

## Supporting Information

### “Molecular Dynamics Simulation of Atomic Interactions in the Vancomycin Binding Site”

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Table S1: Cartesian coordinates for V<sub>N</sub>-Ala complex

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	<u><i>x</i></u>	<u><i>y</i></u>	<u><i>z</i></u>
H	-3.23000000	-5.21300000	2.24900000
H	-3.60800000	-6.88700000	2.65600000
H	-4.91100000	-5.74000000	2.34600000
H	-4.57500000	-7.21300000	0.34800000
H	-3.72600000	-4.93200000	-0.97400000
O	-1.58700000	-6.87900000	0.97500000
O	-2.27900000	-7.09700000	-1.06100000
C	-2.47200000	-6.82700000	0.12400000
C	-3.90900000	-6.04000000	2.04000000
C	-3.87900000	-6.40700000	0.55700000
N	-4.31200000	-5.28600000	-0.24900000
H	-6.42800000	-4.83800000	-2.63200000
H	-4.71400000	-4.42600000	-2.66400000
H	-5.92000000	-3.22400000	-3.12400000
H	-5.05800000	-2.78500000	-0.79100000
H	-7.85700000	-3.58400000	-0.33300000
O	-6.32700000	-5.10500000	0.81600000
C	-5.52100000	-4.74000000	-0.03100000
C	-5.70900000	-4.04200000	-2.43700000
C	-5.79600000	-3.57200000	-0.97900000
N	-7.12700000	-3.03100000	-0.73500000
O	-6.45100000	-1.05100000	-1.59000000
C	-7.32300000	-1.75300000	-1.10100000
C	-8.74500000	-1.21200000	-0.86300000
H	-8.92900000	-1.14500000	0.18900000
H	-8.83600000	-0.24100000	-1.30300000
H	-9.45800000	-1.87400000	-1.30800000
N	-3.38600000	-11.86300000	-0.17800000
C	-2.78200000	-12.15600000	1.11600000
C	-2.79600000	-10.65900000	-0.75200000
C	-1.28700000	-10.83300000	-0.93600000
O	-0.82800000	-11.67700000	-1.69500000
C	-3.40500000	-10.31500000	-2.11000000

C	-4.92700000	-10.19300000	-2.05900000
C	-5.35800000	-9.01500000	-1.18700000
C	-5.49100000	-10.04500000	-3.47300000
H	-3.22600000	-12.66500000	-0.82200000
H	-3.23700000	-13.05800000	1.52500000
H	-1.71100000	-12.31000000	0.98200000
H	-2.95500000	-11.31600000	1.78800000
H	-2.97500000	-9.84200000	-0.05500000
H	-3.13300000	-11.09000000	-2.82700000
H	-2.97500000	-9.38300000	-2.47800000
H	-5.32500000	-11.10800000	-1.62000000
H	-5.00000000	-8.07400000	-1.60600000
H	-6.44400000	-8.95900000	-1.11800000
H	-4.96000000	-9.11200000	-0.17700000
H	-5.11300000	-9.14100000	-3.94900000
H	-5.21000000	-10.89600000	-4.09400000
H	-6.57900000	-9.98700000	-3.45300000
N	-0.54900000	-9.98300000	-0.19800000
C	0.89700000	-10.07300000	-0.31800000
C	1.42700000	-8.95900000	-1.24400000
O	2.44200000	-9.14200000	-1.90600000
C	1.56200000	-10.09900000	1.06700000
O	1.16300000	-11.25100000	1.76500000
C	1.17700000	-8.89300000	1.85900000
C	2.03000000	-7.73400000	1.85500000
C	-0.07200000	-8.86700000	2.58200000
C	1.59200000	-6.53800000	2.51300000
Cl	2.60200000	-5.13500000	2.49000000
C	-0.49900000	-7.66000000	3.24400000
C	0.31700000	-6.47800000	3.16700000
O	-0.15600000	-5.24000000	3.60000000
H	-0.98100000	-9.31000000	0.40200000
H	1.09400000	-11.02200000	-0.81900000
H	2.64700000	-10.13300000	0.96600000
H	1.60800000	-11.23000000	2.60200000
H	2.98000000	-7.75800000	1.34300000
H	-0.70000000	-9.74500000	2.60800000
H	-1.44700000	-7.62900000	3.76100000
N	0.71300000	-7.80600000	-1.28100000
C	1.21300000	-6.79600000	-2.20600000
C	1.10600000	-5.35800000	-1.67600000
O	2.09600000	-4.72200000	-1.33100000
C	0.42700000	-6.89500000	-3.51300000
C	0.42200000	-8.33600000	-4.02500000
O	1.44000000	-8.88700000	-4.42600000
N	-0.80000000	-8.89800000	-3.98200000
H	-0.12300000	-7.64400000	-0.75700000

H	2.25900000	-7.02800000	-2.39600000
H	-0.60500000	-6.57900000	-3.35300000
H	0.85400000	-6.24600000	-4.27800000
H	-1.58300000	-8.37900000	-3.64100000
H	-0.95200000	-9.83900000	-4.28700000
N	-0.15300000	-4.88100000	-1.67300000
C	-0.35500000	-3.50700000	-1.23100000
C	-1.51400000	-2.86100000	-2.00900000
O	-2.51300000	-3.48600000	-2.34300000
C	-0.59800000	-3.35400000	0.25800000
C	-1.22200000	-2.17600000	0.78900000
C	-1.45800000	-1.98500000	2.21400000
C	-1.07500000	-3.06100000	3.10100000
O	-1.33300000	-3.00100000	4.45700000
C	-0.45300000	-4.26500000	2.61100000
C	-0.21300000	-4.37800000	1.17600000
H	-0.91100000	-5.49100000	-1.90800000
H	0.56600000	-2.98300000	-1.48700000
H	-1.56400000	-1.42100000	0.09400000
H	0.26000000	-5.26800000	0.79200000
N	-1.28500000	-1.55600000	-2.25400000
C	-2.30700000	-0.76600000	-2.90700000
C	-1.92000000	0.72200000	-2.94900000
O	-0.75700000	1.02800000	-3.16900000
C	-2.74700000	-1.17900000	-4.27700000
C	-4.13800000	-1.45900000	-4.44400000
C	-4.71500000	-1.70000000	-5.71300000
C	-3.87100000	-1.71000000	-6.86900000
O	-4.41200000	-1.96300000	-8.11300000
C	-2.45300000	-1.45100000	-6.74100000
C	-1.89200000	-1.18000000	-5.43800000
H	-0.42800000	-1.13200000	-1.96200000
H	-3.13300000	-0.91600000	-2.22300000
H	-4.77600000	-1.45800000	-3.57400000
H	-5.34500000	-2.11000000	-8.02700000
H	-1.81900000	-1.45700000	-7.61600000
H	-0.83900000	-0.96300000	-5.33600000
N	-2.89100000	1.65500000	-2.74800000
C	-4.31200000	1.44300000	-2.47900000
O	-2.02900000	-0.82000000	2.79700000
C	-2.25800000	1.37200000	1.64300000
C	-3.93600000	-0.42600000	1.33200000
C	-2.74500000	0.05400000	1.96600000
C	-4.07000000	1.62700000	-0.06400000
C	-2.91700000	2.15900000	0.62500000
C	-4.60100000	0.34900000	0.32800000
C	-4.69400000	2.29200000	-1.26400000

Cl	-4.55800000	-1.98400000	1.75500000
O	-5.04200000	2.67300000	-4.44900000
C	-5.14900000	1.67100000	-3.75100000
O	-4.25700000	3.62400000	-1.41700000
H	-2.59000000	2.60900000	-2.78300000
H	-4.46300000	0.40400000	-2.21400000
H	-1.38000000	1.74800000	2.14200000
H	-2.53100000	3.13400000	0.36200000
H	-5.48000000	-0.03900000	-0.15500000
H	-5.77600000	2.26800000	-1.15800000
H	-4.66800000	4.25600000	-0.68600000
N	-5.97700000	0.62600000	-3.97700000
O	-5.58200000	-4.21800000	-6.36900000
C	-6.55800000	-3.28200000	-6.09200000
C	-6.17900000	-1.94500000	-5.77200000
C	-7.93600000	-3.66900000	-6.11900000
C	-8.95700000	-2.70500000	-5.83200000
O	-10.28700000	-3.07400000	-5.85400000
C	-8.58600000	-1.35600000	-5.51500000
C	-7.19500000	-0.94800000	-5.47600000
C	-6.83800000	0.50800000	-5.12300000
C	-8.05900000	1.40100000	-4.81900000
O	-8.62700000	1.96300000	-5.75400000
O	-8.41400000	1.52000000	-3.64100000
H	-5.97500000	-0.12600000	-3.32400000
H	-6.23600000	0.93300000	-5.92100000
H	-4.72800000	-3.81200000	-6.30700000
H	-8.18500000	-4.69700000	-6.32800000
H	-10.82600000	-2.32400000	-5.64100000
H	-9.35500000	-0.63600000	-5.27800000
C	-1.08900000	-1.98300000	6.56800000
C	-0.26500000	-1.02300000	7.41900000
C	1.22200000	-1.28100000	7.20500000
C	1.55700000	-1.31200000	5.71200000
C	3.02200000	-1.70800000	5.49800000
C	-0.63600000	-1.96700000	5.10700000
O	-2.45400000	-1.64400000	6.65600000
O	-0.59500000	-1.22600000	8.77000000
O	1.96400000	-0.24700000	7.80100000
O	0.74300000	-2.26000000	5.05700000
O	3.28900000	-2.93400000	6.13000000
H	-0.95700000	-2.99500000	6.95000000
H	-0.50300000	0.00700000	7.16200000
H	1.51400000	-2.22200000	7.67100000
H	1.36100000	-0.32400000	5.29100000
H	3.69200000	-0.95900000	5.91800000
H	3.26200000	-1.82400000	4.44000000

H	-0.83600000	-1.00800000	4.63000000
H	-1.25500000	-0.58100000	8.98900000
H	2.20300000	-0.54700000	8.66700000
H	4.20300000	-3.12900000	5.97100000
C	-3.12500000	-2.41200000	7.62800000
C	-4.56400000	-1.92000000	7.81700000
C	-5.43700000	-2.19300000	6.59100000
N	-6.83600000	-1.97400000	6.94000000
C	-5.06700000	-1.24400000	5.45100000
C	-5.24800000	-3.64400000	6.15300000
O	-5.93000000	-3.86500000	4.94400000
C	-3.76200000	-3.94800000	5.98100000
O	-3.13200000	-3.76200000	7.22600000
C	-3.51200000	-5.37600000	5.49300000
H	-2.58600000	-2.32500000	8.57100000
H	-4.99600000	-2.43400000	8.67500000
H	-4.57200000	-0.85600000	8.05500000
H	-7.41500000	-2.57800000	6.39200000
H	-4.02800000	-1.37600000	5.15000000
H	-5.69400000	-1.42500000	4.57700000
H	-5.20300000	-0.20600000	5.75200000
H	-5.67300000	-4.31600000	6.89800000
H	-6.78300000	-4.21200000	5.17200000
H	-3.34500000	-3.24500000	5.26400000
H	-3.98700000	-5.54500000	4.52700000
H	-2.44500000	-5.56700000	5.38300000
H	-3.91400000	-6.10300000	6.19800000
H	-6.97200000	-2.17200000	7.91100000

Table S2: Cartesian coordinates for V<sub>N</sub>-Lac complex

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	<u><i>x</i></u>	<u><i>y</i></u>	<u><i>z</i></u>
H	-3.23000000	-5.21300000	2.24900000
H	-3.60800000	-6.88700000	2.65600000
H	-4.91100000	-5.74000000	2.34600000
H	-4.57500000	-7.21300000	0.34800000
O	-1.58700000	-6.87900000	0.97500000
O	-2.27900000	-7.09700000	-1.06100000
C	-2.47200000	-6.82700000	0.12400000
C	-3.90900000	-6.04000000	2.04000000
C	-3.87900000	-6.40700000	0.55700000
O	-4.31200000	-5.28600000	-0.24900000
H	-6.42800000	-4.83800000	-2.63200000
H	-4.71400000	-4.42600000	-2.66400000
H	-5.92000000	-3.22400000	-3.12400000

H	-5.05800000	-2.78500000	-0.79100000
H	-7.85700000	-3.58400000	-0.33300000
O	-6.32700000	-5.10500000	0.81600000
C	-5.52100000	-4.74000000	-0.03100000
C	-5.70900000	-4.04200000	-2.43700000
C	-5.79600000	-3.57200000	-0.97900000
N	-7.12700000	-3.03100000	-0.73500000
O	-6.45100000	-1.05100000	-1.59000000
C	-7.32300000	-1.75300000	-1.10100000
C	-8.74500000	-1.21200000	-0.86300000
H	-8.92900000	-1.14500000	0.18900000
H	-8.83600000	-0.24100000	-1.30300000
H	-9.45800000	-1.87400000	-1.30800000
N	-3.38600000	-11.86300000	-0.17800000
C	-2.78200000	-12.15600000	1.11600000
C	-2.79600000	-10.65900000	-0.75200000
C	-1.28700000	-10.83300000	-0.93600000
O	-0.82800000	-11.67700000	-1.69500000
C	-3.40500000	-10.31500000	-2.11000000
C	-4.92700000	-10.19300000	-2.05900000
C	-5.35800000	-9.01500000	-1.18700000
C	-5.49100000	-10.04500000	-3.47300000
H	-3.22600000	-12.66500000	-0.82200000
H	-3.23700000	-13.05800000	1.52500000
H	-1.71100000	-12.31000000	0.98200000
H	-2.95500000	-11.31600000	1.78800000
H	-2.97500000	-9.84200000	-0.05500000
H	-3.13300000	-11.09000000	-2.82700000
H	-2.97500000	-9.38300000	-2.47800000
H	-5.32500000	-11.10800000	-1.62000000
H	-5.00000000	-8.07400000	-1.60600000
H	-6.44400000	-8.95900000	-1.11800000
H	-4.96000000	-9.11200000	-0.17700000
H	-5.11300000	-9.14100000	-3.94900000
H	-5.21000000	-10.89600000	-4.09400000
H	-6.57900000	-9.98700000	-3.45300000
N	-0.54900000	-9.98300000	-0.19800000
C	0.89700000	-10.07300000	-0.31800000
C	1.42700000	-8.95900000	-1.24400000
O	2.44200000	-9.14200000	-1.90600000
C	1.56200000	-10.09900000	1.06700000
O	1.16300000	-11.25100000	1.76500000
C	1.17700000	-8.89300000	1.85900000
C	2.03000000	-7.73400000	1.85500000
C	-0.07200000	-8.86700000	2.58200000
C	1.59200000	-6.53800000	2.51300000
Cl	2.60200000	-5.13500000	2.49000000

C	-0.49900000	-7.66000000	3.24400000
C	0.31700000	-6.47800000	3.16700000
O	-0.15600000	-5.24000000	3.60000000
H	-0.98100000	-9.31000000	0.40200000
H	1.09400000	-11.02200000	-0.81900000
H	2.64700000	-10.13300000	0.96600000
H	1.60800000	-11.23000000	2.60200000
H	2.98000000	-7.75800000	1.34300000
H	-0.70000000	-9.74500000	2.60800000
H	-1.44700000	-7.62900000	3.76100000
N	0.71300000	-7.80600000	-1.28100000
C	1.21300000	-6.79600000	-2.20600000
C	1.10600000	-5.35800000	-1.67600000
O	2.09600000	-4.72200000	-1.33100000
C	0.42700000	-6.89500000	-3.51300000
C	0.42200000	-8.33600000	-4.02500000
O	1.44000000	-8.88700000	-4.42600000
N	-0.80000000	-8.89800000	-3.98200000
H	-0.12300000	-7.64400000	-0.75700000
H	2.25900000	-7.02800000	-2.39600000
H	-0.60500000	-6.57900000	-3.35300000
H	0.85400000	-6.24600000	-4.27800000
H	-1.58300000	-8.37900000	-3.64100000
H	-0.95200000	-9.83900000	-4.28700000
N	-0.15300000	-4.88100000	-1.67300000
C	-0.35500000	-3.50700000	-1.23100000
C	-1.51400000	-2.86100000	-2.00900000
O	-2.51300000	-3.48600000	-2.34300000
C	-0.59800000	-3.35400000	0.25800000
C	-1.22200000	-2.17600000	0.78900000
C	-1.45800000	-1.98500000	2.21400000
C	-1.07500000	-3.06100000	3.10100000
O	-1.33300000	-3.00100000	4.45700000
C	-0.45300000	-4.26500000	2.61100000
C	-0.21300000	-4.37800000	1.17600000
H	-0.91100000	-5.49100000	-1.90800000
H	0.56600000	-2.98300000	-1.48700000
H	-1.56400000	-1.42100000	0.09400000
H	0.26000000	-5.26800000	0.79200000
N	-1.28500000	-1.55600000	-2.25400000
C	-2.30700000	-0.76600000	-2.90700000
C	-1.92000000	0.72200000	-2.94900000
O	-0.75700000	1.02800000	-3.16900000
C	-2.74700000	-1.17900000	-4.27700000
C	-4.13800000	-1.45900000	-4.44400000
C	-4.71500000	-1.70000000	-5.71300000
C	-3.87100000	-1.71000000	-6.86900000

O	-4.41200000	-1.96300000	-8.11300000
C	-2.45300000	-1.45100000	-6.74100000
C	-1.89200000	-1.18000000	-5.43800000
H	-0.42800000	-1.13200000	-1.96200000
H	-3.13300000	-0.91600000	-2.22300000
H	-4.77600000	-1.45800000	-3.57400000
H	-5.34500000	-2.11000000	-8.02700000
H	-1.81900000	-1.45700000	-7.61600000
H	-0.83900000	-0.96300000	-5.33600000
N	-2.89100000	1.65500000	-2.74800000
C	-4.31200000	1.44300000	-2.47900000
O	-2.02900000	-0.82000000	2.79700000
C	-2.25800000	1.37200000	1.64300000
C	-3.93600000	-0.42600000	1.33200000
C	-2.74500000	0.05400000	1.96600000
C	-4.07000000	1.62700000	-0.06400000
C	-2.91700000	2.15900000	0.62500000
C	-4.60100000	0.34900000	0.32800000
C	-4.69400000	2.29200000	-1.26400000
Cl	-4.55800000	-1.98400000	1.75500000
O	-5.04200000	2.67300000	-4.44900000
C	-5.14900000	1.67100000	-3.75100000
O	-4.25700000	3.62400000	-1.41700000
H	-2.59000000	2.60900000	-2.78300000
H	-4.46300000	0.40400000	-2.21400000
H	-1.38000000	1.74800000	2.14200000
H	-2.53100000	3.13400000	0.36200000
H	-5.48000000	-0.03900000	-0.15500000
H	-5.77600000	2.26800000	-1.15800000
H	-4.66800000	4.25600000	-0.68600000
N	-5.97700000	0.62600000	-3.97700000
O	-5.58200000	-4.21800000	-6.36900000
C	-6.55800000	-3.28200000	-6.09200000
C	-6.17900000	-1.94500000	-5.77200000
C	-7.93600000	-3.66900000	-6.11900000
C	-8.95700000	-2.70500000	-5.83200000
O	-10.28700000	-3.07400000	-5.85400000
C	-8.58600000	-1.35600000	-5.51500000
C	-7.19500000	-0.94800000	-5.47600000
C	-6.83800000	0.50800000	-5.12300000
C	-8.05900000	1.40100000	-4.81900000
O	-8.62700000	1.96300000	-5.75400000
O	-8.41400000	1.52000000	-3.64100000
H	-5.97500000	-0.12600000	-3.32400000
H	-6.23600000	0.93300000	-5.92100000
H	-4.72800000	-3.81200000	-6.30700000
H	-8.18500000	-4.69700000	-6.32800000



H	-10.82600000	-2.32400000	-5.64100000
H	-9.35500000	-0.63600000	-5.27800000
C	-1.08900000	-1.98300000	6.56800000
C	-0.26500000	-1.02300000	7.41900000
C	1.22200000	-1.28100000	7.20500000
C	1.55700000	-1.31200000	5.71200000
C	3.02200000	-1.70800000	5.49800000
C	-0.63600000	-1.96700000	5.10700000
O	-2.45400000	-1.64400000	6.65600000
O	-0.59500000	-1.22600000	8.77000000
O	1.96400000	-0.24700000	7.80100000
O	0.74300000	-2.26000000	5.05700000
O	3.28900000	-2.93400000	6.13000000
H	-0.95700000	-2.99500000	6.95000000
H	-0.50300000	0.00700000	7.16200000
H	1.51400000	-2.22200000	7.67100000
H	1.36100000	-0.32400000	5.29100000
H	3.69200000	-0.95900000	5.91800000
H	3.26200000	-1.82400000	4.44000000
H	-0.83600000	-1.00800000	4.63000000
H	-1.25500000	-0.58100000	8.98900000
H	2.20300000	-0.54700000	8.66700000
H	4.20300000	-3.12900000	5.97100000
C	-3.12500000	-2.41200000	7.62800000
C	-4.56400000	-1.92000000	7.81700000
C	-5.43700000	-2.19300000	6.59100000
N	-6.83600000	-1.97400000	6.94000000
C	-5.06700000	-1.24400000	5.45100000
C	-5.24800000	-3.64400000	6.15300000
O	-5.93000000	-3.86500000	4.94400000
C	-3.76200000	-3.94800000	5.98100000
O	-3.13200000	-3.76200000	7.22600000
C	-3.51200000	-5.37600000	5.49300000
H	-2.58600000	-2.32500000	8.57100000
H	-4.99600000	-2.43400000	8.67500000
H	-4.57200000	-0.85600000	8.05500000
H	-7.41500000	-2.57800000	6.39200000
H	-4.02800000	-1.37600000	5.15000000
H	-5.69400000	-1.42500000	4.57700000
H	-5.20300000	-0.20600000	5.75200000
H	-5.67300000	-4.31600000	6.89800000
H	-6.78300000	-4.21200000	5.17200000
H	-3.34500000	-3.24500000	5.26400000
H	-3.98700000	-5.54500000	4.52700000
H	-2.44500000	-5.56700000	5.38300000
H	-3.91400000	-6.10300000	6.19800000
H	-6.97200000	-2.17200000	7.91100000

Table S3: Cartesian coordinates for V<sub>D</sub>-Lac complex

	<i>x</i>	<i>y</i>	<i>z</i>
H	-3.23000000	-5.21300000	2.24900000
H	-3.60800000	-6.88700000	2.65600000
H	-4.91100000	-5.74000000	2.34600000
H	-4.57500000	-7.21300000	0.34800000
O	-1.58700000	-6.87900000	0.97500000
O	-2.27900000	-7.09700000	-1.06100000
C	-2.47200000	-6.82700000	0.12400000
C	-3.90900000	-6.04000000	2.04000000
C	-3.87900000	-6.40700000	0.55700000
O	-4.31200000	-5.28600000	-0.24900000
H	-6.42800000	-4.83800000	-2.63200000
H	-4.71400000	-4.42600000	-2.66400000
H	-5.92000000	-3.22400000	-3.12400000
H	-5.05800000	-2.78500000	-0.79100000
H	-7.85700000	-3.58400000	-0.33300000
O	-6.32700000	-5.10500000	0.81600000
C	-5.52100000	-4.74000000	-0.03100000
C	-5.70900000	-4.04200000	-2.43700000
C	-5.79600000	-3.57200000	-0.97900000
N	-7.12700000	-3.03100000	-0.73500000
O	-6.45100000	-1.05100000	-1.59000000
C	-7.32300000	-1.75300000	-1.10100000
C	-8.74500000	-1.21200000	-0.86300000
H	-8.92900000	-1.14500000	0.18900000
H	-8.83600000	-0.24100000	-1.30300000
H	-9.45800000	-1.87400000	-1.30800000
N	-3.38600000	-11.86300000	-0.17800000
C	-2.78200000	-12.15600000	1.11600000
C	-2.79600000	-10.65900000	-0.75200000
C	-1.28700000	-10.83300000	-0.93600000
O	-0.82800000	-11.67700000	-1.69500000
C	-3.40500000	-10.31500000	-2.11000000
C	-4.92700000	-10.19300000	-2.05900000
C	-5.35800000	-9.01500000	-1.18700000
C	-5.49100000	-10.04500000	-3.47300000
H	-3.22600000	-12.66500000	-0.82200000
H	-3.23700000	-13.05800000	1.52500000
H	-1.71100000	-12.31000000	0.98200000
H	-2.95500000	-11.31600000	1.78800000
H	-2.97500000	-9.84200000	-0.05500000
H	-3.13300000	-11.09000000	-2.82700000

H	-2.97500000	-9.38300000	-2.47800000
H	-5.32500000	-11.10800000	-1.62000000
H	-5.00000000	-8.07400000	-1.60600000
H	-6.44400000	-8.95900000	-1.11800000
H	-4.96000000	-9.11200000	-0.17700000
H	-5.11300000	-9.14100000	-3.94900000
H	-5.21000000	-10.89600000	-4.09400000
H	-6.57900000	-9.98700000	-3.45300000
N	-0.54900000	-9.98300000	-0.19800000
C	0.89700000	-10.07300000	-0.31800000
C	1.42700000	-8.95900000	-1.24400000
O	2.44200000	-9.14200000	-1.90600000
C	1.56200000	-10.09900000	1.06700000
O	1.16300000	-11.25100000	1.76500000
C	1.17700000	-8.89300000	1.85900000
C	2.03000000	-7.73400000	1.85500000
C	-0.07200000	-8.86700000	2.58200000
C	1.59200000	-6.53800000	2.51300000
C1	2.60200000	-5.13500000	2.49000000
C	-0.49900000	-7.66000000	3.24400000
C	0.31700000	-6.47800000	3.16700000
O	-0.15600000	-5.24000000	3.60000000
H	-0.98100000	-9.31000000	0.40200000
H	1.09400000	-11.02200000	-0.81900000
H	2.64700000	-10.13300000	0.96600000
H	1.60800000	-11.23000000	2.60200000
H	2.98000000	-7.75800000	1.34300000
H	-0.70000000	-9.74500000	2.60800000
H	-1.44700000	-7.62900000	3.76100000
N	0.71300000	-7.80600000	-1.28100000
C	1.21300000	-6.79600000	-2.20600000
C	1.10600000	-5.35800000	-1.67600000
O	2.09600000	-4.72200000	-1.33100000
C	0.42700000	-6.89500000	-3.51300000
C	0.42200000	-8.33600000	-4.02500000
O	1.44000000	-8.88700000	-4.42600000
H	-0.12300000	-7.64400000	-0.75700000
H	2.25900000	-7.02800000	-2.39600000
H	-0.60500000	-6.57900000	-3.35300000
H	0.85400000	-6.24600000	-4.27800000
N	-0.15300000	-4.88100000	-1.67300000
C	-0.35500000	-3.50700000	-1.23100000
C	-1.51400000	-2.86100000	-2.00900000
O	-2.51300000	-3.48600000	-2.34300000
C	-0.59800000	-3.35400000	0.25800000
C	-1.22200000	-2.17600000	0.78900000
C	-1.45800000	-1.98500000	2.21400000

C	-1.07500000	-3.06100000	3.10100000
O	-1.33300000	-3.00100000	4.45700000
C	-0.45300000	-4.26500000	2.61100000
C	-0.21300000	-4.37800000	1.17600000
H	-0.91100000	-5.49100000	-1.90800000
H	0.56600000	-2.98300000	-1.48700000
H	-1.56400000	-1.42100000	0.09400000
H	0.26000000	-5.26800000	0.79200000
N	-1.28500000	-1.55600000	-2.25400000
C	-2.30700000	-0.76600000	-2.90700000
C	-1.92000000	0.72200000	-2.94900000
O	-0.75700000	1.02800000	-3.16900000
C	-2.74700000	-1.17900000	-4.27700000
C	-4.13800000	-1.45900000	-4.44400000
C	-4.71500000	-1.70000000	-5.71300000
C	-3.87100000	-1.71000000	-6.86900000
O	-4.41200000	-1.96300000	-8.11300000
C	-2.45300000	-1.45100000	-6.74100000
C	-1.89200000	-1.18000000	-5.43800000
H	-0.42800000	-1.13200000	-1.96200000
H	-3.13300000	-0.91600000	-2.22300000
H	-4.77600000	-1.45800000	-3.57400000
H	-5.34500000	-2.11000000	-8.02700000
H	-1.81900000	-1.45700000	-7.61600000
H	-0.83900000	-0.96300000	-5.33600000
N	-2.89100000	1.65500000	-2.74800000
C	-4.31200000	1.44300000	-2.47900000
O	-2.02900000	-0.82000000	2.79700000
C	-2.25800000	1.37200000	1.64300000
C	-3.93600000	-0.42600000	1.33200000
C	-2.74500000	0.05400000	1.96600000
C	-4.07000000	1.62700000	-0.06400000
C	-2.91700000	2.15900000	0.62500000
C	-4.60100000	0.34900000	0.32800000
C	-4.69400000	2.29200000	-1.26400000
Cl	-4.55800000	-1.98400000	1.75500000
O	-5.04200000	2.67300000	-4.44900000
C	-5.14900000	1.67100000	-3.75100000
O	-4.25700000	3.62400000	-1.41700000
H	-2.59000000	2.60900000	-2.78300000
H	-4.46300000	0.40400000	-2.21400000
H	-1.38000000	1.74800000	2.14200000
H	-2.53100000	3.13400000	0.36200000
H	-5.48000000	-0.03900000	-0.15500000
H	-5.77600000	2.26800000	-1.15800000
H	-4.66800000	4.25600000	-0.68600000
N	-5.97700000	0.62600000	-3.97700000

O	-5.58200000	-4.21800000	-6.36900000
C	-6.55800000	-3.28200000	-6.09200000
C	-6.17900000	-1.94500000	-5.77200000
C	-7.93600000	-3.66900000	-6.11900000
C	-8.95700000	-2.70500000	-5.83200000
O	-10.28700000	-3.07400000	-5.85400000
C	-8.58600000	-1.35600000	-5.51500000
C	-7.19500000	-0.94800000	-5.47600000
C	-6.83800000	0.50800000	-5.12300000
C	-8.05900000	1.40100000	-4.81900000
O	-8.62700000	1.96300000	-5.75400000
O	-8.41400000	1.52000000	-3.64100000
H	-5.97500000	-0.12600000	-3.32400000
H	-6.23600000	0.93300000	-5.92100000
H	-4.72800000	-3.81200000	-6.30700000
H	-8.18500000	-4.69700000	-6.32800000
H	-10.82600000	-2.32400000	-5.64100000
H	-9.35500000	-0.63600000	-5.27800000
C	-1.08900000	-1.98300000	6.56800000
C	-0.26500000	-1.02300000	7.41900000
C	1.22200000	-1.28100000	7.20500000
C	1.55700000	-1.31200000	5.71200000
C	3.02200000	-1.70800000	5.49800000
C	-0.63600000	-1.96700000	5.10700000
O	-2.45400000	-1.64400000	6.65600000
O	-0.59500000	-1.22600000	8.77000000
O	1.96400000	-0.24700000	7.80100000
O	0.74300000	-2.26000000	5.05700000
O	3.28900000	-2.93400000	6.13000000
H	-0.95700000	-2.99500000	6.95000000
H	-0.50300000	0.00700000	7.16200000
H	1.51400000	-2.22200000	7.67100000
H	1.36100000	-0.32400000	5.29100000
H	3.69200000	-0.95900000	5.91800000
H	3.26200000	-1.82400000	4.44000000
H	-0.83600000	-1.00800000	4.63000000
H	-1.25500000	-0.58100000	8.98900000
H	2.20300000	-0.54700000	8.66700000
H	4.20300000	-3.12900000	5.97100000
C	-3.12500000	-2.41200000	7.62800000
C	-4.56400000	-1.92000000	7.81700000
C	-5.43700000	-2.19300000	6.59100000
N	-6.83600000	-1.97400000	6.94000000
C	-5.06700000	-1.24400000	5.45100000
C	-5.24800000	-3.64400000	6.15300000
O	-5.93000000	-3.86500000	4.94400000
C	-3.76200000	-3.94800000	5.98100000

O	-3.13200000	-3.76200000	7.22600000
C	-3.51200000	-5.37600000	5.49300000
H	-2.58600000	-2.32500000	8.57100000
H	-4.99600000	-2.43400000	8.67500000
H	-4.57200000	-0.85600000	8.05500000
H	-7.41500000	-2.57800000	6.39200000
H	-4.02800000	-1.37600000	5.15000000
H	-5.69400000	-1.42500000	4.57700000
H	-5.20300000	-0.20600000	5.75200000
H	-5.67300000	-4.31600000	6.89800000
H	-6.78300000	-4.21200000	5.17200000
H	-3.34500000	-3.24500000	5.26400000
H	-3.98700000	-5.54500000	4.52700000
H	-2.44500000	-5.56700000	5.38300000
H	-3.91400000	-6.10300000	6.19800000
H	-6.97200000	-2.17200000	7.91100000
O	-0.76000000	-8.87900000	-3.98300000

Table S4: Cartesian coordinates for V<sub>D</sub>-Ala complex

	<u><u>x</u></u>	<u><u>y</u></u>	<u><u>z</u></u>
H	-3.23000000	-5.21300000	2.24900000
H	-3.60800000	-6.88700000	2.65600000
H	-4.91100000	-5.74000000	2.34600000
H	-4.57500000	-7.21300000	0.34800000
H	-3.72600000	-4.93200000	-0.97400000
O	-1.58700000	-6.87900000	0.97500000
O	-2.27900000	-7.09700000	-1.06100000
C	-2.47200000	-6.82700000	0.12400000
C	-3.90900000	-6.04000000	2.04000000
C	-3.87900000	-6.40700000	0.55700000
N	-4.31200000	-5.28600000	-0.24900000
H	-6.42800000	-4.83800000	-2.63200000
H	-4.71400000	-4.42600000	-2.66400000
H	-5.92000000	-3.22400000	-3.12400000
H	-5.05800000	-2.78500000	-0.79100000
H	-7.85700000	-3.58400000	-0.33300000
O	-6.32700000	-5.10500000	0.81600000
C	-5.52100000	-4.74000000	-0.03100000
C	-5.70900000	-4.04200000	-2.43700000
C	-5.79600000	-3.57200000	-0.97900000
N	-7.12700000	-3.03100000	-0.73500000
O	-6.45100000	-1.05100000	-1.59000000
C	-7.32300000	-1.75300000	-1.10100000
C	-8.74500000	-1.21200000	-0.86300000

H	-8.92900000	-1.14500000	0.18900000
H	-8.83600000	-0.24100000	-1.30300000
H	-9.45800000	-1.87400000	-1.30800000
N	-3.38600000	-11.86300000	-0.17800000
C	-2.78200000	-12.15600000	1.11600000
C	-2.79600000	-10.65900000	-0.75200000
C	-1.28700000	-10.83300000	-0.93600000
O	-0.82800000	-11.67700000	-1.69500000
C	-3.40500000	-10.31500000	-2.11000000
C	-4.92700000	-10.19300000	-2.05900000
C	-5.35800000	-9.01500000	-1.18700000
C	-5.49100000	-10.04500000	-3.47300000
H	-3.22600000	-12.66500000	-0.82200000
H	-3.23700000	-13.05800000	1.52500000
H	-1.71100000	-12.31000000	0.98200000
H	-2.95500000	-11.31600000	1.78800000
H	-2.97500000	-9.84200000	-0.05500000
H	-3.13300000	-11.09000000	-2.82700000
H	-2.97500000	-9.38300000	-2.47800000
H	-5.32500000	-11.10800000	-1.62000000
H	-5.00000000	-8.07400000	-1.60600000
H	-6.44400000	-8.95900000	-1.11800000
H	-4.96000000	-9.11200000	-0.17700000
H	-5.11300000	-9.14100000	-3.94900000
H	-5.21000000	-10.89600000	-4.09400000
H	-6.57900000	-9.98700000	-3.45300000
N	-0.54900000	-9.98300000	-0.19800000
C	0.89700000	-10.07300000	-0.31800000
C	1.42700000	-8.95900000	-1.24400000
O	2.44200000	-9.14200000	-1.90600000
C	1.56200000	-10.09900000	1.06700000
O	1.16300000	-11.25100000	1.76500000
C	1.17700000	-8.89300000	1.85900000
C	2.03000000	-7.73400000	1.85500000
C	-0.07200000	-8.86700000	2.58200000
C	1.59200000	-6.53800000	2.51300000
C1	2.60200000	-5.13500000	2.49000000
C	-0.49900000	-7.66000000	3.24400000
C	0.31700000	-6.47800000	3.16700000
O	-0.15600000	-5.24000000	3.60000000
H	-0.98100000	-9.31000000	0.40200000
H	1.09400000	-11.02200000	-0.81900000
H	2.64700000	-10.13300000	0.96600000
H	1.60800000	-11.23000000	2.60200000
H	2.98000000	-7.75800000	1.34300000
H	-0.70000000	-9.74500000	2.60800000
H	-1.44700000	-7.62900000	3.76100000

N	0.71300000	-7.80600000	-1.28100000
C	1.21300000	-6.79600000	-2.20600000
C	1.10600000	-5.35800000	-1.67600000
O	2.09600000	-4.72200000	-1.33100000
C	0.42700000	-6.89500000	-3.51300000
C	0.42200000	-8.33600000	-4.02500000
O	1.44000000	-8.88700000	-4.42600000
H	-0.12300000	-7.64400000	-0.75700000
H	2.25900000	-7.02800000	-2.39600000
H	-0.60500000	-6.57900000	-3.35300000
H	0.85400000	-6.24600000	-4.27800000
N	-0.15300000	-4.88100000	-1.67300000
C	-0.35500000	-3.50700000	-1.23100000
C	-1.51400000	-2.86100000	-2.00900000
O	-2.51300000	-3.48600000	-2.34300000
C	-0.59800000	-3.35400000	0.25800000
C	-1.22200000	-2.17600000	0.78900000
C	-1.45800000	-1.98500000	2.21400000
C	-1.07500000	-3.06100000	3.10100000
O	-1.33300000	-3.00100000	4.45700000
C	-0.45300000	-4.26500000	2.61100000
C	-0.21300000	-4.37800000	1.17600000
H	-0.91100000	-5.49100000	-1.90800000
H	0.56600000	-2.98300000	-1.48700000
H	-1.56400000	-1.42100000	0.09400000
H	0.26000000	-5.26800000	0.79200000
N	-1.28500000	-1.55600000	-2.25400000
C	-2.30700000	-0.76600000	-2.90700000
C	-1.92000000	0.72200000	-2.94900000
O	-0.75700000	1.02800000	-3.16900000
C	-2.74700000	-1.17900000	-4.27700000
C	-4.13800000	-1.45900000	-4.44400000
C	-4.71500000	-1.70000000	-5.71300000
C	-3.87100000	-1.71000000	-6.86900000
O	-4.41200000	-1.96300000	-8.11300000
C	-2.45300000	-1.45100000	-6.74100000
C	-1.89200000	-1.18000000	-5.43800000
H	-0.42800000	-1.13200000	-1.96200000
H	-3.13300000	-0.91600000	-2.22300000
H	-4.77600000	-1.45800000	-3.57400000
H	-5.34500000	-2.11000000	-8.02700000
H	-1.81900000	-1.45700000	-7.61600000
H	-0.83900000	-0.96300000	-5.33600000
N	-2.89100000	1.65500000	-2.74800000
C	-4.31200000	1.44300000	-2.47900000
O	-2.02900000	-0.82000000	2.79700000
C	-2.25800000	1.37200000	1.64300000



C	-3.93600000	-0.42600000	1.33200000
C	-2.74500000	0.05400000	1.96600000
C	-4.07000000	1.62700000	-0.06400000
C	-2.91700000	2.15900000	0.62500000
C	-4.60100000	0.34900000	0.32800000
C	-4.69400000	2.29200000	-1.26400000
Cl	-4.55800000	-1.98400000	1.75500000
O	-5.04200000	2.67300000	-4.44900000
C	-5.14900000	1.67100000	-3.75100000
O	-4.25700000	3.62400000	-1.41700000
H	-2.59000000	2.60900000	-2.78300000
H	-4.46300000	0.40400000	-2.21400000
H	-1.38000000	1.74800000	2.14200000
H	-2.53100000	3.13400000	0.36200000
H	-5.48000000	-0.03900000	-0.15500000
H	-5.77600000	2.26800000	-1.15800000
H	-4.66800000	4.25600000	-0.68600000
N	-5.97700000	0.62600000	-3.97700000
O	-5.58200000	-4.21800000	-6.36900000
C	-6.55800000	-3.28200000	-6.09200000
C	-6.17900000	-1.94500000	-5.77200000
C	-7.93600000	-3.66900000	-6.11900000
C	-8.95700000	-2.70500000	-5.83200000
O	-10.28700000	-3.07400000	-5.85400000
C	-8.58600000	-1.35600000	-5.51500000
C	-7.19500000	-0.94800000	-5.47600000
C	-6.83800000	0.50800000	-5.12300000
C	-8.05900000	1.40100000	-4.81900000
O	-8.62700000	1.96300000	-5.75400000
O	-8.41400000	1.52000000	-3.64100000
H	-5.97500000	-0.12600000	-3.32400000
H	-6.23600000	0.93300000	-5.92100000
H	-4.72800000	-3.81200000	-6.30700000
H	-8.18500000	-4.69700000	-6.32800000
H	-10.82600000	-2.32400000	-5.64100000
H	-9.35500000	-0.63600000	-5.27800000
C	-1.08900000	-1.98300000	6.56800000
C	-0.26500000	-1.02300000	7.41900000
C	1.22200000	-1.28100000	7.20500000
C	1.55700000	-1.31200000	5.71200000
C	3.02200000	-1.70800000	5.49800000
C	-0.63600000	-1.96700000	5.10700000
O	-2.45400000	-1.64400000	6.65600000
O	-0.59500000	-1.22600000	8.77000000
O	1.96400000	-0.24700000	7.80100000
O	0.74300000	-2.26000000	5.05700000
O	3.28900000	-2.93400000	6.13000000

H	-0.95700000	-2.99500000	6.95000000
H	-0.50300000	0.00700000	7.16200000
H	1.51400000	-2.22200000	7.67100000
H	1.36100000	-0.32400000	5.29100000
H	3.69200000	-0.95900000	5.91800000
H	3.26200000	-1.82400000	4.44000000
H	-0.83600000	-1.00800000	4.63000000
H	-1.25500000	-0.58100000	8.98900000
H	2.20300000	-0.54700000	8.66700000
H	4.20300000	-3.12900000	5.97100000
C	-3.12500000	-2.41200000	7.62800000
C	-4.56400000	-1.92000000	7.81700000
C	-5.43700000	-2.19300000	6.59100000
N	-6.83600000	-1.97400000	6.94000000
C	-5.06700000	-1.24400000	5.45100000
C	-5.24800000	-3.64400000	6.15300000
O	-5.93000000	-3.86500000	4.94400000
C	-3.76200000	-3.94800000	5.98100000
O	-3.13200000	-3.76200000	7.22600000
C	-3.51200000	-5.37600000	5.49300000
H	-2.58600000	-2.32500000	8.57100000
H	-4.99600000	-2.43400000	8.67500000
H	-4.57200000	-0.85600000	8.05500000
H	-7.41500000	-2.57800000	6.39200000
H	-4.02800000	-1.37600000	5.15000000
H	-5.69400000	-1.42500000	4.57700000
H	-5.20300000	-0.20600000	5.75200000
H	-5.67300000	-4.31600000	6.89800000
H	-6.78300000	-4.21200000	5.17200000
H	-3.34500000	-3.24500000	5.26400000
H	-3.98700000	-5.54500000	4.52700000
H	-2.44500000	-5.56700000	5.38300000
H	-3.91400000	-6.10300000	6.19800000
H	-6.97200000	-2.17200000	7.91100000
O	-0.76000000	-8.87900000	-3.98300000