

Dataset S1. DFT coordinates**Relaxed coordinates of Complex 2**

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.46320	30.42890	50.80920
C	30.29080	30.73800	49.89190
O	29.82090	31.87440	49.79440
O	29.87110	29.67260	49.23530
H	33.70520	29.79390	51.83460
H	32.69630	29.90030	49.10730
H	31.33160	29.41690	51.21570
H	31.46590	31.15580	51.63260
H	29.05410	29.84880	48.62640
N	33.63800	32.82200	50.35700
H	33.88250	32.60970	51.31960
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.81190	34.70740	46.47970
C	30.99590	35.92790	46.08200
O	30.90170	33.77310	47.09090
H	33.48010	32.73540	46.68870
H	31.74040	33.67540	44.58110
H	32.58680	34.99730	47.21560
H	31.43560	33.11480	47.58960
H	30.49690	36.33610	46.97120
H	30.23390	35.64980	45.34060
H	31.63030	36.70810	45.64280
N	34.61300	35.31200	44.78500
H	35.05150	34.70490	45.47020
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.57100	28.80890	45.58060

C	27.57550	30.01170	46.52430
O	27.36760	31.16380	46.01180
O	27.79320	29.82030	47.75570
H	25.46860	28.05610	46.85190
H	25.88590	29.38280	44.30400
H	27.90390	27.92000	46.13420
H	28.30260	29.01290	44.78440
N	26.43600	26.10900	44.22600
H	26.15480	25.82150	45.15760
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.02640	33.78580	51.29570
C	24.77450	33.00110	49.99780
C	26.05670	32.48790	49.31350
C	26.84850	33.58150	48.59250
N	28.05980	32.99730	47.92690
H	23.49660	35.52290	50.27890
H	23.07610	33.42890	52.20090
H	25.67380	34.65930	51.10480
H	25.57570	33.14380	52.00200
H	24.13650	32.13560	50.23490
H	24.20340	33.60590	49.27420
H	26.70450	31.99230	50.05580
H	25.78610	31.72060	48.57350
H	26.23390	34.03610	47.80390
H	27.19480	34.36340	49.28180
H	28.65540	32.48020	48.61770
H	28.67630	33.70380	47.49750
H	27.77660	32.29910	47.16970
N	24.74100	35.92700	53.53200
H	24.85570	36.57440	52.75890
O	25.02000	32.63400	45.94200
H	25.77730	32.00510	45.92680
H	25.01390	32.99680	45.03920
O	27.76100	32.56500	43.56800
H	27.92580	31.98250	42.80770
H	27.68420	31.95400	44.33640
H	35.81620	29.27140	51.07360
H	33.84670	33.74950	50.00060
H	34.49820	31.23070	45.31360
H	35.20960	35.82390	44.14210
H	23.26620	27.63570	46.32800

H	26.53700	25.39970	43.50750
H	21.65580	36.76440	50.95380
H	24.88670	36.28040	54.47230

Step 19 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.48110	30.49190	50.83310
C	30.30680	30.93800	49.95250
O	29.79320	32.06940	50.14620
O	29.96270	30.08600	49.06470
H	33.69840	29.78390	51.83300
H	32.65940	29.89680	49.11590
H	31.27400	29.47170	51.18750
H	31.56070	31.16550	51.69860
H	28.81210	29.94560	48.38000
N	33.63800	32.82200	50.35700
H	33.85820	32.61530	51.32650
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.84400	34.72470	46.49240
C	31.00480	35.93290	46.10410
O	30.96800	33.80130	47.15670
H	33.46900	32.72700	46.68870
H	31.72900	33.67980	44.59220
H	32.64710	35.03730	47.18850
H	31.52580	33.16250	47.65870
H	30.56480	36.37300	47.00880
H	30.19040	35.62350	45.43480
H	31.60520	36.69590	45.59320
N	34.61300	35.31200	44.78500
H	35.05070	34.71040	45.47550
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400

C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.59240	28.71570	45.56520
C	27.74890	29.82520	46.59030
O	27.64440	31.02480	46.26760
O	28.05290	29.39060	47.78040
H	25.47340	28.02160	46.84630
H	25.90830	29.39820	44.31670
H	27.90090	27.77130	46.03260
H	28.31110	28.94220	44.76240
N	26.43600	26.10900	44.22600
H	26.15180	25.81730	45.15530
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.04120	33.80230	51.31440
C	24.83180	33.04100	49.99810
C	26.14120	32.53180	49.36810
C	27.01800	33.63990	48.77940
N	28.24140	33.03720	48.16140
H	23.49690	35.52320	50.27920
H	23.08110	33.42440	52.19660
H	25.68760	34.68210	51.15340
H	25.57830	33.15220	52.02280
H	24.17650	32.17750	50.19220
H	24.30240	33.66550	49.25940
H	26.71890	31.96020	50.11380
H	25.89290	31.83060	48.55520
H	26.46780	34.17550	47.99520
H	27.35600	34.35010	49.54550
H	28.84520	32.59090	48.92810
H	28.84050	33.70900	47.65430
H	27.97780	32.29190	47.47130
N	24.74100	35.92700	53.53200
H	24.86110	36.57330	52.75890
O	25.64500	33.31530	45.88490
H	25.71890	32.35200	46.00520
H	26.51920	33.54550	45.48800
O	28.32850	33.50680	45.08060
H	28.72650	33.79930	44.24300
H	28.40160	32.53060	45.07660
H	35.81760	29.27250	51.07320

H	33.82540	33.75690	50.00850
H	34.49740	31.23040	45.31340
H	35.20880	35.83150	44.14760
H	23.26740	27.63110	46.32730
H	26.54560	25.40130	43.50720
H	21.65630	36.76480	50.95400
H	24.89350	36.27710	54.47240

**Step 18 of the relaxed surface scan for
proton transfer from complex 2 to
complex 3 with explicit waters.**

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.43520	30.40690	50.74560
C	30.29540	30.74800	49.77500
O	29.80860	31.89880	49.79120
O	29.94030	29.77580	49.00140
H	33.70460	29.79340	51.83460
H	32.72360	29.90670	49.09980
H	31.28630	29.38050	51.10910
H	31.39980	31.10290	51.59550
H	28.92300	29.89540	48.31760
N	33.63800	32.82200	50.35700
H	33.86950	32.61100	51.32300
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.82090	34.70930	46.48620
C	30.98410	35.91740	46.09280
O	30.93180	33.77440	47.11880
H	33.47350	32.73190	46.68920
H	31.73700	33.67660	44.58440
H	32.60690	35.01530	47.20390
H	31.47580	33.13120	47.62840
H	30.52250	36.34680	46.99190
H	30.18640	35.61030	45.40210
H	31.59140	36.68800	45.60170
N	34.61300	35.31200	44.78500

H	35.04980	34.71140	45.47700
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.56460	28.80540	45.59950
C	27.57730	30.02800	46.51570
O	27.24790	31.14440	46.05090
O	27.91230	29.84820	47.75260
H	25.47190	28.02860	46.84750
H	25.89100	29.38560	44.30680
H	27.88490	27.92190	46.16860
H	28.31430	28.99230	44.81490
N	26.43600	26.10900	44.22600
H	26.15080	25.82030	45.15600
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.03170	33.79360	51.30450
C	24.79210	33.03470	49.99190
C	26.07940	32.52040	49.32460
C	26.95220	33.62800	48.72910
N	28.10150	33.01930	47.98710
H	23.49680	35.52370	50.27920
H	23.07800	33.42700	52.19900
H	25.68300	34.66820	51.13400
H	25.57150	33.13900	52.00640
H	24.13770	32.17380	50.20050
H	24.24700	33.66230	49.26750
H	26.67030	31.92980	50.04410
H	25.80300	31.83270	48.51000
H	26.37140	34.22090	48.01080
H	27.37000	34.28820	49.50050
H	28.73270	32.49130	48.65870
H	28.69290	33.70290	47.48950
H	27.74620	32.33610	47.27010
N	24.74100	35.92700	53.53200
H	24.85860	36.57370	52.75880
O	25.37060	33.54270	45.88800
H	25.45930	32.57440	45.95450
H	26.21750	33.79800	45.45490

O	28.06560	33.62130	44.98720	H	30.48710	36.32110	46.98200
H	28.49360	33.86720	44.14970	H	30.20780	35.61780	45.36150
H	28.00470	32.64260	44.97240	H	31.59670	36.69410	45.63410
H	35.81620	29.27030	51.07330	N	34.61300	35.31200	44.78500
H	33.84230	33.75180	50.00420	H	35.05080	34.70760	45.47310
H	34.49770	31.23050	45.31340	C	23.94400	27.94100	45.50200
H	35.20960	35.82920	44.14660	O	23.57900	28.09500	44.33100
H	23.26670	27.63250	46.32740	N	25.20400	28.15800	45.87400
H	26.53460	25.40030	43.50640	C	26.22300	28.52000	44.89200
H	21.65610	36.76450	50.95380	C	26.47000	27.38700	43.85800
H	24.89020	36.27880	54.47230	O	26.67800	27.71100	42.68900

Step 17 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400	H	25.47050	28.02560	46.84740
O	35.29000	29.74100	49.12000	H	25.89660	29.39110	44.31100
N	33.82600	29.84000	50.82400	H	27.91670	27.81210	46.03880
C	32.80700	30.46300	50.04700	H	28.30510	28.96050	44.74560
C	33.11400	31.92700	49.53200	N	26.43600	26.10900	44.22600
O	32.91300	32.28500	48.36700	H	26.15430	25.81770	45.15630
C	31.46960	30.49900	50.81100	C	22.02800	35.96100	51.62100
C	30.30440	30.96330	49.92280	O	21.52500	35.67200	52.73400
O	29.61670	31.95340	50.28400	N	23.04900	35.23800	51.14800
O	30.12730	30.27520	48.85950	C	23.74700	34.28100	52.02300
H	33.70240	29.79140	51.83400	C	24.10700	34.76800	53.38500
H	32.66470	29.89970	49.11390	O	23.80400	34.05500	54.34000
H	31.23780	29.47610	51.14620	C	25.03350	33.79260	51.30630
H	31.53940	31.15220	51.69210	C	24.80620	33.03170	49.99110
H	28.93090	30.04270	48.25510	C	26.10590	32.50380	49.35410
N	33.63800	32.82200	50.35700	C	26.96380	33.59310	48.70400
H	33.86770	32.61190	51.32360	N	28.24250	32.99880	48.19510
C	33.90300	32.02700	44.81800	H	23.49700	35.52360	50.27940
O	33.71700	32.08700	43.59100	H	23.07800	33.42700	52.19870
N	33.39200	32.93300	45.68900	H	25.68710	34.66650	51.14180
C	32.51000	34.06700	45.26000	H	25.56850	33.13710	52.01100
C	33.32800	35.05900	44.40200	H	24.14420	32.17530	50.19240
O	32.77200	35.51900	43.37500	H	24.27540	33.65770	49.25510
C	31.81410	34.70360	46.48360	H	26.70410	31.97640	50.11570
C	30.97760	35.91070	46.08910	H	25.84860	31.76390	48.58040
O	30.92500	33.75530	47.10620	H	26.43330	34.04330	47.85350
H	33.47710	32.73250	46.68900	H	27.23370	34.38250	49.41770
H	31.73980	33.67570	44.58160	H	28.77520	32.53530	49.00640
H	32.59130	35.00600	47.21140	H	28.89220	33.68060	47.76800
H	31.47780	33.10690	47.60190	H	28.03870	32.26990	47.46740
				N	24.74100	35.92700	53.53200

H	24.86020	36.57340	52.75890	H	33.47690	32.73240	46.68890
O	25.02000	32.63400	45.94200	H	31.74040	33.67540	44.58110
H	25.77700	32.01550	45.99180	H	32.58780	35.00610	47.21180
H	25.08730	32.99230	45.03900	H	31.47520	33.10690	47.60070
O	27.76100	32.56500	43.56800	H	30.48330	36.31990	46.97900
H	28.12660	32.02800	42.84460	H	30.20580	35.61500	45.35890
H	27.81400	31.98460	44.35470	H	31.59360	36.69280	45.63160
H	35.81760	29.27260	51.07330	N	34.61300	35.31200	44.78500
H	33.83570	33.75390	50.00600	H	35.05080	34.70710	45.47270
H	34.49750	31.23060	45.31370	C	23.94400	27.94100	45.50200
H	35.20980	35.82520	44.14340	O	23.57900	28.09500	44.33100
H	23.26750	27.63290	46.32770	N	25.20400	28.15800	45.87400
H	26.54430	25.40100	43.50720	C	26.22300	28.52000	44.89200
H	21.65600	36.76460	50.95390	C	26.47000	27.38700	43.85800
H	24.89220	36.27780	54.47240	O	26.67800	27.71100	42.68900

Step 16 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400	C	27.58830	28.74780	45.55800
O	35.29000	29.74100	49.12000	C	27.74250	29.88630	46.55170
N	33.82600	29.84000	50.82400	O	27.55360	31.07900	46.21890
C	32.80700	30.46300	50.04700	O	28.14100	29.49980	47.72700
C	33.11400	31.92700	49.53200	H	25.47020	28.02800	46.84790
O	32.91300	32.28500	48.36700	H	25.89530	29.39010	44.31000
C	31.46680	30.49150	50.80610	H	27.91550	27.82180	46.04870
C	30.29840	30.92780	49.91000	H	28.30520	28.96330	44.74940
O	29.60230	31.91680	50.24780	N	26.43600	26.10900	44.22600
O	30.12890	30.20950	48.86130	H	26.15590	25.81800	45.15680
H	33.70330	29.79290	51.83420	C	22.02800	35.96100	51.62100
H	32.66980	29.90000	49.11270	O	21.52500	35.67200	52.73400
H	31.24740	29.46980	51.15310	N	23.04900	35.23800	51.14800
H	31.52420	31.15640	51.67920	C	23.74700	34.28100	52.02300
H	28.96880	30.03910	48.26920	C	24.10700	34.76800	53.38500
N	33.63800	32.82200	50.35700	O	23.80400	34.05500	54.34000
H	33.87240	32.61040	51.32220	C	25.03110	33.79050	51.30360
C	33.90300	32.02700	44.81800	C	24.79750	33.02910	49.98940
O	33.71700	32.08700	43.59100	C	26.09360	32.49980	49.34630
N	33.39200	32.93300	45.68900	C	26.94310	33.58590	48.67950
C	32.51000	34.06700	45.26000	N	28.22250	32.98960	48.17260
C	33.32800	35.05900	44.40200	H	23.49640	35.52310	50.27890
O	32.77200	35.51900	43.37500	H	23.07730	33.42770	52.19960
C	31.81190	34.70310	46.48270	H	25.68600	34.66310	51.13660
C	30.97480	35.90930	46.08680	H	25.56700	33.13420	52.00700
O	30.92230	33.75420	47.10430	H	24.13570	32.17340	50.19450
				H	24.26320	33.65480	49.25560
				H	26.69930	31.98060	50.10770
				H	25.83310	31.75190	48.58150
				H	26.40690	34.02150	47.82510
				H	27.21240	34.38530	49.38240

H	28.74570	32.51970	48.98310	O	32.77200	35.51900	43.37500
H	28.87850	33.67020	47.75350	C	31.81330	34.70560	46.48170
H	28.01720	32.26250	47.44060	C	30.97970	35.91400	46.08470
N	24.74100	35.92700	53.53200	O	30.92070	33.76000	47.10360
H	24.85840	36.57410	52.75920	H	33.47820	32.73280	46.68870
O	25.02000	32.63400	45.94200	H	31.74010	33.67550	44.58150
H	25.77420	32.01090	45.98190	H	32.58960	35.00740	47.21090
H	25.08810	33.00510	45.04430	H	31.47160	33.11410	47.60340
O	27.76100	32.56500	43.56800	H	30.48700	36.32470	46.97620
H	28.12320	32.02230	42.84730	H	30.21190	35.62220	45.35460
H	27.80380	31.98600	44.35680	H	31.60110	36.69680	45.63180
H	35.81750	29.27250	51.07340	N	34.61300	35.31200	44.78500
H	33.83980	33.75260	50.00480	H	35.05120	34.70660	45.47200
H	34.49720	31.23030	45.31370	C	23.94400	27.94100	45.50200
H	35.20990	35.82460	44.14300	O	23.57900	28.09500	44.33100
H	23.26740	27.63300	46.32770	N	25.20400	28.15800	45.87400
H	26.54450	25.40080	43.50750	C	26.22300	28.52000	44.89200
H	21.65610	36.76460	50.95390	C	26.47000	27.38700	43.85800
H	24.89070	36.27850	54.47240	O	26.67800	27.71100	42.68900

Step 15 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400	O	27.58520	28.76290	45.56260
O	35.29000	29.74100	49.12000	C	27.71370	29.91460	46.54870
N	33.82600	29.84000	50.82400	O	27.53310	31.10140	46.17880
C	32.80700	30.46300	50.04700	O	28.06380	29.56320	47.74450
C	33.11400	31.92700	49.53200	H	25.47050	28.03120	46.84820
O	32.91300	32.28500	48.36700	H	25.89250	29.38810	44.30840
C	31.46210	30.47530	50.79930	H	27.91550	27.84430	46.06520
C	30.29120	30.87850	49.89270	H	28.30330	28.97780	44.75530
O	29.63890	31.91580	50.15320	N	26.43600	26.10900	44.22600
O	30.07760	30.07300	48.91230	H	26.15630	25.81870	45.15720
H	33.70330	29.79230	51.83420	C	22.02800	35.96100	51.62100
H	32.67870	29.89990	49.11100	O	21.52500	35.67200	52.73400
H	31.26410	29.45390	51.15830	N	23.04900	35.23800	51.14800
H	31.50210	31.15500	51.66170	C	23.74700	34.28100	52.02300
H	28.96810	30.01010	48.31120	C	24.10700	34.76800	53.38500
N	33.63800	32.82200	50.35700	O	23.80400	34.05500	54.34000
H	33.87200	32.61070	51.32230	C	25.03030	33.78960	51.30240
C	33.90300	32.02700	44.81800	C	24.79330	33.02270	49.99190
O	33.71700	32.08700	43.59100	C	26.08720	32.50020	49.33890
N	33.39200	32.93300	45.68900	C	26.92370	33.59120	48.66480
C	32.51000	34.06700	45.26000	N	28.19180	33.00100	48.12380
C	33.32800	35.05900	44.40200	H	23.49680	35.52340	50.27920
				H	23.07700	33.42800	52.19980
				H	25.68320	34.66260	51.13010
				H	25.56930	33.13670	52.00660
				H	24.13860	32.16340	50.20440
				H	24.24930	33.64310	49.26070

H	26.70220	31.98360	50.09460	O	33.71700	32.08700	43.59100
H	25.82480	31.75090	48.57630	N	33.39200	32.93300	45.68900
H	26.37080	34.03330	47.82460	C	32.51000	34.06700	45.26000
H	27.20670	34.38490	49.36890	C	33.32800	35.05900	44.40200
H	28.73390	32.52230	48.91110	O	32.77200	35.51900	43.37500
H	28.83720	33.68960	47.70320	C	31.81980	34.70890	46.48570
H	27.97300	32.27970	47.38640	C	30.98300	35.91670	46.09150
N	24.74100	35.92700	53.53200	O	30.93030	33.77330	47.11680
H	24.85900	36.57370	52.75890	H	33.47360	32.73210	46.68910
O	25.02000	32.63400	45.94200	H	31.73730	33.67650	44.58410
H	25.77800	32.01410	45.97130	H	32.60490	35.01480	47.20440
H	25.07480	33.00680	45.04420	H	31.47420	33.13030	47.62670
O	27.76100	32.56500	43.56800	H	30.51880	36.34480	46.98990
H	28.06720	32.00620	42.83380	H	30.18750	35.61010	45.39810
H	27.78470	31.97620	44.35150	H	31.59120	36.68830	45.60310
H	35.81700	29.27160	51.07330	N	34.61300	35.31200	44.78500
H	33.84040	33.75240	50.00460	H	35.04980	34.71140	45.47690
H	34.49760	31.23060	45.31370	C	23.94400	27.94100	45.50200
H	35.20970	35.82480	44.14300	O	23.57900	28.09500	44.33100
H	23.26720	27.63330	46.32770	N	25.20400	28.15800	45.87400
H	26.54280	25.40060	43.50750	C	26.22300	28.52000	44.89200
H	21.65590	36.76450	50.95380	C	26.47000	27.38700	43.85800
H	24.89090	36.27850	54.47230	O	26.67800	27.71100	42.68900

Step 14 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400	C	27.57600	30.02970	46.51910
O	35.29000	29.74100	49.12000	O	27.24000	31.14560	46.05080
N	33.82600	29.84000	50.82400	O	27.91900	29.85180	47.75100
C	32.80700	30.46300	50.04700	H	25.47220	28.02910	46.84750
C	33.11400	31.92700	49.53200	H	25.88990	29.38510	44.30660
O	32.91300	32.28500	48.36700	H	27.88730	27.92370	46.16670
C	31.43500	30.40620	50.74630	H	28.31310	28.99660	44.81440
C	30.29530	30.74690	49.77710	N	26.43600	26.10900	44.22600
O	29.80500	31.89330	49.78970	H	26.15080	25.82050	45.15610
O	29.94260	29.76860	49.00310	C	22.02800	35.96100	51.62100
H	33.70530	29.79490	51.83480	O	21.52500	35.67200	52.73400
H	32.72430	29.90660	49.09980	N	23.04900	35.23800	51.14800
H	31.28630	29.37970	51.10980	C	23.74700	34.28100	52.02300
H	31.39930	31.10170	51.59620	C	24.10700	34.76800	53.38500
H	28.96730	29.89610	48.33870	O	23.80400	34.05500	54.34000
N	33.63800	32.82200	50.35700	C	25.03080	33.79250	51.30360
H	33.87070	32.61070	51.32270	C	24.78900	33.03200	49.99240
C	33.90300	32.02700	44.81800	C	26.07470	32.51720	49.32260
				C	26.94510	33.62420	48.72300
				N	28.09270	33.01510	47.97800
				H	23.49710	35.52420	50.27950
				H	23.07760	33.42740	52.19930

H	25.68230	34.66660	51.13150
H	25.57110	33.13840	52.00570
H	24.13520	32.17110	50.20340
H	24.24200	33.65850	49.26840
H	26.66770	31.92810	50.04160
H	25.79670	31.82800	48.51000
H	26.36170	34.21520	48.00510
H	27.36510	34.28610	49.49190
H	28.72130	32.48690	48.64820
H	28.68420	33.69990	47.48240
H	27.73600	32.33140	47.26010
N	24.74100	35.92700	53.53200
H	24.85830	36.57380	52.75880
O	25.35790	33.53290	45.89090
H	25.45070	32.56480	45.95850
H	26.20270	33.78960	45.45460
O	28.04890	33.61210	44.98370
H	28.47590	33.85590	44.14500
H	27.98750	32.63290	44.97210
H	35.81620	29.27040	51.07340
H	33.84350	33.75140	50.00380
H	34.49770	31.23050	45.31330
H	35.20970	35.82910	44.14650
H	23.26650	27.63290	46.32740
H	26.53480	25.40020	43.50660
H	21.65590	36.76430	50.95370
H	24.88990	36.27900	54.47230

Step 13 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.45540	30.45790	50.78860
C	30.28990	30.83670	49.86620
O	29.69890	31.92560	50.03000
O	30.01920	29.94780	48.96960
H	33.70420	29.79370	51.83440
H	32.69090	29.90080	49.10830
H	31.27470	29.43670	51.15510
H	31.47630	31.14860	51.64280

H	28.97500	29.97390	48.35100
N	33.63800	32.82200	50.35700
H	33.87300	32.61070	51.32210
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.81780	34.71010	46.48230
C	30.99120	35.92350	46.08520
O	30.91980	33.77320	47.10790
H	33.47770	32.73370	46.68890
H	31.73850	33.67620	44.58290
H	32.59740	35.00860	47.20950
H	31.46510	33.12250	47.60680
H	30.50000	36.33590	46.97670
H	30.22240	35.63640	45.35420
H	31.61680	36.70350	45.63330
N	34.61300	35.31200	44.78500
H	35.05170	34.70490	45.47020
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.58220	28.77240	45.56940
C	27.68670	29.94120	46.54120
O	27.49620	31.11770	46.13350
O	28.00860	29.63420	47.75130
H	25.47060	28.03380	46.84860
H	25.89180	29.38720	44.30750
H	27.90980	27.86150	46.08790
H	28.30570	28.97920	44.76490
N	26.43600	26.10900	44.22600
H	26.15680	25.81910	45.15740
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.03070	33.78970	51.30210
C	24.79360	33.01470	49.99620
C	26.08770	32.50140	49.33530

C	26.90390	33.59730	48.64480	H	33.70440	29.79330	51.83450
N	28.15690	33.01450	48.06200	H	32.70070	29.90220	49.10580
H	23.49670	35.52340	50.27920	H	31.28480	29.42030	51.15240
H	23.07720	33.42790	52.19970	H	31.45160	31.14070	51.62550
H	25.68050	34.66390	51.12390	H	28.99690	29.93720	48.37490
H	25.57340	33.14220	52.00840	N	33.63800	32.82200	50.35700
H	24.14840	32.15030	50.21680	H	33.87440	32.61030	51.32170
H	24.23850	33.62650	49.26610	C	33.90300	32.02700	44.81800
H	26.71600	31.99650	50.08790	O	33.71700	32.08700	43.59100
H	25.82670	31.74380	48.58060	N	33.39200	32.93300	45.68900
H	26.32680	34.04070	47.82170	C	32.51000	34.06700	45.26000
H	27.20470	34.38870	49.34390	C	33.32800	35.05900	44.40200
H	28.72550	32.52790	48.81980	O	32.77200	35.51900	43.37500
H	28.78700	33.71070	47.63250	C	31.81550	34.70890	46.48140
H	27.91950	32.29910	47.32180	C	30.99200	35.92430	46.08410
N	24.74100	35.92700	53.53200	O	30.91380	33.77210	47.10170
H	24.85830	36.57400	52.75900	H	33.47850	32.73420	46.68880
O	25.02000	32.63400	45.94200	H	31.73920	33.67600	44.58220
H	25.77700	32.01140	45.96070	H	32.59320	35.00460	47.21170
H	25.05490	32.99600	45.03880	H	31.45590	33.11990	47.60160
O	27.76100	32.56500	43.56800	H	30.49810	36.33520	46.97490
H	28.00350	31.99140	42.82160	H	30.22560	35.64010	45.34960
H	27.75500	31.96750	44.34620	H	31.62040	36.70460	45.63650
H	35.81670	29.27130	51.07340	N	34.61300	35.31200	44.78500
H	33.84130	33.75200	50.00390	H	35.05080	34.70730	45.47280
H	34.49780	31.23060	45.31360	C	23.94400	27.94100	45.50200
H	35.20950	35.82450	44.14250	O	23.57900	28.09500	44.33100
H	23.26710	27.63350	46.32770	N	25.20400	28.15800	45.87400
H	26.54200	25.40040	43.50750	C	26.22300	28.52000	44.89200
H	21.65600	36.76450	50.95380	C	26.47000	27.38700	43.85800
H	24.89010	36.27880	54.47240	O	26.67800	27.71100	42.68900

Step 12 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400	H	25.47030	28.03720	46.84910
O	35.29000	29.74100	49.12000	H	25.89290	29.38780	44.30780
N	33.82600	29.84000	50.82400	H	27.90060	27.87460	46.11320
C	32.80700	30.46300	50.04700	H	28.31050	28.97350	44.77770
C	33.11400	31.92700	49.53200	N	26.43600	26.10900	44.22600
O	32.91300	32.28500	48.36700	H	26.15600	25.81960	45.15740
C	31.44970	30.44120	50.77850	C	22.02800	35.96100	51.62100
C	30.28750	30.79530	49.84460	O	21.52500	35.67200	52.73400
O	29.72440	31.90320	49.94550	N	23.04900	35.23800	51.14800
O	29.98840	29.85840	49.00040	C	23.74700	34.28100	52.02300
				C	24.10700	34.76800	53.38500

O	23.80400	34.05500	54.34000	C	31.43500	30.39620	50.74760
C	25.02970	33.78870	51.30050	C	30.29530	30.72640	49.77980
C	24.78860	33.01070	49.99700	O	29.86350	31.89040	49.70580
C	26.07940	32.49870	49.32870	O	29.87490	29.70600	49.08890
C	26.89000	33.59590	48.63410	H	33.70480	29.79300	51.83460
N	28.12860	33.01300	48.02120	H	32.72790	29.90750	49.09870
H	23.49710	35.52370	50.27950	H	31.29720	29.37090	51.11730
H	23.07680	33.42820	52.20000	H	31.39360	31.09740	51.59290
H	25.67840	34.66300	51.11850	H	28.95890	29.87050	48.42230
H	25.57440	33.14330	52.00720	N	33.63800	32.82200	50.35700
H	24.14620	32.14540	50.22250	H	33.87300	32.61070	51.32210
H	24.22840	33.62030	49.26900	C	33.90300	32.02700	44.81800
H	26.71260	31.99280	50.07650	O	33.71700	32.08700	43.59100
H	25.81480	31.74170	48.57490	N	33.39200	32.93300	45.68900
H	26.30120	34.04930	47.82510	C	32.51000	34.06700	45.26000
H	27.20790	34.37920	49.33490	C	33.32800	35.05900	44.40200
H	28.70810	32.51150	48.75620	O	32.77200	35.51900	43.37500
H	28.75530	33.71290	47.59380	C	31.81620	34.70720	46.48450
H	27.87470	32.30760	47.27500	C	30.98000	35.91500	46.08830
N	24.74100	35.92700	53.53200	O	30.92360	33.77180	47.11140
H	24.85780	36.57400	52.75890	H	33.47610	32.73440	46.68930
O	25.02000	32.63400	45.94200	H	31.73870	33.67580	44.58290
H	25.77440	32.00670	45.94810	H	32.59890	35.01240	47.20600
H	25.04690	33.00280	45.04150	H	31.46350	33.12470	47.61950
O	27.76100	32.56500	43.56800	H	30.51420	36.34330	46.98580
H	27.98350	31.99050	42.81620	H	30.18570	35.60740	45.39380
H	27.73560	31.96070	44.34140	H	31.58860	36.68660	45.60030
H	35.81640	29.27100	51.07340	N	34.61300	35.31200	44.78500
H	33.84270	33.75150	50.00350	H	35.04970	34.71080	45.47650
H	34.49790	31.23070	45.31370	C	23.94400	27.94100	45.50200
H	35.20970	35.82510	44.14320	O	23.57900	28.09500	44.33100
H	23.26680	27.63380	46.32770	N	25.20400	28.15800	45.87400
H	26.54050	25.40020	43.50740	C	26.22300	28.52000	44.89200
H	21.65590	36.76440	50.95380	C	26.47000	27.38700	43.85800
H	24.88950	36.27910	54.47240	O	26.67800	27.71100	42.68900

Step 11 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400	C	27.56030	28.81900	45.60060
O	35.29000	29.74100	49.12000	C	27.55180	30.04500	46.51650
N	33.82600	29.84000	50.82400	O	27.17510	31.15050	46.04050
C	32.80700	30.46300	50.04700	O	27.91900	29.89530	47.73600
C	33.11400	31.92700	49.53200	H	25.47100	28.03330	46.84830
O	32.91300	32.28500	48.36700	H	25.88710	29.38340	44.30560
				H	27.89020	27.94040	46.17250
				H	28.30970	29.01250	44.81750
				N	26.43600	26.10900	44.22600
				H	26.14880	25.82110	45.15570
				C	22.02800	35.96100	51.62100

O	21.52500	35.67200	52.73400	N	33.82600	29.84000	50.82400
N	23.04900	35.23800	51.14800	C	32.80700	30.46300	50.04700
C	23.74700	34.28100	52.02300	C	33.11400	31.92700	49.53200
C	24.10700	34.76800	53.38500	O	32.91300	32.28500	48.36700
O	23.80400	34.05500	54.34000	C	31.44670	30.42870	50.77300
C	25.03140	33.79250	51.30440	C	30.28710	30.76680	49.83200
C	24.78980	33.02210	49.99900	O	29.74510	31.88600	49.88530
C	26.07610	32.51020	49.32760	O	29.96690	29.79680	49.02770
C	26.93170	33.61820	48.70830	H	33.70470	29.79350	51.83460
N	28.06770	33.01320	47.94300	H	32.70730	29.90320	49.10410
H	23.49550	35.52190	50.27800	H	31.29330	29.40780	51.15080
H	23.07790	33.42720	52.19940	H	31.43580	31.13290	51.61610
H	25.67980	34.66750	51.12550	H	29.01520	29.90550	48.39720
H	25.57510	33.14460	52.00970	N	33.63800	32.82200	50.35700
H	24.14180	32.15890	50.21800	H	33.87550	32.61010	51.32140
H	24.23630	33.64040	49.27290	C	33.90300	32.02700	44.81800
H	26.67850	31.93470	50.04980	O	33.71700	32.08700	43.59100
H	25.79910	31.80900	48.52510	N	33.39200	32.93300	45.68900
H	26.33210	34.20020	47.99650	C	32.51000	34.06700	45.26000
H	27.35980	34.28830	49.46540	C	33.32800	35.05900	44.40200
H	28.71940	32.49340	48.59130	O	32.77200	35.51900	43.37500
H	28.63730	33.69830	47.42320	C	31.81480	34.70830	46.48120
H	27.69620	32.32030	47.23810	C	30.99420	35.92590	46.08440
N	24.74100	35.92700	53.53200	O	30.91000	33.77260	47.09870
H	24.85720	36.57410	52.75890	H	33.47920	32.73520	46.68890
O	25.29160	33.47740	45.90310	H	31.73950	33.67590	44.58200
H	25.47030	32.52040	45.97220	H	32.59180	35.00160	47.21320
H	26.09710	33.79740	45.43910	H	31.44910	33.11780	47.59800
O	27.99540	33.60870	44.96220	H	30.49870	36.33550	46.97480
H	28.43090	33.80750	44.11610	H	30.22920	35.64440	45.34730
H	27.90330	32.63120	44.98590	H	31.62480	36.70610	45.64000
H	35.81600	29.27050	51.07350	N	34.61300	35.31200	44.78500
H	33.84470	33.75070	50.00270	H	35.05080	34.70720	45.47270
H	34.49790	31.23060	45.31330	C	23.94400	27.94100	45.50200
H	35.20990	35.82810	44.14580	O	23.57900	28.09500	44.33100
H	23.26620	27.63380	46.32760	N	25.20400	28.15800	45.87400
H	26.53180	25.40020	43.50620	C	26.22300	28.52000	44.89200
H	21.65600	36.76440	50.95370	C	26.47000	27.38700	43.85800
H	24.88910	36.27930	54.47230	O	26.67800	27.71100	42.68900
				C	27.57800	28.78190	45.58220
				C	27.65020	29.97840	46.52720
				O	27.41820	31.13360	46.06620
				O	27.96150	29.74990	47.74870
				H	25.46990	28.03950	46.84940
				H	25.89380	29.38810	44.30790
				H	27.89650	27.88260	46.12670
Step 10 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.							
C	35.07600	29.61800	50.32400				
O	35.29000	29.74100	49.12000				

H	28.31280	28.97120	44.78410
N	26.43600	26.10900	44.22600
H	26.15580	25.81990	45.15740
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.02920	33.78850	51.29930
C	24.78560	33.00940	49.99680
C	26.07380	32.49760	49.32310
C	26.88120	33.59440	48.62430
N	28.10800	33.00960	47.98960
H	23.49740	35.52410	50.27970
H	23.07680	33.42820	52.20010
H	25.67740	34.66290	51.11540
H	25.57520	33.14380	52.00560
H	24.14480	32.14360	50.22510
H	24.22190	33.61770	49.27040
H	26.71030	31.99110	50.06760
H	25.80550	31.74100	48.57040
H	26.28440	34.05480	47.82520
H	27.21240	34.37220	49.32520
H	28.69430	32.49850	48.70830
H	28.73230	33.71080	47.56140
H	27.84120	32.31010	47.24040
N	24.74100	35.92700	53.53200
H	24.85750	36.57410	52.75890
O	25.02000	32.63400	45.94200
H	25.77140	32.00220	45.93840
H	25.04160	33.00830	45.04380
O	27.76100	32.56500	43.56800
H	27.94370	31.98650	42.80860
H	27.71780	31.95610	44.33760
H	35.81630	29.27090	51.07350
H	33.84440	33.75090	50.00280
H	34.49800	31.23070	45.31360
H	35.20980	35.82480	44.14300
H	23.26680	27.63390	46.32770
H	26.53960	25.40010	43.50740
H	21.65600	36.76450	50.95380
H	24.88900	36.27930	54.47230

Step 9 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.43720	30.39770	50.75300
C	30.29580	30.72580	49.78920
O	29.86770	31.88770	49.70040
O	29.86810	29.69500	49.11130
H	33.70490	29.79310	51.83460
H	32.72570	29.90700	49.09920
H	31.30060	29.37370	51.12630
H	31.39860	31.10180	51.59600
H	28.98120	29.86550	48.45400
N	33.63800	32.82200	50.35700
H	33.87420	32.61070	51.32180
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.81440	34.70610	46.48380
C	30.97780	35.91350	46.08710
O	30.92150	33.76950	47.10850
H	33.47650	32.73450	46.68930
H	31.73930	33.67550	44.58230
H	32.59580	35.01150	47.20680
H	31.46110	33.12270	47.61710
H	30.51060	36.34120	46.98420
H	30.18470	35.60560	45.39140
H	31.58650	36.68560	45.60010
N	34.61300	35.31200	44.78500
H	35.04990	34.71050	45.47600
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.55950	28.82260	45.59940

C	27.54530	30.04720	46.51850	H	26.53140	25.40010	43.50630
O	27.16710	31.15330	46.03820	H	21.65590	36.76430	50.95370
O	27.91050	29.89850	47.73550	H	24.88880	36.27940	54.47230
H	25.47140	28.03420	46.84840				
H	25.88560	29.38260	44.30520				
H	27.89240	27.94440	46.17020	Step 8 of the relaxed surface scan for			
H	28.30710	29.02000	44.81570	proton transfer from complex 2 to			
N	26.43600	26.10900	44.22600	complex 3 with explicit waters.			
H	26.14890	25.82150	45.15580	C	35.07600	29.61800	50.32400
C	22.02800	35.96100	51.62100	O	35.29000	29.74100	49.12000
O	21.52500	35.67200	52.73400	N	33.82600	29.84000	50.82400
N	23.04900	35.23800	51.14800	C	32.80700	30.46300	50.04700
C	23.74700	34.28100	52.02300	C	33.11400	31.92700	49.53200
C	24.10700	34.76800	53.38500	O	32.91300	32.28500	48.36700
O	23.80400	34.05500	54.34000	C	31.44630	30.42250	50.77310
C	25.03070	33.79180	51.30370	C	30.28660	30.74870	49.83030
C	24.78750	33.01940	49.99970	O	29.76610	31.87730	49.84280
C	26.07280	32.50730	49.32670	O	29.94180	29.75260	49.06380
C	26.92460	33.61490	48.70140	H	33.70500	29.79380	51.83460
N	28.05890	33.01010	47.93370	H	32.71000	29.90360	49.10350
H	23.49520	35.52160	50.27770	H	31.30110	29.40280	51.15680
H	23.07760	33.42740	52.19960	H	31.43020	31.13190	51.61170
H	25.67900	34.66660	51.12290	H	29.02120	29.88080	48.43170
H	25.57530	33.14490	52.00930	N	33.63800	32.82200	50.35700
H	24.14040	32.15630	50.22120	H	33.87680	32.60990	51.32100
H	24.23240	33.63630	49.27360	C	33.90300	32.02700	44.81800
H	26.67810	31.93510	50.04920	O	33.71700	32.08700	43.59100
H	25.79540	31.80290	48.52720	N	33.39200	32.93300	45.68900
H	26.32130	34.19310	47.98960	C	32.51000	34.06700	45.26000
H	27.35370	34.28840	49.45490	C	33.32800	35.05900	44.40200
H	28.71080	32.49110	48.57920	O	32.77200	35.51900	43.37500
H	28.62710	33.69580	47.41330	C	31.81420	34.70790	46.48090
H	27.68600	32.31550	47.22880	C	30.99580	35.92720	46.08430
N	24.74100	35.92700	53.53200	O	30.90690	33.77310	47.09590
H	24.85700	36.57410	52.75890	H	33.47940	32.73520	46.68890
O	25.28010	33.46610	45.90150	H	31.73970	33.67580	44.58180
H	25.46640	32.51040	45.97130	H	32.59070	34.99910	47.21430
H	26.08230	33.79010	45.43450	H	31.44360	33.11620	47.59450
O	27.98320	33.60310	44.95460	H	30.49900	36.33600	46.97430
H	28.41790	33.79670	44.10690	H	30.23200	35.64780	45.34520
H	27.88930	32.62550	44.98380	H	31.62840	36.70730	45.64240
H	35.81610	29.27080	51.07350	N	34.61300	35.31200	44.78500
H	33.84500	33.75050	50.00240	H	35.05070	34.70680	45.47240
H	34.49800	31.23060	45.31330	C	23.94400	27.94100	45.50200
H	35.20980	35.82800	44.14570	O	23.57900	28.09500	44.33100
H	23.26620	27.63360	46.32750	N	25.20400	28.15800	45.87400

C	26.22300	28.52000	44.89200	H	33.84570	33.75030	50.00210
C	26.47000	27.38700	43.85800	H	34.49810	31.23070	45.31360
O	26.67800	27.71100	42.68900	H	35.20980	35.82440	44.14270
C	27.57670	28.78420	45.58550	H	23.26660	27.63410	46.32770
C	27.63930	29.98830	46.52280	H	26.53910	25.40010	43.50740
O	27.39480	31.13710	46.04720	H	21.65590	36.76450	50.95380
O	27.94900	29.78130	47.74530	H	24.88870	36.27950	54.47230
H	25.46970	28.04140	46.84970				
H	25.89420	29.38820	44.30800				
H	27.89220	27.88820	46.13730				
H	28.31510	28.96830	44.78960				
N	26.43600	26.10900	44.22600				
H	26.15530	25.82010	45.15730	C	35.07600	29.61800	50.32400
C	22.02800	35.96100	51.62100	O	35.29000	29.74100	49.12000
O	21.52500	35.67200	52.73400	N	33.82600	29.84000	50.82400
N	23.04900	35.23800	51.14800	C	32.80700	30.46300	50.04700
C	23.74700	34.28100	52.02300	C	33.11400	31.92700	49.53200
C	24.10700	34.76800	53.38500	O	32.91300	32.28500	48.36700
O	23.80400	34.05500	54.34000	C	31.44790	30.42320	50.77660
C	25.02910	33.78830	51.29860	C	30.28710	30.74870	49.83730
C	24.78430	33.00820	49.99680	O	29.76740	31.87580	49.84230
C	26.07130	32.49610	49.32060	O	29.93920	29.74560	49.07650
C	26.87690	33.59260	48.61920	H	33.70500	29.79370	51.83460
N	28.09520	33.00690	47.96940	H	32.70840	29.90320	49.10400
H	23.49720	35.52370	50.27950	H	31.30350	29.40420	51.16240
H	23.07690	33.42820	52.20010	H	31.43350	31.13450	51.61360
H	25.67670	34.66280	51.11350	H	29.03570	29.88090	48.45090
H	25.57580	33.14430	52.00490	N	33.63800	32.82200	50.35700
H	24.14420	32.14230	50.22660	H	33.87740	32.61000	51.32090
H	24.21930	33.61590	49.27100	C	33.90300	32.02700	44.81800
H	26.70940	31.98990	50.06390	O	33.71700	32.08700	43.59100
H	25.80150	31.73920	48.56900	N	33.39200	32.93300	45.68900
H	26.27470	34.05830	47.82730	C	32.51000	34.06700	45.26000
H	27.21720	34.36640	49.32020	C	33.32800	35.05900	44.40200
H	28.68820	32.49020	48.67590	O	32.77200	35.51900	43.37500
H	28.71680	33.70910	47.53930	C	31.81370	34.70790	46.48060
H	27.81890	32.31120	47.21880	C	30.99600	35.92740	46.08380
N	24.74100	35.92700	53.53200	O	30.90560	33.77300	47.09450
H	24.85720	36.57410	52.75890	H	33.47930	32.73510	46.68880
O	25.02000	32.63400	45.94200	H	31.73980	33.67580	44.58160
H	25.76960	31.99930	45.93210	H	32.58970	34.99860	47.21470
H	25.03510	33.00850	45.04380	H	31.44200	33.11600	47.59310
O	27.76100	32.56500	43.56800	H	30.49830	36.33590	46.97350
H	27.92770	31.98460	42.80640	H	30.23290	35.64860	45.34370
H	27.70670	31.95490	44.33640	H	31.62900	36.70780	45.64300
H	35.81620	29.27080	51.07350	N	34.61300	35.31200	44.78500

Step 7 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

H	35.05070	34.70680	45.47240
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.57640	28.78790	45.58390
C	27.63400	29.99090	46.52370
O	27.38970	31.14060	46.04510
O	27.93980	29.78550	47.74500
H	25.46970	28.04290	46.84990
H	25.89280	29.38740	44.30750
H	27.89540	27.89250	46.13470
H	28.31270	28.97540	44.78700
N	26.43600	26.10900	44.22600
H	26.15540	25.82030	45.15740
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.02830	33.78770	51.29780
C	24.78150	33.00680	49.99670
C	26.06700	32.49430	49.31810
C	26.87130	33.59030	48.61470
N	28.08880	33.00440	47.96320
H	23.49720	35.52370	50.27950
H	23.07660	33.42840	52.20040
H	25.67600	34.66190	51.11150
H	25.57560	33.14370	52.00380
H	24.14180	32.14110	50.22820
H	24.21500	33.61410	49.27160
H	26.70640	31.98810	50.06030
H	25.79580	31.73700	48.56730
H	26.26810	34.05510	47.82300
H	27.21230	34.36480	49.31460
H	28.68060	32.48790	48.66830
H	28.71060	33.70700	47.53400
H	27.81180	32.30790	47.21120
N	24.74100	35.92700	53.53200
H	24.85720	36.57410	52.75890
O	25.02000	32.63400	45.94200
H	25.76990	31.99910	45.93170
H	25.03320	33.00690	45.04320

O	27.76100	32.56500	43.56800
H	27.91950	31.98260	42.80610
H	27.70320	31.95560	44.33700
H	35.81630	29.27120	51.07360
H	33.84560	33.75030	50.00200
H	34.49810	31.23070	45.31360
H	35.20980	35.82430	44.14270
H	23.26660	27.63420	46.32770
H	26.53870	25.40000	43.50740
H	21.65600	36.76450	50.95380
H	24.88850	36.27960	54.47230

Step 6 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.43970	30.39980	50.75880
C	30.29650	30.72550	49.79920
O	29.87170	31.88560	49.69620
O	29.86170	29.68530	49.13440
H	33.70490	29.79300	51.83460
H	32.72330	29.90640	49.09990
H	31.30430	29.37710	51.13590
H	31.40450	31.10670	51.59940
H	28.99800	29.86110	48.48470
N	33.63800	32.82200	50.35700
H	33.87520	32.61060	51.32160
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.81270	34.70490	46.48330
C	30.97570	35.91190	46.08630
O	30.91960	33.76690	47.10580
H	33.47700	32.73480	46.68920
H	31.74000	33.67520	44.58180
H	32.59280	35.01020	47.20770
H	31.45900	33.12050	47.61500

H	30.50720	36.33890	46.98300
H	30.18360	35.60370	45.38950
H	31.58440	36.68460	45.60030
N	34.61300	35.31200	44.78500
H	35.04970	34.71070	45.47630
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.55860	28.82650	45.59800
C	27.53680	30.04970	46.51960
O	27.15910	31.15640	46.03460
O	27.89530	29.90120	47.73590
H	25.47140	28.03550	46.84860
H	25.88420	29.38170	44.30460
H	27.89540	27.94900	46.16770
H	28.30420	29.02820	44.81370
N	26.43600	26.10900	44.22600
H	26.14890	25.82170	45.15590
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.03040	33.79120	51.30380
C	24.78600	33.01620	50.00160
C	26.07090	32.50460	49.32730
C	26.91840	33.61200	48.69580
N	28.05110	33.00700	47.92580
H	23.49500	35.52120	50.27750
H	23.07750	33.42760	52.19980
H	25.67780	34.66610	51.12060
H	25.57600	33.14600	52.01020
H	24.14060	32.15250	50.22590
H	24.22860	33.63110	49.27580
H	26.67920	31.93640	50.05050
H	25.79380	31.79650	48.53120
H	26.31150	34.18620	47.98390
H	27.34850	34.28950	49.44520
H	28.70300	32.48840	48.56880
H	28.61840	33.69300	47.40480
H	27.67670	32.31140	47.22060
N	24.74100	35.92700	53.53200

H	24.85680	36.57420	52.75890
O	25.26980	33.45560	45.89820
H	25.46280	32.50100	45.96830
H	26.06920	33.78400	45.42950
O	27.97230	33.60030	44.94820
H	28.40680	33.79040	44.09970
H	27.87710	32.62250	44.98110
H	35.81600	29.27070	51.07350
H	33.84530	33.75040	50.00210
H	34.49800	31.23060	45.31330
H	35.20990	35.82780	44.14560
H	23.26620	27.63370	46.32760
H	26.53110	25.40000	43.50640
H	21.65590	36.76430	50.95360
H	24.88860	36.27950	54.47230

Step 5 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.45010	30.42220	50.78170
C	30.28660	30.74150	49.84560
O	29.78420	31.87500	49.82160
O	29.91630	29.72110	49.11540
H	33.70520	29.79420	51.83470
H	32.70760	29.90290	49.10420
H	31.31030	29.40450	51.17210
H	31.43730	31.13670	51.61600
H	29.03320	29.86720	48.49090
N	33.63800	32.82200	50.35700
H	33.87860	32.60980	51.32060
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.81290	34.70690	46.48060
C	30.99620	35.92730	46.08430
O	30.90370	33.77170	47.09230

H	33.47950	32.73560	46.68890
H	31.74000	33.67570	44.58140
H	32.58820	34.99650	47.21590
H	31.43870	33.11340	47.59060
H	30.49790	36.33520	46.97400
H	30.23360	35.64960	45.34330
H	31.63020	36.70770	45.64490
N	34.61300	35.31200	44.78500
H	35.05130	34.70540	45.47080
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.57520	28.78970	45.58500
C	27.62670	29.99630	46.52110
O	27.38110	31.14380	46.03410
O	27.92700	29.79980	47.74300
H	25.46960	28.04440	46.85010
H	25.89240	29.38720	44.30730
H	27.89340	27.89610	46.13940
H	28.31340	28.97530	44.78940
N	26.43600	26.10900	44.22600
H	26.15540	25.82050	45.15740
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.02840	33.78750	51.29780
C	24.78170	33.00560	49.99730
C	26.06720	32.49290	49.31850
C	26.86960	33.58860	48.61230
N	28.08280	33.00260	47.95290
H	23.49720	35.52360	50.27940
H	23.07660	33.42840	52.20030
H	25.67590	34.66180	51.11080
H	25.57590	33.14430	52.00430
H	24.14230	32.13990	50.22950
H	24.21490	33.61220	49.27200
H	26.70770	31.98860	50.06110
H	25.79620	31.73410	48.56930
H	26.26280	34.05430	47.82400
H	27.21490	34.36220	49.31100

H	28.67920	32.48450	48.65130
H	28.70200	33.70620	47.52190
H	27.80110	32.30700	47.20090
N	24.74100	35.92700	53.53200
H	24.85680	36.57420	52.75890
O	25.02000	32.63400	45.94200
H	25.76980	31.99850	45.92670
H	25.02980	33.00980	45.04440
O	27.76100	32.56500	43.56800
H	27.89030	31.98160	42.80140
H	27.69540	31.95370	44.33540
H	35.81610	29.27080	51.07350
H	33.84600	33.75010	50.00160
H	34.49810	31.23070	45.31360
H	35.20970	35.82390	44.14220
H	23.26650	27.63440	46.32770
H	26.53890	25.39990	43.50750
H	21.65590	36.76440	50.95380
H	24.88820	36.27970	54.47230

Step 4 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.44240	30.40280	50.76550
C	30.29700	30.72670	49.81070
O	29.87650	31.88470	49.69260
O	29.85240	29.67670	49.16060
H	33.70470	29.79270	51.83450
H	32.71990	29.90550	49.10080
H	31.30760	29.38190	51.14720
H	31.41140	31.11360	51.60290
H	29.00920	29.85850	48.51580
N	33.63800	32.82200	50.35700
H	33.87620	32.61070	51.32130
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200

O	32.77200	35.51900	43.37500	H	26.68150	31.93950	50.05230
C	31.81080	34.70350	46.48290	H	25.79380	31.78970	48.53580
C	30.97370	35.91020	46.08580	H	26.30050	34.17800	47.97610
O	30.91730	33.76360	47.10230	H	27.34330	34.29250	49.43280
H	33.47730	32.73490	46.68910	H	28.69510	32.48690	48.55780
H	31.74060	33.67490	44.58120	H	28.60970	33.69060	47.39510
H	32.58950	35.00820	47.20900	H	27.66750	32.30760	47.21180
H	31.45620	33.11770	47.61230	N	24.74100	35.92700	53.53200
H	30.50360	36.33620	46.98220	H	24.85670	36.57410	52.75880
H	30.18280	35.60230	45.38760	O	25.25940	33.44660	45.89610
H	31.58280	36.68370	45.60150	H	25.45870	32.49290	45.96530
N	34.61300	35.31200	44.78500	H	26.05630	33.77870	45.42600
H	35.04980	34.71060	45.47620	O	27.96210	33.59820	44.94260
C	23.94400	27.94100	45.50200	H	28.39660	33.78560	44.09350
O	23.57900	28.09500	44.33100	H	27.86520	32.62040	44.97800
N	25.20400	28.15800	45.87400	H	35.81610	29.27130	51.07370
C	26.22300	28.52000	44.89200	H	33.84510	33.75030	50.00180
C	26.47000	27.38700	43.85800	H	34.49810	31.23060	45.31330
O	26.67800	27.71100	42.68900	H	35.20990	35.82760	44.14550
C	27.55780	28.83160	45.59600	H	23.26610	27.63410	46.32760
C	27.52620	30.05310	46.52050	H	26.53070	25.39980	43.50640
O	27.15000	31.16000	46.02980	H	21.65590	36.76430	50.95360
O	27.87430	29.90490	47.73730	H	24.88850	36.27960	54.47230
H	25.47120	28.03830	46.84900				
H	25.88230	29.38060	44.30390				
H	27.89980	27.95530	46.16440				
H	28.30020	29.03900	44.81030				
N	26.43600	26.10900	44.22600				
H	26.14890	25.82200	45.15600	C	35.07600	29.61800	50.32400
C	22.02800	35.96100	51.62100	O	35.29000	29.74100	49.12000
O	21.52500	35.67200	52.73400	N	33.82600	29.84000	50.82400
N	23.04900	35.23800	51.14800	C	32.80700	30.46300	50.04700
C	23.74700	34.28100	52.02300	C	33.11400	31.92700	49.53200
C	24.10700	34.76800	53.38500	O	32.91300	32.28500	48.36700
O	23.80400	34.05500	54.34000	C	31.44600	30.40720	50.77360
C	25.03010	33.79080	51.30370	C	30.29860	30.72790	49.82290
C	24.78500	33.01300	50.00320	O	29.88030	31.88370	49.69170
C	26.06970	32.50250	49.32810	O	29.84880	29.66970	49.18500
C	26.91180	33.60970	48.68910	H	33.70500	29.79320	51.83460
N	28.04330	33.00460	47.91700	H	32.71590	29.90460	49.10190
H	23.49500	35.52110	50.27740	H	31.31180	29.38840	51.16110
H	23.07740	33.42770	52.19990	H	31.42030	31.12240	51.60730
H	25.67690	34.66580	51.11810	H	29.02150	29.85440	48.54490
H	25.57670	33.14720	52.01060	N	33.63800	32.82200	50.35700
H	24.14130	32.14870	50.23020	H	33.87670	32.61090	51.32130
H	24.22530	33.62570	49.27720	C	33.90300	32.02700	44.81800

Step 3 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

O	33.71700	32.08700	43.59100	H	25.67660	34.66550	51.11710
N	33.39200	32.93300	45.68900	H	25.57700	33.14780	52.01110
C	32.51000	34.06700	45.26000	H	24.14210	32.14670	50.23210
C	33.32800	35.05900	44.40200	H	24.22400	33.62290	49.27780
O	32.77200	35.51900	43.37500	H	26.68380	31.94300	50.05480
C	31.80930	34.70210	46.48260	H	25.79570	31.78620	48.53950
C	30.97200	35.90880	46.08570	H	26.29480	34.17310	47.97120
O	30.91560	33.76060	47.09950	H	27.34190	34.29670	49.42390
H	33.47750	32.73490	46.68910	H	28.69020	32.48440	48.55160
H	31.74100	33.67470	44.58080	H	28.60540	33.68740	47.38950
H	32.58670	35.00640	47.21020	H	27.66120	32.30500	47.20670
H	31.45430	33.11530	47.61020	N	24.74100	35.92700	53.53200
H	30.50060	36.33370	46.98190	H	24.85670	36.57410	52.75880
H	30.18210	35.60110	45.38620	O	25.25410	33.44310	45.89480
H	31.58130	36.68300	45.60270	H	25.45620	32.48960	45.96260
N	34.61300	35.31200	44.78500	H	26.05010	33.77730	45.42490
H	35.04980	34.71060	45.47620	O	27.95670	33.59880	44.94150
C	23.94400	27.94100	45.50200	H	28.39180	33.78550	44.09270
O	23.57900	28.09500	44.33100	H	27.85790	32.62080	44.97710
N	25.20400	28.15800	45.87400	H	35.81610	29.27120	51.07360
C	26.22300	28.52000	44.89200	H	33.84470	33.75040	50.00170
C	26.47000	27.38700	43.85800	H	34.49810	31.23060	45.31330
O	26.67800	27.71100	42.68900	H	35.21000	35.82740	44.14540
C	27.55670	28.83580	45.59410	H	23.26600	27.63450	46.32770
C	27.51590	30.05590	46.52030	H	26.53060	25.39980	43.50650
O	27.14220	31.16360	46.02570	H	21.65580	36.76420	50.95360
O	27.85340	29.90620	47.73780	H	24.88850	36.27950	54.47230
H	25.47100	28.04030	46.84930				
H	25.88040	29.37940	44.30320				
H	27.90250	27.96070	46.16220				
H	28.29750	29.04700	44.80810				
N	26.43600	26.10900	44.22600				
H	26.14880	25.82220	45.15600	C	35.07600	29.61800	50.32400
C	22.02800	35.96100	51.62100	O	35.29000	29.74100	49.12000
O	21.52500	35.67200	52.73400	N	33.82600	29.84000	50.82400
N	23.04900	35.23800	51.14800	C	32.80700	30.46300	50.04700
C	23.74700	34.28100	52.02300	C	33.11400	31.92700	49.53200
C	24.10700	34.76800	53.38500	O	32.91300	32.28500	48.36700
O	23.80400	34.05500	54.34000	C	31.45110	30.41320	50.78390
C	25.03000	33.79070	51.30370	C	30.30130	30.72800	49.83640
C	24.78460	33.01160	50.00430	O	29.88670	31.88220	49.68960
C	26.06990	32.50230	49.32940	O	29.84650	29.66130	49.21280
C	26.90840	33.60880	48.68550	H	33.70580	29.79500	51.83480
N	28.03880	33.00210	47.91210	H	32.71120	29.90330	49.10330
H	23.49470	35.52050	50.27700	H	31.31790	29.39730	51.17910
H	23.07740	33.42770	52.20000	H	31.43220	31.13400	51.61270

Step 2 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

H	29.03400	29.84600	48.57590	C	26.91080	33.61100	48.67940
N	33.63800	32.82200	50.35700	N	28.03860	32.99890	47.90680
H	33.87650	32.61120	51.32140	H	23.49450	35.52030	50.27690
C	33.90300	32.02700	44.81800	H	23.07880	33.42650	52.19910
O	33.71700	32.08700	43.59100	H	25.67660	34.67090	51.11930
N	33.39200	32.93300	45.68900	H	25.57990	33.15310	52.01350
C	32.51000	34.06700	45.26000	H	24.14990	32.14780	50.23390
C	33.32800	35.05900	44.40200	H	24.22860	33.62330	49.27850
O	32.77200	35.51900	43.37500	H	26.69410	31.95410	50.06160
C	31.80710	34.70010	46.48200	H	25.80440	31.78610	48.54900
C	30.96840	35.90590	46.08580	H	26.29590	34.16960	47.96140
O	30.91380	33.75580	47.09540	H	27.35070	34.30830	49.40220
H	33.47760	32.73490	46.68900	H	28.68950	32.48150	48.54540
H	31.74160	33.67440	44.58020	H	28.60590	33.68240	47.38300
H	32.58280	35.00390	47.21150	H	27.65790	32.30120	47.20320
H	31.45260	33.11140	47.60740	N	24.74100	35.92700	53.53200
H	30.49450	36.32840	46.98190	H	24.85650	36.57420	52.75890
H	30.18020	35.59800	45.38450	O	25.25470	33.43890	45.89710
H	31.57720	36.68190	45.60500	H	25.45790	32.48560	45.96370
N	34.61300	35.31200	44.78500	H	26.05000	33.77440	45.42650
H	35.04960	34.71100	45.47670	O	27.95450	33.59640	44.94340
C	23.94400	27.94100	45.50200	H	28.39040	33.78240	44.09480
O	23.57900	28.09500	44.33100	H	27.85300	32.61840	44.97840
N	25.20400	28.15800	45.87400	H	35.81600	29.27050	51.07340
C	26.22300	28.52000	44.89200	H	33.84470	33.75030	50.00160
C	26.47000	27.38700	43.85800	H	34.49810	31.23060	45.31330
O	26.67800	27.71100	42.68900	H	35.21010	35.82680	44.14500
C	27.55530	28.83780	45.59270	H	23.26590	27.63460	46.32770
C	27.50650	30.05620	46.52010	H	26.53080	25.39970	43.50660
O	27.13540	31.16510	46.02320	H	21.65600	36.76430	50.95370
O	27.83370	29.90280	47.73890	H	24.88900	36.27930	54.47230
H	25.47100	28.04130	46.84950				
H	25.87890	29.37840	44.30260				
H	27.90340	27.96360	46.16070				
H	28.29650	29.05190	44.80770				
N	26.43600	26.10900	44.22600				
H	26.14850	25.82230	45.15590	C	35.07600	29.61800	50.32400
C	22.02800	35.96100	51.62100	O	35.29000	29.74100	49.12000
O	21.52500	35.67200	52.73400	N	33.82600	29.84000	50.82400
N	23.04900	35.23800	51.14800	C	32.80700	30.46300	50.04700
C	23.74700	34.28100	52.02300	C	33.11400	31.92700	49.53200
C	24.10700	34.76800	53.38500	O	32.91300	32.28500	48.36700
O	23.80400	34.05500	54.34000	C	31.46520	30.44600	50.81140
C	25.03200	33.79430	51.30520	C	30.30320	30.77930	49.88810
C	24.79030	33.01450	50.00620	O	29.83990	31.92040	49.80990
C	26.07730	32.50780	49.33440	O	29.89280	29.73020	49.20430

Step 1 of the relaxed surface scan for proton transfer from complex 2 to complex 3 with explicit waters.

H	33.70130	29.78520	51.83350	O	23.80400	34.05500	54.34000
H	32.69010	29.89950	49.10890	C	25.02530	33.78520	51.30000
H	31.31480	29.43490	51.21390	C	24.77110	32.99730	50.00600
H	31.47960	31.16990	51.63690	C	26.05390	32.49060	49.32320
H	29.07560	29.90700	48.58700	C	26.86270	33.59660	48.64210
N	33.63800	32.82200	50.35700	N	28.04570	33.00550	47.93920
H	33.87760	32.61110	51.32110	H	23.49930	35.52670	50.28140
C	33.90300	32.02700	44.81800	H	23.07480	33.43000	52.20170
O	33.71700	32.08700	43.59100	H	25.67210	34.65830	51.10480
N	33.39200	32.93300	45.68900	H	25.57560	33.14600	52.00830
C	32.51000	34.06700	45.26000	H	24.13490	32.13100	50.24630
C	33.32800	35.05900	44.40200	H	24.19900	33.60210	49.28280
O	32.77200	35.51900	43.37500	H	26.68810	31.96440	50.05650
C	31.81410	34.70660	46.48300	H	25.78450	31.74740	48.55730
C	30.97520	35.91190	46.08670	H	26.24930	34.09640	47.88000
O	30.92420	33.76720	47.10960	H	27.23870	34.33980	49.35870
H	33.47950	32.73590	46.68890	H	28.69360	32.54880	48.62340
H	31.73960	33.67520	44.58220	H	28.59900	33.68990	47.40160
H	32.59560	35.01420	47.20510	H	27.72750	32.25620	47.25070
H	31.47100	33.12320	47.61350	N	24.74100	35.92700	53.53200
H	30.50950	36.34010	46.98420	H	24.85730	36.57380	52.75870
H	30.18090	35.60260	45.39320	O	25.29280	33.34540	45.78310
H	31.58220	36.68400	45.59760	H	25.57750	32.41520	45.87750
N	34.61300	35.31200	44.78500	H	26.07320	33.73950	45.33680
H	35.05030	34.71020	45.47560	O	28.04520	33.57770	44.95180
C	23.94400	27.94100	45.50200	H	28.52250	33.73430	44.11940
O	23.57900	28.09500	44.33100	H	27.95100	32.60120	45.01960
N	25.20400	28.15800	45.87400	H	35.81640	29.27160	51.07350
C	26.22300	28.52000	44.89200	H	33.84010	33.75180	50.00270
C	26.47000	27.38700	43.85800	H	34.49840	31.23080	45.31320
O	26.67800	27.71100	42.68900	H	35.20970	35.82790	44.14550
C	27.55890	28.82400	45.58890	H	23.26590	27.63480	46.32780
C	27.52750	30.01760	46.54900	H	26.53380	25.39970	43.50700
O	27.22500	31.15750	46.06930	H	21.65580	36.76420	50.95360
O	27.81280	29.80950	47.76840	H	24.88740	36.28030	54.47220
H	25.47270	28.03770	46.84870				
H	25.88040	29.37980	44.30350				
H	27.90700	27.93550	46.13420				
H	28.29390	29.05310	44.80240				
N	26.43600	26.10900	44.22600				
H	26.15000	25.82190	45.15630	C	35.07600	29.61800	50.32400
C	22.02800	35.96100	51.62100	O	35.29000	29.74100	49.12000
O	21.52500	35.67200	52.73400	N	33.82600	29.84000	50.82400
N	23.04900	35.23800	51.14800	C	32.80700	30.46300	50.04700
C	23.74700	34.28100	52.02300	C	33.11400	31.92700	49.53200
C	24.10700	34.76800	53.38500	O	32.91300	32.28500	48.36700

Step 8 of the relaxed surface scan for proton transfer from complex 2 to complex 3 without explicit waters.

C	31.48460	30.49620	50.83720	O	21.52500	35.67200	52.73400
C	30.29740	30.92260	49.96630	N	23.04900	35.23800	51.14800
O	29.62900	31.93650	50.29930	C	23.74700	34.28100	52.02300
O	30.08810	30.18350	48.94610	C	24.10700	34.76800	53.38500
H	33.70050	29.78780	51.83340	O	23.80400	34.05500	54.34000
H	32.65410	29.89670	49.11750	C	25.03350	33.79120	51.31040
H	31.27670	29.47630	51.19610	C	24.80670	33.03090	49.99570
H	31.56560	31.16760	51.70370	C	26.10370	32.48740	49.36850
H	28.90100	29.92610	48.34590	C	27.00220	33.56570	48.75400
N	33.63800	32.82200	50.35700	N	28.24930	32.93580	48.22000
H	33.86840	32.61160	51.32340	H	23.50160	35.53050	50.28410
C	33.90300	32.02700	44.81800	H	23.07720	33.42780	52.19920
O	33.71700	32.08700	43.59100	H	25.68960	34.66330	51.14690
N	33.39200	32.93300	45.68900	H	25.56540	33.13430	52.01630
C	32.51000	34.06700	45.26000	H	24.13270	32.18290	50.19330
C	33.32800	35.05900	44.40200	H	24.28720	33.66570	49.25820
O	32.77200	35.51900	43.37500	H	26.67810	31.93390	50.12980
C	31.82690	34.71310	46.48660	H	25.84780	31.76350	48.57890
C	30.99620	35.92500	46.09410	H	26.49050	34.08010	47.92870
O	30.93810	33.77580	47.12450	H	27.30390	34.31710	49.49610
H	33.47400	32.72980	46.68860	H	28.78410	32.47870	49.03570
H	31.73620	33.67750	44.58500	H	28.90070	33.59700	47.76570
H	32.61330	35.01500	47.20490	H	28.00870	32.18620	47.51150
H	31.49240	33.12900	47.62100	N	24.74100	35.92700	53.53200
H	30.51240	36.33940	46.98880	H	24.86230	36.57340	52.75920
H	30.22120	35.63610	45.37020	H	35.81770	29.27180	51.07290
H	31.61760	36.70400	45.63480	H	33.83590	33.75370	50.00580
N	34.61300	35.31200	44.78500	H	34.49680	31.23010	45.31380
H	35.05070	34.70560	45.47150	H	35.20980	35.82470	44.14290
C	23.94400	27.94100	45.50200	H	23.26690	27.63170	46.32740
O	23.57900	28.09500	44.33100	H	26.55280	25.40060	43.50910
N	25.20400	28.15800	45.87400	H	21.65660	36.76530	50.95430
C	26.22300	28.52000	44.89200	H	24.89450	36.27670	54.47240
C	26.47000	27.38700	43.85800				
O	26.67800	27.71100	42.68900				
C	27.58940	28.71530	45.57010				
C	27.74460	29.80340	46.62220				
O	27.56830	31.00260	46.35800				
O	28.14340	29.32980	47.77990	C	35.07600	29.61800	50.32400
H	25.47230	28.02430	46.84680	O	35.29000	29.74100	49.12000
H	25.90710	29.39840	44.31830	N	33.82600	29.84000	50.82400
H	27.90990	27.76440	46.01610	C	32.80700	30.46300	50.04700
H	28.30890	28.96620	44.77500	C	33.11400	31.92700	49.53200
N	26.43600	26.10900	44.22600	O	32.91300	32.28500	48.36700
H	26.16100	25.81720	45.15800	C	31.43500	30.40890	50.74680
C	22.02800	35.96100	51.62100	C	30.28820	30.72500	49.77380

Step 7 of the relaxed surface scan for proton transfer from complex 2 to complex 3 without explicit waters.

O	29.75220	31.85530	49.82280	C	23.74700	34.28100	52.02300
O	29.97610	29.76540	48.97060	C	24.10700	34.76800	53.38500
H	33.70370	29.79140	51.83430	O	23.80400	34.05500	54.34000
H	32.72220	29.90620	49.10040	C	25.02890	33.78780	51.30290
H	31.29180	29.38590	51.12320	C	24.78240	33.01640	49.99820
H	31.39660	31.11360	51.58880	C	26.06390	32.48660	49.32980
H	28.92560	29.86080	48.31450	C	26.93990	33.57880	48.70860
N	33.63800	32.82200	50.35700	N	28.09690	32.95900	47.99030
H	33.87330	32.60950	51.32180	H	23.50200	35.53080	50.28440
C	33.90300	32.02700	44.81800	H	23.07610	33.42880	52.20020
O	33.71700	32.08700	43.59100	H	25.68060	34.66030	51.12300
N	33.39200	32.93300	45.68900	H	25.57100	33.13820	52.00760
C	32.51000	34.06700	45.26000	H	24.12570	32.16020	50.21840
C	33.32800	35.05900	44.40200	H	24.23240	33.63980	49.27310
O	32.77200	35.51900	43.37500	H	26.66110	31.91590	50.05960
C	31.82200	34.70880	46.48550	H	25.78630	31.77750	48.53500
C	31.01650	35.93940	46.09760	H	26.36710	34.17210	47.98170
O	30.90790	33.78030	47.09860	H	27.34640	34.26070	49.46750
H	33.47360	32.73190	46.68920	H	28.69750	32.40610	48.67710
H	31.73740	33.67780	44.58330	H	28.73050	33.64430	47.55090
H	32.60340	34.98890	47.21790	H	27.74760	32.29280	47.24020
H	31.43810	33.11750	47.59740	N	24.74100	35.92700	53.53200
H	30.52110	36.34520	46.98980	H	24.86020	36.57370	52.75910
H	30.25230	35.67510	45.35320	H	35.81620	29.26970	51.07310
H	31.65800	36.71710	45.66440	H	33.84530	33.75070	50.00320
N	34.61300	35.31200	44.78500	H	34.49740	31.23040	45.31360
H	35.05060	34.70590	45.47180	H	35.21010	35.82380	44.14260
C	23.94400	27.94100	45.50200	H	23.26630	27.63290	46.32740
O	23.57900	28.09500	44.33100	H	26.54020	25.39960	43.50810
N	25.20400	28.15800	45.87400	H	21.65650	36.76520	50.95430
C	26.22300	28.52000	44.89200	H	24.89210	36.27790	54.47240
C	26.47000	27.38700	43.85800				
O	26.67800	27.71100	42.68900				
C	27.56090	28.81000	45.60630				
C	27.55000	30.01740	46.54830				
O	27.21040	31.13340	46.11170				
O	27.88160	29.80270	47.79390	C	35.07600	29.61800	50.32400
H	25.47200	28.03040	46.84780	O	35.29000	29.74100	49.12000
H	25.88960	29.38570	44.30780	N	33.82600	29.84000	50.82400
H	27.89090	27.92030	46.16040	C	32.80700	30.46300	50.04700
H	28.31020	29.02130	44.82820	C	33.11400	31.92700	49.53200
N	26.43600	26.10900	44.22600	O	32.91300	32.28500	48.36700
H	26.16160	25.82020	45.15910	C	31.43370	30.40030	50.74340
C	22.02800	35.96100	51.62100	C	30.28880	30.71410	49.77260
O	21.52500	35.67200	52.73400	O	29.75750	31.84220	49.79650
N	23.04900	35.23800	51.14800	O	29.96900	29.73510	48.98410

Step 6 of the relaxed surface scan for proton transfer from complex 2 to complex 3 without explicit waters.

H	33.70490	29.79290	51.83460	O	23.80400	34.05500	54.34000
H	32.72630	29.90710	49.09920	C	25.02570	33.78380	51.30000
H	31.29640	29.37610	51.11800	C	24.76990	33.00920	49.99860
H	31.38680	31.10480	51.58520	C	26.04500	32.47700	49.32010
H	28.98250	29.85250	48.34640	C	26.91580	33.56840	48.69060
N	33.63800	32.82200	50.35700	N	28.06620	32.94950	47.96090
H	33.87540	32.60930	51.32120	H	23.50140	35.53020	50.28390
C	33.90300	32.02700	44.81800	H	23.07480	33.43000	52.20150
O	33.71700	32.08700	43.59100	H	25.67810	34.65460	51.11490
N	33.39200	32.93300	45.68900	H	25.56940	33.13470	52.00390
C	32.51000	34.06700	45.26000	H	24.11440	32.15400	50.22620
C	33.32800	35.05900	44.40200	H	24.21450	33.63100	49.27630
O	32.77200	35.51900	43.37500	H	26.64780	31.90610	50.04510
C	31.81810	34.70610	46.48420	H	25.76070	31.76760	48.52790
C	31.01480	35.93830	46.09650	H	26.33680	34.16100	47.96810
O	30.90060	33.77550	47.08960	H	27.32840	34.25110	49.44560
H	33.47390	32.73230	46.68920	H	28.66730	32.39590	48.63710
H	31.73870	33.67730	44.58210	H	28.69740	33.63730	47.52270
H	32.59610	34.98360	47.22110	H	27.71030	32.28030	47.20840
H	31.42840	33.11250	47.58970	N	24.74100	35.92700	53.53200
H	30.51530	36.34120	46.98770	H	24.85990	36.57370	52.75900
H	30.25410	35.67670	45.34750	H	35.81600	29.27010	51.07340
H	31.65880	36.71720	45.66910	H	33.84720	33.75000	50.00240
N	34.61300	35.31200	44.78500	H	34.49750	31.23040	45.31360
H	35.05060	34.70570	45.47160	H	35.21010	35.82370	44.14240
C	23.94400	27.94100	45.50200	H	23.26600	27.63330	46.32750
O	23.57900	28.09500	44.33100	H	26.53910	25.39930	43.50820
N	25.20400	28.15800	45.87400	H	21.65660	36.76520	50.95430
C	26.22300	28.52000	44.89200	H	24.89140	36.27830	54.47240
C	26.47000	27.38700	43.85800				
O	26.67800	27.71100	42.68900				
C	27.55910	28.81460	45.60780				
C	27.54220	30.02320	46.55250				
O	27.17200	31.13240	46.10840				
O	27.90270	29.82690	47.78340	C	35.07600	29.61800	50.32400
H	25.47190	28.03380	46.84820	O	35.29000	29.74100	49.12000
H	25.88930	29.38570	44.30810	N	33.82600	29.84000	50.82400
H	27.89220	27.92550	46.16160	C	32.80700	30.46300	50.04700
H	28.30760	29.02870	44.82960	C	33.11400	31.92700	49.53200
N	26.43600	26.10900	44.22600	O	32.91300	32.28500	48.36700
H	26.16150	25.82090	45.15930	C	31.43930	30.40570	50.75590
C	22.02800	35.96100	51.62100	C	30.28920	30.70260	49.79060
O	21.52500	35.67200	52.73400	O	29.76590	31.83070	49.77120
N	23.04900	35.23800	51.14800	O	29.95540	29.69030	49.04240
C	23.74700	34.28100	52.02300	H	33.70460	29.79210	51.83450
C	24.10700	34.76800	53.38500	H	32.72120	29.90570	49.10070

Step 5 of the relaxed surface scan for proton transfer from complex 2 to complex 3 without explicit waters.

H	31.30730	29.38690	51.14630	C	24.76430	32.99960	50.00280
H	31.39810	31.12240	51.58760	C	26.03700	32.46800	49.31890
H	29.02700	29.83040	48.39890	C	26.89590	33.55850	48.67190
N	33.63800	32.82200	50.35700	N	28.04060	32.94050	47.93290
H	33.87730	32.60920	51.32080	H	23.50240	35.53130	50.28470
C	33.90300	32.02700	44.81800	H	23.07390	33.43080	52.20210
O	33.71700	32.08700	43.59100	H	25.67580	34.65150	51.10770
N	33.39200	32.93300	45.68900	H	25.57040	33.13610	52.00480
C	32.51000	34.06700	45.26000	H	24.11270	32.14370	50.23830
C	33.32800	35.05900	44.40200	H	24.20230	33.61640	49.28130
O	32.77200	35.51900	43.37500	H	26.64930	31.90740	50.04420
C	31.81590	34.70420	46.48380	H	25.75040	31.75010	48.53540
C	31.01430	35.93760	46.09670	H	26.30620	34.14110	47.94990
O	30.89640	33.77290	47.08550	H	27.31140	34.25070	49.41660
H	33.47510	32.73310	46.68920	H	28.63850	32.37810	48.59760
H	31.73950	33.67690	44.58140	H	28.67370	33.63090	47.50210
H	32.59250	34.97980	47.22290	H	27.67690	32.27140	47.17570
H	31.42260	33.10900	47.58560	N	24.74100	35.92700	53.53200
H	30.51240	36.33860	46.98740	H	24.85930	36.57370	52.75900
H	30.25570	35.67840	45.34480	H	35.81610	29.27020	51.07340
H	31.66010	36.71720	45.67310	H	33.84890	33.74930	50.00150
N	34.61300	35.31200	44.78500	H	34.49750	31.23030	45.31350
H	35.05070	34.70540	45.47130	H	35.21020	35.82320	44.14220
C	23.94400	27.94100	45.50200	H	23.26590	27.63350	46.32750
O	23.57900	28.09500	44.33100	H	26.53800	25.39920	43.50820
N	25.20400	28.15800	45.87400	H	21.65650	36.76510	50.95430
C	26.22300	28.52000	44.89200	H	24.89060	36.27880	54.47230
C	26.47000	27.38700	43.85800				
O	26.67800	27.71100	42.68900				
C	27.55550	28.82140	45.60730				
C	27.53320	30.03350	46.54840				
O	27.12820	31.13510	46.10280				
O	27.93080	29.85740	47.76210	C	35.07600	29.61800	50.32400
H	25.47140	28.03610	46.84850	O	35.29000	29.74100	49.12000
H	25.88690	29.38410	44.30710	N	33.82600	29.84000	50.82400
H	27.89240	27.93570	46.16460	C	32.80700	30.46300	50.04700
H	28.30540	29.03570	44.83040	C	33.11400	31.92700	49.53200
N	26.43600	26.10900	44.22600	O	32.91300	32.28500	48.36700
H	26.16060	25.82140	45.15920	C	31.44240	30.40850	50.76290
C	22.02800	35.96100	51.62100	C	30.28950	30.70150	49.80300
O	21.52500	35.67200	52.73400	O	29.76380	31.82540	49.77340
N	23.04900	35.23800	51.14800	O	29.95520	29.67820	49.06280
C	23.74700	34.28100	52.02300	H	33.70470	29.79220	51.83450
C	24.10700	34.76800	53.38500	H	32.71810	29.90500	49.10160
O	23.80400	34.05500	54.34000	H	31.31200	29.39140	51.15840
C	25.02430	33.78130	51.29920	H	31.40480	31.12900	51.59130

Step 4 of the relaxed surface scan for proton transfer from complex 2 to complex 3 without explicit waters.

H	29.05630	29.82300	48.43040
N	33.63800	32.82200	50.35700
H	33.87840	32.60920	51.32050
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.81500	34.70390	46.48330
C	31.01350	35.93730	46.09580
O	30.89520	33.77210	47.08380
H	33.47560	32.73330	46.68910
H	31.73990	33.67680	44.58110
H	32.59090	34.97950	47.22320
H	31.42140	33.10840	47.58390
H	30.51070	36.33790	46.98620
H	30.25560	35.67810	45.34320
H	31.65950	36.71710	45.67300
N	34.61300	35.31200	44.78500
H	35.05080	34.70530	45.47110
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.55410	28.82590	45.60630
C	27.52480	30.03630	46.55100
O	27.11710	31.13820	46.10130
O	27.92130	29.86120	47.76160
H	25.47130	28.03850	46.84890
H	25.88520	29.38310	44.30650
H	27.89540	27.94090	46.16210
H	28.30200	29.04510	44.82880
N	26.43600	26.10900	44.22600
H	26.16030	25.82180	45.15920
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.02260	33.77930	51.29780
C	24.75870	32.99530	50.00330
C	26.02880	32.46210	49.31600

C	26.88430	33.55150	48.66260
N	28.02890	32.93400	47.92360
H	23.50260	35.53150	50.28490
H	23.07320	33.43140	52.20270
H	25.67450	34.64850	51.10340
H	25.56970	33.13470	52.00340
H	24.10750	32.14000	50.24260
H	24.19430	33.61090	49.28270
H	26.64430	31.90390	50.04040
H	25.74030	31.74150	48.53570
H	26.29190	34.12970	47.93940
H	27.29910	34.24790	49.40390
H	28.62300	32.36940	48.58570
H	28.66360	33.62490	47.49660
H	27.66660	32.26290	47.16260
N	24.74100	35.92700	53.53200
H	24.85920	36.57370	52.75890
H	35.81610	29.27040	51.07340
H	33.84910	33.74910	50.00110
H	34.49750	31.23030	45.31350
H	35.21020	35.82310	44.14210
H	23.26570	27.63390	46.32750
H	26.53750	25.39910	43.50820
H	21.65640	36.76510	50.95420
H	24.89030	36.27900	54.47230

Step 3 of the relaxed surface scan for proton transfer from complex 2 to complex 3 without explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.44590	30.41170	50.77040
C	30.28980	30.70050	49.81620
O	29.76220	31.82090	49.77640
O	29.95420	29.66670	49.08480
H	33.70460	29.79200	51.83450
H	32.71470	29.90410	49.10250
H	31.31720	29.39660	51.17140
H	31.41240	31.13640	51.59520
H	29.07790	29.81520	48.46160
N	33.63800	32.82200	50.35700

H	33.87940	32.60920	51.32030	H	23.50270	35.53160	50.28500
C	33.90300	32.02700	44.81800	H	23.07280	33.43180	52.20300
O	33.71700	32.08700	43.59100	H	25.67400	34.64650	51.10100
N	33.39200	32.93300	45.68900	H	25.56870	33.13300	52.00140
C	32.51000	34.06700	45.26000	H	24.10280	32.13960	50.24320
C	33.32800	35.05900	44.40200	H	24.18920	33.61000	49.28270
O	32.77200	35.51900	43.37500	H	26.63940	31.90140	50.03570
C	31.81440	34.70390	46.48290	H	25.73170	31.73730	48.53380
C	31.01300	35.93720	46.09490	H	26.28300	34.12320	47.93120
O	30.89410	33.77220	47.08290	H	27.29180	34.24550	49.39430
H	33.47610	32.73350	46.68900	H	28.60960	32.36010	48.57520
H	31.74000	33.67660	44.58100	H	28.65810	33.62000	47.49350
H	32.58990	34.97960	47.22320	H	27.65760	32.25840	47.14990
H	31.42050	33.10850	47.58280	N	24.74100	35.92700	53.53200
H	30.50970	36.33790	46.98490	H	24.85900	36.57370	52.75890
H	30.25550	35.67780	45.34200	H	35.81610	29.27040	51.07340
H	31.65910	36.71700	45.67230	H	33.84920	33.74900	50.00090
N	34.61300	35.31200	44.78500	H	34.49760	31.23040	45.31350
H	35.05090	34.70520	45.47100	H	35.21020	35.82300	44.14200
C	23.94400	27.94100	45.50200	H	23.26560	27.63420	46.32760
O	23.57900	28.09500	44.33100	H	26.53680	25.39900	43.50820
N	25.20400	28.15800	45.87400	H	21.65650	36.76510	50.95430
C	26.22300	28.52000	44.89200	H	24.88990	36.27920	54.47230
C	26.47000	27.38700	43.85800				
O	26.67800	27.71100	42.68900				
C	27.55290	28.83050	45.60500				
C	27.51620	30.04020	46.55130				
O	27.11240	31.14340	46.09500				
O	27.90350	29.86550	47.76180				
H	25.47120	28.04070	46.84920	C	35.07600	29.61800	50.32400
H	25.88350	29.38210	44.30580	O	35.29000	29.74100	49.12000
H	27.89770	27.94680	46.16070	N	33.82600	29.84000	50.82400
H	28.29890	29.05320	44.82690	C	32.80700	30.46300	50.04700
N	26.43600	26.10900	44.22600	C	33.11400	31.92700	49.53200
H	26.16000	25.82210	45.15920	O	32.91300	32.28500	48.36700
C	22.02800	35.96100	51.62100	C	31.44980	30.41670	50.77910
O	21.52500	35.67200	52.73400	C	30.28980	30.70160	49.83140
N	23.04900	35.23800	51.14800	O	29.76000	31.81810	49.78250
C	23.74700	34.28100	52.02300	O	29.95150	29.65740	49.10890
C	24.10700	34.76800	53.38500	H	33.70460	29.79190	51.83440
O	23.80400	34.05500	54.34000	H	32.71020	29.90300	49.10380
C	25.02140	33.77800	51.29650	H	31.32180	29.40420	51.18690
C	24.75440	32.99400	50.00240	H	31.42170	31.14640	51.59940
C	26.02230	32.45900	49.31230	H	29.09340	29.80900	48.49320
C	26.87660	33.54700	48.65510	N	33.63800	32.82200	50.35700
N	28.02040	32.92880	47.91540	H	33.88030	32.60920	51.32000
				C	33.90300	32.02700	44.81800

Step 2 of the relaxed surface scan for proton transfer from complex 2 to complex 3 without explicit waters.

O	33.71700	32.08700	43.59100	H	25.67360	34.64420	51.09910
N	33.39200	32.93300	45.68900	H	25.56700	33.13000	51.99850
C	32.51000	34.06700	45.26000	H	24.09560	32.14100	50.24230
C	33.32800	35.05900	44.40200	H	24.18420	33.61140	49.28220
O	32.77200	35.51900	43.37500	H	26.63230	31.89780	50.02980
C	31.81410	34.70430	46.48270	H	25.72110	31.73420	48.53030
C	31.01260	35.93720	46.09400	H	26.27450	34.11780	47.92350
O	30.89380	33.77260	47.08260	H	27.28400	34.24220	49.38600
H	33.47670	32.73360	46.68900	H	28.59480	32.35000	48.56520
H	31.73970	33.67660	44.58140	H	28.65250	33.61520	47.49150
H	32.58940	34.98010	47.22320	H	27.64880	32.25510	47.13650
H	31.42020	33.10890	47.58220	N	24.74100	35.92700	53.53200
H	30.50910	36.33840	46.98360	H	24.85880	36.57360	52.75880
H	30.25540	35.67710	45.34110	H	35.81620	29.27070	51.07340
H	31.65860	36.71700	45.67120	H	33.84900	33.74900	50.00070
N	34.61300	35.31200	44.78500	H	34.49770	31.23040	45.31340
H	35.05100	34.70490	45.47070	H	35.21020	35.82300	44.14190
C	23.94400	27.94100	45.50200	H	23.26550	27.63460	46.32760
O	23.57900	28.09500	44.33100	H	26.53590	25.39890	43.50820
N	25.20400	28.15800	45.87400	H	21.65640	36.76510	50.95420
C	26.22300	28.52000	44.89200	H	24.88960	36.27940	54.47230
C	26.47000	27.38700	43.85800				
O	26.67800	27.71100	42.68900				
C	27.55180	28.83640	45.60300				
C	27.50600	30.04550	46.55050				
O	27.10820	31.14980	46.08590				
O	27.87970	29.87170	47.76270	C	35.07600	29.61800	50.32400
H	25.47110	28.04330	46.84960	O	35.29000	29.74100	49.12000
H	25.88130	29.38090	44.30510	N	33.82600	29.84000	50.82400
H	27.90150	27.95460	46.15890	C	32.80700	30.46300	50.04700
H	28.29470	29.06330	44.82330	C	33.11400	31.92700	49.53200
N	26.43600	26.10900	44.22600	O	32.91300	32.28500	48.36700
H	26.15950	25.82240	45.15920	C	31.45510	30.42310	50.78900
C	22.02800	35.96100	51.62100	C	30.29180	30.70380	49.84620
O	21.52500	35.67200	52.73400	O	29.76050	31.81790	49.78970
N	23.04900	35.23800	51.14800	O	29.95470	29.65170	49.13070
C	23.74700	34.28100	52.02300	H	33.70510	29.79300	51.83450
C	24.10700	34.76800	53.38500	H	32.70600	29.90200	49.10510
O	23.80400	34.05500	54.34000	H	31.32700	29.41340	51.20380
C	25.02000	33.77660	51.29490	H	31.43330	31.15650	51.60610
C	24.74920	32.99380	50.00070	H	29.11010	29.80360	48.52270
C	26.01430	32.45600	49.30750	N	33.63800	32.82200	50.35700
C	26.86840	33.54260	48.64790	H	33.88040	32.60920	51.32000
N	28.01140	32.92370	47.90780	C	33.90300	32.02700	44.81800
H	23.50250	35.53130	50.28480	O	33.71700	32.08700	43.59100
H	23.07230	33.43230	52.20360	N	33.39200	32.93300	45.68900

Step 1 of the relaxed surface scan for proton transfer from complex 2 to complex 3 without explicit waters.

C	32.51000	34.06700	45.26000	H	24.08940	32.14590	50.23840
C	33.32800	35.05900	44.40200	H	24.18420	33.61690	49.28000
O	32.77200	35.51900	43.37500	H	26.62640	31.89530	50.02610
C	31.81460	34.70490	46.48320	H	25.71410	31.73470	48.52680
C	31.01210	35.93680	46.09350	H	26.27320	34.11650	47.92040
O	30.89410	33.77280	47.08350	H	27.28190	34.23880	49.38370
H	33.47720	32.73370	46.68890	H	28.58760	32.34250	48.56140
H	31.73810	33.67730	44.58280	H	28.65170	33.61120	47.49220
H	32.58990	34.98030	47.22370	H	27.64530	32.25450	47.13010
H	31.42080	33.10900	47.58270	N	24.74100	35.92700	53.53200
H	30.50810	36.33890	46.98250	H	24.85880	36.57340	52.75860
H	30.25550	35.67450	45.34090	H	35.81620	29.27050	51.07330
H	31.65760	36.71680	45.67040	H	33.84920	33.74890	50.00060
N	34.61300	35.31200	44.78500	H	34.49780	31.23040	45.31340
H	35.05100	34.70450	45.47030	H	35.21010	35.82330	44.14210
C	23.94400	27.94100	45.50200	H	23.26530	27.63480	46.32760
O	23.57900	28.09500	44.33100	H	26.53540	25.39880	43.50820
N	25.20400	28.15800	45.87400	H	21.65640	36.76500	50.95420
C	26.22300	28.52000	44.89200	H	24.88930	36.27960	54.47220
C	26.47000	27.38700	43.85800	Optimized transition state for proton transfer from complex 2 to complex 3 without explicit waters.			
O	26.67800	27.71100	42.68900	C	35.07600	29.61800	50.32400
C	27.54980	28.84190	45.60150	O	35.29000	29.74100	49.12000
C	27.49540	30.05140	46.54790	N	33.82600	29.84000	50.82400
O	27.10520	31.15750	46.07750	C	32.80700	30.46300	50.04700
O	27.85650	29.87670	47.76240	C	33.11400	31.92700	49.53200
H	25.47090	28.04520	46.84990	O	32.91300	32.28500	48.36700
H	25.87900	29.37990	44.30480	C	31.47330	30.47550	50.81740
H	27.90260	27.96220	46.15860	C	30.28040	30.84350	49.93000
H	28.29210	29.07170	44.82210	O	29.55910	31.81980	50.23890
N	26.43600	26.10900	44.22600	O	30.11780	30.07280	48.91190
H	26.15890	25.82260	45.15910	H	33.70340	29.79240	51.83420
C	22.02800	35.96100	51.62100	H	32.67030	29.89860	49.11350
O	21.52500	35.67200	52.73400	H	31.29110	29.45780	51.19650
N	23.04900	35.23800	51.14800	H	31.51770	31.16710	51.67000
C	23.74700	34.28100	52.02300	H	29.00660	29.94880	48.35060
C	24.10700	34.76800	53.38500	N	33.63800	32.82200	50.35700
O	23.80400	34.05500	54.34000	H	33.87760	32.60880	51.32060
C	25.01930	33.77630	51.29390	C	33.90300	32.02700	44.81800
C	24.74640	32.99640	49.99820	O	33.71700	32.08700	43.59100
C	26.00970	32.45520	49.30410	N	33.39200	32.93300	45.68900
C	26.86610	33.54030	48.64480	C	32.51000	34.06700	45.26000
N	28.00840	32.91980	47.90510	C	33.32800	35.05900	44.40200
H	23.50230	35.53090	50.28460				
H	23.07210	33.43250	52.20390				
H	25.67410	34.64330	51.09970				
H	25.56520	33.12700	51.99600				

O	32.77200	35.51900	43.37500	H	26.66010	31.91260	50.11040
C	31.82030	34.70510	46.48620	H	25.81390	31.75130	48.56830
C	30.99450	35.92160	46.09860	H	26.45070	34.08090	47.93240
O	30.92460	33.76280	47.10850	H	27.30510	34.28500	49.48300
H	33.47900	32.73260	46.68860	H	28.73540	32.42340	48.93940
H	31.73840	33.67660	44.58290	H	28.85740	33.58390	47.72200
H	32.60140	34.99890	47.21350	H	27.93770	32.18710	47.42360
H	31.47510	33.09570	47.58030	N	24.74100	35.92700	53.53200
H	30.50330	36.32810	46.99290	H	24.86240	36.57300	52.75900
H	30.22600	35.64180	45.36450	H	35.81760	29.27260	51.07330
H	31.62210	36.70380	45.65320	H	33.84430	33.75100	50.00320
N	34.61300	35.31200	44.78500	H	34.49740	31.23050	45.31370
H	35.05120	34.70470	45.47030	H	35.20980	35.82340	44.14190
C	23.94400	27.94100	45.50200	H	23.26650	27.63220	46.32730
O	23.57900	28.09500	44.33100	H	26.55440	25.39990	43.51020
N	25.20400	28.15800	45.87400	H	21.65650	36.76520	50.95430
C	26.22300	28.52000	44.89200	H	24.89390	36.27710	54.47240
C	26.47000	27.38700	43.85800				
O	26.67800	27.71100	42.68900	Step 8 of the nudged elastic band for			
C	27.58280	28.73750	45.57950	proton transfer from complex 2 to			
C	27.71020	29.85710	46.60950	complex 3 without explicit waters.			
O	27.50970	31.04410	46.28550				
O	28.08940	29.45000	47.78810	C	35.07600	29.61800	50.32400
H	25.47230	28.03040	46.84770	O	35.29000	29.74100	49.12000
H	25.90310	29.39550	44.31570	N	33.82600	29.84000	50.82400
H	27.90370	27.79910	46.05170	C	32.80700	30.46300	50.04700
H	28.30910	28.97540	44.78680	C	33.11400	31.92700	49.53200
N	26.43600	26.10900	44.22600	O	32.91300	32.28500	48.36700
H	26.16840	25.81840	45.16050	C	31.48550	30.51210	50.83560
C	22.02800	35.96100	51.62100	C	30.32150	31.02180	49.97500
O	21.52500	35.67200	52.73400	O	29.56850	31.92100	50.44330
N	23.04900	35.23800	51.14800	O	30.21010	30.48410	48.82700
C	23.74700	34.28100	52.02300	H	33.70250	29.79240	51.83390
C	24.10700	34.76800	53.38500	H	32.64830	29.89930	49.11790
O	23.80400	34.05500	54.34000	H	31.23230	29.48790	51.15330
C	25.02980	33.78660	51.30650	H	31.58660	31.13920	51.73300
C	24.79160	33.02010	49.99690	H	29.01870	29.94660	48.21560
C	26.08040	32.47170	49.35750	N	33.63800	32.82200	50.35700
C	26.97620	33.54860	48.73740	H	33.86820	32.61150	51.32340
N	28.20150	32.91540	48.15800	C	33.90300	32.02700	44.81800
H	23.50240	35.53150	50.28490	O	33.71700	32.08700	43.59100
H	23.07560	33.42920	52.20030	N	33.39200	32.93300	45.68900
H	25.68590	34.65710	51.13460	C	32.51000	34.06700	45.26000
H	25.56520	33.13220	52.01190	C	33.32800	35.05900	44.40200
H	24.11870	32.17370	50.20510	O	32.77200	35.51900	43.37500
H	24.26480	33.65190	49.26190	C	31.81220	34.69150	46.48910

C	30.98370	35.90830	46.10860
O	30.91770	33.73560	47.09350
H	33.47180	32.72920	46.68900
H	31.74050	33.67620	44.58050
H	32.58730	34.98000	47.22450
H	31.46320	33.08240	47.59200
H	30.48950	36.30810	47.00420
H	30.21740	35.63110	45.37120
H	31.61030	36.69490	45.66930
N	34.61300	35.31200	44.78500
H	35.05010	34.70500	45.47150
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.59360	28.68800	45.56490
C	27.78990	29.75100	46.62780
O	27.46440	30.93420	46.47920
O	28.41780	29.25840	47.67940
H	25.47010	28.02710	46.84750
H	25.91410	29.40290	44.32200
H	27.91100	27.72550	45.98780
H	28.31650	28.93980	44.77150
N	26.43600	26.10900	44.22600
H	26.15410	25.81660	45.15570
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.03180	33.79120	51.31160
C	24.80320	33.03660	49.99490
C	26.10050	32.48760	49.37730
C	27.01220	33.56200	48.77600
N	28.27570	32.92370	48.29460
H	23.50210	35.53110	50.28450
H	23.07670	33.42820	52.19930
H	25.69060	34.66190	51.15150
H	25.56140	33.13040	52.01550
H	24.12240	32.19280	50.18730
H	24.29200	33.67680	49.25640
H	26.66490	31.92990	50.14320
H	25.85010	31.76800	48.58210

H	26.52590	34.06330	47.92770
H	27.29350	34.32410	49.51430
H	28.78150	32.48510	49.14060
H	28.94270	33.57130	47.84120
H	28.05310	32.15900	47.60690
N	24.74100	35.92700	53.53200
H	24.86330	36.57300	52.75910
H	35.81810	29.27230	51.07290
H	33.83790	33.75310	50.00550
H	34.49640	31.22980	45.31370
H	35.21070	35.82170	44.14130
H	23.26700	27.63180	46.32750
H	26.55100	25.40130	43.50810
H	21.65670	36.76540	50.95440
H	24.89590	36.27620	54.47240

Step 7 of the nudged elastic band for proton transfer from complex 2 to complex 3 without explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.48310	30.50080	50.83220
C	30.31280	30.94830	49.94730
O	29.59010	31.90970	50.32440
O	30.17220	30.28460	48.86720
H	33.70280	29.79410	51.83400
H	32.65300	29.89790	49.11760
H	31.26270	29.47900	51.17960
H	31.56300	31.15990	51.70850
H	28.96540	29.96260	48.26550
N	33.63800	32.82200	50.35700
H	33.87540	32.60930	51.32110
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.81970	34.69630	46.49030
C	30.99820	35.91860	46.11280
O	30.92160	33.74850	47.10030

H	33.47770	32.73300	46.68910
H	31.73810	33.67740	44.58280
H	32.60030	34.98070	47.22200
H	31.46870	33.08090	47.57680
H	30.50370	36.31630	47.00910
H	30.23280	35.64880	45.37180
H	31.63040	36.70390	45.67940
N	34.61300	35.31200	44.78500
H	35.05000	34.70810	45.47390
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.58390	28.71540	45.57210
C	27.73230	29.80290	46.62030
O	27.44990	30.98720	46.39410
O	28.25050	29.33860	47.73610
H	25.47070	28.02500	46.84720
H	25.90640	29.39800	44.31810
H	27.90900	27.76580	46.01730
H	28.31000	28.97200	44.78410
N	26.43600	26.10900	44.22600
H	26.16650	25.81680	45.15940
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.03180	33.78850	51.31270
C	24.79860	33.02220	50.00360
C	26.09160	32.47670	49.37220
C	26.98980	33.55520	48.75800
N	28.23250	32.92410	48.21440
H	23.50430	35.53450	50.28680
H	23.07570	33.42890	52.19940
H	25.68830	34.65940	51.14450
H	25.56390	33.13460	52.02120
H	24.12630	32.17500	50.21030
H	24.27340	33.65340	49.26700
H	26.66750	31.92090	50.13060
H	25.83110	31.75580	48.58140
H	26.47540	34.07350	47.93670
H	27.29800	34.30290	49.50080

H	28.77350	32.46440	49.02260
H	28.88240	33.58530	47.75830
H	27.97900	32.17840	47.50830
N	24.74100	35.92700	53.53200
H	24.86830	36.57130	52.75850
H	35.81790	29.27210	51.07310
H	33.84330	33.75120	50.00360
H	34.49750	31.23040	45.31340
H	35.21000	35.82460	44.14320
H	23.26640	27.63190	46.32710
H	26.55780	25.40030	43.51020
H	21.65740	36.76610	50.95500
H	24.90090	36.27420	54.47210

Step 6 of the nudged elastic band for proton transfer from complex 2 to complex 3 without explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.47570	30.49440	50.82220
C	30.30450	30.91200	49.92040
O	29.60440	31.90680	50.24530
O	30.13960	30.18610	48.88200
H	33.70010	29.79180	51.83360
H	32.65570	29.89790	49.11660
H	31.26930	29.47490	51.18390
H	31.53980	31.16870	51.68840
H	28.92570	29.96120	48.27380
N	33.63800	32.82200	50.35700
H	33.87130	32.61090	51.32240
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.81390	34.69800	46.48580
C	30.99380	35.92060	46.10400
O	30.91190	33.75100	47.09190
H	33.47280	32.73060	46.68920
H	31.73940	33.67750	44.58080

H	32.59070	34.98290	47.22080
H	31.45620	33.08530	47.57310
H	30.49670	36.31880	46.99880
H	30.22990	35.65230	45.36070
H	31.62720	36.70600	45.67260
N	34.61300	35.31200	44.78500
H	35.05050	34.70510	45.47110
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.57780	28.73030	45.56910
C	27.69490	29.83020	46.60460
O	27.42700	31.01270	46.34480
O	28.15920	29.38190	47.74810
H	25.46950	28.02390	46.84750
H	25.89900	29.39330	44.31450
H	27.90570	27.78990	46.03070
H	28.30450	28.98740	44.78260
N	26.43600	26.10900	44.22600
H	26.16040	25.81710	45.15780
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.02630	33.78560	51.30620
C	24.78390	33.01670	49.99960
C	26.07310	32.47300	49.35830
C	26.96450	33.55370	48.73820
N	28.19690	32.92620	48.16770
H	23.50020	35.53160	50.28370
H	23.07270	33.43100	52.19930
H	25.68100	34.65630	51.13110
H	25.56200	33.13260	52.01240
H	24.11460	32.16850	50.21210
H	24.25170	33.64510	49.26550
H	26.65570	31.91710	50.11150
H	25.80690	31.75210	48.56940
H	26.43740	34.07890	47.92930
H	27.28580	34.29550	49.48120
H	28.75300	32.45440	48.95780
H	28.83980	33.59320	47.71110

H	27.92940	32.19070	47.45330
N	24.74100	35.92700	53.53200
H	24.86050	36.57230	52.75800
H	35.81710	29.27010	51.07270
H	33.83810	33.75230	50.00320
H	34.49470	31.22830	45.31300
H	35.20860	35.82330	44.14080
H	23.26460	27.63250	46.32580
H	26.54720	25.40120	43.50760
H	21.65410	36.76310	50.95310
H	24.89340	36.27820	54.47200

Step 5 of the nudged elastic band for proton transfer from complex 2 to complex 3 without explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.47270	30.48730	50.81570
C	30.29670	30.89550	49.92580
O	29.58250	31.87090	50.24290
O	30.14530	30.14680	48.88570
H	33.70240	29.78930	51.83380
H	32.66820	29.89860	49.11410
H	31.26620	29.46670	51.17350
H	31.52550	31.16300	51.68060
H	29.06150	29.99050	48.34310
N	33.63800	32.82200	50.35700
H	33.87200	32.61190	51.32260
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.81020	34.69850	46.48310
C	30.98760	35.91770	46.09640
O	30.90920	33.75010	47.08940
H	33.47540	32.73100	46.68870
H	31.74220	33.67550	44.57920
H	32.58350	34.98740	47.22050
H	31.45560	33.08310	47.56530

H	30.48830	36.31770	46.98920
H	30.22580	35.64460	45.35290
H	31.61960	36.70330	45.66310
N	34.61300	35.31200	44.78500
H	35.05200	34.70220	45.46760
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.58210	28.73970	45.57700
C	27.69980	29.84480	46.62470
O	27.42280	31.02610	46.33490
O	28.15430	29.43490	47.77180
H	25.47230	28.02840	46.84740
H	25.90020	29.39420	44.31560
H	27.91660	27.79670	46.03030
H	28.30280	28.99930	44.78530
N	26.43600	26.10900	44.22600
H	26.15210	25.81870	45.15580
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.02510	33.78480	51.30200
C	24.77890	33.01920	49.99350
C	26.06590	32.47380	49.34970
C	26.95670	33.55290	48.72660
N	28.18430	32.92030	48.15130
H	23.49930	35.52750	50.28190
H	23.07430	33.43040	52.20160
H	25.68110	34.65470	51.12650
H	25.56320	33.12930	52.00420
H	24.10780	32.17200	50.20420
H	24.24810	33.65050	49.26100
H	26.64900	31.91770	50.10240
H	25.80080	31.75230	48.56120
H	26.43010	34.07850	47.91790
H	27.28140	34.29510	49.46830
H	28.73160	32.45410	48.93750
H	28.82940	33.58540	47.69550
H	27.91260	32.17320	47.43680
N	24.74100	35.92700	53.53200

H	24.85710	36.57420	52.75900
H	35.81690	29.27040	51.07310
H	33.83800	33.75290	50.00450
H	34.49540	31.22910	45.31400
H	35.21010	35.82010	44.13950
H	23.26640	27.63260	46.32740
H	26.54180	25.40100	43.50700
H	21.65450	36.76310	50.95300
H	24.88890	36.28010	54.47210

Step 4 of the nudged elastic band for proton transfer from complex 2 to complex 3 without explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.46610	30.48340	50.80690
C	30.28880	30.88460	49.91900
O	29.57020	31.85460	50.22100
O	30.13900	30.11380	48.88390
H	33.69790	29.78570	51.83200
H	32.67000	29.89960	49.11090
H	31.25920	29.46280	51.16440
H	31.50910	31.16130	51.67010
H	29.11880	30.01320	48.38360
N	33.63800	32.82200	50.35700
H	33.86420	32.61370	51.32330
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.79900	34.69880	46.47580
C	30.97390	35.91500	46.08270
O	30.89630	33.74890	47.07830
H	33.46910	32.72860	46.68720
H	31.74260	33.67470	44.57490
H	32.56620	34.99130	47.21710
H	31.44180	33.08160	47.55350
H	30.47160	36.31660	46.97320
H	30.21400	35.63840	45.33850

H	31.60440	36.70120	45.64860
N	34.61300	35.31200	44.78500
H	35.04990	34.69710	45.46250
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.57940	28.74880	45.57150
C	27.67810	29.85610	46.62210
O	27.40300	31.03890	46.30890
O	28.10160	29.46770	47.77840
H	25.47000	28.03070	46.84680
H	25.89360	29.39160	44.31230
H	27.91760	27.80700	46.02510
H	28.29430	29.01020	44.77610
N	26.43600	26.10900	44.22600
H	26.13530	25.82000	45.15020
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.01720	33.78250	51.29250
C	24.76260	33.01950	49.98320
C	26.04650	32.47310	49.33420
C	26.93590	33.55160	48.70850
N	28.15880	32.91660	48.12550
H	23.49150	35.52210	50.27570
H	23.06990	33.43220	52.20010
H	25.67310	34.65160	51.11370
H	25.55770	33.12470	51.98980
H	24.09050	32.17320	50.19430
H	24.23060	33.65240	49.25270
H	26.63160	31.91630	50.08490
H	25.78000	31.75150	48.54650
H	26.40720	34.07850	47.90210
H	27.26460	34.29300	49.44930
H	28.70440	32.45060	48.90540
H	28.80380	33.58210	47.67050
H	27.88140	32.16520	47.40770
N	24.74100	35.92700	53.53200
H	24.84530	36.57570	52.75730
H	35.81370	29.26880	51.07130

H	33.82900	33.75440	50.00280
H	34.49020	31.22690	45.31210
H	35.20680	35.81680	44.13380
H	23.26290	27.63320	46.32470
H	26.52610	25.40250	43.50230
H	21.64900	36.76010	50.94930
H	24.87590	36.28480	54.47100

Step 3 of the nudged elastic band for proton transfer from complex 2 to complex 3 without explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.46590	30.47650	50.80600
C	30.29110	30.86360	49.91480
O	29.57050	31.84170	50.19040
O	30.14010	30.06680	48.89500
H	33.69650	29.78370	51.83190
H	32.67360	29.90010	49.10940
H	31.26580	29.45540	51.16690
H	31.50240	31.15880	51.66560
H	29.15330	30.01770	48.41020
N	33.63800	32.82200	50.35700
H	33.86090	32.61240	51.32430
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.79150	34.69830	46.47090
C	30.96540	35.91210	46.07190
O	30.88770	33.74750	47.07070
H	33.46790	32.72820	46.68740
H	31.74430	33.67390	44.57250
H	32.55400	34.99360	47.21500
H	31.43280	33.08080	47.54640
H	30.45950	36.31580	46.95950
H	30.20860	35.63120	45.32610
H	31.59570	36.69810	45.63710
N	34.61300	35.31200	44.78500

H	35.04820	34.69200	45.45980
C	23.94400	27.94100	45.50200
O	23.57900	28.09500	44.33100
N	25.20400	28.15800	45.87400
C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.57650	28.76340	45.57290
C	27.65120	29.88000	46.61810
O	27.38000	31.05950	46.27170
O	28.04130	29.52270	47.78970
H	25.46960	28.03380	46.84790
H	25.89110	29.39000	44.31030
H	27.92430	27.82680	46.02890
H	28.28780	29.02820	44.77620
N	26.43600	26.10900	44.22600
H	26.12440	25.82200	45.14740
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.01290	33.78020	51.28560
C	24.75020	33.01870	49.97660
C	26.03010	32.47120	49.32050
C	26.91660	33.54900	48.68970
N	28.13140	32.91070	48.09390
H	23.48780	35.51810	50.27240
H	23.06890	33.43310	52.19980
H	25.66970	34.64760	51.10370
H	25.55560	33.12090	51.97890
H	24.07790	32.17310	50.18970
H	24.21600	33.65370	49.24970
H	26.61900	31.91360	50.06750
H	25.76020	31.74940	48.53430
H	26.38300	34.07870	47.88860
H	27.25340	34.28860	49.42890
H	28.67890	32.44020	48.86340
H	28.77540	33.57650	47.63840
H	27.84390	32.15940	47.37100
N	24.74100	35.92700	53.53200
H	24.83840	36.57660	52.75730
H	35.81320	29.26820	51.07060
H	33.82500	33.75490	50.00170
H	34.48950	31.22650	45.31090

H	35.20550	35.81420	44.13000
H	23.26190	27.63340	46.32330
H	26.51570	25.40350	43.50040
H	21.64810	36.75970	50.94810
H	24.86790	36.28690	54.47190

Step 2 of the nudged elastic band for proton transfer from complex 2 to complex 3 without explicit waters.

C	35.07600	29.61800	50.32400
O	35.29000	29.74100	49.12000
N	33.82600	29.84000	50.82400
C	32.80700	30.46300	50.04700
C	33.11400	31.92700	49.53200
O	32.91300	32.28500	48.36700
C	31.46170	30.46750	50.79950
C	30.28850	30.83590	49.89910
O	29.59900	31.83810	50.11230
O	30.11010	29.97150	48.93050
H	33.69900	29.78050	51.83250
H	32.68270	29.89960	49.11010
H	31.27170	29.44790	51.16730
H	31.48020	31.16030	51.65080
H	29.15700	29.99880	48.43420
N	33.63800	32.82200	50.35700
H	33.86080	32.61830	51.32590
C	33.90300	32.02700	44.81800
O	33.71700	32.08700	43.59100
N	33.39200	32.93300	45.68900
C	32.51000	34.06700	45.26000
C	33.32800	35.05900	44.40200
O	32.77200	35.51900	43.37500
C	31.78940	34.70030	46.46950
C	30.96560	35.91520	46.06690
O	30.88090	33.75070	47.06390
H	33.46470	32.72410	46.68740
H	31.74880	33.67230	44.57190
H	32.54790	34.99580	47.21900
H	31.42140	33.08460	47.54440
H	30.45820	36.31850	46.95370
H	30.20910	35.63720	45.31960
H	31.59690	36.70140	45.63400
N	34.61300	35.31200	44.78500
H	35.05390	34.69160	45.45620
C	23.94400	27.94100	45.50200

O	23.57900	28.09500	44.33100	H	26.50950	25.40370	43.49950
N	25.20400	28.15800	45.87400	H	21.64630	36.75550	50.94800
C	26.22300	28.52000	44.89200	H	24.86390	36.29130	54.47090
C	26.47000	27.38700	43.85800				
O	26.67800	27.71100	42.68900	Step 1 of the nudged elastic band for			
C	27.57460	28.77900	45.57050	proton transfer from complex 2 to			
C	27.61270	29.91320	46.60120	complex 3 without explicit waters.			
O	27.32900	31.08240	46.22570				
O	27.96630	29.58580	47.79000	C	35.07600	29.61800	50.32400
H	25.47210	28.03710	46.84800	O	35.29000	29.74100	49.12000
H	25.88450	29.38480	44.30890	N	33.82600	29.84000	50.82400
H	27.92350	27.85210	46.04730	C	32.80700	30.46300	50.04700
H	28.28550	29.03590	44.76990	C	33.11400	31.92700	49.53200
N	26.43600	26.10900	44.22600	O	32.91300	32.28500	48.36700
H	26.11920	25.82190	45.14600	C	31.45380	30.41880	50.78830
C	22.02800	35.96100	51.62100	C	30.29160	30.69780	49.84450
O	21.52500	35.67200	52.73400	O	29.77380	31.81690	49.76990
N	23.04900	35.23800	51.14800	O	29.93900	29.63870	49.14650
C	23.74700	34.28100	52.02300	H	33.70520	29.79340	51.83460
C	24.10700	34.76800	53.38500	H	32.70690	29.90220	49.10470
O	23.80400	34.05500	54.34000	H	31.33020	29.40830	51.20180
C	25.01050	33.77750	51.28190	H	31.43020	31.15300	51.60470
C	24.74040	33.01330	49.97470	H	29.10140	29.79500	48.53190
C	26.01730	32.46840	49.31070	N	33.63800	32.82200	50.35700
C	26.89710	33.54770	48.67340	H	33.88100	32.60950	51.31990
N	28.09870	32.91130	48.05000	C	33.90300	32.02700	44.81800
H	23.48700	35.51320	50.27110	O	33.71700	32.08700	43.59100
H	23.06940	33.43410	52.20480	N	33.39200	32.93300	45.68900
H	25.66510	34.64560	51.09290	C	32.51000	34.06700	45.26000
H	25.55850	33.11850	51.97260	C	33.32800	35.05900	44.40200
H	24.07100	32.16640	50.19200	O	32.77200	35.51900	43.37500
H	24.20000	33.64470	49.24890	C	31.81240	34.70260	46.48210
H	26.61240	31.91210	50.05380	C	31.01250	35.93690	46.09420
H	25.74520	31.74540	48.52650	O	30.89010	33.76950	47.07700
H	26.35140	34.08480	47.88510	H	33.47540	32.73340	46.68900
H	27.24790	34.28140	49.41220	H	31.74080	33.67640	44.58010
H	28.65700	32.42740	48.80130	H	32.58590	34.97680	47.22500
H	28.73970	33.58130	47.59790	H	31.41500	33.10580	47.57790
H	27.79550	32.16990	47.31850	H	30.50650	36.33560	46.98360
N	24.74100	35.92700	53.53200	H	30.25750	35.67970	45.33820
H	24.83500	36.57850	52.75870	H	31.66050	36.71740	45.67570
H	35.81420	29.26590	51.07260	N	34.61300	35.31200	44.78500
H	33.82450	33.75620	50.00560	H	35.05090	34.70520	45.47100
H	34.48810	31.22450	45.31450	C	23.94400	27.94100	45.50200
H	35.20890	35.81150	44.13150	O	23.57900	28.09500	44.33100
H	23.26490	27.63390	46.32710	N	25.20400	28.15800	45.87400

C	26.22300	28.52000	44.89200
C	26.47000	27.38700	43.85800
O	26.67800	27.71100	42.68900
C	27.55000	28.84110	45.60180
C	27.49270	30.04670	46.55400
O	27.10990	31.15610	46.08420
O	27.84180	29.86490	47.77040
H	25.47130	28.04480	46.84980
H	25.87880	29.37920	44.30400
H	27.90310	27.96000	46.15660
H	28.29250	29.07370	44.82370
N	26.43600	26.10900	44.22600
H	26.16120	25.82240	45.15970
C	22.02800	35.96100	51.62100
O	21.52500	35.67200	52.73400
N	23.04900	35.23800	51.14800
C	23.74700	34.28100	52.02300
C	24.10700	34.76800	53.38500
O	23.80400	34.05500	54.34000
C	25.02000	33.77640	51.29550
C	24.74960	32.98580	50.00600
C	26.01590	32.45190	49.31220
C	26.86190	33.53990	48.64520
N	28.00640	32.92530	47.90380
H	23.50280	35.53160	50.28500
H	23.07210	33.43250	52.20360
H	25.67100	34.64470	51.09410
H	25.57010	33.13520	52.00180
H	24.10220	32.13030	50.25420
H	24.17840	33.59690	49.28680
H	26.63840	31.90050	50.03590
H	25.72580	31.72420	48.53960
H	26.26250	34.10810	47.91970
H	27.27570	34.24690	49.37730
H	28.60210	32.36520	48.56040
H	28.63660	33.62030	47.47740
H	27.64430	32.24720	47.13820
N	24.74100	35.92700	53.53200
H	24.85880	36.57370	52.75890
H	35.81630	29.27130	51.07360
H	33.84900	33.74890	50.00040
H	34.49770	31.23040	45.31340
H	35.21020	35.82310	44.14210
H	23.26540	27.63500	46.32770
H	26.53750	25.39870	43.50860
H	21.65640	36.76500	50.95420

H	24.88970	36.27920	54.47230
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Optimized structure in the forward direction from the intrinsic reaction coordinate derived from the transition state optimization for proton transfer from complex 2 to complex 3 without explicit waters.

C	35.07590	29.61810	50.32390
O	35.29100	29.74080	49.11940
N	33.82760	29.84070	50.82330
C	32.80470	30.46380	50.05000
C	33.11290	31.92590	49.53220
O	32.91430	32.28590	48.36660
C	31.47110	30.48280	50.82100
C	30.28000	30.87240	49.93250
O	29.57780	31.86430	50.26140
O	30.09440	30.12740	48.91100
H	33.70480	29.79030	51.83330
H	32.66280	29.89870	49.11740
H	31.28050	29.46420	51.19350
H	31.52360	31.16810	51.67840
H	28.87560	29.93220	48.31760
N	33.63780	32.82180	50.35660
H	33.87120	32.61120	51.32230
C	33.90280	32.02720	44.81830
O	33.71690	32.08710	43.59090
N	33.39200	32.93280	45.68930
C	32.51010	34.06680	45.26020
C	33.32800	35.05880	44.40210
O	32.77200	35.51900	43.37490
C	31.81960	34.70380	46.48640
C	30.99440	35.92090	46.09900
O	30.92340	33.76030	47.10580
H	33.47730	32.73210	46.68930
H	31.73870	33.67640	44.58290
H	32.59990	34.99670	47.21500
H	31.47280	33.09620	47.58370
H	30.50290	36.32730	46.99320
H	30.22610	35.64150	45.36450
H	31.62230	36.70310	45.65420
N	34.61290	35.31190	44.78500
H	35.05110	34.70490	45.47070
C	23.94250	27.94050	45.50150
O	23.57960	28.09560	44.33070

N	25.20300	28.15830	45.87450
C	26.22070	28.51900	44.89180
C	26.47030	27.38550	43.85710
O	26.67820	27.71180	42.68940
C	27.58230	28.72870	45.57110
C	27.71310	29.83830	46.60110
O	27.54560	31.02990	46.30030
O	28.07110	29.39630	47.78660
H	25.47200	28.02160	46.84680
H	25.90140	29.39430	44.31490
H	27.90380	27.78840	46.03840
H	28.30550	28.97070	44.77690
N	26.43600	26.10860	44.22600
H	26.16510	25.81840	45.15970
C	22.02800	35.96110	51.62110
O	21.52490	35.67200	52.73390
N	23.04890	35.23790	51.14790
C	23.74680	34.28100	52.02300
C	24.10710	34.76800	53.38510
O	23.80390	34.05500	54.33990
C	25.02990	33.78670	51.30700
C	24.79350	33.02030	49.99710
C	26.08410	32.47300	49.35980
C	26.98310	33.55200	48.74770
N	28.21970	32.92490	48.18670
H	23.50280	35.53190	50.28510
H	23.07540	33.42920	52.20050
H	25.68590	34.65730	51.13560
H	25.56520	33.13250	52.01270
H	24.12080	32.17350	50.20410
H	24.26740	33.65210	49.26160
H	26.66090	31.91150	50.11320
H	25.81870	31.75530	48.56750
H	26.46430	34.08140	47.93620
H	27.29980	34.29040	49.49630
H	28.75370	32.43540	48.98080
H	28.87770	33.59630	47.75790
H	27.97150	32.20170	47.45270
N	24.74090	35.92700	53.53200
H	24.86340	36.57270	52.75880
H	35.81700	29.27110	51.07310
H	33.84210	33.75100	50.00270
H	34.49680	31.23030	45.31370
H	35.20990	35.82340	44.14210
H	23.26500	27.63020	46.32600
H	26.55530	25.39860	43.51110

H	21.65690	36.76570	50.95460
H	24.89500	36.27680	54.47230

Optimized structure in the backward direction from the intrinsic reaction coordinate derived from the transition state optimization for proton transfer from complex 2 to complex 3 without explicit waters.

C	35.07610	29.61790	50.32410
O	35.28900	29.74120	49.12060
N	33.82440	29.83930	50.82470
C	32.80930	30.46220	50.04400
C	33.11510	31.92810	49.53180
O	32.91170	32.28410	48.36740
C	31.48030	30.45950	50.82380
C	30.27940	30.77320	49.94610
O	29.54400	31.74260	50.17720
O	30.12620	29.91090	48.97140
H	33.70350	29.79730	51.83530
H	32.67960	29.89750	49.10990
H	31.32750	29.44660	51.22700
H	31.50940	31.17330	51.65770
H	29.18180	29.94510	48.46600
N	33.63820	32.82220	50.35740
H	33.88320	32.60700	51.31920
C	33.90320	32.02680	44.81770
O	33.71710	32.08690	43.59110
N	33.39200	32.93320	45.68870
C	32.50990	34.06720	45.25980
C	33.32800	35.05920	44.40190
O	32.77200	35.51900	43.37510
C	31.81820	34.70530	46.48430
C	30.99320	35.92200	46.09580
O	30.92100	33.76260	47.10420
H	33.48390	32.73700	46.68820
H	31.73910	33.67620	44.58210
H	32.59780	34.99890	47.21360
H	31.47200	33.09600	47.57440
H	30.50080	36.32820	46.98950
H	30.22570	35.64230	45.36070
H	31.62150	36.70430	45.65160
N	34.61310	35.31210	44.78500
H	35.05200	34.70330	45.46850
C	23.94550	27.94150	45.50250

O	23.57840	28.09440	44.33130	H	26.54840	25.40080	43.50880
N	25.20500	28.15770	45.87350	H	21.65610	36.76460	50.95390
C	26.22530	28.52100	44.89220	H	24.89060	36.27840	54.47250
C	26.46970	27.38850	43.85890				
O	26.67780	27.71020	42.68860				
C	27.57490	28.77880	45.58840	Relaxed coordinates of the	Asparagine		
C	27.63180	29.92990	46.60400	mutant.			
O	27.38450	31.10090	46.20700	C	34.16400	35.32800	47.73900
O	27.96920	29.61470	47.80010	O	34.37300	35.13800	46.49800
H	25.47280	28.04430	46.84920	N	33.27400	34.56400	48.36300
H	25.89630	29.39100	44.31200	C	32.37400	33.54700	47.83100
H	27.90860	27.85780	46.08720	C	31.56500	34.13100	46.69700
H	28.30380	29.01620	44.79850	O	31.29200	33.51100	45.64200
N	26.43600	26.10940	44.22600	C	31.48830	32.94060	48.93320
H	26.16780	25.81970	45.16060	C	30.49190	31.96140	48.30420
C	22.02800	35.96090	51.62090	N	30.94050	30.73260	48.02900
O	21.52510	35.67200	52.73410	O	29.33880	32.35830	48.03610
N	23.04910	35.23810	51.14810	H	33.17260	34.73570	49.36440
C	23.74720	34.28100	52.02300	H	32.97350	32.74640	47.36850
C	24.10690	34.76800	53.38490	H	32.13260	32.44040	49.67070
O	23.80410	34.05500	54.34010	H	30.90830	33.72650	49.43510
C	25.02800	33.78480	51.30360	H	30.37270	30.02760	47.50780
C	24.78140	33.01710	49.99610	H	31.89620	30.47540	48.25280
C	26.06210	32.46300	49.34660	N	31.19000	35.39400	46.84300
C	26.95170	33.53280	48.70630	H	31.43430	35.94540	47.65840
N	28.14590	32.88480	48.07980	C	33.13900	33.20200	42.26000
H	23.50080	35.52890	50.28310	O	33.28000	32.46600	41.26400
H	23.07550	33.42940	52.20060	N	31.90000	33.53500	42.72600
H	25.68480	34.65430	51.12830	C	30.62400	33.09900	41.98400
H	25.56450	33.13020	52.00800	C	30.59000	33.89900	40.66500
H	24.10720	32.17320	50.20990	O	30.13700	33.42700	39.68600
H	24.25150	33.64960	49.26400	C	29.38420	33.33110	42.86680
H	26.65040	31.90790	50.09580	C	28.09090	33.01540	42.12880
H	25.78920	31.73610	48.56620	O	29.42330	32.47900	44.02290
H	26.41010	34.07590	47.91950	H	31.81360	33.94330	43.65870
H	27.31240	34.26200	49.44500	H	30.71400	32.04070	41.71140
H	28.67380	32.36550	48.82700	H	29.38150	34.39100	43.18890
H	28.80990	33.55240	47.65660	H	30.12020	32.81240	44.64240
H	27.84020	32.16890	47.32350	H	28.07870	31.96050	41.82230
N	24.74110	35.92700	53.53200	H	27.97550	33.63700	41.23280
H	24.85870	36.57420	52.75920	H	27.23840	33.19730	42.79740
H	35.81720	29.27140	51.07310	N	31.23400	35.10100	40.60500
H	33.84730	33.75060	50.00320	H	31.76250	35.47450	41.38390
H	34.49810	31.23070	45.31360	C	25.45200	25.96200	45.80200
H	35.20990	35.82270	44.14120	O	24.99200	25.97400	44.64800
H	23.26780	27.63510	46.32890	N	26.77100	26.02300	46.06800

C	27.87900	25.94800	45.01400	H	30.64990	35.83640	46.10640
C	28.12200	24.48400	44.51500	H	33.97550	33.61690	42.85860
O	28.39800	24.25300	43.35800	H	31.29740	35.55080	39.69870
C	29.14910	26.60200	45.54590	H	24.81870	25.94960	46.71270
C	29.02610	28.09540	45.91510	H	27.98190	22.49700	44.97410
O	29.89860	28.55560	46.68770	H	19.60560	35.22520	45.27080
O	28.05000	28.76300	45.41330	H	22.84430	37.58690	48.04450
H	27.05590	26.09660	47.04250				
H	27.50640	26.48550	44.13420				
H	29.53340	26.06440	46.42550				
H	29.92620	26.52440	44.76920				
N	27.88500	23.43300	45.35200				
H	27.56060	23.55220	46.30510				
C	20.19600	35.11900	46.20900				
O	19.76000	35.39100	47.31500				
N	21.46900	34.65800	45.96700				
C	22.43600	34.38200	47.08200				
C	22.62100	35.57700	48.07800				
O	22.54900	35.51400	49.30900				
C	23.77690	33.95380	46.45030				
C	24.89130	33.68970	47.46970				
C	26.24520	33.30250	46.84600				
C	26.29400	31.87040	46.30590				
N	27.69930	31.46110	45.98400				
H	21.74210	34.42460	45.01610				
H	22.03280	33.56550	47.70040				
H	23.59270	33.05210	45.84360				
H	24.10760	34.74540	45.75500				
H	25.04100	34.59640	48.07630				
H	24.57270	32.90410	48.17440				
H	26.51060	34.01830	46.04880				
H	27.02020	33.39810	47.62200				
H	25.93240	31.15940	47.05990				
H	25.68950	31.73120	45.39990				
H	28.32960	31.68290	46.79870				
H	28.10460	31.96320	45.16160				
H	27.80600	30.42250	45.78460				
N	22.81500	36.74500	47.47800				
H	22.72830	36.84970	46.47210				
O	26.04800	28.80300	47.33100				
H	26.76110	28.68370	46.65920				
H	25.25430	28.82460	46.76480				
O	25.52300	28.90400	44.13600				
H	26.46270	28.76350	44.39320				
H	25.17640	27.99100	44.06690				
H	34.68230	36.07640	48.36600				