Supporting Information

Neutral histidine and photoinduced electron transfer in DNA photolyases

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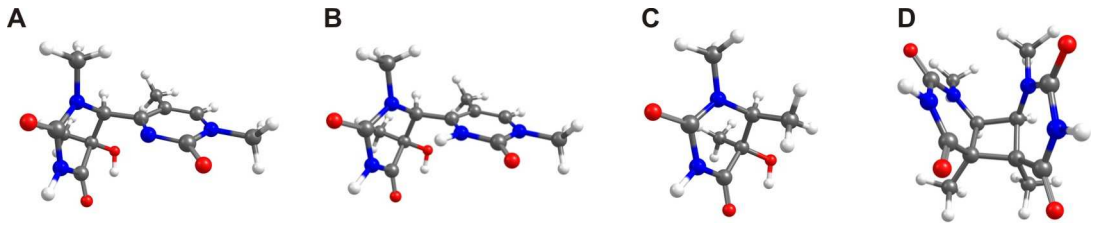

Figure S1. Models of the thymine-thymine photoproducts used to calculate vertical electron affinities. **A**: 3'base (6-4) photoproduct; **B**: N3' protonated 3'base (6-4) photoproduct; **C**: 5'base (6-4) photoproduct; and **D**: CPD photoproduct.

Geometry optimization

The geometries of the (6-4) models were optimized in delocalized intrinsic coordinates (*dlc*) without imposing any restrains to allow for unbiased structure relaxation. However, increasing deviations of the optimized structure from the initial pdb model were observed upon progression of the optimization runs due to the lack of restraining protein environment. Therefore, structures obtained after 25 steps of the *dlc*-geometry optimization were considered in this study. These structures (maximum energy gradient in the range 0.004-0.006 a.u.; *rms* gradient of 0.001 a.u.) are characterized by relaxed geometry configurations of the molecular fragments and hydrogen bonds. At the same time, the models display the relative arrangement of the fragments which is in good agreement with the parent pdb structure as demonstrated in Table S1.

Structures (6-4)Int and (6-4)Repaired were derived from the starting structure (6-4) by transferring the OH-group from the 5'base to the 3'base. The geometry of the modified structure was optimized by using the CASSCF(2,2)2 method in the electronic ground biradical state. The local biradical minimum was found and its structure was further optimized with the broken-symmetry unrestricted U-B3LYP/6-31G(d) method. In the optimization course, the (6-4)Int geometry relaxes into a minimum corresponding to the repaired structure (6-4)Repaired occurred. The geometry (6-4)Int obtained after 7 steps of the UB3LYP geometry optimization was used to compute the excitation spectrum of the OH-transfer repair

intermediate. The (6-4)Repaired structure corresponds to the local minimum computed by the (restricted) B3LYP/6-31G(d) method. The terminal carbon atoms of all the molecular fragments were kept fixed while optimizing models (6-4)Int and (6-4)Repaired.

In the CPD active site model, the "repaired" pair of thymine basis present in the crystal structure was modified in the CPD photoproduct. Upon the *dlc*-geometry optimization of the CPD model, a significant structural change was observed even at the early steps. To prevent rearrangements, the Cartesian coordinates of the terminal atoms (one carbon atom in each molecular fragment) were restraint to the corresponding pdb values and the coordinates of all other atoms were optimized (maximum energy gradient of 0.0005 a.u.; *rms* energy gradient of 0.0001 a.u.). Somewhat larger deviations between the optimized and crystallographic distances were found for the CPD model (Table S1), which could be explained by the presence of the repaired DNA in the pdb structure and the CPD product in the computational model. In all models, the optimized geometry of the flavin ring-system was found to be planar.

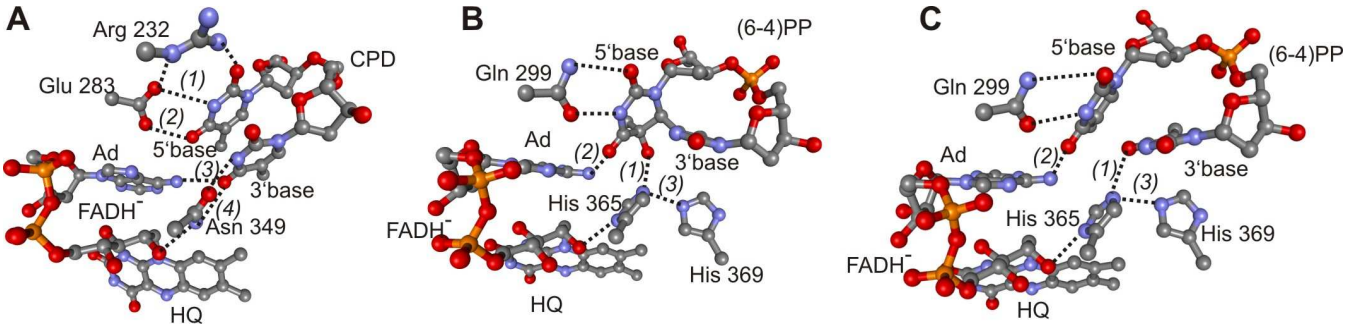

Figure S2. Enzymatic active sites according to crystal structures **A**: CPD photolyase with the repaired CPD photoproduct, pdb 1tez chain A, **B**: (6-4) photolyase with the (6-4) photoproduct, pdb 3cvu, **C**: (6-4) photolyase with the repaired (6-4) photoproduct, pdb 3cvy. Dashed lines indicate hydrogen bonds. Distances *(1)-(4)* are listed in Table S1.

Table S1. Comparison of the optimized geometries with the parent pdb models according to selected hydrogen bonding distances [Å] indicated in Figure S2.

Model	*(1)* His365-(6-4)PP	*(2)* Ad- (6-4)PP	*(3)* His365-His369	
(6-4)	2.79	2.92	2.95	
(6-4)I	2.90	2.93	3.30	
(6-4)II	2.83	2.88	2.96	
(6-4)III	2.62	2.78	3.05	
(6-4)IV	2.88	2.96	2.65	
pdb 3vcu	2.75	2.68	2.75	
(6-4)Repaired	2.59	2.92	3.42	
pdb 3cvy	2.78	2.71	2.86	
	(1) Glu283-CPD	*(2)* Glu283-CPD	*(3)* Asn349-CPD	*(4)* Asn349-CPD
CPD	2.88	2.83	2.81	2.89
pdb 1tez chain A	3.53	2.88	3.00	3.36

Electronic excitation spectra

Figure S3 shows the excitation energies of the CPD and (6-4) models obtained by the CIS, CASSCF and XMCQDPT2 calculations. The excitation energies and the oscillator strengths are collected in Table S2 and S3. The CASSCF-optimized active-space MOs describing the electronic transitions are presented in Figure S4. The HOMOs (the HF reference configuration) of the supra-molecular clusters are localized on the flavin hydroquinone anion. The LUMOs are localized on the photoproducts. With the CIS method, 7 and 11 excited states were required to compute the two ET states of the CPD and (6-4) photoproducts, respectively. The CIS excitation spectrum consists of the LE states of hydroquinone (HQ), adenine (Ad), and the 3'base of the (6-4) photoproduct, and ET states, most of which have flavin HQ as an electron donor. There are two exceptions in Figure S3 and Table S3, the (ET Ad-3'base) and (ET Ad-5'base) states, which describe electron transfer from adenine to the photoproduct. All states have a $\pi\pi^*$ character, except for the (LE 3'base 2) state which has an $n\pi^*$ character.

In Figure S3 and Tables S2-S3, states corresponding to the excitations from the HOMO are indicated. These states, in fact, are the states of interest in this study. Their excitation energies were computed with the CASSCF method. The HOMO and the five unoccupied MOs were included in the active space. The CASSCF(2,6)6 (two electrons in six MOs for six electronic states) state-averaged calculations were performed. The obtained CASSCF excitation energies are lowered compared to the CIS ones. The trend is more pronounced for the ET states than for the LE states. Further decrease of the excitation energies is observed upon the XMCQDPT2 correction. The energy shift of 0.02 hartree was applied to avoid the intruder-state problem.

For models (6-4)I-IV, (6-4)Int and (6-4)Repaired, the same computational protocol - CIS-CASSCF-XMCQDPT2 - was applied. The CASSCF and XMCQDPT2 and the transition oscillator strengths are collected in Tables S4-S9 and the CASSCF-optimized active-space MOs are presented in Figures S4, S6-S8. The data in Tables S4-S7 show only a small dependence on the number of electronic states included in the state-averaged CASSCF calculations, which must not affect any conclusions of this work.

Excitation spectrum of model (6-4)Int was computed in two different ways with the active spaces including only two electrons and two molecular orbitals, CASSCF(2,2)2, and four electrons and six orbitals averaging the energies of the six states, CASSCF(4,6)6. The CASSCF-optimized active-space MOs are shown in Figure S8. The excitation spectrum (Table S8) contains the locally excited states of the radical fragments as well as of the singlet open-shell photoproduct. The later state interacts with the closed-shell photoproduct as well as with the 5'radical of the photoproduct. Thus, the electronically excited (6-4)Int has a more complex structure in comparison to the other models, which is related to the transient (as opposed to chemically stable) character of this model.

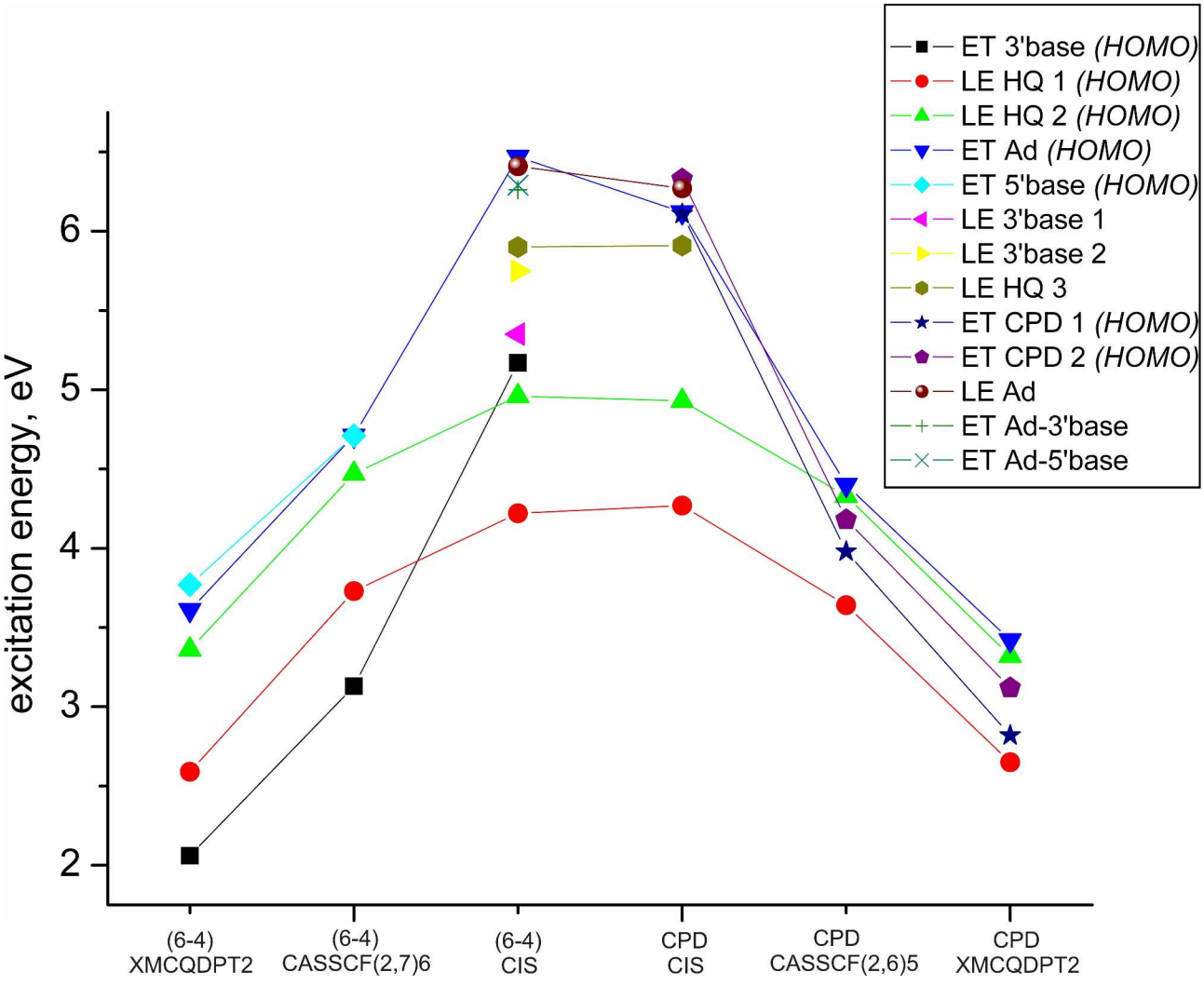

Figure S3. The electronic excitation spectrum of the (6-4) and CPD models computed by the CIS, CASSCF(2,6)6 and XMCQDPT2 methods. In the legend, "*HOMO*" indicates excitations from the HOMO.

Table S2. Model CPD. Excitation energies [eV], oscillator strengths (in brackets).

Electronic States	CIS	CASSCF(2,6)6 Fig. S4A	XMCQDPT2
LE HQ 1 *(HOMO)*	4.27 (0.00)	3.64	**2.65/ 468 nm (0.07)**
LE HQ 2 *(HOMO)*	4.93 (0.29)	4.33	**3.32/ 373 nm (0.28)**
LE HQ 3	5.91 (0.47)		
ET CPD 1 *(HOMO)*	6.11 (0.00)	3.98	2.82 (0.00)
ET Ad *(HOMO)*	6.12 (0.00)	4.40	3.42 (0.01)
LE Ad	6.27 (0.27)		
ET CPD 2 *(HOMO)*	6.33 (0.00)	4.18	3.12 (0.00)

Table S3. Model (6-4). Excitation energies [eV], oscillator strengths (in brackets).

Electronic States	CIS	CASSCF(2,6)6 Fig. S4B	XMCQDPT2
LE HQ 1 *(HOMO)*	4.22 (0.01)	3.73	**2.59/ 479 nm (0.07)**
LE HQ 2 *(HOMO)*	4.96 (0.26)	4.47	**3.36/ 369 nm (0.28)**
ET 3'base *(HOMO)*	5.16 (0.00)	3.13	2.06 (0.00)
LE 3'base 1	5.35 (0.22)		
LE 3'base 2	5.71 (0.01)		
LE HQ 3	5.90 (0.50)		
ET Ad-3'base	6.26 (0.12)		
ET Ad-5'base	6.29 (0.15)		
LE Ad	6.41 (0.04)		
ET Ad *(HOMO)*	6.48 (0.00)	4.71	3.61 (0.02)
ET 5'base *(HOMO)*		4.98	3.77 (0.01)
		CASSCF(2,5)5	XMCQDPT2
ET 3'base		3.36	1.99 (0.00)
LE HQ 1		3.77	**2.57/ 482 nm (0.07)**
LE HQ 2		4.51	**3.30/ 376 nm (0.28)**
ET Ad		4.91	3.57 (0.02)
		CASSCF(2,2)2 Fig. S4B	XMCQDPT2
ET 3'base		2.88	1.98

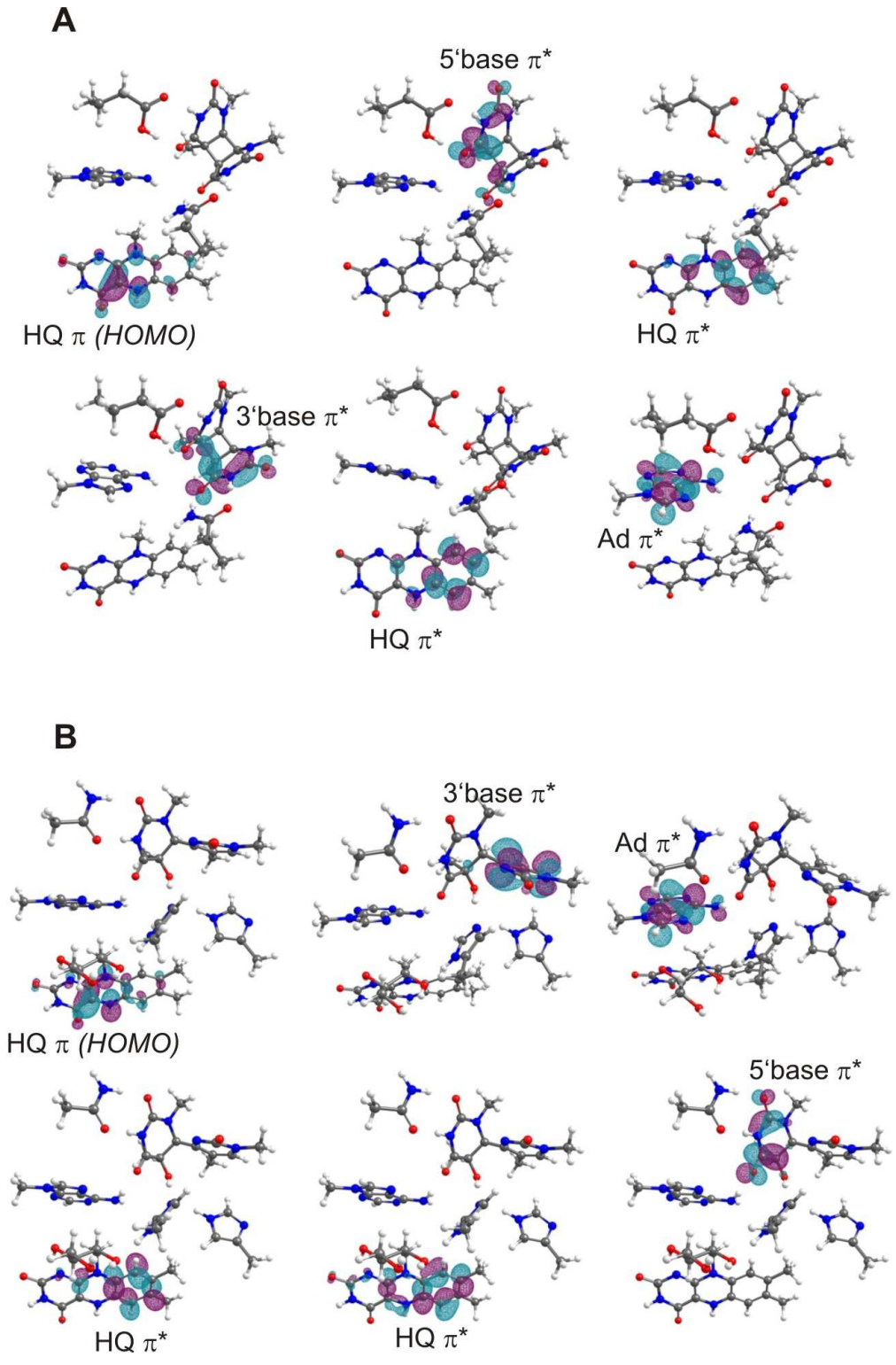

Figure S4. CASSCF-optimized active space MOs. **A**: model CPD, CASSCF(2,6)6 and **B**: model (6-4), CASSCF (2,6)6.

Table S4. Model (6-4)I. Excitation energies [eV], oscillator strengths (in brackets).

Electronic states	Excitation energy, eV (oscillator strength)	
	CASSCF(2,2)2 (Fig. S6A)	XMCQDPT2
ET 3'base	1.89	1.04
	CASSCF(2,5)5	XMCQDPT2
ET 3'base	1.81	1.11 (0.00)
ET His365	2.96	2.53 (0.00)
LE HQ 1	3.48	**2.58/ 481 nm (0.03)**
ET 5'base	3.63	2.66 (0.01)
	CASSCF(2,6)6 (Fig. S6A)	XMCQDPT2
ET 3'base	2.02	1.12 (0.00)
ET His365	3.14	2.56 (0.01)
LE HQ 1	3.58	**2.63/ 471 nm (0.08)**
ET 5'base	3.70	2.70 (0.01)
LE HQ 2	4.19	**3.27/ 379 nm (0.26)**

Table S5. Model (6-4)II. Excitation energies [eV], oscillator strengths (in brackets).

Electronic state	Excitation energy, eV (oscillator strength)	
	CASSCF(2,2)2 (Fig. S6B)	XMCQDPT2
ET 3'base (biradical)	0.0	
Closed-shell (CS)	2.66	3.02
	CASSCF(2,5)5	XMCQDPT2
ET 3'base (biradical)	0.0	
Closed-shell (CS)	3.56	2.34 (0.00)
LE SQ 1	3.77	**2.35/ 527 nm (0.05)**
LE 3'base	4.24	**2.87/ 432 nm (0.14)**
LE SQ 2	5.05	3.16 (0.20)
	CASSCF(2,6)6 (Fig. S6B)	XMCQDPT2
ET 3'base (biradical)	0.0	
LE SQ 1	3.93	**2.31/ 537 nm(0.04)**
Closed-shell (CS)	3.45	2.43 (0.00)
LE 3'base	4.35	**2.93/ 423 nm (0.14)**
LE SQ 2	5.27	**3.12/ 397 nm (0.20)**
ET 3'base -5'base	5.27	3.82 (0.05)

Table S6. Model (6-4)III. Excitation energies [eV], oscillator strengths (in brackets).

Electronic state	Excitation energy, eV (oscillator strength)	
	CASSCF(2,5)5	XMCQDPT2
ET Ad 1	2.02	1.52 (0.01)
ET 3'base	3.13	2.07 (0.00)
LE HQ 1	3.31	**2.60/ 477 nm (0.06)**
ET Ad 2	3.82	2.75 (0.01)
	CASSCF(2,7)7 (Fig. S6C)	XMCQDPT2
ET Ad 1	1.82	1.61 (0.01)
ET 3'base	2.89	2.16 (0.00)
LE HQ 1	3.19	**2.69/ 461 nm (0.05)**
ET Ad 2	3.57	2.82 (0.01)
ET Ad 3	3.69	3.01 (0.03)
ET 5'base	3.90	3.26 (0.07)

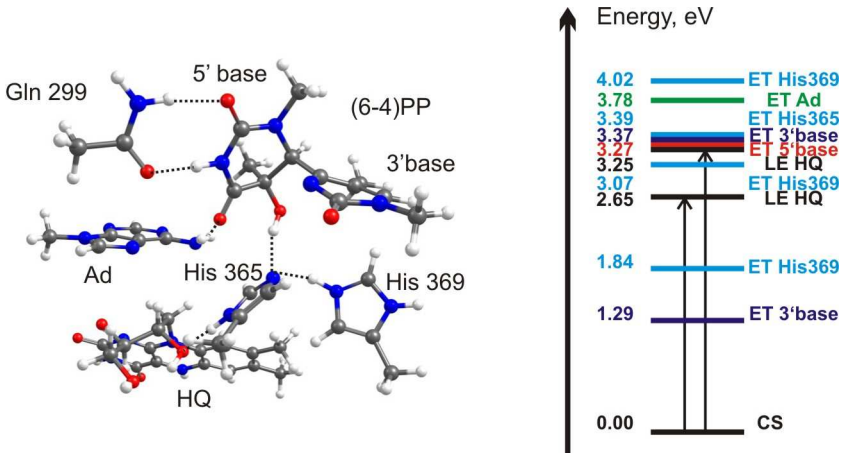

Figure S5. Optimized geometry and vertical excitation spectrum of model (6-4)IV, containing protonated His 369 (see also Table S7).

Table S7. Model (6-4)IV (see Fig.S5). Excitation energies [eV], oscillator strengths (in brackets).

Electronic state	Excitation energy, eV (oscillator strength)	
	CASSCF(2,11)11 (Fig. S7)	XMCQDPT2
ET 3'base 1	1.46	1.29 (0.00)
ET His369 1	1.90	1.84 (0.00)
LE HQ 1	3.37	**2.65/ 468 nm (0.08)**
ET His369 2	3.22	3.07 (0.01)
LE HQ 2	3.90	**3.25/ 382 nm (0.26)**
ET 5'base	4.09	3.27 (0.03)
ET 3'base 3	3.96	3.37 (0.01)
ET His365	4.05	3.39 (0.01)
ET Ad	4.32	3.78 (0.01)
ET His369 3	3.87	4.02 (0.00)

Table S8. Model (6-4)Int. Excitation energies [eV], oscillator strengths (in brackets).

Electronic state	Excitation energy, eV (oscillator strength)	
	CASSCF(2,2)2 (Fig. S8A)	XMCQDPT2
ET 5'base (biradical)	0.0	
ET 5'base to SQ (CS)	2.70	3.27
	CASSCF(4,6)6 (Fig. S8A)	XMCQDPT2
ET 5'base (biradical)	0.0	0.0
(CS*) 1	3.62	1.88 (0.02)
LE SQ 1	4.33	**2.08/ 596 nm (0.08)**
(CS*) 2	4.87	2.89 (0.02)
LE SQ	5.11	**3.04/ 408 nm (0.21)**
2 LE 3'base	4.08	4.43 (0.00)

* the CS* states are multiconfigurational with two major configurations contributing: i) photoproduct and hydroquinone both in the closed-shell singlet state and ii) the ππ*-excited photoproduct and the closed-shell hydroquinone.

Table S9. Model (6-4)Repaired. Excitation energies [eV], oscillator strengths (in brackets).

Electronic state	Excitation energy, eV (oscillator strength)	
	CASSCF(2,6)6 (Fig. S8B)	XMCQDPT2
LE HQ 1	3.80	**2.65/ 468 nm (0.07)**
ET (3'base; 5'base)	3.94	3.39 (0.00)
ET (3'base; 5'base)	4.28	3.34 (0.04)
LE HQ 2	4.48	**3.34/ 371 nm (0.25)**
ET Ad	4.81	3.71 (0.01)

Table S10. Total electronic energies [hartree] of the (6-4)I-III models.

Model	R/U-B3LYP	CASSCF(2,2)2	XMCQDPT2
(6-4)I	-3448.695770	Ground state (closed shell): -3429.850497 Excited state (open shell): -3429.780912	Ground state (closed shell): -3440.263309 Excited state (open shell): -3440.225193
(6-3)II	-3448.740858	Ground state (open shell): -3429.885695 Excited state (closed shell): -3429.798079	Ground state (open shell): -3440.325768 Excited state (closed shell): -3440.214933
(6-4)III	-3448.691270		
(6-4)IV	-3448.695765		

Table S11. Total electronic energies [hartree] of the (6-4), (6-4)Int and (6-4)Repaired models.

Model	R/U-B3LYP	CASSCF(2,2)2	XMCQDPT2
(6-4)	-3448.232460	Ground state (closed shell): -3429.386003 Excited state (open shell): -3429.280118	Ground state (closed shell): -3439.835798 Excited state (open shell): -3439.762879
(6-3)Int	-3448.145464	Ground state (open shell): -3429.282261 Excited state (closed shell): -3429.183163	Ground state (open shell): -3439.768282 Excited state (closed shell): -3439.648146
(6-4)Repaired	-3448.261541		

Table S12. Charge and spin distribution in the photoproduct repair intermediate in model (6-4)Int computed with the U-B3LYP/6-31G(d) method. Atom numbering is shown in Chart S1.

Atom	Atomic spin densities	Mulliken Charge	Free valences
3'base			
N1	0.002	-0.449	0.000
C	0.000	-0.282	0.000
H	0.000	0.163	0.000
H	0.000	0.150	0.000
H	0.000	0.118	0.000
C2	-0.004	0.667	0.000
O2	0.000	-0.605	0.000
N3	-0.005	-0.589	0.000
C4	-0.048	0.378	0.003
O4	0.005	-0.704	0.000
H	0.000	0.445	0.000
C5	0.000	0.101	0.000
C	0.000	-0.527	0.000
H	0.000	0.121	0.000
H	0.001	0.164	0.000
H	0.000	0.126	0.000
C6	-0.004	0.024	0.000
H	0.000	0.108	0.000
5'base			
N1	-0.009	-0.433	0.000
C	-0.002	-0.294	0.000
H	0.000	0.180	0.000
H	0.000	0.149	0.000
H	0.000	0.141	0.000

C2	0.002	0.820	0.000
O2	0.000	-0.590	0.000
N3	-0.006	-0.715	0.002
H	0.001	0.388	0.000
C4	0.021	0.593	0.002
O4	-0.021	-0.553	0.017
C5	-0.083	0.083	0.401
C	0.000	-0.516	0.002
H	-0.020	0.187	0.002
H	-0.010	0.132	0.000
H	-0.002	0.146	0.000
C6	0.022	-0.052	0.002
H	-0.007	0.123	0.000

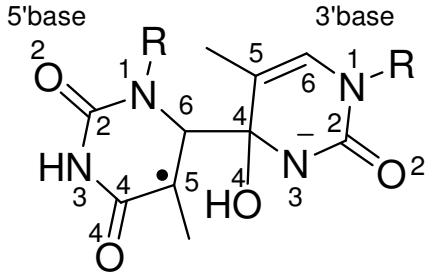

Chart S1. Atom numbering in the OH-transfer repair intermediate.

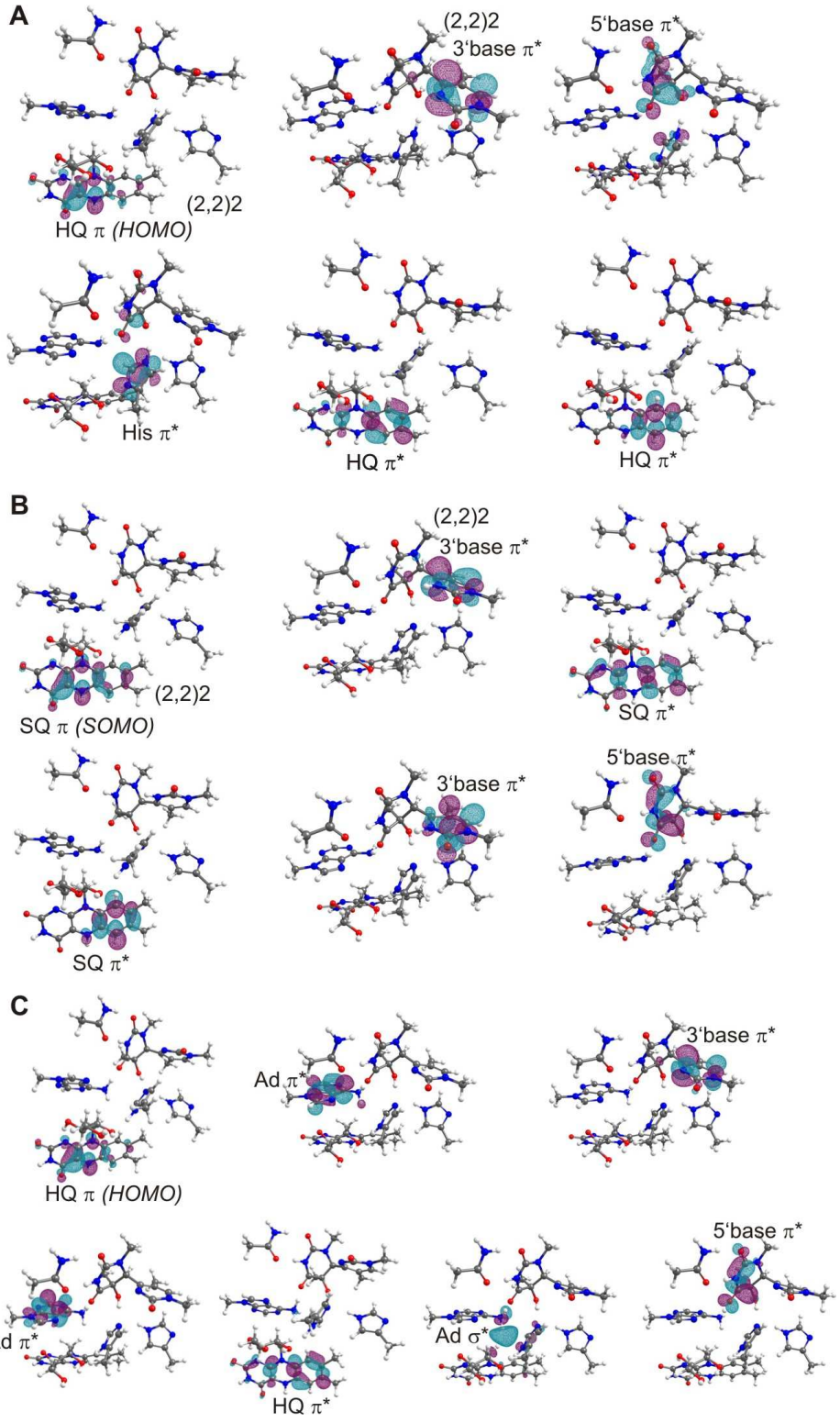

Figure S6. CASSCF-optimized active space MOs. **A**: model (6-4)I CASSCF(2,6)6; **B**: model (6-4)II, CASSCF (2,6)6; and **C**: model (6-4)III, CASSCF(2,7)7. The active space MOs of the CASSCF(2,2)2 calculations (Table S10) are indicated by "(2,2)2".

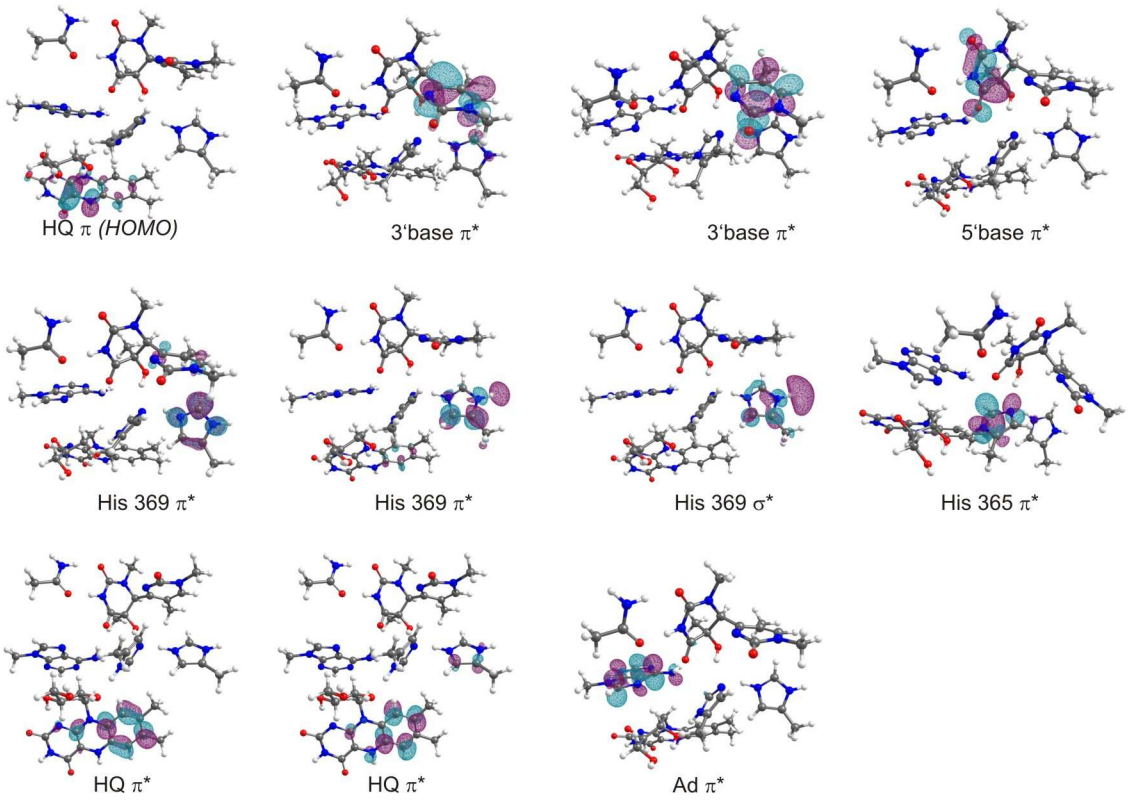

Figure S7. CASSCF-optimized active space MOs of model (6-4)IV, CASSCF(2,11)11.

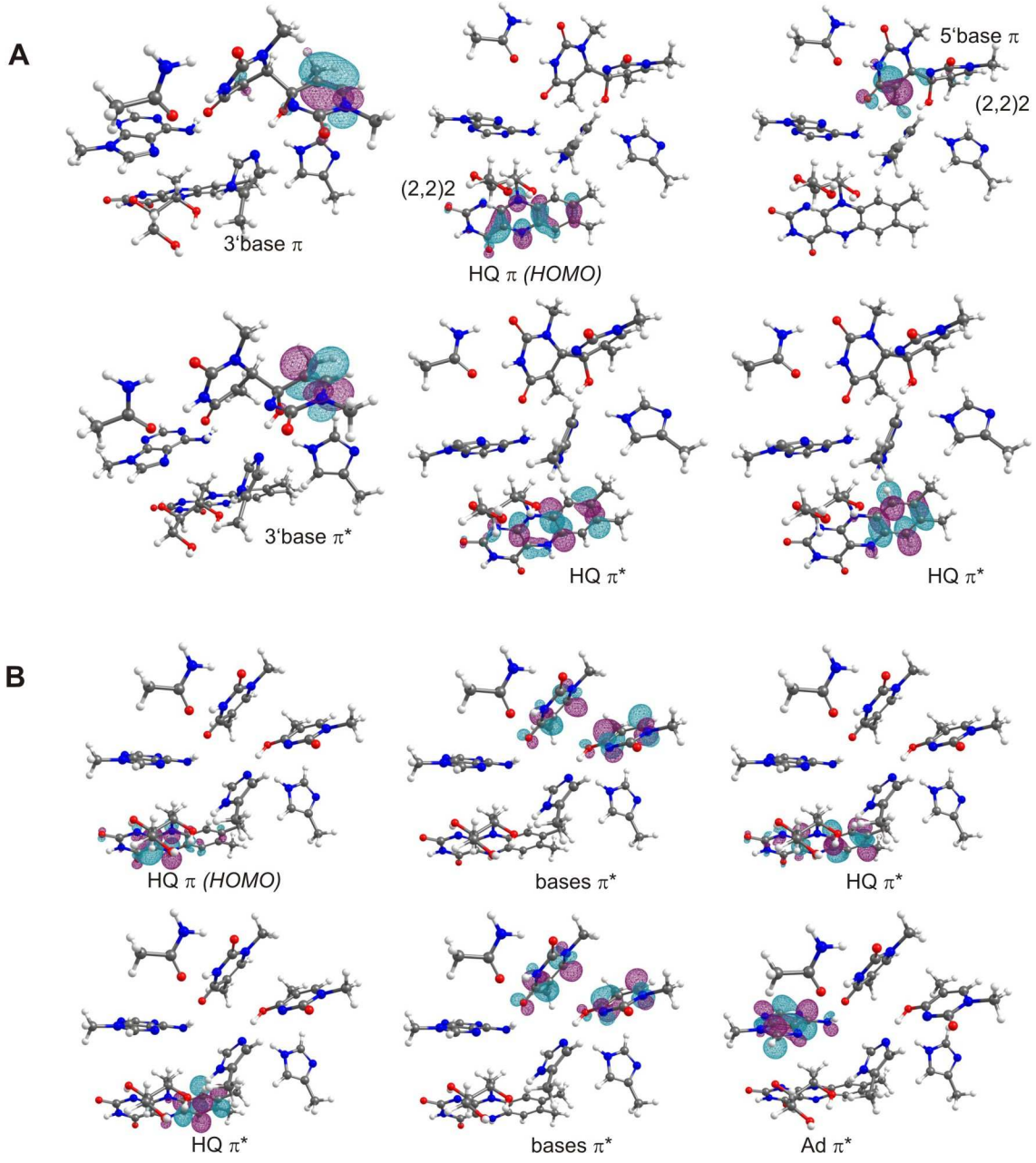

Figure S8. CASSCF-optimized active space MOs. **A:** model (6-4)Int, CASSCF(4,6)6; **B**: model (6-4)Repaired, . The active space MOs of the CASSCF(2,2)2 calculations (Table S11) are indicated by "(2,2)2".

Cartesian coordinates of model CPD

H	72.165	0.570	24.648
C	71.137	0.209	24.777
H	70.795	0.505	25.774
C	71.062	-1.314	24.602
C	71.623	-1.834	23.268
C	70.801	-1.625	22.004
O	69.503	-1.431	22.219
H	70.502	0.719	24.043
H	71.631	-1.793	25.411
H	70.024	-1.647	24.708
H	72.617	-1.419	23.063
H	71.765	-2.923	23.328
O	71.309	-1.694	20.891
H	69.023	-1.379	21.351
H	63.829	-8.047	21.193
C	64.065	-7.173	20.576
H	64.390	-7.521	19.591
C	65.172	-6.331	21.229
C	65.539	-5.174	20.314
O	66.173	-5.386	19.267
N	65.102	-3.955	20.675
H	63.145	-6.590	20.450
H	64.855	-5.972	22.215
H	66.072	-6.940	21.366
H	64.553	-3.814	21.512
H	65.201	-3.181	20.018
N	65.806	0.517	21.518
N	66.746	-0.764	25.883
C	66.886	-0.793	27.333
C	66.501	0.352	25.111
N	66.435	1.630	25.508
C	66.135	2.437	24.487
N	65.914	2.125	23.198
C	66.003	0.833	22.832
C	66.317	-0.131	23.809
N	66.432	-1.509	23.768
C	66.675	-1.837	25.016
H	65.275	1.183	20.973
H	65.716	-0.455	21.258
H	66.050	3.496	24.727
H	66.812	-2.849	25.376
H	65.906	-0.868	27.816
H	67.368	0.133	27.651
H	67.505	-1.647	27.617
O	57.430	-1.376	25.602
C	58.674	-1.442	25.508
C	62.889	-1.987	23.082
H	63.229	-2.982	22.745
N	61.451	-1.917	23.098
C	60.780	-1.705	24.333
C	59.396	-1.679	24.311
N	58.671	-1.902	23.116
C	59.307	-1.992	21.906
C	60.735	-2.019	21.888
C	58.622	-2.094	20.692
C	59.280	-2.218	19.454
C	60.676	-2.248	19.429
C	61.373	-2.151	20.656
C	61.471	-2.363	18.144
C	58.437	-2.316	18.199
N	59.515	-1.280	26.614
C	60.927	-1.340	26.622
N	61.543	-1.549	25.419
O	61.519	-1.199	27.700
H	57.679	-1.719	23.181
H	63.326	-1.232	22.412
H	63.238	-1.818	24.099
H	61.188	-3.247	17.553
H	62.543	-2.447	18.356
H	61.338	-1.488	17.488
H	57.783	-1.439	18.089
H	57.779	-3.197	18.225
H	59.042	-2.386	17.291
H	57.533	-2.083	20.717
H	62.457	-2.172	20.624
H	59.070	-1.115	27.507
H	71.695	1.064	15.852
H	70.256	1.294	14.820
C	70.888	0.555	15.321
N	70.073	-0.198	16.264
C	70.753	-0.790	17.300
O	71.968	-0.894	17.327
N	69.969	-1.236	18.381
C	68.670	-0.905	18.655
O	68.161	-1.158	19.746
C	67.904	-0.128	17.579
C	67.572	1.239	18.189
C	68.636	-0.131	16.219
H	71.343	-0.089	14.558
H	68.374	0.778	15.669
H	66.974	1.849	17.506
H	67.035	1.119	19.134
H	68.498	1.788	18.402
H	70.515	-1.580	19.186
H	69.435	-2.402	13.911
O	65.406	-1.993	18.573
C	66.275	-2.142	17.716
N	66.906	-3.332	17.494
C	67.736	-3.677	16.411
O	68.054	-4.841	16.242
N	68.148	-2.653	15.567
C	67.676	-1.284	15.675
C	66.735	-0.966	16.882
C	65.523	-0.126	16.468
C	68.648	-3.083	14.249
H	67.835	-3.083	13.508
H	66.646	-4.130	18.117
H	67.230	-1.007	14.710
H	64.837	-0.736	15.870
H	65.817	0.735	15.860
H	64.979	0.222	17.347
H	69.048	-4.089	14.349

Cartesian coordinates of model (6-4)

N	88.351	10.322	8.090
C	88.239	11.272	9.079
C	88.180	10.892	10.524
C	88.219	12.479	8.424
N	88.317	12.279	7.057
C	88.386	10.963	6.902
H	88.022	11.775	11.149
H	87.359	10.188	10.717
H	88.124	13.468	8.852
H	88.443	10.435	5.959
H	88.350	9.290	8.240
H	89.108	10.406	10.853
C	91.510	14.589	5.782
N	90.890	13.462	6.221
C	91.766	12.840	7.084
C	92.893	13.630	7.117
N	92.721	14.726	6.290
C	94.141	13.436	7.927
H	94.801	14.293	7.783
H	91.045	15.271	5.082
H	89.915	13.184	6.118
H	91.517	11.911	7.578
H	94.688	12.529	7.643
H	93.912	13.354	8.997
C	82.836	7.619	6.048
C	81.120	6.602	7.592
N	82.180	7.533	7.259
C	82.814	8.425	8.097
N	83.794	9.087	7.535
C	83.824	8.592	6.238
N	82.584	6.922	4.930
C	83.434	7.254	3.955
N	84.420	8.162	3.978
C	84.642	8.853	5.115
N	85.678	9.737	5.129
H	81.489	5.575	7.534
H	80.285	6.723	6.896
H	80.783	6.815	8.610
H	82.489	8.537	9.123
H	83.316	6.722	3.012
H	86.090	9.910	4.222
H	85.669	10.514	5.784
C	84.153	17.400	5.262
O	82.568	15.831	6.754
N	84.414	15.973	5.423
C	83.592	15.308	6.304
N	83.931	14.003	6.628
C	85.021	13.311	6.168
C	85.742	15.485	5.051
C	85.755	13.928	4.966
O	85.326	12.221	6.622
O	87.079	13.477	4.862
C	85.002	13.457	3.702
C	88.511	16.381	3.985
C	88.063	16.576	5.413
C	86.838	16.059	5.963
N	86.538	16.122	7.238
C	87.393	16.705	8.150
N	88.493	17.422	7.603
C	88.833	17.287	6.295
O	87.242	16.685	9.363
C	89.267	18.241	8.534
H	84.435	17.962	6.160
H	83.092	17.553	5.074
H	84.739	17.767	4.414
H	83.354	13.535	7.356
H	85.929	15.842	4.032
H	85.567	13.769	2.818
H	83.988	13.866	3.642
H	84.944	12.365	3.711
H	87.744	16.675	3.259
H	88.744	15.329	3.794
H	89.402	16.983	3.779
H	89.751	17.784	5.985
H	89.771	17.606	9.265
H	88.587	18.905	9.074
H	90.001	18.832	7.977
H	87.421	13.118	5.727
C	88.335	2.025	5.564
N	87.034	1.768	6.010
C	86.142	2.705	6.561
N	86.584	3.999	6.641
C	87.826	4.313	6.214
C	88.705	3.390	5.682
O	89.067	1.130	5.095
O	85.029	2.335	6.947
N	89.979	3.774	5.221
C	90.414	5.068	5.313
C	89.547	6.038	5.902
N	88.243	5.659	6.338
C	91.675	5.468	4.858
C	92.126	6.794	4.958
C	91.291	7.748	5.548
C	90.021	7.341	6.011
C	93.503	7.150	4.431
C	91.706	9.195	5.726
C	87.225	6.689	6.550
C	86.977	7.157	7.990
O	88.207	7.652	8.570
C	86.353	6.078	8.907
O	85.171	5.568	8.346
C	85.968	6.646	10.277
O	87.171	7.030	10.986
H	86.707	0.813	5.951
H	92.319	4.711	4.409
H	89.407	8.082	6.506
H	93.551	7.088	3.334
H	94.269	6.465	4.818
H	93.800	8.165	4.708
H	91.915	9.701	4.774
H	92.607	9.302	6.344
H	90.912	9.761	6.221
H	86.273	6.314	6.175
H	87.486	7.560	5.940
H	86.251	7.984	7.920
H	88.110	7.568	9.541
H	87.107	5.293	9.070
H	85.310	7.516	10.143
H	86.929	7.653	11.690
H	85.490	4.909	7.660
H	85.425	5.868	10.826
H	90.511	3.047	4.751
C	80.132	11.936	9.216
C	81.119	12.911	8.589
O	82.303	12.600	8.442
N	80.634	14.123	8.221
H	79.652	14.339	8.298
H	81.254	14.790	7.752
H	79.262	11.773	8.568
H	79.767	12.308	10.181
H	80.643	10.983	9.372

Cartesian coordinates of model (6-4)I

N	88.299	10.283	8.213	O	82.614	15.868	6.769	C	90.389	5.097	5.261
C	88.219	11.216	9.234	N	84.427	16.002	5.396	C	89.537	6.060	5.880
C	88.247	10.803	10.670	C	83.619	15.345	6.295	N	88.246	5.683	6.338
C	88.105	12.439	8.631	N	83.954	14.029	6.615	C	91.651	5.489	4.809
N	88.125	12.214	7.267	C	85.035	13.350	6.144	C	92.115	6.804	4.932
C	88.217	10.901	7.038	C	85.751	15.514	5.001	C	91.286	7.755	5.539
H	88.079	11.667	11.315	C	85.720	13.964	4.904	C	90.020	7.356	6.009
H	87.474	10.054	10.871	O	85.391	12.272	6.597	C	93.484	7.158	4.394
H	87.998	13.427	9.052	O	87.057	13.451	4.874	C	91.702	9.197	5.712
H	88.173	10.408	6.081	C	84.952	13.473	3.666	C	87.225	6.707	6.547
H	88.316	9.217	8.348	C	88.528	16.475	3.947	C	86.978	7.186	7.983
H	89.212	10.357	10.933	C	88.060	16.625	5.376	O	88.223	7.693	8.553
H	87.843	12.879	6.542	C	86.862	16.056	5.914	C	86.351	6.121	8.913
C	91.520	14.568	5.749	N	86.592	16.022	7.204	O	85.161	5.632	8.352
N	90.972	13.357	6.050	C	87.450	16.579	8.125	C	85.966	6.694	10.282
C	91.829	12.737	6.941	N	88.484	17.406	7.593	O	87.149	7.211	10.931
C	92.863	13.620	7.136	C	88.820	17.336	6.278	H	86.668	0.860	5.839
N	92.653	14.764	6.385	O	87.364	16.441	9.335	H	92.278	4.736	4.330
C	94.076	13.459	8.004	C	89.230	18.232	8.543	H	89.419	8.084	6.538
H	94.735	14.317	7.863	H	84.436	17.988	6.148	H	93.514	7.074	3.299
H	91.056	15.260	5.056	H	83.104	17.581	5.047	H	94.253	6.480	4.784
H	90.119	12.965	5.683	H	84.753	17.812	4.404	H	93.781	8.177	4.653
H	91.640	11.747	7.332	H	83.369	13.560	7.345	H	91.926	9.688	4.756
H	94.636	12.550	7.754	H	85.928	15.891	3.987	H	92.594	9.309	6.344
H	93.812	13.399	9.066	H	85.448	13.816	2.746	H	90.895	9.763	6.191
C	82.864	7.604	6.058	H	83.925	13.848	3.647	H	86.273	6.318	6.185
C	81.125	6.610	7.591	H	84.923	12.379	3.668	H	87.475	7.573	5.925
N	82.204	7.526	7.264	H	87.743	16.681	3.213	H	86.258	8.018	7.914
C	82.827	8.426	8.099	H	88.897	15.460	3.750	H	88.171	7.569	9.523
N	83.812	9.089	7.539	H	89.356	17.159	3.739	H	87.089	5.322	9.069
C	83.851	8.583	6.248	H	89.715	17.875	5.979	H	85.224	7.494	10.150
N	82.621	6.907	4.942	H	89.733	17.597	9.273	H	86.962	7.392	11.866
C	83.464	7.241	3.964	H	88.533	18.885	9.077	H	85.463	4.935	7.700
N	84.447	8.158	3.989	H	89.957	18.839	7.998	H	85.520	5.884	10.868
C	84.660	8.841	5.125	H	87.396	13.540	3.968	H	90.546	3.064	4.830
N	85.698	9.749	5.139	C	88.295	2.069	5.448	N	80.609	14.114	8.205
H	81.479	5.579	7.532	N	87.017	1.804	5.946	C	81.131	12.914	8.552
H	80.299	6.750	6.890	C	86.153	2.733	6.554	O	82.316	12.626	8.361
H	80.787	6.827	8.607	N	86.610	4.021	6.673	C	80.181	11.919	9.204
H	82.495	8.541	9.122	C	87.830	4.338	6.205	H	81.207	14.817	7.766
H	83.345	6.711	3.020	C	88.686	3.430	5.612	H	79.635	14.330	8.361
H	86.020	9.959	4.201	O	89.007	1.200	4.915	H	79.303	11.732	8.574
H	85.579	10.560	5.741	O	85.044	2.372	6.957	H	79.824	12.293	10.171
C	84.165	17.434	5.243	N	89.940	3.811	5.106	H	80.713	10.979	9.361

Cartesian coordinates of model (6-4)II

N	88.335	10.343	8.091	N	84.448	15.953	5.410	C	90.378	5.103	5.278
C	88.252	11.278	9.102	C	83.619	15.317	6.288	C	89.508	6.056	5.864
C	88.197	10.892	10.543	N	83.998	14.029	6.686	N	88.205	5.683	6.264
C	88.232	12.495	8.464	C	84.995	13.254	6.139	C	91.645	5.476	4.821
N	88.294	12.318	7.094	C	85.781	15.422	5.045	C	92.109	6.783	4.932
C	88.349	11.007	6.912	C	85.725	13.862	4.931	C	91.269	7.738	5.545
H	88.043	11.780	11.162	O	85.237	12.138	6.577	C	90.001	7.356	5.999
H	87.371	10.195	10.740	O	87.013	13.329	4.786	C	93.480	7.136	4.398
H	88.178	13.479	8.909	C	84.930	13.449	3.676	C	91.705	9.170	5.722
H	88.371	10.509	5.951	C	88.490	16.477	3.980	C	87.183	6.713	6.563
H	88.346	9.318	8.226	C	88.054	16.593	5.422	C	86.988	7.136	8.024
H	89.125	10.407	10.874	C	86.877	16.001	5.903	O	88.252	7.574	8.556
C	91.506	14.574	5.767	N	86.674	16.045	7.296	C	86.318	6.078	8.936
N	90.888	13.440	6.200	C	87.454	16.732	8.216	O	85.095	5.654	8.378
C	91.762	12.818	7.066	N	88.511	17.435	7.659	C	85.969	6.667	10.309
C	92.887	13.611	7.105	C	88.862	17.277	6.312	O	87.189	7.065	10.968
N	92.715	14.706	6.280	O	87.222	16.722	9.415	H	86.742	0.804	5.838
C	94.124	13.443	7.937	C	89.306	18.255	8.570	H	92.271	4.715	4.359
H	94.773	14.311	7.797	H	84.426	17.970	6.070	H	89.397	8.096	6.500
H	91.030	15.264	5.083	H	83.134	17.513	4.937	H	93.512	7.071	3.303
H	89.908	13.185	6.102	H	84.812	17.709	4.349	H	94.241	6.449	4.785
H	91.503	11.897	7.568	H	83.382	13.566	7.382	H	93.778	8.150	4.672
H	94.698	12.543	7.678	H	85.974	15.765	4.026	H	91.929	9.650	4.761
H	93.876	13.374	9.005	H	85.480	13.771	2.787	H	92.610	9.243	6.338
C	82.845	7.603	6.050	H	83.927	13.886	3.659	H	90.926	9.760	6.211
C	81.099	6.617	7.588	H	84.842	12.358	3.650	H	86.224	6.346	6.194
N	82.178	7.532	7.254	H	87.689	16.750	3.283	H	87.425	7.599	5.972
C	82.831	8.408	8.093	H	88.790	15.451	3.737	H	86.288	7.986	7.976
N	83.835	9.043	7.541	H	89.334	17.145	3.781	H	88.178	7.519	9.534
C	83.860	8.553	6.245	H	89.809	17.713	6.021	H	87.011	5.237	9.083
N	82.588	6.912	4.932	H	89.816	17.636	9.314	H	85.301	7.530	10.173
C	83.449	7.234	3.963	H	88.661	18.959	9.101	H	86.967	7.582	11.757
N	84.457	8.122	3.991	H	90.041	18.808	7.984	H	85.322	4.947	7.734
C	84.682	8.811	5.126	H	85.937	15.502	7.727	H	85.445	5.905	10.897
N	85.730	9.692	5.146	H	87.422	13.144	5.668	H	90.521	3.066	4.769
H	81.451	5.583	7.538	C	88.338	2.035	5.425	N	80.575	14.101	8.202
H	80.263	6.747	6.895	N	87.067	1.766	5.890	C	81.096	12.912	8.588
H	80.762	6.834	8.605	C	86.189	2.691	6.501	O	82.291	12.635	8.446
H	82.496	8.535	9.113	N	86.596	4.009	6.580	C	80.137	11.915	9.225
H	83.322	6.713	3.018	C	87.804	4.355	6.167	H	81.183	14.792	7.752
H	86.075	9.913	4.218	C	88.711	3.423	5.610	H	79.593	14.308	8.308
H	85.653	10.495	5.770	O	89.087	1.206	4.906	H	79.265	11.729	8.586
C	84.188	17.372	5.181	O	85.115	2.300	6.940	H	79.775	12.282	10.192
O	82.588	15.829	6.735	N	89.943	3.801	5.166	H	80.673	10.978	9.379

Cartesian coordinates of model (6-4)III

N	88.455	10.336	8.120	O	82.670	15.822	6.862	C	90.390	5.085	5.267
C	88.207	11.271	9.101	N	84.449	15.920	5.438	C	89.556	6.055	5.894
C	88.153	10.894	10.546	C	83.656	15.290	6.353	N	88.255	5.690	6.351
C	88.071	12.468	8.437	N	83.959	13.952	6.647	C	91.653	5.471	4.807
N	88.225	12.279	7.075	C	84.913	13.208	6.049	C	92.125	6.785	4.925
C	88.453	10.978	6.927	C	85.766	15.406	5.048	C	91.313	7.742	5.542
H	87.971	11.776	11.165	C	85.710	13.854	4.898	C	90.049	7.348	6.023
H	87.358	10.164	10.748	O	85.073	12.028	6.367	C	93.491	7.133	4.373
H	87.869	13.443	8.861	O	86.995	13.300	4.798	C	91.746	9.180	5.715
H	88.668	10.476	5.991	C	84.969	13.485	3.595	C	87.263	6.724	6.584
H	88.529	9.310	8.278	C	88.496	16.366	3.977	C	87.036	7.196	8.029
H	89.100	10.443	10.872	C	88.064	16.517	5.414	O	88.273	7.645	8.609
C	91.526	14.597	5.767	C	86.868	15.955	5.971	C	86.346	6.121	8.911
N	90.899	13.467	6.201	N	86.579	15.984	7.247	O	85.155	5.691	8.297
C	91.765	12.847	7.078	C	87.422	16.590	8.161	C	85.962	6.655	10.294
C	92.892	13.636	7.121	N	88.481	17.368	7.607	O	87.163	7.060	10.984
N	92.729	14.730	6.289	C	88.813	17.257	6.299	H	86.623	0.883	5.831
C	94.133	13.437	7.940	O	87.292	16.537	9.374	H	92.273	4.716	4.324
H	94.799	14.292	7.804	C	89.242	18.211	8.531	H	89.465	8.079	6.568
H	91.071	15.277	5.058	H	84.479	17.918	6.149	H	93.509	7.051	3.279
H	89.926	13.201	6.075	H	83.136	17.504	5.062	H	94.262	6.455	4.757
H	91.515	11.919	7.574	H	84.784	17.703	4.404	H	93.790	8.152	4.630
H	94.677	12.529	7.655	H	83.351	13.472	7.347	H	91.947	9.672	4.755
H	93.897	13.353	9.007	H	85.958	15.792	4.043	H	92.656	9.276	6.320
C	82.840	7.621	6.084	H	85.572	13.810	2.743	H	90.967	9.757	6.221
C	81.116	6.570	7.594	H	83.978	13.946	3.528	H	86.298	6.361	6.223
N	82.189	7.501	7.285	H	84.855	12.399	3.542	H	87.549	7.594	5.969
C	82.814	8.377	8.144	H	87.721	16.682	3.269	H	86.330	8.048	7.974
N	83.797	9.067	7.613	H	88.735	15.322	3.748	H	88.177	7.570	9.578
C	83.835	8.609	6.316	H	89.384	16.976	3.779	H	87.053	5.292	9.049
N	82.613	6.978	4.942	H	89.700	17.802	5.982	H	85.274	7.507	10.188
C	83.443	7.340	3.958	H	89.755	17.588	9.267	H	86.926	7.461	11.834
N	84.434	8.249	4.038	H	88.555	18.877	9.063	H	85.459	4.982	7.654
C	84.618	8.861	5.196	H	89.965	18.803	7.965	H	85.449	5.851	10.835
N	85.770	9.770	5.229	H	87.374	13.073	5.691	H	90.527	3.044	4.823
H	81.486	5.544	7.535	C	88.261	2.080	5.449	N	80.631	14.103	8.211
H	80.298	6.709	6.882	N	86.973	1.829	5.931	C	81.097	12.877	8.546
H	80.764	6.780	8.607	C	86.107	2.767	6.516	O	82.259	12.521	8.318
H	82.480	8.466	9.170	N	86.575	4.052	6.641	C	80.114	11.932	9.222
H	83.323	6.851	2.998	C	87.814	4.351	6.193	H	81.264	14.789	7.793
H	86.136	9.809	4.273	C	88.664	3.436	5.609	H	79.684	14.380	8.426
H	85.551	10.761	5.599	O	88.970	1.197	4.929	H	79.234	11.753	8.593
H	86.511	9.390	5.840	O	84.984	2.420	6.897	H	79.765	12.344	10.176
C	84.197	17.351	5.256	N	89.921	3.810	5.107	H	80.618	10.982	9.410

Cartesian coordinates of model (6-4)IV

N	88.319	10.318	8.064	N	84.436	15.981	5.425	C	89.545	6.056	5.914
C	88.261	11.269	9.058	C	83.624	15.315	6.311	N	88.245	5.677	6.346
C	88.147	10.886	10.498	N	83.966	14.001	6.625	C	91.677	5.485	4.875
C	88.373	12.477	8.412	C	85.071	13.336	6.176	C	92.125	6.810	4.960
N	88.502	12.265	7.045	C	85.757	15.493	5.035	C	91.286	7.765	5.546
C	88.457	10.943	6.887	C	85.768	13.942	4.945	C	90.014	7.363	6.008
H	87.985	11.766	11.124	O	85.449	12.278	6.659	C	93.498	7.160	4.422
H	87.314	10.191	10.655	O	87.102	13.494	4.850	C	91.700	9.208	5.729
H	88.355	13.470	8.836	C	85.013	13.457	3.692	C	87.214	6.695	6.543
H	88.521	10.417	5.942	C	88.530	16.383	3.974	C	86.962	7.166	7.980
H	88.275	9.277	8.220	C	88.078	16.579	5.401	O	88.199	7.676	8.538
H	89.059	10.382	10.848	C	86.861	16.045	5.947	C	86.344	6.095	8.910
C	91.297	14.543	5.813	N	86.573	16.074	7.229	O	85.148	5.604	8.364
N	90.772	13.410	6.282	C	87.429	16.645	8.142	C	85.976	6.677	10.280
C	91.698	12.784	7.090	N	88.491	17.428	7.597	O	87.185	7.102	10.951
C	92.824	13.548	7.125	C	88.834	17.312	6.281	H	86.716	0.834	5.905
N	92.551	14.642	6.308	O	87.322	16.568	9.357	H	92.322	4.726	4.438
C	94.094	13.406	7.911	C	89.227	18.276	8.528	H	89.394	8.104	6.491
H	94.753	14.268	7.763	H	84.431	17.970	6.168	H	93.536	7.085	3.328
H	90.814	15.262	5.165	H	83.118	17.564	5.044	H	94.264	6.480	4.813
H	89.749	13.073	6.292	H	84.778	17.779	4.428	H	93.798	8.178	4.687
H	91.483	11.850	7.574	H	83.391	13.534	7.355	H	91.919	9.715	4.779
H	94.650	12.505	7.638	H	85.938	15.861	4.021	H	92.596	9.310	6.359
H	93.866	13.344	8.979	H	85.563	13.776	2.801	H	90.896	9.767	6.219
C	82.850	7.622	6.060	H	83.994	13.853	3.644	H	86.270	6.301	6.162
C	81.112	6.619	7.587	H	84.970	12.364	3.699	H	87.466	7.564	5.928
N	82.180	7.546	7.263	H	87.755	16.639	3.244	H	86.233	7.991	7.912
C	82.815	8.432	8.102	H	88.788	15.333	3.790	H	88.129	7.581	9.515
N	83.813	9.083	7.551	H	89.400	17.013	3.751	H	87.087	5.300	9.065
C	83.850	8.584	6.255	H	89.723	17.854	5.971	H	85.293	7.528	10.146
N	82.602	6.930	4.938	H	89.733	17.665	9.280	H	86.944	7.571	11.764
C	83.460	7.257	3.972	H	88.524	18.932	9.050	H	85.437	4.931	7.689
N	84.457	8.159	4.002	H	89.950	18.881	7.975	H	85.468	5.898	10.859
C	84.670	8.842	5.143	H	87.366	13.062	5.696	H	90.512	3.083	4.763
N	85.713	9.734	5.166	C	88.352	2.042	5.554	C	80.143	11.911	9.217
H	81.476	5.590	7.524	N	87.044	1.788	5.978	C	81.113	12.891	8.574
H	80.277	6.749	6.892	C	86.152	2.722	6.537	O	82.299	12.593	8.402
H	80.774	6.824	8.606	N	86.592	4.020	6.631	N	80.607	14.097	8.214
H	82.478	8.557	9.122	C	87.836	4.330	6.224	H	79.630	14.316	8.343
H	83.340	6.732	3.026	C	88.726	3.409	5.708	H	81.217	14.784	7.768
H	86.081	9.948	4.252	O	89.087	1.162	5.077	H	79.270	11.736	8.576
H	85.656	10.512	5.820	O	85.044	2.354	6.917	H	79.781	12.293	10.179
C	84.174	17.410	5.262	N	90.013	3.780	5.293	H	80.663	10.966	9.379
O	82.612	15.834	6.786	C	90.420	5.085	5.346	H	93.201	15.393	6.109

Cartesian coordinates of model (6-4)Int

N	88.361	10.198	8.233
C	88.252	11.161	9.218
C	88.180	10.819	10.666
C	88.200	12.360	8.549
N	88.271	12.149	7.188
C	88.360	10.841	7.034
H	88.044	11.731	11.254
H	87.330	10.153	10.874
H	88.090	13.359	8.951
H	88.396	10.316	6.090
H	88.413	9.182	8.374
H	89.093	10.317	11.019
C	91.503	14.638	5.819
N	90.845	13.538	6.266
C	91.705	12.865	7.103
C	92.871	13.600	7.107
N	92.737	14.706	6.291
C	94.129	13.362	7.887
H	94.799	14.215	7.742
H	91.022	15.359	5.174
H	89.847	13.365	6.158
H	91.410	11.967	7.623
H	94.659	12.452	7.573
H	93.923	13.268	8.962
C	82.815	7.588	6.053
C	81.070	6.644	7.588
N	82.152	7.547	7.255
C	82.842	8.402	8.096
N	83.868	8.993	7.535
C	83.865	8.496	6.243
N	82.532	6.895	4.941
C	83.416	7.165	3.975
N	84.464	8.005	4.000
C	84.707	8.699	5.131
N	85.791	9.530	5.173
H	81.417	5.607	7.533
H	80.240	6.778	6.887
H	80.732	6.862	8.603
H	82.521	8.549	9.118
H	83.269	6.637	3.034
H	86.146	9.729	4.244
H	85.660	10.377	5.740
C	88.392	2.009	5.517
N	87.104	1.756	5.953
C	86.194	2.697	6.494
N	86.613	4.001	6.595
C	87.833	4.331	6.190
C	88.751	3.396	5.661
O	89.150	1.152	5.051
O	85.086	2.316	6.853
N	89.988	3.782	5.233
C	90.404	5.090	5.327
C	89.516	6.048	5.877
N	88.218	5.656	6.270
C	91.672	5.471	4.888
C	92.111	6.787	4.976
C	91.251	7.746	5.548
C	89.981	7.359	5.987
C	93.480	7.132	4.442
C	91.667	9.187	5.714
C	87.188	6.664	6.574
C	87.022	7.044	8.049
O	88.334	7.341	8.569
C	86.294	6.021	8.952
O	85.054	5.626	8.400
C	85.935	6.648	10.301
O	87.143	7.043	10.983
H	86.766	0.805	5.885
H	92.319	4.704	4.463
H	89.357	8.100	6.461
H	93.491	7.083	3.345
H	94.231	6.421	4.808
H	93.796	8.136	4.730
H	91.892	9.659	4.750
H	92.565	9.278	6.338
H	90.876	9.771	6.191
H	86.236	6.293	6.194
H	87.430	7.563	6.008
H	86.402	7.953	8.039
H	88.257	7.296	9.544
H	86.957	5.160	9.124
H	85.288	7.516	10.118
H	86.910	7.688	11.666
H	85.263	4.934	7.738
H	85.382	5.911	10.897
H	90.577	3.053	4.845
N	80.678	14.078	8.172
C	80.060	11.960	9.229
C	81.120	12.876	8.624
O	82.295	12.526	8.556
H	79.720	14.364	8.308
H	81.357	14.762	7.816
H	79.200	11.841	8.557
H	79.695	12.368	10.180
H	80.516	10.986	9.410
O	88.038	14.550	5.718
C	84.404	17.431	5.352
O	82.846	15.958	7.007
N	84.605	16.003	5.538
C	83.800	15.391	6.453
N	84.045	14.042	6.684
C	84.873	13.228	5.936
C	85.822	15.373	5.019
C	85.636	13.905	4.909
O	84.885	12.005	6.142
C	86.277	13.107	3.826
C	88.480	16.761	3.888
C	88.006	16.831	5.313
C	87.178	15.720	5.906
N	86.774	15.841	7.248
C	87.372	16.691	8.092
N	88.323	17.634	7.542
C	88.587	17.668	6.198
O	87.199	16.754	9.320
C	89.121	18.400	8.479
H	84.648	17.989	6.263
H	83.358	17.625	5.091
H	85.051	17.772	4.539
H	83.484	13.585	7.412
H	85.999	15.787	4.021
H	87.362	13.043	3.982
H	86.115	13.581	2.846
H	85.858	12.096	3.802
H	87.682	16.912	3.144
H	88.922	15.775	3.683
H	89.253	17.518	3.696
H	89.329	18.398	5.881
H	89.624	17.730	9.187
H	88.501	19.090	9.063
H	89.874	18.964	7.920
H	87.765	13.897	6.392

Cartesian coordinates of model (6-4)Repaired

N	88.212	10.371	8.156
C	88.124	11.283	9.191
C	88.127	10.872	10.627
C	88.040	12.513	8.591
N	88.072	12.360	7.218
C	88.170	11.055	6.994
H	87.895	11.733	11.260
H	87.378	10.092	10.818
H	87.944	13.498	9.024
H	88.193	10.572	6.027
H	88.241	9.336	8.265
H	89.102	10.474	10.939
C	91.857	14.668	5.851
N	91.125	13.681	6.438
C	91.965	13.021	7.308
C	93.186	13.648	7.197
N	93.104	14.680	6.280
C	94.467	13.333	7.912
H	95.119	14.212	7.903
H	91.430	15.352	5.129
H	90.142	13.482	6.296
H	91.624	12.189	7.905
H	95.017	12.507	7.439
H	94.285	13.048	8.955
C	82.775	7.432	5.957
C	81.129	6.498	7.620
N	82.181	7.404	7.198
C	82.888	8.304	7.969
N	83.854	8.920	7.334
C	83.802	8.381	6.059
N	82.451	6.706	4.879
C	83.269	6.973	3.858
N	84.286	7.850	3.798
C	84.572	8.579	4.894
N	85.622	9.454	4.840
H	81.505	5.472	7.676
H	80.300	6.537	6.908
H	80.771	6.807	8.607
H	82.631	8.460	9.010
H	83.089	6.412	2.943
H	85.972	9.598	3.901
H	85.528	10.297	5.404
C	88.364	1.935	5.549
N	87.057	1.688	5.981
C	86.178	2.615	6.563
N	86.629	3.902	6.681
C	87.880	4.206	6.277
C	88.763	3.285	5.746
O	89.066	1.046	5.030
O	85.060	2.242	6.938
N	90.083	3.644	5.388
C	90.461	4.967	5.398
C	89.591	5.937	5.972
N	88.294	5.553	6.429
C	91.704	5.378	4.906
C	92.147	6.707	4.976
C	91.315	7.660	5.572
C	90.059	7.246	6.062
C	93.499	7.064	4.398
C	91.720	9.113	5.704
C	87.255	6.575	6.581
C	86.961	7.073	8.004
O	88.170	7.636	8.572
C	86.352	6.001	8.935
O	85.168	5.484	8.378
C	85.947	6.571	10.296
O	87.119	7.039	11.000
H	86.713	0.742	5.885
H	92.349	4.623	4.458
H	89.449	7.981	6.568
H	93.431	7.334	3.332
H	94.193	6.218	4.474
H	93.957	7.916	4.913
H	91.894	9.590	4.729
H	92.646	9.242	6.284
H	90.942	9.693	6.213
H	86.318	6.178	6.184
H	87.522	7.437	5.962
H	86.209	7.869	7.898
H	88.100	7.536	9.544
H	87.102	5.210	9.097
H	85.234	7.395	10.145
H	86.830	7.558	11.764
H	85.483	4.802	7.716
H	85.451	5.778	10.870
H	90.547	2.981	4.782
N	80.736	14.339	8.361
C	80.016	12.165	9.220
C	81.121	13.093	8.734
O	82.295	12.724	8.691
H	79.768	14.621	8.387
H	81.449	15.016	8.077
H	79.158	12.172	8.537
H	79.661	12.475	10.210
H	80.416	11.153	9.286
O	87.996	14.420	5.656
C	84.164	17.414	5.380
O	82.938	15.990	7.313
N	84.298	15.963	5.478
C	83.642	15.341	6.533
N	83.833	13.985	6.612
C	84.585	13.187	5.737
C	84.947	15.223	4.506
C	85.106	13.883	4.561
O	84.740	11.996	5.972
C	85.801	13.088	3.495
C	88.748	16.664	4.111
C	88.534	16.710	5.600
C	88.127	15.542	6.346
N	87.912	15.532	7.645
C	88.126	16.648	8.408
N	88.592	17.810	7.717
C	88.757	17.816	6.366
O	87.955	16.720	9.620
C	88.836	18.999	8.522
H	84.529	17.892	6.293
H	83.115	17.691	5.241
H	84.756	17.763	4.531
H	83.382	13.502	7.410
H	85.332	15.805	3.676
H	86.769	12.703	3.844
H	85.988	13.703	2.606
H	85.193	12.224	3.200
H	87.801	16.597	3.558
H	89.332	15.780	3.829
H	89.281	17.557	3.763
H	89.083	18.761	5.939
H	89.447	18.736	9.389
H	87.889	19.409	8.889
H	89.350	19.743	7.906
H	87.899	13.592	6.309