
H	6.579000000	-1.547000000	-7.629000000
H	7.150000000	1.275000000	-3.305000000

P	8.767000000	-2.794000000	-6.402000000
C	6.556000000	-4.177000000	-6.759000000
O	7.612000000	-3.434000000	-7.417000000
C	5.592000000	-4.625000000	-7.853000000
O	4.643000000	-3.539000000	-8.089000000
C	6.285000000	-4.930000000	-9.212000000
O	6.088000000	-6.349000000	-9.344000000
C	5.600000000	-4.013000000	-10.232000000
C	4.355000000	-3.481000000	-9.516000000
N	0.458000000	-0.162000000	-10.247000000
C	0.450000000	-1.570000000	-10.144000000
N	-0.738000000	-2.229000000	-10.327000000
N	1.582000000	-2.319000000	-9.940000000
C	2.736000000	-1.587000000	-9.946000000
C	2.850000000	-0.170000000	-10.116000000
C	1.660000000	0.621000000	-10.245000000
O	1.518000000	1.839000000	-10.335000000
N	4.209000000	0.197000000	-10.116000000
C	4.902000000	-0.929000000	-9.919000000
N	4.043000000	-2.077000000	-9.814000000
O	9.370000000	-3.858000000	-5.517000000
O	9.616000000	-1.914000000	-7.284000000
H	-0.475000000	0.351000000	-10.357000000
H	5.978000000	-1.028000000	-9.860000000
H	3.437000000	-4.116000000	-9.690000000
H	6.301000000	-3.212000000	-10.542000000
H	-0.765000000	-3.235000000	-10.135000000
H	7.389000000	-4.782000000	-9.184000000
H	-1.638000000	-1.719000000	-10.336000000
H	4.965000000	-5.499000000	-7.502000000
H	6.038000000	-3.522000000	-6.016000000
H	5.332000000	-4.511000000	-11.186000000
H	6.992000000	-5.060000000	-6.246000000
P	5.897000000	-7.080000000	-10.821000000
C	3.295000000	-6.853000000	-10.376000000
O	4.382000000	-6.593000000	-11.295000000
C	2.180000000	-7.575000000	-11.139000000
O	1.234000000	-6.582000000	-11.626000000
C	2.632000000	-8.348000000	-12.407000000
O	1.847000000	-9.555000000	-12.413000000
C	2.415000000	-7.362000000	-13.562000000
C	1.480000000	-6.277000000	-13.004000000
N	0.512000000	-1.127000000	-13.366000000
C	-0.338000000	-2.200000000	-13.223000000
N	0.003000000	-3.506000000	-13.128000000
C	1.362000000	-3.722000000	-13.146000000
C	2.348000000	-2.681000000	-13.249000000
C	1.881000000	-1.339000000	-13.385000000
N	2.708000000	-0.272000000	-13.571000000
N	3.640000000	-3.236000000	-13.211000000

C	3.463000000	-4.557000000	-13.091000000
N	2.080000000	-4.923000000	-13.084000000
O	5.962000000	-8.556000000	-10.516000000
O	6.807000000	-6.483000000	-11.872000000
H	-1.415000000	-1.946000000	-13.185000000
H	4.244000000	-5.311000000	-13.003000000
H	0.454000000	-6.241000000	-13.455000000
H	3.398000000	-6.970000000	-13.897000000
H	3.675000000	-8.726000000	-12.357000000
H	1.562000000	-8.207000000	-10.457000000
H	2.938000000	-5.840000000	-10.059000000
H	2.337000000	0.690000000	-13.557000000
H	3.708000000	-0.380000000	-13.453000000
H	2.004000000	-7.822000000	-14.483000000
H	3.608000000	-7.424000000	-9.478000000
P	0.764000000	-9.957000000	-13.613000000
C	-1.164000000	-8.411000000	-12.676000000
O	-0.265000000	-8.655000000	-13.777000000
C	-2.517000000	-7.984000000	-13.245000000
O	-2.476000000	-6.555000000	-13.530000000
C	-2.948000000	-8.688000000	-14.552000000
O	-4.158000000	-9.381000000	-14.204000000
C	-3.234000000	-7.565000000	-15.563000000
C	-2.746000000	-6.271000000	-14.910000000
N	-1.480000000	-5.745000000	-15.525000000
C	-1.344000000	-4.310000000	-15.725000000
O	-2.332000000	-3.597000000	-15.522000000
N	-0.148000000	-3.797000000	-16.177000000
C	0.931000000	-4.631000000	-16.397000000
N	2.109000000	-4.054000000	-16.742000000
C	0.792000000	-6.056000000	-16.235000000
C	-0.393000000	-6.575000000	-15.788000000
O	0.048000000	-11.141000000	-13.011000000
O	1.441000000	-10.033000000	-14.956000000
H	-4.445000000	-9.969000000	-14.944000000
H	1.626000000	-6.712000000	-16.479000000
H	-0.522000000	-7.660000000	-15.606000000
H	-3.493000000	-5.436000000	-14.892000000
H	-2.782000000	-7.767000000	-16.552000000
H	-2.213000000	-9.428000000	-14.929000000
H	-3.311000000	-8.072000000	-12.461000000
H	2.938000000	-4.608000000	-16.920000000
H	-0.710000000	-7.569000000	-12.080000000
H	2.214000000	-3.026000000	-16.808000000
H	-4.322000000	-7.509000000	-15.781000000
H	-1.290000000	-9.303000000	-12.030000000
P	3.040000000	5.300000000	-19.690000000
C	0.415000000	5.500000000	-19.397000000
O	1.704000000	5.589000000	-18.747000000
C	-0.620000000	5.718000000	-18.287000000

O	-0.971000000	4.429000000	-17.709000000
C	-0.093000000	6.582000000	-17.109000000
O	-1.159000000	7.466000000	-16.743000000
C	0.374000000	5.562000000	-16.065000000
C	-0.307000000	4.241000000	-16.440000000
N	0.180000000	-0.949000000	-16.473000000
C	-0.936000000	-0.141000000	-16.141000000
N	-2.109000000	-0.774000000	-15.787000000
N	-0.930000000	1.225000000	-16.232000000
C	0.298000000	1.763000000	-16.544000000
C	1.490000000	1.023000000	-16.813000000
C	1.466000000	-0.408000000	-16.790000000
O	2.372000000	-1.213000000	-17.017000000
N	2.557000000	1.915000000	-17.050000000
C	2.044000000	3.143000000	-16.944000000
N	0.648000000	3.118000000	-16.603000000
O	3.124000000	6.273000000	-20.843000000
O	4.153000000	5.136000000	-18.689000000
H	0.098000000	-2.013000000	-16.370000000
H	2.574000000	4.086000000	-17.083000000
H	-1.136000000	3.915000000	-15.751000000
H	1.484000000	5.500000000	-16.104000000
H	-2.744000000	-0.252000000	-15.159000000
H	0.717000000	7.279000000	-17.427000000
H	-2.108000000	-1.807000000	-15.660000000
H	-1.581000000	6.091000000	-18.704000000
H	0.288000000	4.496000000	-19.852000000
H	0.153000000	5.864000000	-15.012000000
H	0.334000000	6.280000000	-20.177000000
P	-2.001000000	7.386000000	-15.298000000
C	-3.569000000	5.397000000	-16.101000000
O	-2.557000000	5.827000000	-15.167000000
C	-4.605000000	4.581000000	-15.322000000
O	-4.010000000	3.331000000	-14.884000000
C	-5.142000000	5.267000000	-14.037000000
O	-6.541000000	4.936000000	-14.035000000
C	-4.292000000	4.672000000	-12.910000000
C	-3.766000000	3.342000000	-13.461000000
N	-2.303000000	3.124000000	-13.250000000
C	-1.830000000	1.773000000	-13.364000000
O	-2.614000000	0.843000000	-13.484000000
N	-0.440000000	1.587000000	-13.247000000
C	0.508000000	2.648000000	-13.209000000
O	1.695000000	2.367000000	-13.337000000
C	-0.055000000	3.988000000	-13.049000000
C	-1.397000000	4.192000000	-13.135000000
C	0.886000000	5.114000000	-12.796000000
O	-3.118000000	8.366000000	-15.547000000
O	-1.063000000	7.501000000	-14.125000000
H	-0.092000000	0.571000000	-13.302000000

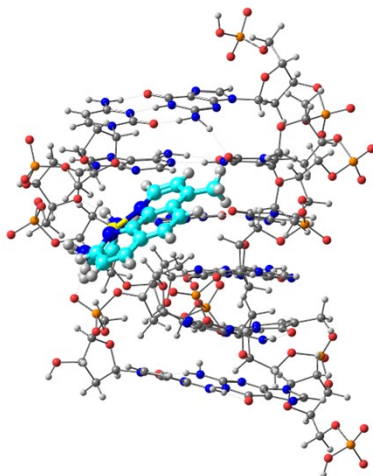
H	-1.842000000	5.206000000	-13.093000000
H	-4.310000000	2.427000000	-13.085000000
H	-3.477000000	5.392000000	-12.662000000
H	-5.109000000	6.378000000	-14.074000000
H	-5.434000000	4.257000000	-15.994000000
H	-3.040000000	4.752000000	-16.839000000
H	0.995000000	5.312000000	-11.720000000
H	1.892000000	4.905000000	-13.190000000
H	0.538000000	6.051000000	-13.271000000
H	-4.834000000	4.539000000	-11.951000000
H	-4.052000000	6.240000000	-16.629000000
P	-7.360000000	4.393000000	-12.686000000
C	-6.801000000	1.855000000	-13.208000000
O	-6.623000000	2.953000000	-12.287000000
C	-7.190000000	0.603000000	-12.420000000
O	-5.979000000	-0.081000000	-12.000000000
C	-8.019000000	0.837000000	-11.129000000
O	-9.038000000	-0.176000000	-11.250000000
C	-7.037000000	0.624000000	-9.968000000
C	-5.749000000	0.074000000	-10.587000000
N	-4.552000000	0.953000000	-10.417000000
C	-3.246000000	0.302000000	-10.424000000
O	-3.218000000	-0.922000000	-10.547000000
N	-2.116000000	1.075000000	-10.275000000
C	-2.207000000	2.443000000	-10.136000000
N	-1.040000000	3.131000000	-10.040000000
C	-3.496000000	3.087000000	-10.102000000
C	-4.628000000	2.335000000	-10.272000000
O	-8.745000000	4.170000000	-13.240000000
O	-7.095000000	5.267000000	-11.490000000
H	-3.561000000	4.164000000	-9.972000000
H	-5.635000000	2.790000000	-10.291000000
H	-5.472000000	-0.961000000	-10.233000000
H	-6.904000000	1.565000000	-9.399000000
H	-8.529000000	1.821000000	-11.095000000
H	-7.685000000	-0.142000000	-13.090000000
H	-1.032000000	4.139000000	-9.973000000
H	-5.797000000	1.709000000	-13.677000000
H	-0.117000000	2.651000000	-10.108000000
H	-7.412000000	-0.102000000	-9.209000000
H	-7.550000000	2.072000000	-13.994000000
P	-9.977000000	-0.642000000	-9.954000000
C	-8.244000000	-2.617000000	-9.841000000
O	-8.954000000	-1.619000000	-9.068000000
C	-7.200000000	-3.238000000	-8.913000000
O	-6.062000000	-2.336000000	-8.823000000
C	-7.693000000	-3.496000000	-7.459000000
O	-7.427000000	-4.887000000	-7.215000000
C	-6.945000000	-2.465000000	-6.608000000
C	-5.682000000	-2.182000000	-7.420000000

N	-1.149000000	0.176000000	-7.134000000
C	-1.476000000	-1.195000000	-7.249000000
N	-0.453000000	-2.116000000	-7.300000000
N	-2.758000000	-1.651000000	-7.367000000
C	-3.707000000	-0.668000000	-7.267000000
C	-3.477000000	0.730000000	-7.074000000
C	-2.128000000	1.223000000	-7.072000000
O	-1.710000000	2.376000000	-7.014000000
N	-4.711000000	1.395000000	-6.955000000
C	-5.660000000	0.459000000	-7.076000000
N	-5.098000000	-0.843000000	-7.289000000
O	-11.050000000	-1.463000000	-10.629000000
O	-10.311000000	0.498000000	-9.030000000
H	-0.117000000	0.466000000	-7.123000000
H	-6.732000000	0.609000000	-7.013000000
H	-4.852000000	-2.936000000	-7.243000000
H	-7.581000000	-1.566000000	-6.476000000
H	-0.694000000	-3.098000000	-7.113000000
H	-8.798000000	-3.426000000	-7.355000000
H	0.507000000	-1.824000000	-7.031000000
H	-6.793000000	-4.172000000	-9.371000000
H	-7.749000000	-2.145000000	-10.718000000
H	-6.725000000	-2.804000000	-5.574000000
H	-8.963000000	-3.388000000	-10.185000000
P	-6.302000000	-5.485000000	-6.136000000
C	-3.889000000	-5.410000000	-7.377000000
O	-4.863000000	-4.764000000	-6.538000000
C	-2.768000000	-6.064000000	-6.560000000
O	-1.888000000	-5.042000000	-6.016000000
C	-3.228000000	-6.913000000	-5.346000000
O	-2.351000000	-8.054000000	-5.367000000
C	-3.108000000	-5.956000000	-4.153000000
C	-2.107000000	-4.883000000	-4.607000000
N	-0.719000000	0.100000000	-3.899000000
C	0.044000000	-1.024000000	-4.094000000
N	-0.409000000	-2.288000000	-4.259000000
C	-1.786000000	-2.382000000	-4.228000000
C	-2.678000000	-1.269000000	-4.042000000
C	-2.099000000	0.021000000	-3.873000000
N	-2.810000000	1.169000000	-3.648000000
N	-4.014000000	-1.708000000	-4.110000000
C	-3.953000000	-3.027000000	-4.331000000
N	-2.606000000	-3.505000000	-4.381000000
O	-6.321000000	-6.963000000	-6.434000000
O	-6.555000000	-4.927000000	-4.757000000
H	1.138000000	-0.851000000	-4.144000000
H	-4.805000000	-3.703000000	-4.466000000
H	-1.081000000	-4.971000000	-4.155000000
H	-4.105000000	-5.546000000	-3.892000000
H	-4.243000000	-7.354000000	-5.456000000

H	-2.075000000	-6.650000000	-7.218000000
H	-3.466000000	-4.542000000	-7.941000000
H	-2.337000000	2.087000000	-3.731000000
H	-3.808000000	1.169000000	-3.834000000
H	-2.791000000	-6.439000000	-3.207000000
H	-4.353000000	-6.134000000	-8.071000000
P	-1.552000000	-8.584000000	-4.005000000
C	0.639000000	-7.113000000	-4.244000000
O	-0.607000000	-7.294000000	-3.537000000
C	1.794000000	-7.120000000	-3.241000000
O	2.086000000	-5.732000000	-2.859000000
C	1.565000000	-7.882000000	-1.918000000
O	2.656000000	-8.816000000	-1.847000000
C	1.673000000	-6.836000000	-0.790000000
C	1.803000000	-5.480000000	-1.481000000
N	0.549000000	-4.651000000	-1.392000000
C	0.679000000	-3.211000000	-1.271000000
O	1.814000000	-2.717000000	-1.326000000
N	-0.441000000	-2.441000000	-1.063000000
C	-1.696000000	-3.020000000	-1.047000000
N	-2.755000000	-2.204000000	-0.824000000
C	-1.840000000	-4.433000000	-1.287000000
C	-0.727000000	-5.209000000	-1.463000000
O	-0.755000000	-9.769000000	-4.466000000
O	-2.533000000	-8.722000000	-2.858000000
H	2.601000000	-9.347000000	-1.019000000
H	-2.834000000	-4.877000000	-1.316000000
H	-0.795000000	-6.295000000	-1.675000000
H	2.653000000	-4.844000000	-1.125000000
H	0.835000000	-6.904000000	-0.073000000
H	0.618000000	-8.453000000	-1.869000000
H	2.745000000	-7.452000000	-3.735000000
H	-3.705000000	-2.559000000	-0.810000000
H	0.560000000	-6.112000000	-4.735000000
H	-2.638000000	-1.186000000	-0.673000000
H	2.567000000	-7.039000000	-0.162000000
H	0.804000000	-7.893000000	-5.024000000
O	2.709000000	3.792000000	-20.333000000
O	-1.519000000	5.682000000	2.745000000
H	2.426000000	3.782000000	-21.288000000
H	-1.122000000	5.548000000	3.649000000
N	2.186000000	-5.643000000	-7.066000000
N	4.696000000	-5.133000000	-3.933000000
N	2.862000000	-3.467000000	-5.212000000
N	3.966000000	-7.298000000	-5.998000000
C	3.406000000	-10.116000000	-5.895000000
C	2.596000000	-9.322000000	-6.649000000
C	2.841000000	-7.886000000	-6.674000000
C	1.956000000	-7.029000000	-7.277000000
C	1.472000000	-4.741000000	-7.786000000

C	0.440000000	-5.143000000	-8.627000000
C	0.080000000	-6.515000000	-8.740000000
C	-1.071000000	-6.864000000	-9.625000000
C	4.850000000	-3.643000000	-3.756000000
C	3.471000000	-2.994000000	-3.919000000
C	0.824000000	-7.478000000	-8.072000000
C	0.609000000	-8.910000000	-8.064000000
C	4.660000000	-8.152000000	-5.131000000
C	1.431000000	-9.771000000	-7.412000000
C	4.464000000	-9.501000000	-5.111000000
Pt	3.456000000	-5.402000000	-5.552000000
H	5.611000000	-5.583000000	-4.019000000
H	4.221000000	-5.540000000	-3.107000000
H	3.146000000	-2.844000000	-6.000000000
H	1.832000000	-3.420000000	-5.145000000
H	3.273000000	-11.184000000	-5.824000000
H	1.748000000	-3.678000000	-7.684000000
H	-0.059000000	-4.413000000	-9.255000000
H	-0.735000000	-6.822000000	-10.687000000
H	-1.900000000	-6.150000000	-9.535000000
H	-1.471000000	-7.868000000	-9.442000000
H	5.291000000	-3.388000000	-2.768000000
H	5.565000000	-3.251000000	-4.534000000
H	2.798000000	-3.274000000	-3.068000000
H	3.575000000	-1.880000000	-3.905000000
H	-0.260000000	-9.281000000	-8.611000000
H	5.436000000	-7.673000000	-4.529000000
H	1.230000000	-10.836000000	-7.405000000
H	5.069000000	-10.146000000	-4.490000000

[Pt(en)(4-Mephen)]²⁺ minor groove
Dock_ID: 96-cl3_4-Mephen



EDA for 96-cl3_4-Mephen in kcal mol⁻¹.

Electrostatic interaction	-810
Orbital interaction	-95.8
Dispersion energy	-71.4
Pauli repulsion	137.9
Total Bonding Energy	-839.3

Contributions of the solvation energies for 96-cl3_4-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1732.5
E _{solv} (intercalator)	-161.7
E _{solv} (duplex DNA)	-2349.5
ΔE _{solv}	778.7
ΔE _{int} (EDA)	-839.3
ΔE _{aq}	-60.6

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 96-cl3_4-Mephen system.
([Pt(en)(4-Mephen)]²⁺ minor groove)

P	-1.326000000	7.099000000	2.841000000
C	1.216000000	6.769000000	2.194000000
O	-0.125000000	6.987000000	1.697000000
C	2.144000000	6.890000000	0.979000000
O	2.349000000	5.566000000	0.408000000
C	1.571000000	7.762000000	-0.170000000
O	2.668000000	8.556000000	-0.641000000
C	0.961000000	6.755000000	-1.150000000
C	1.548000000	5.389000000	-0.777000000
N	0.277000000	0.316000000	-0.768000000
C	1.470000000	0.951000000	-1.188000000
N	2.486000000	0.157000000	-1.672000000
N	1.690000000	2.299000000	-1.081000000
C	0.615000000	3.007000000	-0.595000000
C	-0.634000000	2.447000000	-0.181000000
C	-0.851000000	1.034000000	-0.260000000
O	-1.845000000	0.372000000	0.045000000
N	-1.505000000	3.478000000	0.223000000
C	-0.830000000	4.617000000	0.063000000
N	0.489000000	4.394000000	-0.470000000
O	-0.951000000	8.060000000	3.944000000
O	-2.586000000	7.240000000	2.030000000
H	0.173000000	-0.743000000	-0.912000000
H	-1.177000000	5.625000000	0.288000000
H	2.269000000	4.942000000	-1.519000000
H	-0.146000000	6.792000000	-1.058000000
H	3.157000000	0.596000000	-2.314000000
H	0.833000000	8.515000000	0.194000000
H	2.324000000	-0.861000000	-1.807000000
H	3.168000000	7.202000000	1.286000000
H	1.281000000	5.748000000	2.627000000
H	1.141000000	7.005000000	-2.222000000
H	1.470000000	7.523000000	2.963000000
P	3.222000000	8.557000000	-2.220000000
C	4.772000000	6.482000000	-1.664000000
O	3.734000000	7.007000000	-2.521000000
C	5.420000000	5.328000000	-2.433000000
O	4.432000000	4.281000000	-2.630000000
C	5.938000000	5.703000000	-3.851000000
O	7.132000000	4.912000000	-3.984000000
C	4.778000000	5.320000000	-4.773000000
C	4.097000000	4.165000000	-4.037000000
N	2.615000000	4.143000000	-4.127000000
C	2.008000000	2.850000000	-3.986000000
O	2.681000000	1.831000000	-4.008000000
N	0.606000000	2.838000000	-3.917000000

C	-0.211000000	3.995000000	-3.823000000
O	-1.392000000	3.829000000	-3.531000000
C	0.476000000	5.262000000	-4.083000000
C	1.835000000	5.311000000	-4.153000000
C	-0.361000000	6.484000000	-4.231000000
O	4.370000000	9.529000000	-2.124000000
O	2.100000000	8.723000000	-3.212000000
H	0.161000000	1.863000000	-3.816000000
H	2.395000000	6.262000000	-4.260000000
H	4.474000000	3.139000000	-4.337000000
H	4.108000000	6.206000000	-4.887000000
H	6.255000000	6.763000000	-3.945000000
H	6.214000000	4.844000000	-1.818000000
H	4.282000000	6.104000000	-0.739000000
H	-0.864000000	6.507000000	-5.211000000
H	-1.149000000	6.534000000	-3.464000000
H	0.232000000	7.411000000	-4.143000000
H	5.076000000	5.053000000	-5.806000000
H	5.520000000	7.254000000	-1.401000000
P	7.594000000	4.169000000	-5.407000000
C	6.459000000	1.855000000	-4.742000000
O	6.459000000	2.973000000	-5.657000000
C	6.518000000	0.540000000	-5.525000000
O	5.163000000	0.089000000	-5.794000000
C	7.219000000	0.605000000	-6.907000000
O	7.987000000	-0.613000000	-6.932000000
C	6.076000000	0.742000000	-7.919000000
C	4.805000000	0.300000000	-7.176000000
N	3.699000000	1.300000000	-7.206000000
C	2.325000000	0.821000000	-7.072000000
O	2.132000000	-0.391000000	-6.988000000
N	1.304000000	1.746000000	-7.064000000
C	1.565000000	3.093000000	-7.151000000
N	0.501000000	3.942000000	-7.116000000
C	2.920000000	3.572000000	-7.250000000
C	3.947000000	2.668000000	-7.235000000
O	8.929000000	3.583000000	-5.024000000
O	7.417000000	5.080000000	-6.591000000
H	3.118000000	4.640000000	-7.312000000
H	5.007000000	2.990000000	-7.260000000
H	4.392000000	-0.694000000	-7.510000000
H	6.036000000	1.793000000	-8.281000000
H	7.975000000	1.414000000	-6.993000000
H	6.936000000	-0.276000000	-4.889000000
H	0.630000000	4.946000000	-7.108000000
H	5.470000000	1.933000000	-4.215000000
H	-0.461000000	3.591000000	-6.951000000
H	6.213000000	0.155000000	-8.852000000
H	7.277000000	1.910000000	-4.001000000
P	8.073000000	-1.638000000	-8.238000000

C	5.817000000	-2.938000000	-7.652000000
O	6.491000000	-2.054000000	-8.567000000
C	5.436000000	-4.240000000	-8.371000000
O	4.027000000	-4.176000000	-8.737000000
C	6.207000000	-4.520000000	-9.688000000
O	6.585000000	-5.901000000	-9.533000000
C	5.202000000	-4.243000000	-10.816000000
C	3.873000000	-3.889000000	-10.143000000
N	-0.008000000	-0.379000000	-10.238000000
C	-0.082000000	-1.786000000	-10.136000000
N	-1.323000000	-2.357000000	-10.162000000
N	1.027000000	-2.607000000	-10.101000000
C	2.219000000	-1.925000000	-10.187000000
C	2.378000000	-0.508000000	-10.283000000
C	1.228000000	0.348000000	-10.245000000
O	1.155000000	1.574000000	-10.248000000
N	3.745000000	-0.179000000	-10.364000000
C	4.404000000	-1.337000000	-10.358000000
N	3.512000000	-2.466000000	-10.282000000
O	8.851000000	-2.800000000	-7.678000000
O	8.498000000	-0.900000000	-9.481000000
H	-0.920000000	0.187000000	-10.194000000
H	5.481000000	-1.478000000	-10.386000000
H	3.008000000	-4.523000000	-10.465000000
H	5.578000000	-3.459000000	-11.503000000
H	-1.457000000	-3.329000000	-9.918000000
H	7.144000000	-3.937000000	-9.803000000
H	-2.193000000	-1.784000000	-10.214000000
H	5.476000000	-5.117000000	-7.681000000
H	4.895000000	-2.373000000	-7.368000000
H	5.054000000	-5.127000000	-11.478000000
H	6.413000000	-3.149000000	-6.744000000
P	7.101000000	-6.808000000	-10.838000000
C	4.632000000	-7.648000000	-10.608000000
O	5.641000000	-7.207000000	-11.547000000
C	3.377000000	-7.947000000	-11.428000000
O	2.706000000	-6.696000000	-11.745000000
C	3.661000000	-8.671000000	-12.771000000
O	2.847000000	-9.848000000	-12.754000000
C	3.392000000	-7.625000000	-13.857000000
C	2.544000000	-6.545000000	-13.186000000
N	0.940000000	-1.580000000	-13.337000000
C	0.270000000	-2.746000000	-13.077000000
N	0.788000000	-4.001000000	-13.044000000
C	2.124000000	-4.045000000	-13.361000000
C	2.937000000	-2.903000000	-13.654000000
C	2.304000000	-1.619000000	-13.612000000
N	2.940000000	-0.450000000	-13.874000000
N	4.253000000	-3.315000000	-13.935000000
C	4.257000000	-4.650000000	-13.821000000

N	2.963000000	-5.166000000	-13.488000000
O	7.726000000	-8.007000000	-10.169000000
O	7.835000000	-6.000000000	-11.871000000
H	-0.813000000	-2.639000000	-12.860000000
H	5.109000000	-5.306000000	-13.967000000
H	1.435000000	-6.639000000	-13.371000000
H	4.360000000	-7.245000000	-14.248000000
H	4.695000000	-9.084000000	-12.828000000
H	2.636000000	-8.509000000	-10.810000000
H	4.436000000	-6.842000000	-9.866000000
H	2.468000000	0.456000000	-13.702000000
H	3.947000000	-0.425000000	-13.986000000
H	2.899000000	-8.043000000	-14.762000000
H	4.975000000	-8.567000000	-10.089000000
P	1.465000000	-10.061000000	-13.673000000
C	-0.344000000	-8.545000000	-12.403000000
O	0.607000000	-8.649000000	-13.482000000
C	-1.753000000	-8.352000000	-12.969000000
O	-1.862000000	-6.983000000	-13.457000000
C	-2.152000000	-9.270000000	-14.143000000
O	-3.354000000	-9.924000000	-13.695000000
C	-2.448000000	-8.340000000	-15.334000000
C	-2.097000000	-6.927000000	-14.861000000
N	-0.859000000	-6.359000000	-15.507000000
C	-0.797000000	-4.916000000	-15.688000000
O	-1.810000000	-4.256000000	-15.444000000
N	0.359000000	-4.337000000	-16.167000000
C	1.454000000	-5.118000000	-16.476000000
N	2.567000000	-4.481000000	-16.929000000
C	1.395000000	-6.544000000	-16.310000000
C	0.258000000	-7.128000000	-15.812000000
O	0.794000000	-11.216000000	-12.975000000
O	1.806000000	-10.065000000	-15.138000000
H	-3.652000000	-10.587000000	-14.363000000
H	2.248000000	-7.160000000	-16.590000000
H	0.200000000	-8.217000000	-15.637000000
H	-2.914000000	-6.170000000	-14.983000000
H	-1.917000000	-8.656000000	-16.250000000
H	-1.415000000	-10.057000000	-14.391000000
H	-2.513000000	-8.386000000	-12.137000000
H	3.416000000	-4.991000000	-17.141000000
H	-0.034000000	-7.610000000	-11.863000000
H	2.619000000	-3.448000000	-16.984000000
H	-3.519000000	-8.405000000	-15.618000000
H	-0.317000000	-9.414000000	-11.718000000
P	2.514000000	4.596000000	-19.986000000
C	-0.104000000	4.773000000	-19.519000000
O	1.217000000	5.220000000	-19.148000000
C	-0.980000000	4.951000000	-18.274000000
O	-1.097000000	3.670000000	-17.595000000

C	-0.404000000	5.940000000	-17.224000000
O	-1.506000000	6.752000000	-16.802000000
C	0.272000000	5.051000000	-16.174000000
C	-0.294000000	3.646000000	-16.393000000
N	0.524000000	-1.484000000	-16.468000000
C	-0.615000000	-0.746000000	-16.059000000
N	-1.734000000	-1.456000000	-15.660000000
N	-0.692000000	0.615000000	-16.125000000
C	0.475000000	1.228000000	-16.524000000
C	1.681000000	0.563000000	-16.903000000
C	1.742000000	-0.868000000	-16.900000000
O	2.665000000	-1.620000000	-17.216000000
N	2.673000000	1.519000000	-17.202000000
C	2.101000000	2.714000000	-17.036000000
N	0.741000000	2.603000000	-16.581000000
O	2.649000000	5.289000000	-21.322000000
O	3.628000000	4.595000000	-18.973000000
H	0.505000000	-2.553000000	-16.385000000
H	2.572000000	3.685000000	-17.202000000
H	-1.012000000	3.298000000	-15.599000000
H	1.373000000	5.103000000	-16.315000000
H	-2.330000000	-0.999000000	-14.946000000
H	0.295000000	6.683000000	-17.675000000
H	-1.643000000	-2.486000000	-15.529000000
H	-2.029000000	5.193000000	-18.558000000
H	-0.103000000	3.708000000	-19.833000000
H	0.119000000	5.399000000	-15.118000000
H	-0.454000000	5.410000000	-20.354000000
P	-2.222000000	6.694000000	-15.291000000
C	-3.632000000	4.530000000	-15.905000000
O	-2.646000000	5.108000000	-15.023000000
C	-4.679000000	3.793000000	-15.067000000
O	-4.172000000	2.467000000	-14.743000000
C	-5.075000000	4.461000000	-13.725000000
O	-6.509000000	4.562000000	-13.829000000
C	-4.597000000	3.501000000	-12.630000000
C	-3.911000000	2.332000000	-13.334000000
N	-2.430000000	2.297000000	-13.124000000
C	-1.796000000	1.017000000	-13.229000000
O	-2.462000000	-0.006000000	-13.323000000
N	-0.392000000	0.999000000	-13.152000000
C	0.422000000	2.166000000	-13.149000000
O	1.631000000	2.019000000	-13.306000000
C	-0.296000000	3.429000000	-12.989000000
C	-1.656000000	3.469000000	-13.036000000
C	0.512000000	4.660000000	-12.772000000
O	-3.440000000	7.557000000	-15.502000000
O	-1.206000000	6.972000000	-14.217000000
H	0.079000000	0.040000000	-13.190000000
H	-2.212000000	4.422000000	-12.997000000

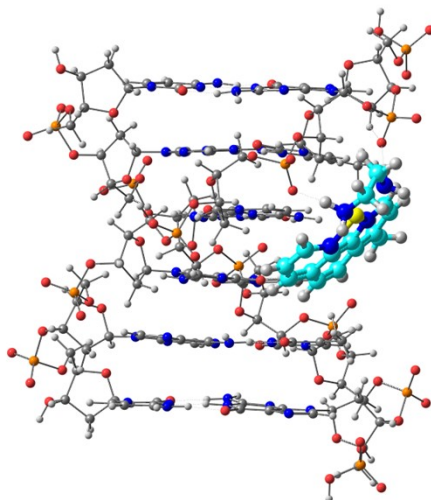
H	-4.328000000	1.321000000	-13.070000000
H	-3.956000000	4.030000000	-11.896000000
H	-4.676000000	5.492000000	-13.613000000
H	-5.583000000	3.578000000	-15.689000000
H	-3.067000000	3.806000000	-16.539000000
H	0.411000000	5.035000000	-11.744000000
H	1.582000000	4.491000000	-12.960000000
H	0.191000000	5.480000000	-13.448000000
H	-5.450000000	3.097000000	-12.029000000
H	-4.119000000	5.283000000	-16.552000000
P	-7.443000000	4.866000000	-12.472000000
C	-7.911000000	2.293000000	-12.647000000
O	-7.523000000	3.361000000	-11.748000000
C	-7.864000000	0.991000000	-11.851000000
O	-6.483000000	0.577000000	-11.691000000
C	-8.499000000	1.057000000	-10.437000000
O	-9.490000000	0.011000000	-10.521000000
C	-7.363000000	0.771000000	-9.453000000
C	-6.165000000	0.336000000	-10.298000000
N	-4.911000000	1.092000000	-10.032000000
C	-3.655000000	0.347000000	-10.144000000
O	-3.720000000	-0.858000000	-10.337000000
N	-2.472000000	1.048000000	-10.019000000
C	-2.465000000	2.402000000	-9.786000000
N	-1.253000000	3.012000000	-9.729000000
C	-3.703000000	3.116000000	-9.588000000
C	-4.891000000	2.451000000	-9.728000000
O	-8.772000000	5.240000000	-13.081000000
O	-6.750000000	5.741000000	-11.466000000
H	-3.686000000	4.173000000	-9.329000000
H	-5.865000000	2.959000000	-9.620000000
H	-5.932000000	-0.772000000	-10.231000000
H	-7.172000000	1.664000000	-8.825000000
H	-9.021000000	2.019000000	-10.238000000
H	-8.330000000	0.167000000	-12.450000000
H	-1.170000000	4.006000000	-9.575000000
H	-7.203000000	2.247000000	-13.503000000
H	-0.376000000	2.488000000	-9.928000000
H	-7.606000000	-0.036000000	-8.718000000
H	-8.940000000	2.476000000	-13.019000000
P	-10.349000000	-0.479000000	-9.181000000
C	-8.576000000	-2.429000000	-9.201000000
O	-9.263000000	-1.456000000	-8.375000000
C	-7.395000000	-2.942000000	-8.377000000
O	-6.357000000	-1.924000000	-8.385000000
C	-7.734000000	-3.243000000	-6.886000000
O	-7.476000000	-4.639000000	-6.699000000
C	-6.900000000	-2.240000000	-6.081000000
C	-5.781000000	-1.839000000	-7.045000000
N	-1.404000000	0.856000000	-6.860000000

C	-1.632000000	-0.519000000	-7.111000000
N	-0.542000000	-1.331000000	-7.346000000
N	-2.876000000	-1.075000000	-7.165000000
C	-3.894000000	-0.189000000	-6.924000000
C	-3.762000000	1.207000000	-6.644000000
C	-2.458000000	1.805000000	-6.669000000
O	-2.139000000	2.986000000	-6.540000000
N	-5.036000000	1.763000000	-6.421000000
C	-5.913000000	0.761000000	-6.557000000
N	-5.267000000	-0.473000000	-6.887000000
O	-11.452000000	-1.306000000	-9.798000000
O	-10.647000000	0.644000000	-8.223000000
H	-0.398000000	1.230000000	-6.899000000
H	-6.989000000	0.825000000	-6.440000000
H	-4.893000000	-2.544000000	-7.040000000
H	-7.535000000	-1.383000000	-5.781000000
H	-0.687000000	-2.339000000	-7.248000000
H	-8.821000000	-3.159000000	-6.669000000
H	0.417000000	-0.987000000	-7.139000000
H	-6.939000000	-3.838000000	-8.870000000
H	-8.219000000	-1.959000000	-10.144000000
H	-6.508000000	-2.646000000	-5.124000000
H	-9.277000000	-3.256000000	-9.431000000
P	-6.187000000	-5.254000000	-5.827000000
C	-4.087000000	-4.857000000	-7.511000000
O	-4.845000000	-4.441000000	-6.359000000
C	-2.767000000	-5.515000000	-7.112000000
O	-1.831000000	-4.536000000	-6.556000000
C	-2.898000000	-6.604000000	-6.018000000
O	-1.851000000	-7.524000000	-6.386000000
C	-2.640000000	-5.846000000	-4.704000000
C	-1.808000000	-4.624000000	-5.122000000
N	-0.444000000	0.227000000	-3.799000000
C	0.310000000	-0.847000000	-4.196000000
N	-0.137000000	-2.099000000	-4.469000000
C	-1.502000000	-2.231000000	-4.324000000
C	-2.383000000	-1.183000000	-3.893000000
C	-1.813000000	0.099000000	-3.635000000
N	-2.527000000	1.184000000	-3.217000000
N	-3.710000000	-1.653000000	-3.883000000
C	-3.651000000	-2.925000000	-4.293000000
N	-2.311000000	-3.351000000	-4.553000000
O	-6.213000000	-6.727000000	-6.090000000
O	-6.263000000	-4.727000000	-4.403000000
H	1.390000000	-0.645000000	-4.330000000
H	-4.508000000	-3.602000000	-4.416000000
H	-0.711000000	-4.708000000	-4.872000000
H	-3.600000000	-5.576000000	-4.223000000
H	-3.855000000	-7.172000000	-6.056000000
H	-2.213000000	-5.899000000	-8.020000000

H	-3.888000000	-3.890000000	-8.033000000
H	-2.099000000	2.128000000	-3.227000000
H	-3.541000000	1.147000000	-3.228000000
H	-2.121000000	-6.443000000	-3.931000000
H	-4.673000000	-5.532000000	-8.164000000
P	-1.145000000	-8.560000000	-5.323000000
C	0.819000000	-6.812000000	-4.957000000
O	-0.250000000	-7.530000000	-4.330000000
C	2.081000000	-6.934000000	-4.093000000
O	2.422000000	-5.580000000	-3.671000000
C	1.943000000	-7.780000000	-2.807000000
O	2.973000000	-8.775000000	-2.910000000
C	2.226000000	-6.815000000	-1.641000000
C	2.275000000	-5.416000000	-2.251000000
N	1.027000000	-4.622000000	-2.000000000
C	1.148000000	-3.202000000	-1.723000000
O	2.257000000	-2.672000000	-1.856000000
N	0.044000000	-2.497000000	-1.301000000
C	-1.193000000	-3.109000000	-1.220000000
N	-2.230000000	-2.364000000	-0.774000000
C	-1.343000000	-4.488000000	-1.625000000
C	-0.243000000	-5.206000000	-2.000000000
O	-0.224000000	-9.314000000	-6.264000000
O	-2.041000000	-9.243000000	-4.330000000
H	2.914000000	-9.413000000	-2.156000000
H	-2.332000000	-4.946000000	-1.621000000
H	-0.318000000	-6.262000000	-2.323000000
H	3.155000000	-4.788000000	-1.951000000
H	1.501000000	-6.923000000	-0.813000000
H	0.962000000	-8.299000000	-2.709000000
H	2.965000000	-7.254000000	-4.693000000
H	-3.170000000	-2.741000000	-0.709000000
H	0.486000000	-5.742000000	-4.998000000
H	-2.112000000	-1.371000000	-0.506000000
H	3.200000000	-7.063000000	-1.165000000
H	1.029000000	-7.171000000	-5.991000000
O	2.061000000	3.018000000	-20.279000000
O	-1.335000000	5.557000000	3.487000000
H	1.796000000	2.815000000	-21.220000000
H	-0.865000000	5.446000000	4.359000000
N	-2.473000000	-5.939000000	-10.851000000
N	0.229000000	-8.090000000	-8.737000000
N	0.442000000	-5.714000000	-10.119000000
N	-2.708000000	-8.257000000	-9.587000000
C	-5.183000000	-8.937000000	-8.305000000
C	-5.166000000	-7.868000000	-9.147000000
C	-3.906000000	-7.482000000	-9.772000000
C	-3.793000000	-6.309000000	-10.470000000
C	-2.306000000	-4.881000000	-11.686000000
C	-3.358000000	-4.020000000	-11.977000000

C	-4.657000000	-4.242000000	-11.427000000
C	-5.677000000	-3.164000000	-11.577000000
C	1.427000000	-7.216000000	-8.448000000
C	1.086000000	-5.754000000	-8.760000000
C	-4.912000000	-5.419000000	-10.741000000
C	-6.178000000	-5.858000000	-10.179000000
C	-2.770000000	-9.240000000	-8.593000000
C	-6.304000000	-6.992000000	-9.449000000
C	-3.944000000	-9.637000000	-8.021000000
Pt	-1.147000000	-7.021000000	-9.842000000
H	0.524000000	-8.933000000	-9.242000000
H	-0.178000000	-8.420000000	-7.816000000
H	1.098000000	-6.042000000	-10.849000000
H	0.194000000	-4.743000000	-10.370000000
H	-6.078000000	-9.245000000	-7.783000000
H	-1.300000000	-4.740000000	-12.106000000
H	-3.188000000	-3.147000000	-12.594000000
H	-5.588000000	-2.625000000	-12.529000000
H	-5.506000000	-2.393000000	-10.786000000
H	-6.709000000	-3.515000000	-11.486000000
H	1.720000000	-7.319000000	-7.369000000
H	2.307000000	-7.559000000	-9.036000000
H	0.347000000	-5.350000000	-8.017000000
H	2.000000000	-5.113000000	-8.698000000
H	-7.049000000	-5.227000000	-10.367000000
H	-1.818000000	-9.724000000	-8.355000000
H	-7.254000000	-7.275000000	-9.005000000
H	-3.974000000	-10.460000000	-7.323000000

[Pt(en)(4-Mephen)]²⁺ major groove
Dock_ID: 284-cl8_4-Mephen



EDA for 284-cl8_4-Mephen in kcal mol⁻¹.

Electrostatic interaction	-765.0
Orbital interaction	-87.3
Dispersion energy	-54.2
Pauli repulsion	110.3
Total Bonding Energy	-796.2

Contributions of the solvation energies for 284-cl8_4-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1743.7
E _{solv} (intercalator)	-161.0
E _{solv} (duplex DNA)	-2320.3
ΔE _{solv}	737.6
ΔE _{int} (EDA)	-796.2
ΔE _{aq}	-58.5

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 284-cl8_4-Mephen system.
([Pt(en)(4-Mephen)]²⁺ major groove)

P	-1.226000000	7.572000000	1.810000000
C	1.384000000	7.085000000	1.918000000
O	0.276000000	7.501000000	1.090000000
C	2.564000000	6.866000000	0.967000000
O	2.635000000	5.458000000	0.603000000
C	2.457000000	7.637000000	-0.376000000
O	3.796000000	8.112000000	-0.593000000
C	1.908000000	6.613000000	-1.371000000
C	2.112000000	5.241000000	-0.725000000
N	0.133000000	0.434000000	-0.608000000
C	1.466000000	0.866000000	-0.802000000
N	2.440000000	-0.095000000	-0.982000000
N	1.850000000	2.179000000	-0.746000000
C	0.808000000	3.063000000	-0.569000000
C	-0.566000000	2.712000000	-0.402000000
C	-0.959000000	1.335000000	-0.385000000
O	-2.069000000	0.836000000	-0.208000000
N	-1.347000000	3.883000000	-0.322000000
C	-0.498000000	4.906000000	-0.431000000
N	0.861000000	4.461000000	-0.598000000
O	-1.280000000	8.676000000	2.838000000
O	-2.162000000	7.503000000	0.633000000
H	-0.080000000	-0.615000000	-0.649000000
H	-0.746000000	5.969000000	-0.405000000
H	2.896000000	4.589000000	-1.218000000
H	0.840000000	6.843000000	-1.574000000
H	3.283000000	0.190000000	-1.489000000
H	1.835000000	8.559000000	-0.306000000
H	2.159000000	-1.086000000	-1.133000000
H	3.535000000	7.047000000	1.485000000
H	1.139000000	6.140000000	2.448000000
H	2.395000000	6.669000000	-2.377000000
H	1.609000000	7.883000000	2.651000000
P	4.650000000	8.136000000	-2.014000000
C	5.645000000	5.869000000	-0.975000000
O	5.919000000	7.118000000	-1.632000000
C	5.871000000	4.689000000	-1.921000000
O	4.591000000	4.019000000	-2.127000000
C	6.421000000	5.024000000	-3.337000000
O	7.474000000	4.053000000	-3.451000000
C	5.233000000	4.797000000	-4.279000000
C	4.465000000	3.692000000	-3.552000000
N	3.016000000	3.581000000	-3.809000000
C	2.456000000	2.260000000	-3.702000000
O	3.172000000	1.274000000	-3.611000000

N	1.056000000	2.169000000	-3.779000000
C	0.183000000	3.290000000	-3.809000000
O	-1.021000000	3.079000000	-3.703000000
C	0.832000000	4.596000000	-3.963000000
C	2.186000000	4.712000000	-3.935000000
C	-0.078000000	5.763000000	-4.118000000
O	5.284000000	9.501000000	-2.050000000
O	3.932000000	7.605000000	-3.234000000
H	0.640000000	1.176000000	-3.731000000
H	2.710000000	5.689000000	-4.021000000
H	4.933000000	2.677000000	-3.690000000
H	4.639000000	5.740000000	-4.382000000
H	6.878000000	6.041000000	-3.412000000
H	6.515000000	3.918000000	-1.428000000
H	4.634000000	5.831000000	-0.518000000
H	-0.560000000	5.762000000	-5.114000000
H	-0.877000000	5.752000000	-3.362000000
H	0.446000000	6.724000000	-4.025000000
H	5.516000000	4.544000000	-5.329000000
H	6.388000000	5.853000000	-0.148000000
P	8.276000000	3.683000000	-4.866000000
C	7.140000000	1.316000000	-4.548000000
O	8.385000000	2.043000000	-4.577000000
C	7.298000000	0.120000000	-5.500000000
O	5.963000000	-0.390000000	-5.742000000
C	7.899000000	0.459000000	-6.890000000
O	8.811000000	-0.630000000	-7.119000000
C	6.690000000	0.564000000	-7.825000000
C	5.507000000	-0.068000000	-7.081000000
N	4.326000000	0.823000000	-6.947000000
C	2.997000000	0.228000000	-6.932000000
O	2.907000000	-1.003000000	-6.930000000
N	1.893000000	1.052000000	-6.928000000
C	2.040000000	2.421000000	-6.898000000
N	0.915000000	3.186000000	-6.880000000
C	3.351000000	3.009000000	-6.794000000
C	4.454000000	2.211000000	-6.838000000
O	9.686000000	4.189000000	-4.732000000
O	7.443000000	3.988000000	-6.084000000
H	3.457000000	4.095000000	-6.718000000
H	5.477000000	2.635000000	-6.808000000
H	5.168000000	-1.057000000	-7.496000000
H	6.517000000	1.626000000	-8.111000000
H	8.534000000	1.373000000	-6.897000000
H	7.837000000	-0.730000000	-5.023000000
H	0.981000000	4.197000000	-6.969000000
H	6.256000000	1.934000000	-4.811000000
H	-0.027000000	2.765000000	-6.940000000
H	6.839000000	0.072000000	-8.811000000
H	7.024000000	0.972000000	-3.499000000

P	9.052000000	-1.339000000	-8.609000000
C	7.176000000	-3.064000000	-7.924000000
O	7.606000000	-2.103000000	-8.917000000
C	6.488000000	-4.217000000	-8.662000000
O	5.083000000	-3.887000000	-8.831000000
C	7.032000000	-4.486000000	-10.092000000
O	6.949000000	-5.919000000	-10.206000000
C	6.100000000	-3.676000000	-10.998000000
C	4.804000000	-3.501000000	-10.198000000
N	0.568000000	-0.489000000	-10.085000000
C	0.674000000	-1.895000000	-10.058000000
N	-0.493000000	-2.615000000	-10.154000000
N	1.871000000	-2.566000000	-10.016000000
C	2.966000000	-1.741000000	-10.113000000
C	2.948000000	-0.314000000	-10.211000000
C	1.703000000	0.396000000	-10.137000000
O	1.464000000	1.595000000	-10.143000000
N	4.260000000	0.175000000	-10.340000000
C	5.058000000	-0.891000000	-10.306000000
N	4.314000000	-2.115000000	-10.177000000
O	10.148000000	-2.328000000	-8.299000000
O	9.168000000	-0.323000000	-9.713000000
H	-0.406000000	-0.041000000	-10.039000000
H	6.145000000	-0.905000000	-10.353000000
H	3.964000000	-4.188000000	-10.509000000
H	6.595000000	-2.708000000	-11.243000000
H	-0.461000000	-3.622000000	-10.052000000
H	8.104000000	-4.230000000	-10.222000000
H	-1.412000000	-2.154000000	-10.006000000
H	6.466000000	-5.142000000	-8.041000000
H	6.441000000	-2.532000000	-7.275000000
H	5.914000000	-4.129000000	-11.992000000
H	8.016000000	-3.440000000	-7.311000000
P	6.545000000	-6.699000000	-11.620000000
C	3.965000000	-6.680000000	-10.992000000
O	4.973000000	-6.225000000	-11.921000000
C	2.782000000	-7.245000000	-11.782000000
O	1.810000000	-6.181000000	-11.991000000
C	3.130000000	-7.780000000	-13.198000000
O	2.298000000	-8.948000000	-13.311000000
C	2.803000000	-6.610000000	-14.136000000
C	1.843000000	-5.706000000	-13.351000000
N	0.333000000	-0.667000000	-13.293000000
C	-0.403000000	-1.823000000	-13.280000000
N	0.069000000	-3.098000000	-13.292000000
C	1.443000000	-3.172000000	-13.313000000
C	2.317000000	-2.032000000	-13.346000000
C	1.718000000	-0.735000000	-13.325000000
N	2.436000000	0.423000000	-13.381000000
N	3.659000000	-2.455000000	-13.357000000

C	3.622000000	-3.791000000	-13.328000000
N	2.282000000	-4.296000000	-13.327000000
O	6.613000000	-8.147000000	-11.202000000
O	7.307000000	-6.155000000	-12.799000000
H	-1.502000000	-1.688000000	-13.244000000
H	4.479000000	-4.466000000	-13.295000000
H	0.770000000	-5.754000000	-13.686000000
H	3.750000000	-6.105000000	-14.425000000
H	4.175000000	-8.138000000	-13.307000000
H	2.212000000	-7.996000000	-11.185000000
H	3.645000000	-5.757000000	-10.439000000
H	1.960000000	1.332000000	-13.247000000
H	3.428000000	0.404000000	-13.159000000
H	2.373000000	-6.914000000	-15.109000000
H	4.351000000	-7.430000000	-10.276000000
P	1.588000000	-9.415000000	-14.744000000
C	-0.576000000	-8.031000000	-14.086000000
O	0.498000000	-8.178000000	-15.038000000
C	-1.898000000	-7.902000000	-14.851000000
O	-2.247000000	-6.485000000	-14.878000000
C	-1.884000000	-8.380000000	-16.321000000
O	-2.932000000	-9.362000000	-16.391000000
C	-2.230000000	-7.144000000	-17.170000000
C	-2.231000000	-5.955000000	-16.212000000
N	-1.015000000	-5.085000000	-16.348000000
C	-1.177000000	-3.643000000	-16.244000000
O	-2.316000000	-3.202000000	-16.054000000
N	-0.082000000	-2.823000000	-16.387000000
C	1.177000000	-3.361000000	-16.576000000
N	2.218000000	-2.499000000	-16.660000000
C	1.350000000	-4.791000000	-16.644000000
C	0.263000000	-5.612000000	-16.525000000
O	0.873000000	-10.681000000	-14.349000000
O	2.539000000	-9.339000000	-15.905000000
H	-2.947000000	-9.787000000	-17.283000000
H	2.344000000	-5.208000000	-16.808000000
H	0.361000000	-6.715000000	-16.555000000
H	-3.138000000	-5.300000000	-16.268000000
H	-1.552000000	-7.027000000	-18.036000000
H	-0.935000000	-8.861000000	-16.637000000
H	-2.741000000	-8.366000000	-14.282000000
H	3.166000000	-2.827000000	-16.811000000
H	-0.355000000	-7.080000000	-13.540000000
H	2.086000000	-1.472000000	-16.589000000
H	-3.227000000	-7.268000000	-17.643000000
H	-0.625000000	-8.871000000	-13.367000000
P	1.276000000	7.186000000	-18.922000000
C	-1.297000000	6.604000000	-18.817000000
O	-0.113000000	6.913000000	-18.046000000
C	-2.460000000	6.555000000	-17.822000000

O	-2.685000000	5.175000000	-17.415000000
C	-2.226000000	7.355000000	-16.512000000
O	-3.464000000	8.060000000	-16.328000000
C	-1.865000000	6.297000000	-15.462000000
C	-2.163000000	4.934000000	-16.095000000
N	-0.397000000	0.030000000	-16.247000000
C	-1.711000000	0.513000000	-16.028000000
N	-2.682000000	-0.405000000	-15.758000000
N	-2.040000000	1.849000000	-16.056000000
C	-0.964000000	2.684000000	-16.237000000
C	0.392000000	2.278000000	-16.440000000
C	0.728000000	0.887000000	-16.469000000
O	1.812000000	0.339000000	-16.671000000
N	1.213000000	3.415000000	-16.590000000
C	0.408000000	4.471000000	-16.475000000
N	-0.957000000	4.085000000	-16.225000000
O	1.067000000	8.252000000	-19.971000000
O	2.350000000	7.278000000	-17.872000000
H	-0.230000000	-1.026000000	-16.249000000
H	0.684000000	5.522000000	-16.557000000
H	-2.975000000	4.333000000	-15.584000000
H	-0.801000000	6.417000000	-15.152000000
H	-3.627000000	-0.095000000	-15.541000000
H	-1.448000000	8.145000000	-16.619000000
H	-2.522000000	-1.422000000	-15.870000000
H	-3.419000000	6.834000000	-18.319000000
H	-1.167000000	5.615000000	-19.307000000
H	-2.427000000	6.406000000	-14.506000000
H	-1.469000000	7.382000000	-19.585000000
P	-4.218000000	8.254000000	-14.849000000
C	-5.346000000	5.911000000	-15.280000000
O	-4.552000000	6.696000000	-14.361000000
C	-5.781000000	4.664000000	-14.511000000
O	-4.669000000	3.723000000	-14.448000000
C	-6.228000000	4.948000000	-13.050000000
O	-7.477000000	4.239000000	-12.967000000
C	-5.088000000	4.401000000	-12.186000000
C	-4.418000000	3.342000000	-13.065000000
N	-2.944000000	3.261000000	-12.905000000
C	-2.336000000	1.959000000	-12.997000000
O	-3.021000000	0.951000000	-13.018000000
N	-0.929000000	1.929000000	-12.993000000
C	-0.103000000	3.086000000	-12.988000000
O	1.110000000	2.935000000	-13.085000000
C	-0.800000000	4.371000000	-12.855000000
C	-2.158000000	4.424000000	-12.868000000
C	0.041000000	5.597000000	-12.787000000
O	-5.468000000	9.001000000	-15.238000000
O	-3.269000000	8.761000000	-13.798000000
H	-0.472000000	0.956000000	-13.084000000

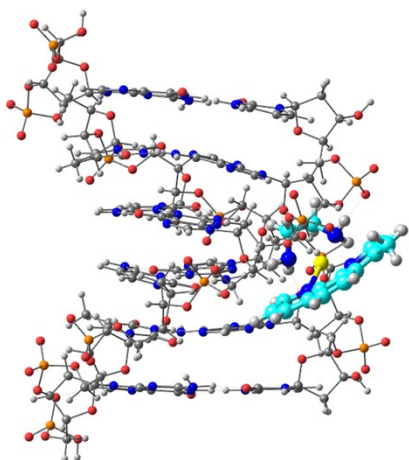
H	-2.713000000	5.381000000	-12.832000000
H	-4.853000000	2.306000000	-12.944000000
H	-4.407000000	5.242000000	-11.923000000
H	-6.452000000	6.021000000	-12.858000000
H	-6.574000000	4.117000000	-15.079000000
H	-4.722000000	5.642000000	-16.159000000
H	1.082000000	5.364000000	-12.508000000
H	0.085000000	6.110000000	-13.765000000
H	-0.340000000	6.326000000	-12.058000000
H	-5.410000000	3.985000000	-11.210000000
H	-6.233000000	6.481000000	-15.622000000
P	-8.045000000	3.615000000	-11.530000000
C	-7.048000000	1.247000000	-12.198000000
O	-7.001000000	2.338000000	-11.258000000
C	-7.337000000	-0.061000000	-11.454000000
O	-6.076000000	-0.742000000	-11.201000000
C	-8.017000000	0.086000000	-10.068000000
O	-8.981000000	-0.985000000	-10.093000000
C	-6.880000000	-0.075000000	-9.048000000
C	-5.663000000	-0.578000000	-9.832000000
N	-4.498000000	0.358000000	-9.824000000
C	-3.163000000	-0.220000000	-9.930000000
O	-3.070000000	-1.443000000	-10.043000000
N	-2.072000000	0.617000000	-9.876000000
C	-2.231000000	1.979000000	-9.765000000
N	-1.100000000	2.734000000	-9.749000000
C	-3.547000000	2.560000000	-9.691000000
C	-4.640000000	1.737000000	-9.719000000
O	-9.421000000	3.131000000	-11.904000000
O	-7.791000000	4.534000000	-10.366000000
H	-3.664000000	3.636000000	-9.597000000
H	-5.672000000	2.137000000	-9.667000000
H	-5.299000000	-1.599000000	-9.520000000
H	-6.714000000	0.879000000	-8.509000000
H	-8.586000000	1.030000000	-9.938000000
H	-7.887000000	-0.780000000	-12.107000000
H	-1.134000000	3.738000000	-9.645000000
H	-6.019000000	1.219000000	-12.642000000
H	-0.157000000	2.298000000	-9.823000000
H	-7.126000000	-0.798000000	-8.237000000
H	-7.784000000	1.410000000	-13.008000000
P	-9.665000000	-1.599000000	-8.701000000
C	-7.746000000	-3.377000000	-8.935000000
O	-8.407000000	-2.462000000	-8.025000000
C	-6.646000000	-4.069000000	-8.133000000
O	-5.459000000	-3.225000000	-8.120000000
C	-7.017000000	-4.365000000	-6.652000000
O	-6.759000000	-5.779000000	-6.562000000
C	-6.116000000	-3.444000000	-5.825000000
C	-4.958000000	-3.083000000	-6.759000000

N	-0.756000000	-0.028000000	-6.880000000
C	-0.853000000	-1.435000000	-6.961000000
N	0.310000000	-2.143000000	-7.096000000
N	-2.045000000	-2.120000000	-6.940000000
C	-3.138000000	-1.313000000	-6.760000000
C	-3.129000000	0.111000000	-6.625000000
C	-1.894000000	0.832000000	-6.727000000
O	-1.687000000	2.041000000	-6.700000000
N	-4.436000000	0.583000000	-6.404000000
C	-5.226000000	-0.492000000	-6.412000000
N	-4.482000000	-1.702000000	-6.633000000
O	-10.721000000	-2.523000000	-9.257000000
O	-9.992000000	-0.530000000	-7.694000000
H	0.219000000	0.424000000	-6.908000000
H	-6.299000000	-0.514000000	-6.255000000
H	-4.075000000	-3.786000000	-6.679000000
H	-6.701000000	-2.559000000	-5.496000000
H	0.288000000	-3.156000000	-7.043000000
H	-8.097000000	-4.228000000	-6.429000000
H	1.241000000	-1.680000000	-7.050000000
H	-6.319000000	-5.003000000	-8.656000000
H	-7.320000000	-2.814000000	-9.794000000
H	-5.757000000	-3.885000000	-4.873000000
H	-8.474000000	-4.126000000	-9.308000000
P	-6.216000000	-6.527000000	-5.179000000
C	-3.734000000	-6.221000000	-6.085000000
O	-4.664000000	-5.927000000	-5.022000000
C	-2.510000000	-6.942000000	-5.511000000
O	-1.435000000	-5.972000000	-5.342000000
C	-2.714000000	-7.583000000	-4.114000000
O	-1.972000000	-8.813000000	-4.230000000
C	-2.112000000	-6.573000000	-3.124000000
C	-1.309000000	-5.574000000	-3.966000000
N	-0.055000000	-0.479000000	-3.680000000
C	0.727000000	-1.586000000	-3.868000000
N	0.315000000	-2.878000000	-3.957000000
C	-1.049000000	-3.028000000	-3.827000000
C	-1.970000000	-1.943000000	-3.635000000
C	-1.435000000	-0.619000000	-3.575000000
N	-2.194000000	0.493000000	-3.420000000
N	-3.286000000	-2.435000000	-3.562000000
C	-3.187000000	-3.761000000	-3.695000000
N	-1.827000000	-4.192000000	-3.847000000
O	-6.199000000	-7.977000000	-5.589000000
O	-6.918000000	-6.035000000	-3.943000000
H	1.812000000	-1.391000000	-3.971000000
H	-4.009000000	-4.479000000	-3.704000000
H	-0.203000000	-5.569000000	-3.768000000
H	-2.918000000	-6.104000000	-2.526000000
H	-3.766000000	-7.839000000	-3.877000000

H	-2.077000000	-7.669000000	-6.240000000
H	-3.432000000	-5.212000000	-6.476000000
H	-1.778000000	1.437000000	-3.479000000
H	-3.206000000	0.428000000	-3.416000000
H	-1.458000000	-7.050000000	-2.361000000
H	-4.190000000	-6.811000000	-6.902000000
P	-1.672000000	-9.754000000	-2.884000000
C	0.671000000	-8.571000000	-2.984000000
O	-0.455000000	-8.887000000	-2.129000000
C	1.656000000	-7.760000000	-2.147000000
O	1.316000000	-6.345000000	-2.299000000
C	1.651000000	-8.034000000	-0.626000000
O	2.807000000	-8.856000000	-0.400000000
C	1.822000000	-6.656000000	0.033000000
C	1.636000000	-5.625000000	-1.081000000
N	0.489000000	-4.700000000	-0.842000000
C	0.727000000	-3.265000000	-0.870000000
O	1.881000000	-2.873000000	-1.064000000
N	-0.328000000	-2.405000000	-0.668000000
C	-1.603000000	-2.892000000	-0.451000000
N	-2.591000000	-1.987000000	-0.253000000
C	-1.841000000	-4.316000000	-0.419000000
C	-0.797000000	-5.180000000	-0.598000000
O	-1.125000000	-11.022000000	-3.492000000
O	-2.809000000	-9.755000000	-1.902000000
H	2.811000000	-9.195000000	0.527000000
H	-2.847000000	-4.692000000	-0.228000000
H	-0.929000000	-6.276000000	-0.577000000
H	2.549000000	-5.013000000	-1.305000000
H	1.133000000	-6.521000000	0.888000000
H	0.748000000	-8.576000000	-0.273000000
H	2.691000000	-7.864000000	-2.562000000
H	-3.560000000	-2.275000000	-0.157000000
H	0.324000000	-7.982000000	-3.863000000
H	-2.418000000	-0.968000000	-0.330000000
H	2.829000000	-6.571000000	0.496000000
H	1.150000000	-9.513000000	-3.322000000
O	1.480000000	5.725000000	-19.711000000
O	-1.311000000	6.114000000	2.619000000
H	1.225000000	5.712000000	-20.673000000
H	-1.202000000	6.159000000	3.609000000
N	3.315000000	7.010000000	-7.025000000
N	7.334000000	6.628000000	-6.983000000
N	5.588000000	8.197000000	-5.452000000
N	5.021000000	5.607000000	-8.527000000
C	4.022000000	3.469000000	-10.128000000
C	3.149000000	4.426000000	-9.713000000
C	3.621000000	5.457000000	-8.791000000
C	2.749000000	6.221000000	-8.069000000
C	2.473000000	7.707000000	-6.201000000

C	1.108000000	7.713000000	-6.404000000
C	0.503000000	6.922000000	-7.446000000
C	-0.988000000	6.904000000	-7.520000000
C	7.929000000	7.739000000	-6.160000000
C	7.010000000	8.067000000	-4.977000000
C	1.304000000	6.186000000	-8.283000000
C	0.868000000	5.298000000	-9.362000000
C	5.821000000	4.506000000	-8.829000000
C	1.718000000	4.474000000	-10.014000000
C	5.392000000	3.510000000	-9.667000000
Pt	5.295000000	6.830000000	-6.985000000
H	7.735000000	6.652000000	-7.930000000
H	7.553000000	5.677000000	-6.585000000
H	5.412000000	9.158000000	-5.771000000
H	4.919000000	7.999000000	-4.654000000
H	3.706000000	2.631000000	-10.749000000
H	2.933000000	8.248000000	-5.364000000
H	0.471000000	8.291000000	-5.748000000
H	-1.370000000	6.463000000	-8.450000000
H	-1.412000000	7.915000000	-7.441000000
H	-1.401000000	6.324000000	-6.676000000
H	8.070000000	8.640000000	-6.804000000
H	8.946000000	7.469000000	-5.790000000
H	7.360000000	8.999000000	-4.475000000
H	7.072000000	7.259000000	-4.197000000
H	-0.193000000	5.334000000	-9.612000000
H	6.831000000	4.510000000	-8.405000000
H	1.379000000	3.782000000	-10.792000000
H	6.047000000	2.697000000	-9.955000000

[Pt(en)(4-Mephen)]²⁺ minor groove
Dock_ID: 186-cl6_4-Mephen



EDA for 186-cl6_4-Mephen in kcal mol⁻¹.

Electrostatic interaction	-808.4
Orbital interaction	-98.8
Dispersion energy	-68.5
Pauli repulsion	135.5
Total Bonding Energy	-840.1

Contributions of the solvation energies for 186-cl6_4-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1732.1
E _{solv} (intercalator)	-161.9
E _{solv} (duplex DNA)	-2352.6
ΔE _{solv}	782.4
ΔE _{int} (EDA)	-840.1
ΔE _{aq}	-57.7

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 186-cl6_4-Mephen system.
([Pt(en)(4-Mephen)]²⁺ minor groove)

P	-1.25200000	7.37600000	2.03300000
C	1.34400000	6.97800000	1.70300000
O	0.07200000	7.18300000	1.04600000
C	2.39800000	6.97100000	0.59100000
O	2.64000000	5.59800000	0.17000000
C	1.97300000	7.73900000	-0.69000000
O	3.14000000	8.48200000	-1.07200000
C	1.48200000	6.65000000	-1.65100000
C	1.96800000	5.31400000	-1.07200000
N	0.50800000	0.30400000	-0.78500000
C	1.76600000	0.86300000	-1.11800000
N	2.77500000	0.00000000	-1.45600000
N	2.03100000	2.21000000	-1.08000000
C	0.93800000	2.98700000	-0.77600000
C	-0.36900000	2.50200000	-0.45100000
C	-0.62900000	1.09500000	-0.43100000
O	-1.66900000	0.49000000	-0.16100000
N	-1.23800000	3.58900000	-0.23100000
C	-0.51000000	4.69000000	-0.41900000
N	0.84900000	4.38300000	-0.78600000
O	-1.01500000	8.44000000	3.07800000
O	-2.40800000	7.42200000	1.06900000
H	0.37900000	-0.75800000	-0.85300000
H	-0.84100000	5.72300000	-0.32200000
H	2.74800000	4.77100000	-1.68300000
H	0.37500000	6.71300000	-1.73100000
H	3.56900000	0.36200000	-1.99200000
H	1.20100000	8.51700000	-0.48600000
H	2.60500000	-1.02300000	-1.49900000
H	3.39100000	7.30000000	0.97500000
H	1.33200000	5.99900000	2.22800000
H	1.83200000	6.78500000	-2.69900000
H	1.53700000	7.79300000	2.42700000
P	3.77800000	8.48200000	-2.61800000
C	5.13100000	6.30400000	-2.00400000
O	4.17400000	6.89500000	-2.91300000
C	5.69200000	5.07500000	-2.72000000
O	4.65600000	4.05300000	-2.78200000
C	6.14000000	5.34900000	-4.18300000
O	7.35400000	4.58700000	-4.29600000
C	4.96700000	4.84500000	-5.02800000
C	4.33300000	3.75000000	-4.16700000
N	2.85400000	3.66900000	-4.25400000
C	2.26700000	2.37100000	-4.06500000
O	2.95600000	1.36600000	-4.02300000
N	0.86200000	2.33500000	-4.00500000

C	0.02500000	3.48000000	-3.98200000
O	-1.16500000	3.31400000	-3.73000000
C	0.69500000	4.75300000	-4.26700000
C	2.05100000	4.82100000	-4.33400000
C	-0.17600000	5.94300000	-4.46800000
O	5.00000000	9.34800000	-2.43800000
O	2.72800000	8.78000000	-3.65400000
H	0.41900000	1.36100000	-3.87700000
H	2.59700000	5.77500000	-4.47700000
H	4.76000000	2.71900000	-4.35500000
H	4.27300000	5.69900000	-5.21300000
H	6.40200000	6.41200000	-4.37300000
H	6.50600000	4.60500000	-2.12000000
H	4.59100000	6.00800000	-1.07800000
H	-1.02400000	5.71200000	-5.13400000
H	-0.60900000	6.29300000	-3.51700000
H	0.36300000	6.79500000	-4.90600000
H	5.25000000	4.47700000	-6.03300000
H	5.94300000	7.01400000	-1.74800000
P	7.89400000	3.97800000	-5.75600000
C	6.88100000	1.61700000	-5.14400000
O	6.83700000	2.72900000	-6.06700000
C	6.89800000	0.30600000	-5.93500000
O	5.52800000	-0.10500000	-6.17200000
C	7.55200000	0.38100000	-7.34100000
O	8.25000000	-0.86900000	-7.48700000
C	6.37800000	0.65100000	-8.29000000
C	5.13100000	0.17500000	-7.53400000
N	4.01600000	1.16300000	-7.46400000
C	2.68000000	0.62000000	-7.22600000
O	2.56700000	-0.59600000	-7.10600000
N	1.61900000	1.49800000	-7.15800000
C	1.80800000	2.85100000	-7.30000000
N	0.70700000	3.64700000	-7.19300000
C	3.12800000	3.39000000	-7.51100000
C	4.19600000	2.53300000	-7.56300000
O	9.26300000	3.46200000	-5.38900000
O	7.67200000	4.94000000	-6.89100000
H	3.26800000	4.46300000	-7.61700000
H	5.23500000	2.89600000	-7.69200000
H	4.70100000	-0.80300000	-7.90200000
H	6.35900000	1.73700000	-8.53000000
H	8.36000000	1.13900000	-7.41800000
H	7.31900000	-0.52500000	-5.32200000
H	0.77900000	4.65400000	-7.23800000
H	5.92400000	1.69100000	-4.56300000
H	-0.23800000	3.24500000	-7.02900000
H	6.47000000	0.16200000	-9.28200000
H	7.74000000	1.67100000	-4.44900000
P	7.91100000	-1.99900000	-8.66500000

C	5.73600000	-3.11400000	-7.57200000
O	6.27100000	-2.27500000	-8.60900000
C	5.16900000	-4.40900000	-8.16700000
O	3.79500000	-4.18900000	-8.58400000
C	5.90000000	-4.95000000	-9.42300000
O	5.92000000	-6.36900000	-9.15700000
C	5.01900000	-4.53900000	-10.61300000
C	3.70400000	-4.02500000	-10.01500000
N	0.02000000	-0.32300000	-10.26900000
C	-0.13000000	-1.72300000	-10.13500000
N	-1.41200000	-2.21200000	-10.18600000
N	0.93000000	-2.60000000	-10.07800000
C	2.15900000	-1.99300000	-10.21900000
C	2.38700000	-0.59400000	-10.40500000
C	1.29300000	0.32800000	-10.33500000
O	1.29600000	1.55800000	-10.34800000
N	3.76500000	-0.34300000	-10.55500000
C	4.36600000	-1.53000000	-10.47600000
N	3.42400000	-2.60200000	-10.28300000
O	8.68900000	-3.20300000	-8.20000000
O	8.08900000	-1.39500000	-10.03600000
H	-0.85200000	0.29900000	-10.20800000
H	5.43300000	-1.72700000	-10.53400000
H	2.80700000	-4.63100000	-10.31600000
H	5.54200000	-3.79500000	-11.24300000
H	-1.61200000	-3.16400000	-9.89500000
H	6.95300000	-4.61600000	-9.52000000
H	-2.23000000	-1.57000000	-10.12600000
H	5.06900000	-5.19600000	-7.38100000
H	4.90200000	-2.49500000	-7.15100000
H	4.80600000	-5.39000000	-11.30100000
H	6.47100000	-3.33400000	-6.77700000
P	6.37600000	-7.45900000	-10.33300000
C	3.78700000	-7.85900000	-10.42500000
O	4.96300000	-7.59700000	-11.22100000
C	2.58200000	-7.73500000	-11.35400000
O	2.31500000	-6.31900000	-11.57200000
C	2.79200000	-8.37900000	-12.75600000
O	1.80600000	-9.42100000	-12.76900000
C	2.64500000	-7.22500000	-13.75400000
C	1.94100000	-6.11400000	-12.97200000
N	0.34800000	-1.16800000	-13.40200000
C	-0.34900000	-2.32900000	-13.18700000
N	0.16100000	-3.58400000	-13.10600000
C	1.51800000	-3.63500000	-13.30100000
C	2.35700000	-2.50100000	-13.56000000
C	1.72300000	-1.22000000	-13.59600000
N	2.38700000	-0.05900000	-13.85100000
N	3.69100000	-2.91900000	-13.72400000
C	3.68800000	-4.24600000	-13.55700000

N	2.37500000	-4.75000000	-13.28400000
O	6.63200000	-8.71400000	-9.53500000
O	7.38300000	-6.90100000	-11.30000000
H	-1.44200000	-2.21900000	-13.03800000
H	4.54800000	-4.90600000	-13.61600000
H	0.81000000	-6.16900000	-13.01300000
H	3.64600000	-6.92700000	-14.12800000
H	3.76900000	-8.90300000	-12.85800000
H	1.64800000	-8.13300000	-10.86900000
H	3.71300000	-7.11700000	-9.58800000
H	1.91800000	0.85100000	-13.70600000
H	3.40100000	-0.04500000	-13.85200000
H	2.09600000	-7.49000000	-14.68100000
H	3.84700000	-8.88800000	-10.01400000
P	0.77000000	-9.71500000	-14.04300000
C	-0.95800000	-7.89000000	-13.14700000
O	-0.06400000	-8.28800000	-14.21200000
C	-2.38000000	-7.74200000	-13.69100000
O	-2.58400000	-6.35400000	-14.09000000
C	-2.71600000	-8.59300000	-14.93300000
O	-3.98600000	-9.19900000	-14.62300000
C	-2.85500000	-7.59800000	-16.10300000
C	-2.61300000	-6.20800000	-15.50500000
N	-1.31100000	-5.57600000	-15.93500000
C	-1.24900000	-4.12700000	-15.99700000
O	-2.29000000	-3.48700000	-15.81600000
N	-0.05700000	-3.50500000	-16.30700000
C	1.08200000	-4.25300000	-16.53100000
N	2.22500000	-3.57900000	-16.82100000
C	1.03600000	-5.68700000	-16.43700000
C	-0.14600000	-6.30900000	-16.13300000
O	-0.10800000	-10.81000000	-13.49800000
O	1.52300000	-9.85500000	-15.33900000
H	-4.25300000	-9.82200000	-15.34200000
H	1.93500000	-6.27200000	-16.62600000
H	-0.21400000	-7.41000000	-16.04000000
H	-3.42500000	-5.46200000	-15.70100000
H	-2.18500000	-7.85500000	-16.94300000
H	-1.99500000	-9.40600000	-15.14700000
H	-3.13300000	-7.86500000	-12.86800000
H	3.09500000	-4.06600000	-17.00100000
H	-0.56900000	-6.88000000	-12.84100000
H	2.25200000	-2.54500000	-16.87400000
H	-3.86600000	-7.66200000	-16.55200000
H	-0.92800000	-8.57500000	-12.27500000
P	1.98300000	6.65700000	-19.04200000
C	-0.54400000	5.82700000	-19.23600000
O	0.35200000	6.95100000	-19.29600000
C	-1.45000000	5.91700000	-17.99800000
O	-1.53000000	4.57300000	-17.44400000

C	-0.94600000	6.82400000	-16.84600000
O	-2.10300000	7.51600000	-16.35300000
C	-0.23100000	5.86600000	-15.88800000
C	-0.77500000	4.47500000	-16.21100000
N	0.09100000	-0.64300000	-16.50500000
C	-1.07600000	0.06400000	-16.13300000
N	-2.21400000	-0.67500000	-15.86200000
N	-1.16100000	1.42800000	-16.11100000
C	0.01500000	2.06800000	-16.43800000
C	1.24200000	1.43200000	-16.79800000
C	1.32000000	0.00300000	-16.85600000
O	2.26700000	-0.72400000	-17.15800000
N	2.22900000	2.41200000	-17.03500000
C	1.63800000	3.59200000	-16.83500000
N	0.26600000	3.44700000	-16.43600000
O	2.66100000	7.74500000	-19.83600000
O	2.28500000	6.42800000	-17.58400000
H	0.07800000	-1.71700000	-16.46500000
H	2.09600000	4.58600000	-16.93800000
H	-1.51900000	4.07200000	-15.46500000
H	0.87200000	5.95300000	-16.05300000
H	-2.89100000	-0.25300000	-15.21000000
H	-0.30100000	7.66100000	-17.20000000
H	-2.12900000	-1.71100000	-15.77300000
H	-2.50100000	6.15000000	-18.27800000
H	-0.01500000	4.85000000	-19.26700000
H	-0.36200000	6.12600000	-14.80600000
H	-1.13800000	5.92100000	-20.16900000
P	-2.80700000	7.25000000	-14.85900000
C	-4.11300000	5.09200000	-15.68900000
O	-3.12800000	5.61900000	-14.77600000
C	-5.17600000	4.32400000	-14.90200000
O	-4.67300000	2.99900000	-14.57300000
C	-5.63300000	4.96200000	-13.56600000
O	-7.06800000	4.91400000	-13.68800000
C	-5.05000000	4.06800000	-12.46300000
C	-4.40600000	2.87100000	-13.16700000
N	-2.92200000	2.78400000	-12.97600000
C	-2.31900000	1.50100000	-13.17700000
O	-3.00900000	0.50000000	-13.34100000
N	-0.91700000	1.43800000	-13.10200000
C	-0.07400000	2.58600000	-13.07700000
O	1.12700000	2.42100000	-13.26000000
C	-0.75700000	3.86100000	-12.85600000
C	-2.11500000	3.93400000	-12.86700000
C	0.08700000	5.06400000	-12.61900000
O	-4.08000000	8.05100000	-14.96800000
O	-1.80600000	7.46200000	-13.75500000
H	-0.47100000	0.46700000	-13.19200000
H	-2.64900000	4.89500000	-12.76900000

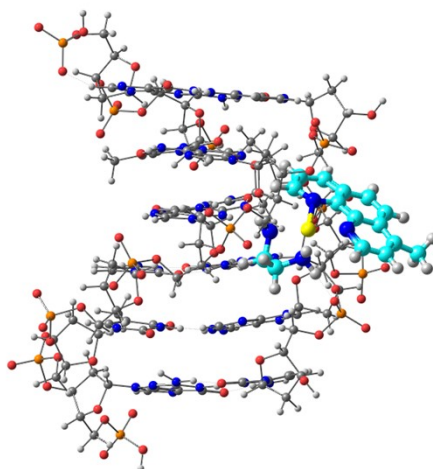
H	-4.85200000	1.87600000	-12.88200000
H	-4.35000000	4.65000000	-11.82700000
H	-5.35000000	6.03200000	-13.46300000
H	-6.05300000	4.10400000	-15.56200000
H	-3.54100000	4.39800000	-16.35000000
H	0.11800000	5.33800000	-11.55500000
H	1.12600000	4.90900000	-12.94600000
H	-0.29700000	5.94900000	-13.16800000
H	-5.83400000	3.69700000	-11.75900000
H	-4.58500000	5.87500000	-16.31200000
P	-8.07400000	5.07400000	-12.36400000
C	-8.10900000	2.44900000	-12.50800000
O	-7.93800000	3.58400000	-11.62400000
C	-7.85700000	1.19700000	-11.66900000
O	-6.42100000	1.00400000	-11.52700000
C	-8.45900000	1.24900000	-10.23600000
O	-9.18800000	0.00900000	-10.17200000
C	-7.24900000	1.37000000	-9.30700000
C	-6.08200000	0.80800000	-10.12100000
N	-4.77600000	1.47400000	-9.92800000
C	-3.57400000	0.64800000	-10.05000000
O	-3.71900000	-0.55700000	-10.21700000
N	-2.34600000	1.26600000	-9.97400000
C	-2.24300000	2.62200000	-9.76400000
N	-0.99100000	3.14600000	-9.76000000
C	-3.42500000	3.42500000	-9.55500000
C	-4.65400000	2.83300000	-9.63700000
O	-9.42500000	5.24100000	-13.01600000
O	-7.55600000	6.05200000	-11.34700000
H	-3.33000000	4.48400000	-9.31800000
H	-5.59100000	3.39700000	-9.48300000
H	-5.94600000	-0.30900000	-9.98900000
H	-7.11300000	2.43700000	-9.02400000
H	-9.20300000	2.06400000	-10.09700000
H	-8.21000000	0.28900000	-12.21800000
H	-0.83200000	4.13000000	-9.60000000
H	-7.38400000	2.51000000	-13.34800000
H	-0.15800000	2.55800000	-9.98100000
H	-7.36600000	0.84300000	-8.33700000
H	-9.14300000	2.44200000	-12.90700000
P	-9.42100000	-0.83700000	-8.75300000
C	-7.33400000	-2.35500000	-9.34500000
O	-7.90600000	-1.41900000	-8.39800000
C	-6.62000000	-3.45900000	-8.55600000
O	-5.27400000	-3.00800000	-8.27000000
C	-7.25700000	-3.78800000	-7.17800000
O	-7.15200000	-5.20700000	-7.00200000
C	-6.48900000	-2.89200000	-6.19600000
C	-5.15500000	-2.60400000	-6.89200000
N	-1.02000000	0.45500000	-6.87600000

C	-1.14100000	-0.94500000	-7.04800000
N	0.00100000	-1.68300000	-7.26100000
N	-2.33400000	-1.60100000	-7.06400000
C	-3.42400000	-0.78100000	-6.91900000
C	-3.40600000	0.64300000	-6.76800000
C	-2.14700000	1.33400000	-6.78700000
O	-1.90800000	2.53900000	-6.72200000
N	-4.72800000	1.11200000	-6.65200000
C	-5.51700000	0.03000000	-6.72800000
N	-4.76300000	-1.17500000	-6.88000000
O	-10.34800000	-1.93900000	-9.20300000
O	-9.75300000	0.07500000	-7.60200000
H	-0.04400000	0.90000000	-6.91800000
H	-6.60300000	0.01400000	-6.70400000
H	-4.27700000	-3.20500000	-6.51100000
H	-7.08500000	-1.97400000	-6.00900000
H	-0.06400000	-2.69200000	-7.15800000
H	-8.35300000	-3.61700000	-7.14900000
H	0.93900000	-1.26900000	-7.09400000
H	-6.46200000	-4.37200000	-9.17600000
H	-6.57500000	-1.76100000	-9.91800000
H	-6.35100000	-3.34400000	-5.19300000
H	-8.08900000	-2.78000000	-10.03000000
P	-6.12600000	-5.95800000	-5.90800000
C	-3.84600000	-5.68800000	-7.29300000
O	-4.61600000	-5.32200000	-6.12400000
C	-2.47200000	-6.18000000	-6.84800000
O	-1.64600000	-5.10000000	-6.31100000
C	-2.51900000	-7.23000000	-5.70600000
O	-1.33000000	-8.00000000	-5.97700000
C	-2.42100000	-6.38100000	-4.42800000
C	-1.61700000	-5.15300000	-4.87400000
N	-0.28700000	-0.25600000	-3.77400000
C	0.47300000	-1.35300000	-4.08800000
N	0.02900000	-2.61500000	-4.30800000
C	-1.33900000	-2.73600000	-4.17900000
C	-2.23000000	-1.67400000	-3.80700000
C	-1.66200000	-0.37400000	-3.63700000
N	-2.38500000	0.74300000	-3.35900000
N	-3.55300000	-2.15700000	-3.76900000
C	-3.48500000	-3.44900000	-4.12100000
N	-2.14000000	-3.87000000	-4.35800000
O	-6.26900000	-7.41300000	-6.23900000
O	-6.44000000	-5.45400000	-4.51000000
H	1.55900000	-1.16000000	-4.19100000
H	-4.32400000	-4.14200000	-4.22000000
H	-0.51900000	-5.20200000	-4.61100000
H	-3.44100000	-6.12300000	-4.07400000
H	-3.38300000	-7.91900000	-5.74100000
H	-1.85700000	-6.53400000	-7.73200000

H	-3.75900000	-4.74400000	-7.88400000
H	-1.94400000	1.67700000	-3.37000000
H	-3.39700000	0.70100000	-3.31100000
H	-1.95100000	-6.89300000	-3.56900000
H	-4.35200000	-6.46800000	-7.90200000
P	-0.53700000	-8.91800000	-4.86900000
C	1.17300000	-6.97600000	-4.25400000
O	0.07500000	-7.76600000	-3.79600000
C	2.37000000	-7.15700000	-3.30800000
O	2.75500000	-5.81600000	-2.88200000
C	2.09200000	-7.96400000	-2.02100000
O	3.10800000	-8.98100000	-2.00200000
C	2.28600000	-6.97400000	-0.85700000
C	2.44800000	-5.59700000	-1.49500000
N	1.20600000	-4.75800000	-1.41600000
C	1.34800000	-3.31700000	-1.31000000
O	2.47900000	-2.82900000	-1.41700000
N	0.23600000	-2.54400000	-1.06700000
C	-1.01800000	-3.11900000	-0.99300000
N	-2.05600000	-2.31600000	-0.65800000
C	-1.18200000	-4.52700000	-1.27400000
C	-0.08000000	-5.30600000	-1.48200000
O	0.58000000	-9.45500000	-5.74400000
O	-1.36900000	-9.77700000	-3.96400000
H	2.96400000	-9.59900000	-1.24500000
H	-2.18300000	-4.95800000	-1.31100000
H	-0.16500000	-6.38400000	-1.70700000
H	3.30700000	-4.98600000	-1.11500000
H	1.47700000	-7.03700000	-0.10600000
H	1.09700000	-8.46300000	-2.00200000
H	3.27600000	-7.53900000	-3.83400000
H	-3.01300000	-2.65700000	-0.65400000
H	0.80500000	-5.91600000	-4.21900000
H	-1.93100000	-1.29700000	-0.51900000
H	3.19400000	-7.24100000	-0.27400000
H	1.48100000	-7.22200000	-5.29700000
O	2.19800000	5.17200000	-19.76800000
O	-1.32300000	5.90000000	2.81400000
H	2.23900000	5.17000000	-20.76400000
H	-0.96700000	5.87900000	3.74300000
N	-1.75100000	-8.81500000	-9.15300000
N	0.62500000	-5.53600000	-9.36300000
N	1.02000000	-7.94700000	-8.08300000
N	-1.88800000	-6.57100000	-10.57600000
C	-4.38300000	-5.32500000	-11.17900000
C	-4.39800000	-6.53400000	-10.55000000
C	-3.12900000	-7.18200000	-10.22300000
C	-3.06100000	-8.33200000	-9.48200000
C	-1.66900000	-9.79900000	-8.19400000
C	-2.77800000	-10.42200000	-7.66700000

C	-4.10200000	-9.95300000	-7.98900000
C	-5.26800000	-10.52800000	-7.25500000
C	1.18800000	-5.47300000	-7.96700000
C	1.91800000	-6.79500000	-7.70200000
C	-4.25600000	-8.95000000	-8.91500000
C	-5.52400000	-8.33400000	-9.29800000
C	-1.94100000	-5.31100000	-11.16800000
C	-5.59500000	-7.22100000	-10.06200000
C	-3.11900000	-4.71200000	-11.51700000
Pt	-0.49100000	-7.22700000	-9.31700000
H	0.08100000	-4.68100000	-9.56600000
H	1.38000000	-5.57100000	-10.07600000
H	0.63500000	-8.40200000	-7.20900000
H	1.56100000	-8.67300000	-8.56400000
H	-5.29500000	-4.79100000	-11.41600000
H	-0.65500000	-10.09700000	-7.90000000
H	-2.67100000	-11.22900000	-6.95800000
H	-6.00100000	-10.99300000	-7.92600000
H	-5.79400000	-9.71800000	-6.71400000
H	-4.98400000	-11.28000000	-6.51100000
H	0.32800000	-5.34000000	-7.25200000
H	1.88800000	-4.60700000	-7.83800000
H	2.20700000	-6.87300000	-6.62300000
H	2.87900000	-6.83400000	-8.27900000
H	-6.42800000	-8.79800000	-8.90500000
H	-0.96600000	-4.87000000	-11.41500000
H	-6.55500000	-6.78000000	-10.31900000
H	-3.12600000	-3.78000000	-12.06700000

[Pt(en)(4-Mephen)]²⁺ minor groove
Dock_ID: 272-cl4_4-Mephen



EDA for 272-cl4_4-Mephen in kcal mol⁻¹.

Electrostatic interaction	-807.7
Orbital interaction	-97.9
Dispersion energy	-68.1
Pauli repulsion	134.3
Total Bonding Energy	-839.3

Contributions of the solvation energies for 272-cl4_4-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1730.7
E _{solv} (intercalator)	-161.9
E _{solv} (duplex DNA)	-2350.8
ΔE _{solv}	781.9
ΔE _{int} (EDA)	-839.3
ΔE _{aq}	-57.4

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 272-cl4_4-Mephen system.
([Pt(en)(4-Mephen)]²⁺ minor groove)

P	-1.879000000	6.645000000	2.257000000
C	0.694000000	5.939000000	2.376000000
O	-0.255000000	7.017000000	2.440000000
C	1.525000000	6.006000000	1.086000000
O	1.546000000	4.660000000	0.532000000
C	0.983000000	6.927000000	-0.036000000
O	2.119000000	7.626000000	-0.564000000
C	0.229000000	5.986000000	-0.980000000
C	0.768000000	4.586000000	-0.688000000
N	-0.132000000	-0.529000000	-0.356000000
C	1.040000000	0.166000000	-0.746000000
N	2.150000000	-0.583000000	-1.054000000
N	1.137000000	1.533000000	-0.767000000
C	-0.034000000	2.183000000	-0.449000000
C	-1.269000000	1.557000000	-0.093000000
C	-1.357000000	0.131000000	-0.022000000
O	-2.311000000	-0.588000000	0.285000000
N	-2.253000000	2.543000000	0.127000000
C	-1.653000000	3.718000000	-0.076000000
N	-0.277000000	3.563000000	-0.460000000
O	-2.573000000	7.639000000	3.157000000
O	-2.248000000	6.506000000	0.803000000
H	-0.129000000	-1.600000000	-0.394000000
H	-2.104000000	4.716000000	0.017000000
H	1.495000000	4.189000000	-1.453000000
H	-0.867000000	6.083000000	-0.780000000
H	2.857000000	-0.160000000	-1.671000000
H	0.353000000	7.760000000	0.353000000
H	2.084000000	-1.621000000	-1.081000000
H	2.596000000	6.215000000	1.309000000
H	0.219000000	4.939000000	2.483000000
H	0.330000000	6.255000000	-2.064000000
H	1.333000000	6.111000000	3.267000000
P	2.794000000	7.346000000	-2.069000000
C	4.108000000	5.189000000	-1.249000000
O	3.108000000	5.714000000	-2.145000000
C	5.165000000	4.430000000	-2.052000000
O	4.671000000	3.097000000	-2.367000000
C	5.590000000	5.067000000	-3.400000000
O	7.027000000	5.040000000	-3.302000000
C	4.993000000	4.163000000	-4.487000000
C	4.369000000	2.965000000	-3.765000000
N	2.881000000	2.874000000	-3.920000000
C	2.285000000	1.589000000	-3.711000000
O	2.981000000	0.593000000	-3.547000000
N	0.883000000	1.521000000	-3.773000000

C	0.035000000	2.664000000	-3.799000000
O	-1.166000000	2.496000000	-3.618000000
C	0.711000000	3.943000000	-4.019000000
C	2.070000000	4.020000000	-4.026000000
C	-0.140000000	5.144000000	-4.238000000
O	4.071000000	8.143000000	-1.991000000
O	1.772000000	7.555000000	-3.155000000
H	0.440000000	0.549000000	-3.675000000
H	2.598000000	4.983000000	-4.134000000
H	4.811000000	1.969000000	-4.057000000
H	4.277000000	4.736000000	-5.113000000
H	5.295000000	6.134000000	-3.502000000
H	6.057000000	4.221000000	-1.408000000
H	3.548000000	4.488000000	-0.584000000
H	-0.203000000	5.409000000	-5.303000000
H	-1.169000000	4.989000000	-3.880000000
H	0.257000000	6.033000000	-3.706000000
H	5.764000000	3.796000000	-5.205000000
H	4.583000000	5.971000000	-0.628000000
P	8.022000000	5.130000000	-4.640000000
C	8.028000000	2.512000000	-4.383000000
O	7.863000000	3.610000000	-5.313000000
C	7.808000000	1.227000000	-5.179000000
O	6.377000000	1.005000000	-5.332000000
C	8.426000000	1.242000000	-6.605000000
O	9.157000000	0.002000000	-6.630000000
C	7.225000000	1.338000000	-7.549000000
C	6.050000000	0.788000000	-6.738000000
N	4.746000000	1.450000000	-6.951000000
C	3.540000000	0.630000000	-6.811000000
O	3.681000000	-0.573000000	-6.627000000
N	2.315000000	1.252000000	-6.894000000
C	2.216000000	2.606000000	-7.116000000
N	0.971000000	3.144000000	-7.081000000
C	3.401000000	3.399000000	-7.353000000
C	4.627000000	2.804000000	-7.266000000
O	9.378000000	5.312000000	-4.003000000
O	7.508000000	6.067000000	-5.698000000
H	3.307000000	4.453000000	-7.610000000
H	5.566000000	3.361000000	-7.437000000
H	5.915000000	-0.331000000	-6.852000000
H	7.087000000	2.398000000	-7.857000000
H	9.169000000	2.055000000	-6.758000000
H	8.167000000	0.344000000	-4.595000000
H	0.811000000	4.117000000	-7.297000000
H	7.284000000	2.599000000	-3.562000000
H	0.132000000	2.556000000	-6.883000000
H	7.355000000	0.790000000	-8.506000000
H	9.053000000	2.531000000	-3.961000000
P	9.418000000	-0.874000000	-8.027000000

C	7.315000000	-2.373000000	-7.450000000
O	7.908000000	-1.456000000	-8.402000000
C	6.599000000	-3.481000000	-8.233000000
O	5.259000000	-3.023000000	-8.536000000
C	7.245000000	-3.830000000	-9.602000000
O	7.129000000	-5.248000000	-9.767000000
C	6.495000000	-2.936000000	-10.599000000
C	5.156000000	-2.634000000	-9.921000000
N	1.033000000	0.436000000	-9.970000000
C	1.150000000	-0.963000000	-9.794000000
N	0.004000000	-1.698000000	-9.589000000
N	2.341000000	-1.621000000	-9.766000000
C	3.432000000	-0.806000000	-9.920000000
C	3.418000000	0.616000000	-10.091000000
C	2.162000000	1.312000000	-10.077000000
O	1.923000000	2.516000000	-10.156000000
N	4.741000000	1.079000000	-10.219000000
C	5.527000000	-0.003000000	-10.129000000
N	4.771000000	-1.204000000	-9.954000000
O	10.328000000	-1.972000000	-7.533000000
O	9.783000000	0.012000000	-9.188000000
H	0.057000000	0.880000000	-9.946000000
H	6.613000000	-0.023000000	-10.159000000
H	4.278000000	-3.236000000	-10.302000000
H	7.100000000	-2.024000000	-10.786000000
H	0.069000000	-2.708000000	-9.682000000
H	8.344000000	-3.668000000	-9.622000000
H	-0.931000000	-1.279000000	-9.751000000
H	6.429000000	-4.385000000	-7.603000000
H	6.554000000	-1.764000000	-6.894000000
H	6.366000000	-3.395000000	-11.601000000
H	8.057000000	-2.797000000	-6.751000000
P	6.096000000	-6.002000000	-10.853000000
C	3.797000000	-5.717000000	-9.497000000
O	4.591000000	-5.350000000	-10.650000000
C	2.429000000	-6.196000000	-9.975000000
O	1.626000000	-5.105000000	-10.525000000
C	2.493000000	-7.242000000	-11.119000000
O	1.293000000	-8.004000000	-10.880000000
C	2.431000000	-6.388000000	-12.396000000
C	1.623000000	-5.158000000	-11.963000000
N	0.348000000	-0.253000000	-13.101000000
C	-0.425000000	-1.342000000	-12.791000000
N	0.005000000	-2.605000000	-12.551000000
C	1.374000000	-2.737000000	-12.661000000
C	2.279000000	-1.685000000	-13.028000000
C	1.724000000	-0.381000000	-13.215000000
N	2.458000000	0.727000000	-13.501000000
N	3.597000000	-2.181000000	-13.051000000
C	3.513000000	-3.471000000	-12.697000000

N	2.162000000	-3.878000000	-12.469000000
O	6.223000000	-7.453000000	-10.498000000
O	6.418000000	-5.517000000	-12.256000000
H	-1.511000000	-1.141000000	-12.712000000
H	4.343000000	-4.173000000	-12.587000000
H	0.530000000	-5.202000000	-12.247000000
H	3.461000000	-6.133000000	-12.724000000
H	3.352000000	-7.938000000	-11.066000000
H	1.791000000	-6.548000000	-9.106000000
H	3.705000000	-4.774000000	-8.905000000
H	2.025000000	1.665000000	-13.493000000
H	3.471000000	0.684000000	-13.505000000
H	1.981000000	-6.894000000	-13.268000000
H	4.284000000	-6.504000000	-8.881000000
P	0.524000000	-8.912000000	-12.014000000
C	-1.158000000	-6.964000000	-12.676000000
O	-0.044000000	-7.752000000	-13.101000000
C	-2.314000000	-7.133000000	-13.672000000
O	-2.678000000	-5.786000000	-14.098000000
C	-1.984000000	-7.926000000	-14.957000000
O	-3.003000000	-8.935000000	-15.033000000
C	-2.122000000	-6.918000000	-16.114000000
C	-2.304000000	-5.548000000	-15.464000000
N	-1.053000000	-4.718000000	-15.470000000
C	-1.185000000	-3.276000000	-15.580000000
O	-2.314000000	-2.783000000	-15.485000000
N	-0.065000000	-2.508000000	-15.803000000
C	1.186000000	-3.092000000	-15.862000000
N	2.231000000	-2.296000000	-16.189000000
C	1.337000000	-4.500000000	-15.573000000
C	0.227000000	-5.274000000	-15.389000000
O	-0.627000000	-9.438000000	-11.177000000
O	1.375000000	-9.779000000	-12.894000000
H	-2.836000000	-9.541000000	-15.794000000
H	2.335000000	-4.936000000	-15.517000000
H	0.302000000	-6.353000000	-15.165000000
H	-3.139000000	-4.926000000	-15.875000000
H	-1.283000000	-6.976000000	-16.832000000
H	-0.992000000	-8.429000000	-14.940000000
H	-3.242000000	-7.518000000	-13.189000000
H	3.187000000	-2.640000000	-16.179000000
H	-0.786000000	-5.904000000	-12.686000000
H	2.112000000	-1.278000000	-16.343000000
H	-3.003000000	-7.170000000	-16.743000000
H	-1.508000000	-7.220000000	-11.650000000
P	1.302000000	7.305000000	-19.110000000
C	-1.292000000	6.953000000	-18.710000000
O	-0.010000000	7.214000000	-18.094000000
C	-2.314000000	6.949000000	-17.568000000
O	-2.506000000	5.580000000	-17.109000000

C	-1.867000000	7.755000000	-16.318000000
O	-3.035000000	8.469000000	-15.892000000
C	-1.293000000	6.700000000	-15.364000000
C	-1.787000000	5.344000000	-15.883000000
N	-0.325000000	0.336000000	-16.107000000
C	-1.583000000	0.899000000	-15.783000000
N	-2.602000000	0.041000000	-15.453000000
N	-1.844000000	2.246000000	-15.828000000
C	-0.753000000	3.018000000	-16.154000000
C	0.551000000	2.528000000	-16.481000000
C	0.813000000	1.121000000	-16.474000000
O	1.853000000	0.510000000	-16.730000000
N	1.415000000	3.613000000	-16.736000000
C	0.684000000	4.715000000	-16.569000000
N	-0.670000000	4.413000000	-16.181000000
O	1.107000000	8.354000000	-20.179000000
O	2.473000000	7.315000000	-18.164000000
H	-0.197000000	-0.725000000	-16.026000000
H	1.013000000	5.748000000	-16.693000000
H	-2.540000000	4.814000000	-15.229000000
H	-0.184000000	6.789000000	-15.366000000
H	-3.374000000	0.406000000	-14.886000000
H	-1.135000000	8.557000000	-16.568000000
H	-2.423000000	-0.980000000	-15.383000000
H	-3.325000000	7.244000000	-17.930000000
H	-1.270000000	5.962000000	-19.211000000
H	-1.571000000	6.857000000	-14.298000000
H	-1.525000000	7.743000000	-19.448000000
P	-3.681000000	8.367000000	-14.352000000
C	-5.007000000	6.184000000	-15.018000000
O	-4.024000000	6.758000000	-14.126000000
C	-5.606000000	4.985000000	-14.281000000
O	-4.592000000	3.948000000	-14.168000000
C	-6.084000000	5.301000000	-12.836000000
O	-7.294000000	4.534000000	-12.723000000
C	-4.922000000	4.831000000	-11.956000000
C	-4.268000000	3.713000000	-12.772000000
N	-2.787000000	3.657000000	-12.675000000
C	-2.186000000	2.364000000	-12.847000000
O	-2.866000000	1.351000000	-12.887000000
N	-0.782000000	2.339000000	-12.888000000
C	0.046000000	3.491000000	-12.926000000
O	1.238000000	3.326000000	-13.168000000
C	-0.639000000	4.762000000	-12.668000000
C	-1.997000000	4.819000000	-12.616000000
C	0.219000000	5.962000000	-12.469000000
O	-4.930000000	9.200000000	-14.496000000
O	-2.640000000	8.648000000	-13.302000000
H	-0.332000000	1.367000000	-13.007000000
H	-2.554000000	5.770000000	-12.499000000

H	-4.678000000	2.682000000	-12.544000000
H	-4.235000000	5.694000000	-11.786000000
H	-6.358000000	6.366000000	-12.681000000
H	-6.414000000	4.513000000	-14.890000000
H	-4.472000000	5.854000000	-15.936000000
H	0.934000000	5.809000000	-11.645000000
H	0.817000000	6.186000000	-13.366000000
H	-0.360000000	6.867000000	-12.233000000
H	-5.220000000	4.493000000	-10.944000000
H	-5.794000000	6.912000000	-15.292000000
P	-7.839000000	3.923000000	-11.266000000
C	-6.789000000	1.559000000	-11.820000000
O	-6.764000000	2.695000000	-10.928000000
C	-6.843000000	0.268000000	-10.996000000
O	-5.488000000	-0.153000000	-10.701000000
C	-7.538000000	0.392000000	-9.612000000
O	-8.261000000	-0.840000000	-9.448000000
C	-6.389000000	0.674000000	-8.634000000
C	-5.125000000	0.173000000	-9.342000000
N	-4.008000000	1.160000000	-9.421000000
C	-2.672000000	0.613000000	-9.642000000
O	-2.558000000	-0.606000000	-9.739000000
N	-1.608000000	1.486000000	-9.719000000
C	-1.796000000	2.843000000	-9.611000000
N	-0.690000000	3.632000000	-9.718000000
C	-3.116000000	3.387000000	-9.426000000
C	-4.187000000	2.534000000	-9.360000000
O	-9.193000000	3.381000000	-11.646000000
O	-7.644000000	4.898000000	-10.136000000
H	-3.257000000	4.463000000	-9.351000000
H	-5.226000000	2.900000000	-9.249000000
H	-4.704000000	-0.791000000	-8.932000000
H	-6.369000000	1.764000000	-8.414000000
H	-8.337000000	1.163000000	-9.579000000
H	-7.255000000	-0.574000000	-11.598000000
H	-0.761000000	4.640000000	-9.697000000
H	-5.812000000	1.611000000	-12.370000000
H	0.252000000	3.225000000	-9.891000000
H	-6.517000000	0.206000000	-7.636000000
H	-7.622000000	1.600000000	-12.547000000
P	-7.950000000	-1.963000000	-8.255000000
C	-5.794000000	-3.126000000	-9.320000000
O	-6.314000000	-2.262000000	-8.293000000
C	-5.220000000	-4.406000000	-8.700000000
O	-3.849000000	-4.174000000	-8.275000000
C	-5.958000000	-4.936000000	-7.443000000
O	-5.967000000	-6.357000000	-7.693000000
C	-5.089000000	-4.501000000	-6.252000000
C	-3.767000000	-4.000000000	-6.845000000
N	-0.064000000	-0.315000000	-6.592000000

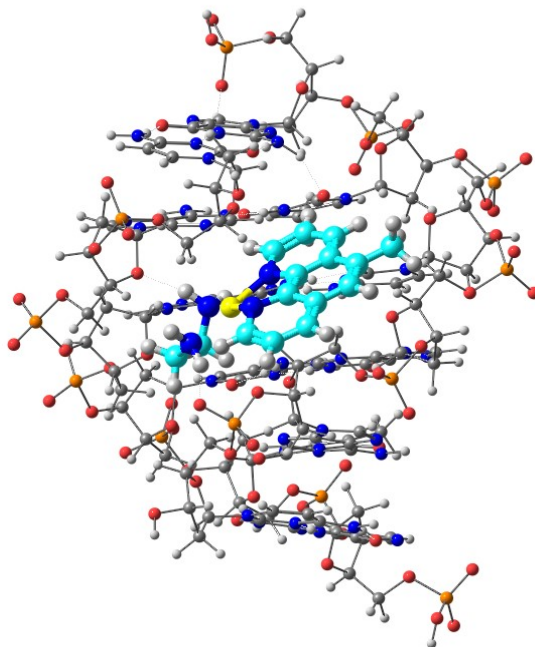
C	0.080000000	-1.718000000	-6.711000000
N	1.359000000	-2.210000000	-6.649000000
N	-0.985000000	-2.589000000	-6.774000000
C	-2.211000000	-1.977000000	-6.639000000
C	-2.433000000	-0.575000000	-6.461000000
C	-1.334000000	0.341000000	-6.528000000
O	-1.333000000	1.571000000	-6.523000000
N	-3.810000000	-0.317000000	-6.313000000
C	-4.418000000	-1.500000000	-6.397000000
N	-3.480000000	-2.577000000	-6.583000000
O	-8.739000000	-3.160000000	-8.719000000
O	-8.137000000	-1.340000000	-6.894000000
H	0.812000000	0.302000000	-6.646000000
H	-5.486000000	-1.692000000	-6.345000000
H	-2.875000000	-4.610000000	-6.534000000
H	-5.620000000	-3.744000000	-5.644000000
H	1.554000000	-3.173000000	-6.903000000
H	-7.015000000	-4.609000000	-7.359000000
H	2.182000000	-1.575000000	-6.717000000
H	-5.109000000	-5.203000000	-9.476000000
H	-4.971000000	-2.520000000	-9.773000000
H	-4.888000000	-5.334000000	-5.541000000
H	-6.542000000	-3.369000000	-10.097000000
P	-6.364000000	-7.449000000	-6.498000000
C	-3.763000000	-7.783000000	-6.438000000
O	-4.935000000	-7.535000000	-5.632000000
C	-2.556000000	-7.655000000	-5.513000000
O	-2.302000000	-6.237000000	-5.286000000
C	-2.758000000	-8.310000000	-4.115000000
O	-1.738000000	-9.320000000	-4.103000000
C	-2.640000000	-7.155000000	-3.112000000
C	-1.939000000	-6.036000000	-3.884000000
N	-0.386000000	-1.079000000	-3.446000000
C	0.323000000	-2.237000000	-3.636000000
N	-0.175000000	-3.497000000	-3.708000000
C	-1.536000000	-3.556000000	-3.539000000
C	-2.387000000	-2.426000000	-3.304000000
C	-1.764000000	-1.139000000	-3.270000000
N	-2.438000000	0.020000000	-3.040000000
N	-3.721000000	-2.852000000	-3.163000000
C	-3.706000000	-4.180000000	-3.322000000
N	-2.383000000	-4.678000000	-3.562000000
O	-6.601000000	-8.717000000	-7.281000000
O	-7.369000000	-6.913000000	-5.517000000
H	1.417000000	-2.120000000	-3.771000000
H	-4.561000000	-4.845000000	-3.275000000
H	-0.807000000	-6.084000000	-3.834000000
H	-3.651000000	-6.870000000	-2.757000000
H	-3.722000000	-8.857000000	-4.019000000
H	-1.615000000	-8.038000000	-6.005000000

H	-3.704000000	-7.039000000	-7.271000000
H	-1.969000000	0.932000000	-3.175000000
H	-3.451000000	0.028000000	-3.048000000
H	-2.102000000	-7.414000000	-2.178000000
H	-3.817000000	-8.812000000	-6.854000000
P	-0.793000000	-9.663000000	-2.774000000
C	0.951000000	-7.814000000	-3.560000000
O	0.047000000	-8.250000000	-2.520000000
C	2.367000000	-7.678000000	-2.994000000
O	2.582000000	-6.288000000	-2.608000000
C	2.662000000	-8.516000000	-1.733000000
O	3.933000000	-9.139000000	-1.998000000
C	2.775000000	-7.507000000	-0.572000000
C	2.564000000	-6.123000000	-1.194000000
N	1.252000000	-5.478000000	-0.819000000
C	1.196000000	-4.027000000	-0.785000000
O	2.243000000	-3.394000000	-0.958000000
N	0.001000000	-3.395000000	-0.515000000
C	-1.147000000	-4.131000000	-0.301000000
N	-2.289000000	-3.447000000	-0.034000000
C	-1.109000000	-5.567000000	-0.379000000
C	0.077000000	-6.200000000	-0.644000000
O	0.107000000	-10.759000000	-3.283000000
O	-1.623000000	-9.828000000	-1.529000000
H	4.170000000	-9.760000000	-1.268000000
H	-2.017000000	-6.143000000	-0.210000000
H	0.139000000	-7.303000000	-0.725000000
H	3.374000000	-5.380000000	-0.980000000
H	2.080000000	-7.747000000	0.252000000
H	1.926000000	-9.319000000	-1.526000000
H	3.133000000	-7.823000000	-3.800000000
H	-3.169000000	-3.925000000	0.123000000
H	0.565000000	-6.796000000	-3.843000000
H	-2.310000000	-2.412000000	0.007000000
H	3.773000000	-7.574000000	-0.093000000
H	0.936000000	-8.470000000	-4.454000000
O	1.273000000	5.810000000	-19.857000000
O	-1.982000000	5.110000000	2.895000000
H	0.955000000	5.802000000	-20.801000000
H	-1.993000000	5.048000000	3.891000000
N	1.582000000	-8.828000000	-7.714000000
N	-0.729000000	-5.503000000	-7.581000000
N	-1.139000000	-7.918000000	-8.862000000
N	1.703000000	-6.599000000	-6.268000000
C	4.197000000	-5.402000000	-5.566000000
C	4.213000000	-6.602000000	-6.209000000
C	2.947000000	-7.227000000	-6.584000000
C	2.886000000	-8.372000000	-7.334000000
C	1.514000000	-9.823000000	-8.659000000
C	2.630000000	-10.469000000	-9.145000000

C	3.949000000	-10.015000000	-8.788000000
C	5.129000000	-10.606000000	-9.486000000
C	-1.274000000	-5.439000000	-8.982000000
C	-2.017000000	-6.754000000	-9.254000000
C	4.089000000	-9.009000000	-7.861000000
C	5.352000000	-8.410000000	-7.439000000
C	1.757000000	-5.344000000	-5.666000000
C	5.415000000	-7.302000000	-6.667000000
C	2.932000000	-4.771000000	-5.264000000
Pt	0.342000000	-7.223000000	-7.584000000
H	-0.158000000	-4.664000000	-7.383000000
H	-1.491000000	-5.502000000	-6.874000000
H	-0.734000000	-8.371000000	-9.728000000
H	-1.700000000	-8.642000000	-8.401000000
H	5.109000000	-4.884000000	-5.292000000
H	0.505000000	-10.108000000	-8.986000000
H	2.532000000	-11.282000000	-9.848000000
H	4.859000000	-11.368000000	-10.225000000
H	5.844000000	-11.065000000	-8.791000000
H	5.672000000	-9.807000000	-10.027000000
H	-1.967000000	-4.569000000	-9.119000000
H	-0.405000000	-5.319000000	-9.688000000
H	-2.983000000	-6.782000000	-8.685000000
H	-2.296000000	-6.830000000	-10.335000000
H	6.261000000	-8.885000000	-7.806000000
H	0.781000000	-4.884000000	-5.455000000
H	6.372000000	-6.875000000	-6.379000000
H	2.933000000	-3.850000000	-4.696000000

[Pt(en)(5-Mephen)]²⁺ systems

[Pt(en)(5-Mephen)]²⁺ minor groove
Dock_ID: 62-cl2_5-Mephen



EDA for 62-cl2_5-Mephen in kcal mol⁻¹.

Electrostatic interaction	-801.9
Orbital interaction	-95.5
Dispersion energy	-66.8
Pauli repulsion	127.3
Total Bonding Energy	-836.7

Contributions of the solvation energies for 62-cl2_5-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1735.4
E _{solv} (intercalator)	-162.5
E _{solv} (duplex DNA)	-2347.6
ΔE _{solv}	774.7
ΔE _{int} (EDA)	-836.7
ΔE _{aq}	-62.1

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 62-cl2_5-Mephen system.
([Pt(en)(5-Mephen)]²⁺ minor groove)

P	-1.48900000	7.15200000	2.69500000
C	1.07100000	6.72000000	2.20700000
O	-0.22700000	6.97700000	1.62400000
C	2.08500000	6.81400000	1.06200000
O	2.34700000	5.47700000	0.54600000
C	1.60900000	7.65500000	-0.15400000
O	2.74100000	8.47300000	-0.48200000
C	1.16000000	6.62300000	-1.19600000
C	1.66200000	5.26100000	-0.70000000
N	0.24000000	0.23500000	-0.74100000
C	1.46900000	0.83200000	-1.10500000
N	2.48200000	0.00700000	-1.54300000
N	1.72400000	2.17400000	-0.98800000
C	0.64800000	2.91400000	-0.55600000
C	-0.63500000	2.39300000	-0.19900000
C	-0.88600000	0.98600000	-0.27500000
O	-1.90600000	0.35000000	-0.00400000
N	-1.49800000	3.45400000	0.14700000
C	-0.78400000	4.57200000	0.01100000
N	0.55300000	4.30700000	-0.45500000
O	-1.15200000	8.13500000	3.79000000
O	-2.69500000	7.30100000	1.80800000
H	0.11200000	-0.82000000	-0.88800000
H	-1.11200000	5.59200000	0.20900000
H	2.43800000	4.76000000	-1.35400000
H	0.05500000	6.66800000	-1.31000000
H	3.19500000	0.42400000	-2.15300000
H	0.80500000	8.37900000	0.11300000
H	2.28700000	-1.00200000	-1.70300000
H	3.08200000	7.14300000	1.43800000
H	1.07700000	5.69800000	2.64200000
H	1.53600000	6.83400000	-2.22300000
H	1.29600000	7.46600000	2.99300000
P	3.35300000	8.65100000	-2.02900000
C	4.76600000	6.46500000	-1.61600000
O	3.80800000	7.11800000	-2.48200000
C	5.31100000	5.27600000	-2.40600000
O	4.26800000	4.26700000	-2.52200000
C	5.75800000	5.63100000	-3.85300000
O	6.98000000	4.89000000	-4.00400000
C	4.58400000	5.17400000	-4.72400000
C	3.95800000	4.03000000	-3.92400000
N	2.48200000	3.92800000	-4.02200000
C	1.92800000	2.60800000	-3.89900000
O	2.64600000	1.62000000	-3.92100000
N	0.52700000	2.53200000	-3.83400000

C	-0.33700000	3.65200000	-3.72800000
O	-1.51800000	3.44000000	-3.46900000
C	0.29800000	4.95700000	-3.94400000
C	1.65200000	5.06300000	-4.02400000
C	-0.60000000	6.14000000	-4.02800000
O	4.54300000	9.54400000	-1.77700000
O	2.27800000	9.00700000	-3.01900000
H	0.11200000	1.53800000	-3.77100000
H	2.17200000	6.03600000	-4.11800000
H	4.39900000	3.01300000	-4.15800000
H	3.88700000	6.03400000	-4.85500000
H	6.01800000	6.70300000	-3.98600000
H	6.12500000	4.76700000	-1.83700000
H	4.23500000	6.12000000	-0.70200000
H	-1.53700000	5.90100000	-4.55800000
H	-0.88600000	6.50200000	-3.02700000
H	-0.13700000	6.98800000	-4.55300000
H	4.86500000	4.87000000	-5.75200000
H	5.58400000	7.15500000	-1.33000000
P	7.46600000	4.21900000	-5.45400000
C	6.48500000	1.85900000	-4.73100000
O	6.41400000	2.94600000	-5.67800000
C	6.58500000	0.53100000	-5.48700000
O	5.24700000	0.05600000	-5.79000000
C	7.31500000	0.59100000	-6.85500000
O	8.04900000	-0.64600000	-6.89800000
C	6.18900000	0.78200000	-7.87900000
C	4.91000000	0.31000000	-7.17100000
N	3.79200000	1.29900000	-7.17600000
C	2.44000000	0.78200000	-6.99700000
O	2.28900000	-0.43400000	-6.88600000
N	1.39100000	1.67700000	-6.97300000
C	1.60700000	3.02800000	-7.09300000
N	0.51900000	3.84600000	-7.01700000
C	2.94100000	3.54300000	-7.26100000
C	3.99500000	2.66900000	-7.26900000
O	8.85300000	3.73600000	-5.11900000
O	7.18200000	5.12400000	-6.62100000
H	3.10400000	4.61300000	-7.36400000
H	5.04300000	3.01800000	-7.36300000
H	4.50600000	-0.67700000	-7.54100000
H	6.15600000	1.85500000	-8.17500000
H	8.09900000	1.37500000	-6.91300000
H	6.99800000	-0.26900000	-4.82800000
H	0.61600000	4.85200000	-7.06400000
H	5.50700000	1.90600000	-4.18100000
H	-0.43100000	3.46800000	-6.82900000
H	6.34100000	0.24700000	-8.83800000
H	7.31800000	1.96900000	-4.01300000
P	7.99500000	-1.72000000	-8.16900000

C	5.72600000	-2.97400000	-7.51100000
O	6.38100000	-2.06100000	-8.41100000
C	5.31300000	-4.25400000	-8.25100000
O	3.91600000	-4.14000000	-8.64700000
C	6.10100000	-4.55900000	-9.55100000
O	6.42300000	-5.95300000	-9.38800000
C	5.13000000	-4.25000000	-10.70200000
C	3.79600000	-3.86200000	-10.05800000
N	0.02100000	-0.22300000	-10.16300000
C	-0.10700000	-1.62900000	-10.11800000
N	-1.37400000	-2.14600000	-10.21600000
N	0.97000000	-2.49200000	-10.08200000
C	2.18900000	-1.85400000	-10.13300000
C	2.39800000	-0.44200000	-10.20100000
C	1.28300000	0.45600000	-10.16500000
O	1.26300000	1.68400000	-10.14800000
N	3.77500000	-0.15300000	-10.26600000
C	4.39700000	-1.33100000	-10.26300000
N	3.46900000	-2.43300000	-10.21300000
O	8.73900000	-2.90700000	-7.61500000
O	8.39200000	-1.04000000	-9.45400000
H	-0.86500000	0.38100000	-10.14700000
H	5.46900000	-1.50500000	-10.27800000
H	2.92700000	-4.48000000	-10.39700000
H	5.54500000	-3.47400000	-11.37500000
H	-1.56500000	-3.10300000	-9.94500000
H	7.06000000	-4.00900000	-9.64600000
H	-2.21000000	-1.52200000	-10.22100000
H	5.30700000	-5.13400000	-7.56400000
H	4.81700000	-2.40800000	-7.18700000
H	4.97500000	-5.12700000	-11.37100000
H	6.34100000	-3.21300000	-6.62400000
P	6.99500000	-6.85500000	-10.67300000
C	4.50300000	-7.65700000	-10.60900000
O	5.56900000	-7.20100000	-11.47500000
C	3.27900000	-7.86200000	-11.50200000
O	2.65300000	-6.57200000	-11.74500000
C	3.61300000	-8.48500000	-12.88600000
O	2.85300000	-9.69500000	-12.96500000
C	3.32200000	-7.38500000	-13.90900000
C	2.46300000	-6.35400000	-13.17600000
N	0.80800000	-1.38600000	-13.26900000
C	0.13800000	-2.56400000	-13.06200000
N	0.66200000	-3.81700000	-13.03700000
C	2.01000000	-3.84800000	-13.30100000
C	2.82400000	-2.69400000	-13.54200000
C	2.17900000	-1.41600000	-13.50400000
N	2.82300000	-0.24300000	-13.74100000
N	4.15300000	-3.08600000	-13.78300000
C	4.16400000	-4.42300000	-13.69800000

N	2.86700000	-4.95800000	-13.41300000
O	7.54500000	-8.08100000	-9.98800000
O	7.80900000	-6.05000000	-11.64800000
H	-0.95200000	-2.47200000	-12.88100000
H	5.02700000	-5.06700000	-13.83100000
H	1.35300000	-6.45400000	-13.35000000
H	4.27900000	-6.97000000	-14.28900000
H	4.66500000	-8.85100000	-12.95100000
H	2.50200000	-8.46000000	-10.97000000
H	4.29800000	-6.89000000	-9.82800000
H	2.34800000	0.65900000	-13.56400000
H	3.83400000	-0.21800000	-13.79800000
H	2.82700000	-7.75900000	-14.83200000
H	4.79200000	-8.61600000	-10.13100000
P	1.46400000	-9.87800000	-13.88000000
C	-0.37400000	-8.48300000	-12.51100000
O	0.59300000	-8.49500000	-13.58300000
C	-1.76100000	-8.20200000	-13.09200000
O	-1.79600000	-6.79500000	-13.46900000
C	-2.17000000	-9.00700000	-14.34400000
O	-3.34000000	-9.74200000	-13.93600000
C	-2.52900000	-7.96700000	-15.42100000
C	-2.11700000	-6.61100000	-14.84500000
N	-0.89500000	-6.03100000	-15.51500000
C	-0.83500000	-4.59000000	-15.69400000
O	-1.85100000	-3.93000000	-15.45800000
N	0.32300000	-4.00600000	-16.16800000
C	1.42300000	-4.78500000	-16.46700000
N	2.54500000	-4.14600000	-16.89000000
C	1.35800000	-6.21300000	-16.32300000
C	0.21900000	-6.79800000	-15.83300000
O	0.82500000	-11.09100000	-13.25500000
O	1.79100000	-9.78200000	-15.34400000
H	-3.62000000	-10.35900000	-14.65400000
H	2.20900000	-6.82900000	-16.61300000
H	0.15700000	-7.88900000	-15.66800000
H	-2.91400000	-5.82200000	-14.85500000
H	-2.07000000	-8.20200000	-16.39800000
H	-1.41800000	-9.73800000	-14.69500000
H	-2.54300000	-8.28200000	-12.28400000
H	3.39300000	-4.65800000	-17.10300000
H	-0.05800000	-7.61800000	-11.86600000
H	2.60500000	-3.11200000	-16.92400000
H	-3.62000000	-7.99000000	-15.62600000
H	-0.37700000	-9.41700000	-11.92000000
P	2.27000000	5.52500000	-19.59600000
C	-0.37400000	5.10800000	-19.49600000
O	0.68500000	6.06800000	-19.64400000
C	-1.08100000	5.27800000	-18.14400000
O	-1.07500000	3.98000000	-17.49000000

C	-0.43600000	6.27800000	-17.15000000
O	-1.50000000	7.10000000	-16.66000000
C	0.31600000	5.40700000	-16.13900000
C	-0.25700000	3.99700000	-16.29300000
N	0.50700000	-1.15300000	-16.41500000
C	-0.62900000	-0.41300000	-16.00400000
N	-1.76200000	-1.12000000	-15.64000000
N	-0.69300000	0.95100000	-16.03800000
C	0.47900000	1.56300000	-16.42200000
C	1.68500000	0.89300000	-16.79400000
C	1.73900000	-0.53800000	-16.80700000
O	2.66600000	-1.28900000	-17.11200000
N	2.69300000	1.84300000	-17.06200000
C	2.12900000	3.03900000	-16.88700000
N	0.76100000	2.93700000	-16.46000000
O	2.93800000	6.27000000	-20.72800000
O	2.80100000	5.58600000	-18.18900000
H	0.47900000	-2.22500000	-16.34700000
H	2.60500000	4.01800000	-17.02900000
H	-0.96700000	3.68600000	-15.47600000
H	1.40900000	5.46000000	-16.36500000
H	-2.36700000	-0.67100000	-14.93000000
H	0.22100000	7.02500000	-17.65500000
H	-1.68400000	-2.15300000	-15.52900000
H	-2.16500000	5.49200000	-18.29900000
H	-0.03000000	4.05800000	-19.62400000
H	0.23500000	5.77200000	-15.08300000
H	-1.05600000	5.34900000	-20.33700000
P	-2.21600000	6.97400000	-15.15200000
C	-3.60200000	4.81000000	-15.82400000
O	-2.61500000	5.37300000	-14.93600000
C	-4.69100000	4.11600000	-15.00400000
O	-4.23600000	2.77900000	-14.65000000
C	-5.10500000	4.80800000	-13.68100000
O	-6.53300000	4.92200000	-13.83000000
C	-4.65700000	3.86200000	-12.56000000
C	-3.99300000	2.66300000	-13.23800000
N	-2.51400000	2.59100000	-13.01600000
C	-1.90600000	1.30200000	-13.15500000
O	-2.59300000	0.29600000	-13.29100000
N	-0.50500000	1.24500000	-13.04800000
C	0.33600000	2.39400000	-13.04200000
O	1.54400000	2.22400000	-13.17300000
C	-0.35400000	3.67700000	-12.90300000
C	-1.71200000	3.74700000	-12.93700000
C	0.48800000	4.88800000	-12.70700000
O	-3.45100000	7.82000000	-15.33500000
O	-1.20400000	7.23600000	-14.07100000
H	-0.05800000	0.27700000	-13.09800000
H	-2.24600000	4.71100000	-12.89300000

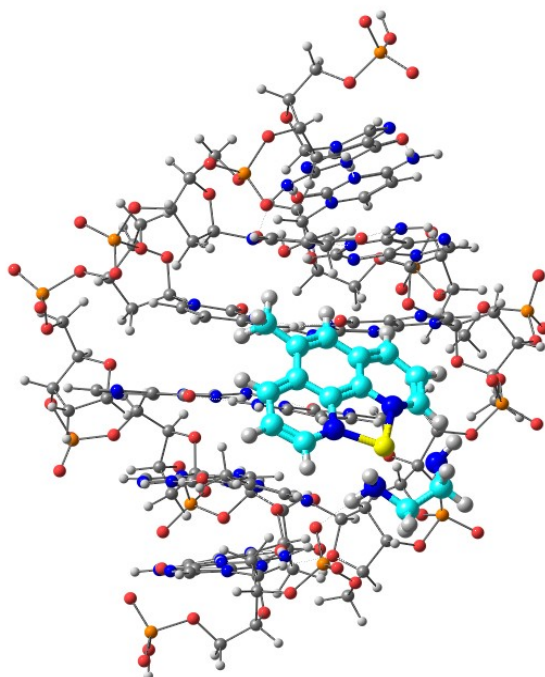
H	-4.44000000	1.66900000	-12.95600000
H	-4.00700000	4.39000000	-11.83400000
H	-4.70200000	5.83800000	-13.57400000
H	-5.58500000	3.91800000	-15.64700000
H	-3.04300000	4.05600000	-16.42900000
H	0.41600000	5.27100000	-11.67900000
H	1.55000000	4.69200000	-12.91400000
H	0.17800000	5.71500000	-13.37900000
H	-5.51800000	3.48700000	-11.95200000
H	-4.05200000	5.56200000	-16.49800000
P	-7.52700000	5.23400000	-12.52200000
C	-7.91400000	2.64000000	-12.67900000
O	-7.63700000	3.74100000	-11.78100000
C	-7.75300000	1.35300000	-11.87300000
O	-6.34000000	1.10100000	-11.65200000
C	-8.44600000	1.36500000	-10.48200000
O	-9.24000000	0.16500000	-10.54600000
C	-7.30300000	1.35400000	-9.46400000
C	-6.08900000	0.83600000	-10.23800000
N	-4.80300000	1.50200000	-9.94100000
C	-3.58300000	0.69600000	-10.06900000
O	-3.70600000	-0.50100000	-10.27600000
N	-2.36800000	1.33900000	-9.95200000
C	-2.29700000	2.69100000	-9.71100000
N	-1.06300000	3.25700000	-9.72400000
C	-3.49700000	3.46300000	-9.48600000
C	-4.71300000	2.85500000	-9.61400000
O	-8.82500000	5.59500000	-13.20300000
O	-6.89200000	6.13300000	-11.49900000
H	-3.42300000	4.51600000	-9.21300000
H	-5.66200000	3.40100000	-9.47300000
H	-5.95200000	-0.28600000	-10.15400000
H	-7.16200000	2.37900000	-9.05800000
H	-9.14600000	2.21700000	-10.34300000
H	-8.10400000	0.48000000	-12.48100000
H	-0.92500000	4.22400000	-9.46900000
H	-7.20500000	2.65400000	-13.53600000
H	-0.20900000	2.68200000	-9.88400000
H	-7.50200000	0.72500000	-8.56900000
H	-8.95300000	2.73000000	-13.05700000
P	-9.74500000	-0.66300000	-9.19000000
C	-7.62300000	-2.20900000	-9.45500000
O	-8.33300000	-1.29600000	-8.58400000
C	-6.85600000	-3.18800000	-8.55800000
O	-5.57000000	-2.59900000	-8.25700000
C	-7.54100000	-3.47900000	-7.19500000
O	-7.43500000	-4.88400000	-6.94600000
C	-6.83900000	-2.53000000	-6.21100000
C	-5.48800000	-2.23200000	-6.86200000
N	-1.29000000	0.72100000	-6.84300000

C	-1.44800000	-0.66800000	-7.05700000
N	-0.32100000	-1.42500000	-7.32700000
N	-2.65500000	-1.29200000	-7.06800000
C	-3.72100000	-0.45000000	-6.87700000
C	-3.66700000	0.96700000	-6.68200000
C	-2.39000000	1.62500000	-6.68900000
O	-2.11800000	2.81800000	-6.56900000
N	-4.97300000	1.46400000	-6.52500000
C	-5.79000000	0.40300000	-6.60900000
N	-5.07000000	-0.81300000	-6.81600000
O	-10.61300000	-1.73800000	-9.79700000
O	-10.25000000	0.26200000	-8.11500000
H	-0.30100000	1.13400000	-6.85800000
H	-6.87300000	0.41700000	-6.53600000
H	-4.62500000	-2.84800000	-6.46600000
H	-7.46600000	-1.62400000	-6.07900000
H	-0.41600000	-2.43600000	-7.22400000
H	-8.64200000	-3.32600000	-7.22100000
H	0.61600000	-1.04600000	-7.08800000
H	-6.59500000	-4.12500000	-9.10600000
H	-6.89200000	-1.59300000	-10.03900000
H	-6.72800000	-2.95500000	-5.19200000
H	-8.30800000	-2.74600000	-10.13500000
P	-6.29400000	-5.59400000	-5.94300000
C	-4.11300000	-5.27300000	-7.49700000
O	-4.82700000	-4.92000000	-6.29100000
C	-2.75700000	-5.86600000	-7.12000000
O	-1.86000000	-4.85700000	-6.55900000
C	-2.83000000	-6.97200000	-6.03600000
O	-1.73500000	-7.82800000	-6.41800000
C	-2.59300000	-6.22000000	-4.71500000
C	-1.80200000	-4.97100000	-5.13000000
N	-0.52500000	-0.10200000	-3.76800000
C	0.24600000	-1.15700000	-4.18200000
N	-0.17800000	-2.41100000	-4.47700000
C	-1.53700000	-2.58000000	-4.30800000
C	-2.43400000	-1.56500000	-3.83300000
C	-1.89200000	-0.26500000	-3.59200000
N	-2.63300000	0.80900000	-3.21000000
N	-3.74300000	-2.08000000	-3.76900000
C	-3.66000000	-3.34600000	-4.20100000
N	-2.32000000	-3.72000000	-4.52900000
O	-6.41000000	-7.05600000	-6.24500000
O	-6.49600000	-5.08100000	-4.52600000
H	1.32200000	-0.93200000	-4.31400000
H	-4.49700000	-4.04600000	-4.30300000
H	-0.69700000	-5.03000000	-4.90200000
H	-3.56600000	-5.98100000	-4.24100000
H	-3.75800000	-7.58000000	-6.06800000
H	-2.19000000	-6.20900000	-8.03700000

H	-3.98500000	-4.29900000	-8.02900000
H	-2.22100000	1.75600000	-3.18400000
H	-3.64100000	0.73200000	-3.13300000
H	-2.05500000	-6.80800000	-3.94800000
H	-4.68300000	-5.98000000	-8.13500000
P	-1.01100000	-8.90200000	-5.40500000
C	0.86200000	-7.10100000	-4.86800000
O	-0.18700000	-7.90700000	-4.32100000
C	2.06200000	-7.13600000	-3.91300000
O	2.30700000	-5.74900000	-3.53300000
C	1.87000000	-7.93300000	-2.60400000
O	2.89700000	-8.93700000	-2.63200000
C	2.11700000	-6.92800000	-1.46500000
C	2.17000000	-5.54800000	-2.11700000
N	0.92700000	-4.74100000	-1.88400000
C	1.06300000	-3.31600000	-1.64300000
O	2.18000000	-2.80500000	-1.78600000
N	-0.03400000	-2.58600000	-1.24600000
C	-1.27300000	-3.18700000	-1.13400000
N	-2.29400000	-2.43000000	-0.66700000
C	-1.43900000	-4.57400000	-1.50400000
C	-0.34900000	-5.31300000	-1.86600000
O	-0.03800000	-9.54900000	-6.37200000
O	-1.90300000	-9.68700000	-4.48500000
H	2.81700000	-9.53500000	-1.84900000
H	-2.43300000	-5.02200000	-1.48600000
H	-0.43300000	-6.37500000	-2.15700000
H	3.05300000	-4.91700000	-1.83400000
H	1.37600000	-7.01900000	-0.65000000
H	0.88300000	-8.44400000	-2.52600000
H	3.00000000	-7.44300000	-4.43200000
H	-3.24500000	-2.78500000	-0.63000000
H	0.45800000	-6.05500000	-4.93400000
H	-2.17400000	-1.42000000	-0.46800000
H	3.07900000	-7.15500000	-0.95700000
H	1.17800000	-7.44300000	-5.88300000
O	2.13900000	3.91000000	-19.98400000
O	-1.57000000	5.62900000	3.38000000
H	2.04700000	3.70300000	-20.95700000
H	-1.18000000	5.53900000	4.29200000
N	-2.42700000	-6.03500000	-10.74600000
N	0.42600000	-8.09000000	-8.73400000
N	0.44800000	-5.63900000	-9.97800000
N	-2.47300000	-8.46000000	-9.63400000
C	-4.92900000	-9.44200000	-8.52400000
C	-4.97900000	-8.35300000	-9.34000000
C	-3.73100000	-7.80800000	-9.86100000
C	-3.71000000	-6.59900000	-10.50300000
C	-4.91000000	-5.88100000	-10.91100000
C	-4.75100000	-4.73100000	-11.64800000

C	-3.45400000	-4.28000000	-12.01600000
C	-2.32400000	-4.96100000	-11.57400000
C	-6.16800000	-6.49000000	-10.47300000
C	-7.46000000	-5.85400000	-10.88400000
C	1.52800000	-7.12900000	-8.35100000
C	1.06400000	-5.68900000	-8.60500000
C	-2.48500000	-9.47700000	-8.67100000
C	-6.18800000	-7.62900000	-9.73000000
C	-3.63900000	-10.00900000	-8.17600000
Pt	-1.02900000	-7.06900000	-9.79000000
H	0.80500000	-8.85900000	-9.29600000
H	0.03400000	-8.53200000	-7.85500000
H	1.13700000	-5.89500000	-10.70600000
H	0.13400000	-4.68000000	-10.19400000
H	-5.81600000	-9.87300000	-8.08200000
H	-5.61600000	-4.14300000	-11.95700000
H	-3.34500000	-3.39500000	-12.62700000
H	-1.31000000	-4.65700000	-11.86900000
H	-7.34400000	-4.81500000	-11.22100000
H	-8.19500000	-5.85300000	-10.06700000
H	-7.91900000	-6.40500000	-11.71800000
H	1.78900000	-7.26500000	-7.26800000
H	2.46000000	-7.35600000	-8.91400000
H	0.27200000	-5.39100000	-7.86300000
H	1.91600000	-4.97500000	-8.48600000
H	-1.50000000	-9.86800000	-8.39400000
H	-7.12300000	-8.03500000	-9.35700000
H	-3.62100000	-10.85000000	-7.49800000

[Pt(en)(5-Mephen)]²⁺ major groove
Dock_ID: 5-cl3_5-Mephen



EDA for 5-cl3_5-Mephen in kcal mol⁻¹.

Electrostatic interaction	-775.9
Orbital interaction	-92.5
Dispersion energy	-55.6
Pauli repulsion	119.5
Total Bonding Energy	-804.4

Contributions of the solvation energies for 5-cl3_5-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1749.6
E _{solv} (intercalator)	-161.7
E _{solv} (duplex DNA)	-2333.0
ΔE _{solv}	745.1
ΔE _{int} (EDA)	-804.4
ΔE _{aq}	-59.4

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 5-cl3_5-Mephen system.
([Pt(en)(5-Mephen)]²⁺ major groove)

P	-2.33200000	6.81900000	2.85900000
C	0.27000000	6.33500000	2.78800000
O	-0.87600000	6.80500000	2.04400000
C	1.43600000	6.27900000	1.79800000
O	1.53500000	4.93800000	1.24300000
C	1.29700000	7.22600000	0.57600000
O	2.59800000	7.81400000	0.42800000
C	0.78700000	6.33800000	-0.55900000
C	1.01900000	4.89500000	-0.10600000
N	-0.79700000	0.04000000	-0.51100000
C	0.49100000	0.55300000	-0.79400000
N	1.45100000	-0.31900000	-1.23700000
N	0.83700000	1.86900000	-0.60400000
C	-0.21300000	2.67600000	-0.23600000
C	-1.55700000	2.25000000	-0.00300000
C	-1.89300000	0.86200000	-0.09400000
O	-2.96100000	0.29000000	0.13100000
N	-2.36500000	3.36800000	0.29000000
C	-1.55900000	4.43000000	0.25300000
N	-0.20800000	4.07000000	-0.09300000
O	-2.29200000	7.77400000	4.02700000
O	-3.34000000	6.93000000	1.74700000
H	-0.97300000	-1.01200000	-0.63200000
H	-1.83200000	5.46900000	0.44200000
H	1.82200000	4.33500000	-0.67900000
H	-0.28500000	6.56300000	-0.74800000
H	2.26300000	0.06200000	-1.73400000
H	0.63600000	8.10100000	0.77800000
H	1.21300000	-1.31100000	-1.43100000
H	2.40800000	6.41200000	2.33000000
H	0.06900000	5.32300000	3.20000000
H	1.28700000	6.54800000	-1.53600000
H	0.48700000	7.03800000	3.61500000
P	3.59600000	7.86100000	-0.89300000
C	4.54600000	5.50200000	0.02000000
O	4.83000000	6.82200000	-0.46400000
C	4.83300000	4.43400000	-1.03800000
O	3.55600000	3.84500000	-1.43300000
C	5.52400000	4.91800000	-2.34300000
O	6.70200000	4.10200000	-2.42400000
C	4.45700000	4.76400000	-3.43000000
C	3.57200000	3.64500000	-2.88300000
N	2.16300000	3.63500000	-3.32400000
C	1.54700000	2.34000000	-3.44900000

O	2.23000000	1.32900000	-3.50700000
N	0.14600000	2.31700000	-3.57300000
C	-0.67100000	3.47900000	-3.46800000
O	-1.88400000	3.32600000	-3.39300000
C	0.04000000	4.76100000	-3.47800000
C	1.39300000	4.81300000	-3.37000000
C	-0.80700000	5.97900000	-3.58100000
O	4.24800000	9.21500000	-0.78200000
O	3.00400000	7.42700000	-2.21500000
H	-0.31900000	1.34700000	-3.65400000
H	1.96300000	5.76800000	-3.31900000
H	3.99300000	2.60800000	-3.03400000
H	3.89000000	5.72800000	-3.53700000
H	5.92800000	5.96200000	-2.26100000
H	5.40600000	3.58800000	-0.58300000
H	3.51600000	5.40100000	0.41700000
H	-1.16200000	6.13300000	-4.61300000
H	-1.69400000	5.91200000	-2.93400000
H	-0.26800000	6.89600000	-3.29900000
H	4.84800000	4.59700000	-4.46300000
H	5.25100000	5.39800000	0.87500000
P	7.24600000	3.30300000	-3.78100000
C	5.34600000	1.69800000	-4.69400000
O	6.36800000	1.88000000	-3.70100000
C	5.74900000	0.51500000	-5.58000000
O	4.54100000	-0.27600000	-5.77700000
C	6.24100000	0.92100000	-6.99500000
O	7.47000000	0.20100000	-7.14400000
C	5.14500000	0.43600000	-7.96000000
C	3.99600000	-0.07600000	-7.09600000
N	2.85500000	0.89000000	-6.99200000
C	1.49400000	0.37900000	-6.91200000
O	1.32900000	-0.84000000	-6.99100000
N	0.44700000	1.26800000	-6.78600000
C	0.68300000	2.61700000	-6.64400000
N	-0.38600000	3.46000000	-6.57000000
C	2.03000000	3.11000000	-6.57300000
C	3.07100000	2.25700000	-6.78800000
O	8.65200000	2.93500000	-3.39200000
O	6.90600000	4.06500000	-5.03500000
H	2.21500000	4.17800000	-6.41000000
H	4.11100000	2.62400000	-6.81200000
H	3.58300000	-1.07600000	-7.38100000
H	4.85100000	1.24200000	-8.67100000
H	6.44600000	2.01400000	-7.09000000
H	6.46000000	-0.17000000	-5.06900000
H	-0.24400000	4.45800000	-6.43900000
H	5.15500000	2.62400000	-5.28400000
H	-1.35800000	3.10400000	-6.53900000
H	5.52400000	-0.38400000	-8.61000000

H	4.42600000	1.43600000	-4.10300000
P	8.40000000	0.51300000	-8.50600000
C	7.93600000	-2.04600000	-8.70000000
O	8.01100000	-0.80700000	-9.45100000
C	7.55200000	-3.15700000	-9.67700000
O	6.12300000	-3.11500000	-9.92400000
C	8.23900000	-3.08000000	-11.06700000
O	8.76800000	-4.38900000	-11.31700000
C	7.16200000	-2.56100000	-12.02400000
C	5.83700000	-2.64300000	-11.25800000
N	1.34100000	-0.23900000	-10.19700000
C	1.65400000	-1.60900000	-10.17600000
N	0.63800000	-2.49800000	-9.83600000
N	2.90700000	-2.10300000	-10.40900000
C	3.83200000	-1.14200000	-10.75400000
C	3.59600000	0.26700000	-10.81100000
C	2.30800000	0.79600000	-10.46900000
O	1.91900000	1.95200000	-10.37500000
N	4.77200000	0.93600000	-11.19500000
C	5.69800000	-0.01200000	-11.36000000
N	5.16600000	-1.32900000	-11.13400000
O	9.81900000	0.37500000	-7.99900000
O	7.96200000	1.74700000	-9.23900000
H	0.33000000	0.06100000	-9.98500000
H	6.74400000	0.13300000	-11.61100000
H	5.10100000	-3.39300000	-11.65100000
H	7.42100000	-1.53200000	-12.35500000
H	0.75800000	-3.46200000	-10.15200000
H	9.15100000	-2.43900000	-11.05900000
H	-0.34500000	-2.15000000	-9.90100000
H	7.70400000	-4.15500000	-9.19700000
H	7.15600000	-1.95200000	-7.91100000
H	7.10900000	-3.11500000	-12.98500000
H	8.92100000	-2.26500000	-8.24200000
P	8.16100000	-5.47200000	-12.43700000
C	5.95300000	-6.11800000	-11.10000000
O	6.51200000	-5.47100000	-12.26400000
C	4.77900000	-6.98800000	-11.55800000
O	3.64000000	-6.14400000	-11.86800000
C	5.04800000	-7.82100000	-12.84300000
O	4.49300000	-9.11900000	-12.57700000
C	4.41100000	-7.00900000	-13.97600000
C	3.44200000	-6.03600000	-13.29200000
N	1.47500000	-1.16100000	-13.43900000
C	0.91500000	-2.35100000	-13.04100000
N	1.49400000	-3.57400000	-13.03400000
C	2.78500000	-3.57000000	-13.51500000
C	3.46900000	-2.40000000	-13.98700000
C	2.77400000	-1.15400000	-13.92700000
N	3.30900000	0.01800000	-14.36900000

N	4.76700000	-2.73600000	-14.41400000
C	4.88600000	-4.05400000	-14.21200000
N	3.68700000	-4.63100000	-13.68500000
O	8.77800000	-6.76700000	-11.96800000
O	8.35200000	-4.93500000	-13.83200000
H	-0.12800000	-2.28500000	-12.67500000
H	5.77100000	-4.66100000	-14.40000000
H	2.34900000	-6.26200000	-13.42500000
H	5.21500000	-6.50100000	-14.55200000
H	6.12400000	-8.03200000	-13.02000000
H	4.40800000	-7.63000000	-10.72300000
H	5.58900000	-5.28600000	-10.45100000
H	2.84800000	0.91500000	-14.14000000
H	4.29400000	0.06200000	-14.60400000
H	3.90700000	-7.62100000	-14.75200000
H	6.69500000	-6.72900000	-10.55300000
P	3.26100000	-9.80700000	-13.47100000
C	1.33300000	-8.46700000	-12.25200000
O	2.04000000	-8.67200000	-13.49600000
C	-0.15100000	-8.29400000	-12.57500000
O	-0.38700000	-6.90200000	-12.93500000
C	-0.69000000	-9.15400000	-13.74200000
O	-1.67200000	-10.01200000	-13.13700000
C	-1.35800000	-8.17000000	-14.71700000
C	-0.97200000	-6.77100000	-14.23800000
N	0.03800000	-6.10500000	-15.12800000
C	-0.09700000	-4.68200000	-15.38900000
O	-1.11000000	-4.10600000	-14.97700000
N	0.87200000	-4.02900000	-16.12000000
C	1.97100000	-4.71700000	-16.59700000
N	2.89700000	-4.01200000	-17.29200000
C	2.10700000	-6.13000000	-16.34500000
C	1.16000000	-6.78100000	-15.60400000
O	2.88700000	-10.99200000	-12.61600000
O	3.65200000	-9.94700000	-14.91700000
H	-1.96800000	-10.70300000	-13.77800000
H	2.96300000	-6.67000000	-16.74800000
H	1.25600000	-7.85400000	-15.35000000
H	-1.82900000	-6.06000000	-14.10100000
H	-1.08900000	-8.37600000	-15.76900000
H	0.07800000	-9.78500000	-14.23100000
H	-0.76900000	-8.43900000	-11.65200000
H	3.74400000	-4.44900000	-17.64100000
H	1.74800000	-7.52700000	-11.81400000
H	2.81600000	-2.98800000	-17.42300000
H	-2.46200000	-8.30300000	-14.70400000
H	1.47300000	-9.30900000	-11.54400000
P	1.70400000	5.80700000	-20.55200000
C	-0.61400000	5.16500000	-19.48200000
O	0.76800000	5.50600000	-19.21100000

C	-1.36400000	5.29600000	-18.15200000
O	-1.43200000	3.98500000	-17.52300000
C	-0.67800000	6.23100000	-17.11800000
O	-1.70800000	7.02900000	-16.53100000
C	0.08700000	5.28600000	-16.18500000
C	-0.49400000	3.89100000	-16.42800000
N	0.68800000	-1.18600000	-16.53100000
C	-0.38000000	-0.51700000	-15.88700000
N	-1.33200000	-1.27900000	-15.23600000
N	-0.56000000	0.83800000	-15.94100000
C	0.40300000	1.51000000	-16.65400000
C	1.50600000	0.91300000	-17.33900000
C	1.69600000	-0.50500000	-17.28700000
O	2.58000000	-1.20000000	-17.79300000
N	2.27300000	1.91600000	-17.96700000
C	1.67700000	3.07500000	-17.67500000
N	0.52900000	2.89500000	-16.82700000
O	0.98300000	6.68700000	-21.54600000
O	3.06100000	6.15200000	-19.99800000
H	0.77800000	-2.24900000	-16.42300000
H	1.97200000	4.06800000	-18.01000000
H	-1.10200000	3.47200000	-15.57800000
H	1.17300000	5.34900000	-16.40600000
H	-1.81300000	-0.82300000	-14.43300000
H	-0.02100000	6.99000000	-17.60300000
H	-1.16200000	-2.29800000	-15.12700000
H	-2.43300000	5.55700000	-18.32600000
H	-0.65300000	4.11600000	-19.84600000
H	0.01700000	5.57700000	-15.11100000
H	-1.04400000	5.84000000	-20.24600000
P	-2.32500000	6.82700000	-14.98300000
C	-3.73800000	4.64200000	-15.52900000
O	-2.62800000	5.20600000	-14.80100000
C	-4.57100000	3.80500000	-14.55400000
O	-3.82200000	2.62800000	-14.15300000
C	-4.96800000	4.52900000	-13.23900000
O	-6.34600000	4.19200000	-13.03100000
C	-3.96200000	4.02600000	-12.19800000
C	-3.37200000	2.73800000	-12.78800000
N	-1.87300000	2.70300000	-12.78600000
C	-1.25800000	1.42300000	-12.99500000
O	-1.92800000	0.39600000	-12.99000000
N	0.14400000	1.41000000	-13.10400000
C	0.93900000	2.58100000	-13.25300000
O	2.11000000	2.44800000	-13.59400000
C	0.24800000	3.84600000	-13.01000000
C	-1.10200000	3.87700000	-12.86200000
C	1.08300000	5.07600000	-12.94700000
O	-3.59800000	7.63100000	-15.06300000
O	-1.26100000	7.08700000	-13.95200000

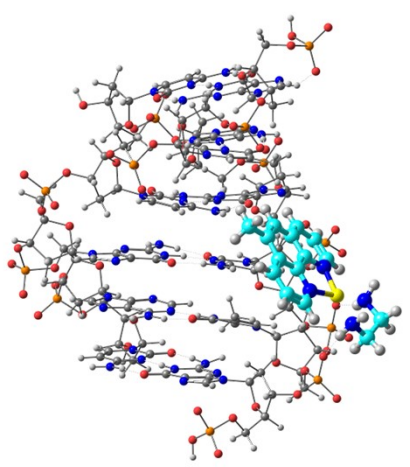
H	0.60900000	0.45200000	-13.21300000
H	-1.65500000	4.83200000	-12.76400000
H	-3.73300000	1.78800000	-12.30600000
H	-3.20000000	4.81800000	-12.02400000
H	-4.98400000	5.63800000	-13.33100000
H	-5.46300000	3.38400000	-15.07600000
H	-3.27600000	3.98900000	-16.30500000
H	1.55000000	5.17400000	-11.95000000
H	1.90100000	5.05400000	-13.68200000
H	0.49100000	5.99000000	-13.13800000
H	-4.39900000	3.85400000	-11.19000000
H	-4.36600000	5.40700000	-16.02300000
P	-6.91900000	3.33200000	-11.71600000
C	-6.28400000	0.89900000	-12.59800000
O	-5.99700000	1.94500000	-11.64800000
C	-6.51100000	-0.41000000	-11.83700000
O	-5.22100000	-1.06800000	-11.65000000
C	-7.14200000	-0.27100000	-10.42900000
O	-8.32800000	-1.08400000	-10.49300000
C	-6.11600000	-0.86500000	-9.45400000
C	-4.84700000	-1.12300000	-10.26300000
N	-3.77900000	-0.09900000	-10.02000000
C	-2.38100000	-0.51100000	-10.08400000
O	-2.12200000	-1.70300000	-10.26200000
N	-1.40500000	0.44200000	-9.89500000
C	-1.72900000	1.76100000	-9.67900000
N	-0.70700000	2.65000000	-9.60000000
C	-3.10700000	2.16100000	-9.55300000
C	-4.09200000	1.23400000	-9.76000000
O	-8.33500000	3.05000000	-12.14400000
O	-6.56500000	4.03900000	-10.43800000
H	-3.36200000	3.18900000	-9.30800000
H	-5.16100000	1.51600000	-9.72400000
H	-4.39400000	-2.13800000	-10.13400000
H	-5.97100000	-0.19900000	-8.58500000
H	-7.41600000	0.77700000	-10.17000000
H	-7.08200000	-1.13500000	-12.46600000
H	-0.86600000	3.61500000	-9.34800000
H	-5.36600000	0.82700000	-13.22700000
H	0.27600000	2.37500000	-9.79400000
H	-6.48600000	-1.81200000	-8.99100000
H	-7.15600000	1.13200000	-13.23800000
P	-9.52100000	-0.75100000	-9.36300000
C	-8.77900000	-3.14300000	-8.56000000
O	-9.18500000	-1.82300000	-8.13300000
C	-7.99400000	-3.76800000	-7.40500000
O	-6.69600000	-3.12900000	-7.30100000
C	-8.68000000	-3.64100000	-6.01700000
O	-8.75900000	-4.96700000	-5.47600000
C	-7.84700000	-2.61500000	-5.24600000

C	-6.51100000	-2.53600000	-5.98900000
N	-2.25200000	0.34000000	-6.71100000
C	-2.42600000	-1.06100000	-6.81100000
N	-1.33300000	-1.81500000	-7.14100000
N	-3.63400000	-1.69000000	-6.63700000
C	-4.67700000	-0.83100000	-6.40200000
C	-4.60400000	0.59800000	-6.37500000
C	-3.33500000	1.25300000	-6.49900000
O	-3.06200000	2.45000000	-6.44500000
N	-5.89200000	1.13800000	-6.19100000
C	-6.72300000	0.09700000	-6.09500000
N	-6.02500000	-1.15700000	-6.19100000
O	-10.78400000	-1.17800000	-10.08000000
O	-9.38000000	0.62100000	-8.77100000
H	-1.25600000	0.74200000	-6.79200000
H	-7.80200000	0.13000000	-5.97500000
H	-5.67600000	-3.13700000	-5.52800000
H	-8.39600000	-1.64800000	-5.22500000
H	-1.39500000	-2.82700000	-7.08600000
H	-9.75400000	-3.35000000	-6.09300000
H	-0.37900000	-1.40100000	-7.15700000
H	-7.76000000	-4.83300000	-7.65200000
H	-8.14600000	-3.09800000	-9.47400000
H	-7.71600000	-2.86200000	-4.17100000
H	-9.69200000	-3.73300000	-8.77700000
P	-7.73000000	-5.56800000	-4.30200000
C	-5.57800000	-5.81400000	-5.87100000
O	-6.19900000	-5.11900000	-4.77000000
C	-4.31900000	-6.52900000	-5.37900000
O	-3.22100000	-5.57500000	-5.28100000
C	-4.44400000	-7.19300000	-3.98400000
O	-3.82100000	-8.47500000	-4.18400000
C	-3.70600000	-6.24300000	-3.03100000
C	-2.90900000	-5.27100000	-3.91000000
N	-1.17200000	-0.29100000	-3.66300000
C	-0.52700000	-1.45100000	-4.00000000
N	-1.05600000	-2.70200000	-4.07400000
C	-2.39300000	-2.75700000	-3.74300000
C	-3.17400000	-1.61000000	-3.37600000
C	-2.53500000	-0.33200000	-3.38400000
N	-3.20300000	0.83200000	-3.18800000
N	-4.49600000	-1.99700000	-3.08500000
C	-4.53500000	-3.32000000	-3.26400000
N	-3.26100000	-3.85600000	-3.65200000
O	-7.93600000	-7.05500000	-4.42600000
O	-7.91000000	-4.81500000	-3.01000000
H	0.54800000	-1.34400000	-4.24700000
H	-5.40700000	-3.96500000	-3.14700000
H	-1.79100000	-5.38000000	-3.84300000
H	-4.43300000	-5.74100000	-2.36100000

H	-5.49000000	-7.40000000	-3.67100000
H	-3.95000000	-7.25500000	-6.14600000
H	-5.30500000	-4.99700000	-6.58100000
H	-2.71300000	1.74000000	-3.19500000
H	-4.17500000	0.82300000	-2.89800000
H	-3.03300000	-6.77700000	-2.32600000
H	-6.26100000	-6.52700000	-6.37000000
P	-3.18200000	-9.35000000	-2.91100000
C	-0.94400000	-8.29900000	-3.76300000
O	-1.78400000	-8.48600000	-2.59600000
C	0.39900000	-7.76700000	-3.27200000
O	0.30800000	-6.31200000	-3.19500000
C	0.83900000	-8.26300000	-1.87500000
O	1.95600000	-9.12900000	-2.13500000
C	1.28800000	-7.01000000	-1.10900000
C	0.85600000	-5.81400000	-1.95600000
N	-0.23200000	-5.00700000	-1.31900000
C	-0.06400000	-3.56700000	-1.21400000
O	1.02700000	-3.09100000	-1.53900000
N	-1.10500000	-2.80000000	-0.74400000
C	-2.29300000	-3.39100000	-0.35400000
N	-3.28300000	-2.57300000	0.07600000
C	-2.43800000	-4.82600000	-0.39700000
C	-1.41700000	-5.59500000	-0.88100000
O	-2.86900000	-10.67600000	-3.55500000
O	-3.99700000	-9.23900000	-1.65300000
H	2.20800000	-9.62000000	-1.31700000
H	-3.35600000	-5.28600000	-0.02800000
H	-1.49600000	-6.69600000	-0.96900000
H	1.68600000	-5.11800000	-2.25100000
H	0.88800000	-6.99100000	-0.07700000
H	0.05500000	-8.84000000	-1.34000000
H	1.19700000	-7.95800000	-4.03400000
H	-4.20100000	-2.93600000	0.31700000
H	-1.43600000	-7.56800000	-4.44400000
H	-3.19000000	-1.54100000	0.03900000
H	2.39000000	-7.02000000	-0.96300000
H	-0.79600000	-9.26300000	-4.29200000
O	1.82500000	4.27300000	-21.21100000
O	-2.41300000	5.26800000	3.47100000
H	1.29400000	4.11100000	-22.03600000
H	-2.24400000	5.17900000	4.45100000
N	2.91600000	7.10700000	-6.03800000
N	6.91600000	6.77300000	-5.54000000
N	4.94300000	8.21600000	-4.15200000
N	4.79300000	5.76400000	-7.37700000
C	4.04600000	3.91600000	-9.40400000
C	3.12400000	4.83500000	-8.99900000
C	3.46100000	5.71900000	-7.88600000
C	2.50400000	6.44100000	-7.23000000

C	1.11800000	6.51500000	-7.68700000
C	0.22900000	7.22600000	-6.93300000
C	0.66500000	7.87800000	-5.73000000
C	1.97700000	7.78500000	-5.30900000
C	0.83900000	5.79400000	-8.94000000
C	-0.50600000	5.99500000	-9.56400000
C	7.36100000	7.87400000	-4.61500000
C	6.30700000	8.10500000	-3.52600000
C	5.63300000	4.71600000	-7.71800000
C	1.76800000	4.99200000	-9.51900000
C	5.32400000	3.84800000	-8.73800000
Pt	4.87600000	6.92700000	-5.76800000
H	7.41000000	6.85900000	-6.43800000
H	7.15300000	5.81900000	-5.16500000
H	4.76900000	9.18600000	-4.44600000
H	4.18900000	7.95600000	-3.45300000
H	3.83100000	3.19700000	-10.19700000
H	-0.82100000	7.32000000	-7.20500000
H	-0.05500000	8.42500000	-5.13900000
H	2.31300000	8.23500000	-4.36400000
H	-0.58300000	5.55200000	-10.56700000
H	-0.72800000	7.06700000	-9.68800000
H	-1.31400000	5.58900000	-8.93900000
H	7.52500000	8.80800000	-5.20600000
H	8.34600000	7.63800000	-4.14800000
H	6.56200000	9.01700000	-2.93800000
H	6.31200000	7.25400000	-2.78900000
H	6.57600000	4.64900000	-7.16200000
H	1.55100000	4.42300000	-10.43100000
H	6.03200000	3.08100000	-9.05000000

[Pt(en)(5-Mephen)]²⁺ major groove
Dock_ID: 82-cl4_5-Mephen



EDE for 82-cl4_5-Mephen in kcal mol⁻¹.

Electrostatic interaction	-775.8
Orbital interaction	-94.4
Dispersion energy	-53.9
Pauli repulsion	122.4
Total Bonding Energy	-801.7

Contributions of the solvation energies for 82-cl4_5-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1754.8
E _{solv} (intercalator)	-161.7
E _{solv} (duplex DNA)	-2336.3
ΔE _{solv}	743.2
ΔE _{int} (EDA)	-801.7
ΔE _{aq}	-58.5

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 82-cl4_5-Mephen system.
([Pt(en)(5-Mephen)]²⁺ major groove)

P	-1.277000000	6.163000000	2.635000000
C	1.355000000	5.764000000	2.326000000
O	0.298000000	6.719000000	2.511000000
C	1.834000000	5.718000000	0.870000000
O	1.642000000	4.357000000	0.391000000
C	1.103000000	6.654000000	-0.128000000
O	2.110000000	7.394000000	-0.825000000
C	0.205000000	5.733000000	-0.958000000
C	0.746000000	4.317000000	-0.748000000
N	-0.336000000	-0.788000000	-0.477000000
C	0.790000000	-0.131000000	-1.029000000
N	1.800000000	-0.917000000	-1.551000000
N	0.958000000	1.227000000	-1.010000000
C	-0.110000000	1.923000000	-0.489000000
C	-1.299000000	1.337000000	0.043000000
C	-1.450000000	-0.086000000	0.084000000
O	-2.372000000	-0.768000000	0.535000000
N	-2.204000000	2.351000000	0.420000000
C	-1.593000000	3.506000000	0.154000000
N	-0.295000000	3.313000000	-0.435000000
O	-1.833000000	6.906000000	3.828000000
O	-1.952000000	6.224000000	1.291000000
H	-0.388000000	-1.858000000	-0.518000000
H	-1.985000000	4.515000000	0.331000000
H	1.381000000	3.921000000	-1.592000000
H	-0.848000000	5.851000000	-0.605000000
H	2.362000000	-0.498000000	-2.312000000
H	0.538000000	7.468000000	0.386000000
H	1.643000000	-1.943000000	-1.636000000
H	2.939000000	5.861000000	0.831000000
H	1.078000000	4.744000000	2.672000000
H	0.166000000	6.011000000	-2.041000000
H	2.154000000	6.152000000	2.993000000
P	2.671000000	7.048000000	-2.367000000
C	4.041000000	4.877000000	-1.654000000
O	2.933000000	5.410000000	-2.406000000
C	4.837000000	3.951000000	-2.577000000
O	4.028000000	2.794000000	-2.909000000
C	5.257000000	4.585000000	-3.930000000
O	6.604000000	4.130000000	-4.137000000
C	4.196000000	4.103000000	-4.924000000
C	3.587000000	2.849000000	-4.284000000
N	2.092000000	2.819000000	-4.291000000
C	1.482000000	1.543000000	-4.030000000

O	2.152000000	0.521000000	-4.005000000
N	0.080000000	1.534000000	-3.921000000
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C	1.320000000	3.994000000	-4.238000000
C	-0.853000000	5.205000000	-4.145000000
O	3.960000000	7.828000000	-2.402000000
O	1.577000000	7.235000000	-3.383000000
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H	1.870000000	4.948000000	-4.360000000
H	3.946000000	1.877000000	-4.726000000
H	3.453000000	4.918000000	-5.076000000
H	5.356000000	5.693000000	-3.892000000
H	5.710000000	3.520000000	-2.033000000
H	3.574000000	4.289000000	-0.831000000
H	-1.132000000	5.450000000	-5.181000000
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H	-0.305000000	6.076000000	-3.735000000
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H	4.690000000	5.659000000	-1.221000000
P	7.104000000	3.248000000	-5.462000000
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C	6.645000000	-0.461000000	-5.280000000
O	5.373000000	-1.116000000	-5.557000000
C	7.369000000	-0.327000000	-6.644000000
O	8.430000000	-1.297000000	-6.541000000
C	6.331000000	-0.718000000	-7.706000000
C	5.044000000	-1.063000000	-6.957000000
N	3.947000000	-0.057000000	-7.130000000
C	2.566000000	-0.513000000	-6.999000000
O	2.360000000	-1.714000000	-6.830000000
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C	1.824000000	1.747000000	-7.287000000
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C	3.181000000	2.197000000	-7.446000000
C	4.205000000	1.295000000	-7.341000000
O	8.519000000	2.896000000	-5.081000000
O	6.748000000	3.954000000	-6.741000000
H	3.393000000	3.243000000	-7.653000000
H	5.262000000	1.609000000	-7.428000000
H	4.623000000	-2.076000000	-7.186000000
H	6.219000000	0.076000000	-8.464000000
H	7.811000000	0.676000000	-6.823000000
H	7.168000000	-1.190000000	-4.614000000
H	0.906000000	3.604000000	-7.398000000
H	5.424000000	0.777000000	-3.959000000
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H	6.660000000	-1.606000000	-8.304000000

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N	5.607000000	0.779000000	-10.955000000
C	6.414000000	-0.286000000	-11.032000000
N	5.701000000	-1.512000000	-10.817000000
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O	5.431000000	-5.477000000	-11.977000000
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C	2.055000000	-0.451000000	-13.524000000
N	2.785000000	0.677000000	-13.709000000

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C	-0.273000000	-3.179000000	-15.894000000
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N	0.772000000	-2.357000000	-16.247000000
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C	2.232000000	-4.313000000	-16.478000000
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O	1.710000000	-10.784000000	-13.036000000
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O	0.514000000	7.327000000	-18.494000000

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N	0.356000000	0.486000000	-16.437000000
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O	2.537000000	0.826000000	-16.972000000
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P	-3.956000000	8.431000000	-15.662000000
C	-4.783000000	5.975000000	-16.237000000
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O	-2.601000000	1.319000000	-13.376000000
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O	1.540000000	3.242000000	-13.446000000
C	-0.351000000	4.704000000	-13.135000000
C	-1.707000000	4.786000000	-13.193000000
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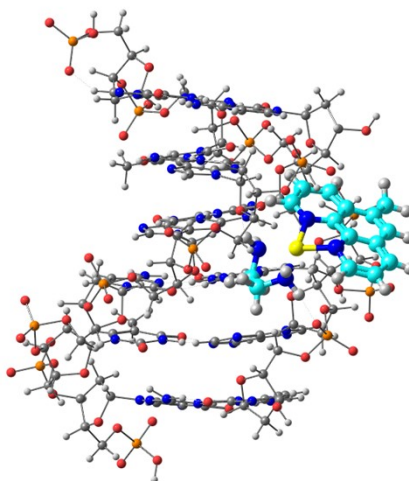
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C	-7.783000000	-2.485000000	-8.189000000
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C	-5.256000000	-6.380000000	-5.630000000
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C	1.669000000	-6.493000000	-2.134000000
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C	0.624000000	-4.336000000	-1.282000000
O	1.634000000	-3.758000000	-1.694000000
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H	0.761000000	6.952000000	-7.422000000
H	1.285000000	5.811000000	-8.651000000
H	0.858000000	5.237000000	-7.024000000
H	-8.830000000	7.468000000	-12.284000000
H	-8.185000000	8.729000000	-11.211000000
H	-6.751000000	7.409000000	-13.651000000
H	-7.282000000	9.109000000	-13.488000000
H	-6.728000000	4.618000000	-9.465000000
H	-1.370000000	4.325000000	-6.792000000
H	-5.957000000	2.995000000	-7.714000000

[Pt(en)(5-Mephen)]²⁺ minor groove
Dock_ID: 227-cl1_5-Mephen



EDA for 227-cl1_5-Mephen in kcal mol⁻¹.

Electrostatic interaction	-802.1
Orbital interaction	-99.3
Dispersion energy	-67.0
Pauli repulsion	134.3
Total Bonding Energy	-834.2

Contributions of the solvation energies for 227-cl1_5-Mephen in kcal mol⁻¹.

E _{solv} (total system)	-1733.0
E _{solv} (intercalator)	-162.7
E _{solv} (duplex DNA)	-2348.4
ΔE _{solv}	778.1
ΔE _{int} (EDA)	-834.2
ΔE _{aq}	-56.0

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 227-cl1_5-Mephen system.
([Pt(en)(5-Mephen)]²⁺ minor groove)

P	-1.950000000	6.392000000	2.206000000
C	0.699000000	5.986000000	2.313000000
O	-0.373000000	6.941000000	2.339000000
C	1.419000000	5.963000000	0.957000000
O	1.374000000	4.593000000	0.470000000
C	0.825000000	6.854000000	-0.163000000
O	1.925000000	7.577000000	-0.732000000
C	0.066000000	5.888000000	-1.077000000
C	0.612000000	4.497000000	-0.759000000
N	-0.214000000	-0.626000000	-0.403000000
C	0.956000000	0.086000000	-0.758000000
N	2.104000000	-0.649000000	-0.998000000
N	1.032000000	1.450000000	-0.790000000
C	-0.156000000	2.087000000	-0.503000000
C	-1.390000000	1.443000000	-0.180000000
C	-1.458000000	0.016000000	-0.097000000
O	-2.404000000	-0.716000000	0.198000000
N	-2.398000000	2.413000000	-0.004000000
C	-1.811000000	3.597000000	-0.198000000
N	-0.421000000	3.462000000	-0.530000000
O	-2.707000000	7.222000000	3.216000000
O	-2.372000000	6.345000000	0.761000000
H	-0.193000000	-1.699000000	-0.435000000
H	-2.280000000	4.587000000	-0.129000000
H	1.351000000	4.097000000	-1.513000000
H	-1.029000000	5.982000000	-0.867000000
H	2.794000000	-0.229000000	-1.637000000
H	0.186000000	7.677000000	0.234000000
H	2.024000000	-1.685000000	-1.085000000
H	2.509000000	6.155000000	1.099000000
H	0.365000000	4.962000000	2.590000000
H	0.158000000	6.131000000	-2.166000000
H	1.375000000	6.356000000	3.112000000
P	2.638000000	7.233000000	-2.207000000
C	3.940000000	5.112000000	-1.268000000
O	2.956000000	5.599000000	-2.203000000
C	5.032000000	4.351000000	-2.023000000
O	4.560000000	3.009000000	-2.332000000
C	5.492000000	4.973000000	-3.365000000
O	6.925000000	4.962000000	-3.220000000
C	4.946000000	4.043000000	-4.457000000
C	4.305000000	2.853000000	-3.737000000
N	2.823000000	2.750000000	-3.938000000
C	2.229000000	1.465000000	-3.719000000

O	2.928000000	0.475000000	-3.526000000
N	0.830000000	1.385000000	-3.814000000
C	-0.024000000	2.524000000	-3.863000000
O	-1.225000000	2.353000000	-3.691000000
C	0.648000000	3.802000000	-4.103000000
C	2.006000000	3.888000000	-4.081000000
C	-0.210000000	4.990000000	-4.362000000
O	3.914000000	8.034000000	-2.137000000
O	1.640000000	7.391000000	-3.320000000
H	0.391000000	0.411000000	-3.703000000
H	2.530000000	4.852000000	-4.198000000
H	4.761000000	1.857000000	-3.999000000
H	4.251000000	4.598000000	-5.121000000
H	5.185000000	6.034000000	-3.494000000
H	5.903000000	4.163000000	-1.347000000
H	3.373000000	4.414000000	-0.606000000
H	-0.243000000	5.246000000	-5.430000000
H	-1.247000000	4.827000000	-4.033000000
H	0.161000000	5.888000000	-3.825000000
H	5.751000000	3.666000000	-5.132000000
H	4.385000000	5.915000000	-0.653000000
P	7.945000000	5.137000000	-4.531000000
C	8.052000000	2.517000000	-4.342000000
O	7.863000000	3.631000000	-5.248000000
C	7.848000000	1.246000000	-5.163000000
O	6.419000000	1.008000000	-5.317000000
C	8.466000000	1.293000000	-6.588000000
O	9.247000000	0.084000000	-6.616000000
C	7.266000000	1.340000000	-7.537000000
C	6.097000000	0.783000000	-6.722000000
N	4.788000000	1.437000000	-6.940000000
C	3.587000000	0.610000000	-6.805000000
O	3.731000000	-0.587000000	-6.598000000
N	2.356000000	1.223000000	-6.904000000
C	2.252000000	2.573000000	-7.149000000
N	1.000000000	3.097000000	-7.197000000
C	3.434000000	3.373000000	-7.370000000
C	4.664000000	2.787000000	-7.268000000
O	9.280000000	5.356000000	-3.863000000
O	7.414000000	6.085000000	-5.570000000
H	3.338000000	4.426000000	-7.633000000
H	5.600000000	3.350000000	-7.434000000
H	5.972000000	-0.338000000	-6.834000000
H	7.108000000	2.388000000	-7.874000000
H	9.171000000	2.141000000	-6.734000000
H	8.219000000	0.356000000	-4.595000000
H	0.856000000	4.093000000	-7.288000000
H	7.313000000	2.573000000	-3.513000000
H	0.165000000	2.518000000	-6.965000000
H	7.415000000	0.768000000	-8.478000000

H	9.080000000	2.546000000	-3.927000000
P	9.610000000	-0.727000000	-8.028000000
C	7.549000000	-2.289000000	-7.512000000
O	8.149000000	-1.386000000	-8.472000000
C	6.791000000	-3.370000000	-8.291000000
O	5.446000000	-2.892000000	-8.528000000
C	7.376000000	-3.701000000	-9.692000000
O	7.223000000	-5.114000000	-9.875000000
C	6.599000000	-2.777000000	-10.638000000
C	5.281000000	-2.504000000	-9.909000000
N	1.089000000	0.460000000	-9.997000000
C	1.238000000	-0.931000000	-9.787000000
N	0.109000000	-1.692000000	-9.562000000
N	2.446000000	-1.557000000	-9.735000000
C	3.516000000	-0.717000000	-9.904000000
C	3.468000000	0.699000000	-10.106000000
C	2.195000000	1.361000000	-10.122000000
O	1.930000000	2.557000000	-10.241000000
N	4.779000000	1.192000000	-10.246000000
C	5.591000000	0.132000000	-10.138000000
N	4.865000000	-1.082000000	-9.928000000
O	10.565000000	-1.787000000	-7.535000000
O	9.962000000	0.212000000	-9.151000000
H	0.102000000	0.875000000	-10.005000000
H	6.677000000	0.138000000	-10.177000000
H	4.401000000	-3.124000000	-10.259000000
H	7.199000000	-1.858000000	-10.807000000
H	0.205000000	-2.701000000	-9.660000000
H	8.476000000	-3.557000000	-9.752000000
H	-0.830000000	-1.309000000	-9.783000000
H	6.644000000	-4.298000000	-7.673000000
H	6.814000000	-1.674000000	-6.929000000
H	6.443000000	-3.202000000	-11.651000000
H	8.297000000	-2.740000000	-6.836000000
P	6.128000000	-5.822000000	-10.928000000
C	3.873000000	-5.633000000	-9.486000000
O	4.637000000	-5.173000000	-10.624000000
C	2.506000000	-6.120000000	-9.961000000
O	1.683000000	-5.029000000	-10.482000000
C	2.569000000	-7.150000000	-11.119000000
O	1.391000000	-7.941000000	-10.860000000
C	2.456000000	-6.284000000	-12.385000000
C	1.651000000	-5.064000000	-11.920000000
N	0.326000000	-0.173000000	-13.101000000
C	-0.436000000	-1.264000000	-12.770000000
N	0.006000000	-2.520000000	-12.514000000
C	1.375000000	-2.647000000	-12.630000000
C	2.269000000	-1.590000000	-13.006000000
C	1.702000000	-0.294000000	-13.219000000
N	2.432000000	0.810000000	-13.526000000

N	3.593000000	-2.071000000	-13.021000000
C	3.522000000	-3.359000000	-12.661000000
N	2.174000000	-3.780000000	-12.431000000
O	6.250000000	-7.284000000	-10.624000000
O	6.374000000	-5.293000000	-12.331000000
H	-1.522000000	-1.072000000	-12.680000000
H	4.362000000	-4.051000000	-12.544000000
H	0.552000000	-5.114000000	-12.180000000
H	3.470000000	-6.021000000	-12.750000000
H	3.448000000	-7.823000000	-11.092000000
H	1.880000000	-6.502000000	-9.097000000
H	3.772000000	-4.729000000	-8.840000000
H	1.995000000	1.742000000	-13.544000000
H	3.446000000	0.770000000	-13.545000000
H	1.981000000	-6.789000000	-13.246000000
H	4.392000000	-6.443000000	-8.929000000
P	0.677000000	-8.906000000	-11.984000000
C	-1.058000000	-7.000000000	-12.621000000
O	0.045000000	-7.786000000	-13.079000000
C	-2.218000000	-7.119000000	-13.618000000
O	-2.571000000	-5.753000000	-13.987000000
C	-1.904000000	-7.869000000	-14.932000000
O	-2.910000000	-8.891000000	-15.015000000
C	-2.084000000	-6.832000000	-16.056000000
C	-2.271000000	-5.483000000	-15.366000000
N	-1.044000000	-4.621000000	-15.422000000
C	-1.215000000	-3.184000000	-15.527000000
O	-2.355000000	-2.720000000	-15.412000000
N	-0.120000000	-2.389000000	-15.778000000
C	1.146000000	-2.939000000	-15.846000000
N	2.165000000	-2.116000000	-16.186000000
C	1.338000000	-4.342000000	-15.556000000
C	0.252000000	-5.143000000	-15.348000000
O	-0.448000000	-9.505000000	-11.163000000
O	1.588000000	-9.717000000	-12.860000000
H	-2.748000000	-9.475000000	-15.795000000
H	2.348000000	-4.749000000	-15.507000000
H	0.355000000	-6.220000000	-15.123000000
H	-3.141000000	-4.875000000	-15.726000000
H	-1.260000000	-6.858000000	-16.793000000
H	-0.904000000	-8.357000000	-14.947000000
H	-3.147000000	-7.514000000	-13.143000000
H	3.128000000	-2.437000000	-16.195000000
H	-0.681000000	-5.942000000	-12.590000000
H	2.017000000	-1.104000000	-16.352000000
H	-2.975000000	-7.082000000	-16.671000000
H	-1.409000000	-7.294000000	-11.606000000
P	1.104000000	7.553000000	-19.058000000
C	-1.472000000	7.126000000	-18.656000000
O	-0.196000000	7.394000000	-18.030000000

C	-2.507000000	7.097000000	-17.526000000
O	-2.737000000	5.714000000	-17.129000000
C	-2.076000000	7.845000000	-16.236000000
O	-3.238000000	8.597000000	-15.859000000
C	-1.610000000	6.742000000	-15.277000000
C	-2.064000000	5.413000000	-15.894000000
N	-0.466000000	0.447000000	-16.099000000
C	-1.737000000	0.977000000	-15.779000000
N	-2.736000000	0.093000000	-15.442000000
N	-2.036000000	2.314000000	-15.832000000
C	-0.969000000	3.115000000	-16.171000000
C	0.345000000	2.659000000	-16.503000000
C	0.647000000	1.259000000	-16.485000000
O	1.700000000	0.676000000	-16.748000000
N	1.179000000	3.766000000	-16.760000000
C	0.421000000	4.850000000	-16.588000000
N	-0.924000000	4.512000000	-16.200000000
O	0.838000000	8.580000000	-20.133000000
O	2.285000000	7.633000000	-18.129000000
H	-0.307000000	-0.612000000	-16.014000000
H	0.719000000	5.890000000	-16.718000000
H	-2.834000000	4.837000000	-15.297000000
H	-0.507000000	6.809000000	-15.141000000
H	-3.492000000	0.440000000	-14.841000000
H	-1.291000000	8.613000000	-16.428000000
H	-2.518000000	-0.920000000	-15.347000000
H	-3.508000000	7.426000000	-17.891000000
H	-1.435000000	6.141000000	-19.168000000
H	-2.009000000	6.854000000	-14.244000000
H	-1.709000000	7.923000000	-19.387000000
P	-3.874000000	8.629000000	-14.312000000
C	-5.200000000	6.425000000	-14.892000000
O	-4.260000000	7.045000000	-13.984000000
C	-5.697000000	5.162000000	-14.188000000
O	-4.621000000	4.179000000	-14.161000000
C	-6.134000000	5.393000000	-12.714000000
O	-7.326000000	4.597000000	-12.606000000
C	-4.937000000	4.904000000	-11.894000000
C	-4.296000000	3.838000000	-12.784000000
N	-2.818000000	3.761000000	-12.700000000
C	-2.231000000	2.462000000	-12.880000000
O	-2.923000000	1.457000000	-12.908000000
N	-0.827000000	2.423000000	-12.945000000
C	0.010000000	3.568000000	-12.986000000
O	1.199000000	3.397000000	-13.233000000
C	-0.659000000	4.846000000	-12.723000000
C	-2.015000000	4.914000000	-12.639000000
C	0.209000000	6.046000000	-12.572000000
O	-5.101000000	9.482000000	-14.511000000
O	-2.826000000	8.952000000	-13.283000000

H	-0.384000000	1.446000000	-13.052000000
H	-2.560000000	5.868000000	-12.502000000
H	-4.717000000	2.799000000	-12.624000000
H	-4.259000000	5.770000000	-11.706000000
H	-6.423000000	6.444000000	-12.498000000
H	-6.503000000	4.672000000	-14.785000000
H	-4.665000000	6.169000000	-15.831000000
H	1.163000000	5.797000000	-12.080000000
H	0.464000000	6.484000000	-13.552000000
H	-0.268000000	6.842000000	-11.982000000
H	-5.197000000	4.516000000	-10.891000000
H	-6.046000000	7.104000000	-15.121000000
P	-7.819000000	3.908000000	-11.166000000
C	-6.767000000	1.588000000	-11.905000000
O	-6.732000000	2.664000000	-10.943000000
C	-6.817000000	0.246000000	-11.167000000
O	-5.459000000	-0.194000000	-10.908000000
C	-7.505000000	0.276000000	-9.775000000
O	-8.198000000	-0.983000000	-9.701000000
C	-6.352000000	0.507000000	-8.789000000
C	-5.088000000	0.057000000	-9.534000000
N	-3.979000000	1.053000000	-9.557000000
C	-2.630000000	0.538000000	-9.777000000
O	-2.489000000	-0.678000000	-9.902000000
N	-1.584000000	1.432000000	-9.822000000
C	-1.799000000	2.782000000	-9.677000000
N	-0.716000000	3.600000000	-9.789000000
C	-3.129000000	3.295000000	-9.478000000
C	-4.184000000	2.421000000	-9.452000000
O	-9.187000000	3.386000000	-11.522000000
O	-7.576000000	4.812000000	-9.990000000
H	-3.289000000	4.363000000	-9.361000000
H	-5.231000000	2.767000000	-9.335000000
H	-4.661000000	-0.929000000	-9.184000000
H	-6.335000000	1.585000000	-8.510000000
H	-8.315000000	1.032000000	-9.689000000
H	-7.231000000	-0.555000000	-11.822000000
H	-0.801000000	4.603000000	-9.697000000
H	-5.794000000	1.677000000	-12.460000000
H	0.240000000	3.218000000	-9.928000000
H	-6.464000000	-0.019000000	-7.820000000
H	-7.606000000	1.678000000	-12.618000000
P	-7.991000000	-2.096000000	-8.480000000
C	-5.743000000	-3.222000000	-9.380000000
O	-6.354000000	-2.385000000	-8.381000000
C	-5.177000000	-4.495000000	-8.738000000
O	-3.801000000	-4.259000000	-8.329000000
C	-5.909000000	-4.994000000	-7.467000000
O	-5.957000000	-6.417000000	-7.702000000
C	-5.016000000	-4.570000000	-6.290000000

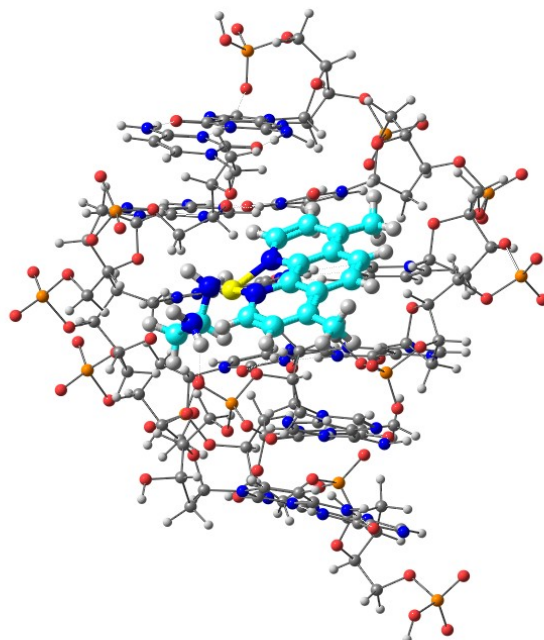
C	-3.703000000	-4.070000000	-6.902000000
N	-0.022000000	-0.355000000	-6.629000000
C	0.134000000	-1.756000000	-6.719000000
N	1.414000000	-2.243000000	-6.616000000
N	-0.924000000	-2.638000000	-6.791000000
C	-2.156000000	-2.031000000	-6.701000000
C	-2.394000000	-0.627000000	-6.561000000
C	-1.300000000	0.296000000	-6.611000000
O	-1.301000000	1.525000000	-6.621000000
N	-3.777000000	-0.375000000	-6.480000000
C	-4.372000000	-1.566000000	-6.542000000
N	-3.423000000	-2.640000000	-6.667000000
O	-8.726000000	-3.301000000	-9.008000000
O	-8.301000000	-1.473000000	-7.142000000
H	0.853000000	0.265000000	-6.657000000
H	-5.441000000	-1.764000000	-6.528000000
H	-2.806000000	-4.671000000	-6.590000000
H	-5.532000000	-3.818000000	-5.663000000
H	1.619000000	-3.201000000	-6.883000000
H	-6.955000000	-4.638000000	-7.371000000
H	2.233000000	-1.602000000	-6.679000000
H	-5.075000000	-5.309000000	-9.496000000
H	-4.905000000	-2.591000000	-9.770000000
H	-4.802000000	-5.416000000	-5.595000000
H	-6.431000000	-3.474000000	-10.208000000
P	-6.400000000	-7.478000000	-6.493000000
C	-3.814000000	-7.910000000	-6.444000000
O	-4.970000000	-7.604000000	-5.633000000
C	-2.593000000	-7.800000000	-5.534000000
O	-2.304000000	-6.389000000	-5.316000000
C	-2.796000000	-8.449000000	-4.133000000
O	-1.783000000	-9.465000000	-4.115000000
C	-2.679000000	-7.291000000	-3.136000000
C	-1.967000000	-6.179000000	-3.909000000
N	-0.428000000	-1.216000000	-3.492000000
C	0.284000000	-2.373000000	-3.680000000
N	-0.213000000	-3.633000000	-3.762000000
C	-1.573000000	-3.695000000	-3.594000000
C	-2.428000000	-2.566000000	-3.370000000
C	-1.808000000	-1.277000000	-3.330000000
N	-2.489000000	-0.122000000	-3.104000000
N	-3.762000000	-2.993000000	-3.231000000
C	-3.742000000	-4.323000000	-3.375000000
N	-2.417000000	-4.819000000	-3.605000000
O	-6.685000000	-8.746000000	-7.258000000
O	-7.383000000	-6.887000000	-5.522000000
H	1.379000000	-2.254000000	-3.803000000
H	-4.595000000	-4.992000000	-3.320000000
H	-0.837000000	-6.225000000	-3.842000000
H	-3.692000000	-6.998000000	-2.788000000

H	-3.760000000	-8.994000000	-4.035000000
H	-1.669000000	-8.204000000	-6.034000000
H	-3.738000000	-7.186000000	-7.295000000
H	-2.025000000	0.792000000	-3.237000000
H	-3.502000000	-0.120000000	-3.122000000
H	-2.148000000	-7.548000000	-2.197000000
H	-3.906000000	-8.945000000	-6.835000000
P	-0.784000000	-9.756000000	-2.813000000
C	0.955000000	-7.913000000	-3.651000000
O	0.028000000	-8.314000000	-2.621000000
C	2.360000000	-7.765000000	-3.058000000
O	2.559000000	-6.369000000	-2.687000000
C	2.640000000	-8.586000000	-1.782000000
O	3.900000000	-9.234000000	-2.037000000
C	2.771000000	-7.560000000	-0.638000000
C	2.541000000	-6.186000000	-1.275000000
N	1.222000000	-5.557000000	-0.898000000
C	1.149000000	-4.107000000	-0.856000000
O	2.187000000	-3.462000000	-1.034000000
N	-0.052000000	-3.490000000	-0.574000000
C	-1.192000000	-4.243000000	-0.365000000
N	-2.348000000	-3.573000000	-0.123000000
C	-1.134000000	-5.678000000	-0.440000000
C	0.058000000	-6.296000000	-0.713000000
O	0.127000000	-10.839000000	-3.328000000
O	-1.568000000	-9.904000000	-1.538000000
H	4.133000000	-9.835000000	-1.288000000
H	-2.034000000	-6.266000000	-0.265000000
H	0.134000000	-7.397000000	-0.794000000
H	3.342000000	-5.429000000	-1.075000000
H	2.093000000	-7.791000000	0.203000000
H	1.892000000	-9.373000000	-1.562000000
H	3.144000000	-7.920000000	-3.844000000
H	-3.213000000	-4.065000000	0.069000000
H	0.574000000	-6.903000000	-3.967000000
H	-2.379000000	-2.539000000	-0.063000000
H	3.778000000	-7.616000000	-0.176000000
H	0.959000000	-8.599000000	-4.523000000
O	1.144000000	6.050000000	-19.787000000
O	-1.864000000	4.813000000	2.724000000
H	0.822000000	6.012000000	-20.729000000
H	-1.866000000	4.677000000	3.713000000
N	1.833000000	-6.546000000	-6.433000000
N	-1.063000000	-8.051000000	-8.833000000
N	-0.704000000	-5.598000000	-7.618000000
N	1.633000000	-8.917000000	-7.647000000
C	3.991000000	-10.175000000	-8.685000000
C	4.143000000	-9.097000000	-7.868000000
C	2.952000000	-8.426000000	-7.355000000
C	3.052000000	-7.237000000	-6.679000000

C	4.323000000	-6.634000000	-6.294000000
C	4.293000000	-5.465000000	-5.576000000
C	3.048000000	-4.854000000	-5.239000000
C	1.861000000	-5.393000000	-5.700000000
C	5.514000000	-7.322000000	-6.805000000
C	6.844000000	-6.679000000	-6.572000000
C	-1.980000000	-6.921000000	-9.238000000
C	-1.271000000	-5.580000000	-9.011000000
C	1.559000000	-9.929000000	-8.605000000
C	5.419000000	-8.475000000	-7.517000000
C	2.658000000	-10.600000000	-9.063000000
Pt	0.413000000	-7.308000000	-7.621000000
H	-1.594000000	-8.781000000	-8.347000000
H	-0.655000000	-8.507000000	-9.699000000
H	-1.455000000	-5.618000000	-6.901000000
H	-0.161000000	-4.738000000	-7.443000000
H	4.835000000	-10.701000000	-9.109000000
H	5.211000000	-4.971000000	-5.265000000
H	3.035000000	-3.980000000	-4.601000000
H	0.888000000	-4.926000000	-5.478000000
H	7.681000000	-7.279000000	-6.951000000
H	7.035000000	-6.486000000	-5.509000000
H	6.894000000	-5.708000000	-7.107000000
H	-2.937000000	-6.964000000	-8.655000000
H	-2.272000000	-7.034000000	-10.314000000
H	-1.987000000	-4.731000000	-9.165000000
H	-0.415000000	-5.453000000	-9.730000000
H	0.547000000	-10.197000000	-8.927000000
H	6.307000000	-8.944000000	-7.932000000
H	2.563000000	-11.437000000	-9.738000000

[Pt(en)(4,7-Me₂phen)]²⁺ systems

[Pt(en)(4,7-Me₂phen)]²⁺ minor groove
Dock_ID: 161-cl1_4,7-Me₂phen



EDA for 161-cl1_4,7-Me₂phen in kcal mol⁻¹.

Electrostatic interaction	-802.7
Orbital interaction	-94.5
Dispersion energy	-70.6
Pauli repulsion	130.5
Total Bonding Energy	-837.3

Contributions of the solvation energies for 161-cl1_4,7-Me₂phen in kcal mol⁻¹.

E _{solv} (total system)	-1737.6
E _{solv} (intercalator)	-159.3
E _{solv} (duplex DNA)	-2353.2
ΔE _{solv}	774.8
ΔE _{int} (EDA)	-837.3
ΔE _{aq}	-62.5

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 161-cl1_4,7-Me₂phen system.
([Pt(en)(4,7-Me₂phen)]²⁺ minor groove)

P	-2.59200000	5.48200000	2.70500000
C	-0.01700000	4.79000000	2.83000000
O	-0.98000000	5.84600000	2.98500000
C	0.86300000	5.01600000	1.59000000
O	0.96300000	3.73200000	0.91400000
C	0.32800000	6.01600000	0.53200000
O	1.46600000	6.77700000	0.10200000
C	-0.36700000	5.13900000	-0.51200000
C	0.21200000	3.73700000	-0.32500000
N	-0.54700000	-1.40900000	-0.36200000
C	0.61700000	-0.66000000	-0.65300000
N	1.78800000	-1.35800000	-0.91700000
N	0.67200000	0.70300000	-0.59000000
C	-0.52700000	1.30200000	-0.26900000
C	-1.75300000	0.62300000	0.00000000
C	-1.79900000	-0.80700000	-0.01600000
O	-2.74100000	-1.56400000	0.22500000
N	-2.77600000	1.56500000	0.23900000
C	-2.20400000	2.76600000	0.12800000
N	-0.81100000	2.67300000	-0.21100000
O	-3.32800000	6.40300000	3.64800000
O	-2.90000000	5.45200000	1.23100000
H	-0.52000000	-2.48100000	-0.44700000
H	-2.68800000	3.74200000	0.26300000
H	0.97100000	3.42200000	-1.09800000
H	-1.47100000	5.18300000	-0.33600000
H	2.47700000	-0.86500000	-1.50800000
H	-0.33600000	6.79700000	0.96800000
H	1.69700000	-2.36500000	-1.17700000
H	1.91400000	5.24600000	1.87900000
H	-0.48500000	3.78200000	2.79600000
H	-0.25000000	5.50200000	-1.56600000
H	0.58400000	4.85200000	3.76100000
P	2.14700000	6.69500000	-1.42400000
C	3.53800000	4.51500000	-0.82400000
O	2.53800000	5.10000000	-1.68700000
C	4.45200000	3.63000000	-1.67500000
O	3.79700000	2.34100000	-1.86100000
C	4.80800000	4.17200000	-3.08100000
O	6.24100000	4.29600000	-3.04400000
C	4.32800000	3.09900000	-4.06600000
C	3.55700000	2.06500000	-3.25300000
N	2.08500000	2.10800000	-3.50900000
C	1.39300000	0.85500000	-3.51500000

O	1.98700000	-0.21200000	-3.47100000
N	-0.00900000	0.91300000	-3.60800000
C	-0.77300000	2.10800000	-3.59000000
O	-1.99400000	1.99600000	-3.48600000
C	0.00800000	3.34300000	-3.67000000
C	1.36700000	3.31500000	-3.57900000
C	-0.73700000	4.61600000	-3.86000000
O	3.38300000	7.54000000	-1.24400000
O	1.11700000	6.97900000	-2.48500000
H	-0.50800000	-0.03400000	-3.62400000
H	1.96800000	4.24100000	-3.55600000
H	3.90200000	1.00300000	-3.39100000
H	3.73300000	3.56100000	-4.87900000
H	4.37400000	5.17600000	-3.28000000
H	5.37600000	3.37700000	-1.09900000
H	2.97600000	3.89400000	-0.08800000
H	-0.69200000	4.95800000	-4.90500000
H	-1.79800000	4.51800000	-3.58800000
H	-0.32400000	5.43400000	-3.23600000
H	5.18400000	2.59500000	-4.57900000
H	4.13100000	5.27800000	-0.28700000
P	7.05300000	4.73100000	-4.44700000
C	7.81300000	2.23400000	-4.40000000
O	7.21500000	3.26300000	-5.22700000
C	7.91500000	0.96300000	-5.24100000
O	6.60500000	0.36600000	-5.39700000
C	8.50800000	1.14700000	-6.66300000
O	9.57800000	0.17800000	-6.64800000
C	7.36400000	0.84500000	-7.63200000
C	6.20400000	0.31700000	-6.78300000
N	4.94500000	1.11100000	-6.89800000
C	3.68600000	0.38400000	-6.70400000
O	3.74500000	-0.81900000	-6.50200000
N	2.50400000	1.09900000	-6.76000000
C	2.50300000	2.45200000	-6.98800000
N	1.29400000	3.07700000	-7.02700000
C	3.74000000	3.16100000	-7.20700000
C	4.92700000	2.48100000	-7.13700000
O	8.38300000	5.20300000	-3.90800000
O	6.21800000	5.57800000	-5.36400000
H	3.72700000	4.22800000	-7.41300000
H	5.90000000	2.98900000	-7.25500000
H	5.94800000	-0.76900000	-6.97000000
H	7.11700000	1.74900000	-8.22500000
H	8.96500000	2.14700000	-6.82300000
H	8.49200000	0.18800000	-4.67300000
H	1.23200000	4.08400000	-7.06400000
H	7.16600000	2.05300000	-3.51400000
H	0.41900000	2.56000000	-6.80400000
H	7.62700000	0.08100000	-8.40400000

H	8.82300000	2.55500000	-4.07100000
P	10.31500000	-0.37900000	-8.03100000
C	8.54600000	-2.32600000	-7.81000000
O	9.16400000	-1.37200000	-8.71200000
C	7.40700000	-2.97600000	-8.59900000
O	6.28000000	-2.06200000	-8.60800000
C	7.76500000	-3.28300000	-10.08300000
O	7.61200000	-4.69500000	-10.25100000
C	6.87000000	-2.35300000	-10.91000000
C	5.73600000	-1.97000000	-9.95600000
N	1.39900000	0.81200000	-9.92800000
C	1.60700000	-0.56700000	-9.70000000
N	0.50500000	-1.35700000	-9.43400000
N	2.84100000	-1.15000000	-9.70300000
C	3.86800000	-0.28400000	-9.97500000
C	3.75300000	1.12100000	-10.22000000
C	2.46300000	1.74500000	-10.14800000
O	2.15600000	2.93100000	-10.25700000
N	5.02200000	1.65300000	-10.51400000
C	5.88200000	0.63000000	-10.44400000
N	5.22900000	-0.59700000	-10.09900000
O	11.45900000	-1.18800000	-7.46500000
O	10.54800000	0.69900000	-9.05600000
H	0.39800000	1.19700000	-9.87300000
H	6.95100000	0.67200000	-10.62100000
H	4.84800000	-2.67500000	-9.98600000
H	7.45800000	-1.48000000	-11.25300000
H	0.63300000	-2.36600000	-9.52500000
H	8.84600000	-3.12900000	-10.30100000
H	-0.44700000	-1.00400000	-9.66500000
H	7.03800000	-3.88900000	-8.06900000
H	8.15600000	-1.80500000	-6.90900000
H	6.49200000	-2.81600000	-11.84700000
H	9.29500000	-3.08400000	-7.51200000
P	6.33400000	-5.42400000	-11.05200000
C	4.26700000	-5.06300000	-9.32200000
O	4.97000000	-4.66200000	-10.51700000
C	2.91100000	-5.67200000	-9.67200000
O	2.00900000	-4.67100000	-10.23900000
C	2.97600000	-6.79600000	-10.73700000
O	1.89400000	-7.65800000	-10.32800000
C	2.72600000	-6.06300000	-12.06700000
C	1.93900000	-4.80700000	-11.66500000
N	0.65200000	0.05600000	-12.99500000
C	-0.11500000	-0.99300000	-12.55600000
N	0.31200000	-2.25000000	-12.28500000
C	1.66600000	-2.42000000	-12.48500000
C	2.55700000	-1.40300000	-12.96900000
C	2.00800000	-0.11100000	-13.21800000
N	2.73100000	0.95400000	-13.67200000

N	3.86200000	-1.92400000	-13.06900000
C	3.78400000	-3.19000000	-12.64000000
N	2.45000000	-3.56300000	-12.28700000
O	6.47800000	-6.87900000	-10.72800000
O	6.34300000	-4.96000000	-12.50200000
H	-1.18500000	-0.75900000	-12.37800000
H	4.62200000	-3.89900000	-12.56600000
H	0.83200000	-4.87100000	-11.88200000
H	3.69000000	-5.83200000	-12.56100000
H	3.90600000	-7.40400000	-10.70300000
H	2.35800000	-6.00200000	-8.74200000
H	4.12800000	-4.10000000	-8.77500000
H	2.32800000	1.90800000	-13.64900000
H	3.74300000	0.89100000	-13.70100000
H	2.18200000	-6.66200000	-12.82100000
H	4.86200000	-5.76400000	-8.70500000
P	1.13200000	-8.69400000	-11.34900000
C	-0.76700000	-6.88300000	-11.75000000
O	0.26600000	-7.66200000	-12.36500000
C	-2.03500000	-6.96700000	-12.60800000
O	-2.32400000	-5.60600000	-13.04600000
C	-1.93500000	-7.83500000	-13.88400000
O	-2.99700000	-8.79300000	-13.75600000
C	-2.19200000	-6.87500000	-15.05900000
C	-2.18400000	-5.46600000	-14.46900000
N	-0.91000000	-4.72100000	-14.74300000
C	-0.98400000	-3.30000000	-15.03600000
O	-2.07000000	-2.72800000	-14.89000000
N	0.13700000	-2.64500000	-15.49100000
C	1.34700000	-3.30600000	-15.59200000
N	2.39400000	-2.61400000	-16.09900000
C	1.45500000	-4.68200000	-15.16400000
C	0.33700000	-5.35300000	-14.75800000
O	0.19200000	-9.39100000	-10.38400000
O	1.98600000	-9.44300000	-12.33300000
H	-2.99600000	-9.41500000	-14.52400000
H	2.42600000	-5.17600000	-15.17900000
H	0.37900000	-6.40500000	-14.41900000
H	-3.04200000	-4.81300000	-14.77000000
H	-1.48000000	-7.02300000	-15.89300000
H	-0.97400000	-8.38900000	-13.98100000
H	-2.92900000	-7.24500000	-12.00100000
H	3.32300000	-3.01900000	-16.15800000
H	-0.38700000	-5.82700000	-11.73100000
H	2.30900000	-1.61600000	-16.36300000
H	-3.17600000	-7.09300000	-15.52700000
H	-0.98800000	-7.20800000	-10.70700000
P	1.33400000	6.40900000	-20.01800000
C	-1.19500000	6.42100000	-19.21900000
O	0.17800000	6.69600000	-18.85900000

C	-2.00000000	6.57000000	-17.92300000
O	-2.04600000	5.28400000	-17.24400000
C	-1.36500000	7.56100000	-16.90900000
O	-2.44400000	8.31400000	-16.34300000
C	-0.55000000	6.66900000	-15.96600000
C	-1.11900000	5.25700000	-16.13600000
N	0.00500000	0.17100000	-16.04100000
C	-1.15300000	0.85700000	-15.60300000
N	-2.18500000	0.10800000	-15.07300000
N	-1.32600000	2.20900000	-15.73200000
C	-0.24500000	2.86500000	-16.27600000
C	0.96600000	2.25100000	-16.72500000
C	1.13800000	0.83500000	-16.60800000
O	2.09700000	0.12900000	-16.92900000
N	1.85500000	3.24300000	-17.18600000
C	1.22000000	4.40900000	-17.03900000
N	-0.08100000	4.24400000	-16.44800000
O	1.13000000	7.30000000	-21.22000000
O	2.61600000	6.39400000	-19.22900000
H	0.07300000	-0.88800000	-15.88500000
H	1.59800000	5.39600000	-17.31300000
H	-1.74400000	4.88200000	-15.27700000
H	0.52100000	6.73900000	-16.25500000
H	-2.79200000	0.57900000	-14.38500000
H	-0.74700000	8.34100000	-17.40900000
H	-2.04600000	-0.91100000	-14.92300000
H	-3.06900000	6.79300000	-18.13700000
H	-1.28900000	5.38700000	-19.61300000
H	-0.56500000	7.00400000	-14.89700000
H	-1.52800000	7.15000000	-19.98200000
P	-2.94000000	8.20100000	-14.74800000
C	-4.40200000	6.02400000	-15.16000000
O	-3.27200000	6.60000000	-14.47000000
C	-5.14300000	5.12300000	-14.16700000
O	-4.31000000	3.98300000	-13.83900000
C	-5.49800000	5.79200000	-12.81100000
O	-6.81200000	5.31500000	-12.48800000
C	-4.36000000	5.37500000	-11.87400000
C	-3.79500000	4.09300000	-12.49200000
N	-2.30500000	4.04600000	-12.57400000
C	-1.73700000	2.74400000	-12.76800000
O	-2.42800000	1.73600000	-12.73500000
N	-0.33800000	2.69600000	-12.89300000
C	0.49800000	3.83000000	-13.06600000
O	1.67000000	3.62400000	-13.37700000
C	-0.15900000	5.12100000	-12.86900000
C	-1.50700000	5.19600000	-12.68600000
C	0.68700000	6.34500000	-12.88100000
O	-4.19100000	9.04300000	-14.76600000
O	-1.79400000	8.46900000	-13.80700000

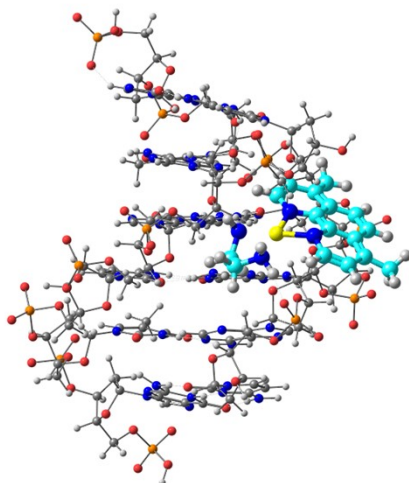
H	0.08000000	1.71000000	-12.97900000
H	-2.03500000	6.16600000	-12.59300000
H	-4.13300000	3.13900000	-11.99200000
H	-3.61100000	6.20000000	-11.83100000
H	-5.62900000	6.89400000	-12.88300000
H	-6.03900000	4.67100000	-14.65300000
H	-3.96700000	5.41700000	-15.98700000
H	0.96400000	6.65300000	-11.86200000
H	1.62100000	6.19600000	-13.44200000
H	0.15900000	7.20000000	-13.34900000
H	-4.67200000	5.23300000	-10.81700000
H	-5.08100000	6.78700000	-15.58400000
P	-7.18800000	4.38100000	-11.15100000
C	-6.47000000	2.03700000	-12.19800000
O	-6.20100000	3.04500000	-11.20000000
C	-6.48300000	0.66400000	-11.52100000
O	-5.12500000	0.23300000	-11.23900000
C	-7.23500000	0.60200000	-10.16500000
O	-7.93300000	-0.65600000	-10.25200000
C	-6.13100000	0.71000000	-9.10700000
C	-4.83300000	0.31200000	-9.82400000
N	-3.70900000	1.27400000	-9.65300000
C	-2.34300000	0.77900000	-9.80200000
O	-2.16100000	-0.42800000	-9.95600000
N	-1.30800000	1.68900000	-9.75300000
C	-1.54300000	3.02800000	-9.55500000
N	-0.47300000	3.86800000	-9.59400000
C	-2.88500000	3.51200000	-9.34500000
C	-3.92800000	2.63200000	-9.44500000
O	-8.62500000	4.02800000	-11.43800000
O	-6.75600000	5.06900000	-9.88300000
H	-3.06300000	4.56800000	-9.15600000
H	-4.98100000	2.96400000	-9.34700000
H	-4.45800000	-0.72000000	-9.56200000
H	-6.11200000	1.75300000	-8.71500000
H	-8.02700000	1.37200000	-10.05100000
H	-6.85600000	-0.11200000	-12.23100000
H	-0.58500000	4.86700000	-9.48400000
H	-5.61500000	2.10500000	-12.91200000
H	0.47800000	3.52000000	-9.82300000
H	-6.29400000	0.08900000	-8.20200000
H	-7.41700000	2.21400000	-12.74000000
P	-8.16800000	-1.66800000	-8.95400000
C	-5.85600000	-2.94300000	-9.29300000
O	-6.62600000	-2.06700000	-8.44900000
C	-5.48100000	-4.21200000	-8.51400000
O	-4.06300000	-4.13700000	-8.18500000
C	-6.22800000	-4.41300000	-7.16800000
O	-6.67000000	-5.78000000	-7.25800000
C	-5.18300000	-4.14200000	-6.07600000

C	-3.87200000	-3.81000000	-6.79200000
N	0.02800000	-0.32700000	-6.56200000
C	0.09800000	-1.73700000	-6.64500000
N	1.33400000	-2.31400000	-6.55700000
N	-1.01500000	-2.55000000	-6.72000000
C	-2.20400000	-1.85900000	-6.70000000
C	-2.35800000	-0.43900000	-6.62400000
C	-1.20200000	0.40900000	-6.59300000
O	-1.12300000	1.63400000	-6.56900000
N	-3.72300000	-0.09900000	-6.62900000
C	-4.39100000	-1.25100000	-6.67700000
N	-3.50600000	-2.38600000	-6.70100000
O	-8.86800000	-2.84000000	-9.59000000
O	-8.73500000	-0.92800000	-7.77100000
H	0.94200000	0.23300000	-6.56900000
H	-5.46900000	-1.38400000	-6.72200000
H	-2.99900000	-4.43700000	-6.48000000
H	-5.52400000	-3.35000000	-5.38100000
H	1.47900000	-3.28200000	-6.81800000
H	-7.13300000	-3.78000000	-7.05400000
H	2.20200000	-1.74000000	-6.49500000
H	-5.54400000	-5.12300000	-9.15400000
H	-4.93600000	-2.35100000	-9.53200000
H	-5.02700000	-5.02800000	-5.41900000
H	-6.37800000	-3.20000000	-10.23400000
P	-7.19600000	-6.61100000	-5.90600000
C	-4.79700000	-7.61600000	-6.18100000
O	-5.74100000	-7.07500000	-5.22500000
C	-3.55300000	-8.02400000	-5.39300000
O	-2.77900000	-6.83900000	-5.06300000
C	-3.85400000	-8.75700000	-4.05900000
O	-3.08400000	-9.96300000	-4.10500000
C	-3.52800000	-7.74400000	-2.95800000
C	-2.67900000	-6.66000000	-3.62400000
N	-1.24400000	-1.65000000	-3.48900000
C	-0.52500000	-2.79000000	-3.72200000
N	-1.00400000	-4.06100000	-3.76500000
C	-2.34400000	-4.14200000	-3.46900000
C	-3.20100000	-3.02500000	-3.19400000
C	-2.61100000	-1.72100000	-3.25000000
N	-3.29500000	-0.55900000	-3.10800000
N	-4.50300000	-3.48000000	-2.92000000
C	-4.46200000	-4.81500000	-3.03000000
N	-3.14900000	-5.28800000	-3.35300000
O	-7.90800000	-7.79300000	-6.51800000
O	-7.85000000	-5.73200000	-4.87800000
H	0.56100000	-2.64300000	-3.90300000
H	-5.29600000	-5.50000000	-2.90500000
H	-1.57500000	-6.72300000	-3.40800000
H	-4.47400000	-7.35700000	-2.52300000

H	-4.90400000	-9.12700000	-3.99800000
H	-2.86700000	-8.62400000	-6.04000000
H	-4.54600000	-6.83400000	-6.93200000
H	-2.82200000	0.36000000	-3.20300000
H	-4.28500000	-0.55900000	-2.89800000
H	-3.01700000	-8.18900000	-2.07600000
H	-5.23300000	-8.50200000	-6.68700000
P	-1.74200000	-10.26500000	-3.15100000
C	0.07100000	-8.78400000	-4.42500000
O	-0.80500000	-8.89700000	-3.28000000
C	1.46700000	-8.40100000	-3.93100000
O	1.41500000	-6.99200000	-3.56100000
C	1.99700000	-9.16800000	-2.70100000
O	3.10900000	-9.93300000	-3.19600000
C	2.47200000	-8.08800000	-1.71100000
C	1.92700000	-6.76400000	-2.24800000
N	0.77200000	-6.23400000	-1.43900000
C	0.72200000	-4.80500000	-1.17600000
O	1.73500000	-4.14000000	-1.40600000
N	-0.42500000	-4.25200000	-0.64900000
C	-1.52100000	-5.04700000	-0.37500000
N	-2.65200000	-4.42400000	0.04300000
C	-1.45000000	-6.47200000	-0.56500000
C	-0.32500000	-7.02600000	-1.11900000
O	-1.11300000	-11.43300000	-3.86700000
O	-2.13400000	-10.30200000	-1.70000000
H	3.42400000	-10.56100000	-2.50300000
H	-2.28600000	-7.10000000	-0.26600000
H	-0.25800000	-8.10500000	-1.34600000
H	2.68100000	-5.94000000	-2.35900000
H	2.16800000	-8.31000000	-0.67400000
H	1.26700000	-9.86800000	-2.24900000
H	2.20800000	-8.43200000	-4.78200000
H	-3.48100000	-4.94600000	0.29900000
H	-0.35300000	-7.94600000	-5.03200000
H	-2.70800000	-3.39300000	0.11000000
H	3.58100000	-8.07200000	-1.66700000
H	0.11500000	-9.71400000	-5.02400000
O	1.00200000	4.84200000	-20.49400000
O	-2.70700000	3.90300000	3.22300000
H	0.56400000	4.74500000	-21.38500000
H	-2.74500000	3.76700000	4.21200000
N	2.46700000	-5.93400000	-5.93800000
N	-0.29700000	-8.10100000	-7.94900000
N	-0.44600000	-5.73200000	-6.57200000
N	2.67100000	-8.25900000	-7.20200000
C	5.15400000	-9.07700000	-8.35700000
C	5.15600000	-7.98100000	-7.53500000
C	3.88700000	-7.53300000	-6.96600000
C	3.78300000	-6.35000000	-6.28800000

C	4.92200000	-5.48800000	-5.99000000
C	4.69200000	-4.31800000	-5.30300000
C	3.38000000	-4.05600000	-4.77000000
C	2.31400000	-4.86800000	-5.09900000
C	5.73300000	-3.26600000	-5.10700000
C	6.19200000	-5.96800000	-6.52900000
C	-1.46900000	-7.19800000	-8.26000000
C	-1.10000000	-5.74500000	-7.92700000
C	2.72700000	-9.30400000	-8.09900000
C	6.30200000	-7.11900000	-7.23100000
C	6.39100000	-9.55800000	-9.04100000
C	3.90800000	-9.76600000	-8.62400000
Pt	1.11100000	-7.03100000	-6.87900000
H	-0.61500000	-8.92300000	-7.42500000
H	0.10500000	-8.46500000	-8.85800000
H	-1.09500000	-6.06400000	-5.84000000
H	-0.18000000	-4.76700000	-6.31000000
H	3.22900000	-3.17700000	-4.15600000
H	1.30100000	-4.69800000	-4.70700000
H	6.73100000	-3.56800000	-5.44000000
H	5.80500000	-2.93700000	-4.06500000
H	5.44500000	-2.36500000	-5.69200000
H	7.07000000	-5.35100000	-6.33600000
H	-2.36900000	-7.52300000	-7.69300000
H	-1.73900000	-7.28700000	-9.34400000
H	-2.00300000	-5.08900000	-7.97300000
H	-0.35900000	-5.34500000	-8.67000000
H	1.76900000	-9.78300000	-8.33600000
H	7.25800000	-7.43500000	-7.64100000
H	6.24000000	-10.47600000	-9.61500000
H	7.21800000	-9.73600000	-8.34400000
H	6.73000000	-8.77900000	-9.75200000
H	3.92300000	-10.62200000	-9.27900000

[Pt(en)(4,7-Me₂phen)]²⁺ minor groove
Dock_ID: 166-cl2_4,7-Me₂phen



EDA for 166-cl2_4,7-Me₂phen in kcal mol⁻¹.

Electrostatic interaction	-810.4
Orbital interaction	-99.0
Dispersion energy	-71.1
Pauli repulsion	141.4
Total Bonding Energy	-839.1

Contributions of the solvation energies for 166-cl2_4,7-Me₂phen in kcal mol⁻¹.

E _{solv} (total system)	-1730.2
E _{solv} (intercalator)	-159.1
E _{solv} (duplex DNA)	-2349.4
ΔE _{solv}	778.3
ΔE _{int} (EDA)	-839.1
ΔE _{aq}	-60.8

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 166-cl2_4,7-Me₂phen system.
([Pt(en)(4,7-Me₂phen)]²⁺ minor groove)

P	-1.35700000	7.33900000	2.49400000
C	1.19600000	6.95000000	1.94000000
O	-0.12500000	7.16700000	1.39000000
C	2.16400000	6.98900000	0.75300000
O	2.38400000	5.63000000	0.27700000
C	1.64300000	7.79200000	-0.46900000
O	2.76000000	8.57800000	-0.90600000
C	1.10400000	6.72800000	-1.43300000
C	1.64600000	5.38200000	-0.93400000
N	0.23600000	0.34500000	-0.79900000
C	1.47400000	0.92800000	-1.16400000
N	2.47400000	0.08900000	-1.58200000
N	1.73000000	2.27500000	-1.08600000
C	0.65200000	3.02900000	-0.68600000
C	-0.63100000	2.51800000	-0.31100000
C	-0.88700000	1.11000000	-0.35600000
O	-1.91400000	0.48800000	-0.07800000
N	-1.49000000	3.58700000	0.01600000
C	-0.77700000	4.70100000	-0.15400000
N	0.55700000	4.42300000	-0.61900000
O	-1.01300000	8.35400000	3.55700000
O	-2.59300000	7.44300000	1.64000000
H	0.11100000	-0.71500000	-0.91000000
H	-1.10400000	5.72600000	0.02000000
H	2.39700000	4.87500000	-1.60800000
H	-0.00700000	6.77600000	-1.43400000
H	3.22200000	0.48000000	-2.16500000
H	0.87400000	8.54800000	-0.18600000
H	2.30400000	-0.93300000	-1.66700000
H	3.17900000	7.31500000	1.07700000
H	1.22800000	5.95500000	2.43200000
H	1.37400000	6.90600000	-2.49800000
H	1.44000000	7.74100000	2.67500000
P	3.37300000	8.54900000	-2.46300000
C	4.80700000	6.41900000	-1.84900000
O	3.79900000	6.96700000	-2.73000000
C	5.41400000	5.22900000	-2.59200000
O	4.40600000	4.18500000	-2.70500000
C	5.87700000	5.55900000	-4.03900000
O	7.10300000	4.81800000	-4.16200000
C	4.71600000	5.07900000	-4.91400000
C	4.08600000	3.94600000	-4.10100000
N	2.60700000	3.85600000	-4.19500000
C	2.04100000	2.54600000	-4.03100000
O	2.74900000	1.55200000	-4.01500000
N	0.63800000	2.48400000	-3.97700000

C	-0.21600000	3.61500000	-3.90400000
O	-1.39600000	3.41900000	-3.63000000
C	0.43100000	4.90400000	-4.17000000
C	1.78600000	4.99700000	-4.23800000
C	-0.46100000	6.08300000	-4.34100000
O	4.57800000	9.44600000	-2.32300000
O	2.29800000	8.79300000	-3.48600000
H	0.21400000	1.49900000	-3.87300000
H	2.31600000	5.96300000	-4.35700000
H	4.51600000	2.92300000	-4.33100000
H	4.01500000	5.93300000	-5.06900000
H	6.13500000	6.62900000	-4.19000000
H	6.22900000	4.76100000	-1.99200000
H	4.29800000	6.08500000	-0.91900000
H	-1.21500000	5.90300000	-5.12400000
H	-1.01600000	6.31000000	-3.41700000
H	0.08500000	6.99600000	-4.62000000
H	5.01000000	4.75700000	-5.93200000
H	5.58400000	7.16700000	-1.59700000
P	7.62000000	4.16200000	-5.60800000
C	6.63400000	1.80300000	-4.91500000
O	6.57200000	2.89200000	-5.86200000
C	6.70500000	0.47600000	-5.67600000
O	5.35400000	0.02300000	-5.95200000
C	7.40800000	0.53800000	-7.05800000
O	8.14200000	-0.69800000	-7.12800000
C	6.26300000	0.74400000	-8.05800000
C	4.99700000	0.26900000	-7.33000000
N	3.87300000	1.25000000	-7.32400000
C	2.52500000	0.72100000	-7.13500000
O	2.38700000	-0.49500000	-7.02100000
N	1.47000000	1.60900000	-7.10400000
C	1.67500000	2.96000000	-7.23700000
N	0.57800000	3.77000000	-7.18400000
C	3.00400000	3.48600000	-7.41300000
C	4.06600000	2.62000000	-7.41700000
O	9.00000000	3.67400000	-5.24900000
O	7.36100000	5.07700000	-6.77400000
H	3.15900000	4.55800000	-7.51500000
H	5.11100000	2.97500000	-7.51300000
H	4.59100000	-0.72200000	-7.69000000
H	6.22900000	1.82000000	-8.34100000
H	8.19500000	1.32000000	-7.12700000
H	7.12300000	-0.33100000	-5.03100000
H	0.67600000	4.77600000	-7.17100000
H	5.66300000	1.86100000	-4.35500000
H	-0.36500000	3.38500000	-6.96900000
H	6.39700000	0.21700000	-9.02500000
H	7.47600000	1.89800000	-4.20500000
P	7.99300000	-1.79800000	-8.36800000

C	5.74500000	-2.99200000	-7.54000000
O	6.36300000	-2.12000000	-8.50300000
C	5.26500000	-4.28000000	-8.22200000
O	3.87700000	-4.11900000	-8.63100000
C	6.04300000	-4.67700000	-9.50300000
O	6.28400000	-6.08100000	-9.28500000
C	5.09900000	-4.35800000	-10.67300000
C	3.77400000	-3.90200000	-10.05500000
N	0.04500000	-0.22900000	-10.27500000
C	-0.09600000	-1.63200000	-10.19500000
N	-1.36700000	-2.13700000	-10.29500000
N	0.97400000	-2.50200000	-10.13600000
C	2.19900000	-1.88000000	-10.21100000
C	2.42200000	-0.47000000	-10.32100000
C	1.31500000	0.43800000	-10.29000000
O	1.29900000	1.66700000	-10.28500000
N	3.80100000	-0.20100000	-10.40600000
C	4.41000000	-1.38600000	-10.37000000
N	3.47200000	-2.47400000	-10.26700000
O	8.75200000	-2.98700000	-7.84000000
O	8.31300000	-1.15000000	-9.69100000
H	-0.83800000	0.38000000	-10.25100000
H	5.48000000	-1.57200000	-10.39000000
H	2.89300000	-4.51300000	-10.37600000
H	5.55100000	-3.61400000	-11.35700000
H	-1.56800000	-3.09000000	-10.01100000
H	7.03200000	-4.18600000	-9.60700000
H	-2.19900000	-1.50700000	-10.28300000
H	5.21400000	-5.12700000	-7.49600000
H	4.86700000	-2.39800000	-7.18200000
H	4.91200000	-5.24900000	-11.31800000
H	6.40700000	-3.22400000	-6.68600000
P	6.87300000	-7.04100000	-10.51900000
C	4.36400000	-7.78700000	-10.52100000
O	5.46200000	-7.35800000	-11.35800000
C	3.14400000	-7.88800000	-11.43400000
O	2.63500000	-6.55100000	-11.69000000
C	3.44600000	-8.54400000	-12.81100000
O	2.62000000	-9.71200000	-12.85000000
C	3.20600000	-7.44300000	-13.84700000
C	2.39900000	-6.36500000	-13.12200000
N	0.78500000	-1.40200000	-13.37100000
C	0.10100000	-2.57100000	-13.16200000
N	0.62000000	-3.82500000	-13.10600000
C	1.97300000	-3.86700000	-13.33600000
C	2.79900000	-2.72400000	-13.58700000
C	2.16000000	-1.44200000	-13.58200000
N	2.81200000	-0.27500000	-13.81200000
N	4.12900000	-3.13300000	-13.79600000
C	4.13000000	-4.46800000	-13.67700000

N	2.82500000	-4.98500000	-13.39500000
O	7.35300000	-8.26700000	-9.78200000
O	7.75100000	-6.29500000	-11.48400000
H	-0.99300000	-2.47000000	-13.00600000
H	4.99000000	-5.12100000	-13.77800000
H	1.28200000	-6.44500000	-13.26400000
H	4.18100000	-7.07700000	-14.23100000
H	4.47700000	-8.96300000	-12.87400000
H	2.30900000	-8.42000000	-10.91700000
H	4.18200000	-7.04500000	-9.70800000
H	2.33100000	0.63000000	-13.68300000
H	3.82400000	-0.25100000	-13.87300000
H	2.69300000	-7.80200000	-14.76500000
H	4.59800000	-8.78000000	-10.08300000
P	1.27000000	-9.87900000	-13.82100000
C	-0.54200000	-8.34300000	-12.58100000
O	0.44900000	-8.44900000	-13.62700000
C	-1.92600000	-8.14600000	-13.20200000
O	-2.04200000	-6.74900000	-13.60100000
C	-2.26600000	-8.98600000	-14.45200000
O	-3.45600000	-9.71300000	-14.08700000
C	-2.56900000	-7.97800000	-15.57700000
C	-2.24400000	-6.59700000	-14.99900000
N	-0.99100000	-5.99300000	-15.58900000
C	-0.95000000	-4.55400000	-15.78600000
O	-1.98600000	-3.90800000	-15.60600000
N	0.21800000	-3.95400000	-16.21400000
C	1.34300000	-4.71600000	-16.45600000
N	2.46700000	-4.06400000	-16.85500000
C	1.30300000	-6.14200000	-16.28400000
C	0.15300000	-6.74100000	-15.83500000
O	0.54400000	-11.03400000	-13.18100000
O	1.67600000	-9.86900000	-15.27000000
H	-3.71600000	-10.32900000	-14.81200000
H	2.17800000	-6.74400000	-16.52200000
H	0.10500000	-7.83000000	-15.65200000
H	-3.05800000	-5.83200000	-15.09000000
H	-2.02700000	-8.21700000	-16.50800000
H	-1.49800000	-9.72600000	-14.74300000
H	-2.72100000	-8.25400000	-12.41100000
H	3.33600000	-4.56100000	-17.01000000
H	-0.24500000	-7.41000000	-12.02400000
H	2.50900000	-3.03000000	-16.90100000
H	-3.63700000	-8.03800000	-15.87100000
H	-0.54000000	-9.20900000	-11.89200000
P	2.15300000	5.76800000	-19.45200000
C	-0.49900000	5.38700000	-19.51000000
O	0.58000000	6.33000000	-19.59900000
C	-1.21500000	5.46600000	-18.15400000
O	-1.22300000	4.12300000	-17.59500000

C	-0.58000000	6.39200000	-17.08500000
O	-1.64600000	7.19900000	-16.57100000
C	0.13100000	5.44700000	-16.11200000
C	-0.45400000	4.05700000	-16.36800000
N	0.36300000	-1.09800000	-16.47900000
C	-0.80500000	-0.37100000	-16.14300000
N	-1.93500000	-1.09600000	-15.81600000
N	-0.89000000	0.99300000	-16.19600000
C	0.29400000	1.62000000	-16.52200000
C	1.52400000	0.96100000	-16.82600000
C	1.59700000	-0.46800000	-16.83700000
O	2.54500000	-1.20800000	-17.10700000
N	2.53400000	1.92000000	-17.04800000
C	1.95000000	3.11100000	-16.90200000
N	0.56000000	2.99500000	-16.55700000
O	2.91200000	6.53500000	-20.50700000
O	2.58200000	5.78300000	-18.01000000
H	0.34400000	-2.17000000	-16.41400000
H	2.42100000	4.09600000	-17.01800000
H	-1.19700000	3.70900000	-15.59700000
H	1.23100000	5.49900000	-16.30800000
H	-2.59300000	-0.64600000	-15.15900000
H	0.10000000	7.15800000	-17.52600000
H	-1.84600000	-2.12700000	-15.68600000
H	-2.29600000	5.69600000	-18.30400000
H	-0.17400000	4.34300000	-19.71600000
H	0.03200000	5.74700000	-15.03800000
H	-1.17200000	5.70400000	-20.33300000
P	-2.35200000	7.01700000	-15.06500000
C	-3.76300000	4.90000000	-15.83000000
O	-2.75400000	5.40800000	-14.93100000
C	-4.80100000	4.12100000	-15.02200000
O	-4.28800000	2.78600000	-14.75200000
C	-5.19900000	4.73400000	-13.65600000
O	-6.63100000	4.83700000	-13.76900000
C	-4.72600000	3.73000000	-12.59800000
C	-4.04400000	2.58700000	-13.34900000
N	-2.56400000	2.52300000	-13.13000000
C	-1.94800000	1.23700000	-13.26500000
O	-2.62900000	0.22800000	-13.39500000
N	-0.54500000	1.19100000	-13.17800000
C	0.28500000	2.34700000	-13.16000000
O	1.49200000	2.19100000	-13.31600000
C	-0.41300000	3.62000000	-12.98200000
C	-1.77200000	3.68200000	-13.02100000
C	0.42200000	4.82900000	-12.75000000
O	-3.58000000	7.88100000	-15.19200000
O	-1.33100000	7.21800000	-13.97900000
H	-0.08700000	0.22500000	-13.23000000
H	-2.31400000	4.64100000	-12.95800000

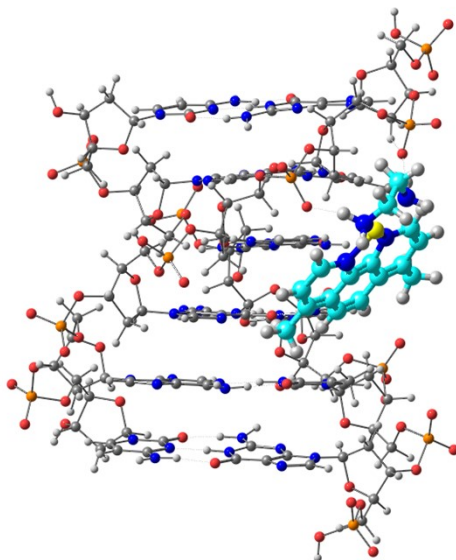
H	-4.47600000	1.57200000	-13.12800000
H	-4.08000000	4.22800000	-11.84800000
H	-4.79900000	5.75900000	-13.49900000
H	-5.70600000	3.92700000	-15.65100000
H	-3.21600000	4.21200000	-16.51800000
H	0.41500000	5.13000000	-11.69200000
H	1.47200000	4.66700000	-13.03600000
H	0.05900000	5.69900000	-13.33400000
H	-5.58000000	3.30300000	-12.01100000
H	-4.25300000	5.69700000	-16.41900000
P	-7.56800000	5.20800000	-12.43300000
C	-8.04800000	2.62800000	-12.54300000
O	-7.70400000	3.72900000	-11.66800000
C	-7.83900000	1.34400000	-11.74200000
O	-6.41400000	1.10400000	-11.59700000
C	-8.45700000	1.36000000	-10.31700000
O	-9.25700000	0.16300000	-10.33200000
C	-7.26200000	1.34100000	-9.36100000
C	-6.08900000	0.82900000	-10.20100000
N	-4.79000000	1.49500000	-9.96200000
C	-3.57700000	0.68100000	-10.11000000
O	-3.71200000	-0.51800000	-10.29900000
N	-2.35500000	1.31800000	-10.02700000
C	-2.27100000	2.66800000	-9.78600000
N	-1.03400000	3.22500000	-9.81900000
C	-3.46200000	3.44700000	-9.53600000
C	-4.68500000	2.84500000	-9.63200000
O	-8.87800000	5.60200000	-13.07000000
O	-6.86500000	6.09900000	-11.44900000
H	-3.37600000	4.49700000	-9.26100000
H	-5.62800000	3.39700000	-9.46800000
H	-5.94800000	-0.29200000	-10.13200000
H	-7.09800000	2.36100000	-8.95300000
H	-9.14300000	2.21700000	-10.14200000
H	-8.21800000	0.46700000	-12.32600000
H	-0.88600000	4.19100000	-9.56500000
H	-7.40000000	2.63100000	-13.44700000
H	-0.18500000	2.64900000	-10.00200000
H	-7.41800000	0.70500000	-8.46300000
H	-9.10900000	2.72400000	-12.84900000
P	-9.73500000	-0.61500000	-8.93500000
C	-7.68000000	-2.21000000	-9.32900000
O	-8.32400000	-1.31000000	-8.39300000
C	-6.89600000	-3.24400000	-8.51200000
O	-5.56800000	-2.71500000	-8.28700000
C	-7.48800000	-3.54900000	-7.10900000
O	-7.38300000	-4.96400000	-6.90900000
C	-6.69700000	-2.63700000	-6.16300000
C	-5.38900000	-2.34900000	-6.90300000
N	-1.20100000	0.62800000	-6.91600000

C	-1.35000000	-0.76300000	-7.12400000
N	-0.21900000	-1.51500000	-7.38400000
N	-2.55500000	-1.39400000	-7.13500000
C	-3.62400000	-0.55800000	-6.94400000
C	-3.57700000	0.86000000	-6.75500000
C	-2.30600000	1.52800000	-6.77300000
O	-2.04100000	2.72400000	-6.67100000
N	-4.88500000	1.34900000	-6.58200000
C	-5.69600000	0.28300000	-6.66000000
N	-4.97100000	-0.92800000	-6.87700000
O	-10.68600000	-1.65700000	-9.47400000
O	-10.13500000	0.35000000	-7.85100000
H	-0.21800000	1.04700000	-6.93700000
H	-6.77900000	0.28800000	-6.58400000
H	-4.50500000	-2.97000000	-6.56800000
H	-7.29400000	-1.72300000	-5.96500000
H	-0.30700000	-2.52600000	-7.28900000
H	-8.58500000	-3.37600000	-7.05400000
H	0.72000000	-1.12800000	-7.17000000
H	-6.71200000	-4.17500000	-9.10000000
H	-6.96200000	-1.58900000	-9.92400000
H	-6.52400000	-3.08000000	-5.16000000
H	-8.41100000	-2.70600000	-9.99400000
P	-6.26100000	-5.70700000	-5.90800000
C	-4.07600000	-5.40900000	-7.46900000
O	-4.77800000	-5.06700000	-6.25100000
C	-2.69300000	-5.94600000	-7.11400000
O	-1.81800000	-4.90500000	-6.57300000
C	-2.71200000	-7.04600000	-6.02200000
O	-1.57900000	-7.85400000	-6.40200000
C	-2.50200000	-6.26800000	-4.71100000
C	-1.72900000	-5.01300000	-5.14400000
N	-0.44300000	-0.13800000	-3.83300000
C	0.33000000	-1.20700000	-4.20700000
N	-0.09600000	-2.46500000	-4.48200000
C	-1.46000000	-2.62000000	-4.33700000
C	-2.35900000	-1.59100000	-3.90000000
C	-1.81300000	-0.28800000	-3.68000000
N	-2.55300000	0.80100000	-3.34700000
N	-3.67200000	-2.09800000	-3.84900000
C	-3.58900000	-3.37300000	-4.25100000
N	-2.24400000	-3.76300000	-4.54200000
O	-6.43800000	-7.16400000	-6.21000000
O	-6.44700000	-5.19300000	-4.48900000
H	1.41100000	-0.99200000	-4.31900000
H	-4.42300000	-4.07600000	-4.35100000
H	-0.62000000	-5.06400000	-4.93400000
H	-3.48400000	-6.03500000	-4.25500000
H	-3.61100000	-7.69500000	-6.04000000
H	-2.13000000	-6.27300000	-8.04100000

H	-3.99700000	-4.44400000	-8.02500000
H	-2.13200000	1.74500000	-3.32700000
H	-3.56300000	0.73600000	-3.28700000
H	-1.96400000	-6.83200000	-3.92700000
H	-4.63400000	-6.14900000	-8.08100000
P	-0.83400000	-8.90800000	-5.38300000
C	0.98300000	-7.06400000	-4.76000000
O	-0.08100000	-7.88700000	-4.27300000
C	2.13400000	-7.09600000	-3.74500000
O	2.36700000	-5.70800000	-3.36100000
C	1.86900000	-7.88300000	-2.44200000
O	2.88400000	-8.89800000	-2.41100000
C	2.07300000	-6.87400000	-1.29800000
C	2.17500000	-5.49800000	-1.95200000
N	0.93800000	-4.67000000	-1.76900000
C	1.08300000	-3.24100000	-1.56200000
O	2.20800000	-2.74200000	-1.67500000
N	-0.01900000	-2.49000000	-1.22000000
C	-1.27000000	-3.07200000	-1.14100000
N	-2.29800000	-2.29200000	-0.73200000
C	-1.44000000	-4.46500000	-1.49200000
C	-0.34600000	-5.22200000	-1.80100000
O	0.18600000	-9.51600000	-6.32800000
O	-1.70700000	-9.73400000	-4.48400000
H	2.73300000	-9.51400000	-1.65400000
H	-2.44000000	-4.89700000	-1.51100000
H	-0.43400000	-6.28700000	-2.07700000
H	3.05600000	-4.88200000	-1.63600000
H	1.28900000	-6.95200000	-0.52200000
H	0.87300000	-8.38100000	-2.41000000
H	3.09700000	-7.41100000	-4.21300000
H	-3.25300000	-2.63800000	-0.71100000
H	0.56900000	-6.02300000	-4.83500000
H	-2.17100000	-1.28500000	-0.53000000
H	3.00200000	-7.11200000	-0.73700000
H	1.35200000	-7.39300000	-5.76100000
O	2.03100000	4.16600000	-19.89400000
O	-1.38200000	5.83100000	3.21500000
H	2.03000000	3.98400000	-20.87600000
H	-0.97800000	5.77600000	4.12300000
N	-2.29300000	-6.09200000	-10.75100000
N	0.60600000	-8.03800000	-8.69000000
N	0.51400000	-5.57400000	-9.88000000
N	-2.30700000	-8.50300000	-9.63900000
C	-4.73300000	-9.46900000	-8.43500000
C	-4.81300000	-8.40700000	-9.29100000
C	-3.58100000	-7.86700000	-9.85900000
C	-3.57100000	-6.65100000	-10.48700000
C	-4.77700000	-5.90600000	-10.83100000
C	-4.63700000	-4.72000000	-11.51900000

C	-3.33300000	-4.28000000	-11.92500000
C	-2.20500000	-4.97900000	-11.53800000
C	-5.79200000	-3.83300000	-11.85600000
C	-6.01000000	-6.50600000	-10.33700000
C	1.63100000	-7.01700000	-8.24400000
C	1.07800000	-5.60600000	-8.48400000
C	-2.29100000	-9.50500000	-8.67200000
C	-6.02900000	-7.65900000	-9.63100000
C	-5.93000000	-10.01400000	-7.72900000
C	-3.42900000	-10.03900000	-8.13600000
Pt	-0.88900000	-7.07600000	-9.76100000
H	1.05000000	-8.76100000	-9.26400000
H	0.22500000	-8.52700000	-7.83400000
H	1.24500000	-5.77900000	-10.58400000
H	0.15200000	-4.63000000	-10.09600000
H	-3.24200000	-3.38600000	-12.52800000
H	-1.19400000	-4.67700000	-11.84500000
H	-5.77200000	-3.52200000	-12.90800000
H	-5.72900000	-2.91000000	-11.25200000
H	-6.76700000	-4.29500000	-11.67300000
H	-6.93800000	-5.97800000	-10.56000000
H	1.86300000	-7.16500000	-7.15700000
H	2.59800000	-7.16100000	-8.77900000
H	0.23700000	-5.38300000	-7.76900000
H	1.87300000	-4.83700000	-8.32000000
H	-1.29800000	-9.89000000	-8.41200000
H	-6.96200000	-8.06200000	-9.24300000
H	-6.72900000	-10.30900000	-8.41800000
H	-6.34500000	-9.22700000	-7.06900000
H	-5.70400000	-10.87900000	-7.09800000
H	-3.38300000	-10.86800000	-7.44600000

[Pt(en)(4,7-Me₂phen)]²⁺ major groove
Dock_ID: 189-cl3_4,7-Me₂phen



EDA for 189-cl3_4,7-Me₂phen in kcal mol⁻¹.

Electrostatic interaction	-759.4
Orbital interaction	-88.1
Dispersion energy	-55.5
Pauli repulsion	118.4
Total Bonding Energy	-784.6

Contributions of the solvation energies for 189-cl3_4,7-Me₂phen in kcal mol⁻¹.

E _{solv} (total system)	-1748.8
E _{solv} (intercalator)	-158.3
E _{solv} (duplex DNA)	-2316.31
ΔE _{solv}	725.8
ΔE _{int} (EDA)	-784.6
ΔE _{aq}	-58.76

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 189-cl3_4,7-Me₂phen system.
([Pt(en)(4,7-Me₂phen)]²⁺ major groove)

P	-1.55600000	6.81800000	2.47500000
C	1.06100000	6.46500000	2.31100000
O	-0.13600000	6.85500000	1.60300000
C	2.19300000	6.48100000	1.28100000
O	2.38200000	5.14100000	0.74800000
C	1.93000000	7.38400000	0.04500000
O	3.18800000	8.04700000	-0.16500000
C	1.44900000	6.42900000	-1.04800000
C	1.79200000	5.01900000	-0.56400000
N	0.14900000	0.07900000	-0.63400000
C	1.41400000	0.62000000	-0.97600000
N	2.39000000	-0.24200000	-1.40300000
N	1.72100000	1.95100000	-0.84400000
C	0.64700000	2.74400000	-0.51700000
C	-0.68400000	2.28900000	-0.26500000
C	-0.97700000	0.88800000	-0.27800000
O	-2.03200000	0.30500000	-0.02700000
N	-1.53100000	3.39400000	-0.03800000
C	-0.76100000	4.47700000	-0.13300000
N	0.60600000	4.14200000	-0.44600000
O	-1.50800000	7.78400000	3.63400000
O	-2.61500000	6.88000000	1.40600000
H	-0.00700000	-0.97400000	-0.73500000
H	-1.06700000	5.51600000	-0.00500000
H	2.58600000	4.48000000	-1.16200000
H	0.36100000	6.58000000	-1.21600000
H	3.16900000	0.14300000	-1.94900000
H	1.21300000	8.21100000	0.25200000
H	2.18900000	-1.25600000	-1.51700000
H	3.17100000	6.70500000	1.76900000
H	0.94000000	5.44200000	2.72900000
H	1.90100000	6.63900000	-2.04900000
H	1.26000000	7.18500000	3.12800000
P	4.01600000	8.25100000	-1.58500000
C	5.27200000	6.02900000	-0.74300000
O	5.39200000	7.34600000	-1.30500000
C	5.61200000	4.95100000	-1.77300000
O	4.39000000	4.20700000	-2.06200000
C	6.17000000	5.43600000	-3.14000000
O	7.37500000	4.65700000	-3.25000000
C	5.05500000	5.14600000	-4.14800000
C	4.30900000	3.97800000	-3.50500000
N	2.87100000	3.85100000	-3.80600000
C	2.32600000	2.51800000	-3.75200000
O	3.05800000	1.54100000	-3.73700000

N	0.92500000	2.42100000	-3.80200000
C	0.04700000	3.54000000	-3.74300000
O	-1.14600000	3.32400000	-3.57200000
C	0.68100000	4.85100000	-3.91100000
C	2.03300000	4.97900000	-3.91000000
C	-0.23300000	6.01700000	-4.06000000
O	4.51300000	9.67100000	-1.52000000
O	3.33500000	7.75300000	-2.84000000
H	0.51400000	1.42500000	-3.78800000
H	2.54800000	5.96200000	-4.00200000
H	4.80200000	2.97500000	-3.69000000
H	4.40000000	6.05300000	-4.26100000
H	6.49700000	6.50700000	-3.13500000
H	6.30200000	4.19400000	-1.32100000
H	4.27700000	5.84100000	-0.28700000
H	-0.62000000	6.08800000	-5.09100000
H	-1.09400000	5.94800000	-3.38100000
H	0.26900000	6.97300000	-3.85400000
H	5.40000000	4.95900000	-5.19300000
H	6.02500000	6.03600000	0.07500000
P	8.08300000	4.14100000	-4.66300000
C	6.49800000	2.11800000	-5.28600000
O	7.70600000	2.51000000	-4.61100000
C	6.74900000	0.70100000	-5.81900000
O	5.46200000	0.02900000	-5.86100000
C	7.29000000	0.65800000	-7.27400000
O	8.18100000	-0.46900000	-7.23300000
C	6.04200000	0.46700000	-8.14400000
C	4.91300000	0.03200000	-7.20400000
N	3.73900000	0.94600000	-7.19200000
C	2.39800000	0.38800000	-7.09600000
O	2.27600000	-0.84000000	-7.13700000
N	1.32000000	1.23900000	-6.99100000
C	1.50600000	2.60300000	-6.91900000
N	0.41500000	3.40500000	-6.82100000
C	2.83700000	3.15200000	-6.91400000
C	3.90600000	2.33000000	-7.08600000
O	9.55700000	4.18600000	-4.36200000
O	7.47000000	4.79700000	-5.87300000
H	2.97700000	4.23200000	-6.79600000
H	4.93300000	2.73100000	-7.15700000
H	4.55200000	-1.01700000	-7.36300000
H	5.80200000	1.37700000	-8.73300000
H	7.89000000	1.55000000	-7.55500000
H	7.36500000	0.09300000	-5.12100000
H	0.52300000	4.41700000	-6.79900000
H	6.22400000	2.83300000	-6.09800000
H	-0.54800000	3.02500000	-6.77900000
H	6.19500000	-0.30100000	-8.93500000
H	5.68100000	2.08400000	-4.51700000

P	8.72300000	-1.24400000	-8.61000000
C	6.85200000	-3.05400000	-8.18500000
O	7.38800000	-2.09800000	-9.12900000
C	6.35000000	-4.27100000	-8.97100000
O	4.94900000	-4.07100000	-9.30200000
C	7.06100000	-4.52500000	-10.32700000
O	7.14400000	-5.96100000	-10.39800000
C	6.16700000	-3.83000000	-11.35900000
C	4.79600000	-3.67900000	-10.68700000
N	0.62600000	-0.58000000	-10.16900000
C	0.70400000	-1.98700000	-10.17500000
N	-0.47200000	-2.70000000	-10.01100000
N	1.87700000	-2.68500000	-10.27300000
C	2.98500000	-1.88900000	-10.45600000
C	2.98900000	-0.45900000	-10.51400000
C	1.77300000	0.27600000	-10.31900000
O	1.57700000	1.48400000	-10.28000000
N	4.28700000	0.00500000	-10.78900000
C	5.05600000	-1.07900000	-10.88100000
N	4.30400000	-2.29000000	-10.69000000
O	9.76900000	-2.17200000	-8.03900000
O	9.01900000	-0.28200000	-9.72700000
H	-0.33300000	-0.10600000	-10.06600000
H	6.12700000	-1.11300000	-11.06100000
H	3.99400000	-4.36400000	-11.07300000
H	6.63000000	-2.85600000	-11.63800000
H	-0.48400000	-3.67100000	-10.31400000
H	8.11400000	-4.17200000	-10.35500000
H	-1.38000000	-2.19800000	-10.09100000
H	6.33400000	-5.18600000	-8.33300000
H	5.99700000	-2.55000000	-7.68000000
H	6.09200000	-4.35700000	-12.33000000
H	7.60200000	-3.36600000	-7.43200000
P	6.76300000	-6.84000000	-11.76400000
C	4.19900000	-6.98600000	-11.09900000
O	5.15900000	-6.50100000	-12.06400000
C	3.01200000	-7.58300000	-11.86100000
O	2.04900000	-6.53100000	-12.14700000
C	3.37200000	-8.21400000	-13.23300000
O	2.62800000	-9.44100000	-13.27400000
C	3.01700000	-7.13300000	-14.26100000
C	2.08400000	-6.15400000	-13.53600000
N	0.73900000	-1.06000000	-13.40200000
C	-0.01800000	-2.19400000	-13.25600000
N	0.40900000	-3.48200000	-13.27900000
C	1.76300000	-3.60500000	-13.50300000
C	2.65500000	-2.49400000	-13.68800000
C	2.10400000	-1.17700000	-13.62700000
N	2.83900000	-0.04600000	-13.81800000
N	3.96900000	-2.95600000	-13.88800000

C	3.89700000	-4.29100000	-13.82500000
N	2.56000000	-4.75400000	-13.61500000
O	6.94400000	-8.25500000	-11.27400000
O	7.47000000	-6.30300000	-12.98000000
H	-1.09900000	-2.02400000	-13.08300000
H	4.72800000	-4.99200000	-13.90700000
H	1.00900000	-6.18800000	-13.85600000
H	3.95600000	-6.66500000	-14.63000000
H	4.43100000	-8.54300000	-13.31200000
H	2.43400000	-8.29100000	-11.21800000
H	3.87100000	-6.08500000	-10.52600000
H	2.42100000	0.88400000	-13.63800000
H	3.85100000	-0.09800000	-13.77800000
H	2.56100000	-7.52400000	-15.19300000
H	4.63300000	-7.73400000	-10.40700000
P	1.54000000	-9.83100000	-14.47700000
C	-0.45400000	-8.42100000	-13.43400000
O	0.48200000	-8.54000000	-14.52600000
C	-1.86100000	-8.23700000	-14.00900000
O	-2.11300000	-6.80700000	-14.15400000
C	-2.11500000	-8.87200000	-15.39600000
O	-3.22000000	-9.76700000	-15.18600000
C	-2.51700000	-7.71200000	-16.32400000
C	-2.29300000	-6.42900000	-15.52600000
N	-1.07300000	-5.66600000	-15.95700000
C	-1.12200000	-4.21100000	-15.95900000
O	-2.18100000	-3.66600000	-15.63100000
N	-0.01500000	-3.49500000	-16.35400000
C	1.15200000	-4.14300000	-16.70800000
N	2.21400000	-3.37700000	-17.05900000
C	1.21200000	-5.58300000	-16.69600000
C	0.11200000	-6.30400000	-16.31900000
O	0.87300000	-11.05900000	-13.91300000
O	2.19400000	-9.81200000	-15.83100000
H	-3.39700000	-10.29600000	-16.00100000
H	2.12700000	-6.08900000	-17.00000000
H	0.13100000	-7.41000000	-16.27400000
H	-3.16000000	-5.71800000	-15.51300000
H	-1.98400000	-7.74400000	-17.29200000
H	-1.26400000	-9.45700000	-15.79700000
H	-2.63400000	-8.56200000	-13.26900000
H	3.11200000	-3.79100000	-17.29100000
H	-0.13900000	-7.50600000	-12.87700000
H	2.17700000	-2.34300000	-17.01400000
H	-3.58300000	-7.80800000	-16.62500000
H	-0.42900000	-9.29700000	-12.75600000
P	1.83200000	6.32500000	-19.59800000
C	-0.71800000	5.83200000	-19.14000000
O	0.56200000	6.14100000	-18.53900000
C	-1.76200000	5.96000000	-18.02700000

O	-2.06200000	4.63400000	-17.50400000
C	-1.31500000	6.81100000	-16.80700000
O	-2.44200000	7.65800000	-16.54400000
C	-0.94200000	5.78800000	-15.72600000
C	-1.42100000	4.42300000	-16.23200000
N	-0.10600000	-0.62000000	-16.39600000
C	-1.30700000	-0.01300000	-15.95400000
N	-2.30900000	-0.82700000	-15.50500000
N	-1.52300000	1.34500000	-15.98700000
C	-0.43000000	2.07500000	-16.38800000
C	0.83700000	1.54400000	-16.78200000
C	1.04500000	0.12800000	-16.80700000
O	2.03800000	-0.52000000	-17.13900000
N	1.72300000	2.59900000	-17.08500000
C	1.03500000	3.72500000	-16.90000000
N	-0.30500000	3.46900000	-16.43500000
O	1.48000000	7.26000000	-20.73100000
O	3.02200000	6.54400000	-18.70300000
H	-0.02500000	-1.68500000	-16.37000000
H	1.38100000	4.74400000	-17.06200000
H	-2.21800000	3.92500000	-15.60200000
H	0.15400000	5.82600000	-15.52800000
H	-3.05800000	-0.42300000	-14.93200000
H	-0.48200000	7.51000000	-17.05000000
H	-2.20600000	-1.85800000	-15.50800000
H	-2.74100000	6.29800000	-18.44000000
H	-0.69300000	4.79200000	-19.52800000
H	-1.38800000	6.00800000	-14.73000000
H	-0.93600000	6.53400000	-19.96800000
P	-3.11000000	7.90000000	-15.02900000
C	-4.47800000	5.67600000	-15.37900000
O	-3.55300000	6.37900000	-14.51800000
C	-5.05600000	4.53500000	-14.54400000
O	-4.06100000	3.47800000	-14.42200000
C	-5.46500000	4.95300000	-13.10500000
O	-6.79100000	4.40500000	-12.98800000
C	-4.39700000	4.33400000	-12.20100000
C	-3.80700000	3.18300000	-13.02100000
N	-2.33500000	3.02800000	-12.87900000
C	-1.79900000	1.69700000	-13.02100000
O	-2.53800000	0.72800000	-13.03100000
N	-0.39600000	1.59800000	-13.06900000
C	0.48600000	2.71300000	-13.14600000
O	1.67400000	2.50300000	-13.35400000
C	-0.13900000	4.03200000	-12.98600000
C	-1.49000000	4.15200000	-12.91400000
C	0.77500000	5.20700000	-12.97900000
O	-4.30800000	8.75100000	-15.36600000
O	-2.07500000	8.32800000	-14.02500000
H	0.01000000	0.60900000	-13.16300000

H	-1.99500000	5.13500000	-12.86600000
H	-4.29900000	2.18600000	-12.82400000
H	-3.64700000	5.11600000	-11.94800000
H	-5.56300000	6.05400000	-12.97700000
H	-5.90600000	4.05300000	-15.08500000
H	-3.91900000	5.28400000	-16.25600000
H	1.77600000	4.94000000	-12.59900000
H	0.93000000	5.60500000	-13.99800000
H	0.39800000	6.03400000	-12.36200000
H	-4.77600000	3.98400000	-11.21800000
H	-5.28700000	6.34600000	-15.73200000
P	-7.41600000	3.91200000	-11.52400000
C	-6.72600000	1.43800000	-12.20200000
O	-6.57200000	2.50000000	-11.23800000
C	-7.14700000	0.15500000	-11.47700000
O	-5.95600000	-0.61600000	-11.16000000
C	-7.88400000	0.36000000	-10.12700000
O	-8.93400000	-0.62500000	-10.20700000
C	-6.82500000	0.09000000	-9.04800000
C	-5.59500000	-0.46700000	-9.77300000
N	-4.39100000	0.41900000	-9.72400000
C	-3.08400000	-0.19200000	-9.95000000
O	-3.03000000	-1.40600000	-10.14100000
N	-1.96500000	0.61000000	-9.89900000
C	-2.07200000	1.96800000	-9.71100000
N	-0.91700000	2.68700000	-9.69700000
C	-3.36000000	2.58100000	-9.52600000
C	-4.48200000	1.79700000	-9.54800000
O	-8.85900000	3.63600000	-11.86000000
O	-7.00200000	4.80500000	-10.38700000
H	-3.43900000	3.65200000	-9.35800000
H	-5.49200000	2.22600000	-9.41200000
H	-5.28800000	-1.49800000	-9.44200000
H	-6.63300000	1.01100000	-8.46000000
H	-8.37000000	1.35200000	-10.02200000
H	-7.71500000	-0.52200000	-12.15800000
H	-0.90900000	3.68500000	-9.52900000
H	-5.70300000	1.31000000	-12.64100000
H	0.00200000	2.23700000	-9.87000000
H	-7.16500000	-0.64700000	-8.28400000
H	-7.44100000	1.69000000	-13.00700000
P	-9.82000000	-1.08500000	-8.87000000
C	-8.10200000	-3.07300000	-8.84900000
O	-8.75800000	-2.06700000	-8.03900000
C	-7.08100000	-3.76200000	-7.94400000
O	-5.89700000	-2.92500000	-7.84300000
C	-7.58100000	-4.02500000	-6.49500000
O	-7.34100000	-5.42900000	-6.29900000
C	-6.80100000	-3.03800000	-5.62300000
C	-5.55600000	-2.70000000	-6.44300000

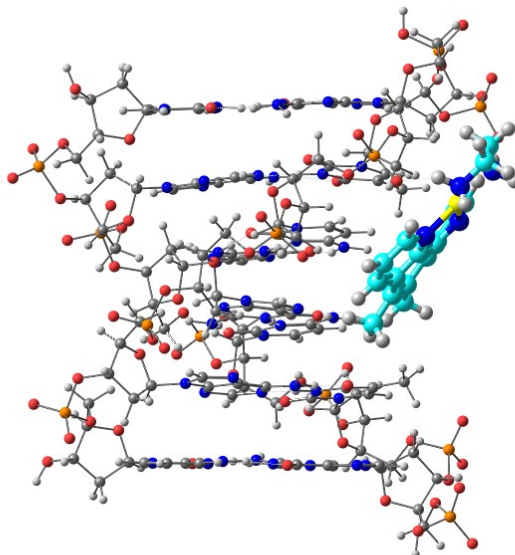
N	-1.36600000	0.29000000	-6.78900000
C	-1.50300000	-1.11500000	-6.91300000
N	-0.37000000	-1.85200000	-7.08700000
N	-2.71100000	-1.76600000	-6.82400000
C	-3.76200000	-0.93700000	-6.54900000
C	-3.71600000	0.48500000	-6.39500000
C	-2.46700000	1.17200000	-6.54100000
O	-2.22100000	2.37500000	-6.48800000
N	-5.00500000	0.97500000	-6.11200000
C	-5.81400000	-0.08900000	-6.09000000
N	-5.10100000	-1.30800000	-6.34700000
O	-10.92500000	-1.90000000	-9.49700000
O	-10.10800000	0.05700000	-7.93300000
H	-0.38500000	0.71200000	-6.89100000
H	-6.88000000	-0.08900000	-5.88900000
H	-4.67100000	-3.37300000	-6.23900000
H	-7.43900000	-2.15200000	-5.42000000
H	-0.44000000	-2.85600000	-7.22000000
H	-8.68300000	-3.91900000	-6.38500000
H	0.56100000	-1.41000000	-7.19500000
H	-6.71900000	-4.70500000	-8.42400000
H	-7.59600000	-2.59400000	-9.71800000
H	-6.55100000	-3.41800000	-4.61000000
H	-8.85300000	-3.80400000	-9.20900000
P	-6.42900000	-6.06800000	-5.05800000
C	-4.08800000	-5.77600000	-6.31700000
O	-4.93000000	-5.35700000	-5.22200000
C	-2.86200000	-6.53800000	-5.80400000
O	-1.76900000	-5.59100000	-5.61300000
C	-3.03500000	-7.26300000	-4.44700000
O	-2.34700000	-8.51100000	-4.66400000
C	-2.36400000	-6.34000000	-3.41800000
C	-1.56800000	-5.30200000	-4.21800000
N	-0.17700000	-0.24500000	-3.75300000
C	0.56500000	-1.35100000	-4.06400000
N	0.12800000	-2.63600000	-4.16200000
C	-1.22400000	-2.77400000	-3.93200000
C	-2.10400000	-1.68600000	-3.60700000
C	-1.54300000	-0.37500000	-3.52800000
N	-2.26900000	0.73700000	-3.25400000
N	-3.42100000	-2.15800000	-3.45500000
C	-3.36500000	-3.47200000	-3.68500000
N	-2.03000000	-3.92000000	-3.96200000
O	-6.37900000	-7.53100000	-5.41800000
O	-6.90800000	-5.57000000	-3.72100000
H	1.63900000	-1.16600000	-4.26300000
H	-4.20300000	-4.16900000	-3.68500000
H	-0.45400000	-5.34700000	-4.07800000
H	-3.12700000	-5.89600000	-2.74800000
H	-4.08500000	-7.50900000	-4.19000000

H	-2.45900000	-7.22600000	-6.58800000
H	-3.76100000	-4.80200000	-6.76600000
H	-1.85000000	1.68200000	-3.30100000
H	-3.27200000	0.67700000	-3.12800000
H	-1.69200000	-6.88800000	-2.72100000
H	-4.63600000	-6.36700000	-7.07400000
P	-1.91700000	-9.47700000	-3.36700000
C	0.43500000	-8.41900000	-3.79800000
O	-0.57600000	-8.66200000	-2.78800000
C	1.65000000	-7.82500000	-3.09100000
O	1.48800000	-6.37300000	-3.06500000
C	1.85900000	-8.27000000	-1.62600000
O	2.97900000	-9.16800000	-1.67200000
C	2.21700000	-6.99000000	-0.85600000
C	1.90100000	-5.82400000	-1.79300000
N	0.75500000	-4.98600000	-1.32200000
C	0.91300000	-3.54100000	-1.25400000
O	2.02000000	-3.06400000	-1.51600000
N	-0.16200000	-2.76700000	-0.88100000
C	-1.37400000	-3.34800000	-0.56500000
N	-2.39300000	-2.52400000	-0.22200000
C	-1.52500000	-4.78400000	-0.60500000
C	-0.46700000	-5.56300000	-0.97800000
O	-1.51900000	-10.76700000	-4.03900000
O	-2.91900000	-9.43000000	-2.24700000
H	3.11200000	-9.59700000	-0.79300000
H	-2.47600000	-5.23400000	-0.31800000
H	-0.54000000	-6.66500000	-1.04200000
H	2.76800000	-5.15000000	-2.01300000
H	1.69600000	-6.93300000	0.11800000
H	0.98800000	-8.80800000	-1.19300000
H	2.57800000	-7.99900000	-3.69300000
H	-3.31800000	-2.88400000	-0.01300000
H	0.03300000	-7.70500000	-4.55300000
H	-2.28700000	-1.49300000	-0.23400000
H	3.29100000	-6.99700000	-0.57200000
H	0.71800000	-9.37400000	-4.28900000
O	1.96900000	4.78200000	-20.22900000
O	-1.55200000	5.27000000	3.10200000
H	1.62900000	4.65900000	-21.15600000
H	-1.33400000	5.19600000	4.07200000
N	2.92800000	7.12200000	-6.61700000
N	6.97400000	7.45600000	-6.46500000
N	4.92000000	8.67100000	-4.98700000
N	4.87600000	5.99900000	-8.02400000
C	4.32700000	4.08600000	-10.05300000
C	3.27800000	4.83700000	-9.56400000
C	3.54300000	5.78100000	-8.48600000
C	2.54400000	6.41100000	-7.79700000
C	1.14500000	6.34200000	-8.21900000

C	0.22600000	7.11100000	-7.56100000
C	0.67500000	7.96300000	-6.47200000
C	1.98100000	7.96700000	-6.05900000
C	-1.23300000	7.10800000	-7.88100000
C	0.89200000	5.42200000	-9.33000000
C	7.32700000	8.62800000	-5.59000000
C	6.32100000	8.72100000	-4.43700000
C	5.85400000	5.14700000	-8.44800000
C	1.87600000	4.70900000	-9.92800000
C	4.14100000	3.12200000	-11.16600000
C	5.62800000	4.22900000	-9.46100000
Pt	4.90600000	7.30400000	-6.53000000
H	7.38100000	7.59100000	-7.40000000
H	7.37500000	6.55800000	-6.09700000
H	4.63000000	9.60600000	-5.29900000
H	4.24400000	8.36200000	-4.22900000
H	-0.05900000	8.57400000	-5.96400000
H	2.31400000	8.57300000	-5.21100000
H	-1.45000000	6.68400000	-8.87000000
H	-1.65200000	8.12400000	-7.86700000
H	-1.79500000	6.52300000	-7.13800000
H	-0.14600000	5.32200000	-9.64300000
H	7.31500000	9.56400000	-6.20000000
H	8.36300000	8.54000000	-5.18800000
H	6.49800000	9.65200000	-3.85000000
H	6.47300000	7.86800000	-3.71600000
H	6.83700000	5.23300000	-7.96300000
H	1.64600000	3.97300000	-10.70600000
H	5.02800000	2.51700000	-11.38100000
H	3.81400000	3.59600000	-12.09800000
H	3.35100000	2.37700000	-10.91200000
H	6.43600000	3.60100000	-9.80900000

[Pt(en)(5,6-Me₂phen)]²⁺ systems

[Pt(en)(5,6-Me₂phen)]²⁺ major groove
Dock_ID: 277-cl3_5,6-Me₂phen



EDA for 277-cl3_5,6-Me₂phen in kcal mol⁻¹.

Electrostatic interaction	-770.0
Orbital interaction	-95.0
Dispersion energy	-55.8
Pauli repulsion	130.6
Total Bonding Energy	-790.2

Contributions of the solvation energies for 277-cl3_5,6-Me₂phen in kcal mol⁻¹.

E _{solv} (total system)	-1746.7
E _{solv} (intercalator)	-160.0
E _{solv} (duplex DNA)	-2314.3
ΔE _{solv}	727.6
ΔE _{int} (EDA)	-790.2
ΔE _{aq}	-62.6

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 227-cl3_5,6-Me₂phen system.
([Pt(en)(5,6-Me₂phen)]²⁺ major groove)

P	-1.23400000	7.58000000	1.98400000
C	1.36800000	7.16700000	1.74800000
O	0.14100000	7.46900000	1.04700000
C	2.47300000	7.10800000	0.68600000
O	2.69400000	5.71300000	0.33000000
C	2.13200000	7.84600000	-0.63700000
O	3.15000000	8.78800000	-0.95200000
C	1.88100000	6.74300000	-1.67600000
C	2.15000000	5.41100000	-0.96800000
N	0.24600000	0.55600000	-0.71200000
C	1.56300000	1.00100000	-0.97400000
N	2.53500000	0.04700000	-1.20000000
N	1.93400000	2.31900000	-0.94900000
C	0.89500000	3.19600000	-0.72800000
C	-0.46400000	2.82900000	-0.48200000
C	-0.84200000	1.44900000	-0.43900000
O	-1.93900000	0.93700000	-0.21300000
N	-1.25200000	3.99100000	-0.35200000
C	-0.42300000	5.02300000	-0.51600000
N	0.92800000	4.59500000	-0.77100000
O	-1.06900000	8.61700000	3.06900000
O	-2.34300000	7.63400000	0.96900000
H	0.03900000	-0.49400000	-0.74900000
H	-0.67300000	6.08300000	-0.46700000
H	2.94400000	4.76000000	-1.45300000
H	0.85100000	6.82400000	-2.07800000
H	3.33400000	0.32900000	-1.78200000
H	1.24800000	8.52500000	-0.51800000
H	2.25100000	-0.95000000	-1.31300000
H	3.44600000	7.42200000	1.12600000
H	1.27700000	6.18300000	2.25700000
H	2.54300000	6.84300000	-2.56500000
H	1.57900000	7.95900000	2.49200000
P	4.62100000	8.52700000	-1.71000000
C	5.39900000	6.04400000	-1.25100000
O	4.71300000	6.93600000	-2.16200000
C	5.78400000	4.81300000	-2.06400000
O	4.60500000	3.99100000	-2.29600000
C	6.40300000	5.10900000	-3.46100000
O	7.59200000	4.30600000	-3.40800000
C	5.32000000	4.71400000	-4.46900000
C	4.51900000	3.65300000	-3.71500000
N	3.07100000	3.54000000	-4.01000000
C	2.52100000	2.22000000	-3.86900000
O	3.24600000	1.24000000	-3.76500000
N	1.12200000	2.11400000	-3.93000000

C	0.24100000	3.22700000	-3.95300000
O	-0.95800000	3.01400000	-3.79900000
C	0.87500000	4.53200000	-4.16300000
C	2.23000000	4.65900000	-4.15800000
C	-0.06000000	5.67600000	-4.34200000
O	5.66600000	8.88800000	-0.69300000
O	4.51400000	9.25300000	-3.03500000
H	0.71300000	1.11800000	-3.87000000
H	2.74100000	5.62700000	-4.30600000
H	4.96900000	2.61900000	-3.81300000
H	4.72800000	5.62100000	-4.74300000
H	6.75300000	6.16400000	-3.58800000
H	6.46400000	4.16100000	-1.45900000
H	4.70300000	5.77500000	-0.42600000
H	-0.63700000	5.57600000	-5.27500000
H	-0.78500000	5.73000000	-3.51500000
H	0.45600000	6.64800000	-4.38500000
H	5.71300000	4.35100000	-5.44500000
H	6.30100000	6.52600000	-0.82000000
P	8.23400000	3.41000000	-4.65000000
C	6.77800000	1.19700000	-4.49700000
O	6.98800000	2.44100000	-5.19200000
C	7.10900000	0.01900000	-5.42200000
O	5.86800000	-0.68100000	-5.71400000
C	7.73100000	0.38100000	-6.79800000
O	8.84000000	-0.53300000	-6.86900000
C	6.60900000	0.16900000	-7.82300000
C	5.41500000	-0.41000000	-7.05500000
N	4.25400000	0.52300000	-6.97700000
C	2.91300000	-0.03100000	-6.94500000
O	2.78600000	-1.25800000	-6.87400000
N	1.83200000	0.82100000	-7.01500000
C	2.01600000	2.18500000	-7.04900000
N	0.91100000	2.97800000	-7.08400000
C	3.34100000	2.74200000	-6.97300000
C	4.42200000	1.91300000	-6.93400000
O	9.29000000	2.59800000	-3.94200000
O	8.57400000	4.30000000	-5.81500000
H	3.47600000	3.82800000	-6.95900000
H	5.45600000	2.30200000	-6.86800000
H	5.05000000	-1.40800000	-7.43000000
H	6.38500000	1.11500000	-8.35900000
H	8.16000000	1.40500000	-6.85400000
H	7.71900000	-0.75100000	-4.89400000
H	1.00300000	3.97900000	-7.21500000
H	5.67900000	1.21000000	-4.25600000
H	-0.04200000	2.57700000	-7.11600000
H	6.89600000	-0.52900000	-8.64300000
H	7.35100000	1.13100000	-3.55200000
P	9.49100000	-1.06200000	-8.31100000

C	7.77200000	-3.02000000	-7.93700000
O	8.30500000	-2.07600000	-8.89800000
C	6.78400000	-3.89600000	-8.70600000
O	5.48000000	-3.24300000	-8.72100000
C	7.18800000	-4.15200000	-10.18500000
O	7.04000000	-5.58100000	-10.29200000
C	6.21200000	-3.30600000	-11.00500000
C	5.00300000	-3.09700000	-10.09000000
N	0.53600000	-0.42200000	-10.11800000
C	0.74800000	-1.81700000	-10.05700000
N	-0.36100000	-2.61600000	-10.18000000
N	1.99400000	-2.39300000	-9.97200000
C	3.02400000	-1.49300000	-10.11300000
C	2.89700000	-0.07700000	-10.26100000
C	1.60200000	0.53800000	-10.17200000
O	1.28500000	1.72000000	-10.16800000
N	4.16100000	0.50400000	-10.46800000
C	5.03900000	-0.49700000	-10.42100000
N	4.39900000	-1.76300000	-10.17600000
O	10.68800000	-1.84800000	-7.83100000
O	9.61900000	0.03100000	-9.33500000
H	-0.46200000	-0.03800000	-10.06400000
H	6.11300000	-0.43100000	-10.55500000
H	4.19800000	-3.88000000	-10.21900000
H	6.71000000	-2.35500000	-11.29300000
H	-0.26500000	-3.62000000	-10.08400000
H	8.25400000	-3.91900000	-10.39900000
H	-1.31300000	-2.21900000	-10.05300000
H	6.60300000	-4.85500000	-8.16200000
H	7.26100000	-2.46900000	-7.11500000
H	5.92300000	-3.75500000	-11.97600000
H	8.59000000	-3.64000000	-7.51900000
P	6.72300000	-6.33800000	-11.74100000
C	4.16300000	-6.31600000	-11.04600000
O	5.13700000	-5.90200000	-12.02900000
C	3.00900000	-7.02900000	-11.75900000
O	1.94700000	-6.06600000	-12.00600000
C	3.36800000	-7.61000000	-13.15500000
O	2.63200000	-8.84300000	-13.21100000
C	2.96500000	-6.50200000	-14.13700000
C	1.97600000	-5.61100000	-13.37300000
N	0.31300000	-0.63100000	-13.30700000
C	-0.38400000	-1.81200000	-13.27200000
N	0.13100000	-3.06800000	-13.28000000
C	1.50600000	-3.09300000	-13.32500000
C	2.34100000	-1.92400000	-13.35300000
C	1.69700000	-0.65000000	-13.35400000
N	2.37500000	0.53300000	-13.45900000
N	3.69600000	-2.30200000	-13.38300000
C	3.70200000	-3.63900000	-13.37000000

N	2.38000000	-4.18900000	-13.36300000
O	6.83600000	-7.79500000	-11.37300000
O	7.47700000	-5.72800000	-12.89200000
H	-1.48600000	-1.71200000	-13.21900000
H	4.58100000	-4.28700000	-13.35700000
H	0.90700000	-5.68600000	-13.71100000
H	3.87900000	-5.96500000	-14.47000000
H	4.43100000	-7.91300000	-13.26400000
H	2.52100000	-7.78600000	-11.10400000
H	3.79800000	-5.35900000	-10.58700000
H	1.86500000	1.42200000	-13.34100000
H	3.36100000	0.55800000	-13.20300000
H	2.53400000	-6.87100000	-15.08800000
H	4.59600000	-6.96200000	-10.25900000
P	1.70300000	-9.30300000	-14.51500000
C	-0.44800000	-8.00800000	-13.66100000
O	0.57900000	-8.07700000	-14.67100000
C	-1.81400000	-7.92800000	-14.34800000
O	-2.17600000	-6.51900000	-14.47100000
C	-1.89900000	-8.52900000	-15.77100000
O	-2.95000000	-9.50600000	-15.68600000
C	-2.29900000	-7.36800000	-16.69800000
C	-2.25800000	-6.10300000	-15.84200000
N	-1.07100000	-5.22900000	-16.12600000
C	-1.24600000	-3.78500000	-16.09200000
O	-2.38000000	-3.34700000	-15.86900000
N	-0.17000000	-2.96300000	-16.33300000
C	1.08100000	-3.49800000	-16.57300000
N	2.11700000	-2.63300000	-16.70700000
C	1.26200000	-4.92700000	-16.61500000
C	0.19600000	-5.75200000	-16.37900000
O	1.05600000	-10.56700000	-14.00900000
O	2.48300000	-9.24500000	-15.80000000
H	-3.03700000	-9.99500000	-16.53900000
H	2.24400000	-5.34100000	-16.84200000
H	0.30500000	-6.85300000	-16.36800000
H	-3.18000000	-5.46600000	-15.89100000
H	-1.67000000	-7.32100000	-17.60700000
H	-0.97500000	-9.04000000	-16.10800000
H	-2.61500000	-8.34300000	-13.68800000
H	3.05100000	-2.95700000	-16.94000000
H	-0.24200000	-7.06300000	-13.10300000
H	1.97700000	-1.60900000	-16.67600000
H	-3.31800000	-7.53300000	-17.10800000
H	-0.41800000	-8.86800000	-12.96300000
P	1.07000000	7.24900000	-18.88400000
C	-1.43700000	6.43100000	-18.78200000
O	-0.27300000	6.80400000	-18.00700000
C	-2.61600000	6.38400000	-17.80400000
O	-2.83000000	5.00700000	-17.38300000

C	-2.40500000	7.19800000	-16.49800000
O	-3.66500000	7.86000000	-16.30700000
C	-2.00100000	6.15500000	-15.44900000
C	-2.29200000	4.78200000	-16.06600000
N	-0.50300000	-0.10800000	-16.26500000
C	-1.80400000	0.37000000	-15.96800000
N	-2.75600000	-0.54700000	-15.63800000
N	-2.14100000	1.70400000	-15.99400000
C	-1.07900000	2.54300000	-16.22300000
C	0.27000000	2.14400000	-16.48000000
C	0.60900000	0.75500000	-16.52900000
O	1.68500000	0.20900000	-16.77800000
N	1.08100000	3.28600000	-16.64600000
C	0.27600000	4.33800000	-16.49700000
N	-1.08000000	3.94400000	-16.20600000
O	0.71700000	8.22400000	-19.98000000
O	2.11500000	7.53700000	-17.84000000
H	-0.33000000	-1.16200000	-16.26400000
H	0.54100000	5.39000000	-16.58200000
H	-3.09200000	4.17700000	-15.54100000
H	-0.92900000	6.29400000	-15.17300000
H	-3.66100000	-0.23500000	-15.29100000
H	-1.65700000	8.01500000	-16.61300000
H	-2.58700000	-1.56600000	-15.71800000
H	-3.57200000	6.64600000	-18.31500000
H	-1.26400000	5.42700000	-19.22500000
H	-2.53900000	6.26600000	-14.48000000
H	-1.62400000	7.16700000	-19.58700000
P	-4.41200000	8.01500000	-14.81900000
C	-5.51300000	5.67000000	-15.29400000
O	-4.72600000	6.44500000	-14.35900000
C	-5.94900000	4.41100000	-14.54700000
O	-4.81900000	3.49700000	-14.44200000
C	-6.45800000	4.67800000	-13.10200000
O	-7.66400000	3.89400000	-13.05300000
C	-5.31800000	4.19800000	-12.20100000
C	-4.58100000	3.15600000	-13.04700000
N	-3.11000000	3.13900000	-12.85700000
C	-2.45000000	1.86300000	-12.97600000
O	-3.09300000	0.82900000	-13.00400000
N	-1.04300000	1.89500000	-12.97100000
C	-0.26600000	3.08500000	-12.98900000
O	0.94500000	2.98900000	-13.13800000
C	-1.01400000	4.33500000	-12.81300000
C	-2.37300000	4.33500000	-12.81200000
C	-0.21600000	5.58800000	-12.72500000
O	-5.67400000	8.75500000	-15.18600000
O	-3.46600000	8.51400000	-13.76300000
H	-0.54400000	0.94300000	-13.06100000
H	-2.96900000	5.26600000	-12.75000000

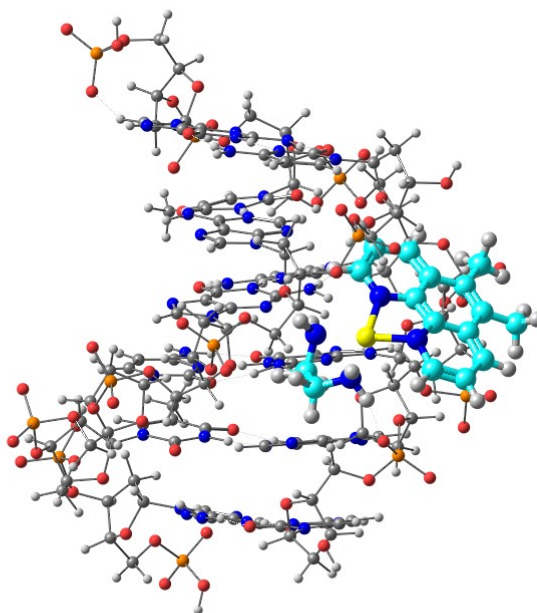
H	-4.97500000	2.10500000	-12.91600000
H	-4.67900000	5.07300000	-11.93800000
H	-6.74800000	5.73600000	-12.92500000
H	-6.70500000	3.84700000	-15.14700000
H	-4.88000000	5.41400000	-16.17100000
H	0.80300000	5.39900000	-12.34500000
H	-0.09300000	6.05700000	-13.71900000
H	-0.68200000	6.34100000	-12.07400000
H	-5.64700000	3.78200000	-11.22700000
H	-6.39900000	6.24200000	-15.63600000
P	-8.25600000	3.26500000	-11.62900000
C	-7.10900000	0.94300000	-12.21500000
O	-7.16500000	2.04500000	-11.28700000
C	-7.34400000	-0.37300000	-11.46900000
O	-6.05400000	-1.00100000	-11.22300000
C	-8.02700000	-0.25600000	-10.08100000
O	-8.98000000	-1.33600000	-10.13000000
C	-6.89700000	-0.43600000	-9.05600000
C	-5.65400000	-0.85300000	-9.84900000
N	-4.54500000	0.14800000	-9.81000000
C	-3.17700000	-0.34300000	-9.92200000
O	-3.00100000	-1.55600000	-10.02900000
N	-2.14200000	0.56600000	-9.87900000
C	-2.39000000	1.91400000	-9.76700000
N	-1.31100000	2.74600000	-9.70200000
C	-3.74000000	2.40800000	-9.69700000
C	-4.77800000	1.51800000	-9.72700000
O	-9.59000000	2.70700000	-12.05200000
O	-8.10000000	4.21400000	-10.47200000
H	-3.92500000	3.47700000	-9.61200000
H	-5.83300000	1.85200000	-9.68800000
H	-5.23700000	-1.85900000	-9.56100000
H	-6.76800000	0.48600000	-8.45600000
H	-8.59700000	0.68600000	-9.93500000
H	-7.86600000	-1.11400000	-12.12000000
H	-1.43100000	3.74800000	-9.76600000
H	-6.06300000	0.97500000	-12.62100000
H	-0.35000000	2.37600000	-9.85000000
H	-7.12400000	-1.21800000	-8.29400000
H	-7.82200000	1.05400000	-13.05400000
P	-9.75100000	-1.88200000	-8.75600000
C	-7.84700000	-3.69700000	-8.83900000
O	-8.55400000	-2.75800000	-7.99100000
C	-6.71900000	-4.28300000	-7.99200000
O	-5.58300000	-3.37100000	-8.01600000
C	-7.09200000	-4.51800000	-6.50000000
O	-6.83100000	-5.92100000	-6.32600000
C	-6.22500000	-3.52900000	-5.71600000
C	-5.07100000	-3.19000000	-6.66100000
N	-0.83300000	-0.21800000	-6.90400000

C	-0.96400000	-1.62000000	-6.99100000
N	0.18100000	-2.35700000	-7.17900000
N	-2.16900000	-2.27600000	-6.94700000
C	-3.24000000	-1.44400000	-6.74200000
C	-3.19700000	-0.02100000	-6.61300000
C	-1.94700000	0.67200000	-6.74200000
O	-1.70800000	1.87500000	-6.72200000
N	-4.48900000	0.47600000	-6.36100000
C	-5.30100000	-0.58300000	-6.34400000
N	-4.58700000	-1.80800000	-6.58200000
O	-10.80800000	-2.79500000	-9.33000000
O	-10.09200000	-0.77500000	-7.79600000
H	0.15100000	0.21500000	-6.95900000
H	-6.37000000	-0.58200000	-6.16000000
H	-4.18700000	-3.88900000	-6.56700000
H	-6.83700000	-2.64100000	-5.44500000
H	0.13600000	-3.36400000	-7.04900000
H	-8.17800000	-4.39700000	-6.29200000
H	1.11900000	-1.91600000	-7.05800000
H	-6.33900000	-5.22500000	-8.46100000
H	-7.44000000	-3.17700000	-9.73400000
H	-5.86900000	-3.90500000	-4.73500000
H	-8.54400000	-4.49800000	-9.16000000
P	-6.02300000	-6.56800000	-5.02000000
C	-3.65400000	-6.26900000	-6.20500000
O	-4.51200000	-5.86600000	-5.12000000
C	-2.40300000	-6.96700000	-5.66200000
O	-1.34800000	-5.97800000	-5.48000000
C	-2.56600000	-7.65400000	-4.28100000
O	-1.76000000	-8.84000000	-4.43300000
C	-2.01000000	-6.63700000	-3.27200000
C	-1.21700000	-5.61300000	-4.09500000
N	0.03600000	-0.52400000	-3.77900000
C	0.81500000	-1.62300000	-4.01500000
N	0.40100000	-2.91500000	-4.10600000
C	-0.95700000	-3.07100000	-3.92700000
C	-1.87100000	-1.99200000	-3.68000000
C	-1.33700000	-0.66900000	-3.61600000
N	-2.09200000	0.43700000	-3.39600000
N	-3.18300000	-2.48700000	-3.55800000
C	-3.08700000	-3.81000000	-3.72300000
N	-1.73400000	-4.23500000	-3.93400000
O	-5.96900000	-8.03300000	-5.36500000
O	-6.56700000	-6.05000000	-3.71600000
H	1.89500000	-1.42300000	-4.16400000
H	-3.90700000	-4.52700000	-3.71100000
H	-0.10900000	-5.60900000	-3.90300000
H	-2.84400000	-6.19200000	-2.69300000
H	-3.60000000	-7.97700000	-4.04900000
H	-1.96500000	-7.66100000	-6.41900000

H	-3.36300000	-5.29600000	-6.68000000
H	-1.68500000	1.38300000	-3.48400000
H	-3.10500000	0.36700000	-3.37100000
H	-1.36200000	-7.09600000	-2.49300000
H	-4.17000000	-6.90600000	-6.94900000
P	-1.37800000	-9.78400000	-3.11100000
C	0.88700000	-8.45900000	-3.22500000
O	-0.20400000	-8.85700000	-2.36000000
C	1.84500000	-7.61900000	-2.38700000
O	1.44500000	-6.21700000	-2.51300000
C	1.86800000	-7.91000000	-0.86800000
O	3.04500000	-8.70800000	-0.66700000
C	2.01500000	-6.53600000	-0.19700000
C	1.78900000	-5.49800000	-1.29900000
N	0.64200000	-4.58600000	-1.02100000
C	0.86900000	-3.14900000	-1.02500000
O	2.01600000	-2.74400000	-1.24000000
N	-0.18500000	-2.30000000	-0.77900000
C	-1.45000000	-2.80000000	-0.53700000
N	-2.43200000	-1.90400000	-0.27000000
C	-1.68200000	-4.22500000	-0.54200000
C	-0.63900000	-5.07800000	-0.77100000
O	-0.76600000	-11.00500000	-3.75200000
O	-2.49400000	-9.86900000	-2.10700000
H	3.06800000	-9.06000000	0.25600000
H	-2.68300000	-4.61200000	-0.34400000
H	-0.76500000	-6.17400000	-0.78100000
H	2.69100000	-4.87600000	-1.54200000
H	1.33300000	-6.42700000	0.66700000
H	0.98300000	-8.47700000	-0.50900000
H	2.88000000	-7.67400000	-2.81100000
H	-3.40100000	-2.19800000	-0.17700000
H	0.49300000	-7.86800000	-4.08300000
H	-2.26700000	-0.88300000	-0.34100000
H	3.02500000	-6.43200000	0.25400000
H	1.41000000	-9.36600000	-3.59700000
O	1.49700000	5.79800000	-19.60000000
O	-1.28600000	6.08000000	2.71600000
H	1.23200000	5.68600000	-20.55200000
H	-1.02000000	6.05800000	3.67700000
N	6.26700000	5.77900000	-7.71000000
N	4.48500000	7.49500000	-6.69500000
N	6.54000000	8.71600000	-4.92300000
N	8.48500000	7.02000000	-6.02700000
C	5.53100000	3.76400000	-9.55600000
C	6.84700000	3.85000000	-9.02500000
C	7.18000000	4.84800000	-8.11600000
C	4.92900000	5.65700000	-8.16900000
C	4.00300000	6.48300000	-7.59300000
C	3.56700000	7.85300000	-5.68500000

C	2.23200000	7.63600000	-5.82900000
C	1.70700000	6.88300000	-6.95800000
C	2.57500000	6.30200000	-7.83100000
C	2.23500000	5.46200000	-8.98900000
C	3.17600000	4.70900000	-9.63500000
C	2.88100000	3.89100000	-10.84200000
C	0.80500000	5.50400000	-9.43300000
C	7.75500000	8.38600000	-4.09800000
C	8.92400000	8.06800000	-5.03900000
C	4.57000000	4.67200000	-9.17500000
Pt	6.41100000	7.19300000	-6.31900000
H	5.69600000	8.82500000	-4.29100000
H	6.66600000	9.62200000	-5.39600000
H	8.71900000	6.05700000	-5.67900000
H	9.00100000	7.13700000	-6.90600000
H	5.30300000	2.95700000	-10.25600000
H	7.59200000	3.12000000	-9.31100000
H	8.19500000	4.93100000	-7.70600000
H	3.98600000	8.39300000	-4.82600000
H	1.52300000	8.01200000	-5.09800000
H	0.63200000	6.79900000	-7.05100000
H	3.47100000	4.20300000	-11.70900000
H	1.81800000	3.89400000	-11.14000000
H	3.11000000	2.82100000	-10.65300000
H	0.59700000	4.74900000	-10.20900000
H	0.55700000	6.48400000	-9.86300000
H	0.10900000	5.33700000	-8.60000000
H	8.02900000	9.21400000	-3.40700000
H	7.51300000	7.49300000	-3.45600000
H	9.25800000	8.98500000	-5.57900000
H	9.80900000	7.72900000	-4.45200000

[Pt(en)(5,6-Me₂phen)]²⁺ minor groove
Dock_ID: 285-cl1_5,6-Me₂phen



EDA for 285-cl1_5,6-Me₂phen in kcal mol⁻¹.

Electrostatic interaction	-798.4
Orbital interaction	-95.2
Dispersion energy	-63.7
Pauli repulsion	119.7
Total Bonding Energy	-837.5

Contributions of the solvation energies for 285-cl1_5,6-Me₂phen in kcal mol⁻¹.

E _{solv} (total system)	-1731.8
E _{solv} (intercalator)	-160.6
E _{solv} (duplex DNA)	-2348.0
ΔE _{solv}	776.9
ΔE _{int} (EDA)	-837.5
ΔE _{aq}	-60.6

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

**Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 285-cl1_5,6-Me₂phen system.
([Pt(en)(5,6-Me₂phen)]²⁺ minor groove)**

P	-1.890000000	6.684000000	2.027000000
C	0.718000000	6.095000000	2.187000000
O	-0.281000000	7.129000000	2.163000000
C	1.495000000	6.030000000	0.866000000
O	1.417000000	4.656000000	0.391000000
C	0.976000000	6.925000000	-0.289000000
O	2.130000000	7.565000000	-0.853000000
C	0.181000000	5.979000000	-1.192000000
C	0.666000000	4.571000000	-0.846000000
N	-0.381000000	-0.506000000	-0.415000000
C	0.824000000	0.149000000	-0.767000000
N	1.937000000	-0.636000000	-0.976000000
N	0.955000000	1.510000000	-0.833000000
C	-0.208000000	2.199000000	-0.569000000
C	-1.471000000	1.614000000	-0.244000000
C	-1.601000000	0.193000000	-0.142000000
O	-2.582000000	-0.494000000	0.149000000
N	-2.436000000	2.631000000	-0.086000000
C	-1.796000000	3.785000000	-0.291000000
N	-0.413000000	3.585000000	-0.615000000
O	-2.603000000	7.617000000	2.976000000
O	-2.292000000	6.582000000	0.579000000
H	-0.404000000	-1.577000000	-0.421000000
H	-2.224000000	4.795000000	-0.238000000
H	1.396000000	4.129000000	-1.585000000
H	-0.909000000	6.125000000	-0.989000000
H	2.680000000	-0.255000000	-1.574000000
H	0.381000000	7.795000000	0.073000000
H	1.831000000	-1.673000000	-1.018000000
H	2.585000000	6.183000000	1.046000000
H	0.296000000	5.097000000	2.438000000
H	0.288000000	6.201000000	-2.284000000
H	1.380000000	6.410000000	3.021000000
P	2.824000000	7.159000000	-2.320000000
C	4.033000000	4.997000000	-1.351000000
O	3.067000000	5.513000000	-2.288000000
C	5.096000000	4.191000000	-2.101000000
O	4.584000000	2.856000000	-2.377000000
C	5.561000000	4.773000000	-3.459000000
O	6.994000000	4.738000000	-3.323000000
C	4.994000000	3.827000000	-4.527000000
C	4.323000000	2.673000000	-3.777000000
N	2.838000000	2.608000000	-3.975000000
C	2.206000000	1.344000000	-3.748000000
O	2.873000000	0.336000000	-3.535000000
N	0.805000000	1.303000000	-3.849000000

C	-0.016000000	2.466000000	-3.914000000
O	-1.223000000	2.328000000	-3.755000000
C	0.696000000	3.723000000	-4.153000000
C	2.054000000	3.770000000	-4.125000000
C	-0.126000000	4.937000000	-4.410000000
O	4.136000000	7.901000000	-2.266000000
O	1.833000000	7.340000000	-3.437000000
H	0.338000000	0.345000000	-3.736000000
H	2.607000000	4.718000000	-4.243000000
H	4.750000000	1.658000000	-4.015000000
H	4.315000000	4.379000000	-5.209000000
H	5.272000000	5.835000000	-3.612000000
H	5.969000000	3.992000000	-1.430000000
H	3.440000000	4.327000000	-0.683000000
H	-0.189000000	5.164000000	-5.484000000
H	-1.156000000	4.820000000	-4.041000000
H	0.297000000	5.835000000	-3.914000000
H	5.791000000	3.412000000	-5.191000000
H	4.508000000	5.787000000	-0.741000000
P	8.007000000	4.897000000	-4.643000000
C	8.085000000	2.280000000	-4.433000000
O	7.899000000	3.387000000	-5.348000000
C	7.892000000	1.003000000	-5.249000000
O	6.467000000	0.751000000	-5.406000000
C	8.514000000	1.053000000	-6.672000000
O	9.307000000	-0.148000000	-6.689000000
C	7.317000000	1.087000000	-7.627000000
C	6.141000000	0.545000000	-6.812000000
N	4.842000000	1.226000000	-7.018000000
C	3.624000000	0.431000000	-6.840000000
O	3.746000000	-0.765000000	-6.611000000
N	2.408000000	1.072000000	-6.933000000
C	2.331000000	2.419000000	-7.204000000
N	1.092000000	2.969000000	-7.228000000
C	3.527000000	3.187000000	-7.459000000
C	4.744000000	2.574000000	-7.364000000
O	9.348000000	5.099000000	-3.982000000
O	7.483000000	5.848000000	-5.682000000
H	3.450000000	4.237000000	-7.740000000
H	5.691000000	3.112000000	-7.552000000
H	5.994000000	-0.571000000	-6.933000000
H	7.165000000	2.131000000	-7.980000000
H	9.212000000	1.907000000	-6.818000000
H	8.270000000	0.119000000	-4.677000000
H	0.953000000	3.947000000	-7.438000000
H	7.338000000	2.338000000	-3.612000000
H	0.245000000	2.409000000	-6.994000000
H	7.468000000	0.498000000	-8.556000000
H	9.108000000	2.314000000	-4.008000000
P	9.712000000	-0.942000000	-8.099000000

C	7.616000000	-2.489000000	-7.686000000
O	8.256000000	-1.567000000	-8.601000000
C	6.812000000	-3.481000000	-8.534000000
O	5.496000000	-2.916000000	-8.742000000
C	7.406000000	-3.742000000	-9.945000000
O	7.281000000	-5.145000000	-10.205000000
C	6.638000000	-2.775000000	-10.856000000
C	5.329000000	-2.501000000	-10.114000000
N	1.139000000	0.458000000	-10.014000000
C	1.300000000	-0.931000000	-9.796000000
N	0.176000000	-1.690000000	-9.519000000
N	2.508000000	-1.552000000	-9.785000000
C	3.571000000	-0.714000000	-10.008000000
C	3.513000000	0.702000000	-10.210000000
C	2.237000000	1.362000000	-10.179000000
O	1.965000000	2.556000000	-10.287000000
N	4.815000000	1.196000000	-10.408000000
C	5.632000000	0.135000000	-10.342000000
N	4.917000000	-1.079000000	-10.097000000
O	10.631000000	-2.026000000	-7.592000000
O	10.124000000	0.010000000	-9.190000000
H	0.151000000	0.874000000	-9.985000000
H	6.713000000	0.144000000	-10.444000000
H	4.442000000	-3.106000000	-10.473000000
H	7.252000000	-1.861000000	-11.001000000
H	0.270000000	-2.698000000	-9.633000000
H	8.506000000	-3.588000000	-9.988000000
H	-0.765000000	-1.311000000	-9.747000000
H	6.610000000	-4.429000000	-7.979000000
H	6.912000000	-1.878000000	-7.064000000
H	6.468000000	-3.168000000	-11.880000000
H	8.346000000	-3.013000000	-7.042000000
P	6.131000000	-5.822000000	-11.214000000
C	3.946000000	-5.568000000	-9.627000000
O	4.664000000	-5.172000000	-10.819000000
C	2.568000000	-6.087000000	-10.037000000
O	1.712000000	-5.012000000	-10.540000000
C	2.612000000	-7.121000000	-11.193000000
O	1.465000000	-7.943000000	-10.904000000
C	2.448000000	-6.263000000	-12.459000000
C	1.655000000	-5.041000000	-11.976000000
N	0.348000000	-0.131000000	-13.113000000
C	-0.417000000	-1.212000000	-12.761000000
N	0.019000000	-2.471000000	-12.512000000
C	1.383000000	-2.613000000	-12.667000000
C	2.277000000	-1.566000000	-13.072000000
C	1.720000000	-0.264000000	-13.266000000
N	2.447000000	0.839000000	-13.585000000
N	3.592000000	-2.066000000	-13.142000000
C	3.516000000	-3.355000000	-12.786000000

N	2.173000000	-3.757000000	-12.499000000
O	6.269000000	-7.297000000	-10.980000000
O	6.296000000	-5.250000000	-12.613000000
H	-1.499000000	-1.008000000	-12.645000000
H	4.352000000	-4.060000000	-12.712000000
H	0.551000000	-5.085000000	-12.213000000
H	3.444000000	-5.998000000	-12.867000000
H	3.506000000	-7.776000000	-11.188000000
H	1.985000000	-6.465000000	-9.143000000
H	3.856000000	-4.623000000	-9.039000000
H	2.016000000	1.779000000	-13.573000000
H	3.459000000	0.790000000	-13.633000000
H	1.944000000	-6.774000000	-13.300000000
H	4.493000000	-6.329000000	-9.035000000
P	0.700000000	-8.883000000	-12.017000000
C	-1.088000000	-6.994000000	-12.550000000
O	0.004000000	-7.761000000	-13.065000000
C	-2.257000000	-7.050000000	-13.544000000
O	-2.552000000	-5.667000000	-13.898000000
C	-1.984000000	-7.799000000	-14.868000000
O	-3.008000000	-8.804000000	-14.935000000
C	-2.167000000	-6.755000000	-15.983000000
C	-2.293000000	-5.403000000	-15.286000000
N	-1.047000000	-4.574000000	-15.381000000
C	-1.189000000	-3.136000000	-15.517000000
O	-2.318000000	-2.647000000	-15.396000000
N	-0.082000000	-2.369000000	-15.801000000
C	1.170000000	-2.949000000	-15.887000000
N	2.202000000	-2.150000000	-16.241000000
C	1.336000000	-4.354000000	-15.586000000
C	0.237000000	-5.126000000	-15.340000000
O	-0.364000000	-9.498000000	-11.127000000
O	1.570000000	-9.686000000	-12.941000000
H	-2.877000000	-9.381000000	-15.727000000
H	2.337000000	-4.786000000	-15.564000000
H	0.319000000	-6.202000000	-15.104000000
H	-3.159000000	-4.772000000	-15.617000000
H	-1.365000000	-6.804000000	-16.743000000
H	-0.993000000	-8.306000000	-14.906000000
H	-3.198000000	-7.411000000	-13.066000000
H	3.155000000	-2.497000000	-16.287000000
H	-0.706000000	-5.941000000	-12.462000000
H	2.072000000	-1.138000000	-16.421000000
H	-3.082000000	-6.977000000	-16.573000000
H	-1.432000000	-7.347000000	-11.549000000
P	1.142000000	7.431000000	-19.271000000
C	-1.438000000	7.124000000	-18.765000000
O	-0.132000000	7.388000000	-18.202000000
C	-2.411000000	7.106000000	-17.580000000
O	-2.587000000	5.730000000	-17.137000000

C	-1.912000000	7.893000000	-16.339000000
O	-3.053000000	8.619000000	-15.863000000
C	-1.317000000	6.824000000	-15.416000000
C	-1.835000000	5.476000000	-15.934000000
N	-0.369000000	0.468000000	-16.150000000
C	-1.624000000	1.030000000	-15.820000000
N	-2.645000000	0.169000000	-15.483000000
N	-1.889000000	2.374000000	-15.868000000
C	-0.809000000	3.147000000	-16.230000000
C	0.487000000	2.658000000	-16.584000000
C	0.756000000	1.251000000	-16.560000000
O	1.793000000	0.643000000	-16.831000000
N	1.340000000	3.741000000	-16.873000000
C	0.612000000	4.844000000	-16.696000000
N	-0.732000000	4.543000000	-16.274000000
O	0.920000000	8.463000000	-20.351000000
O	2.351000000	7.439000000	-18.375000000
H	-0.234000000	-0.593000000	-16.056000000
H	0.935000000	5.876000000	-16.841000000
H	-2.573000000	4.944000000	-15.266000000
H	-0.207000000	6.905000000	-15.449000000
H	-3.390000000	0.536000000	-14.879000000
H	-1.179000000	8.690000000	-16.606000000
H	-2.444000000	-0.845000000	-15.373000000
H	-3.435000000	7.409000000	-17.896000000
H	-1.436000000	6.138000000	-19.276000000
H	-1.560000000	6.970000000	-14.340000000
H	-1.704000000	7.921000000	-19.485000000
P	-3.661000000	8.491000000	-14.309000000
C	-5.036000000	6.346000000	-14.998000000
O	-4.025000000	6.883000000	-14.114000000
C	-5.615000000	5.121000000	-14.290000000
O	-4.584000000	4.097000000	-14.207000000
C	-6.088000000	5.393000000	-12.834000000
O	-7.287000000	4.605000000	-12.734000000
C	-4.913000000	4.922000000	-11.973000000
C	-4.252000000	3.831000000	-12.819000000
N	-2.771000000	3.782000000	-12.731000000
C	-2.171000000	2.491000000	-12.909000000
O	-2.853000000	1.477000000	-12.941000000
N	-0.768000000	2.466000000	-12.969000000
C	0.060000000	3.618000000	-13.009000000
O	1.248000000	3.452000000	-13.266000000
C	-0.623000000	4.887000000	-12.736000000
C	-1.981000000	4.944000000	-12.669000000
C	0.236000000	6.086000000	-12.543000000
O	-4.898000000	9.348000000	-14.402000000
O	-2.589000000	8.726000000	-13.278000000
H	-0.320000000	1.490000000	-13.073000000
H	-2.536000000	5.894000000	-12.540000000

H	-4.653000000	2.792000000	-12.614000000
H	-4.236000000	5.790000000	-11.790000000
H	-6.380000000	6.449000000	-12.651000000
H	-6.419000000	4.654000000	-14.905000000
H	-4.529000000	6.048000000	-15.943000000
H	0.935000000	5.945000000	-11.703000000
H	0.852000000	6.291000000	-13.432000000
H	-0.342000000	6.999000000	-12.335000000
H	-5.198000000	4.561000000	-10.966000000
H	-5.828000000	7.087000000	-15.220000000
P	-7.800000000	3.917000000	-11.301000000
C	-6.726000000	1.590000000	-11.989000000
O	-6.712000000	2.681000000	-11.043000000
C	-6.774000000	0.259000000	-11.233000000
O	-5.415000000	-0.178000000	-10.971000000
C	-7.463000000	0.304000000	-9.843000000
O	-8.169000000	-0.948000000	-9.767000000
C	-6.311000000	0.530000000	-8.856000000
C	-5.047000000	0.069000000	-9.596000000
N	-3.933000000	1.061000000	-9.612000000
C	-2.580000000	0.543000000	-9.795000000
O	-2.432000000	-0.672000000	-9.904000000
N	-1.533000000	1.439000000	-9.830000000
C	-1.751000000	2.791000000	-9.708000000
N	-0.664000000	3.608000000	-9.788000000
C	-3.086000000	3.305000000	-9.545000000
C	-4.140000000	2.430000000	-9.529000000
O	-9.158000000	3.386000000	-11.682000000
O	-7.587000000	4.831000000	-10.125000000
H	-3.249000000	4.376000000	-9.446000000
H	-5.189000000	2.777000000	-9.441000000
H	-4.628000000	-0.919000000	-9.242000000
H	-6.289000000	1.608000000	-8.578000000
H	-8.265000000	1.069000000	-9.762000000
H	-7.187000000	-0.552000000	-11.878000000
H	-0.760000000	4.615000000	-9.756000000
H	-5.747000000	1.679000000	-12.533000000
H	0.288000000	3.226000000	-9.949000000
H	-6.428000000	0.006000000	-7.885000000
H	-7.558000000	1.663000000	-12.713000000
P	-8.001000000	-2.036000000	-8.517000000
C	-5.754000000	-3.206000000	-9.373000000
O	-6.368000000	-2.344000000	-8.398000000
C	-5.249000000	-4.493000000	-8.708000000
O	-3.867000000	-4.306000000	-8.293000000
C	-6.012000000	-4.932000000	-7.433000000
O	-6.135000000	-6.355000000	-7.640000000
C	-5.108000000	-4.527000000	-6.259000000
C	-3.774000000	-4.084000000	-6.870000000
N	-0.002000000	-0.449000000	-6.611000000

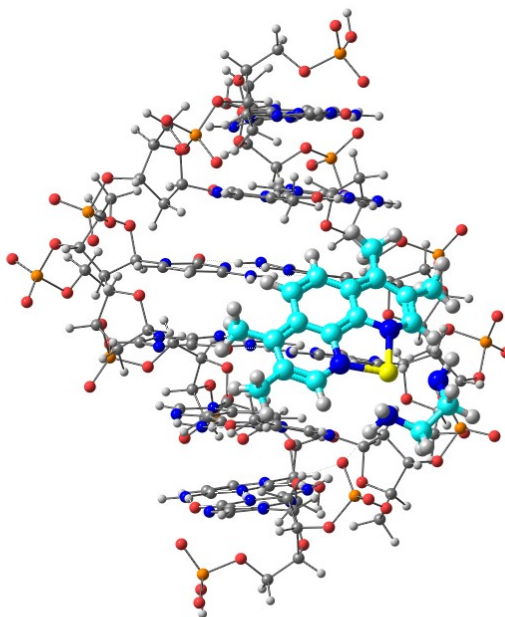
C	0.123000000	-1.855000000	-6.694000000
N	1.390000000	-2.368000000	-6.575000000
N	-0.954000000	-2.713000000	-6.764000000
C	-2.175000000	-2.080000000	-6.693000000
C	-2.380000000	-0.669000000	-6.572000000
C	-1.264000000	0.227000000	-6.625000000
O	-1.244000000	1.457000000	-6.653000000
N	-3.757000000	-0.382000000	-6.503000000
C	-4.381000000	-1.557000000	-6.564000000
N	-3.457000000	-2.657000000	-6.665000000
O	-8.752000000	-3.239000000	-9.026000000
O	-8.315000000	-1.379000000	-7.197000000
H	0.884000000	0.152000000	-6.669000000
H	-5.454000000	-1.731000000	-6.552000000
H	-2.899000000	-4.702000000	-6.537000000
H	-5.597000000	-3.746000000	-5.644000000
H	1.574000000	-3.340000000	-6.800000000
H	-7.040000000	-4.523000000	-7.350000000
H	2.226000000	-1.748000000	-6.649000000
H	-5.177000000	-5.325000000	-9.449000000
H	-4.886000000	-2.601000000	-9.739000000
H	-4.927000000	-5.369000000	-5.550000000
H	-6.424000000	-3.438000000	-10.221000000
P	-6.617000000	-7.365000000	-6.401000000
C	-4.042000000	-7.869000000	-6.355000000
O	-5.189000000	-7.528000000	-5.546000000
C	-2.830000000	-7.800000000	-5.430000000
O	-2.487000000	-6.401000000	-5.209000000
C	-3.068000000	-8.440000000	-4.031000000
O	-2.039000000	-9.440000000	-3.985000000
C	-2.981000000	-7.273000000	-3.040000000
C	-2.211000000	-6.184000000	-3.787000000
N	-0.552000000	-1.256000000	-3.495000000
C	0.132000000	-2.437000000	-3.618000000
N	-0.396000000	-3.687000000	-3.657000000
C	-1.762000000	-3.706000000	-3.527000000
C	-2.591000000	-2.548000000	-3.364000000
C	-1.936000000	-1.276000000	-3.354000000
N	-2.586000000	-0.096000000	-3.157000000
N	-3.937000000	-2.938000000	-3.231000000
C	-3.950000000	-4.271000000	-3.330000000
N	-2.632000000	-4.811000000	-3.506000000
O	-6.962000000	-8.640000000	-7.129000000
O	-7.571000000	-6.706000000	-5.444000000
H	1.232000000	-2.352000000	-3.720000000
H	-4.821000000	-4.915000000	-3.261000000
H	-1.087000000	-6.258000000	-3.671000000
H	-4.006000000	-6.959000000	-2.750000000
H	-4.029000000	-8.992000000	-3.952000000
H	-1.922000000	-8.242000000	-5.917000000

H	-3.933000000	-7.152000000	-7.204000000
H	-2.092000000	0.798000000	-3.316000000
H	-3.598000000	-0.062000000	-3.222000000
H	-2.504000000	-7.530000000	-2.073000000
H	-4.164000000	-8.901000000	-6.748000000
P	-1.109000000	-9.757000000	-2.638000000
C	0.696000000	-7.934000000	-3.355000000
O	-0.310000000	-8.312000000	-2.394000000
C	2.065000000	-7.833000000	-2.671000000
O	2.308000000	-6.434000000	-2.353000000
C	2.217000000	-8.605000000	-1.340000000
O	3.447000000	-9.338000000	-1.484000000
C	2.343000000	-7.531000000	-0.241000000
C	2.204000000	-6.183000000	-0.951000000
N	0.889000000	-5.497000000	-0.689000000
C	0.867000000	-4.045000000	-0.706000000
O	1.933000000	-3.445000000	-0.878000000
N	-0.321000000	-3.378000000	-0.491000000
C	-1.491000000	-4.081000000	-0.284000000
N	-2.619000000	-3.362000000	-0.054000000
C	-1.487000000	-5.520000000	-0.332000000
C	-0.310000000	-6.188000000	-0.542000000
O	-0.169000000	-10.820000000	-3.144000000
O	-1.951000000	-9.927000000	-1.406000000
H	3.605000000	-9.906000000	-0.693000000
H	-2.416000000	-6.069000000	-0.186000000
H	-0.274000000	-7.293000000	-0.600000000
H	3.020000000	-5.445000000	-0.738000000
H	1.622000000	-7.689000000	0.581000000
H	1.410000000	-9.331000000	-1.125000000
H	2.889000000	-8.072000000	-3.388000000
H	-3.515000000	-3.815000000	0.084000000
H	0.369000000	-6.912000000	-3.690000000
H	-2.616000000	-2.326000000	-0.050000000
H	3.326000000	-7.607000000	0.267000000
H	0.737000000	-8.614000000	-4.229000000
O	1.053000000	5.923000000	-19.986000000
O	-1.919000000	5.130000000	2.623000000
H	0.698000000	5.904000000	-20.917000000
H	-1.945000000	5.044000000	3.618000000
N	1.935000000	-6.455000000	-6.251000000
N	2.007000000	-8.740000000	-7.603000000
N	-0.804000000	-8.119000000	-8.724000000
N	-0.686000000	-5.682000000	-7.413000000
C	4.228000000	-5.262000000	-5.138000000
C	2.915000000	-4.816000000	-4.802000000
C	1.808000000	-5.401000000	-5.386000000
C	3.222000000	-6.990000000	-6.502000000
C	3.268000000	-8.120000000	-7.275000000
C	2.046000000	-9.645000000	-8.674000000

C	3.213000000	-10.125000000	-9.191000000
C	4.490000000	-9.588000000	-8.764000000
C	4.528000000	-8.589000000	-7.839000000
C	5.738000000	-7.869000000	-7.390000000
C	5.686000000	-6.837000000	-6.498000000
C	6.923000000	-6.164000000	-5.985000000
C	7.020000000	-8.301000000	-8.028000000
C	-1.825000000	-7.066000000	-9.086000000
C	-1.239000000	-5.675000000	-8.812000000
C	4.409000000	-6.324000000	-5.988000000
Pt	0.621000000	-7.281000000	-7.496000000
H	-1.258000000	-8.904000000	-8.243000000
H	-0.387000000	-8.518000000	-9.610000000
H	-1.436000000	-5.797000000	-6.707000000
H	-0.238000000	-4.772000000	-7.206000000
H	5.078000000	-4.727000000	-4.716000000
H	2.787000000	-4.031000000	-4.067000000
H	0.785000000	-5.057000000	-5.173000000
H	1.069000000	-9.995000000	-9.022000000
H	3.215000000	-10.895000000	-9.950000000
H	5.382000000	-9.969000000	-9.246000000
H	7.803000000	-6.361000000	-6.618000000
H	7.174000000	-6.520000000	-4.977000000
H	6.808000000	-5.073000000	-5.925000000
H	6.905000000	-8.287000000	-9.131000000
H	7.316000000	-9.311000000	-7.731000000
H	7.858000000	-7.626000000	-7.806000000
H	-2.770000000	-7.219000000	-8.511000000
H	-2.107000000	-7.165000000	-10.167000000
H	-2.021000000	-4.885000000	-8.957000000
H	-0.390000000	-5.455000000	-9.517000000

[Pt(en)(3,4,7,8-Me₄phen)]²⁺ systems

[Pt(en)(3,4,7,8-Me₄phen)]²⁺ major groove
Dock_ID: 130-cl5_3,4,7,8-Me₄phen



EDA for 130-cl5_3,4,7,8-Me₄phen in kcal mol⁻¹.

Electrostatic interaction	-755.3
Orbital interaction	-87.2
Dispersion energy	-58.1
Pauli repulsion	108.8
Total Bonding Energy	-791.8

Contributions of the solvation energies for 130-cl5_3,4,7,8-Me₄phen in kcal mol⁻¹.

E _{solv} (total system)	-1746.6
E _{solv} (intercalator)	-154.7
E _{solv} (duplex DNA)	-2320.8
ΔE _{solv}	728.8
ΔE _{int} (EDA)	-791.8
ΔE _{aq}	-63.0

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 130-cl5_3,4,7,8-Me₄phen system.
([Pt(en)(3,4,7,8-Me₄phen)]²⁺ major groove)

P	-1.241000000	6.734000000	2.505000000
C	1.281000000	5.998000000	2.266000000
O	0.083000000	6.393000000	1.556000000
C	2.430000000	6.060000000	1.255000000
O	2.676000000	4.724000000	0.729000000
C	2.165000000	6.963000000	0.019000000
O	3.385000000	7.712000000	-0.099000000
C	1.834000000	5.991000000	-1.121000000
C	2.136000000	4.583000000	-0.597000000
N	0.370000000	-0.320000000	-0.671000000
C	1.664000000	0.178000000	-0.959000000
N	2.597000000	-0.725000000	-1.411000000
N	1.995000000	1.506000000	-0.869000000
C	0.929000000	2.331000000	-0.590000000
C	-0.418000000	1.914000000	-0.361000000
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N	0.927000000	3.730000000	-0.509000000
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H	0.773000000	6.127000000	-1.442000000
H	3.556000000	-0.400000000	-1.534000000
H	1.364000000	7.717000000	0.196000000
H	2.496000000	-1.730000000	-1.167000000
H	3.391000000	6.314000000	1.761000000
H	1.149000000	4.959000000	2.637000000
H	2.419000000	6.181000000	-2.052000000
H	1.473000000	6.678000000	3.118000000
P	4.076000000	8.135000000	-1.560000000
C	5.263000000	5.783000000	-1.438000000
O	4.455000000	6.664000000	-2.251000000
C	5.695000000	4.634000000	-2.348000000
O	4.611000000	3.663000000	-2.448000000
C	6.057000000	5.074000000	-3.793000000
O	7.353000000	4.477000000	-3.975000000
C	4.930000000	4.514000000	-4.667000000
C	4.331000000	3.369000000	-3.845000000
N	2.857000000	3.236000000	-3.963000000
C	2.301000000	1.906000000	-3.944000000
O	3.026000000	0.931000000	-4.020000000
N	0.895000000	1.820000000	-3.912000000

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C	3.481000000	2.878000000	-7.313000000
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O	9.350000000	3.646000000	-5.180000000
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H	3.549000000	3.960000000	-7.383000000
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O	1.193000000	-11.066000000	-12.978000000
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C	-0.845000000	2.701000000	-16.381000000
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O	1.898000000	0.353000000	-16.940000000
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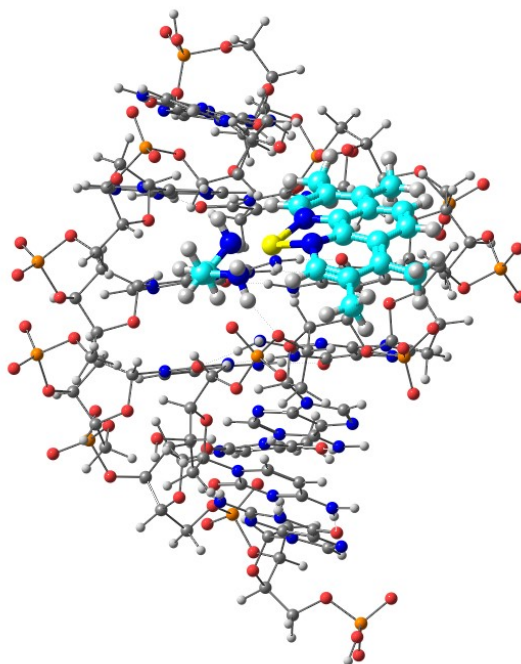
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P	-5.041000000	7.108000000	-10.016000000
H	-7.511000000	7.015000000	-9.121000000
H	-7.332000000	5.995000000	-10.433000000
H	-5.013000000	9.297000000	-11.484000000
H	-4.641000000	7.992000000	-12.478000000
H	-0.408000000	9.053000000	-12.316000000
H	1.022000000	8.415000000	-11.502000000
H	0.198000000	9.830000000	-10.851000000
H	-2.624000000	8.454000000	-11.603000000
H	1.763000000	7.552000000	-10.071000000
H	1.577000000	6.139000000	-9.028000000
H	1.520000000	7.772000000	-8.335000000
H	0.337000000	5.638000000	-7.180000000
H	-8.666000000	7.842000000	-11.263000000
H	-7.692000000	8.995000000	-10.319000000
H	-6.847000000	7.431000000	-12.875000000
H	-7.009000000	9.195000000	-12.675000000
H	-6.668000000	4.994000000	-8.467000000
H	-1.297000000	4.260000000	-5.919000000
H	-2.790000000	3.477000000	-4.753000000
H	-3.406000000	2.184000000	-5.779000000
H	-4.502000000	3.005000000	-4.658000000
H	-7.246000000	3.080000000	-7.163000000
H	-6.584000000	3.156000000	-5.534000000
H	-5.863000000	2.055000000	-6.718000000

[Pt(en)(3,4,7,8-Me₄phen)]²⁺ minor groove
Dock_ID: 56-cl4_3,4,7,8-Me₄phen



EDA analysis for 3,4,7,8-Me₄phen in kcal mol⁻¹.

Electrostatic interaction	-808.7
Orbital interaction	-99.8
Dispersion energy	-78.6
Pauli repulsion	155.7
Total Bonding Energy	-831.4

Contributions of the solvation energies for 3,4,7,8-Me₄phen in kcal mol⁻¹.

E _{solv} (total system)	-1723.3
E _{solv} (intercalator)	-155.68
E _{solv} (duplex DNA)	-2340.7
ΔE _{solv}	773.1
ΔE _{int} (EDA)	-831.4
ΔE _{aq}	-58.3

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 56-cl4_3,4,7,8-Me₄phen system.
([Pt(en)(3,4,7,8-Me₄phen)]²⁺ minor groove)

P	-1.89500000	6.80000000	2.89600000
C	0.65200000	6.48500000	2.26300000
O	-0.68800000	6.68500000	1.75600000
C	1.58900000	6.61000000	1.05600000
O	1.83600000	5.28200000	0.51100000
C	1.00900000	7.44900000	-0.11300000
O	2.08400000	8.28000000	-0.56800000
C	0.45200000	6.41200000	-1.09500000
C	1.07000000	5.06800000	-0.69000000
N	-0.08200000	-0.03700000	-0.71400000
C	1.10000000	0.62500000	-1.12400000
N	2.13000000	-0.14600000	-1.61200000
N	1.29200000	1.97800000	-1.00300000
C	0.19800000	2.66000000	-0.52100000
C	-1.03100000	2.06800000	-0.09200000
C	-1.21300000	0.65100000	-0.17000000
O	-2.18300000	-0.03500000	0.15800000
N	-1.92800000	3.07800000	0.31400000
C	-1.28300000	4.23300000	0.15000000
N	0.03700000	4.04400000	-0.39400000
O	-1.54500000	7.79600000	3.97500000
O	-3.15600000	6.89300000	2.07900000
H	-0.16100000	-1.09700000	-0.85600000
H	-1.65400000	5.23200000	0.37700000
H	1.81800000	4.63700000	-1.41400000
H	-0.65700000	6.41800000	-1.03200000
H	2.79800000	0.30800000	-2.25200000
H	0.23900000	8.18000000	0.22900000
H	1.98100000	-1.16500000	-1.76600000
H	2.60100000	6.95300000	1.37000000
H	0.72500000	5.46900000	2.70500000
H	0.65400000	6.65300000	-2.16500000
H	0.89200000	7.24700000	3.03000000
P	2.71200000	8.24100000	-2.12000000
C	4.29600000	6.21300000	-1.47800000
O	3.24900000	6.68900000	-2.35200000
C	5.06200000	5.14300000	-2.26100000
O	4.17800000	4.01500000	-2.50400000
C	5.57000000	5.60300000	-3.65700000
O	6.84700000	4.95300000	-3.77600000
C	4.48000000	5.12300000	-4.62000000
C	3.87100000	3.90700000	-3.91800000
N	2.39400000	3.79100000	-4.03600000
C	1.86200000	2.46400000	-3.91900000
O	2.59800000	1.48800000	-3.90700000
N	0.46300000	2.36000000	-3.91900000

C	-0.42800000	3.46200000	-3.82000000
O	-1.60300000	3.21500000	-3.56200000
C	0.18800000	4.77600000	-4.02600000
C	1.54200000	4.90800000	-4.06000000
C	-0.72200000	5.94400000	-4.18100000
O	3.84600000	9.22700000	-1.99900000
O	1.63100000	8.36900000	-3.16100000
H	0.06900000	1.35600000	-3.87300000
H	2.04300000	5.89400000	-4.13500000
H	4.32400000	2.91700000	-4.22900000
H	3.74300000	5.94900000	-4.76000000
H	5.77300000	6.69300000	-3.72000000
H	5.88400000	4.71700000	-1.64100000
H	3.79800000	5.76300000	-0.59000000
H	-1.18800000	5.95500000	-5.17800000
H	-1.53800000	5.92500000	-3.44200000
H	-0.19500000	6.90500000	-4.05400000
H	4.84000000	4.88900000	-5.64100000
H	4.97200000	7.02500000	-1.15200000
P	7.41700000	4.28800000	-5.19900000
C	6.52900000	1.87700000	-4.52900000
O	6.44000000	2.96600000	-5.47300000
C	6.63700000	0.55300000	-5.29000000
O	5.30000000	0.06300000	-5.57500000
C	7.36200000	0.61500000	-6.66100000
O	8.14500000	-0.59400000	-6.66200000
C	6.23100000	0.71600000	-7.69200000
C	4.96500000	0.23800000	-6.96800000
N	3.82200000	1.19100000	-7.04600000
C	2.46700000	0.65100000	-6.96200000
O	2.32400000	-0.56400000	-6.83200000
N	1.40600000	1.52700000	-7.04800000
C	1.60900000	2.88300000	-7.14400000
N	0.50800000	3.68400000	-7.16000000
C	2.94400000	3.42100000	-7.19800000
C	4.01000000	2.56600000	-7.11500000
O	8.80900000	3.86900000	-4.79800000
O	7.14600000	5.17900000	-6.38100000
H	3.09700000	4.49500000	-7.28100000
H	5.05500000	2.93300000	-7.11900000
H	4.59900000	-0.78200000	-7.28800000
H	6.16600000	1.76700000	-8.05200000
H	8.10200000	1.43900000	-6.74100000
H	7.06700000	-0.24100000	-4.63300000
H	0.59500000	4.69100000	-7.18800000
H	5.55700000	1.90600000	-3.97100000
H	-0.45000000	3.29400000	-7.06000000
H	6.40300000	0.13600000	-8.62200000
H	7.36900000	1.99400000	-3.81900000
P	8.30600000	-1.59500000	-7.98100000

C	6.08000000	-2.95200000	-7.43200000
O	6.75000000	-2.07100000	-8.35400000
C	5.59500000	-4.20100000	-8.18200000
O	4.16200000	-4.06200000	-8.40800000
C	6.23900000	-4.44200000	-9.57100000
O	6.66000000	-5.81800000	-9.49400000
C	5.12100000	-4.18900000	-10.59300000
C	3.86600000	-3.82400000	-9.79800000
N	-0.02000000	-0.33600000	-10.21400000
C	-0.09400000	-1.74200000	-10.11100000
N	-1.33300000	-2.33000000	-10.23000000
N	1.01200000	-2.56000000	-10.02700000
C	2.20400000	-1.87500000	-10.02000000
C	2.36600000	-0.45800000	-10.13100000
C	1.21500000	0.39400000	-10.19400000
O	1.14500000	1.62000000	-10.24000000
N	3.73400000	-0.12400000	-10.11800000
C	4.39400000	-1.27700000	-10.01600000
N	3.50100000	-2.40600000	-9.95900000
O	9.11700000	-2.73100000	-7.41500000
O	8.72800000	-0.82500000	-9.20600000
H	-0.93200000	0.23500000	-10.20700000
H	5.47100000	-1.41400000	-9.95300000
H	2.96700000	-4.47000000	-10.00400000
H	5.42500000	-3.41000000	-11.32100000
H	-1.49100000	-3.25200000	-9.83000000
H	7.13700000	-3.81700000	-9.76300000
H	-2.19300000	-1.73900000	-10.26400000
H	5.66400000	-5.11300000	-7.54100000
H	5.20200000	-2.35900000	-7.06800000
H	4.91600000	-5.08100000	-11.22600000
H	6.71400000	-3.23300000	-6.57200000
P	7.24700000	-6.57100000	-10.86800000
C	4.85700000	-7.64500000	-10.79400000
O	5.82200000	-6.97600000	-11.64300000
C	3.66900000	-8.01000000	-11.68200000
O	2.80800000	-6.85000000	-11.85400000
C	4.05400000	-8.51300000	-13.09800000
O	3.47800000	-9.81900000	-13.21200000
C	3.56900000	-7.43100000	-14.06700000
C	2.67200000	-6.49400000	-13.25100000
N	1.04900000	-1.47900000	-13.27400000
C	0.36000000	-2.64600000	-13.08900000
N	0.86600000	-3.90700000	-13.05400000
C	2.22200000	-3.96000000	-13.28200000
C	3.05400000	-2.80900000	-13.48600000
C	2.42600000	-1.52200000	-13.47100000
N	3.08700000	-0.35500000	-13.67800000
N	4.38500000	-3.21100000	-13.69800000
C	4.38200000	-4.54800000	-13.62500000

N	3.07200000	-5.07500000	-13.38100000
O	7.93400000	-7.79200000	-10.31000000
O	7.94100000	-5.62100000	-11.80500000
H	-0.74900000	-2.53800000	-12.95200000
H	5.24600000	-5.20100000	-13.72500000
H	1.56600000	-6.59000000	-13.45500000
H	4.44500000	-6.92300000	-14.52200000
H	5.14800000	-8.71200000	-13.19900000
H	3.01900000	-8.75000000	-11.15100000
H	4.54300000	-6.95500000	-9.98000000
H	2.61500000	0.55600000	-13.53300000
H	4.10000000	-0.34100000	-13.72500000
H	3.04000000	-7.83200000	-14.95900000
H	5.30300000	-8.56300000	-10.36000000
P	2.18200000	-10.19300000	-14.20300000
C	0.33000000	-9.04100000	-12.68800000
O	1.07300000	-8.98400000	-13.92500000
C	-1.00100000	-8.34800000	-12.96500000
O	-0.69100000	-6.95400000	-13.27500000
C	-1.77700000	-8.90300000	-14.18000000
O	-2.87600000	-9.63500000	-13.61600000
C	-2.27900000	-7.66300000	-14.93900000
C	-1.47200000	-6.48600000	-14.39300000
N	-0.46800000	-5.95000000	-15.37100000
C	-0.48000000	-4.51900000	-15.63500000
O	-1.49100000	-3.88800000	-15.32400000
N	0.61600000	-3.93300000	-16.23100000
C	1.70300000	-4.70200000	-16.59800000
N	2.80500000	-4.04300000	-17.03400000
C	1.64600000	-6.13800000	-16.48300000
C	0.58700000	-6.72400000	-15.84200000
O	1.72600000	-11.51400000	-13.63800000
O	2.55200000	-10.00000000	-15.64800000
H	-3.30600000	-10.18900000	-14.30800000
H	2.44900000	-6.74500000	-16.89900000
H	0.53700000	-7.81400000	-15.65300000
H	-2.08500000	-5.62700000	-14.00800000
H	-2.19800000	-7.78300000	-16.03300000
H	-1.18200000	-9.58600000	-14.82000000
H	-1.66000000	-8.30600000	-12.04200000
H	3.62800000	-4.53800000	-17.35700000
H	0.92100000	-8.47700000	-11.92300000
H	2.84700000	-3.00600000	-17.05200000
H	-3.36500000	-7.51800000	-14.75000000
H	0.16600000	-10.08200000	-12.34400000
P	2.21000000	5.75900000	-19.65300000
C	-0.40300000	5.18100000	-19.64800000
O	0.60000000	6.19900000	-19.80200000
C	-1.13100000	5.30200000	-18.30200000
O	-1.06800000	3.99400000	-17.66800000

C	-0.55100000	6.31400000	-17.28100000
O	-1.66800000	7.05000000	-16.76700000
C	0.24800000	5.46200000	-16.29000000
C	-0.26900000	4.03400000	-16.45900000
N	0.69600000	-1.07700000	-16.45100000
C	-0.48400000	-0.37300000	-16.11400000
N	-1.60800000	-1.11200000	-15.79300000
N	-0.59300000	0.98900000	-16.16800000
C	0.56800000	1.63300000	-16.53500000
C	1.80900000	0.99900000	-16.85100000
C	1.91200000	-0.42800000	-16.84100000
O	2.86600000	-1.15700000	-17.12000000
N	2.78100000	1.98100000	-17.13500000
C	2.16500000	3.15900000	-17.01500000
N	0.79200000	3.01300000	-16.61700000
O	2.90000000	6.55600000	-20.73400000
O	2.65000000	5.83600000	-18.21600000
H	0.70300000	-2.14700000	-16.38700000
H	2.60200000	4.15300000	-17.17800000
H	-0.97700000	3.68700000	-15.65300000
H	1.33600000	5.56200000	-16.53000000
H	-2.29300000	-0.64900000	-15.17100000
H	0.05700000	7.11400000	-17.76300000
H	-1.48800000	-2.12700000	-15.58500000
H	-2.22300000	5.46500000	-18.46200000
H	0.00500000	4.15300000	-19.77400000
H	0.17100000	5.81000000	-15.22800000
H	-1.09500000	5.38400000	-20.49100000
P	-2.32300000	6.86400000	-15.23800000
C	-3.63200000	4.65300000	-15.91700000
O	-2.64100000	5.24200000	-15.05100000
C	-4.61400000	3.83800000	-15.07400000
O	-4.01400000	2.55100000	-14.75600000
C	-5.05000000	4.47300000	-13.72900000
O	-6.48800000	4.41200000	-13.80800000
C	-4.44800000	3.58000000	-12.63800000
C	-3.73600000	2.43200000	-13.35000000
N	-2.25300000	2.43400000	-13.15100000
C	-1.60300000	1.16000000	-13.23600000
O	-2.25200000	0.12800000	-13.32500000
N	-0.19900000	1.15200000	-13.15000000
C	0.60400000	2.32300000	-13.16700000
O	1.82100000	2.17800000	-13.27000000
C	-0.12700000	3.58700000	-13.08300000
C	-1.48900000	3.61400000	-13.11900000
C	0.67100000	4.83500000	-12.94500000
O	-3.59900000	7.66000000	-15.35600000
O	-1.28900000	7.13700000	-14.18000000
H	0.26600000	0.19000000	-13.15800000
H	-2.05500000	4.56200000	-13.11000000

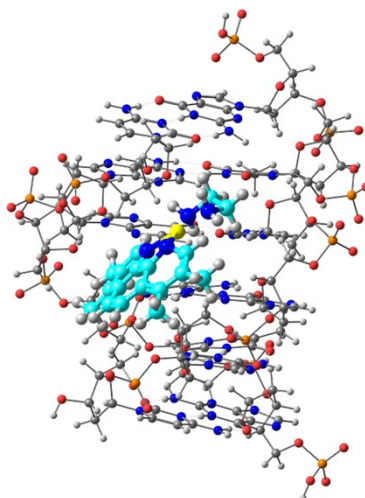
H	-4.11700000	1.40700000	-13.07900000
H	-3.79400000	4.17100000	-11.96600000
H	-4.76700000	5.54200000	-13.63200000
H	-5.50500000	3.55900000	-15.69200000
H	-3.05700000	3.97700000	-16.59400000
H	0.69300000	5.18900000	-11.90400000
H	1.71300000	4.69600000	-13.26800000
H	0.25300000	5.66100000	-13.55700000
H	-5.23400000	3.15800000	-11.96700000
H	-4.17400000	5.40400000	-16.52200000
P	-7.43800000	4.62200000	-12.44400000
C	-7.67400000	2.01500000	-12.59900000
O	-7.36000000	3.12200000	-11.71700000
C	-7.74000000	0.75000000	-11.74200000
O	-6.40100000	0.29800000	-11.42900000
C	-8.48400000	0.91300000	-10.38900000
O	-9.32000000	-0.26000000	-10.36400000
C	-7.37400000	0.98400000	-9.33600000
C	-6.13600000	0.38100000	-10.00600000
N	-4.88500000	1.17400000	-9.86500000
C	-3.62600000	0.44200000	-10.02900000
O	-3.68700000	-0.76800000	-10.17800000
N	-2.44700000	1.15900000	-10.00800000
C	-2.44400000	2.52000000	-9.81700000
N	-1.23500000	3.14000000	-9.84900000
C	-3.67900000	3.23100000	-9.59400000
C	-4.86400000	2.54600000	-9.63900000
O	-8.79900000	4.86400000	-13.05200000
O	-6.82800000	5.56700000	-11.44700000
H	-3.66300000	4.30000000	-9.39200000
H	-5.84000000	3.05000000	-9.50700000
H	-5.91800000	-0.68700000	-9.69700000
H	-7.23600000	2.04400000	-9.02700000
H	-9.16900000	1.78800000	-10.36100000
H	-8.17000000	-0.09200000	-12.34000000
H	-1.15200000	4.13800000	-9.73000000
H	-6.86700000	1.92200000	-13.35800000
H	-0.36300000	2.60300000	-10.03700000
H	-7.61100000	0.45200000	-8.39100000
H	-8.64700000	2.18800000	-13.10100000
P	-9.75900000	-1.04900000	-8.96300000
C	-7.63300000	-2.60200000	-9.15500000
O	-8.33600000	-1.63000000	-8.34200000
C	-6.83500000	-3.50300000	-8.20700000
O	-5.55800000	-2.86400000	-7.97000000
C	-7.48700000	-3.72600000	-6.81600000
O	-7.38000000	-5.12000000	-6.50500000
C	-6.76700000	-2.73000000	-5.89400000
C	-5.43600000	-2.44700000	-6.59300000
N	-1.27600000	0.56300000	-6.91100000

C	-1.42100000	-0.83500000	-7.05600000
N	-0.29100000	-1.57800000	-7.36600000
N	-2.61100000	-1.48200000	-6.95600000
C	-3.68700000	-0.65000000	-6.76700000
C	-3.64700000	0.77700000	-6.65900000
C	-2.38600000	1.45500000	-6.75600000
O	-2.12900000	2.65800000	-6.70900000
N	-4.95200000	1.26700000	-6.47400000
C	-5.75600000	0.19400000	-6.46000000
N	-5.02600000	-1.02400000	-6.62100000
O	-10.61800000	-2.16700000	-9.50600000
O	-10.27000000	-0.08600000	-7.92300000
H	-0.29600000	0.98700000	-6.98900000
H	-6.83400000	0.19700000	-6.34300000
H	-4.56100000	-3.04100000	-6.19200000
H	-7.39900000	-1.82700000	-5.77800000
H	-0.36500000	-2.58800000	-7.23100000
H	-8.58900000	-3.57400000	-6.82700000
H	0.64600000	-1.18600000	-7.13800000
H	-6.56500000	-4.46500000	-8.71200000
H	-6.92000000	-2.02800000	-9.80000000
H	-6.61900000	-3.11300000	-4.86100000
H	-8.32600000	-3.19400000	-9.77900000
P	-6.22400000	-5.78300000	-5.49100000
C	-4.17900000	-5.46600000	-7.25300000
O	-4.75400000	-5.19100000	-5.95800000
C	-2.78000000	-6.04400000	-7.05700000
O	-1.82600000	-5.05400000	-6.56300000
C	-2.73000000	-7.19800000	-6.02700000
O	-1.78300000	-8.10900000	-6.62300000
C	-2.24000000	-6.54000000	-4.72600000
C	-1.57600000	-5.22600000	-5.16200000
N	-0.46700000	-0.29900000	-3.86600000
C	0.33600000	-1.31500000	-4.30900000
N	-0.03400000	-2.59800000	-4.55600000
C	-1.36600000	-2.84300000	-4.30000000
C	-2.28400000	-1.86700000	-3.78200000
C	-1.80900000	-0.53400000	-3.60200000
N	-2.58200000	0.51000000	-3.19500000
N	-3.55500000	-2.45100000	-3.62300000
C	-3.43200000	-3.71800000	-4.03300000
N	-2.09400000	-4.03300000	-4.44100000
O	-6.39800000	-7.26700000	-5.62600000
O	-6.34000000	-5.15500000	-4.11100000
H	1.38800000	-1.03300000	-4.52000000
H	-4.23400000	-4.46300000	-4.05200000
H	-0.45400000	-5.22000000	-5.06600000
H	-3.09600000	-6.38800000	-4.04100000
H	-3.68900000	-7.75000000	-5.91700000
H	-2.33800000	-6.31400000	-8.06200000

H	-4.12000000	-4.46700000	-7.75800000
H	-2.22800000	1.48100000	-3.23600000
H	-3.58000000	0.38400000	-3.07000000
H	-1.53600000	-7.16900000	-4.14400000
H	-4.80100000	-6.15700000	-7.85700000
P	-1.04200000	-9.34800000	-5.80100000
C	0.97900000	-7.70800000	-5.48000000
O	0.00300000	-8.51600000	-4.78800000
C	1.99000000	-7.23300000	-4.43800000
O	1.60500000	-5.87300000	-4.06400000
C	2.04700000	-8.03400000	-3.11700000
O	3.21700000	-8.85700000	-3.23300000
C	2.22300000	-6.97500000	-2.01700000
C	1.92500000	-5.62500000	-2.67100000
N	0.74100000	-4.93400000	-2.08600000
C	0.85000000	-3.52300000	-1.75700000
O	1.93700000	-2.96300000	-1.94200000
N	-0.23600000	-2.86600000	-1.22800000
C	-1.42300000	-3.53900000	-1.00000000
N	-2.44500000	-2.83400000	-0.46400000
C	-1.54100000	-4.93900000	-1.34200000
C	-0.47600000	-5.59300000	-1.89000000
O	-0.28500000	-9.99300000	-6.93600000
O	-1.93000000	-10.10400000	-4.85700000
H	3.29400000	-9.45700000	-2.45200000
H	-2.48600000	-5.45600000	-1.17400000
H	-0.52700000	-6.65200000	-2.19000000
H	2.78900000	-4.90900000	-2.67600000
H	1.60400000	-7.19000000	-1.12600000
H	1.16400000	-8.69000000	-2.95100000
H	3.00900000	-7.14400000	-4.88700000
H	-3.35200000	-3.25500000	-0.29000000
H	0.46300000	-6.83400000	-5.93900000
H	-2.36300000	-1.82200000	-0.26300000
H	3.26000000	-7.00100000	-1.61900000
H	1.49000000	-8.31300000	-6.25900000
O	2.20600000	4.14200000	-20.05500000
O	-1.86600000	5.27400000	3.57900000
H	2.20200000	3.93700000	-21.03300000
H	-1.41900000	5.20200000	4.46500000
N	-3.02600000	-5.60000000	-11.28900000
N	-0.52000000	-7.97200000	-9.17000000
N	-0.09400000	-5.69100000	-10.71900000
N	-3.46300000	-7.88800000	-10.00300000
C	-6.05800000	-8.35700000	-8.84000000
C	-5.93000000	-7.39200000	-9.79800000
C	-4.60200000	-7.06600000	-10.30700000
C	-4.37800000	-5.91200000	-11.01300000
C	-5.44600000	-5.00700000	-11.42200000
C	-5.12100000	-3.82700000	-12.05400000

C	-3.73500000	-3.55000000	-12.35000000
C	-3.34500000	-2.28300000	-13.03000000
C	-2.74700000	-4.42900000	-11.94400000
C	-6.14900000	-2.81500000	-12.43600000
C	-6.78900000	-5.45200000	-11.06600000
C	0.89800000	-7.55400000	-9.46300000
C	0.92800000	-6.03500000	-9.67200000
C	-3.62600000	-8.72400000	-8.89000000
C	-7.01400000	-6.55600000	-10.32000000
C	-7.36900000	-8.70600000	-8.22400000
C	-4.84600000	-9.01200000	-8.34300000
C	-4.94800000	-9.92600000	-7.16600000
Pt	-1.79800000	-6.79600000	-10.28900000
H	-0.62800000	-8.98400000	-9.31600000
H	-0.74400000	-7.82100000	-8.16100000
H	0.24500000	-5.94200000	-11.66500000
H	-0.24200000	-4.67000000	-10.73400000
H	-3.58700000	-1.41200000	-12.38800000
H	-3.86300000	-2.14800000	-13.98400000
H	-2.25800000	-2.23200000	-13.22300000
H	-1.68800000	-4.23200000	-12.15600000
H	-5.92500000	-1.83700000	-11.96200000
H	-7.16600000	-3.09300000	-12.13800000
H	-6.16200000	-2.63800000	-13.52000000
H	-7.62100000	-4.84800000	-11.43100000
H	1.59000000	-7.86000000	-8.64900000
H	1.25200000	-8.07700000	-10.39400000
H	0.67600000	-5.49100000	-8.72900000
H	1.95500000	-5.70100000	-9.98600000
H	-2.71200000	-9.19100000	-8.51500000
H	-8.02500000	-6.86200000	-10.04900000
H	-8.22500000	-8.24700000	-8.73100000
H	-7.37500000	-8.33300000	-7.17900000
H	-7.54400000	-9.78500000	-8.18200000
H	-5.67700000	-10.72800000	-7.32400000
H	-5.29500000	-9.34600000	-6.29000000
H	-4.00000000	-10.40100000	-6.89700000

[Pt(en)(3,4,7,8-Me₄phen)]²⁺ minor groove
Dock_ID: 71-cl2_3,4,7,8-Me₄phen



EDA analysis for 71-cl2_3,4,7,8-Me₄phen in kcal mol⁻¹.

Electrostatic interaction	-799.6
Orbital interaction	-77.2
Dispersion energy	-70.7
Pauli repulsion	113.1
Total Bonding Energy	-814.4

Contributions of the solvation energies for 71-cl2_3,4,7,8-Me₄phen in kcal mol⁻¹.

E _{solv} (total system)	-1752.2
E _{solv} (intercalator)	-155.8
E _{solv} (duplex DNA)	-2352.9
ΔE _{solv}	756.6
ΔE _{int} (EDA)	-814.4
ΔE _{aq}	-57.8

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 71-cl2_3,4,7,8-Me₄phen system.
([Pt(en)(3,4,7,8-Me₄phen)]²⁺ minor groove)

P	-2.378000000	7.215000000	2.034000000
C	0.134000000	6.560000000	1.559000000
O	-1.171000000	6.789000000	0.973000000
C	1.135000000	6.557000000	0.398000000
O	1.362000000	5.181000000	-0.022000000
C	0.646000000	7.311000000	-0.867000000
O	1.777000000	8.049000000	-1.350000000
C	0.079000000	6.213000000	-1.773000000
C	0.643000000	4.890000000	-1.239000000
N	-0.655000000	-0.173000000	-0.923000000
C	0.558000000	0.425000000	-1.347000000
N	1.577000000	-0.406000000	-1.735000000
N	0.778000000	1.781000000	-1.339000000
C	-0.310000000	2.524000000	-0.948000000
C	-1.577000000	2.000000000	-0.540000000
C	-1.803000000	0.587000000	-0.535000000
O	-2.819000000	-0.046000000	-0.241000000
N	-2.452000000	3.060000000	-0.227000000
C	-1.760000000	4.182000000	-0.428000000
N	-0.426000000	3.918000000	-0.900000000
O	-1.887000000	8.201000000	3.066000000
O	-3.573000000	7.479000000	1.157000000
H	-0.756000000	-1.240000000	-0.988000000
H	-2.098000000	5.205000000	-0.265000000
H	1.410000000	4.384000000	-1.892000000
H	-1.031000000	6.257000000	-1.735000000
H	2.307000000	-0.018000000	-2.349000000
H	-0.098000000	8.105000000	-0.627000000
H	1.423000000	-1.433000000	-1.787000000
H	2.142000000	6.892000000	0.737000000
H	0.126000000	5.571000000	2.064000000
H	0.309000000	6.359000000	-2.857000000
H	0.380000000	7.352000000	2.292000000
P	2.489000000	7.796000000	-2.843000000
C	3.913000000	5.760000000	-1.915000000
O	2.927000000	6.197000000	-2.876000000
C	4.631000000	4.564000000	-2.544000000
O	3.678000000	3.487000000	-2.750000000
C	5.271000000	4.855000000	-3.930000000
O	6.520000000	4.144000000	-3.864000000
C	4.244000000	4.328000000	-4.934000000
C	3.482000000	3.244000000	-4.166000000
N	2.016000000	3.234000000	-4.413000000
C	1.351000000	1.972000000	-4.229000000
O	1.998000000	0.938000000	-4.138000000
N	-0.053000000	1.997000000	-4.264000000

C	-0.833000000	3.183000000	-4.325000000
O	-2.040000000	3.089000000	-4.125000000
C	-0.084000000	4.411000000	-4.601000000
C	1.277000000	4.419000000	-4.563000000
C	-0.860000000	5.638000000	-4.927000000
O	3.680000000	8.717000000	-2.767000000
O	1.474000000	7.877000000	-3.955000000
H	-0.548000000	1.045000000	-4.154000000
H	1.870000000	5.348000000	-4.680000000
H	3.875000000	2.197000000	-4.336000000
H	3.587000000	5.174000000	-5.246000000
H	5.535000000	5.924000000	-4.085000000
H	5.375000000	4.137000000	-1.830000000
H	3.361000000	5.447000000	-1.001000000
H	-1.045000000	5.720000000	-6.008000000
H	-1.838000000	5.652000000	-4.423000000
H	-0.327000000	6.556000000	-4.615000000
H	4.679000000	3.943000000	-5.879000000
H	4.630000000	6.562000000	-1.656000000
P	7.181000000	3.331000000	-5.162000000
C	6.052000000	1.010000000	-4.497000000
O	6.108000000	2.086000000	-5.454000000
C	6.323000000	-0.326000000	-5.200000000
O	5.042000000	-0.976000000	-5.443000000
C	7.036000000	-0.239000000	-6.572000000
O	8.106000000	-1.198000000	-6.446000000
C	5.999000000	-0.684000000	-7.611000000
C	4.713000000	-0.993000000	-6.848000000
N	3.637000000	0.016000000	-7.084000000
C	2.241000000	-0.416000000	-7.052000000
O	1.996000000	-1.611000000	-6.909000000
N	1.258000000	0.534000000	-7.233000000
C	1.573000000	1.868000000	-7.357000000
N	0.545000000	2.749000000	-7.460000000
C	2.948000000	2.300000000	-7.374000000
C	3.935000000	1.372000000	-7.206000000
O	8.474000000	2.825000000	-4.576000000
O	7.120000000	4.149000000	-6.422000000
H	3.185000000	3.352000000	-7.515000000
H	5.000000000	1.665000000	-7.172000000
H	4.283000000	-2.012000000	-7.026000000
H	5.878000000	0.070000000	-8.409000000
H	7.462000000	0.765000000	-6.795000000
H	6.846000000	-1.037000000	-4.516000000
H	0.713000000	3.744000000	-7.505000000
H	4.994000000	1.035000000	-4.123000000
H	-0.444000000	2.438000000	-7.381000000
H	6.329000000	-1.597000000	-8.172000000
H	6.746000000	1.156000000	-3.649000000
P	9.326000000	-1.147000000	-7.586000000

C	8.170000000	-3.383000000	-8.326000000
O	8.749000000	-2.141000000	-8.792000000
C	7.270000000	-3.908000000	-9.446000000
O	6.065000000	-3.105000000	-9.510000000
C	7.918000000	-3.882000000	-10.858000000
O	7.956000000	-5.233000000	-11.332000000
C	7.106000000	-2.867000000	-11.669000000
C	5.816000000	-2.657000000	-10.873000000
N	1.553000000	0.188000000	-10.367000000
C	1.753000000	-1.208000000	-10.272000000
N	0.652000000	-2.008000000	-10.161000000
N	2.983000000	-1.809000000	-10.349000000
C	4.007000000	-0.933000000	-10.573000000
C	3.911000000	0.495000000	-10.643000000
C	2.624000000	1.126000000	-10.536000000
O	2.301000000	2.313000000	-10.557000000
N	5.190000000	1.034000000	-10.875000000
C	6.032000000	-0.004000000	-10.951000000
N	5.357000000	-1.258000000	-10.774000000
O	10.476000000	-1.815000000	-6.865000000
O	9.474000000	0.213000000	-8.212000000
H	0.553000000	0.565000000	-10.290000000
H	7.103000000	0.041000000	-11.111000000
H	4.947000000	-3.285000000	-11.232000000
H	7.695000000	-1.936000000	-11.795000000
H	0.781000000	-3.010000000	-10.014000000
H	9.003000000	-3.624000000	-10.824000000
H	-0.290000000	-1.617000000	-10.012000000
H	6.914000000	-4.933000000	-9.176000000
H	7.574000000	-3.226000000	-7.399000000
H	6.901000000	-3.199000000	-12.708000000
H	8.992000000	-4.097000000	-8.122000000
P	6.766000000	-5.950000000	-12.266000000
C	4.548000000	-5.944000000	-10.742000000
O	5.333000000	-5.293000000	-11.758000000
C	3.297000000	-6.590000000	-11.349000000
O	2.379000000	-5.559000000	-11.800000000
C	3.548000000	-7.494000000	-12.585000000
O	2.665000000	-8.613000000	-12.396000000
C	3.269000000	-6.582000000	-13.786000000
C	2.399000000	-5.445000000	-13.233000000
N	1.182000000	-0.376000000	-13.516000000
C	0.404000000	-1.474000000	-13.255000000
N	0.810000000	-2.767000000	-13.214000000
C	2.155000000	-2.920000000	-13.477000000
C	3.062000000	-1.845000000	-13.771000000
C	2.540000000	-0.518000000	-13.750000000
N	3.296000000	0.606000000	-13.880000000
N	4.357000000	-2.355000000	-13.985000000
C	4.253000000	-3.683000000	-13.847000000

N	2.915000000	-4.097000000	-13.564000000
O	6.879000000	-7.412000000	-11.917000000
O	6.882000000	-5.440000000	-13.682000000
H	-0.664000000	-1.256000000	-13.046000000
H	5.071000000	-4.404000000	-13.939000000
H	1.316000000	-5.493000000	-13.529000000
H	4.224000000	-6.229000000	-14.226000000
H	4.557000000	-7.962000000	-12.612000000
H	2.704000000	-7.117000000	-10.559000000
H	4.239000000	-5.084000000	-10.093000000
H	2.864000000	1.542000000	-13.890000000
H	4.264000000	0.545000000	-14.169000000
H	2.786000000	-7.092000000	-14.643000000
H	5.131000000	-6.676000000	-10.155000000
P	1.504000000	-9.077000000	-13.498000000
C	-0.441000000	-7.409000000	-12.800000000
O	0.566000000	-7.734000000	-13.786000000
C	-1.818000000	-7.398000000	-13.466000000
O	-2.108000000	-6.024000000	-13.894000000
C	-1.998000000	-8.274000000	-14.725000000
O	-3.134000000	-9.104000000	-14.420000000
C	-2.324000000	-7.307000000	-15.881000000
C	-2.145000000	-5.898000000	-15.316000000
N	-0.873000000	-5.230000000	-15.765000000
C	-0.851000000	-3.779000000	-15.870000000
O	-1.887000000	-3.160000000	-15.603000000
N	0.293000000	-3.148000000	-16.304000000
C	1.440000000	-3.875000000	-16.564000000
N	2.543000000	-3.189000000	-16.951000000
C	1.444000000	-5.306000000	-16.394000000
C	0.307000000	-5.943000000	-15.982000000
O	0.747000000	-10.133000000	-12.732000000
O	2.134000000	-9.364000000	-14.838000000
H	-3.324000000	-9.718000000	-15.170000000
H	2.352000000	-5.871000000	-16.600000000
H	0.286000000	-7.034000000	-15.805000000
H	-2.989000000	-5.190000000	-15.518000000
H	-1.726000000	-7.515000000	-16.786000000
H	-1.143000000	-8.937000000	-14.960000000
H	-2.624000000	-7.602000000	-12.706000000
H	3.417000000	-3.661000000	-17.153000000
H	-0.174000000	-6.380000000	-12.453000000
H	2.546000000	-2.157000000	-17.026000000
H	-3.370000000	-7.457000000	-16.224000000
H	-0.434000000	-8.098000000	-11.928000000
P	2.327000000	6.000000000	-19.977000000
C	-0.290000000	6.203000000	-19.555000000
O	1.034000000	6.491000000	-19.051000000
C	-1.228000000	6.290000000	-18.346000000
O	-1.377000000	4.962000000	-17.771000000

C	-0.696000000	7.195000000	-17.202000000
O	-1.816000000	7.961000000	-16.737000000
C	-0.045000000	6.222000000	-16.215000000
C	-0.634000000	4.845000000	-16.536000000
N	0.333000000	-0.290000000	-16.550000000
C	-0.843000000	0.412000000	-16.195000000
N	-1.939000000	-0.325000000	-15.804000000
N	-0.970000000	1.775000000	-16.280000000
C	0.182000000	2.426000000	-16.655000000
C	1.429000000	1.797000000	-16.962000000
C	1.541000000	0.372000000	-16.941000000
O	2.508000000	-0.343000000	-17.213000000
N	2.403000000	2.779000000	-17.235000000
C	1.786000000	3.955000000	-17.111000000
N	0.405000000	3.806000000	-16.732000000
O	2.414000000	6.809000000	-21.249000000
O	3.460000000	5.938000000	-18.987000000
H	0.351000000	-1.362000000	-16.463000000
H	2.227000000	4.939000000	-17.267000000
H	-1.400000000	4.457000000	-15.804000000
H	1.057000000	6.264000000	-16.359000000
H	-2.647000000	0.153000000	-15.232000000
H	0.009000000	7.975000000	-17.572000000
H	-1.847000000	-1.351000000	-15.656000000
H	-2.262000000	6.558000000	-18.661000000
H	-0.336000000	5.187000000	-20.000000000
H	-0.189000000	6.505000000	-15.142000000
H	-0.546000000	6.964000000	-20.317000000
P	-2.486000000	7.812000000	-15.210000000
C	-3.912000000	5.690000000	-15.922000000
O	-2.895000000	6.214000000	-15.041000000
C	-4.639000000	4.591000000	-15.144000000
O	-3.709000000	3.515000000	-14.850000000
C	-5.222000000	5.048000000	-13.779000000
O	-6.508000000	4.412000000	-13.720000000
C	-4.176000000	4.605000000	-12.754000000
C	-3.441000000	3.443000000	-13.429000000
N	-1.965000000	3.454000000	-13.248000000
C	-1.309000000	2.179000000	-13.361000000
O	-1.944000000	1.135000000	-13.382000000
N	0.094000000	2.207000000	-13.326000000
C	0.886000000	3.384000000	-13.396000000
O	2.088000000	3.248000000	-13.601000000
C	0.145000000	4.635000000	-13.217000000
C	-1.216000000	4.642000000	-13.219000000
C	0.928000000	5.889000000	-13.041000000
O	-3.697000000	8.702000000	-15.325000000
O	-1.443000000	7.996000000	-14.137000000
H	0.572000000	1.242000000	-13.372000000
H	-1.801000000	5.582000000	-13.168000000

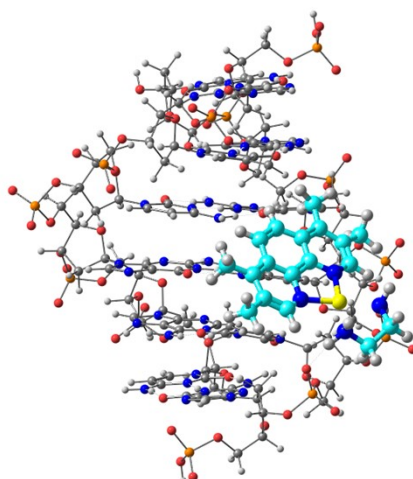
H	-3.812000000	2.419000000	-13.124000000
H	-3.504000000	5.469000000	-12.537000000
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H	-5.415000000	4.111000000	-15.785000000
H	-3.382000000	5.260000000	-16.802000000
H	1.107000000	6.105000000	-11.978000000
H	1.913000000	5.832000000	-13.529000000
H	0.401000000	6.764000000	-13.470000000
H	-4.596000000	4.322000000	-11.766000000
H	-4.619000000	6.470000000	-16.262000000
P	-7.042000000	3.478000000	-12.443000000
C	-5.910000000	1.192000000	-13.243000000
O	-5.919000000	2.259000000	-12.272000000
C	-6.118000000	-0.152000000	-12.541000000
O	-4.823000000	-0.689000000	-12.151000000
C	-6.980000000	-0.112000000	-11.256000000
O	-7.901000000	-1.202000000	-11.467000000
C	-6.015000000	-0.398000000	-10.096000000
C	-4.640000000	-0.637000000	-10.723000000
N	-3.614000000	0.416000000	-10.439000000
C	-2.215000000	0.009000000	-10.439000000
O	-1.959000000	-1.190000000	-10.552000000
N	-1.230000000	0.965000000	-10.299000000
C	-1.554000000	2.298000000	-10.227000000
N	-0.519000000	3.190000000	-10.159000000
C	-2.934000000	2.711000000	-10.202000000
C	-3.923000000	1.771000000	-10.330000000
O	-8.350000000	2.954000000	-12.977000000
O	-6.931000000	4.228000000	-11.144000000
H	-3.183000000	3.763000000	-10.077000000
H	-4.991000000	2.048000000	-10.355000000
H	-4.187000000	-1.634000000	-10.461000000
H	-6.036000000	0.418000000	-9.351000000
H	-7.550000000	0.833000000	-11.124000000
H	-6.498000000	-0.918000000	-13.262000000
H	-0.691000000	4.179000000	-10.279000000
H	-4.879000000	1.239000000	-13.678000000
H	0.455000000	2.875000000	-10.337000000
H	-6.327000000	-1.310000000	-9.524000000
H	-6.658000000	1.338000000	-14.043000000
P	-9.270000000	-1.276000000	-10.516000000
C	-8.090000000	-3.474000000	-9.721000000
O	-8.780000000	-2.278000000	-9.279000000
C	-7.299000000	-3.998000000	-8.521000000
O	-6.117000000	-3.174000000	-8.374000000
C	-8.068000000	-3.958000000	-7.169000000
O	-8.147000000	-5.303000000	-6.686000000
C	-7.312000000	-2.943000000	-6.305000000
C	-5.941000000	-2.815000000	-6.972000000
N	-1.477000000	-0.267000000	-7.246000000

C	-1.748000000	-1.659000000	-7.286000000
N	-0.680000000	-2.520000000	-7.464000000
N	-3.008000000	-2.171000000	-7.227000000
C	-3.995000000	-1.229000000	-7.098000000
C	-3.818000000	0.189000000	-7.034000000
C	-2.494000000	0.733000000	-7.120000000
O	-2.138000000	1.910000000	-7.119000000
N	-5.064000000	0.814000000	-6.853000000
C	-5.975000000	-0.169000000	-6.836000000
N	-5.373000000	-1.457000000	-6.986000000
O	-10.259000000	-1.993000000	-11.408000000
O	-9.605000000	0.043000000	-9.876000000
H	-0.460000000	0.069000000	-7.269000000
H	-7.046000000	-0.053000000	-6.717000000
H	-5.152000000	-3.520000000	-6.567000000
H	-7.874000000	-1.988000000	-6.279000000
H	-0.862000000	-3.514000000	-7.286000000
H	-9.142000000	-3.691000000	-7.299000000
H	0.273000000	-2.196000000	-7.196000000
H	-6.918000000	-5.025000000	-8.740000000
H	-7.399000000	-3.246000000	-10.561000000
H	-7.232000000	-3.243000000	-5.238000000
H	-8.848000000	-4.214000000	-10.046000000
P	-7.086000000	-5.967000000	-5.567000000
C	-4.698000000	-6.179000000	-6.783000000
O	-5.601000000	-5.382000000	-5.984000000
C	-3.615000000	-6.824000000	-5.920000000
O	-2.677000000	-5.818000000	-5.450000000
C	-4.115000000	-7.559000000	-4.652000000
O	-3.354000000	-8.780000000	-4.614000000
C	-3.900000000	-6.547000000	-3.515000000
C	-2.896000000	-5.524000000	-4.070000000
N	-1.346000000	-0.530000000	-3.994000000
C	-0.646000000	-1.698000000	-4.192000000
N	-1.147000000	-2.952000000	-4.216000000
C	-2.511000000	-3.004000000	-4.016000000
C	-3.348000000	-1.856000000	-3.808000000
C	-2.719000000	-0.572000000	-3.816000000
N	-3.393000000	0.601000000	-3.685000000
N	-4.687000000	-2.262000000	-3.662000000
C	-4.678000000	-3.599000000	-3.780000000
N	-3.362000000	-4.116000000	-3.965000000
O	-7.243000000	-7.449000000	-5.771000000
O	-7.340000000	-5.320000000	-4.221000000
H	0.442000000	-1.576000000	-4.358000000
H	-5.555000000	-4.254000000	-3.751000000
H	-1.869000000	-5.579000000	-3.616000000
H	-4.870000000	-6.095000000	-3.224000000
H	-5.164000000	-7.928000000	-4.727000000
H	-2.957000000	-7.483000000	-6.548000000

H	-4.235000000	-5.418000000	-7.458000000
H	-2.906000000	1.507000000	-3.755000000
H	-4.393000000	0.610000000	-3.535000000
H	-3.541000000	-6.995000000	-2.568000000
H	-5.235000000	-6.940000000	-7.381000000
P	-2.412000000	-9.240000000	-3.341000000
C	-0.361000000	-7.773000000	-4.116000000
O	-1.349000000	-7.974000000	-3.086000000
C	1.026000000	-7.718000000	-3.473000000
O	1.367000000	-6.314000000	-3.267000000
C	1.180000000	-8.411000000	-2.098000000
O	2.234000000	-9.370000000	-2.294000000
C	1.617000000	-7.309000000	-1.116000000
C	1.470000000	-5.990000000	-1.876000000
N	0.243000000	-5.217000000	-1.476000000
C	0.314000000	-3.766000000	-1.448000000
O	1.394000000	-3.230000000	-1.715000000
N	-0.798000000	-3.037000000	-1.084000000
C	-1.991000000	-3.670000000	-0.804000000
N	-3.052000000	-2.896000000	-0.464000000
C	-2.082000000	-5.107000000	-0.875000000
C	-0.978000000	-5.839000000	-1.219000000
O	-1.676000000	-10.462000000	-3.822000000
O	-3.211000000	-9.289000000	-2.056000000
H	2.346000000	-9.930000000	-1.490000000
H	-3.025000000	-5.602000000	-0.651000000
H	-1.022000000	-6.940000000	-1.311000000
H	2.349000000	-5.298000000	-1.810000000
H	1.056000000	-7.347000000	-0.165000000
H	0.275000000	-8.952000000	-1.756000000
H	1.812000000	-8.071000000	-4.184000000
H	-3.970000000	-3.297000000	-0.307000000
H	-0.616000000	-6.787000000	-4.584000000
H	-2.990000000	-1.863000000	-0.462000000
H	2.671000000	-7.466000000	-0.804000000
H	-0.394000000	-8.565000000	-4.894000000
O	1.912000000	4.440000000	-20.404000000
O	-2.669000000	5.755000000	2.798000000
H	1.633000000	4.316000000	-21.355000000
H	-2.262000000	5.643000000	3.699000000
N	-3.166000000	-7.505000000	-10.337000000
N	-1.872000000	-3.849000000	-11.628000000
N	-4.219000000	-5.264000000	-12.069000000
N	-0.893000000	-6.134000000	-9.925000000
C	0.953000000	-6.802000000	-7.865000000
C	-0.138000000	-7.621000000	-8.077000000
C	-1.116000000	-7.257000000	-9.093000000
C	-2.292000000	-7.940000000	-9.279000000
C	-2.716000000	-8.973000000	-8.340000000
C	-4.040000000	-9.303000000	-8.260000000

C	-4.987000000	-8.604000000	-9.138000000
C	-6.453000000	-8.821000000	-8.947000000
C	-4.536000000	-7.709000000	-10.065000000
C	-4.567000000	-10.279000000	-7.263000000
C	-1.660000000	-9.456000000	-7.444000000
C	-2.891000000	-3.260000000	-12.569000000
C	-4.280000000	-3.762000000	-12.153000000
C	0.210000000	-5.358000000	-9.688000000
C	-0.473000000	-8.823000000	-7.322000000
C	1.946000000	-7.082000000	-6.783000000
C	1.135000000	-5.636000000	-8.692000000
C	2.271000000	-4.686000000	-8.492000000
Pt	-2.535000000	-5.702000000	-10.970000000
H	-0.956000000	-3.903000000	-12.100000000
H	-1.776000000	-3.219000000	-10.809000000
H	-4.109000000	-5.671000000	-13.010000000
H	-5.082000000	-5.648000000	-11.664000000
H	-7.068000000	-8.260000000	-9.658000000
H	-6.761000000	-8.501000000	-7.934000000
H	-6.728000000	-9.879000000	-9.037000000
H	-5.227000000	-7.156000000	-10.707000000
H	-5.059000000	-11.134000000	-7.737000000
H	-5.310000000	-9.797000000	-6.608000000
H	-3.784000000	-10.662000000	-6.592000000
H	-1.905000000	-10.324000000	-6.831000000
H	-2.873000000	-2.140000000	-12.536000000
H	-2.649000000	-3.564000000	-13.618000000
H	-5.057000000	-3.410000000	-12.867000000
H	-4.559000000	-3.357000000	-11.145000000
H	0.368000000	-4.517000000	-10.380000000
H	0.284000000	-9.198000000	-6.629000000
H	2.979000000	-6.938000000	-7.133000000
H	1.878000000	-8.108000000	-6.398000000
H	1.782000000	-6.395000000	-5.936000000
H	2.685000000	-4.331000000	-9.456000000
H	3.106000000	-5.143000000	-7.947000000
H	1.962000000	-3.798000000	-7.917000000

[Pt(en)(3,4,7,8-Me₄phen)]²⁺ major groove
Dock_ID: 108-cl1_3,4,7,8-Me₄phen



EDA analysis for 108-cl1_3,4,7,8-Me₄phen in kcal mol⁻¹.

Electrostatic interaction	-763.5
Orbital interaction	-93.7
Dispersion energy	-58.5
Pauli repulsion	135.3
Total Bonding Energy	-780.3

Contributions of the solvation energies for 108-cl1_3,4,7,8-Me₄phen in kcal mol⁻¹.

E _{solv} (total system)	-1743.6
E _{solv} (intercalator)	-154.7
E _{solv} (duplex DNA)	-2312.4
ΔE _{solv}	723.4
ΔE _{int} (EDA)	-780.3
ΔE _{aq}	-56.8

$$\Delta E_{\text{solv}} = \Delta E_{\text{solv}}(\text{total system}) - \Delta E_{\text{solv}}(\text{intercalator}) - \Delta E_{\text{solv}}(\text{duplex DNA})$$

$$\Delta E_{\text{aq}} = \Delta E_{\text{int}}(\text{EDA}) + \Delta E_{\text{solv}}$$

Optimized Cartesian coordinates at PM6-DH2 level considering solvation effects
with water within the COSMO approach for the 108-cl1_3,4,7,8-Me₄phen system.
([Pt(en)(3,4,7,8-Me₄phen)]²⁺ major groove)

P	-1.685000000	6.911000000	2.277000000
C	0.913000000	6.535000000	2.023000000
O	-0.308000000	6.894000000	1.337000000
C	2.044000000	6.654000000	0.996000000
O	2.365000000	5.328000000	0.490000000
C	1.712000000	7.519000000	-0.252000000
O	2.797000000	8.446000000	-0.350000000
C	1.504000000	6.523000000	-1.401000000
C	1.825000000	5.136000000	-0.831000000
N	0.123000000	0.209000000	-0.637000000
C	1.401000000	0.714000000	-0.984000000
N	2.378000000	-0.188000000	-1.336000000
N	1.723000000	2.045000000	-0.933000000
C	0.656000000	2.871000000	-0.659000000
C	-0.679000000	2.447000000	-0.379000000
C	-0.992000000	1.051000000	-0.325000000
O	-2.055000000	0.494000000	-0.048000000
N	-1.517000000	3.574000000	-0.242000000
C	-0.735000000	4.640000000	-0.414000000
N	0.628000000	4.271000000	-0.702000000
O	-1.521000000	7.838000000	3.458000000
O	-2.801000000	7.060000000	1.279000000
H	-0.047000000	-0.844000000	-0.696000000
H	-1.030000000	5.688000000	-0.361000000
H	2.637000000	4.563000000	-1.373000000
H	0.471000000	6.605000000	-1.797000000
H	3.135000000	0.154000000	-1.943000000
H	0.827000000	8.180000000	-0.092000000
H	2.143000000	-1.197000000	-1.426000000
H	2.990000000	6.977000000	1.491000000
H	0.838000000	5.489000000	2.390000000
H	2.148000000	6.731000000	-2.287000000
H	1.083000000	7.222000000	2.875000000
P	3.921000000	8.568000000	-1.574000000
C	5.045000000	6.194000000	-1.177000000
O	4.319000000	7.040000000	-2.095000000
C	5.552000000	5.006000000	-1.993000000
O	4.453000000	4.082000000	-2.246000000
C	6.143000000	5.378000000	-3.382000000
O	7.331000000	4.565000000	-3.406000000
C	5.055000000	4.983000000	-4.384000000
C	4.349000000	3.824000000	-3.682000000
N	2.907000000	3.654000000	-3.963000000
C	2.383000000	2.324000000	-3.813000000
O	3.127000000	1.359000000	-3.717000000
N	0.985000000	2.195000000	-3.880000000

C	0.083000000	3.297000000	-3.888000000
O	-1.105000000	3.065000000	-3.703000000
C	0.696000000	4.606000000	-4.130000000
C	2.046000000	4.758000000	-4.131000000
C	-0.235000000	5.743000000	-4.364000000
O	5.067000000	9.238000000	-0.865000000
O	3.290000000	9.160000000	-2.812000000
H	0.591000000	1.196000000	-3.819000000
H	2.541000000	5.736000000	-4.310000000
H	4.866000000	2.829000000	-3.846000000
H	4.381000000	5.869000000	-4.563000000
H	6.449000000	6.450000000	-3.461000000
H	6.280000000	4.412000000	-1.388000000
H	4.353000000	5.852000000	-0.376000000
H	-0.557000000	5.782000000	-5.419000000
H	-1.135000000	5.672000000	-3.738000000
H	0.233000000	6.719000000	-4.159000000
H	5.432000000	4.744000000	-5.401000000
H	5.893000000	6.744000000	-0.722000000
P	8.242000000	4.272000000	-4.771000000
C	6.827000000	2.146000000	-5.365000000
O	8.089000000	2.603000000	-4.846000000
C	7.029000000	0.672000000	-5.738000000
O	5.721000000	0.044000000	-5.643000000
C	7.505000000	0.441000000	-7.197000000
O	8.343000000	-0.720000000	-7.069000000
C	6.217000000	0.184000000	-7.985000000
C	5.133000000	-0.145000000	-6.955000000
N	3.943000000	0.744000000	-7.038000000
C	2.608000000	0.169000000	-6.960000000
O	2.503000000	-1.059000000	-6.907000000
N	1.517000000	1.009000000	-6.970000000
C	1.679000000	2.378000000	-6.989000000
N	0.576000000	3.165000000	-6.963000000
C	3.002000000	2.949000000	-6.988000000
C	4.088000000	2.134000000	-7.043000000
O	9.668000000	4.493000000	-4.349000000
O	7.637000000	4.913000000	-5.992000000
H	3.118000000	4.036000000	-6.950000000
H	5.112000000	2.544000000	-7.102000000
H	4.787000000	-1.210000000	-6.963000000
H	5.961000000	1.048000000	-8.651000000
H	8.117000000	1.275000000	-7.600000000
H	7.660000000	0.134000000	-4.997000000
H	0.664000000	4.178000000	-7.026000000
H	6.508000000	2.761000000	-6.241000000
H	-0.383000000	2.770000000	-6.946000000
H	6.326000000	-0.662000000	-8.703000000
H	6.061000000	2.209000000	-4.548000000
P	8.941000000	-1.496000000	-8.427000000

C	7.022000000	-3.289000000	-8.166000000
O	7.600000000	-2.282000000	-9.032000000
C	6.437000000	-4.390000000	-9.058000000
O	5.040000000	-4.091000000	-9.320000000
C	7.111000000	-4.525000000	-10.449000000
O	7.204000000	-5.945000000	-10.659000000
C	6.205000000	-3.724000000	-11.390000000
C	4.855000000	-3.605000000	-10.672000000
N	0.651000000	-0.560000000	-10.147000000
C	0.747000000	-1.968000000	-10.177000000
N	-0.420000000	-2.681000000	-10.199000000
N	1.941000000	-2.650000000	-10.219000000
C	3.037000000	-1.834000000	-10.365000000
C	3.024000000	-0.403000000	-10.393000000
C	1.791000000	0.311000000	-10.217000000
O	1.573000000	1.514000000	-10.148000000
N	4.323000000	0.084000000	-10.622000000
C	5.106000000	-0.991000000	-10.722000000
N	4.369000000	-2.215000000	-10.566000000
O	9.910000000	-2.477000000	-7.815000000
O	9.340000000	-0.520000000	-9.498000000
H	-0.316000000	-0.104000000	-10.058000000
H	6.179000000	-1.007000000	-10.892000000
H	4.035000000	-4.254000000	-11.085000000
H	6.683000000	-2.740000000	-11.595000000
H	-0.400000000	-3.689000000	-10.296000000
H	8.167000000	-4.177000000	-10.468000000
H	-1.341000000	-2.214000000	-10.117000000
H	6.396000000	-5.367000000	-8.520000000
H	6.209000000	-2.791000000	-7.592000000
H	6.096000000	-4.166000000	-12.401000000
H	7.770000000	-3.715000000	-7.469000000
P	6.625000000	-6.730000000	-12.011000000
C	4.135000000	-6.940000000	-11.105000000
O	5.009000000	-6.341000000	-12.087000000
C	2.926000000	-7.538000000	-11.831000000
O	1.967000000	-6.488000000	-12.129000000
C	3.254000000	-8.204000000	-13.196000000
O	2.452000000	-9.397000000	-13.213000000
C	2.933000000	-7.124000000	-14.236000000
C	2.010000000	-6.127000000	-13.523000000
N	0.682000000	-1.045000000	-13.333000000
C	-0.082000000	-2.181000000	-13.241000000
N	0.345000000	-3.468000000	-13.293000000
C	1.703000000	-3.584000000	-13.481000000
C	2.600000000	-2.471000000	-13.624000000
C	2.050000000	-1.156000000	-13.533000000
N	2.795000000	-0.025000000	-13.685000000
N	3.914000000	-2.933000000	-13.823000000
C	3.839000000	-4.268000000	-13.797000000

N	2.498000000	-4.732000000	-13.615000000
O	6.832000000	-8.176000000	-11.637000000
O	7.181000000	-6.122000000	-13.273000000
H	-1.166000000	-2.011000000	-13.089000000
H	4.668000000	-4.969000000	-13.895000000
H	0.935000000	-6.154000000	-13.845000000
H	3.884000000	-6.670000000	-14.590000000
H	4.296000000	-8.580000000	-13.278000000
H	2.354000000	-8.225000000	-11.163000000
H	3.813000000	-6.094000000	-10.454000000
H	2.376000000	0.900000000	-13.500000000
H	3.806000000	-0.082000000	-13.606000000
H	2.482000000	-7.508000000	-15.172000000
H	4.641000000	-7.712000000	-10.493000000
P	1.394000000	-9.784000000	-14.441000000
C	-0.589000000	-8.323000000	-13.454000000
O	0.356000000	-8.478000000	-14.534000000
C	-1.989000000	-8.136000000	-14.044000000
O	-2.231000000	-6.705000000	-14.194000000
C	-2.230000000	-8.769000000	-15.434000000
O	-3.344000000	-9.656000000	-15.239000000
C	-2.609000000	-7.607000000	-16.368000000
C	-2.387000000	-6.325000000	-15.569000000
N	-1.153000000	-5.572000000	-15.980000000
C	-1.192000000	-4.118000000	-15.973000000
O	-2.254000000	-3.568000000	-15.663000000
N	-0.071000000	-3.406000000	-16.336000000
C	1.098000000	-4.061000000	-16.671000000
N	2.177000000	-3.300000000	-16.980000000
C	1.145000000	-5.502000000	-16.675000000
C	0.033000000	-6.217000000	-16.324000000
O	0.692000000	-10.994000000	-13.879000000
O	2.082000000	-9.795000000	-15.778000000
H	-3.525000000	-10.172000000	-16.061000000
H	2.062000000	-6.012000000	-16.968000000
H	0.043000000	-7.323000000	-16.286000000
H	-3.248000000	-5.608000000	-15.570000000
H	-2.063000000	-7.645000000	-17.328000000
H	-1.378000000	-9.362000000	-15.824000000
H	-2.775000000	-8.455000000	-13.314000000
H	3.076000000	-3.718000000	-17.194000000
H	-0.269000000	-7.398000000	-12.917000000
H	2.153000000	-2.266000000	-16.906000000
H	-3.671000000	-7.696000000	-16.685000000
H	-0.580000000	-9.182000000	-12.754000000
P	2.094000000	6.504000000	-19.098000000
C	-0.486000000	5.991000000	-18.880000000
O	0.735000000	6.286000000	-18.162000000
C	-1.625000000	6.093000000	-17.860000000
O	-1.961000000	4.758000000	-17.386000000

C	-1.283000000	6.919000000	-16.590000000
O	-2.452000000	7.726000000	-16.380000000
C	-0.950000000	5.873000000	-15.520000000
C	-1.396000000	4.519000000	-16.083000000
N	-0.117000000	-0.529000000	-16.312000000
C	-1.336000000	0.080000000	-15.920000000
N	-2.368000000	-0.736000000	-15.555000000
N	-1.536000000	1.440000000	-15.925000000
C	-0.412000000	2.168000000	-16.235000000
C	0.878000000	1.633000000	-16.542000000
C	1.065000000	0.216000000	-16.626000000
O	2.064000000	-0.432000000	-16.937000000
N	1.791000000	2.687000000	-16.752000000
C	1.100000000	3.816000000	-16.589000000
N	-0.277000000	3.562000000	-16.250000000
O	1.844000000	7.484000000	-20.218000000
O	3.202000000	6.681000000	-18.094000000
H	-0.049000000	-1.595000000	-16.312000000
H	1.468000000	4.835000000	-16.690000000
H	-2.229000000	4.008000000	-15.512000000
H	0.139000000	5.913000000	-15.283000000
H	-3.161000000	-0.338000000	-15.044000000
H	-0.458000000	7.649000000	-16.759000000
H	-2.268000000	-1.768000000	-15.560000000
H	-2.568000000	6.435000000	-18.346000000
H	-0.425000000	4.959000000	-19.288000000
H	-1.440000000	6.067000000	-14.539000000
H	-0.634000000	6.710000000	-19.708000000
P	-3.200000000	7.924000000	-14.898000000
C	-4.513000000	5.688000000	-15.358000000
O	-3.633000000	6.382000000	-14.444000000
C	-5.102000000	4.515000000	-14.576000000
O	-4.090000000	3.476000000	-14.435000000
C	-5.577000000	4.890000000	-13.146000000
O	-6.877000000	4.276000000	-13.076000000
C	-4.504000000	4.308000000	-12.222000000
C	-3.880000000	3.167000000	-13.031000000
N	-2.411000000	3.017000000	-12.845000000
C	-1.869000000	1.686000000	-12.969000000
O	-2.604000000	0.716000000	-13.007000000
N	-0.464000000	1.589000000	-12.963000000
C	0.416000000	2.704000000	-13.006000000
O	1.610000000	2.506000000	-13.184000000
C	-0.214000000	4.020000000	-12.834000000
C	-1.567000000	4.142000000	-12.823000000
C	0.709000000	5.186000000	-12.771000000
O	-4.401000000	8.756000000	-15.270000000
O	-2.223000000	8.345000000	-13.836000000
H	-0.054000000	0.596000000	-13.040000000
H	-2.076000000	5.123000000	-12.773000000

H	-4.369000000	2.164000000	-12.858000000
H	-3.776000000	5.115000000	-11.978000000
H	-5.734000000	5.983000000	-13.007000000
H	-5.917000000	4.026000000	-15.163000000
H	-3.913000000	5.329000000	-16.223000000
H	1.700000000	4.892000000	-12.368000000
H	0.898000000	5.607000000	-13.775000000
H	0.320000000	6.005000000	-12.151000000
H	-4.888000000	3.962000000	-11.240000000
H	-5.320000000	6.354000000	-15.724000000
P	-7.509000000	3.714000000	-11.640000000
C	-6.734000000	1.253000000	-12.284000000
O	-6.598000000	2.344000000	-11.353000000
C	-7.125000000	-0.021000000	-11.526000000
O	-5.912000000	-0.752000000	-11.194000000
C	-7.868000000	0.188000000	-10.180000000
O	-8.901000000	-0.816000000	-10.247000000
C	-6.807000000	-0.044000000	-9.095000000
C	-5.562000000	-0.577000000	-9.809000000
N	-4.385000000	0.344000000	-9.759000000
C	-3.060000000	-0.241000000	-9.933000000
O	-2.981000000	-1.459000000	-10.082000000
N	-1.960000000	0.588000000	-9.886000000
C	-2.103000000	1.945000000	-9.733000000
N	-0.960000000	2.688000000	-9.657000000
C	-3.408000000	2.534000000	-9.606000000
C	-4.512000000	1.724000000	-9.631000000
O	-8.925000000	3.368000000	-12.020000000
O	-7.173000000	4.604000000	-10.475000000
H	-3.515000000	3.608000000	-9.479000000
H	-5.537000000	2.134000000	-9.539000000
H	-5.229000000	-1.597000000	-9.467000000
H	-6.640000000	0.884000000	-8.512000000
H	-8.376000000	1.171000000	-10.090000000
H	-7.674000000	-0.729000000	-12.193000000
H	-0.998000000	3.695000000	-9.683000000
H	-5.711000000	1.140000000	-12.725000000
H	-0.032000000	2.253000000	-9.841000000
H	-7.131000000	-0.781000000	-8.324000000
H	-7.457000000	1.466000000	-13.093000000
P	-9.714000000	-1.347000000	-8.890000000
C	-7.938000000	-3.282000000	-8.985000000
O	-8.583000000	-2.309000000	-8.128000000
C	-6.903000000	-4.007000000	-8.125000000
O	-5.709000000	-3.184000000	-8.025000000
C	-7.369000000	-4.319000000	-6.675000000
O	-7.111000000	-5.728000000	-6.539000000
C	-6.563000000	-3.365000000	-5.790000000
C	-5.334000000	-3.011000000	-6.627000000
N	-1.142000000	0.001000000	-6.841000000

C	-1.265000000	-1.401000000	-6.972000000
N	-0.122000000	-2.124000000	-7.200000000
N	-2.463000000	-2.066000000	-6.902000000
C	-3.533000000	-1.246000000	-6.663000000
C	-3.501000000	0.176000000	-6.505000000
C	-2.259000000	0.876000000	-6.636000000
O	-2.031000000	2.083000000	-6.593000000
N	-4.797000000	0.656000000	-6.239000000
C	-5.599000000	-0.412000000	-6.234000000
N	-4.873000000	-1.624000000	-6.491000000
O	-10.814000000	-2.182000000	-9.498000000
O	-10.001000000	-0.242000000	-7.909000000
H	-0.164000000	0.440000000	-6.924000000
H	-6.668000000	-0.423000000	-6.048000000
H	-4.449000000	-3.697000000	-6.466000000
H	-7.190000000	-2.481000000	-5.545000000
H	-0.168000000	-3.137000000	-7.141000000
H	-8.468000000	-4.217000000	-6.534000000
H	0.815000000	-1.688000000	-7.100000000
H	-6.559000000	-4.937000000	-8.645000000
H	-7.445000000	-2.765000000	-9.839000000
H	-6.294000000	-3.776000000	-4.795000000
H	-8.692000000	-4.000000000	-9.367000000
P	-6.277000000	-6.414000000	-5.269000000
C	-3.889000000	-6.080000000	-6.415000000
O	-4.767000000	-5.705000000	-5.334000000
C	-2.656000000	-6.816000000	-5.879000000
O	-1.584000000	-5.850000000	-5.672000000
C	-2.837000000	-7.538000000	-4.521000000
O	-2.101000000	-8.762000000	-4.718000000
C	-2.217000000	-6.589000000	-3.483000000
C	-1.421000000	-5.545000000	-4.276000000
N	-0.103000000	-0.478000000	-3.765000000
C	0.657000000	-1.576000000	-4.066000000
N	0.232000000	-2.861000000	-4.191000000
C	-1.123000000	-3.014000000	-3.990000000
C	-2.021000000	-1.936000000	-3.684000000
C	-1.471000000	-0.622000000	-3.573000000
N	-2.213000000	0.478000000	-3.281000000
N	-3.335000000	-2.423000000	-3.565000000
C	-3.259000000	-3.737000000	-3.798000000
N	-1.914000000	-4.168000000	-4.047000000
O	-6.217000000	-7.863000000	-5.675000000
O	-6.821000000	-5.954000000	-3.943000000
H	1.734000000	-1.380000000	-4.239000000
H	-4.089000000	-4.444000000	-3.818000000
H	-0.309000000	-5.568000000	-4.108000000
H	-3.012000000	-6.152000000	-2.846000000
H	-3.884000000	-7.814000000	-4.283000000
H	-2.227000000	-7.501000000	-6.652000000

H	-3.577000000	-5.092000000	-6.845000000
H	-1.806000000	1.425000000	-3.356000000
H	-3.226000000	0.413000000	-3.246000000
H	-1.555000000	-7.110000000	-2.757000000
H	-4.399000000	-6.678000000	-7.193000000
P	-1.713000000	-9.741000000	-3.422000000
C	0.615000000	-8.556000000	-3.664000000
O	-0.441000000	-8.896000000	-2.731000000
C	1.693000000	-7.818000000	-2.878000000
O	1.378000000	-6.390000000	-2.912000000
C	1.826000000	-8.189000000	-1.383000000
O	2.983000000	-9.038000000	-1.320000000
C	2.082000000	-6.860000000	-0.659000000
C	1.779000000	-5.755000000	-1.673000000
N	0.632000000	-4.888000000	-1.269000000
C	0.828000000	-3.448000000	-1.192000000
O	1.956000000	-3.003000000	-1.424000000
N	-0.235000000	-2.643000000	-0.853000000
C	-1.476000000	-3.188000000	-0.584000000
N	-2.475000000	-2.334000000	-0.263000000
C	-1.669000000	-4.619000000	-0.647000000
C	-0.620000000	-5.429000000	-0.974000000
O	-1.217000000	-10.994000000	-4.099000000
O	-2.777000000	-9.763000000	-2.361000000
H	3.075000000	-9.427000000	-0.417000000
H	-2.646000000	-5.041000000	-0.410000000
H	-0.719000000	-6.527000000	-1.038000000
H	2.652000000	-5.099000000	-1.924000000
H	1.495000000	-6.780000000	0.276000000
H	0.951000000	-8.744000000	-0.982000000
H	2.682000000	-7.914000000	-3.395000000
H	-3.419000000	-2.664000000	-0.086000000
H	0.206000000	-7.910000000	-4.474000000
H	-2.336000000	-1.306000000	-0.259000000
H	3.135000000	-6.807000000	-0.307000000
H	1.038000000	-9.486000000	-4.099000000
O	2.289000000	4.986000000	-19.772000000
O	-1.733000000	5.348000000	2.865000000
H	2.002000000	4.891000000	-20.720000000
H	-1.460000000	5.236000000	3.817000000
N	2.897000000	7.268000000	-6.241000000
N	6.967000000	7.588000000	-6.467000000
N	5.049000000	9.003000000	-4.989000000
N	4.703000000	6.096000000	-7.774000000
C	3.986000000	4.305000000	-9.862000000
C	2.995000000	5.095000000	-9.292000000
C	3.349000000	5.963000000	-8.183000000
C	2.418000000	6.631000000	-7.429000000
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C	0.188000000	7.573000000	-7.180000000

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C	0.664000000	5.821000000	-8.946000000
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C	6.419000000	8.829000000	-4.391000000
C	5.625000000	5.235000000	-8.281000000
C	1.582000000	5.068000000	-9.604000000
C	3.695000000	3.434000000	-11.025000000
C	5.306000000	4.329000000	-9.294000000
C	6.345000000	3.357000000	-9.747000000
Pt	4.871000000	7.483000000	-6.381000000
H	7.304000000	7.791000000	-7.416000000
H	7.364000000	6.652000000	-6.208000000
H	4.974000000	9.925000000	-5.438000000
H	4.310000000	8.981000000	-4.228000000
H	-1.022000000	8.856000000	-4.943000000
H	-0.517000000	10.136000000	-6.045000000
H	0.368000000	9.861000000	-4.543000000
H	2.462000000	8.815000000	-4.857000000
H	-1.560000000	7.079000000	-8.364000000
H	-1.500000000	8.755000000	-7.797000000
H	-1.898000000	7.462000000	-6.667000000
H	-0.389000000	5.800000000	-9.220000000
H	7.583000000	9.618000000	-6.074000000
H	8.442000000	8.409000000	-5.097000000
H	6.704000000	9.687000000	-3.742000000
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H	6.638000000	5.274000000	-7.852000000
H	1.276000000	4.377000000	-10.395000000
H	4.558000000	3.262000000	-11.676000000
H	2.858000000	3.780000000	-11.654000000
H	3.391000000	2.422000000	-10.665000000
H	6.001000000	2.314000000	-9.596000000
H	7.298000000	3.474000000	-9.217000000
H	6.563000000	3.459000000	-10.819000000