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Supporting information for article:

Enzyme catalysis captured using multiple structures from one crystal at varying temperatures

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Table S1 Data collection and crystallographic structure refinement statistics for the selected serial datasets from the nitrite-bound AcNiR structural movie at 190K. Data were processed using $CC_{1/2}$ >0.3 and I/σ(I) >1.0 (outer shell) cutoff.

Structure	$ds1_{190}$	$ds2_{190}$	$ds10_{190}$	$ds18_{190}$	$ds50_{190}$	$ds69_{190}$	$ds75_{190}$
Accumulated Dose (MGy)	0.24	0.48	2.40	4.89	21.65	46.51	59.05
Cell axis (Å)	94.9	94.9	94.9	95.0	95.0	95.0	95.0
Resolution (Å)	42.46-1.08 (1.10-1.08)	42.46-1.08 (1.10-1.08)	42.46-1.27 (1.29-1.27)	42.48-1.34 (1.36-1.34)	42.49-1.68 (1.71-1.68)	42.50-1.77 (1.81-1.77)	42.50-1.84 (1.88-1.84)
Unique reflections	120835	120809	75137	64147	32846	28154	25120
Redundancy	5.9 (3.1)	5.9 (3.2)	6.4 (6.1)	6.5 (6.0)	6.6 (6.3)	6.8 (6.9)	6.8 (7.0)
R_{pim} (%)	2.9 (62.3)	2.9 (72.9)	3.3 (69.7)	3.0 (74.6)	5.1 (79.0)	7.7 (78.0)	9.9 (79.2)
CC-1/2	0.99 (0.32)	0.99 (0.35)	0.99 (0.36)	0.99 (0.29)	0.99 (0.32)	0.99 (0.31)	0.99 (0.37)
I/σ(I)	13.7 (1.1)	13.5 (1.0)	12.2 (1.1)	13.1 (1.0)	10.6 (1.1)	8.3 (1.3)	7.7 (1.3)
Completeness (%)	99.4 (93.9)	99.4 (93.7)	100.0 (100.0)	99.9 (99.9)	99.9 (99.9)	100 (100)	100(100)
Wilson B-factor ($Å^2$)	8.0	8.6	12.1	14.5	29.1	29.7	29.3
Refinement							
R_{work}/R_{free} (%)	11.6/14.3	11.8/14.4	12.4/16.1	12.9/17.3	19.7/22.8	20.1/22.6	20.2/24.5
RMSD Bond Length (Å)	0.015	0.015	0.014	0.014	0.014	0.014	0.013
RMDS Bond Angle (°)	1.814	1.839	1.670	1.627	1.657	1.642	1.611
ML Based ESU (Å)	0.020	0.020	0.042	0.039	0.085	0.100	0.115
Av Protein B-factor ($Å^2$)	11.1	11.7	16.7	19.8	26.1	22.4	22.1
Av Water B-factor ($Å^2$)	25.1	25.8	32.4	34.1	31.2	25.6	25.0
No. waters	459	451	344	283	130	111	108
Ramachandran (%)							
Favoured Regions	99	99	99	99	99	99.7	99.7
Allowed Regions	1	1	1	1	1	0.3	1
PDB Code	5OF5	5OF6	5OF7	5OF8	5OFC	5OFD	5OFE

Table S2 Data collection and crystallographic structure refinement statistics for the selected serial datasets from the nitrite-bound AcNiR structural movie at room temperature. Data were processed using $CC_{1/2}$ ~ 0.5 I/ σ (I) >1.0 (outer shell) cut-off.

Structure	$ds1_{RT}$	$ds2_{RT}$	$ds3_{RT}$	$ds4_{RT}$	$ds5_{RT}$	$ds6_{RT}$	$ds7_{RT}$	$ds8_{RT}$	$ds9_{RT}$	$ds10_{RT}$
Accumulated Dose (MGy)	0.03	0.06	0.09	0.12	0.15	0.18	0.21	0.24	0.27	0.30
Cell axis (Å)	96.2	96.2	96.2	96.2	96.3	96.3	96.3	96.3	96.3	96.3
Resolution (Å) (outer shell)	48.11-1.41 (1.45-1.41)	55.56-1.49 (1.53-1.49)	48.12-1.58 (1.61-1.58)	55.57-1.64 (1.68-1.64)	48.13-1.70 (1.74-1.70)	55.58-1.76 (1.81-1.76)	48.13-1.82 (1.87-1.82)	48.13-1.85 (1.90-1.85)	48.13-1.88 (1.93-1.88)	48.12-1.91 (1.96-1.91)
Unique reflections	57140	48510	40744	36457	32772	29589	26780	25531	24354	23248
Redundancy	3.3 (3.3)	3.3 (3.3)	3.3 (3.3)	3.3 (3.3)	3.3 (3.3)	3.3 (3.2)	3.3 (3.2)	3.3 (3.2)	3.3 (3.1)	3.3 (3.2)
R_{pim} (%)	7.9 (57.0)	7.7 (57.8)	7.9 (53.3)	8.1 (55.2)	8.6 (54.9)	8.9 (51.3)	9.4 (48.7)	9.8 (46.8)	10.4 (46.0)	11.0 (48.7)
CC-1/2	0.99 (0.50)	0.99 (0.50)	0.99 (0.54)	0.99 (0.53)	0.99 (0.54)	0.99 (0.51)	0.99 (0.55)	0.99 (0.55)	0.99 (0.60)	0.99 (0.58)
I/σ(I)	5.1 (1.2)	5.3 (1.2)	5.2 (1.3)	5.2 (1.3)	5.0 (1.3)	4.9 (1.3)	4.9 (1.5)	4.7 (1.4)	4.5 (1.4)	4.4 (1.4)
Completeness (%)	99.7 (99.8)	99.7 (99.8)	99.6 (99.7)	99.6 (99.8)	99.6 (99.6)	99.6 (99.7)	99.5 (99.7)	99.5 (99.3)	99.5 (97.6)	99.6 (97.5)
Wilson B-factor ($Å^2$)	10.9	13.6	17.5	16.3	17.6	20.0	21.8	23.0	22.8	24.7
Refinement										
R_{work}/R_{free} (%)	16.0/18.4	15.9/18.4	15.4/17.8	16.4/19.0	16.6/19.4	17.2/20.3	17.4/20.9	17.7/22.3	18.3/21.6	18.6/23.0
RMSD Bond Length (Å)	0.014	0.014	0.014	0.014	0.014	0.014	0.014	0.013	0.013	0.013
RMDS Bond Angle (°)	1.68	1.67	1.67	1.65	1.68	1.69	1.72	1.65	1.63	1.68
ML Based ESU (Å)	0.055	0.064	0.072	0.083	0.093	0.105	0.118	0.128	0.133	0.144
Av Protein B-factor ($Å^2$)	16.8	19.1	21.5	21.1	21.4	21.9	22.2	22.1	22.0	22.1
Av Water B-factor ($Å^2$)	27.7	29.6	31.7	30.8	29.9	29.5	28.7	28.0	27.2	26.4
No. waters	186	184	159	161	155	150	138	131	124	122
Ramachandran (%)										
Favoured Regions	99	99	98.8	98.8	99	99	98.8	98.5	98.2	99
Allowed Regions	1	1	1.2	1.2	1	1	1.2	1.5	1.8	1
PDB Code	5OFF	5OFG	50FH	5OG2	5OG3	5OG4	5OG5	5OG6	5OGF	5OGG

Table S3 Cu-ligand distances and angles at the T1Cu site for selected frames of the 190K series movie.

Structure	**ds1$_{190}$**	**ds2$_{190}$**	**ds10$_{190}$**	**ds18$_{190}$**	**ds50$_{190}$**	**ds69$_{190}$**	**ds75$_{190}$**
Resolution (Å)	1.08	1.08	1.27	1.34	1.68	1.77	1.84
Bond length (Å)							
T1Cu-His145Nδ1	2.02	2.05	2.09	2.13	2.11	2.10	2.07
T1Cu-His95Nδ1	2.01	2.02	2.04	2.06	2.08	2.13	2.14
T1Cu-Cys136 Sγ	2.19	2.20	2.17	2.15	2.18	2.23	2.19
T1Cu-Met150 Sδ	2.54	2.55	2.59	2.61	2.66	2.58	2.60
Bond angle (°)							
His95Nδ1-T1Cu- His145Nδ1	101.3	101.8	101.7	103.3	102.0	104.1	102.7
His145Nδ1-T1Cu- Cys136 Sγ	107.7	108.6	109.4	107.5	109.1	107.8	109.9
Cys136 Sγ-T1Cu- Met150 Sδ	107.1	107.0	107.4	108.3	108.2	109.8	109.6
Met150 Sδ-T1Cu- His95Nδ1	84.9	85.3	84.8	84.8	84.5	84.6	84.7
Cys136 Sγ-T1Cu- His95Nδ1	131.9	129.9	129.7	130.1	128.9	128.2	128.0
Met150 Sδ-T1Cu- His145Nδ1	124.5	125.1	124.1	121.4	124.4	122.6	121.9

Table S4 Cu-ligand distances and angles at the T1Cu site for selected frames of the RT movie

Structure	$ds1_{RT}$	$ds2_{RT}$	$ds4_{RT}$	$ds6_{RT}$	$ds8_{RT}$	$ds10_{RT}$
Resolution (Å)	1.41	1.49	1.64	1.76	1.85	1.91
Bond length (Å)						
T1Cu-His145Nδ1	2.02	2.04	2.03	2.04	2.02	2.03
T1Cu-His95Nδ1	2.04	2.09	2.06	2.07	2.05	2.05
T1Cu-Cys136 Sγ	2.20	2.20	2.23	2.26	2.23	2.24
T1Cu-Met150 Sδ	2.51	2.50	2.47	2.42	2.41	2.44
Bond angle (°)						
His95Nδ1-T1Cu- His145Nδ1	99.2	99.9	100.5	100.6	97.7	100.7
His145Nδ1-T1Cu- Cys136 Sγ	105.3	106.5	104.2	103.5	103.5	104.4
Cys136 Sγ-T1Cu- Met150 Sδ	106.2	107.1	107.2	109.3	107.3	107.4
Met150 Sγ-T1Cu- His95Nδ1	87.2	86.7	86.1	86.4	89.0	86.0
Cys136 Sγ-T1Cu- His95Nδ1	135.1	132.5	133.9	132.5	131.5	134.1
Met150 Sδ-T1Cu- His145Nδ1	126.8	126.3	128.2	126.3	127.3	127.1

Table S5 T2Cu-ligand distances for selected serial datasets at 190 K for nitrite soaked *Ac*NiR. In $ds1_{190}$ the Asp98 residue is partially (~35%) in the gatekeeper position.

Structure	$ds1_{190}$	$ds2_{190}$	$ds10_{190}$	$ds18_{190}$	$ds50_{190}$	$ds69_{190}$	$ds75_{190}$
Resolution (Å)	1.08	1.08	1.27	1.34	1.68	1.77	1.84
Bond lengths (Å)							
His100Nε2	2.01	2.02	2.05	2.04	2.06	2.07	2.11
His135Nε2	2.06	2.05	2.06	2.07	2.06	2.07	2.05
His306Nε2	2.00	2.01	2.05	2.05	2.09	2.09	2.12
His255Nε2	4.18	4.19	4.20	4.12	4.15	4.12	4.21
NO_2 (O1/O2)	2.03/1.97	2.15/1.98	2.22/2.02	-	-	-	-
O/N (NO)	-	-	2.20/1.98	2.20/1.90	-	-	-
H_2O	-	-	-	-	1.93	-	-
Asp98Oδ2-NO_2	2.26	2.19	2.27	-	-	-	-
Asp98-NO	-	-	2.51	2.69	-	-	-
Asp98-H_2O	-	-	-	-	3.08	-	

Table S6 T2Cu-ligand distances (Å) for selected serial datasets at RT for nitrite soaked *Ac*NiR.

Structure	ds1	ds2	ds4	ds6	ds8	ds10
Resolution (Å)	1.41	1.49	1.64	1.76	1.85	1.91
Bond lengths (Å)						
His100Nε2	2.04	2.04	2.07	2.06	2.05	2.06
His135Nε2	2.08	2.07	2.06	2.06	2.07	2.06
His306Nε2	2.01	2.03	2.08	2.04	2.07	2.03
His255Nε2	4.09	4.07	4.05	4.02	4.02	4.05
NO_2a (O1/O2)	1.97/1.91	1.96/1.91	2.16/2.03	-	-	-
O/N (NO)	-	-		2.35/2.08	2.49/2.00	-
H_2O	-	-	-	-	-	2.04
Asp98Oδ2-NO_2	2.20	2.23	2.22	-	-	-
Asp98Oδ2-NO	-	-	-	2.81	2.63	-

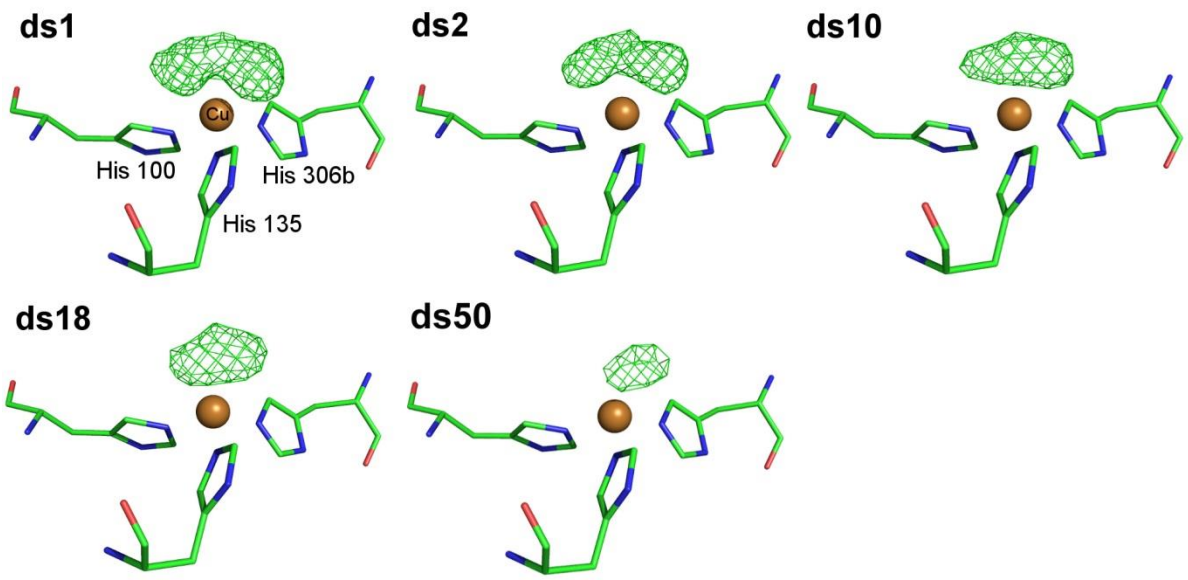

Figure S1 Ligand binding at the T2Cu site for 190 K series. 3σ, weighted electron density Fo-Fc difference maps are shown for the datasets reported in the manuscript and Table S1.

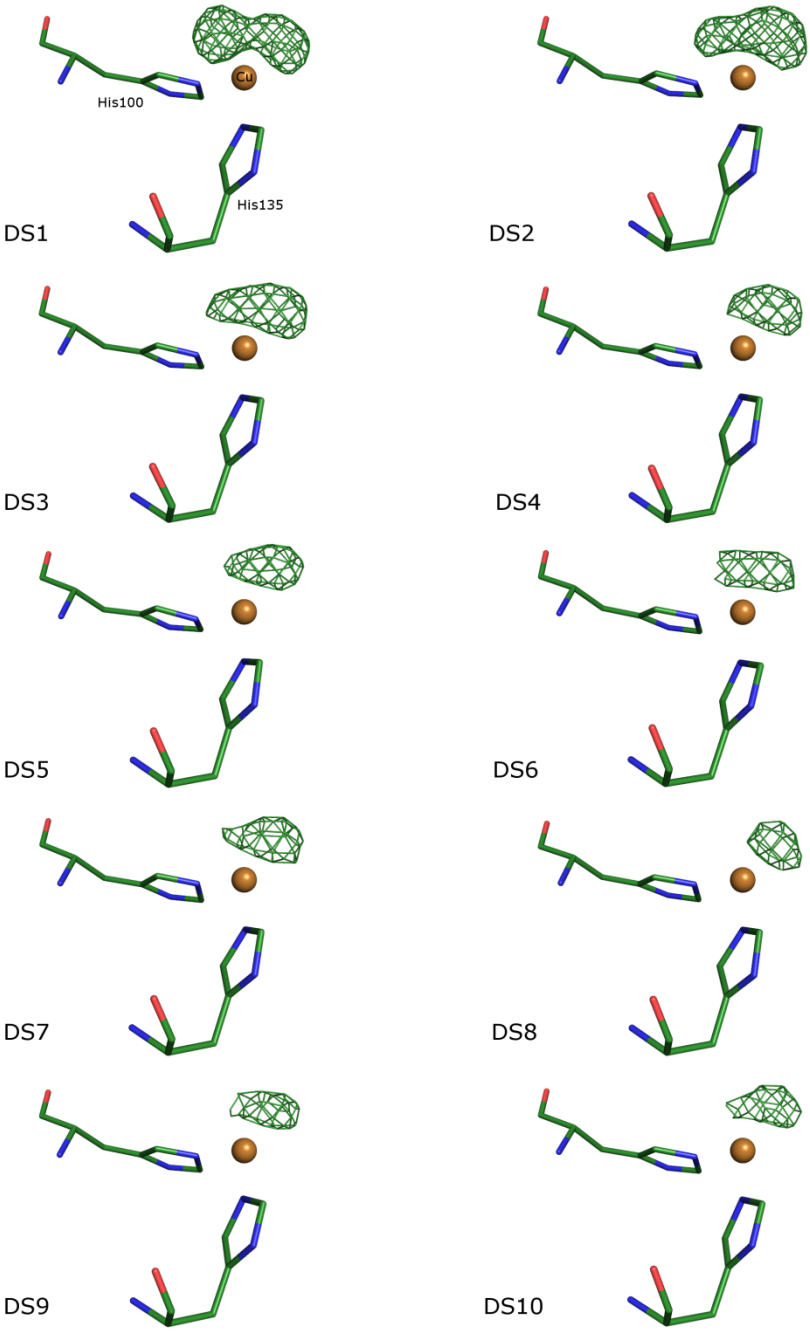

Figure S2 Ligand binding at the T2Cu site for RT series. 3σ, weighted electron density Fo-Fc difference maps are shown for the datasets reported in the manuscript and Table S2.

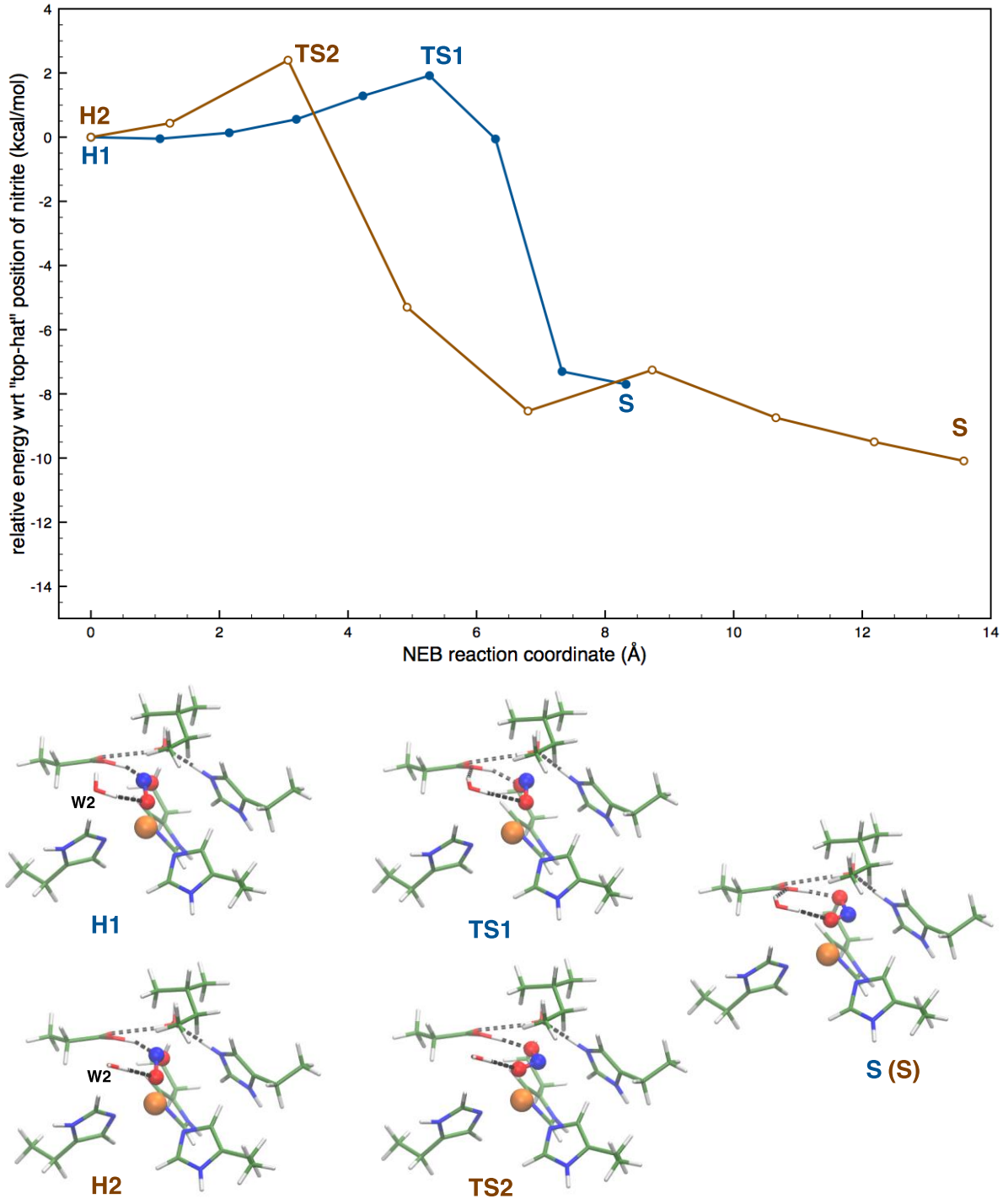

Figure S3 Optimised minimum energy paths between the top-hat and side-on orientation of nitrite at the T2Cu(I) site. Initial top-hat geometries are labelled H1 and H2, with corresponding paths in blue and brown respectively via transition states TS1 and TS2. The structure of the final side-on geometry labelled S is the same for both pathways, while the position of S along the x-axis varies due to the differences in reaction coordinate path lengths. The minimum energy path (MEP) was generated using the geometries in Fig. 5, giving a barrier of 1.9 - 2.4 kcal/mol, depending on the

position of water molecule W2. The barrier is estimated from the initial top-hat orientation of nitrite and the highest point on the path. The barrier to transition is low and hence reorientation of nitrite is likely to take place when the Cu is reduced. Although the barriers calculated from the different top-hat starting geometries are similar, the MEPs are somewhat different. The approximate transition state TS1 in the first path is an early TS and resembles a top-hat orientation, whereas TS2 in the second path is a late TS and is closer to the side-on orientation. The different positioning of W2 influences the nature of the transition state and reorientation of W2 causes the small distortion in the energy pathway observed at a reaction coordinate of approximately 7 Å in TS2. Despite these differences, the barrier is low enough in both cases to suggest that the transition from top-hat to side-on nitrite is straightforward in the Cu(I) state.

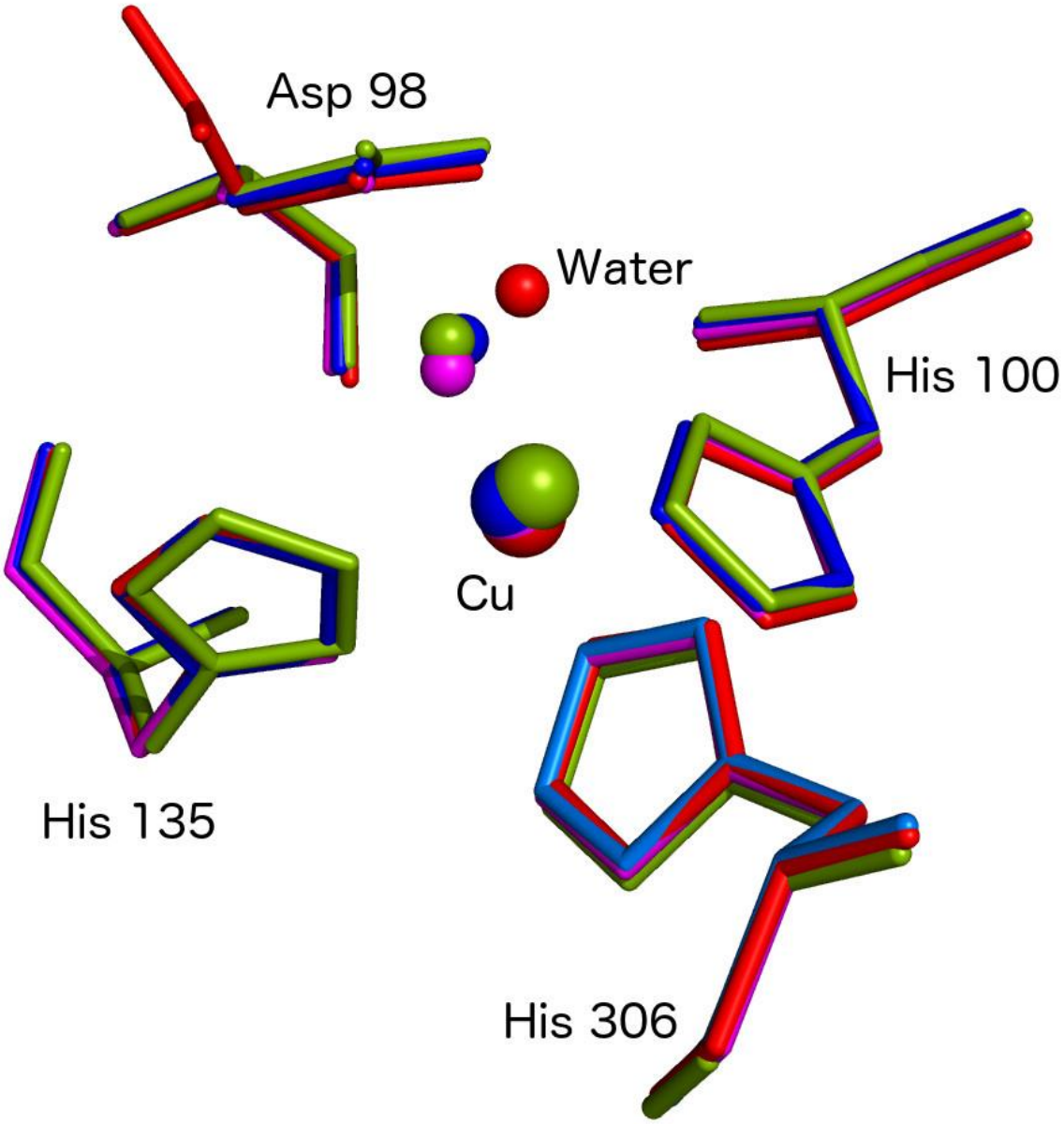

Figure S4 Superposition of the T2Cu-water structures from $ds50_{190}$, ds10RT with previously determined MSOX series at 100K [magenta, PDB 5i6p, (Horrell *et al*., 2017)] and the structure of the resting state enzyme [red, PDB 2bw4 [(Antontyuk *et al*., 2005)], which was also determined at 100K. Note that a longer T2Cu-water separation is observed in the resting state enzyme together with a dual conformation of Asp98, not observed in our MSOX structures.

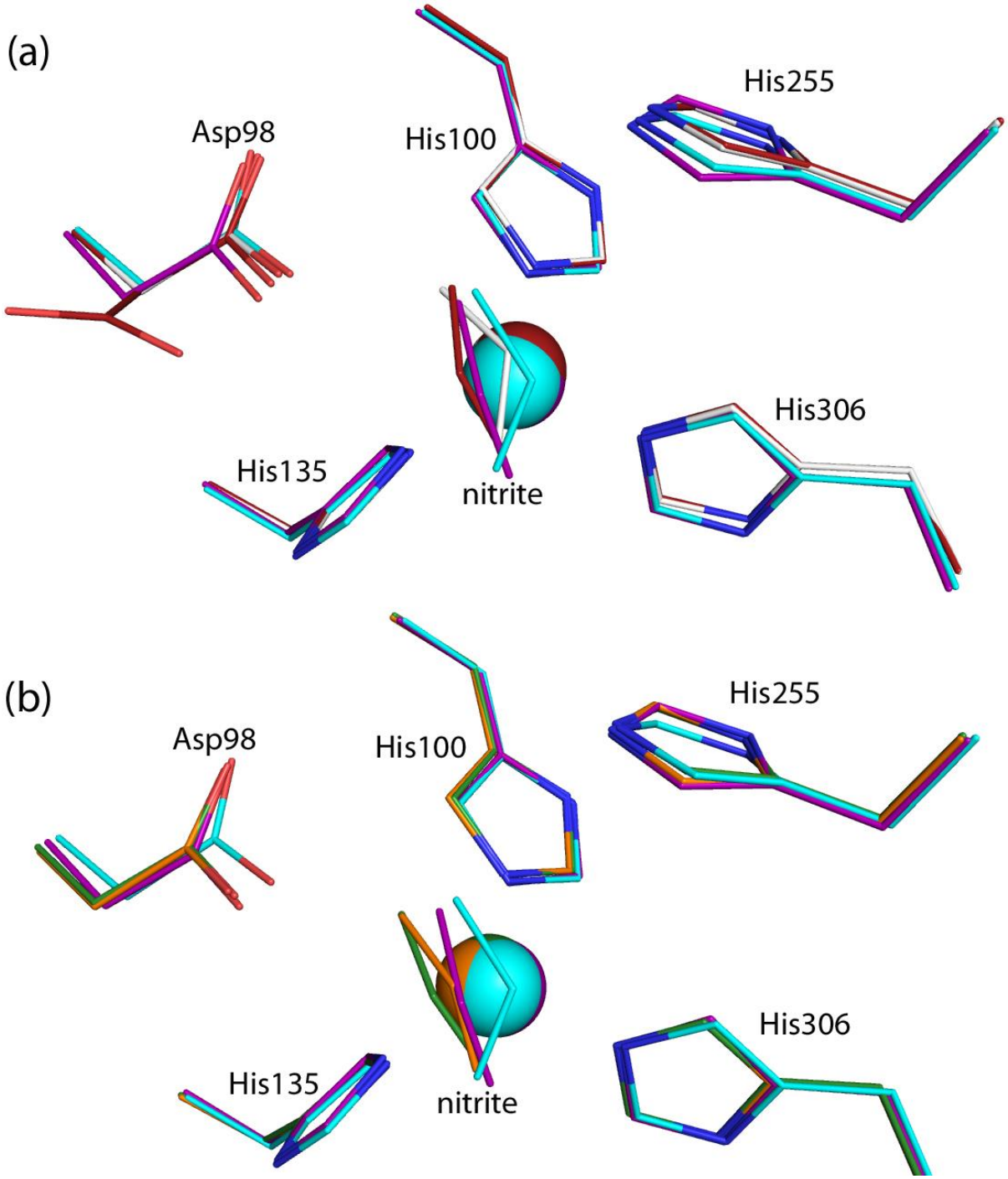

Figure S5 Superposition of T2Cu site structures for nitrite bound *Ac*NiR. The MSOX serial structures at 190K (a) and RT (b) are shown for 'top-hat' $ds1_{190}$ (red)/ $ds1_{RT}$ (green) and 'side-on' $ds3_{190}$ (white)/ $ds3_{RT}$ (orange) and are compared in both panels to the *Af*NiR nitrite bound structures obtained using SFX (purple) and SR methods (cyan) (Fukuda *et al*., 2016).

References

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Antonyuk, S. V., Strange, R. W., Sawers, G., Eady, R. R. & Hasnain, S. S. (2005). *Proc. Natl. Acad. Sci. USA* **102**, 12041-12046.

Fukuda, Y., Tse, K. M., Nakane, T., Nakatsu, T., Suzuki, M., Sugahara, M., Inoue, S., Masuda, T., Yumoto, F., Matsugaki, N., Nango, E., Tono, K., Joti, Y., Kameshima, T., Song, C., Hatsui, T., Yabashi, M., Nureki, O., Murphy, M. E. P., Inoue, T., Iwata, S. & Mizohata, E. (2016). *Proc. Natl. Acad. Sci. USA* **113**, 2928-2933.

Cartesian coordinates of the optimized structures reported in Fig5

Fig 5A. Optimized top-hat NO_2^- binding to T2Cu(II)

C	-82.440002	-40.873001	27.580000
H	-82.534568	-40.833787	26.485481
H	-81.380789	-40.746125	27.847591
H	-82.762839	-41.865092	27.929701
C	-83.307999	-39.764999	28.209999
H	-84.366831	-39.875933	27.910432
H	-83.009083	-38.763289	27.857030
C	-83.325996	-39.710999	29.767000
O	-82.828003	-40.604000	30.461000
O	-83.901001	-38.724998	30.306999
H	-83.949195	-38.792677	31.281376
C	-83.183998	-43.875999	33.056000
H	-82.500061	-44.660753	33.408294
H	-83.141060	-43.868924	31.955544
H	-82.793325	-42.907304	33.408082
C	-84.578003	-44.123001	33.558998
H	-84.580209	-44.216212	34.661323
H	-84.946751	-45.096334	33.184631
C	-85.573997	-43.063999	33.173000
N	-86.836998	-43.075001	33.702000
H	-87.210143	-43.833453	34.266520
C	-87.503998	-42.029999	33.297001
H	-88.533416	-41.799778	33.560534
N	-86.737000	-41.311001	32.509998
C	-85.509003	-41.931000	32.424000
H	-84.690045	-41.543080	31.821110
C	-87.307999	-42.450001	25.966999
H	-87.736139	-43.133447	25.219478
H	-86.733395	-41.676808	25.432876
H	-86.609669	-43.018598	26.600033
C	-88.452003	-41.827000	26.822001
H	-89.017312	-42.639409	27.304658
H	-89.169527	-41.323476	26.150961
C	-88.031998	-40.875000	27.884001
N	-87.778000	-39.547001	27.646999
H	-87.867912	-39.082022	26.749194
C	-87.445999	-38.958000	28.794001
H	-87.206444	-37.898579	28.908071
N	-87.435997	-39.849998	29.747999
C	-87.806999	-41.056999	29.201000
H	-87.886000	-41.965860	29.791713
C	-87.014998	-37.764001	38.837003
H	-87.777313	-37.261613	39.450010
H	-86.634881	-38.630796	39.399242
H	-86.180678	-37.063120	38.686283
C	-87.622001	-38.194001	37.476003
H	-88.511019	-38.824145	37.643228
H	-87.973387	-37.298497	36.939053
C	-86.665999	-38.933000	36.615003
N	-86.716002	-40.285001	36.488000
H	-87.374372	-40.888313	36.971564
C	-85.716002	-40.702001	35.750001
H	-85.490532	-41.734772	35.499421
N	-85.032996	-39.669000	35.336000
H	-84.266561	-39.723655	34.622278
C	-85.624999	-38.539002	35.853002
H	-85.246406	-37.545164	35.637236
C	-82.637999	-36.596002	34.766999
H	-81.538914	-36.629375	34.704321
H	-82.898809	-36.288952	35.794657
H	-83.012472	-37.618572	34.596787
C	-83.222999	-35.639001	33.717000
H	-82.719188	-34.661670	33.840523
C	-84.718001	-35.410001	33.900003
H	-84.866386	-34.937790	34.889504
H	-85.210090	-36.391565	33.958573
C	-85.439002	-34.570001	32.849999
H	-86.486614	-34.404255	33.147131
H	-84.963044	-33.578785	32.749948
H	-85.455685	-35.036792	31.856344
C	-82.869002	-36.174001	32.349000
H	-81.777588	-36.229911	32.210080
H	-83.275749	-37.188568	32.221122
H	-83.268429	-35.557428	31.530148
C	-92.029998	-37.131001	35.453000
H	-92.493683	-36.835159	36.405765
H	-91.448153	-36.276785	35.073520
H	-92.849363	-37.321631	34.741327
C	-91.142997	-38.359001	35.634999
H	-91.744522	-39.211156	35.998990
H	-90.389872	-38.164614	36.412545
C	-90.410003	-38.770000	34.396001
N	-91.042999	-39.223999	33.273000
H	-92.049537	-39.316741	33.168009
C	-90.138000	-39.576000	32.362001
H	-90.369414	-39.970501	31.373727
N	-88.948997	-39.303001	32.834001
C	-89.089996	-38.806000	34.104001
H	-88.235521	-38.487526	34.689357
Cu	-87.226997	-39.501999	31.761000
O	-87.071031	-37.513878	31.518011
N	-85.920404	-37.374236	31.991404
O	-85.465330	-38.443839	32.475076
O	-82.957636	-40.118408	33.394141
H	-82.053469	-39.897154	33.662814
H	-82.879933	-40.346796	32.437524
O	-86.630413	-35.989921	29.152343
H	-87.032050	-35.714498	29.988372
H	-86.274180	-35.179215	28.765219

Figure 5B. Optimized top-hat NO_2^- binding to T2Cu(I)

C -82.440002 -40.873001 27.580000
H -82.553613 -40.854541 26.486182
H -81.376944 -40.734316 27.828036
H -82.747941 -41.861454 27.953165
C -83.307999 -39.764999 28.209999
H -84.368700 -39.882426 27.921739
H -83.017603 -38.762827 27.851337
C -83.325996 -39.710999 29.767000
O -82.828003 -40.604000 30.461000
O -83.901001 -38.724998 30.306999
H -84.276054 -38.783804 31.242805
C -83.183998 -43.875999 33.056000
H -82.498391 -44.667788 33.391032
H -83.146372 -43.843801 31.955569
H -82.790131 -42.912667 33.419941
C -84.578003 -44.123001 33.558998
H -84.572320 -44.222245 34.661810
H -84.939422 -45.100442 33.185084
C -85.573997 -43.063999 33.173000
N -86.836998 -43.075001 33.702000
H -87.204275 -43.837134 34.263634
C -87.503998 -42.029999 33.297001
H -88.534018 -41.796450 33.559755
N -86.737000 -41.311001 32.509998
C -85.509003 -41.931000 32.424000
H -84.695035 -41.543674 31.815725
C -87.307999 -42.450001 25.966999
H -87.727599 -43.139313 25.218624
H -86.734182 -41.674508 25.434537
H -86.606435 -43.010178 26.604421
C -88.452003 -41.827000 26.822001
H -89.014132 -42.642711 27.304021
H -89.171656 -41.329909 26.146916
C -88.031998 -40.875000 27.884001
N -87.778000 -39.547001 27.646999
H -87.871001 -39.087985 26.747460
C -87.445999 -38.958000 28.794001
H -87.193452 -37.903377 28.901189
N -87.435997 -39.849998 29.747999
C -87.806999 -41.056999 29.201000
H -87.885216 -41.960563 29.801509
C -87.014998 -37.764001 38.837003
H -87.771968 -37.254166 39.451377
H -86.638020 -38.631601 39.400964
H -86.175252 -37.069813 38.683872
C -87.622001 -38.194001 37.476003
H -88.511787 -38.823486 37.641024
H -87.972775 -37.299596 36.937529
C -86.665999 -38.933000 36.615003
N -86.716002 -40.285001 36.488000
H -87.394661 -40.888208 36.940017
C -85.716002 -40.702001 35.750001
H -85.514843 -41.731007 35.463275
N -85.032996 -39.669000 35.336000
H -84.278236 -39.723883 34.599361
C -85.624999 -38.539002 35.853002
H -85.256993 -37.545413 35.620241
C -82.637999 -36.596002 34.766999
H -81.537781 -36.623962 34.710746
H -82.908635 -36.297121 35.795032
H -83.013151 -37.617154 34.591591
C -83.222999 -35.639001 33.717000
H -82.714424 -34.663013 33.843840
C -84.718001 -35.410001 33.900003
H -84.870432 -34.947712 34.894868
H -85.208717 -36.392993 33.932781
C -85.439002 -34.570001 32.849999
H -86.496185 -34.440994 33.128748
H -84.986439 -33.564414 32.771946
H -85.424994 -35.020561 31.849881
C -82.869002 -36.174001 32.349000
H -81.777592 -36.272143 32.225750
H -83.320446 -37.164730 32.198005
H -83.232002 -35.530626 31.533784
C -92.029998 -37.131001 35.453000
H -92.512526 -36.840563 36.399045
H -91.442713 -36.275007 35.085403
H -92.834192 -37.318898 34.722963
C -91.142997 -38.359001 35.634999
H -91.748972 -39.205570 36.007648
H -90.389857 -38.162864 36.412712
C -90.410003 -38.770000 34.396001
N -91.042999 -39.223999 33.273000
H -92.048384 -39.319852 33.174504
C -90.138000 -39.576000 32.362001
H -90.364381 -39.971720 31.373151
N -88.948997 -39.303001 32.834001
C -89.089996 -38.806000 34.104001
H -88.230501 -38.483099 34.680597
Cu -87.226997 -39.501999 31.761000
O -87.004383 -37.044176 31.685101
N -85.794727 -37.244349 31.740839
O -85.467335 -38.388612 32.226122
O -83.021031 -40.069877 33.439637
H -82.167434 -39.640285 33.593687
H -83.015653 -40.268520 32.472832
O -86.551797 -35.876980 29.175378
H -86.974811 -35.972348 30.047739
H -85.639361 -36.129279 29.380619

Figure 5C. Optimized side-on NO_2^- binding to T2Cu(I)

C -82.504997 -40.918999 27.530001

H -82.505981 -40.910737 26.429305
H -81.469552 -40.821580 27.889059
H -82.887189 -41.890758 27.879274
C -83.389999 -39.763000 28.087999
H -83.035959 -38.779169 27.736842
H -84.429191 -39.850564 27.722854
C -83.487999 -39.667000 29.632000
O -82.941002 -40.499001 30.406000
O -84.134003 -38.668999 30.097000
H -84.342349 -38.740121 31.104393
C -83.234001 -43.950001 33.138000
H -82.556390 -44.731706 33.509995
H -83.192532 -43.962307 32.037706
H -82.844264 -42.972287 33.465812
C -84.642998 -44.176998 33.646000
H -84.635143 -44.267932 34.749564
H -85.012050 -45.155227 33.281322
C -85.627998 -43.118000 33.257999
N -86.897003 -43.122002 33.780998
H -87.280964 -43.874207 34.343260
C -87.550003 -42.067001 33.328999
H -88.578080 -41.809390 33.576278
N -86.748001 -41.366001 32.562000
C -85.545998 -42.019001 32.474998
H -84.719935 -41.634230 31.875497
C -87.425003 -42.456001 25.958000
H -87.817375 -43.157317 25.205814
H -86.848754 -41.678513 25.431455
H -86.729240 -43.000892 26.614326
C -88.589996 -41.841999 26.781000
H -89.150601 -42.651633 27.273658
H -89.303856 -41.351063 26.096088
C -88.169998 -40.867001 27.841999
N -87.926003 -39.536999 27.610001
H -87.947354 -39.097272 26.696558
C -87.612999 -38.924999 28.750000
H -87.309375 -37.880181 28.858785
N -87.654999 -39.806000 29.724001
C -88.017998 -41.027000 29.186001
H -88.120063 -41.922078 29.794484
C -87.108003 -37.827001 38.902000
H -87.867061 -37.342147 39.533650
H -86.707948 -38.694691 39.450288
H -86.282549 -37.114304 38.754986
C -87.721002 -38.241002 37.553001
H -88.104341 -37.345222 37.039296
H -88.596463 -38.890585 37.721770
C -86.781999 -38.941002 36.636002
N -86.745004 -40.299000 36.528000
H -87.341792 -40.941849 37.037607
C -85.771004 -40.654999 35.721001
H -85.499936 -41.669933 35.439772
N -85.202004 -39.581001 35.259998
H -84.494757 -39.578699 34.485636
C -85.849000 -38.490002 35.793999
H -85.553442 -37.478446 35.534332
C -82.759004 -36.749001 34.784999
H -81.657714 -36.719534 34.776069
H -83.092572 -36.461613 35.797569
H -83.067121 -37.786789 34.589838
C -83.339997 -35.807999 33.698001
H -82.894844 -34.807418 33.864609
C -84.857003 -35.660999 33.801997
H -85.310956 -36.661596 33.722024
H -85.101062 -35.277756 34.813257
C -85.558999 -34.777000 32.762000
H -85.473678 -35.192676 31.750501
H -85.133284 -33.758450 32.755012
H -86.631546 -34.690757 32.998702
C -82.927003 -36.301998 32.339999
H -81.828986 -36.324167 32.236682
H -83.308830 -37.315485 32.141649
H -83.306507 -35.665506 31.526852
C -92.123002 -37.183999 35.490002
H -92.563905 -36.909301 36.460560
H -91.578076 -36.311831 35.096216
H -92.957144 -37.394611 34.800956
C -91.193002 -38.391000 35.625000
H -91.757399 -39.254616 36.022232
H -90.409310 -38.173424 36.365290
C -90.497003 -38.782002 34.352001
N -91.129998 -39.284001 33.244999
H -92.133522 -39.399224 33.149743
C -90.226998 -39.557000 32.308998
H -90.449971 -39.957936 31.321325
N -89.038003 -39.257000 32.768002
C -89.182000 -38.770001 34.040001
H -88.329555 -38.427659 34.615756
Cu -87.295998 -39.577999 31.743999
O -86.395604 -37.631934 31.756515
N -85.974322 -38.316937 32.729109
O -84.818489 -38.848798 32.563189
O -82.909525 -40.425341 33.650048
H -81.964438 -40.357641 33.841974
H -82.970913 -40.294432 32.682010
O -85.940854 -36.397618 29.208814
H -85.241771 -37.064813 29.326426
H -86.289517 -36.351615 30.112342