

Supplementary Information

Capture of Amyloid Precursor Protein Fragments by an Engineered Water-Soluble γ -Secretase Variant

Energetic Components Prot-Prot | Normal | GB | Delta | TOTAL

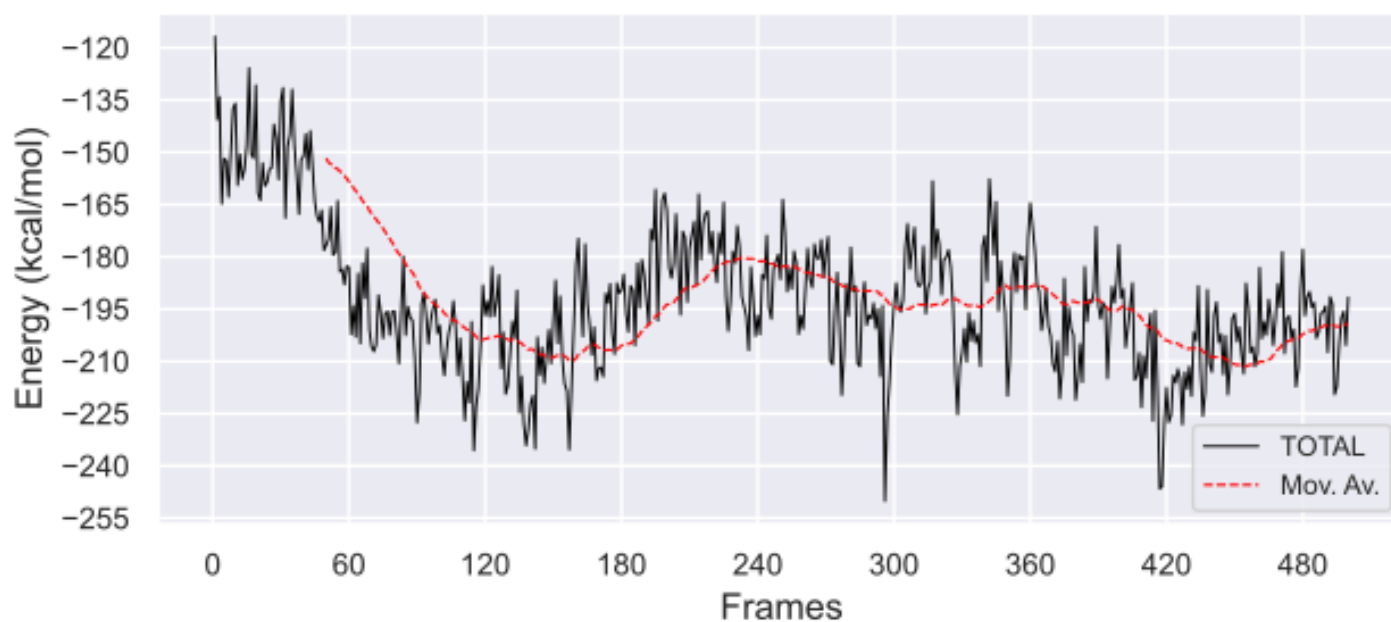


Figure S1. Total Binding Energy Fluctuations Across 250ns full-atom MD simulation.

Energetic Components [Per-residue]
Prot-Prot | NORMAL | GB | Delta | TDC

Receptor Ligand

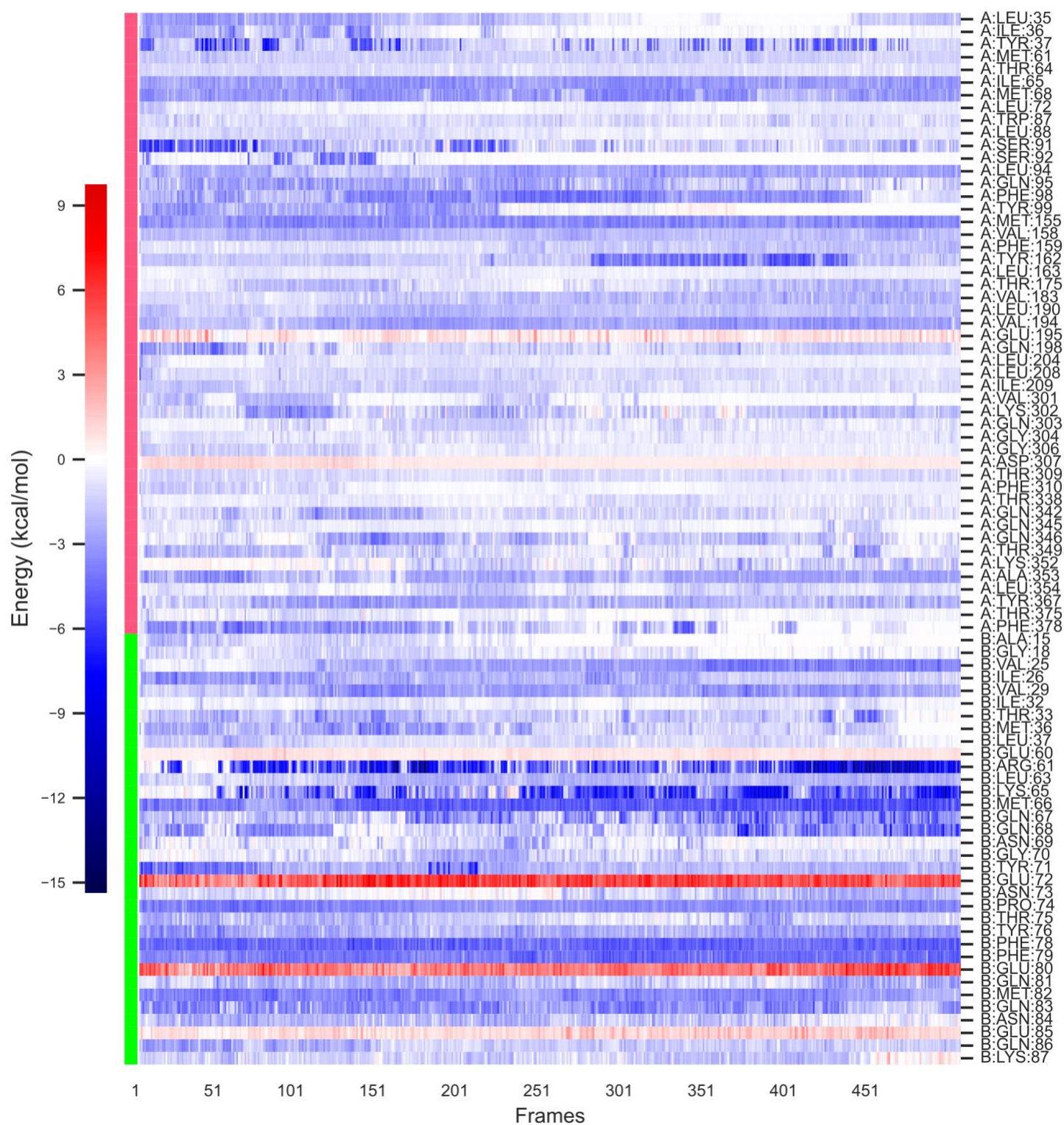


Figure S9. Per-Residue Binding Energy Decomposition. Heatmap visualization of residue-wise MM/PBSA energy components (kcal/mol) across simulation frames.

Table S1. MMGBSA energy terms.

GENERALIZED BORN: Complex Energy Terms															
Frame #	BOND	ANGLE	DIHED	UB	IMP	CMAP	VDWAALS	EEL	1-4 VDW	1-4 EEL	EGB	ESURF	GGAS	GSOLV	TOTAL
1	1554	3647.67	4745.04	419.53	260.3	-79.53	-3006.29	30442.35	1626.05	23539.69	7087.33	247.03	2264.12	-6840.3	4576.18
2	1560.59	3705.86	4739.24	431.93	251.54	103.76	-3109.08	30254.32	1558.54	23299.8	6984.96	246.66	2080.32	6738.31	4657.99
3	1566.27	3726.71	4724.16	434.6	260.48	-99.33	-3108.87	-30074.5	1557.61	23293.75	7191.61	248.16	2280.88	6943.45	4662.57
4	1600.17	3698.39	4702.14	439.65	277.1	-103.8	-3083.49	30386.09	1574.01	23340.64	6885.02	243.21	2058.73	-6641.8	4583.07
5	1549.62	3698.18	4688.81	429.77	262	119.12	-3123.09	30248.37	1537.2	23394.02	7051.49	242.29	2069.02	-6809.2	4740.18
6	1547.8	3679.85	4708.79	437.05	246.02	143.07	-3102.19	-30134.8	1577.27	23347.37	7080.57	240.38	2164.08	6840.18	-4676.1
7	1644.17	3770.27	4684.19	421.12	242.62	-115.6	-3133.4	30072.96	1563.04	23132.28	6993.45	238.47	2135.72	6754.98	4619.26
8	1576.87	3701.82	4716.31	439.69	274.23	120.56	-3116.64	30008.97	1556.79	23274.52	-7186.2	241.4	2294.07	6944.79	4650.72
9	1586.25	3699.82	4703.59	452.1	266.11	109.05	-3065.36	29973.24	1570.83	23134.69	7081.49	244.03	2265.73	6837.46	4571.74
10	1662.02	3721.4	4693.95	454.21	251.09	122.68	-3115.62	29863.46	1538.47	23043.55	7091.04	244.69	2262.93	6846.34	4583.41
11	1589.75	3738.76	4709.83	443.22	255.69	114.76	-3135.13	-30392.2	1552.32	23304.09	6788.93	236.9	1951.56	6552.03	4600.47
12	1577.65	3739.91	4688.95	435.67	259.08	122.37	-3128.12	30104.58	1583.42	23169.97	-6947.5	237.45	2099.58	6710.05	4610.47
13	1578.38	3784.45	4659.23	429.52	251.29	124.36	-3137.71	30213.51	1544.94	23111.73	6817.94	233.37	1883.97	6584.58	4700.61
14	1628.94	3833.2	4683.85	439.42	249.4	139.21	-3132.42	30337.45	1550.55	23090.99	6677.34	231.78	1867.27	6445.56	4578.29
15	1604.14	3762.22	4670.34	419.97	273.92	128.62	-3153.33	30227.95	1521.96	23190.99	6835.53	233.19	1933.65	6602.33	4668.69
16	1595.37	3720.97	4691.05	447.21	262.62	113.16	-3137.23	-30290.6	1569.08	23262.65	-6809	236.58	2007.97	6572.42	4564.45
17	1572.61	3648.68	4637.46	431.33	257.92	116.72	-3167.52	30367.68	1560.94	23382.73	6867.81	234.31	1839.76	-6633.5	4793.75
18	1586.43	3733.14	4632.28	435.99	233.5	118.56	-3151.49	30420.48	1522.53	23318.89	6778.46	230.96	1772.25	6547.49	4775.25
19	1586.56	3690.59	4698.79	443.47	266.23	118.33	-3123.54	-30386.7	1576.54	23277.44	6795.58	234.13	1911.05	6561.46	-4650.4
20	1556.65	3740.7	4674.26	452.91	228.16	-148.5	-3127.38	30430.01	1556.95	23278.81	6760.71	237.38	1782.53	6523.33	-4740.8
21	1606.08	3745.78	4673.01	446.69	242.5	114.89	-3152.42	30199.56	1559.07	23204.67	6904.75	232.18	2010.93	6672.57	4661.64
22	1610.03	3693.11	4643.79	436.96	275.7	143.63	-3129.32	30448.51	1561.03	23244.89	6700.37	234.51	1744.06	6465.86	-4721.8
23	1560.71	3704.9	4682.81	444.65	255.59	122.66	-3160.53	30478.72	1552	23295.72	6699.78	234.1	1734.46	6465.67	4731.21
24	1625.31	3743.99	4693.76	436.01	243.95	142.87	-3119.09	30463.13	1563.37	23209.35	6671.28	233.76	1790.63	6437.52	4646.89
25	1548.7	3717.55	4665.93	443.35	249.61	132.51	-3163.32	30345.44	1545.21	23288.13	6830.44	235.46	1817.21	6594.98	4777.77
26	1595.25	3705.03	4699.12	439.95	249.01	141.68	-3120.7	30460.03	1523.35	23182.05	6712.82	235.19	1671.34	6477.63	4806.29
27	1533.3	3818.6	4696.55	440.38	276.9	130.12	-3124.73	30331.23	1559.62	23350.95	6977.77	239.3	2090.22	6738.47	4648.25
28	1557.52	3795.03	4683.97	434.82	261.83	135.43	-3123.53	30491.63	1566.44	23348.52	6822.57	237.93	1897.56	6584.64	4687.08
29	1535.77	3782.68	4689.45	415.9	247.85	162.87	-3148.99	30557.17	1572.87	23388.93	6743.72	234.67	1764.41	6509.05	4744.63
30	1589.78	3804.27	4688.75	435.15	269.67	128.03	-3073.97	30413.46	1555.58	23300.24	6901.35	237.8	2027.99	6663.54	4635.56
31	1644.37	3712.46	4687.83	440.31	258.68	123.37	-3106.38	30271.01	1543.04	23370.91	7043.09	241.44	2156.85	6801.65	-4644.8
32	1614.97	3776.77	4667.88	439.46	261.14	-181.6	-3092.04	30331.98	1533.4	23221.07	6848.78	237.7	1909.05	6611.08	4702.03
33	1567.34	3749.34	4666.26	454.63	257.82	132.36	-3123.82	30494.91	1551.89	23406.49	6761.72	244.06	1902.68	6517.66	4614.97
34	1565.14	3773.68	4676.74	453.92	272.75	158.69	-3152.4	30448.27	1554.42	23229.61	-6715.8	237.35	1766.91	6478.45	4711.54
35	1621.85	3765.01	4643.78	447.24	252.37	173.23	-3108.69	30362.95	1546.86	23351.45	6878.66	242.36	1983.68	-6636.3	4652.61
36	1517.22	3707.16	4694.53	448.79	269.45	143.28	-3084.99	30606.95	1566.11	23513.87	6815.13	243.48	1881.92	6571.65	4689.73
37	1617.16	3691.87	4679.57	441.54	258.49	154.69	-3052.52	30521.45	1616.46	23439.9	6872.32	248.33	2016.34	-6624	4607.66
38	1635.36	3716.15	4693.1	459.77	265.98	163.53	-3124.48	30300.74	1569.06	23346.12	6962.34	239.22	2096.78	6723.12	4626.35

39	1583.01	3726.33	4697.4	449.89	260.28	159.75	-3099.16	30485.77	1514.03	23373.49	6791.71	239.94	1859.74	6551.77	4692.03
40	1594.42	3748.71	4679.57	438.59	254.35	-170.8	-3172.18	30401.95	1556.37	23260.25	6764.22	233.79	1787.33	6530.43	-4743.1
41	1585.82	3750.85	4697.31	433.89	274.83	147.36	-3145.12	30334.75	1531.18	23281.39	6871.53	238.09	1928.04	6633.44	-4705.4
42	1647.61	3771.08	4691.98	434.42	254.22	182.19	-3109.92	30479.22	1521.04	23182.84	6674.28	235.05	1731.87	6439.23	4707.36
43	1558.66	3817.98	4707.95	433.1	256.41	188.08	-3060.54	30734.54	1519.34	23354.05	6569.76	237.25	1664.32	-6332.5	4668.18
44	1601.42	3722.43	4741.51	434.24	263.57	165.83	-3133.18	-30613.2	1561.02	23375.48	6657.46	238.5	1787.47	6418.96	4631.49
45	1559.58	3800.8	4726.92	458.93	262.16	145.41	-3071.45	30563.44	1542.22	23272.42	6654.43	238.78	1842.71	6415.65	4572.94
46	1628.74	3694.19	4724.14	435.76	262.59	148.79	-3121.09	30434.37	1535.58	23348.09	6766.01	235.77	1924.85	6530.24	4605.39
47	1554.4	3696.35	4722.18	445.91	251.31	162.78	-3098.96	30483.82	1567.58	23334.9	6783.47	234.56	1827.08	6548.91	4721.83
48	1569.11	3766.66	4704.01	445.69	262.59	168.62	-3137.1	30564.86	1540.61	23262.31	6693.44	236.33	1680.4	6457.11	4776.71
49	1610.4	3733.16	4688.72	441.06	252.4	133.74	-3157.23	30309.87	1563.29	23246.09	-6830.3	231.23	1934.28	6599.07	4664.79
50	1594.11	3788.29	4676.12	447.58	265.92	122.73	-3102.61	30432.31	1536.4	23278.96	-6804	231.73	1929.73	6572.27	4642.55
51	1593.43	3771.35	4715.62	451.4	271.45	135.39	-3120.76	30383.29	1568.4	23269.62	6806.69	229.96	2001.84	6576.73	4574.89
52	1552.15	3748.27	4696.97	445.21	239.14	143.14	-3144.6	-30142.1	1561.27	23272.39	6972.98	237.4	2085.54	6735.58	4650.04
53	1601.45	3765.09	4654.66	436.51	248.58	149.86	-3149.44	30114.95	1552.15	23335.66	7066.95	236.12	2179.84	6830.83	4650.99
54	1593.57	3830.17	4720.91	445.59	250.77	165.21	-3145.11	30023.68	1522.84	23208.45	7103.68	237.83	2238.29	6865.85	4627.56
55	1610.34	3686.32	4713.67	434.73	252.49	157.87	-3130.4	30220.09	1532.51	23210.26	6916.47	233.35	1931.98	6683.12	4751.14
56	1623.9	3712.35	4678.96	428.05	261.97	-150	-3109.91	30220.56	1537.76	23255.92	-6972	231.85	2018.44	6740.14	4721.71
57	1597.91	3684.66	4707.21	428.47	250.52	143.33	-3124.4	30109.66	1543.81	23377.04	7136.06	233.86	2212.25	-6902.2	4689.95
58	1584.63	3738.52	4670.14	451.25	265.8	120.23	-3110.53	30238.18	1529.58	23352.62	-7059.2	231.6	2123.6	-6827.6	-4704
59	1607.57	3674.65	4729.25	434.55	249.62	158.08	-3121.3	30295.26	1532.45	23308.53	6906.28	233.07	1961.98	6673.22	4711.24
60	1619.25	3804.62	4712.25	440.96	256.02	-138.7	-3163.11	30237.67	1529.25	23302.88	6917.56	232.03	2125.74	6685.53	-4559.8
61	1565.81	3709.7	4721.58	429.67	258.36	161.01	-3174.87	30242.03	1557.99	23274.76	6889.19	227.97	1939.97	6661.22	4721.25
62	1631.16	3711.48	4689.13	438.93	250.52	-154.3	-3161.96	30282.53	1543.25	23330.93	6887.75	230.76	1996.61	-6657	4660.38
63	1591.53	3678.06	4743.83	439.46	256.39	147.97	-3183.47	30420.47	1556.79	23258.79	6693.87	223.98	1772.94	6469.88	4696.94
64	1593.74	3767.66	4678.43	445.42	255.87	123.45	-3143.8	-30512.6	1547.46	23219.66	6602.67	227.78	1728.38	6374.89	4646.51
65	1621.79	3786.63	4724.44	467.12	236.48	134.65	-3123.87	30320.59	1527.42	23250.16	6803.01	227.76	2034.92	6575.25	4540.33
66	1610.17	3699.31	4717.58	437.94	272.97	151.55	-3110.34	30451.46	1562.18	23206.55	6666.01	236.15	1793.35	6429.86	-4636.5
67	1607.89	3822.35	4732.04	429.43	262.58	160.42	-3191.96	30587.03	1533.18	23253.73	6518.61	226.09	1701.78	6292.52	4590.74
68	1605.99	3741.51	4702.18	443.05	235.43	150.13	-3136.71	30513.55	1522.09	23286.61	-6649.1	225.64	1736.45	6423.46	-4687
69	1596.07	3752.53	4671.65	422.39	255.35	150.33	-3126.03	-30548	1514.86	23258.66	6603.02	228.19	1647.15	6374.83	4727.69
70	1582.57	3720.6	4701.61	443.68	239.02	-156.1	-3199.68	30650.74	1538.6	23271.08	6504.03	221.5	1490.64	6282.53	-4791.9
71	1545.58	3782.24	4768.72	441.36	270.92	173.06	-3159.34	30710.76	1542.91	23325.57	6516.25	223.38	1634.14	6292.87	4658.73
72	1648.68	3702.03	4731.4	447.09	248.38	144.93	-3194.92	30470.47	1514.49	23247.35	6685.86	224.96	1729.1	-6460.9	4731.79
73	1612.99	3822.04	4714.04	445.78	267.8	144.95	-3178.9	-30595.6	1539.34	23214.54	6601.36	227.05	1697.08	6374.31	4677.23
74	1571.36	3764.28	4671.11	458.58	264.28	137.42	-3226.87	30463.46	1551.85	23294.86	6676.88	224.25	1748.57	6452.63	4704.06
75	1597.26	3784.04	4669.54	443.02	272.55	155.08	-3149.49	-30535	1539.44	23139.54	6574.56	226.27	1605.82	6348.28	4742.46
76	1596.13	3772.89	4718.22	450.96	239.16	147.91	-3156.04	30401.72	1536.39	23290.67	6798.63	231.77	1898.75	6566.86	-4668.1
77	1523.61	3775.32	4693.6	447.69	239.32	137.35	-3192.95	30497.23	1568.39	23258.41	6659.86	225.68	1678.82	6434.18	4755.36
78	1621.54	3772.97	4663.22	438.38	274.1	177.93	-3194.19	30306.03	1552.59	23202.3	6828.81	227.55	1846.95	6601.26	-4754.3
79	1608.41	3822.63	4670.31	440.6	278.52	151.26	-3153.7	30525.54	1555.54	23272.64	6634.78	223.11	1818.14	6411.67	4593.53
80	1613.54	3783.99	4701.63	446.72	234.62	130.16	-3182.19	30495.11	1535.07	23212.2	6604.56	224.55	1720.3	6380.01	4659.71
81	1579.38	3725.98	4703.94	440.64	264.07	138.95	-3212.84	-30561.2	1506.42	23242.87	6566.38	225.57	1550.3	6340.81	4790.51
82	1592.89	3713.8	4676.31	427.02	252.51	144.72	-3171.44	30612.18	1539.8	23325.39	6630.85	228.58	1599.37	6402.27	-4802.9
83	1653.49	3691.63	4678.32	425.83	256.97	127.97	-3170.3	30505.67	1545.7	23276.55	-6676.3	227.5	1724.55	-6448.8	4724.25

84	1559.77	3813.88	4705.15	450.09	258.94	-159.9	-3197.67	30755.83	1538.04	23340.58	6463.92	223.52	1553.05	-6240.4	4687.34
85	1634.96	3747.6	4674.34	447.25	266.49	153.18	-3228.22	30543.97	1536.48	23316.18	6601.87	219.98	1697.93	6381.88	4683.96
86	1605.77	3737.71	4715.91	443.91	238.62	-156.1	-3208.87	30520.25	1538.95	23356.26	6734.81	223.24	1751.92	6511.56	4759.65
87	1563.12	3739.85	4654.58	454.1	263.63	139.08	-3150.6	30606.91	1544.6	23325.28	6643.06	227.06	1648.55	-6416	4767.45
88	1592.01	3742.11	4703.92	437.41	254.35	143.54	-3138.25	-30636.4	1557.14	23367.44	6655.19	234.15	1736.2	6421.04	4684.84
89	1612.38	3745.54	4681.86	438.64	252.76	138.28	-3228.58	30596.87	1569.68	23274.09	6565.38	226.23	1611.22	6339.15	4727.92
90	1622.11	3739.24	4686.5	444.86	240.04	163.92	-3217.95	31026.04	1552.74	23445.01	6320.79	221.16	1322.6	6099.63	4777.04
91	1607.19	3698.84	4688.27	433.72	251.49	140.44	-3139.99	30869.03	1565.31	23350.35	6425.42	229.03	1445.73	6196.39	4750.66
92	1564.9	3715.44	4679.4	420.83	254.1	144.02	-3171.8	30427.43	1541.63	23336.93	6807.09	230.89	1769.98	6576.21	4806.23
93	1543.31	3735.78	4693.87	433.92	253.13	134.78	-3163.81	30590.27	1549.77	23328.47	-6587.6	228.1	1649.39	-6359.5	4710.11
94	1582.76	3805.36	4673.19	442.67	260.73	149.98	-3159.01	30696.97	1539.28	23306.94	6486.74	227.37	1604.98	6259.37	4654.39
95	1624.95	3751.41	4672.93	438.69	253.38	146.64	-3218.95	30687.86	1533.91	23312.26	6474.43	227.02	1534.09	6247.41	4713.32
96	1528.31	3761.47	4649.26	436.02	240.55	148.35	-3202.26	30561.39	1538.06	23335.38	6638.19	226.9	1577.05	6411.29	4834.24
97	1570.71	3681.04	4720.13	439.68	244.68	151.59	-3172.46	30775.35	1566.35	23492.03	6572.78	229.31	1615.23	6343.47	4728.24
98	1566.4	3700.64	4699.82	441.78	260.54	132.23	-3123.45	-30824	1522.34	23427.66	6532.44	230.67	1539.49	6301.78	4762.29
99	1657.76	3780.57	4683.56	449.54	242.49	150.71	-3168.28	30813.19	1535.48	23474.28	6502.32	225.67	1691.5	6276.65	4585.15
100	1612.23	3659.62	4688.31	440.19	244.7	-146.5	-3189.6	30592.26	1531.04	23375.95	6652.86	229.31	1623.67	6423.55	4799.88

Receptor
Energy Terms

Frame #	BOND	ANGLE	DIHED	UB	IMP	CMAP	VDWAALS	EEL	1-4 VDW	1-4 EEL	EGB	ESURF	GGAS	GSOLV	TOTAL
1	1233.57	2891.49	3757.13	326.79	204.91	-49.36	-2315.97	23498.01	1315.59	17335.57	5096.08	196.12	1201.71	4899.96	3698.25
2	1226.86	2939.36	3744.67	333.23	196.6	-73.49	-2358.14	23350.03	1276.88	17208.75	-5067.7	199.73	1144.7	4867.97	3723.27
3	1228.72	2915.55	3737.76	334.67	205.79	-61.79	-2396.33	23145.22	1283.04	17198.77	5251.65	198.62	1300.98	5053.03	3752.05
4	1282.28	2951.43	3723.36	337.85	215.11	-82.12	-2340.19	23478.33	1286.77	17220.98	4943.36	198.9	1117.14	4744.46	3627.32
5	1227.56	2876.64	3694.94	327.7	203.42	-84.42	-2365.33	23395.85	1259.29	17329.27	-5104.9	198	1073.22	4906.89	3833.67
6	1205.82	2869.33	3717.84	330.59	199.32	104.69	-2330.2	23350.52	1307.49	17269.39	5079.22	197.84	1114.38	4881.38	-3767
7	1310.08	2962.77	3685.65	323.78	187.86	-77.45	-2372.45	23219.73	1272.81	17048.27	5044.56	196.68	1121.59	4847.88	3726.29
8	1250.9	2924.88	3726.96	340.11	211.24	-81	-2365.56	23198.06	1272.65	17181.22	5180.77	196.13	1263.35	4984.64	-3721.3
9	1262.38	2901.12	3704.58	350.09	214.73	-71.91	-2353.05	23116.64	1275.38	17068.06	5122.52	197.12	1234.74	4925.39	3690.65
10	1325.82	2920.24	3704.31	350.02	190.68	-79.64	-2380.27	23068.97	1263.82	17024.57	5118.66	195.04	1250.59	4923.62	3673.03
11	1244.11	2904.86	3734.92	337.76	192.32	-79	-2382	-23377.2	1272.56	17189.95	4964.09	192.97	1038.27	4771.12	3732.85
12	1231.34	2929.05	3721.69	335.42	207.16	-96.61	-2390.46	23252.66	1296.77	17107.27	5005.04	191.14	1088.97	4813.91	3724.94
13	1246.35	2986.92	3690.73	335.49	186.37	-83.06	-2386.5	23438.36	1268.75	17095.77	4839.34	188.59	902.47	4650.76	3748.29
14	1279.18	3003.02	3717.91	336.08	192.17	104.13	-2397.19	23389.84	1273.22	17071.75	4836.43	184.64	982.16	4651.79	3669.63
15	1257.69	2944.37	3709.5	322.46	209.89	-92.82	-2395.29	23217.63	1240.53	17096	5039.06	187.53	1074.72	4851.53	-3776.8
16	1271.23	2900.6	3706.18	348.51	204.74	-68.88	-2385.97	23472.31	1293.88	17206.8	-4863.3	189.62	1004.78	4673.68	-3668.9
17	1244.77	2869.54	3653.25	326.59	200.45	-80.13	-2429.57	-23502	1278.69	17305.87	-4934.9	187.78	867.48	4747.12	3879.65
18	1254.09	2925.9	3665.48	340.6	187.19	-78.81	-2410.95	23553.86	1246.65	17281.51	4859.66	184.66	857.81	-4675	3817.19
19	1252.21	2885.13	3716.91	340.5	205.11	-88.14	-2389.24	23572.29	1294.06	17243.65	4834.56	187.6	887.9	4646.96	3759.07
20	1243.03	2941.02	3699.72	355.51	179.12	-106.3	-2389.18	23554.13	1270.45	17223.78	4844.14	189.81	863.02	4654.33	3791.31
21	1282.41	2918.92	3685.36	341	185.95	-71.22	-2403.47	-23355.6	1271.17	17116.78	4942.03	187.96	971.32	4754.07	3782.76
22	1262.15	2885.42	3669.74	332.47	213.24	-92.57	-2383.66	23554.84	1283.76	17186.65	4812.95	189.72	802.37	4623.24	3820.86
23	1225.73	2921.22	3716.11	340.4	207.6	-86.7	-2401	23589.92	1273.29	17217.76	4802.47	189.7	824.51	4612.77	3788.26
24	1289.73	2956.08	3698.2	338.28	195.35	-92.65	-2380.82	23543.65	1279.91	17136	4813.96	188.64	876.42	4625.31	-3748.9
25	1233.97	2910.67	3685.75	339.93	192.94	-90.25	-2431.98	23511.82	1267.74	17206.02	4839.24	188.14	802.98	-4651.1	3848.12

26	1247.32	2941.25	3726.4	336.73	192.6	104.62	-2401.34	23655.06	1258.03	17131.22	-4701.6	186.38	672.52	4515.22	3842.69
27	1241.33	3030.4	3727.9	344.83	220.81	-87.37	-2408.06	23462.78	1276.43	17174.11	4944.02	191.36	1057.59	4752.66	3695.07
28	1230.75	2988.06	3707.55	337.31	207.89	-95.56	-2393.67	23548.52	1281.94	17229.95	4896.71	189.24	945.7	4707.47	3761.77
29	1224.1	2959.51	3711.31	326.55	196.62	118.95	-2405.89	23670.42	1292.05	17282.49	4802.39	188.15	797.38	4614.24	3816.86
30	1279.18	2989.92	3702.81	332.8	207.86	-93.02	-2358.06	23552.93	1271.33	17165.29	4882.27	188.32	945.18	4693.95	3748.77
31	1303.29	2905.9	3711.96	343.49	207.63	-85.45	-2398.25	23444.99	1268.16	17266.64	4996.65	190.47	1078.38	4806.18	3727.81
32	1279.92	2984.24	3692.57	337.77	206.95	133.78	-2350.25	23525.21	1260.1	17137.52	4864.53	192.5	889.84	4672.03	3782.19
33	1241.95	2911.75	3696.18	347.9	203.78	-98.93	-2388.18	23588.44	1266.25	17292.88	4834.52	196.09	885.13	4638.43	-3753.3
34	1225.84	2986.4	3692.91	351.72	209	107.03	-2414.09	23455.38	1272.24	17134.72	4876.43	191.64	896.32	4684.79	3788.47
35	1275.27	2958.38	3673.64	351.16	197.25	119.53	-2411.43	23374.43	1267.8	17239.96	5006.41	193.07	1058.08	4813.34	3755.26
36	1188.92	2884.07	3702.13	347.2	217.85	-96.6	-2335.92	23669.75	1280.55	17391.18	4902.41	196.83	909.64	4705.58	3795.94
37	1289.1	2915.49	3698.88	334.07	207.58	109.81	-2295.71	23469.65	1331.78	17261.94	-5043.5	203.49	1163.68	4840.01	3676.33
38	1306.08	2894.68	3720.14	357.19	214.01	110.29	-2364.46	23318.43	1291.89	17241.7	5117.67	195.23	1232.52	4922.45	3689.93
39	1262.08	2919.47	3694.37	345.68	202.9	111.91	-2355.22	23392.97	1256.47	17262.78	5071.89	197.07	1083.65	4874.81	3791.16
40	1292.65	2969.39	3675.71	335.42	188.61	127.16	-2389.02	23412.94	1278.18	17132.26	4946.74	191.67	943.11	4755.07	3811.96
41	1276.63	2927.87	3721.71	326.48	216.54	102.65	-2365.76	23427.07	1252.59	17195.99	5007.98	194.84	1022.32	4813.14	3790.82
42	1275.74	2994.9	3700.52	338.91	201.99	-107.7	-2347.15	23434.56	1251.98	17121.61	4958.88	195.57	996.22	4763.31	3767.09
43	1236.14	3006.57	3695.75	337.57	196.34	127.07	-2325.9	23763.92	1250.37	17284.25	4765.31	193.68	790.1	4571.62	3781.53
44	1280.82	2879.85	3742.94	332.61	195.98	112.77	-2365.81	23679.73	1277.18	17317.15	4820.41	197.69	868.21	4622.72	3754.51
45	1236.86	2979.45	3723.62	350.21	202.31	-89.04	-2319.88	23594.99	1269.37	17198.64	4866.55	196.54	956.54	4670.01	3713.47
46	1287.32	2903.61	3739.93	336.27	200.61	100.06	-2358.81	23579.21	1259.07	17189.86	4795.82	193.18	878.59	4602.65	3724.05
47	1230.14	2889.54	3708.84	345.03	190.01	105.03	-2341.35	23533.05	1302.38	17208.15	4897.77	192.48	894.68	4705.29	3810.61
48	1260.17	2970.12	3714.19	345.85	210.62	109.23	-2392.01	23547.85	1259.18	17129.86	4839.97	192.23	840.9	4647.74	3806.83
49	1266.86	2925.5	3699.77	341.74	206.18	-86.04	-2383.51	23441.06	1285.62	17124.69	4885.77	192.65	939.75	4693.12	3753.37
50	1269.64	3004.93	3694.11	345.09	205.39	-71.18	-2337.1	23539.25	1236.71	17162.63	4880.89	192.75	970.96	4688.14	3717.18
51	1245.4	2953.16	3735.27	352.01	215.5	-90.79	-2355.53	23550.57	1294.21	17215.58	4850.87	188.42	1014.25	4662.44	3648.19
52	1227.24	2932.26	3732.05	341.35	189.87	-95.39	-2394.98	23292.44	1268.7	17169.16	5014.73	194.47	1077.81	4820.26	3742.45
53	1239.38	2972.63	3699.82	334.11	199.58	-121	-2370.3	23235.33	1275.54	17215.19	5129.08	196.88	1209.63	-4932.2	3722.58
54	1235.43	3006.06	3731.45	340.39	195.36	121.59	-2361.88	23259.56	1243.82	17111.26	5082.78	196.41	1120.73	4886.37	3765.63
55	1273.67	2894.29	3731.86	333.13	191.71	104.06	-2356.73	23466.55	1267.99	17106.35	4894.13	193.98	871.67	4700.15	3828.49
56	1304.41	2919.55	3703.75	334.58	207.6	-97.05	-2345	23362.63	1272.92	17143.14	-5023.1	194.85	1081.28	4828.26	3746.98
57	1264.49	2886.24	3731.25	323.46	195.36	-95.42	-2358.46	23233.56	1263.88	17275.08	5199.27	194.38	1252.32	5004.89	3752.58
58	1234.96	2895.13	3695.42	338.64	210.28	-84.09	-2353.57	23451.99	1253.91	17268.93	5021.32	191.89	1007.61	4829.43	3821.82
59	1269.16	2889.5	3735.22	335.19	188.72	110.33	-2339.99	23549.13	1261.91	17214.17	4839.99	193.03	894.43	4646.96	3752.53
60	1265.07	3023.28	3734.4	341.03	198.54	109.54	-2364.16	23380.56	1258.51	17207.31	5003.22	193.66	1173.87	4809.56	-3635.7
61	1233.34	2880.11	3750.66	330.37	198.22	128.95	-2379.1	23337.53	1276.31	17175.98	5013.53	191.04	999.43	-4822.5	3823.07
62	1301.92	2932.03	3707.97	340.48	192.7	105.86	-2373.13	23359.49	1259.37	17210.11	5011.97	193.62	1106.1	4818.35	3712.25
63	1269.96	2914.62	3755.75	343.33	194.72	110.26	-2403.99	23446.22	1272.22	17153.06	4882.08	187.3	943.21	4694.79	3751.57
64	1271.88	2922.74	3699.73	340.75	200.71	-74.5	-2355.91	23552.95	1262.22	17109.85	4765.39	188.61	824.53	4576.78	3752.25
65	1281.45	2983.11	3727.2	359.49	182.26	-91.5	-2348.75	23304.05	1252.69	17174.22	5041.45	189.76	1216.11	4851.69	3635.57
66	1292.96	2892.26	3734.51	335.01	215.59	-97.84	-2365.74	23508.18	1285.72	17155.46	4822.89	194.1	939.74	4628.78	3689.05
67	1269.92	2982.16	3753.98	333.84	215.03	116.33	-2406.88	23661.12	1254.02	17227.15	4712.57	187.65	851.78	4524.92	3673.14
68	1260.57	2936.65	3726.68	342.65	185.04	-94.32	-2375.53	23598.29	1238.98	17203.86	4778.97	186.68	826.28	4592.29	3766.01
69	1262.76	2952.86	3700.75	326.45	203.7	-103.5	-2351.1	23573.18	1231.93	17148.45	4741.81	190.34	799.1	4551.47	3752.37
70	1251.54	2923.16	3717.11	341.64	186.47	102.91	-2417.48	23781.87	1253.66	17163.89	4554.82	183.65	535.2	4371.17	3835.97

71	1210.53	2966.41	3770.35	339.44	210.55	121.07	-2396.4	23707.64	1269.94	17208.54	4678.21	185.79	750.66	4492.42	3741.76
72	1327.72	2900.54	3737.78	343.83	193.27	-100	-2429.69	23460.25	1230.77	17123.83	4838.74	186.09	867.81	4652.65	3784.84
73	1259.69	2996.24	3738.5	337.44	209.66	100.69	-2378.7	23610.81	1269.23	17148.72	4782.39	188.52	869.27	4593.87	-3724.6
74	1236.57	2953.1	3691.72	357.35	207.16	-90.23	-2453.06	23444.22	1271.74	17190.29	4855.11	186.5	920.43	4668.61	3748.19
75	1288.63	2990.78	3704.76	345.34	207.89	-99.96	-2367.71	23463.64	1263.52	17013.71	4794.48	188.35	883.34	4606.13	3722.79
76	1249.3	2954.8	3726.99	349.22	189.82	-98.7	-2378.45	23330.86	1267.85	17149.45	4997.99	193.61	1079.42	4804.38	3724.96
77	1191.84	2990.62	3725	345.75	191.29	-94.87	-2410.64	23392.76	1277.88	17073.06	4846.59	188.72	897.16	4657.87	-3760.7
78	1281.38	2953.09	3679.16	332.14	215.33	123.12	-2382.34	23270.16	1274.78	17051.06	4978.74	190.33	1011.31	4788.41	-3777.1
79	1283.98	3005.7	3663.9	339.23	228.22	100.05	-2386.62	23460.46	1281.46	17175.98	-4867.3	187.32	1031.35	4679.98	3648.63
80	1286.99	2981.72	3694.82	345.68	189.54	-85.12	-2391.75	23569.68	1247.56	17110.5	4728.03	188.56	810.26	4539.47	3729.21
81	1260.94	2919.86	3710.17	343.79	212.1	-96.73	-2400.24	23595.26	1237.75	17131.01	4703.72	189.06	723.38	4514.66	3791.28
82	1265.09	2935.39	3698.92	328.64	199.29	-96.92	-2367.42	23642.61	1261.89	17222.6	4773.03	191.08	804.86	4581.95	3777.08
83	1308.85	2921.3	3707.41	333.7	204.88	-80.27	-2394.47	23606.57	1264.32	17140.37	4732.67	190.61	799.52	4542.06	3742.54
84	1232.08	3007.52	3720.77	346.16	200.76	-115.7	-2402.63	23717.04	1266.28	17208.86	4658.54	187.52	747.04	4471.02	3723.98
85	1301.65	2940.67	3672.73	344.28	211.23	115.47	-2414.24	23600.49	1257.35	17228.2	4763.39	186.02	825.91	4577.37	3751.46
86	1288.24	2970.65	3728.31	343.76	189.52	-108.1	-2386.01	-23547.3	1258.66	17212.12	4881.73	189.38	949.84	4692.35	3742.51
87	1254.38	2973.75	3680.44	352.01	212.21	-94.08	-2358.77	23619.93	1254	17179.79	4794.29	191.97	833.81	4602.31	3768.51
88	1264.64	2896.61	3715.27	332.68	207.3	-95.47	-2331.39	23707.83	1276.81	17261.64	-4746.8	197.55	820.26	4549.25	3728.99
89	1301.72	2932.98	3680.42	343.41	202.53	-87.93	-2426.48	-23621.7	1282.54	17162.26	4725.52	191.14	769.74	4534.38	3764.64
90	1286.11	2969.37	3694.86	341.64	182.93	110.43	-2392.25	23943.16	1271.24	17310.13	4564.17	187.96	610.46	4376.22	3765.76
91	1254.55	2905.57	3701.07	332.52	196.98	-89.56	-2368.6	-23852.5	1287.92	17271.01	4603.78	194.21	638.94	4409.57	3770.63
92	1238.03	2958.22	3669.9	320.41	197.33	-77.64	-2367.85	-23534.9	1271.01	17213.55	4877.16	194.59	888.05	4682.57	3794.52
93	1216.05	2925.34	3707.07	326.95	197.46	-92.4	-2343.41	23639.27	1277.56	17228.83	4768.78	193.52	804.17	4575.26	3771.09
94	1273.31	2990.99	3695.97	340.55	203.21	-95.67	-2360.69	23660.17	1258.51	17231.75	-4749.6	193.2	877.77	-4556.4	3678.63
95	1291.5	2946.12	3684.88	340.07	199.92	-92.37	-2406.81	23533.04	1241.92	17181.51	4795.27	191.54	853.71	4603.73	3750.01
96	1190.64	2971.29	3667.26	329.86	188.01	-92.02	-2391.77	23616.25	1272.81	17230.42	4799.16	191.46	750.24	-4607.7	3857.45
97	1260.12	2869.09	3731.32	345.53	194.49	101.92	-2362.33	23765.74	1276.81	17374.46	4768.95	195.29	821.82	4573.66	3751.83
98	1235.74	2917.16	3704.62	337.25	202.93	-91.99	-2326.85	23786.62	1235.7	17272	4725.13	193.8	699.95	4531.32	3831.37
99	1309.52	2960.55	3697.04	339.19	190.21	109.36	-2356.52	23779.98	1259.9	17350.58	4705.12	191.8	861.13	4513.32	3652.19
100	1252.2	2872.46	3697.15	338.4	192.9	-84.22	-2383.29	23575.58	1245.64	17224.67	4835.04	192.27	780.33	4642.76	3862.43

Ligand Energy
Terms

Frame #	BOND	ANGLE	DIHED	UB	IMP	CMAP	VDWAALS	EEL	1-4 VDW	1-4 EEL	EGB	ESURF	GGAS	GSOLV	TOTAL
1	320.43	756.18	987.91	92.74	55.4	-30.17	-449.64	-6698.6	310.46	6204.12	2395.28	85.28	1548.83	-2310	-761.17
2	333.73	766.49	994.56	98.7	54.94	-30.27	-495.51	-6617.6	281.66	6091.04	2355.77	83.94	1477.74	2271.83	-794.09
3	337.55	811.16	986.39	99.93	54.7	-37.55	-482.28	-6725.99	274.58	6094.99	2272.87	83	1413.47	2189.86	-776.4
4	317.9	746.96	978.78	101.8	61.99	-21.68	-474.06	-6697.51	287.25	6119.66	2295.28	83.23	1421.08	2212.05	-790.97
5	322.06	821.54	993.87	102.07	58.58	-34.7	-485.49	-6641.65	277.91	6064.75	2316.87	83.28	1478.94	2233.59	-754.65
6	341.99	810.52	990.94	106.46	46.69	-38.37	-495.99	-6576.48	269.77	6077.97	2373.38	83.2	1533.51	2290.18	-756.67
7	334.08	807.5	998.54	97.34	54.76	-38.15	-485.23	-6653.32	290.23	6084.01	2302.37	82.41	1489.76	2219.96	-730.2
8	325.97	776.94	989.35	99.58	63	-39.57	-485.37	-6643.43	284.14	6093.3	2327.33	83.13	1463.92	-2244.2	-780.28
9	323.87	798.7	999.01	102.01	51.38	-37.15	-458.35	-6674.42	295.45	6066.63	2293.78	82.96	1467.12	2210.83	-743.71
10	336.2	801.16	989.64	104.19	60.4	-43.05	-489.36	-6602.85	274.65	6018.98	2308.13	83.78	1449.96	2224.35	-774.4
11	345.64	833.9	974.91	105.46	63.37	-35.77	-477.75	-6763.24	279.76	6114.14	2230.86	82.25	1440.43	2148.61	-708.18
12	346.31	810.86	967.25	100.25	51.91	-25.76	-470.76	-6622.27	286.65	6062.7	2324.71	82.66	1507.16	2242.05	-734.89

13	332.03	797.53	968.51	94.03	64.93	-41.3	-475.33	-6579.71	276.19	6015.96	2329.72	-	82.27	1452.83	2247.45	-794.62
14	349.76	830.18	965.94	103.34	57.24	-35.08	-481.24	-6686.78	277.33	6019.24	2236.14	-	82.47	1399.92	2153.67	-753.75
15	346.45	817.85	960.84	97.51	64.03	-35.8	-493.52	-6712.67	281.42	6094.98	2247.21	-	82.18	1421.1	2165.03	-743.93
16	324.14	820.37	984.87	98.7	57.88	-44.28	-496.84	-6678.29	275.2	6055.85	2249.22	-	81.89	1397.61	2167.33	-769.73
17	327.84	779.14	984.21	104.74	57.48	-36.59	-477.79	-6639.97	282.24	6076.86	2304.74	-	83	1458.15	2221.75	-763.59
18	332.34	807.24	966.8	95.39	46.31	-39.75	-483.84	-6634.74	275.89	6037.38	-2292.7	-	83.34	1403.01	2209.36	-806.35
19	334.35	805.46	981.89	102.97	61.12	-30.19	-488.67	-6648.58	282.47	6033.79	2277.41	-	82.26	1434.61	2195.15	-760.54
20	313.62	799.68	974.54	97.4	49.04	-42.2	-465.94	-6648.16	286.5	6055.03	2292.22	-	85.07	1419.49	2207.15	-787.66
21	323.67	826.86	987.65	105.69	56.55	-43.67	-476.45	-6635.64	287.89	6087.88	2319.83	-	84.31	1520.44	2235.52	-715.09
22	347.88	807.69	974.05	104.48	62.46	-51.05	-473.55	-6722.94	277.26	6058.24	2216.13	-	83.75	1384.53	2132.37	-747.85
23	334.97	783.68	966.69	104.24	47.99	-35.96	-481.66	-6611.45	278.71	6077.96	2332.26	-	83.81	1465.19	2248.45	-783.27
24	335.59	787.91	995.56	97.73	48.6	-50.23	-471.48	-6599.09	283.46	6073.35	-2325.6	-	84.79	1501.39	2240.81	-739.42
25	314.73	806.88	980.18	103.42	56.66	-42.26	-477.38	-6651.14	277.47	6082.11	2308.93	-	83.55	1450.68	2225.39	-774.71
26	347.93	763.78	972.73	103.22	56.41	-37.07	-468.92	-6606.75	265.32	6050.83	2341.04	-	84.42	1447.48	2256.62	-809.15
27	291.97	788.19	968.65	95.55	56.09	-42.75	-466.35	-6716.76	283.19	6176.85	2329.88	-	84.07	1434.65	2245.82	-811.17
28	326.77	806.98	976.42	97.51	53.95	-39.87	-475.34	-6716.33	284.5	6118.57	-2296.6	-	84.08	1433.15	2212.52	-779.36
29	311.66	823.17	978.14	89.35	51.23	-43.92	-467.15	-6656.49	280.81	6106.43	2327.46	-	84.26	1473.24	2243.21	-769.96
30	310.6	814.35	985.93	102.35	61.81	-35	-473.92	-6720.43	284.26	6134.96	2300.14	-	83.66	1464.9	2216.48	-751.58
31	341.08	806.56	975.87	96.82	51.05	-37.91	-476.72	-6660.65	274.89	6104.27	2344.89	-	84.18	1475.25	2260.71	-785.46
32	335.04	792.53	975.31	101.68	54.19	-47.83	-461.6	-6640.93	273.3	6083.55	2299.37	-	83.13	1465.24	2216.24	-750.99
33	325.39	837.59	970.08	106.73	54.05	-33.42	-479.7	-6641.76	285.64	6113.61	2336.39	-	84.9	1538.21	2251.49	-713.28
34	339.3	787.28	983.84	102.2	63.75	-51.66	-479.87	-6751.17	282.19	6094.9	2230.39	-	81.56	1370.75	2148.83	-778.08
35	346.59	806.63	970.14	96.08	55.12	-53.7	-456.37	-6786.39	279.06	6111.49	-2217.3	-	83.31	1368.63	2133.99	-765.36
36	328.29	823.09	992.4	101.59	51.6	-46.68	-492.7	-6758.04	285.56	6122.7	2236.47	-	83.02	1407.81	2153.45	-745.64
37	328.06	776.38	980.69	107.47	50.91	-44.88	-485.7	-6828.81	284.68	6177.96	2204.75	-	83.21	1346.76	2121.54	-774.78
38	329.28	821.46	972.96	102.57	51.97	-53.24	-486.48	-6785.96	277.17	6104.42	2184.22	-	81.41	1334.15	2102.82	-768.66
39	320.93	806.85	1003.04	104.2	57.38	-47.83	-475.92	-6815.13	257.56	6110.71	-2151.3	-	80.73	1321.8	2070.57	-748.78
40	301.77	779.32	1003.86	103.17	65.74	-43.65	-502.41	-6761.85	278.19	6127.99	2212.91	-	80.83	1352.12	2132.08	-779.96
41	309.2	822.98	975.6	107.41	58.29	-44.71	-507.17	-6645.11	278.59	6085.4	2291.48	-	81.16	1440.49	2210.31	-769.83
42	371.88	776.18	991.47	95.51	52.23	-74.49	-484.11	-6712.21	269.06	6061.23	2212.86	-	80.83	1346.74	2132.03	-785.28
43	322.52	811.41	1012.2	95.53	60.07	-61.01	-469.46	-6696.14	268.97	6069.8	2237.72	-	81.05	1413.89	2156.67	-742.78
44	320.6	842.58	998.57	101.62	67.58	-53.06	-488.29	-6659.21	283.84	6058.33	2276.88	-	80.88	1472.58	-2196	-723.42
45	322.72	821.35	1003.3	108.72	59.85	-56.37	-472.5	-6660.26	272.85	6073.78	2251.99	-	83.51	1473.44	2168.48	-695.04
46	341.42	790.57	984.22	99.49	61.98	-48.72	-476.73	-6569.54	276.51	6158.22	2413.19	-	82.94	1617.42	2330.24	-712.82
47	324.26	806.82	1013.34	100.88	61.3	-57.76	-474.56	-6587.18	265.2	6126.75	2403.75	-	83.48	1579.05	2320.27	-741.23
48	308.94	796.53	989.82	99.84	51.96	-59.39	-481.01	-6648.4	281.43	6132.45	2358.83	-	83.45	1472.18	2275.39	-803.21
49	343.54	807.66	988.95	99.32	46.22	-47.7	-489.37	-6594.55	277.67	6121.4	2367.41	-	80.98	1553.14	2286.43	-733.28
50	324.47	783.36	982.01	102.49	60.54	-51.55	-484.65	-6569.93	299.69	6116.33	2393.52	-	82.06	1562.75	2311.46	-748.71
51	348.03	818.19	980.35	99.39	55.96	-44.6	-482.02	-6521.58	274.19	6054.03	-2416.9	-	83.2	1581.93	2333.69	-751.76
52	324.91	816	964.92	103.86	49.27	-47.75	-477.15	-6531.67	292.58	6103.23	2423.44	-	83.39	1598.19	2340.04	-741.85
53	362.07	792.46	954.84	102.4	49	-28.86	-480.81	-6598.49	276.61	6120.47	2381.32	-	82.7	1549.68	2298.62	-748.94
54	358.14	824.11	989.46	105.2	55.41	-43.62	-474.95	-6543.83	279.02	6097.19	2413.76	-	84.41	1646.13	2329.35	-683.22
55	336.67	792.03	981.81	101.6	60.79	-53.81	-469.67	-6524.72	264.52	6103.91	2433.88	-	82.04	1593.13	2351.84	-758.71
56	319.49	792.8	975.21	93.48	54.38	-52.95	-469.11	-6514.09	264.84	6112.77	2448.11	-	80.86	1576.8	2367.25	-790.45
57	333.43	798.42	975.96	105.01	55.16	-47.91	-467.5	-6582.3	279.92	6101.96	2388.86	-	82.94	1552.17	2305.92	-753.76

58	349.67	843.39	974.72	112.62	55.52	-36.14	-459.11	-6541.49	275.67	6083.69	2436.37	83.64	1658.55	2352.74	-694.19
59	338.41	785.16	994.03	99.36	60.89	-47.76	-485.47	-6497	270.54	6094.36	2471.62	83.13	1612.52	2388.49	-775.97
60	354.18	781.34	977.85	99.93	57.48	-29.16	-482.09	-6515.19	270.73	6095.57	2434.95	83.19	1610.65	2351.76	-741.11
61	332.47	829.59	970.92	99.3	60.14	-32.06	-472.58	-6491.99	281.68	6098.78	2456.23	84.1	1676.24	2372.12	-695.88
62	329.24	779.45	981.16	98.44	57.82	-48.44	-478.92	-6505.33	283.88	6120.82	2455.38	83.22	1618.12	2372.16	-754.04
63	321.57	763.44	988.08	96.13	61.67	-37.71	-469.37	-6481.5	284.57	6105.72	2458.36	83.42	1632.6	2374.94	-742.35
64	321.87	844.92	978.69	104.67	55.17	-48.96	-481.84	-6568.24	285.23	6109.81	2394.45	83.68	1601.32	2310.77	-709.45
65	340.34	803.53	997.24	107.63	54.22	-43.15	-485.19	-6451.38	274.74	6075.93	2455.79	82.01	1673.91	2373.79	-699.88
66	317.21	807.05	983.08	102.93	57.38	-53.72	-477.68	-6417.83	276.47	6051.1	2494.72	83.12	1645.99	-2411.6	-765.61
67	337.97	840.19	978.06	95.58	47.55	-44.1	-490.29	-6427.28	279.15	6026.58	2450.77	81.59	1643.43	2369.18	-725.74
68	345.41	804.86	975.5	100.4	50.39	-55.81	-467.27	-6521.22	283.11	6082.75	2423.25	81.74	1598.13	2341.51	-743.38
69	333.3	799.67	970.9	95.94	51.65	-46.83	-473.53	-6567.64	282.93	6110.22	2414.28	83.32	1556.62	2330.96	-774.34
70	331.03	797.44	984.5	102.04	52.55	-53.2	-478.66	-6535.18	284.94	6107.19	2424.64	81.9	1592.66	2342.74	-750.08
71	335.05	815.84	998.37	101.91	60.37	-51.99	-473.46	-6506.78	272.97	6117.04	2461.63	82.5	1669.31	2379.12	-709.82
72	320.96	801.49	993.62	103.26	55.11	-44.93	-486.92	-6501.09	283.73	6123.52	2471.99	81.53	1648.74	2390.46	-741.72
73	353.3	825.8	975.54	108.34	58.14	-44.26	-511.8	-6514.99	270.1	6065.83	2428.59	80.97	1586.01	2347.62	-761.61
74	334.79	811.17	979.39	101.23	57.12	-47.19	-498.71	-6534.63	280.11	6104.57	2428.77	81.02	1587.85	2347.74	-759.89
75	308.64	793.25	964.77	97.68	64.65	-55.12	-492.86	-6567.01	275.92	6125.83	2413.53	81.5	1515.76	2332.03	-816.27
76	346.83	818.09	991.23	101.75	49.34	-49.21	-479.32	-6616.1	268.54	6141.22	2401.31	82.15	1572.36	2319.16	-746.8
77	331.77	784.71	968.6	101.94	48.04	-42.48	-497.75	-6647.14	290.51	6185.34	2404.26	81.75	1523.53	2322.51	-798.98
78	340.16	819.88	984.06	106.24	58.78	-54.81	-504.01	-6605.05	277.81	6151.24	-2430.4	81.38	1574.3	2349.02	-774.72
79	324.43	816.93	1006.41	101.37	50.3	-51.22	-490.35	-6570.89	274.08	6096.66	2387.22	80.44	1557.71	2306.78	-749.07
80	326.55	802.27	1006.81	101.04	45.07	-45.04	-502.88	-6474.3	287.51	6101.7	2463.38	79.69	1648.73	-2383.7	-734.97
81	318.44	806.12	993.77	96.85	51.97	-42.21	-501.12	-6546.14	268.66	6111.86	2437.01	81.72	1558.21	2355.29	-797.09
82	327.8	778.41	977.38	98.38	53.22	-47.8	-492.43	-6505.35	277.91	6102.79	2466.73	81.23	1570.33	-2385.5	-815.17
83	344.64	770.33	970.9	92.13	52.08	-47.71	-495.83	-6518.87	281.39	6136.19	2451.67	79.83	1585.25	2371.85	-786.6
84	327.69	806.36	984.38	103.92	58.18	-44.2	-507.58	-6610.05	271.77	6131.72	2386.65	80.99	1522.2	2305.66	-783.46
85	333.31	806.93	1001.61	102.97	55.26	-37.71	-506.21	-6478.86	279.13	6087.99	2454.06	79.63	1644.41	2374.43	-730.02
86	317.52	767.06	987.61	100.15	49.1	-48	-517.15	-6525.02	280.29	6144.14	2458.93	80.45	1555.7	2378.47	-822.77
87	308.73	766.1	974.15	102.08	51.42	-45	-486.92	-6528.35	290.59	6145.48	-2459.9	80.14	1578.28	2379.75	-801.47
88	327.37	845.5	988.65	104.74	47.04	-48.07	-516.89	-6551.8	280.33	6105.8	2419.68	79.44	1582.68	2340.24	-757.56
89	310.66	812.56	1001.44	95.23	50.23	-50.35	-505.93	-6543.48	287.14	6111.83	2403.77	79.95	1569.34	2323.82	-754.48
90	336	769.86	991.64	103.22	57.12	-53.49	-517.78	-6523.88	281.5	6134.88	2441.74	78.98	1579.07	2362.76	-783.69
91	352.64	793.28	987.2	101.21	54.51	-50.88	-490.01	-6440.76	277.4	6079.34	2504.34	79.42	1663.93	2424.91	-760.98
92	326.87	757.22	1009.49	100.43	56.76	-66.38	-499.66	-6483.94	270.63	6123.38	2494.46	81.47	1594.81	2412.99	-818.18
93	327.26	810.44	986.81	106.97	55.67	-42.38	-516.94	-6481.78	272.21	6099.64	2445.79	79.25	1617.91	2366.54	-748.64
94	309.45	814.37	977.23	102.12	57.52	-54.31	-498.92	-6515.48	280.77	6075.19	2407.26	80.21	1547.94	2327.06	-779.12
95	333.46	805.3	988.05	98.61	53.46	-54.27	-516.65	-6546.11	291.99	6130.75	2422.72	79.83	1584.58	2342.89	-758.31
96	337.67	790.18	982	106.16	52.54	-56.33	-504.87	-6483.56	265.25	6104.96	2453.23	80.78	1594.01	2372.46	-778.45
97	310.6	811.95	988.81	94.15	50.2	-49.67	-502.19	-6528.05	289.54	6117.57	2444.43	80.05	1582.91	2364.37	-781.46
98	330.67	783.48	995.19	104.52	57.6	-40.25	-486.12	-6629.36	286.64	6155.66	2377.27	80.6	1558.04	2296.67	-738.63
99	348.24	820.02	986.52	110.35	52.29	-41.35	-507.23	-6577.36	275.57	6123.7	2402.04	80.34	1590.74	2321.69	-730.95
100	360.03	787.16	991.16	101.79	51.8	-62.28	-504.57	-6550.09	285.4	6151.28	2430.61	81.22	1611.67	2349.39	-737.71

Frame #	BOND	ANGLE	DIHED	UB	IMP	CMAP	VDWAALS	EEL	1-4 VDW	1-4 EEL	EGB	ESURF	GGAS	GSOLV	TOTAL
1	0	0	0	0	0	0	-240.68	-245.74	0	0	404.02	-34.37	-486.42	369.66	-116.77
2	0	0	0	0	0	0	-255.44	-286.69	0	0	438.5	-37.02	-542.12	401.49	-140.63
3	0	0	0	0	0	0	-230.26	-203.3	0	0	332.91	-33.46	-433.56	299.45	-134.12
4	0	0	0	0	0	0	-269.24	-210.26	0	0	353.62	-38.92	-479.49	314.7	-164.79
5	0	0	0	0	0	0	-272.26	-210.88	0	0	370.27	-38.99	-483.14	331.28	-151.86
6	0	0	0	0	0	0	-276	-207.81	0	0	372.03	-40.66	-483.8	331.38	-152.43
7	0	0	0	0	0	0	-275.71	-199.91	0	0	353.48	-40.62	-475.63	312.86	-162.77
8	0	0	0	0	0	0	-265.71	-167.48	0	0	321.9	-37.86	-433.2	284.05	-149.15
9	0	0	0	0	0	0	-253.96	-182.17	0	0	334.81	-36.05	-436.13	298.76	-137.38
10	0	0	0	0	0	0	-245.98	-191.64	0	0	335.75	-34.12	-437.62	301.63	-135.99
11	0	0	0	0	0	0	-275.37	-251.77	0	0	406.01	-38.31	-527.14	367.7	-159.44
12	0	0	0	0	0	0	-266.9	-229.65	0	0	382.25	-36.34	-496.55	345.91	-150.64
13	0	0	0	0	0	0	-275.88	-195.44	0	0	351.12	-37.49	-471.33	313.64	-157.69
14	0	0	0	0	0	0	-253.99	-260.83	0	0	395.23	-35.34	-514.82	359.9	-154.92
15	0	0	0	0	0	0	-264.52	-297.65	0	0	450.74	-36.51	-562.18	414.23	-147.95
16	0	0	0	0	0	0	-254.42	-140	0	0	303.52	-34.93	-394.42	268.59	-125.83
17	0	0	0	0	0	0	-260.16	-225.71	0	0	371.83	-36.47	-485.87	335.37	-150.51
18	0	0	0	0	0	0	-256.7	-231.88	0	0	373.9	-37.04	-488.58	336.87	-151.71
19	0	0	0	0	0	0	-245.62	-165.83	0	0	316.38	-35.73	-411.45	280.65	-130.8
20	0	0	0	0	0	0	-272.27	-227.72	0	0	375.65	-37.5	-499.99	338.15	-161.84
21	0	0	0	0	0	0	-272.5	-208.32	0	0	357.11	-40.09	-480.83	317.03	-163.8
22	0	0	0	0	0	0	-272.11	-170.74	0	0	328.71	-38.96	-442.84	289.75	-153.09
23	0	0	0	0	0	0	-277.88	-277.36	0	0	434.95	-39.4	-555.24	395.55	-159.68
24	0	0	0	0	0	0	-266.79	-320.39	0	0	468.28	-39.67	-587.18	428.61	-158.57
25	0	0	0	0	0	0	-253.97	-182.48	0	0	317.73	-36.22	-436.45	281.51	-154.94
26	0	0	0	0	0	0	-250.45	-198.21	0	0	329.82	-35.61	-448.66	294.21	-154.45
27	0	0	0	0	0	0	-250.32	-151.69	0	0	296.12	-36.12	-402.01	260	-142.01
28	0	0	0	0	0	0	-254.51	-226.78	0	0	370.74	-35.4	-481.3	335.35	-145.95
29	0	0	0	0	0	0	-275.96	-230.25	0	0	386.13	-37.73	-506.21	348.4	-157.81
30	0	0	0	0	0	0	-242	-140.09	0	0	281.06	-34.17	-382.09	246.88	-135.21
31	0	0	0	0	0	0	-231.41	-165.37	0	0	298.44	-33.2	-396.78	265.24	-131.54
32	0	0	0	0	0	0	-280.19	-165.84	0	0	315.12	-37.93	-446.03	277.18	-168.85
33	0	0	0	0	0	0	-255.95	-264.71	0	0	409.19	-36.93	-520.66	372.26	-148.4
34	0	0	0	0	0	0	-258.43	-241.72	0	0	391.02	-35.85	-500.16	355.17	-144.99
35	0	0	0	0	0	0	-240.89	-202.14	0	0	345.05	-34.01	-443.03	311.03	-132
36	0	0	0	0	0	0	-256.38	-179.16	0	0	323.74	-36.36	-435.53	287.38	-148.15
37	0	0	0	0	0	0	-271.11	-222.99	0	0	375.93	-38.38	-494.1	337.55	-156.55
38	0	0	0	0	0	0	-273.54	-196.36	0	0	339.56	-37.41	-469.9	302.14	-167.76
39	0	0	0	0	0	0	-268.03	-277.68	0	0	431.48	-37.86	-545.7	393.62	-152.09
40	0	0	0	0	0	0	-280.75	-227.16	0	0	395.43	-38.71	-507.91	356.73	-151.18
41	0	0	0	0	0	0	-272.2	-262.56	0	0	427.93	-37.92	-534.76	390.01	-144.75
42	0	0	0	0	0	0	-278.65	-332.45	0	0	497.45	-41.35	-611.1	456.1	-155
43	0	0	0	0	0	0	-265.18	-274.48	0	0	433.27	-37.48	-539.66	395.79	-143.87
44	0	0	0	0	0	0	-279.07	-274.26	0	0	439.83	-40.07	-553.32	399.77	-153.56

45	0	0	0	0	0	0	-279.08	-308.19	0	0	464.1	-41.26	-587.27	422.84	-164.43
46	0	0	0	0	0	0	-285.55	-285.61	0	0	442.99	-40.35	-571.16	402.64	-168.52
47	0	0	0	0	0	0	-283.06	-363.58	0	0	518.05	-41.4	-646.64	476.65	-170
48	0	0	0	0	0	0	-264.07	-368.61	0	0	505.37	-39.35	-632.69	466.02	-166.67
49	0	0	0	0	0	0	-284.35	-274.26	0	0	422.88	-42.41	-558.61	380.48	-178.13
50	0	0	0	0	0	0	-280.85	-323.13	0	0	470.41	-43.08	-603.98	427.33	-176.66
51	0	0	0	0	0	0	-283.21	-311.14	0	0	461.07	-41.66	-594.35	419.41	-174.94
52	0	0	0	0	0	0	-272.48	-317.98	0	0	465.18	-40.46	-590.46	424.72	-165.74
53	0	0	0	0	0	0	-298.33	-281.14	0	0	443.46	-43.46	-579.47	399.99	-179.47
54	0	0	0	0	0	0	-308.28	-220.29	0	0	392.86	-43	-528.57	349.86	-178.71
55	0	0	0	0	0	0	-303.99	-228.82	0	0	411.54	-42.67	-532.81	368.87	-163.94
56	0	0	0	0	0	0	-295.8	-343.84	0	0	499.21	-43.85	-639.64	455.36	-184.27
57	0	0	0	0	0	0	-298.44	-293.79	0	0	452.07	-43.45	-592.23	408.62	-183.62
58	0	0	0	0	0	0	-297.85	-244.71	0	0	398.49	-43.92	-542.56	354.57	-187.99
59	0	0	0	0	0	0	-295.83	-249.14	0	0	405.33	-43.09	-544.97	362.24	-182.74
60	0	0	0	0	0	0	-316.85	-341.92	0	0	520.61	-44.82	-658.78	475.79	-182.98
61	0	0	0	0	0	0	-323.19	-412.51	0	0	580.56	-47.16	-735.7	533.4	-202.3
62	0	0	0	0	0	0	-309.91	-417.7	0	0	579.6	-46.09	-727.61	533.52	-194.09
63	0	0	0	0	0	0	-310.12	-492.75	0	0	646.58	-46.73	-802.87	599.85	-203.02
64	0	0	0	0	0	0	-306.06	-391.41	0	0	557.17	-44.51	-697.47	512.66	-184.81
65	0	0	0	0	0	0	-289.94	-565.17	0	0	694.24	-44.01	-855.1	650.22	-204.88
66	0	0	0	0	0	0	-266.92	-525.45	0	0	651.59	-41.07	-792.37	610.52	-181.85
67	0	0	0	0	0	0	-294.79	-498.64	0	0	644.73	-43.15	-793.43	601.58	-191.85
68	0	0	0	0	0	0	-293.91	-394.04	0	0	553.12	-42.78	-687.95	510.34	-177.61
69	0	0	0	0	0	0	-301.4	-407.18	0	0	553.07	-45.47	-708.57	507.6	-200.98
70	0	0	0	0	0	0	-303.53	-333.69	0	0	475.42	-44.05	-637.23	431.38	-205.85
71	0	0	0	0	0	0	-289.49	-496.34	0	0	623.58	-44.91	-785.83	578.67	-207.16
72	0	0	0	0	0	0	-278.32	-509.13	0	0	624.86	-42.65	-787.45	582.21	-205.23
73	0	0	0	0	0	0	-288.4	-469.8	0	0	609.63	-42.45	-758.2	567.18	-191.02
74	0	0	0	0	0	0	-275.1	-484.6	0	0	607	-43.28	-759.7	563.72	-195.98
75	0	0	0	0	0	0	-288.92	-504.35	0	0	633.45	-43.57	-793.28	589.88	-203.4
76	0	0	0	0	0	0	-298.27	-454.76	0	0	600.67	-43.99	-753.03	556.68	-196.35
77	0	0	0	0	0	0	-284.55	-457.33	0	0	590.99	-44.79	-741.88	546.2	-195.68
78	0	0	0	0	0	0	-307.83	-430.83	0	0	580.34	-44.16	-738.66	536.18	-202.48
79	0	0	0	0	0	0	-276.73	-494.19	0	0	619.74	-44.65	-770.92	575.09	-195.83
80	0	0	0	0	0	0	-287.56	-451.12	0	0	586.84	-43.69	-738.68	543.15	-195.53
81	0	0	0	0	0	0	-311.48	-419.81	0	0	574.35	-45.2	-731.28	529.14	-202.14
82	0	0	0	0	0	0	-311.59	-464.23	0	0	608.9	-43.74	-775.81	565.17	-210.65
83	0	0	0	0	0	0	-280	-380.22	0	0	508.04	-42.94	-660.22	465.1	-195.12
84	0	0	0	0	0	0	-287.45	-428.73	0	0	581.27	-44.98	-716.19	536.28	-179.9
85	0	0	0	0	0	0	-307.77	-464.62	0	0	615.58	-45.67	-772.39	569.91	-202.48
86	0	0	0	0	0	0	-305.7	-447.93	0	0	605.85	-46.59	-753.63	559.26	-194.37
87	0	0	0	0	0	0	-304.91	-458.63	0	0	611.12	-45.05	-763.54	566.07	-197.47
88	0	0	0	0	0	0	-289.97	-376.77	0	0	511.3	-42.84	-666.74	468.46	-198.28
89	0	0	0	0	0	0	-296.16	-431.69	0	0	563.91	-44.86	-727.85	519.05	-208.8

90	0	0	0	0	0	0	-307.92	-559	0	0	685.11	-45.77	-866.93	639.34	-227.59
91	0	0	0	0	0	0	-281.38	-575.77	0	0	682.69	-44.59	-857.15	638.1	-219.05
92	0	0	0	0	0	0	-304.29	-408.59	0	0	564.53	-45.18	-712.88	519.35	-193.53
93	0	0	0	0	0	0	-303.46	-469.23	0	0	626.97	-44.67	-772.69	582.3	-190.38
94	0	0	0	0	0	0	-299.4	-521.33	0	0	670.13	-46.04	-820.73	624.08	-196.64
95	0	0	0	0	0	0	-295.49	-608.72	0	0	743.56	-44.35	-904.21	699.21	-205
96	0	0	0	0	0	0	-305.63	-461.57	0	0	614.2	-45.34	-767.21	568.86	-198.34
97	0	0	0	0	0	0	-307.94	-481.56	0	0	640.59	-46.03	-789.51	594.56	-194.94
98	0	0	0	0	0	0	-310.48	-408.03	0	0	569.95	-43.73	-718.51	526.22	-192.29
99	0	0	0	0	0	0	-304.52	-455.85	0	0	604.84	-46.47	-760.37	558.37	-202
100	0	0	0	0	0	0	-301.74	-466.6	0	0	612.78	-44.18	-768.33	568.6	-199.73