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Supplementary Data:
Molecular geometries of test systems (units given in parentheses).

Table 1: Cartesian coordinates of the Cd2+-imidazole complex (Bohr).

Atom	x	y	z
Cd	0.000000000	0.000000000	0.000000000
N	0.000000000	0.000000000	-4.270782744
N	-1.295300812	0.000000000	-8.216595657
C	1.277555548	0.000000000	-8.286579686
C	2.050807130	0.000000000	-5.841580898
C	-1.974295739	0.000000000	-5.782977653
H	2.327254176	0.000000000	-10.016981910
H	3.946959286	0.000000000	-5.123193109
H	-3.909370623	0.000000000	-5.152366230
H	-2.481531661	0.000000000	-9.778799182

Table 2: Cartesian coordinates of the 29-residue polyalanine (Angstrom).

Atom	x	y	z
C	-4.89650	-0.57930	2.59220
C	-4.79050	0.56470	1.58380
C	-3.46760	1.56900	-0.21940
C	-2.15200	1.26200	-0.95240
C	-3.46800	2.94290	0.45510
C	0.27460	0.77750	-0.66260
C	0.19760	-0.41950	-1.62360
C	1.22280	0.53720	0.51460
C	-0.57270	-2.77450	-1.88420
C	-1.23250	-2.45770	-3.23580
C	-1.37430	-3.77590	-1.04930
C	-3.17360	-1.35870	-4.34560
C	-2.25360	-0.63780	-5.34380
C	-4.36210	-0.50160	-3.90350
C	-0.62200	1.22300	-5.63060
C	0.37360	0.30040	-6.35170
C	0.06340	2.24470	-4.72010
C	2.02920	-1.53720	-6.05340
C	1.42080	-2.33650	-7.21680
C	2.50010	-2.42690	-4.90050
C	-0.50390	-3.74880	-7.92940
C	-0.67320	-2.94410	-9.22790
C	-1.83820	-4.18960	-7.32270
C	-1.47270	-0.79450	-10.20110
C	-0.17890	-0.62800	-11.01390
C	-2.01300	0.53200	-9.66150
C	2.24080	-0.04700	-10.89260
C	2.62580	-1.27960	-11.72630
C	3.25080	0.26330	-9.78530
C	2.88700	-3.75710	-11.69570
C	2.10070	-3.90240	-13.00830
C	2.60540	-4.88790	-10.70340
C	-0.16450	-3.82960	-14.04300
C	0.33390	-2.92480	-15.18110
C	-1.58180	-3.48160	-13.58160
C	1.03810	-0.61210	-15.78320
C	2.29550	-1.13160	-16.49830
C	1.27690	0.70230	-15.03630
C	4.57300	-2.08820	-16.17400
C	4.30210	-3.20060	-17.19940
C	5.41590	-2.56270	-14.98790
C	3.10510	-5.34770	-17.60500
C	2.56580	-4.84560	-18.95380

C	2.09810	-6.21450	-16.84540
C	0.91080	-3.34120	-20.05160
C	1.98590	-2.76440	-20.98630
C	-0.10660	-2.29320	-19.59430
C	3.95240	-1.24160	-21.13200
C	4.77770	-2.30330	-21.87620
C	4.78830	-0.41590	-20.15110
C	6.03980	-4.43780	-21.63530
C	5.33090	-5.04830	-22.85470
C	6.29120	-5.45560	-20.52010
C	3.19760	-6.02740	-23.69000
C	3.23090	-5.14410	-24.94750
C	1.78330	-6.23110	-23.14150
C	2.89180	-2.83680	-25.82390
C	4.22120	-2.88420	-26.59390
C	2.59670	-1.45830	-25.22780
C	6.70160	-2.78710	-26.38090
C	6.87270	-4.02960	-27.26940
C	7.71290	-2.73060	-25.23340
C	6.65390	-6.50960	-27.36490
C	5.90070	-6.43770	-28.70280
C	6.12670	-7.61090	-26.44200
C	3.72880	-5.88020	-29.78870
C	4.43060	-5.03520	-30.86390
C	2.38900	-5.28800	-29.34510
C	5.58480	-2.87560	-31.32340
C	6.74380	-3.59310	-32.03350
C	6.04430	-1.66910	-30.50140
C	8.78350	-4.98520	-31.70370
C	8.34080	-5.97430	-32.79370
C	9.47810	-5.66940	-30.52380
C	6.77020	-7.82850	-33.34360
C	6.38440	-7.16800	-34.67680
C	5.59000	-8.52010	-32.65710
C	5.08710	-5.32210	-35.73360
C	6.28470	-4.91950	-36.60880
C	4.27360	-4.12060	-35.24660
C	8.51000	-3.79920	-36.62320
C	9.14250	-4.96340	-37.40220
C	9.45360	-3.19790	-35.57880
C	9.96390	-7.31020	-37.24440
C	9.19430	-7.71360	-38.51220
C	9.97680	-8.40940	-36.17940
C	9.04270	-9.33980	-40.34860
H	-3.04660	-0.19650	0.90050
H	-5.82730	-0.46100	3.19080
H	-4.92150	-1.55190	2.05170
H	-4.01300	-0.56330	3.26890
H	-4.29820	1.53990	-0.95960
H	-3.27930	3.73800	-0.30050
H	-4.45490	3.11810	0.93900
H	-2.67240	2.97430	1.23290
H	-1.17190	1.15070	0.85950
H	0.63690	1.66300	-1.23140
H	2.24490	0.30660	0.13930
H	1.25920	1.44800	1.15330
H	0.84970	-0.31700	1.12270
H	-0.76200	-1.52250	-0.16810
H	0.43580	-3.20410	-2.07680
H	-1.51010	-4.72310	-1.61790
H	-0.83080	-3.98730	-0.10130
H	-2.37060	-3.34300	-0.80700
H	-2.76390	-1.48250	-2.25620
H	-3.56530	-2.28080	-4.83030
H	-4.95960	-0.19300	-4.79040
H	-5.00460	-1.08850	-3.20960
H	-3.98970	0.40380	-3.37410
H	-1.66190	0.66200	-3.85510

H	-1.21060	1.77410	-6.39780
H	0.77200	2.86670	-5.31160
H	-0.70560	2.90060	-4.25400
H	0.61970	1.71130	-3.91710
H	0.85570	-0.58210	-4.55040
H	2.90410	-0.96660	-6.43780
H	3.25120	-3.16120	-5.26850
H	2.95770	-1.79450	-4.10720
H	1.62860	-2.97100	-4.47230
H	-0.18500	-2.84310	-6.02510
H	0.09800	-4.65760	-8.15420
H	-2.40680	-4.80200	-8.05780
H	-1.64770	-4.79240	-6.40660
H	-2.43520	-3.29140	-7.04780
H	-1.49920	-1.38910	-8.15310
H	-2.24660	-1.24800	-10.85990
H	-2.20050	1.23680	-10.50220
H	-2.96340	0.34910	-9.11200
H	-1.27040	0.97790	-8.96260
H	0.83280	-0.11060	-9.29210
H	2.18140	0.83280	-11.57170
H	4.26060	0.42340	-10.22500
H	2.93370	1.18090	-9.24090
H	3.28890	-0.58790	-9.06920
H	2.26780	-2.49090	-10.09520
H	3.97420	-3.76050	-11.93420
H	2.84990	-5.87010	-11.16620
H	3.22600	-4.74340	-9.79080
H	1.53010	-4.87050	-10.41690
H	0.34460	-3.52110	-11.99510
H	-0.15990	-4.88280	-14.40270
H	-2.28910	-3.55250	-14.43800
H	-1.89560	-4.18950	-12.78200
H	-1.59530	-2.44590	-13.17440
H	0.39630	-1.32600	-13.87890
H	0.24360	-0.44510	-16.54460
H	1.64050	1.48130	-15.74330
H	0.32550	1.04120	-14.56870
H	2.03610	0.54260	-14.23830
H	3.17230	-1.51620	-14.67100
H	5.11760	-1.26300	-16.68520
H	6.38750	-2.96790	-15.34920
H	5.60350	-1.70750	-14.30070
H	4.86530	-3.35700	-14.43600
H	3.09900	-4.16610	-15.82960
H	4.01900	-5.95410	-17.79490
H	1.80360	-7.08950	-17.46710
H	2.55770	-6.57170	-15.89670
H	1.19510	-5.60970	-16.60530
H	1.21590	-3.64120	-17.96230
H	0.36710	-4.14630	-20.59480
H	-0.60270	-1.83320	-20.47810
H	-0.87330	-2.77760	-18.94910
H	0.41340	-1.50280	-19.00800
H	2.76300	-1.67560	-19.41580
H	3.50720	-0.55140	-21.88310
H	5.62300	0.08540	-20.69040
H	4.14310	0.35300	-19.67000
H	5.20380	-1.08420	-19.36410
H	5.01890	-3.34720	-20.11320
H	7.02060	-4.02890	-21.96640
H	6.90040	-6.30250	-20.90800
H	6.83340	-4.96190	-19.68290
H	5.31730	-5.84130	-20.14380
H	3.61710	-5.29210	-21.73250
H	3.62210	-7.02340	-23.94800
H	1.13410	-6.68660	-23.92250
H	1.82280	-6.90230	-22.25460

H	1.35990	-5.24880	-22.83410
H	2.68050	-3.51210	-23.81200
H	2.06890	-3.10060	-26.52530
H	2.57690	-0.69120	-26.03400
H	1.61020	-1.48050	-24.71290
H	3.38600	-1.19780	-24.48760
H	5.25230	-2.65440	-24.82190
H	6.83530	-1.88100	-27.01310
H	8.74950	-2.74740	-25.63840
H	7.55840	-1.79620	-24.64880
H	7.56250	-3.60640	-24.56320
H	6.23280	-5.22560	-25.71500
H	7.72800	-6.71110	-27.57590
H	6.19480	-8.59860	-26.95050
H	6.73110	-7.63250	-25.50770
H	5.06520	-7.40010	-26.18210
H	4.21560	-5.77380	-27.71510
H	3.54450	-6.89620	-30.20410
H	1.71160	-5.18020	-30.22160
H	1.91780	-5.95930	-28.59280
H	2.55960	-4.28970	-28.88350
H	4.75200	-3.54250	-29.47670
H	4.86400	-2.52250	-32.09450
H	6.57470	-0.94200	-31.15630
H	5.15950	-1.17590	-30.04040
H	6.73060	-2.01010	-29.69420
H	7.46640	-4.22630	-30.20780
H	9.49340	-4.25710	-32.15610
H	10.36630	-6.23670	-30.88180
H	9.80160	-4.90030	-29.78730
H	8.76670	-6.36810	-30.02930
H	6.92810	-6.75400	-31.50820
H	7.55730	-8.58990	-33.54270
H	5.15560	-9.29120	-33.33200
H	5.93940	-9.00410	-31.71770
H	4.81160	-7.76470	-32.40770
H	5.25590	-5.77470	-33.65640
H	4.41870	-5.98040	-36.33260
H	3.90590	-3.53200	-36.11660
H	3.40630	-4.47830	-34.64780
H	4.91440	-3.47430	-34.60590
H	7.20030	-4.07720	-34.96320
H	8.23160	-3.00100	-37.34720
H	10.38710	-2.84180	-36.06940
H	8.95100	-2.34300	-35.07360
H	9.70590	-3.97060	-34.81860
H	9.11780	-6.11720	-35.69220
H	10.44310	-9.29640	-38.75020
H	11.01570	-7.08270	-37.52830
H	10.42590	-9.33840	-36.59660
H	10.57380	-8.07000	-35.30350
H	8.93460	-8.61760	-35.84880
H	8.18490	-8.69100	-40.63490
H	9.79510	-9.35240	-41.16870
H	8.68540	10.37830	-40.16860
N	-3.71640	0.55200	0.79250
N	-1.05150	1.07620	-0.14070
N	-0.41200	-1.54840	-1.11540
N	-2.41280	-1.74600	-3.16600
N	-1.54070	0.42620	-4.82980
N	1.04960	-0.58930	-5.54180
N	0.21540	-2.95140	-6.94610
N	-1.23770	-1.69360	-9.08010
N	0.93220	-0.25110	-10.28750
N	2.55820	-2.48770	-11.06270
N	0.73580	-3.72820	-12.90310
N	0.56410	-1.60920	-14.83390
N	3.31110	-1.56470	-15.67040

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N	3.47040	-4.21380	-16.76780
N	1.54170	-3.92380	-18.87570
N	2.87080	-1.88370	-20.39840
N	5.24230	-3.34430	-21.09840
N	4.02140	-5.43150	-22.64770
N	2.91120	-3.81670	-24.74710
N	5.35780	-2.76370	-25.82060
N	6.55210	-5.23230	-26.67330
N	4.59150	-6.00880	-28.62280
N	4.89590	-3.80680	-30.44100
N	7.62820	-4.25290	-31.20460
N	7.31610	-6.82750	-32.43800
N	5.55340	-6.07090	-34.57520
N	7.30060	-4.25500	-35.95250
N	9.37190	-6.11030	-36.66990
N	9.64690	-8.81000	-39.13460
O	-5.66860	1.42350	1.54160
O	-2.10740	1.19170	-2.18120
O	0.65560	-0.35220	-2.76490
O	-0.72390	-2.82450	-4.29580
O	-2.17470	-1.00280	-6.51740
O	0.53980	0.36890	-7.57010
O	1.98880	-2.40880	-8.30730
O	-0.32150	-3.40480	-10.31460
O	-0.15950	-0.82320	-12.22980
O	2.96820	-1.17170	-12.90440
O	2.67160	-4.15730	-14.06940
O	0.50850	-3.36630	-16.31750
O	2.36870	-1.15050	-17.72760
O	4.80410	-3.16850	-18.32350
O	3.03160	-5.25250	-20.01880
O	2.03450	-3.08140	-22.17540
O	4.99650	-2.21010	-23.08460
O	5.91220	-5.17670	-23.93280
O	3.52570	-5.61160	-26.04810
O	4.24540	-3.02130	-27.81760
O	7.27030	-3.93360	-28.43100
O	6.44910	-6.74700	-29.76130
O	4.55720	-5.44740	-32.01760
O	6.85500	-3.56700	-33.25970
O	8.87880	-5.98600	-33.90150
O	6.80070	-7.60580	-35.75000
O	6.31330	-5.18270	-37.81160
O	9.41720	-4.85650	-38.59800
O	8.23030	-7.05800	-38.90930

Table 3: Cartesian coordinates of the water cluster (Angstrom).

Atom	x	y	z
O	-1.92649	0.41885	0.30394
O	1.19668	-0.04145	0.42587
O	0.10501	1.02169	-2.02618
O	-0.69563	-1.79961	-1.40220
O	1.71889	-0.49832	3.40046
O	-2.90867	0.43623	-2.34864
O	-0.71898	-2.03672	1.58354
O	0.09643	2.56985	1.21862
O	-2.87031	2.81360	1.77031
O	-3.68432	-0.90139	2.38297
O	-1.03513	0.53650	3.06838
O	-2.33220	-0.18777	-5.29366
O	2.14296	-1.47302	-2.09524
O	3.00742	1.68503	-1.26838
O	1.04499	-4.28818	-0.91614

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O	-2.46799	-2.87637	4.17314
O	-3.60449	-2.02869	-0.55900
O	0.09771	-5.02625	1.83533
O	-1.82660	3.19850	-1.23096
O	4.04479	2.32811	1.29971
O	-0.50169	2.04744	-4.77630
O	0.62030	-3.01734	4.16721
O	1.03641	3.91377	-1.31397
O	-0.05917	4.74395	3.30585
O	-2.83116	-4.07081	1.42368
O	-1.95301	-4.59576	-1.42835
O	4.42582	0.55234	3.78459
O	-3.64697	0.54645	4.89899
O	0.34718	-0.90354	-4.48374
O	-0.87243	-0.74261	5.71285
O	4.08936	-0.73356	1.06414
O	4.47484	-0.63613	-3.88752
O	5.54620	0.10720	-1.36956
O	-5.99617	0.40549	-1.90442
O	-3.14909	2.78790	-4.08193
O	-0.03565	-3.72767	-3.63321
O	-4.91873	1.10084	0.65651
O	-4.87902	-4.98060	-0.73006
O	2.03245	2.48733	3.55750
O	-2.87841	-2.50202	-3.51261
O	-3.37965	-1.72519	6.87633
O	-1.90347	3.01107	4.66089
O	2.62625	-5.15843	3.79164
O	3.98989	-2.51678	3.68131
O	-5.77826	-2.57671	-2.48894
O	2.38366	1.57586	-4.02819
O	2.27634	4.63515	1.34743
O	2.14566	-2.86754	1.33590
O	2.55471	-0.29343	-6.31312
O	2.74232	-2.95766	-4.73880
O	-5.05301	-0.38069	-4.44543
H	-2.36868	0.50264	1.13163
H	-1.06528	0.74780	0.49737
H	0.89711	-0.40740	-0.38900
H	1.34550	0.86093	0.19837
H	0.50962	1.59451	-2.65556
H	-0.31153	0.37282	-2.56840
H	-0.56254	-2.70217	-1.16686
H	-1.15946	-1.45903	-0.65616
H	2.01446	-0.42500	2.50883
H	2.52319	-0.55746	3.88747
H	-2.73690	-0.33092	-1.82903
H	-2.49669	1.11492	-1.84132
H	-0.26540	-1.23104	1.76743
H	-1.61073	-1.83078	1.80740
H	-0.61053	3.04711	1.61866
H	0.36054	1.98011	1.90516
H	-3.72085	2.45272	1.95485
H	-2.87204	2.87619	0.82986
H	-4.41784	-0.32146	2.49877
H	-3.23889	-0.84575	3.21144
H	-0.41106	0.34990	3.74908
H	-1.69221	1.04595	3.51140
H	-2.14169	-1.11063	-5.32154
H	-2.03115	0.05675	-4.43400
H	1.83425	-2.34312	-1.90657
H	1.37756	-1.05337	-2.45157
H	2.83559	2.39208	-1.86782
H	2.75778	0.92910	-1.77325
H	0.42812	-4.78525	-0.40541
H	0.88285	-4.58099	-1.79665
H	-1.62708	-3.26447	4.00101
H	-2.96070	-3.08065	3.39654

H	-3.48869	-2.96021	-0.47581
H	-3.53704	-1.73405	0.33294
H	0.75992	-5.36144	2.41528
H	0.02115	-4.12381	2.09595
H	-1.17391	2.57602	-0.95615
H	-1.31212	3.95569	-1.45393
H	3.70730	1.51126	0.97267
H	3.97965	2.89776	0.55177
H	-0.85197	2.75342	-4.25932
H	-1.17776	1.91103	-5.41889
H	0.84254	-2.56742	3.36902
H	0.52220	-2.30801	4.77973
H	1.05873	3.21798	-0.67843
H	1.36061	4.65420	-0.82952
H	0.16378	5.30850	2.58523
H	0.75911	4.33298	3.52708
H	-1.99646	-4.28612	1.04190
H	-3.40489	-4.73170	1.07518
H	-1.65993	-4.57136	-2.32366
H	-2.74944	-5.09721	-1.46961
H	4.85032	-0.27889	3.91529
H	4.73577	0.82828	2.93838
H	-3.33766	1.39731	5.15858
H	-3.91660	0.15055	5.71013
H	0.25170	-0.13156	-5.01585
H	1.17110	-1.25436	-4.77669
H	-1.61967	-0.98300	5.19046
H	-1.20889	-0.78065	6.59199
H	4.11852	-1.53185	1.56374
H	3.36435	-0.87772	0.47896
H	5.36733	-0.42488	-3.67138
H	4.05095	-0.59495	-3.04615
H	5.19230	0.94183	-1.11239
H	5.62799	-0.35209	-0.55128
H	-5.13608	0.47545	-2.28281
H	-6.55999	0.47937	-2.65564
H	-3.19087	2.92811	-3.15101
H	-3.51511	1.92645	-4.19412
H	0.62175	-3.58735	-4.29259
H	-0.52727	-2.92332	-3.65103
H	-5.70457	1.26199	0.16290
H	-4.47494	0.44918	0.13960
H	-5.35684	-4.29006	-1.15685
H	-5.49013	-5.69740	-0.72227
H	1.77327	1.72442	4.04573
H	2.95438	2.34503	3.42264
H	-3.73052	-2.86403	-3.33923
H	-2.54284	-2.31713	-2.65162
H	-3.54438	-2.34308	7.56762
H	-3.36871	-2.25697	6.09847
H	-2.09708	3.33196	3.79610
H	-1.25086	3.61963	4.96276
H	2.05089	-4.71025	4.38863
H	2.81746	-5.97272	4.22484
H	4.36401	-3.35379	3.89810
H	3.14287	-2.74952	3.33927
H	-6.12402	-2.08270	-3.21292
H	-5.58007	-1.91284	-1.84958
H	3.02973	1.06844	-4.48919
H	1.77540	1.81258	-4.70756
H	3.02636	4.76390	1.90309
H	1.96608	3.78115	1.59913
H	1.47967	-2.51892	0.76741
H	2.22262	-3.76212	1.05000
H	3.21827	-0.77605	-5.84882
H	2.53159	-0.70341	-7.16060
H	3.13480	-2.42947	-4.06398
H	3.38390	-3.63061	-4.88946

H	-4.21351	-0.60715	-4.08111
H	-4.85181	-0.23649	-5.35432

Table 4: Cartesian coordinates of insulin (Angstrom).

Atom	x	y	z
C	0.03300	22.18400	14.19400
C	0.11500	20.61100	14.05700
C	0.40400	5.92400	4.31200
C	0.99000	20.37300	15.27700
C	-0.79500	6.52800	4.98300
C	-1.03200	7.33900	8.70500
C	-1.42100	7.28000	7.23900
C	-1.50400	16.50900	8.54300
C	-1.52400	14.05200	5.99500
C	-1.73000	19.01000	13.52400
C	-2.04200	14.72000	4.88600
C	-2.09800	0.43900	5.66600
C	-2.12300	5.93400	4.64500
C	-2.15100	16.22400	9.88800
C	-2.24900	2.00800	7.21400
C	-2.31200	13.12100	6.61900
C	-2.38500	17.38800	7.69700
C	-2.81200	10.71200	3.17200
C	-2.82300	9.74000	0.82400
C	-2.93500	5.93200	9.44500
C	-3.07300	3.83500	-0.69400
C	-3.09400	9.52700	2.28200
C	-3.19600	2.20800	6.29100
C	-3.23200	18.92600	13.22800
C	-3.32500	18.20300	10.91300
C	-3.34000	14.49300	4.38100
C	-3.36400	4.49100	0.66000
C	-3.41900	5.18300	11.80600
C	-3.42600	17.04000	9.94700
C	-3.61800	12.91100	6.18700
C	-3.82400	19.21600	15.71000
C	-3.93000	4.38700	5.22400
C	-3.94900	15.25500	3.27600
C	-3.99300	5.82500	10.55400
C	-4.00800	18.42900	14.43400
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C	-4.22400	3.30000	6.21400
C	-4.37600	13.01700	10.27000
C	-4.45400	17.36000	4.72600
C	-4.57000	9.09200	2.44000
C	-4.73800	18.06300	8.20400
C	-4.73900	18.65200	17.97200
C	-4.76600	18.58700	6.75500
C	-4.89700	4.48700	0.92300
C	-4.95700	16.30800	3.74900
C	-5.03800	8.16200	1.35900
C	-5.08900	18.94800	16.50900
C	-5.12700	5.36100	5.10400
C	-5.15200	20.75000	5.63100
C	-5.37900	12.42800	-1.04600
C	-5.41700	5.87700	0.53800
C	-5.49700	14.52200	14.90300
C	-5.54200	22.66000	-0.05300
C	-5.56500	7.84100	13.61600
C	-5.57800	13.34300	0.00300
C	-5.57900	19.89700	6.82000
C	-5.60300	15.40700	13.66800
C	-5.74000	13.73100	10.28200

C	-5.82800	21.60100	0.81900
C	-5.84600	14.47200	8.94900
C	-5.86700	8.94400	-6.68000
C	-5.93900	8.60400	6.67000
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C	-5.97800	8.20400	4.23700
C	-6.07200	7.68300	-7.14500
C	-6.10800	7.53600	5.62000
C	-6.27900	8.10400	-4.48200
C	-6.30000	12.38100	-2.10400
C	-6.33200	22.84600	-1.20400
C	-6.36700	6.60900	-6.32800
C	-6.38800	5.64600	10.12300
C	-6.42200	9.79900	18.16200
C	-6.47000	6.82800	-4.94300
C	-6.53900	8.24900	-2.96400
C	-6.59200	17.34800	2.28400
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C	-6.99600	12.91600	10.55500
C	-7.20400	2.11000	15.15200
C	-7.24600	19.66000	1.49000
C	-7.25000	7.05100	15.29800
C	-7.36100	21.96300	-1.52100
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C	-7.85400	8.99300	-2.70400
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C	-8.35900	10.90200	1.33700
C	-8.40300	3.70500	14.32500
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C	-8.81300	15.00000	-1.07100
C	-8.81800	15.70300	-5.44800
C	-8.83900	2.51700	13.87100
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O	-18.83600	8.59800	8.01000
O	-18.94600	15.96600	4.48000
O	-18.95200	11.92500	-1.58800
O	-20.22200	11.62900	0.30300
O	-21.24900	1.03200	6.24900
O	-23.38500	5.83300	1.90000
S	-4.20400	6.79300	14.15100
S	-4.52800	5.04100	13.23200
S	-10.92600	9.43700	9.57900
S	-12.02500	13.10100	-1.36800
S	-12.39200	8.04000	9.39800
S	-13.95600	13.76900	-1.58700

Table 5: Cartesian coordinates of the model of vitamin B12 (Angstrom).

Atom	x	y	z
C	-0.33160	-6.46582	-0.86703
C	0.68325	-5.39375	-1.30691
C	0.58372	-4.09773	-0.55870
C	0.61920	-2.68974	1.18678
C	0.29812	-2.80644	-0.97674
C	0.30930	6.40091	-1.16426
C	-0.79941	5.34950	-1.36096
C	-0.60130	4.08425	-0.58053
C	-0.36515	2.75418	1.21067
C	-0.40947	2.77014	-0.97944
C	-2.82487	-0.07719	-0.33258
C	-3.77241	-0.69405	-1.37729

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C	-3.06679	-0.35715	-2.71519
C	-1.61133	-0.23143	-2.30504
C	0.81296	0.03680	-2.74149
C	2.01742	0.13787	-3.65572
C	3.19402	0.36718	-2.69043
C	2.54436	0.34310	-1.32491
C	2.73313	0.45083	1.16116
C	3.56625	0.64514	2.40930
C	2.53847	0.55447	3.55128
C	1.22868	0.27805	2.83880
C	-1.20672	-0.18573	2.79452
C	-2.55254	-0.48463	3.42970
C	-3.52525	-0.39031	2.22731
C	-2.61665	-0.73342	1.03288
C	-0.48490	-0.15946	-3.18186
C	3.26320	0.48972	-0.13141
C	0.01374	0.09887	3.48241
Co	0.01479	0.00525	0.13032
H	-0.20028	-6.75712	0.19533
H	1.71777	-5.79095	-1.20581
H	0.55498	-5.16644	-2.38397
H	1.00949	-4.75528	1.44378
H	0.71521	-2.33385	2.21727
H	0.08004	-2.46098	-1.99074
H	-1.78629	5.78880	-1.09431
H	-0.87531	5.07183	-2.43112
H	-0.67366	4.83742	1.43203
H	-0.30388	2.44287	2.25828
H	-0.37380	2.37521	-1.99830
H	-0.65769	-0.25294	-4.26261
H	4.34683	0.65038	-0.22127
H	-0.00772	0.16194	4.57907
H	-1.37444	-6.11567	-0.99823
H	-0.20241	-7.38382	-1.47200
H	0.38096	6.74237	-0.11127
H	0.09936	7.29599	-1.78094
H	1.30039	6.00595	-1.46273
H	-4.80275	-0.29776	-1.31655
H	-3.82151	-1.79409	-1.23886
H	-3.21566	-1.11426	-3.51039
H	-3.41032	0.61404	-3.13622
H	2.12750	-0.78900	-4.25508
H	1.88488	0.96213	-4.38580
H	3.97982	-0.41360	-2.75970
H	3.71143	1.33594	-2.85289
H	4.35632	-0.13272	2.47066
H	4.09923	1.61767	2.37341
H	2.46805	1.49106	4.14223
H	2.76512	-0.25009	4.27987
H	-2.78946	0.20768	4.26177
H	-2.52905	-1.50711	3.86899
H	-3.90685	0.64700	2.12572
H	-4.39687	-1.06436	2.31776
H	-2.55850	-1.83791	0.88206
H	-3.06665	1.00013	-0.16794
N	0.77712	-3.98489	0.81131
N	0.32895	-1.94647	0.11209
N	-0.56514	4.03491	0.80639
N	-0.26338	1.96012	0.13850
N	-1.50168	-0.14169	-0.99794
N	1.20115	0.16555	-1.41473
N	1.42401	0.23514	1.46643
N	-1.28145	-0.26995	1.48384