Electronic Supplementary Material (ESI)
for *Organic & Biomolecular Chemistry*

Phosphoramidate Hydrolysis Catalyzed by Human Histidine Triad Nucleotide Binding Protein 1 (hHint1): A Cluster-model DFT Computational Study

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Table of Contents

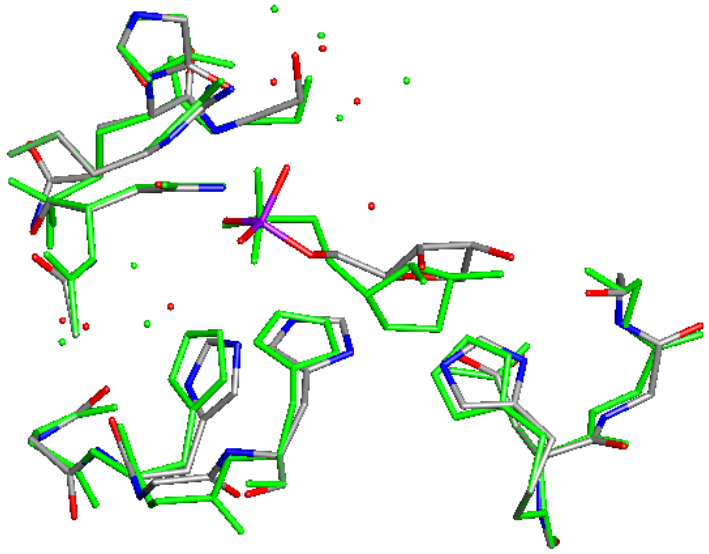


Figure S1. Overlay of the X-ray crystal structure (green) of 3TW2 (enzyme with active-site bound AMP) and the DFT-optimized structure of the phosphoramidate hydrolysis product. Hydrogen atoms are removed for clarity. Color code: purple, P; blue, N; red, O; gray, C; white, H.

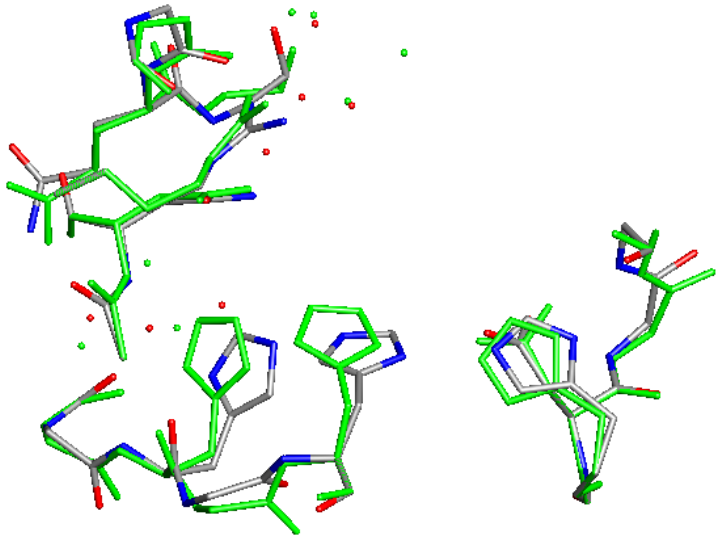


Figure S2. Overlay of the X-ray crystal structure (green) of 3TW2 (with the active-site bound AMP removed) and the DFT-optimized structure of the empty enzyme active site. Hydrogen atoms are removed for clarity. Color code: blue, N; red, O; gray, C; white, H.

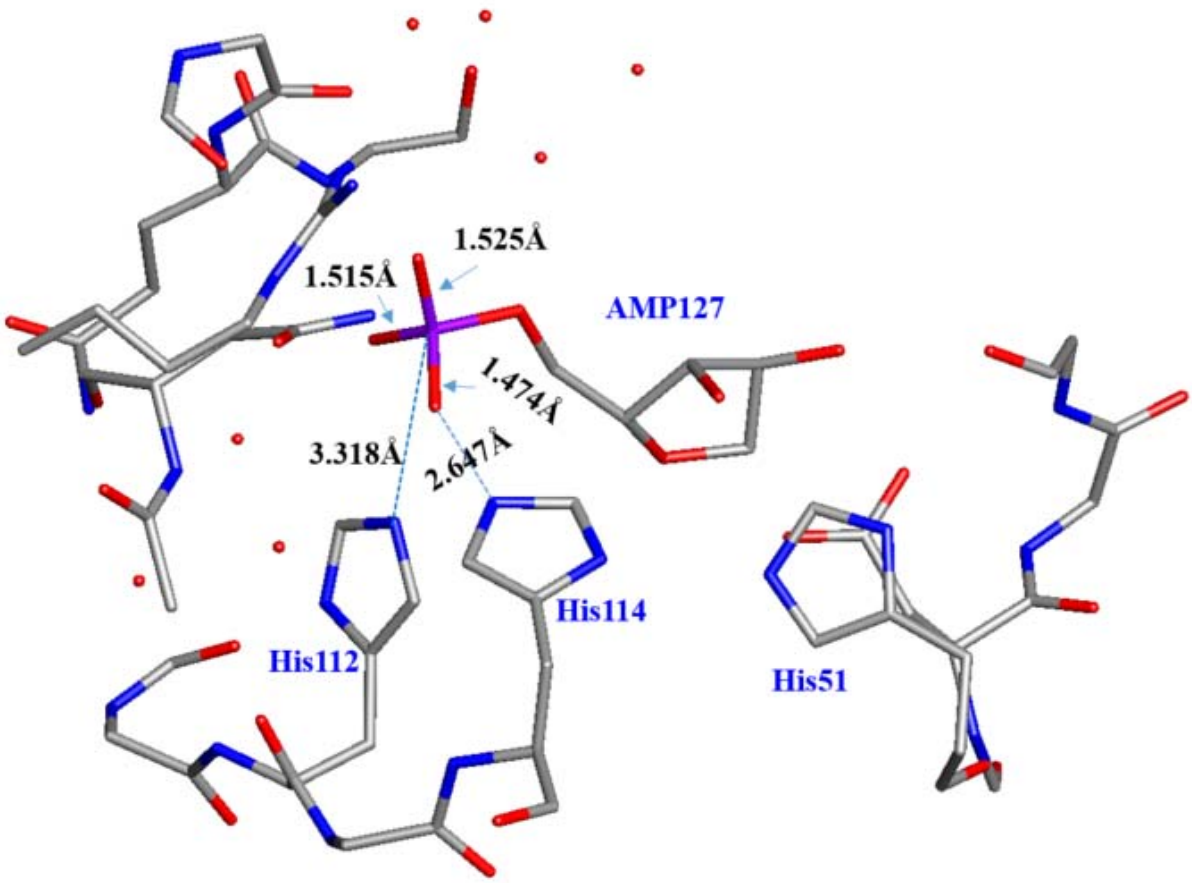
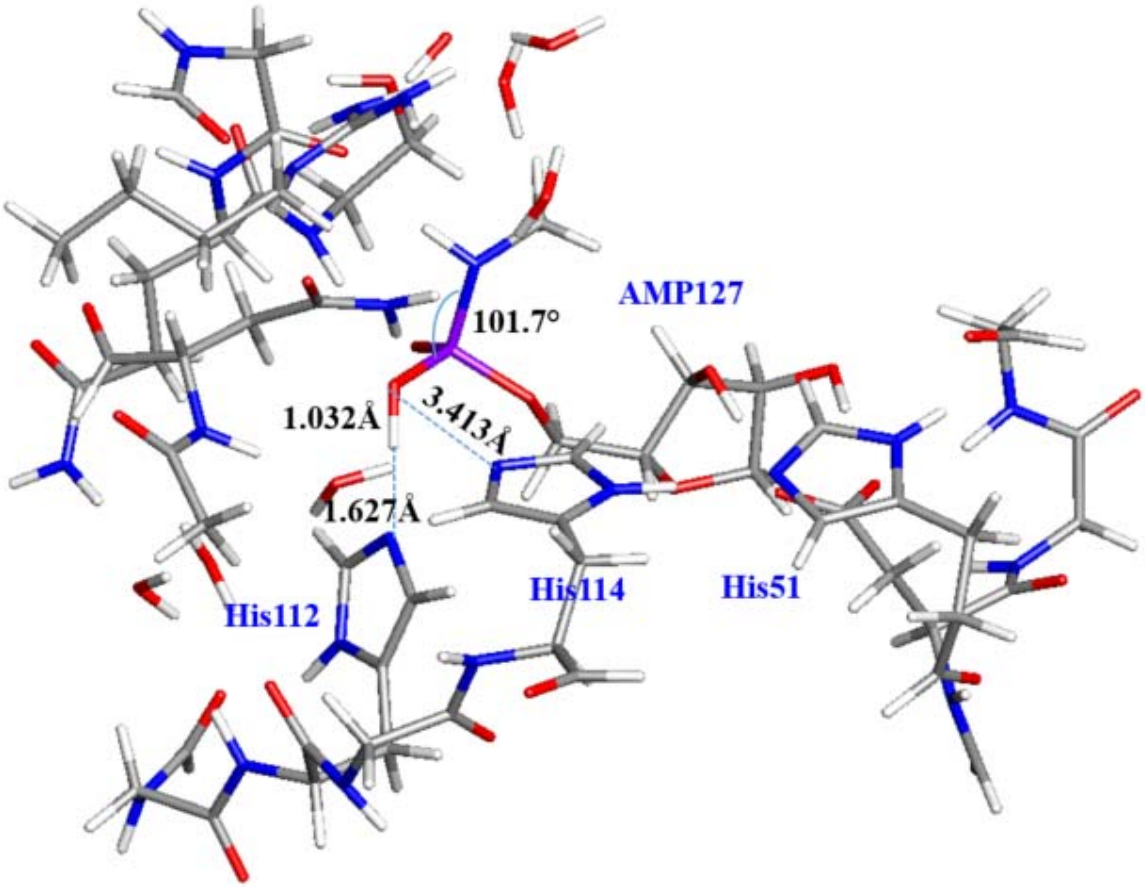


Figure S3. Select distances in native enzyme in 3TW2 X-ray crystal structure. Color code: purple, P; blue, N; red, O; gray, C; white, H.



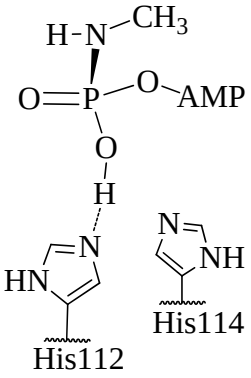


Figure S4. 3D representation of structure **2'** with selected geometric parameters and 2D diagrammatic representation of **2'**. Color code: purple, P; blue, N; red, O; gray, C; white, H.

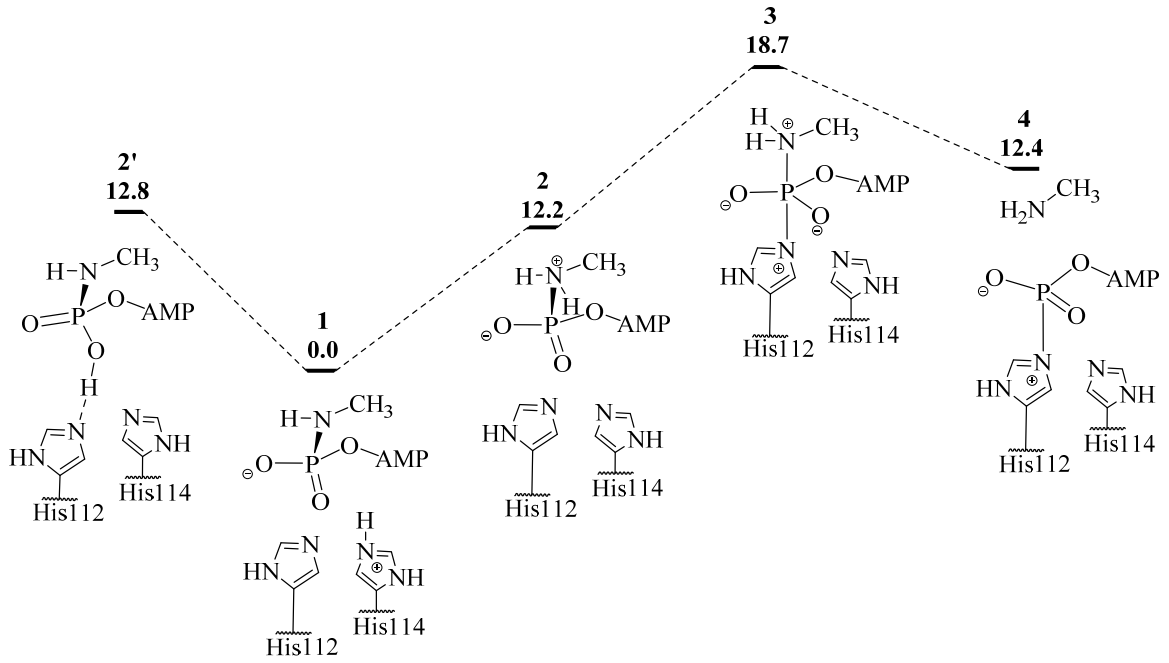


Figure S5. Proposed alternative structure **2'** can be formed from structure **1**. **2'** is a protomer of structure **2**.

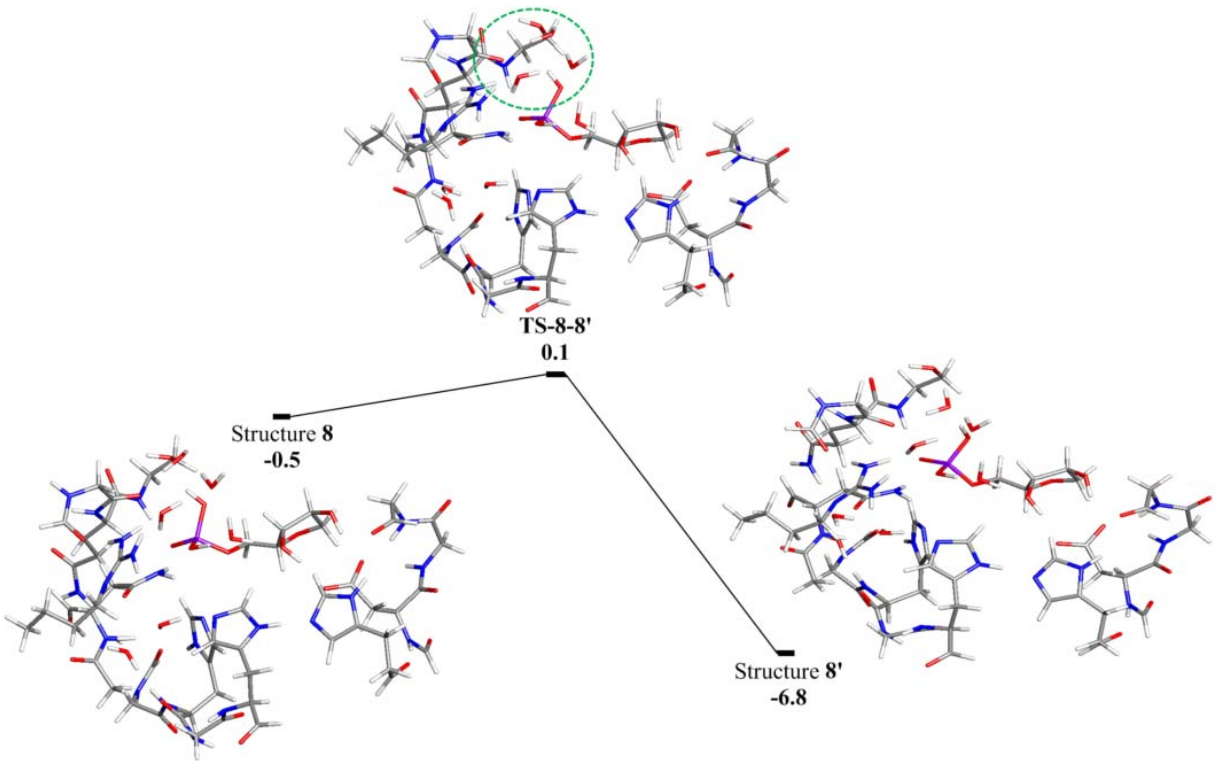


Figure S6. Hydrogen bonding caused transition state of structure **8**.
Hydrogen bonding involved in the transition state of the three solvent waters is circled.

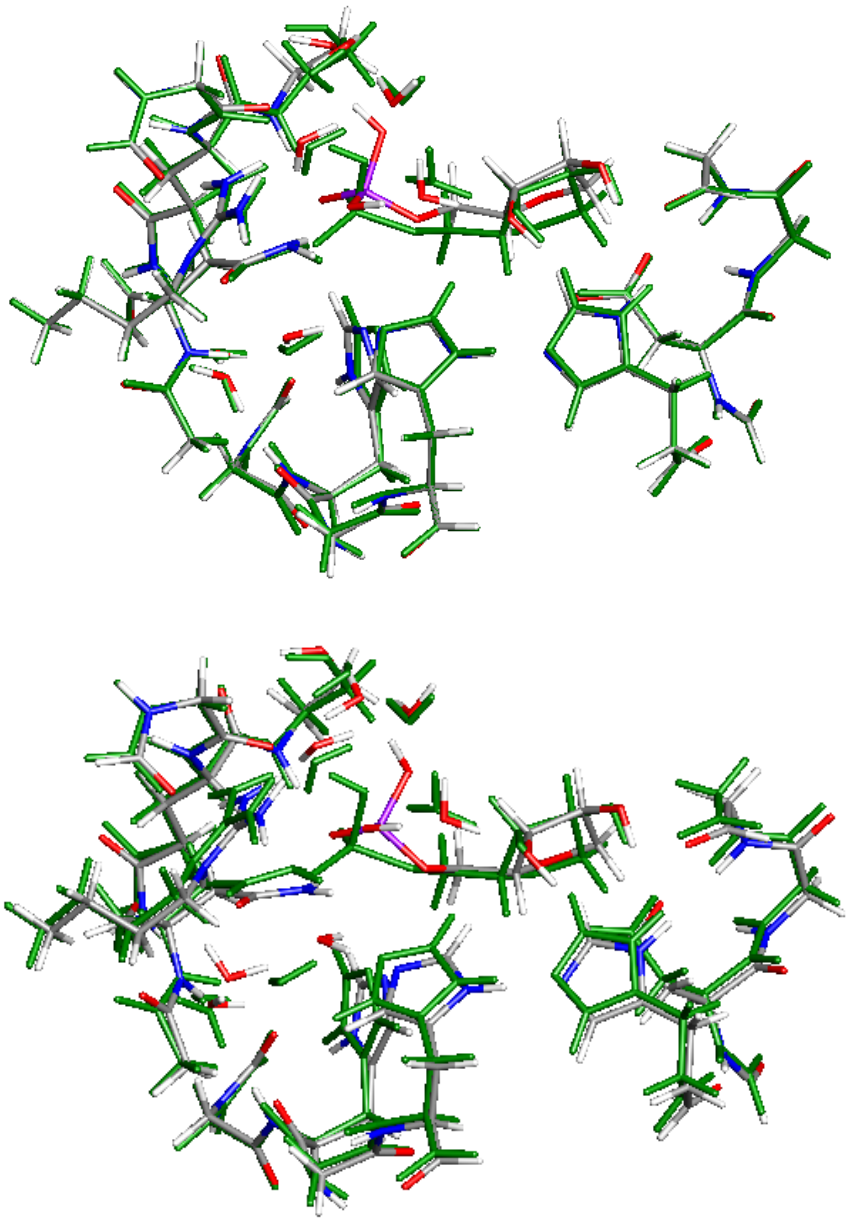


Figure S7. Overlay of structure **7** (green) and structures **8** (top) and **8'** (bottom).

Repeated attempts to locate the transition state between structures **7** and **8** were unsuccessful. The hydrogen bond between the equatorial OH of dihydrogen phosphate substrate and one solvent water molecule in structure **8** caused the hydrogen bonds between the axial OH and residues and other solvent water molecules different from these hydrogen bonds between the axial OH and residues in structures **7**. Hydrogen bonds caused by the fluxional explicit water molecules prevented the location of the transition state between structure **7** and structures **8** and **8'**.

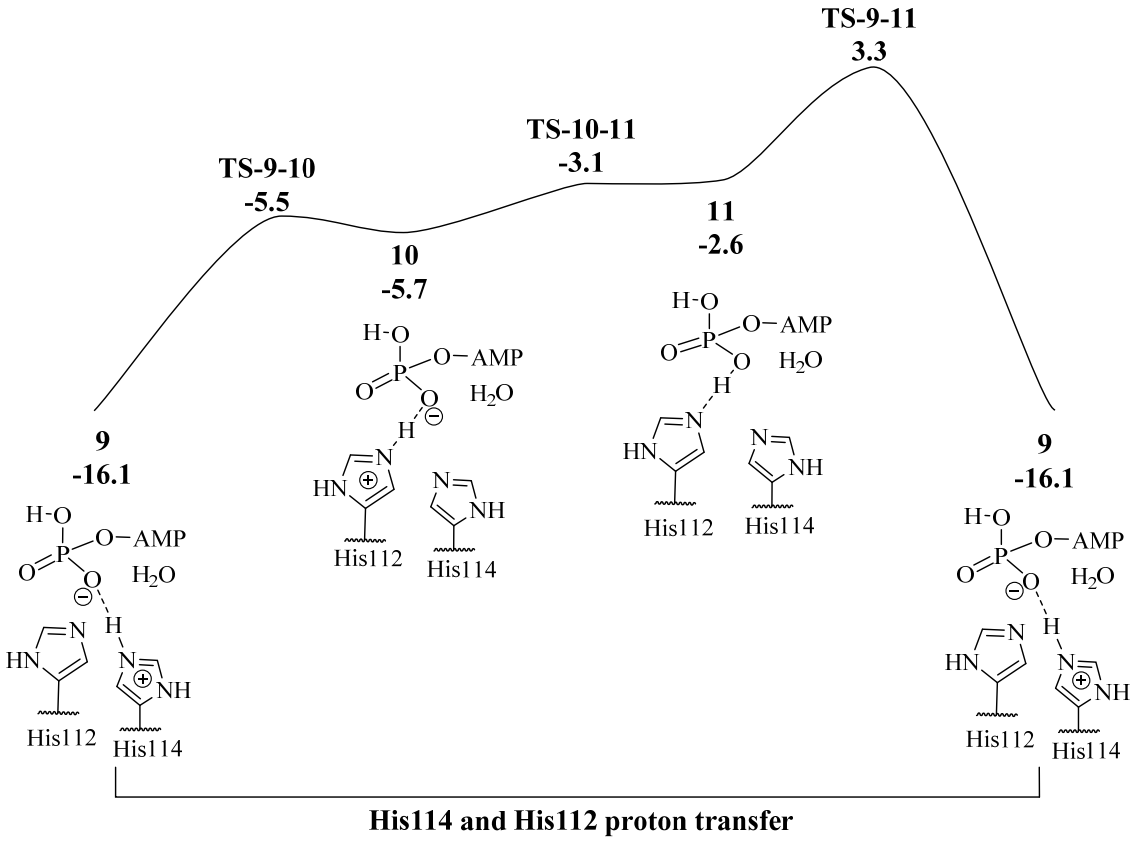


Figure S8. Proton transfer processes between His 11, His 112, and the phosphoryl group.

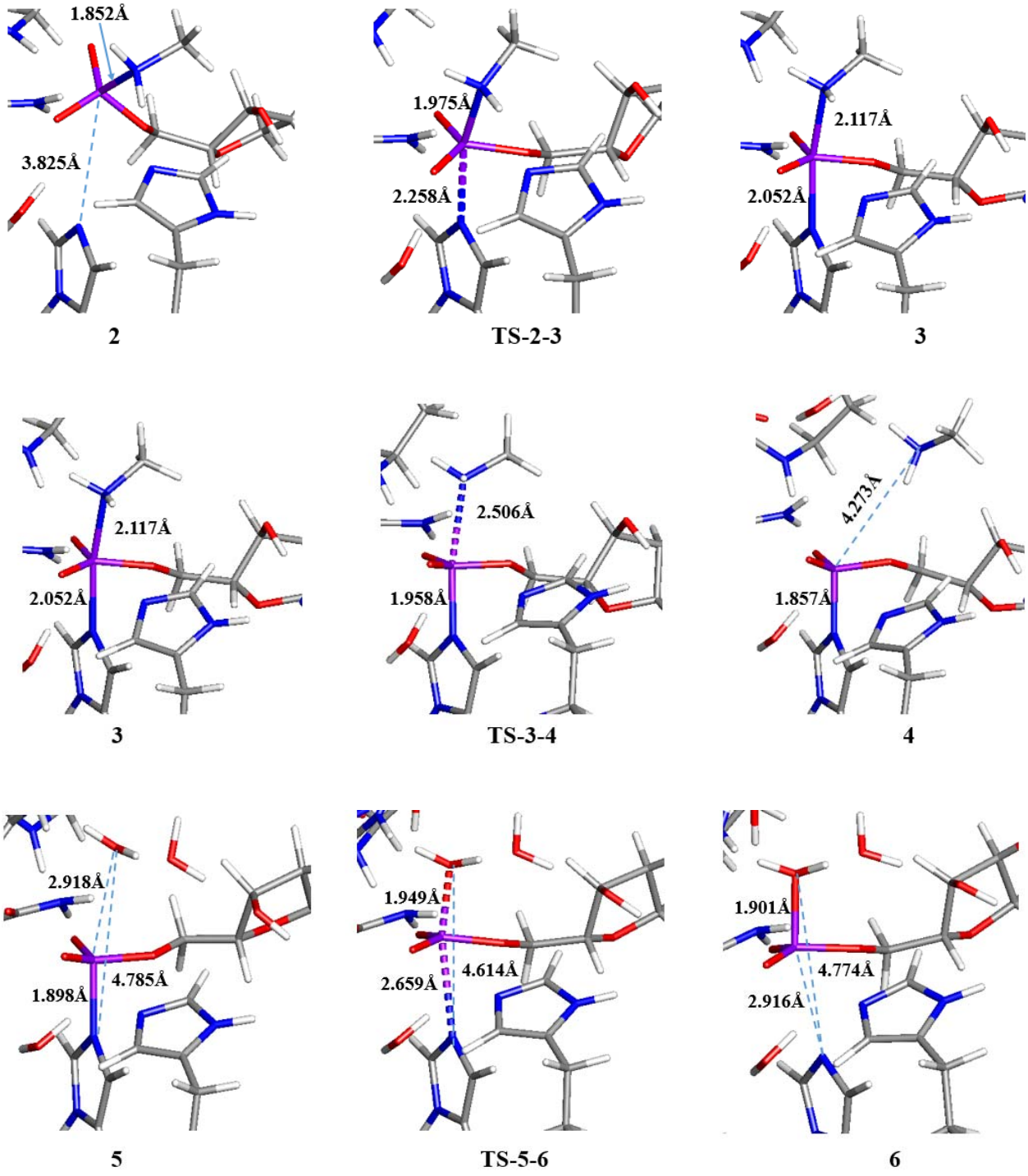


Figure S9. Partial 3D representation of intermediates and transition states with selected geometric parameters.

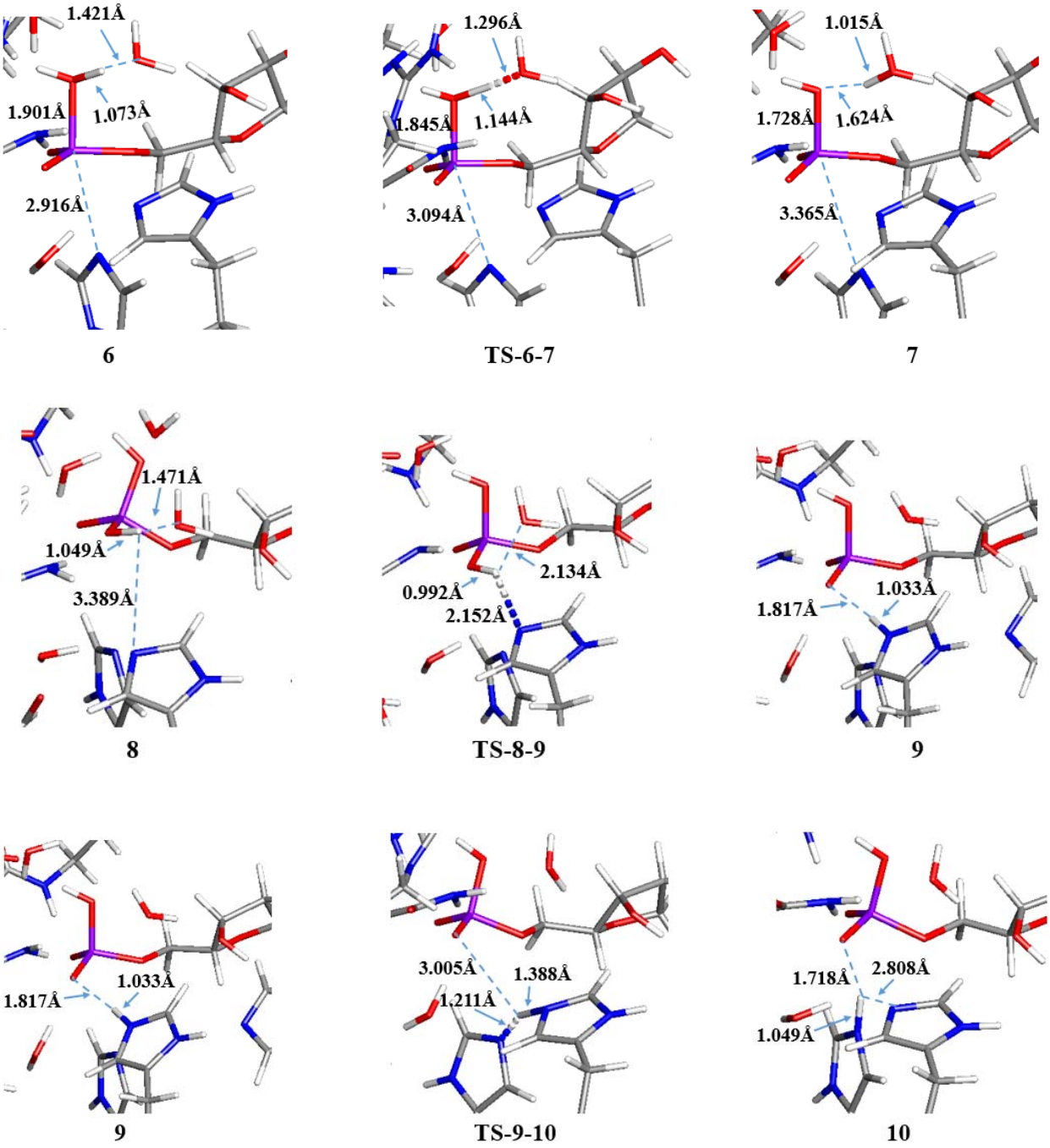


Figure S9. (cont.) Partial 3D representation of intermediates and transition states with selected geometric parameters.

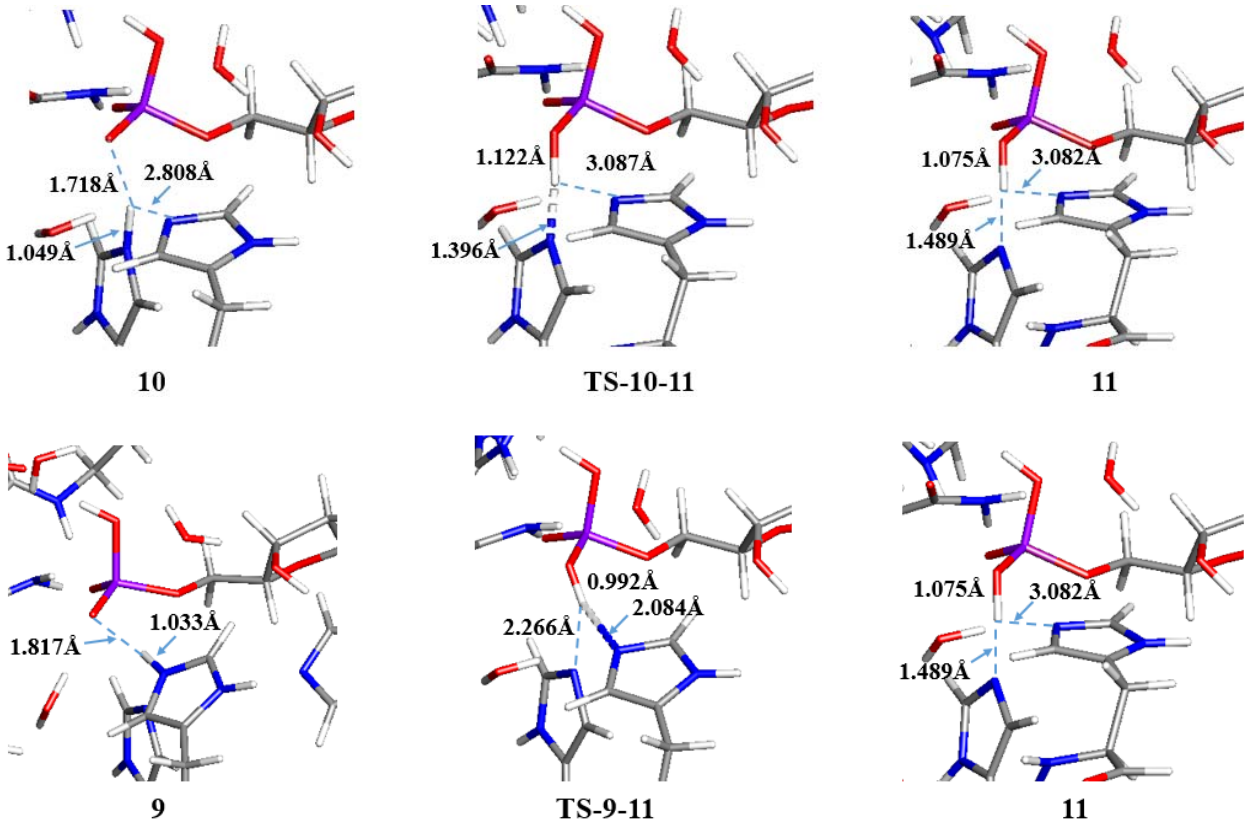


Figure S9. (cont.) Partial 3D representation of intermediates and transition states with selected geometric parameters.

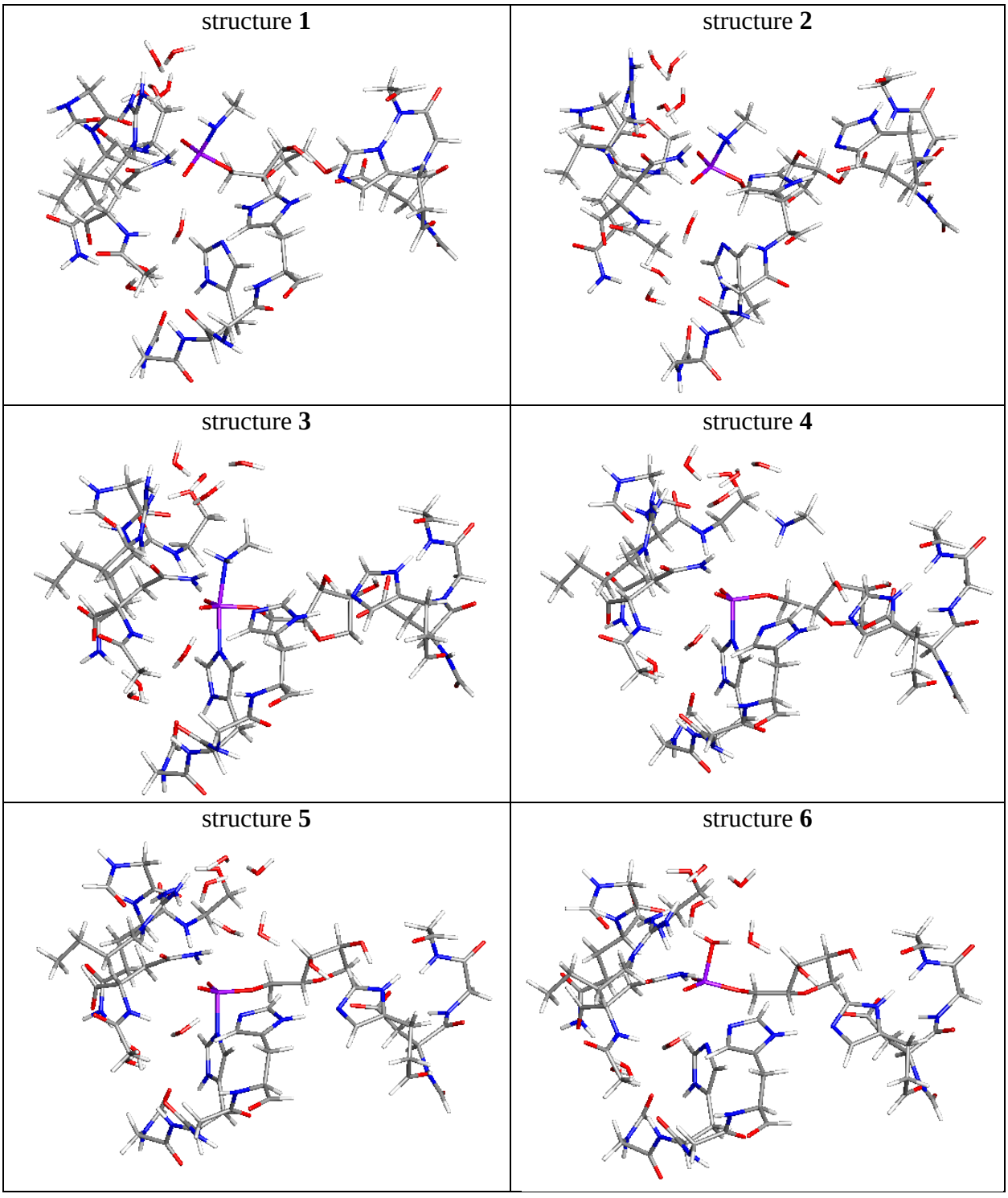


Figure S10. DFT optimized structures of the related intermediates.

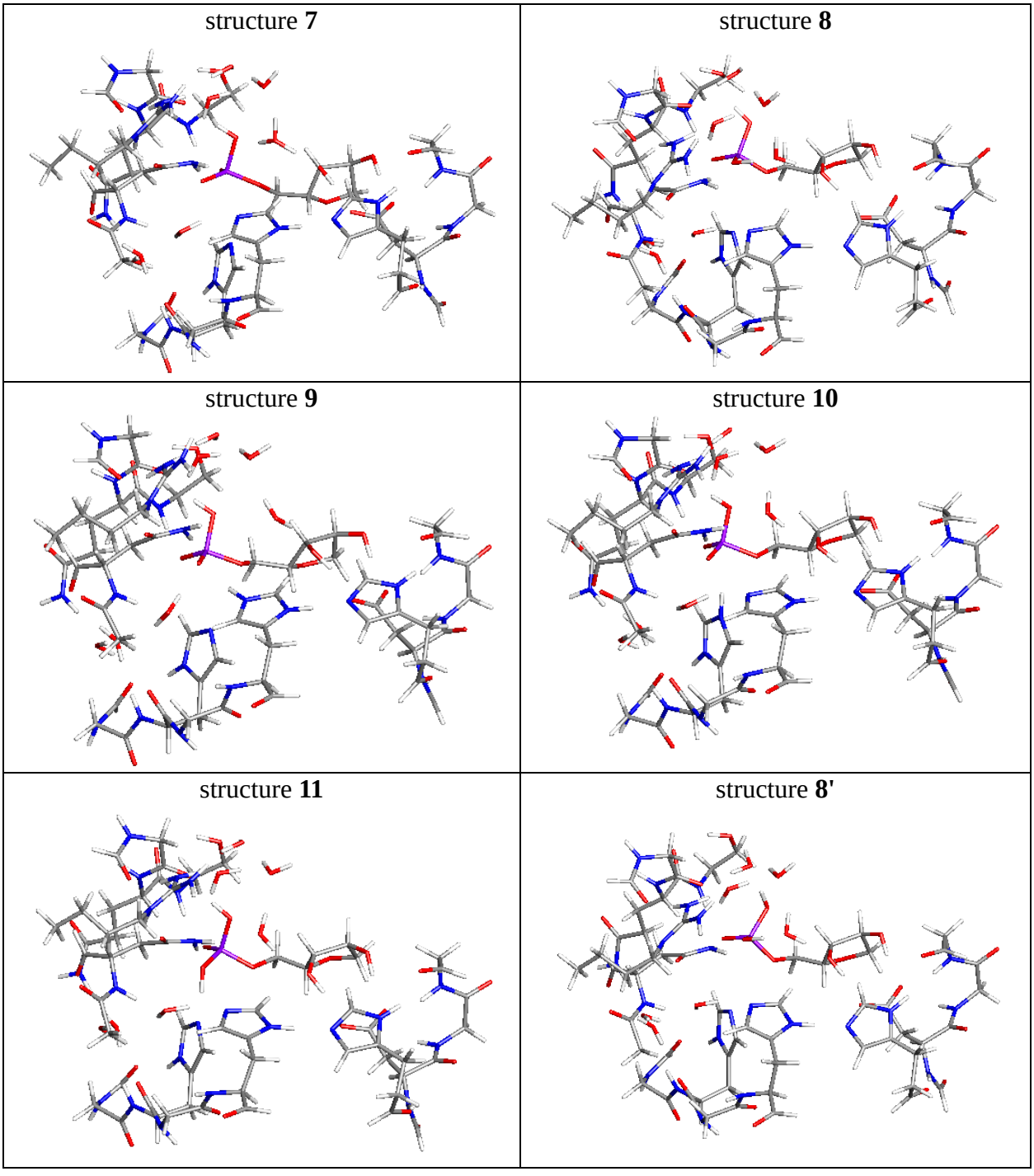


Figure S10. (cont.) DFT optimized structures of the related intermediates.

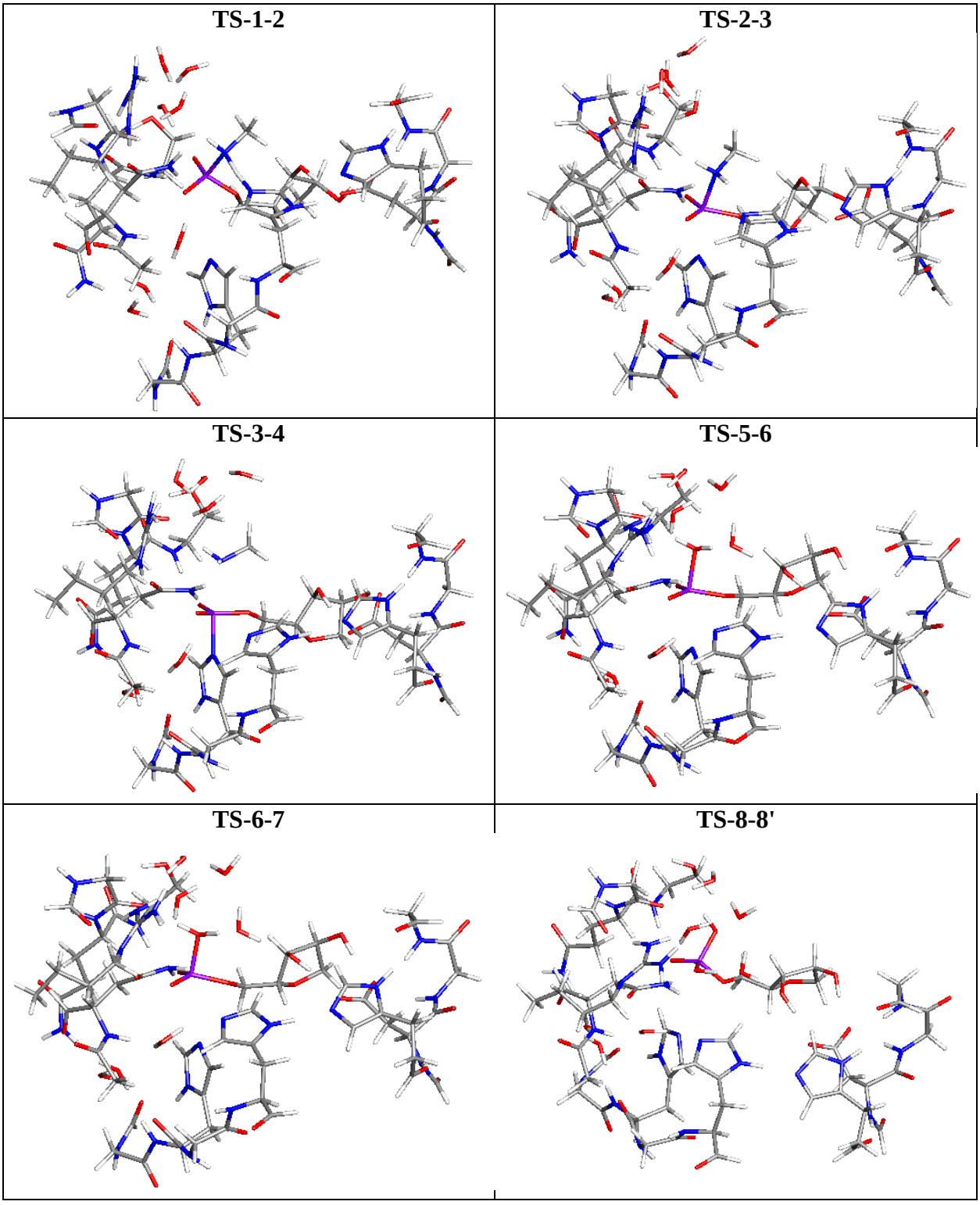


Figure S10. (cont.) DFT optimized structures of the related intermediates.

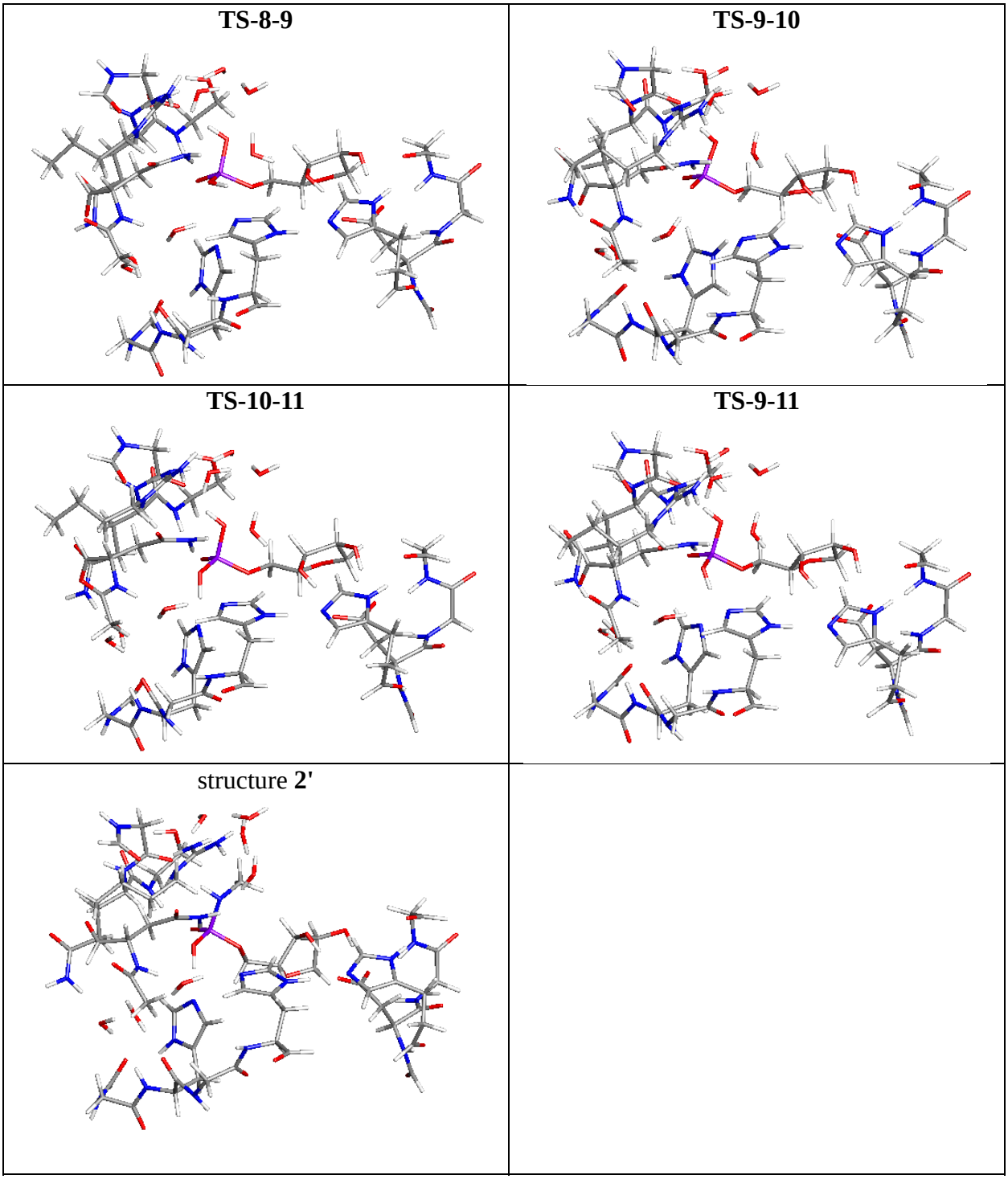


Figure S10. (cont.) DFT optimized structures of the related intermediates.

Table S1. DFT computed energies (in Hartrees) of various species.

Structure	**E**	**E_0**	**$G_{(gas)}$**	**$E_{(soln)}$**
H_2O	-76.403471	-76.382358	-76.400664	-76.408096
CH_3NH_2	-95.850493	-95.786136	-95.809029	-95.852998
methylphosphoramidate substrate model	-749.154580	-748.941015	-748.983795	-749.212242
nucleotide product model	-729.714099	-729.541282	-729.582615	-729.774631
native enzyme model	-5314.754242	-5313.166002	-5313.301815	-5314.849391
structure **1**	-6064.077599	-6062.271587	-6062.426387	-6064.142150
structure **2**	-6064.053942	-6062.248239	-6062.405229	-6064.120242
structure **2'**	-6064.0528287	-6062.248861	-6062.406235	-6064.1179607
structure **3**	-6064.042646	-6062.236992	-6062.392027	-6064.111777
structure **4**	-6064.049688	-6062.244734	-6062.400391	-6064.120394
structure **5**	-6044.620221	-6042.856633	-6043.007778	-6044.685874
structure **6**	-6044.610338	-6042.848080	-6043.000292	-6044.675606
structure **7**	-6044.614218	-6042.852788	-6043.004359	-6044.680677
structure **8**	-6044.629635	-6042.867034	-6043.019540	-6044.695597
structure **8'**	-6044.637149	-6042.875365	-6043.029581	-6044.703173
structure **9**	-6044.649923	-6042.886937	-6043.040570	-6044.719639
structure **10**	-6044.637097	-6042.873553	-6043.025544	-6044.705363
structure **11**	-6044.630957	-6042.870029	-6043.023242	-6044.696624
TS-1-2	-6064.046104	-6062.244699	-6062.400543	-6064.111485
TS-2-3	-6064.040584	-6062.234491	-6062.389716	-6064.107157
TS-3-4	-6064.041918	-6062.237335	-6062.391951	-6064.112007
TS-5-6	-6044.610295	-6042.847421	-6042.996888	-6044.675125
TS-6-7	-6044.610209	-6042.849948	-6043.001149	-6044.675886
TS-8-8'	-6044.628016	-6042.866576	-6043.019120	-6044.693466
TS-8-9	-6044.616652	-6042.855123	-6043.007084	-6044.683447
TS-9-10	-6044.635292	-6042.875928	-6043.025000	-6044.703767
TS-10-11	-6044.630911	-6042.871475	-6043.023718	-6044.696844
TS-9-11	-6044.620472	-6042.859852	-6043.014092	-6044.685783

Table S2. Cartesian coordinates of optimized structures and absolute energies (in Hartrees).

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ch3nh2
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N    -0.050829 -0.760465  0.000000
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H     0.945475  1.185382  0.000000
H    -0.594302  1.063596 -0.882835
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H     0.451956 -1.106405  0.813844
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H    -0.767954 -0.468283  0.000000
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O    -2.511442 -1.647256  1.093062
O    -1.129987 -0.656955 -0.917820
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C     1.164715 -0.851298 -0.058831
O     2.339579 -1.632782 -0.307267
C     1.527611  0.572087 -0.539504
O     0.931401  1.623228  0.178274
C     3.086589  0.636928 -0.319075
O     3.414544  1.559186  0.694972
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O    -3.071207 -1.489227 -0.382446
O    -3.347362  1.208081 -0.188066
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C    -0.281055  1.175788 -0.560776
C     1.157643  0.676179 -0.566808
O     2.071322  1.685579 -0.135041
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C    -3.016007  3.072026  5.399268
C    -9.945837  2.566967 -1.410053
C    -8.510388  0.592562 -1.473418
C    -7.564542 -0.110246 -0.469234
C    -8.364973 -4.713795 -1.005184
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N     3.924326  7.559420 -3.752085
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H	4.140200	8.499046	-4.053951
H	4.397400	6.236117	-2.202644
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O	1.596345	4.554934	1.181385
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N	-0.393945	2.232842	-1.748943
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H	0.961417	2.034236	-3.398628
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C	-9.257020	-3.318337	-3.662866
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N	-8.093096	-3.395116	-2.950228
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H	-7.553754	-2.555656	-2.700790
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O	6.033050	1.370828	3.845831
N	4.510937	1.136273	2.168286
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C	1.982578	-3.695595	-5.681808
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H     1.901553  0.987955  0.773132
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structure 5
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structure 6
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C	4.702319	-4.294809	-0.750574
O	3.486926	-4.162669	-0.956245
H	7.277664	-5.782288	0.404074
H	4.434039	-5.481066	0.987637
H	5.152827	-6.349801	-0.380418
N	5.636168	-3.512314	-1.319172
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O	5.156936	-4.640797	-3.746720
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H     4.549532 -2.172695  4.812100
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H     2.965995 -4.811620  3.586623
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P     1.336751 -0.996285 -2.161480
O     1.117900 -2.867055 -1.904847
O     2.129749 -0.683308 -0.916761
O     1.890486 -0.928833 -3.566934
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O    -3.206999 -0.709497 -4.149630
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O    -3.040587 -2.167806 -0.897611
C    -4.125483 -2.648034 -3.136699
O    -5.191038 -3.135647 -2.377975
C    -4.444591 -1.400727 -3.992739
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H    -5.184466 -0.772146 -3.473416
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H     1.690201  1.080949  0.749295
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H     5.127470 -0.705699 -4.362465
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free energy= -6043.000292

structure 7

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C	-7.357498	0.531691	0.114846
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C	-8.547528	1.684978	4.783966
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C	4.510114	3.247449	3.683989
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C	6.789911	-4.226325	1.728958
C	5.290137	-2.675634	-2.352446
C	5.878363	-0.488512	-3.564408
C	8.187419	-0.576726	5.976226
C	7.252684	-1.654695	6.532181
N	4.317834	6.783756	-4.924851
C	4.478533	6.793393	-3.473629
C	3.149047	7.162058	-2.787552
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H	5.214479	7.563539	-3.221925
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C	0.485530	4.198611	-2.089048
N	1.206026	3.822372	-3.212980
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H	-0.105143	6.200838	-2.578307
H	1.693217	4.420382	-3.870543
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H	1.747732	5.235558	2.705449
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O	-6.738815	-1.143139	-1.480088
O	-5.155196	-0.526323	-0.024998
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C	-10.418965	-1.604666	-2.715374
C	-10.012492	-2.985672	-2.153634
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H	-10.561774	-1.709945	-3.796837
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H     4.455068 -2.068313 -1.979257
H     5.163516 -0.795039 -4.339615
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H    -2.608942  4.109475  3.008079
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structure 8
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C    -8.519747  2.848003  3.310356
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