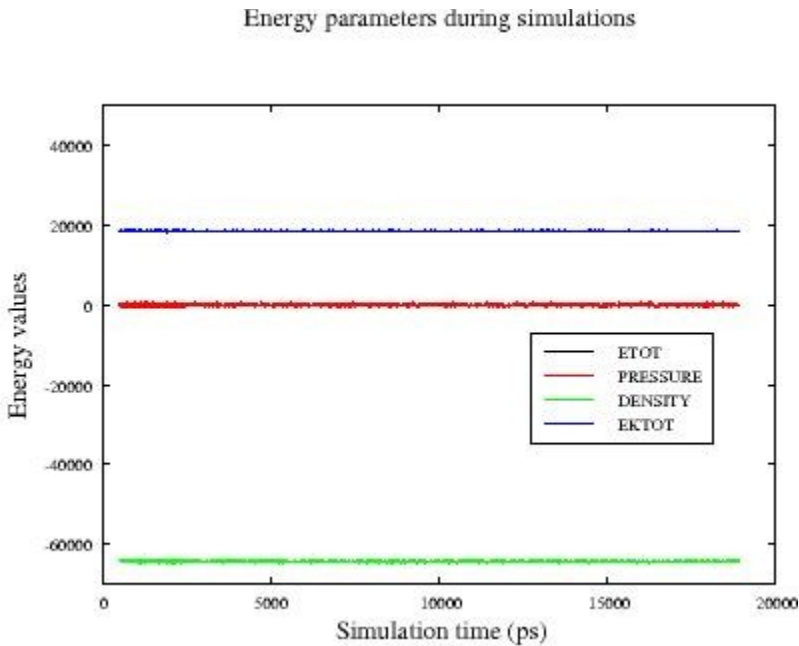


Molecular Docking, MD simulations and Free Energy Calculations of DENV inhibitor for a novel binding Site

Kshatresh Dutta Dubey\*, Gargi Tiwari and Rajendra Prasad Ojha

Supplementary materials

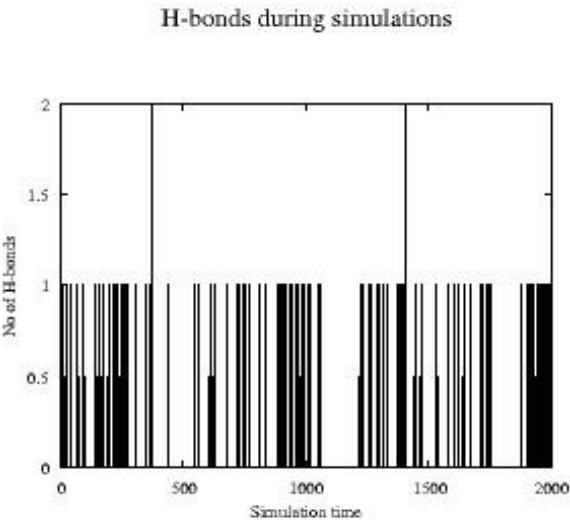
**Figure 1S.** The variation of energy parameters during simulation. We notice that all energy parameters are constant, which represents a well equilibrated system.



**Table 1S.** Details of hydrogen bonds for R1

Donor	acceptor	occupancy
THR176-Main	R1396-Side	14.94%
HIE158-Side	R1396-Side	3.09%
THR176-Side	R1396-Side	6.27%
LYS160-Side	R1396-Side	0.18%
LYS295-Side	R1396-Side	5.04%
SER145-Side	R1396-Side	0.27%

**Figure 2S.** Hydrogen bonds for R1

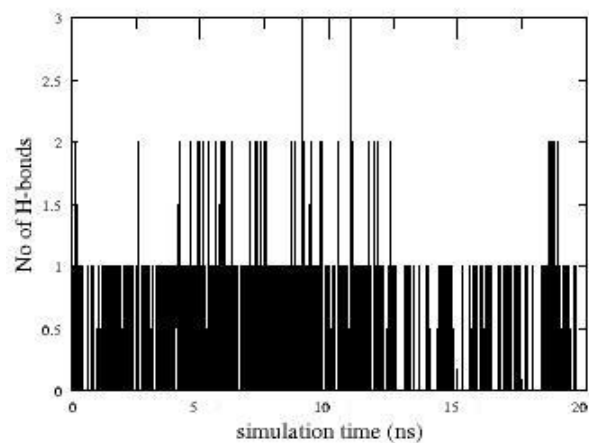


**Table 2S.** Details of hydrogen bonds for R2

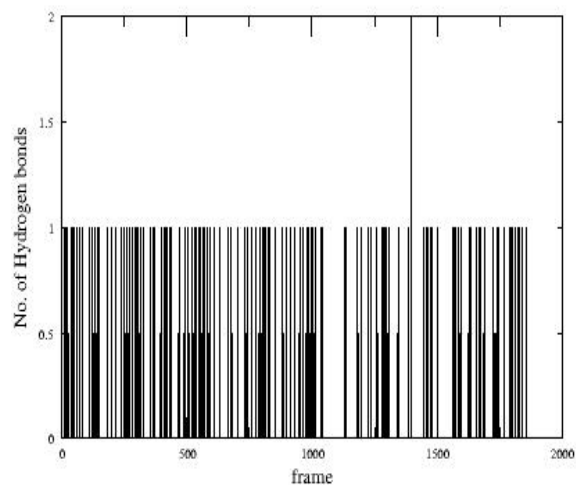
Donor	Acceptor	occupancy
THR176-Main	R2396-Side	9.79%
R2395-Side	LYS157-Main	12.75%
ASN153-Side	R2396-Side	0.20%
HIE149-Side	R2396-Side	0.36%
R2396-Side	ASN153-Side	0.10%
R2396-Side	HIE158-Main	3.11%
R2396-Side	HIE158-Side	0.66%

**Figure 3S.** Variation of hydrogen bond for R2

R2 complex with DENV receptor: H-Bonds vs. Frame

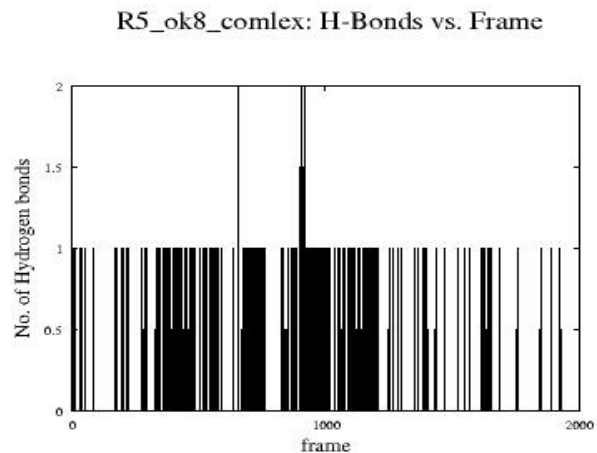
**Hydrogen bonds for R3**

donor	acceptor	occupancy
THR176-Main	R4396-Side	3.37%
LYS295-Side	R4396-Side	0.72%
THR176-Side	R4396-Side	0.50%
R4396-Side	LYS157-Main	0.06%

**R3\_ok8\_complex: H bond Vs frame****R4\_ok8\_complex : H-Bonds vs. Frame****Hydrogen bonds for R4**

donor	acceptor	occupancy
THR359-Side	R5396-Side	0.05%
THR176-Main	R5396-Side	2.19%
SER145-Side	R5396-Side	0.48%
R5396-Side	LYS157-Main	4.55%
R5396-Side	HIE158-Main	0.21%
R5396-Side	GLY159-Main	0.32%
THR176-Side	R5396-Side	0.32%
R5396-Side	THR176-Side	0.11%
HIE160-Side	R5396-Side	0.05%

Hydrogen bonds for R5		
donor	acceptor	occupancy
LYS295-Side	R6396-Side	0.39%
THR359-Side	R6396-Side	0.07%
THR176-Main	R6396-Side	5.23%
R6396-Side	LYS157-Main	1.47%
THR176-Side	R6396-Side	0.85%
R6396-Side	GLY156-Main	0.03%
LYS160-Side	R6396-Side	0.03%
LYS157-Side	R6396-Side	0.13%



#### cavity\_1\_KTNEGHSDVIQRLMCFY

Cavity point -16.043 68.631 -6.310

Volume of the Cavity = 1248

1	ARG	10	2HD	-9.314	72.484	-17.350
2	ARG	10	2HB	-8.482	71.718	-15.077
3	ARG	10	3HD	-7.738	72.544	-18.174
4	ARG	10	3HB	-6.928	72.204	-15.795
5	ARG	10	H	-5.904	71.885	-13.565
6	ARG	10	O	-4.658	70.551	-15.605
7	ASP	11	OD2	-4.155	66.697	-13.291
8	ASP	11	OD1	-2.434	67.598	-14.376
9	LEU	136	3HD2	-14.022	54.754	-0.974
10	GLU	137	O	-17.687	55.350	-4.563
11	TYR	138	HE2	-11.916	56.935	-4.848
12	THR	139	1HG	-21.806	58.757	-7.160
13	THR	139	3HG2	-20.706	60.626	-9.921
14	VAL	141	1HG1	-20.776	64.248	-16.019
15	VAL	141	2HG2	-20.991	64.727	-13.061
16	THR	143	1HG	-19.125	67.243	-18.003
17	VAL	152	O	-19.037	76.893	-19.089
18	GLY	153	O	-18.809	74.763	-15.209
19	ASN	154	1HD2	-25.339	74.473	-17.944
20	ASN	154	OD1	-23.961	73.246	-16.285
21	ASN	154	3HB	-21.910	72.470	-18.042
22	ASN	154	2HB	-21.902	74.147	-18.637
23	ASN	154	HA	-21.513	74.599	-16.003
24	ASN	154	O	-20.815	71.418	-16.167
25	ASN	154	H	-19.637	73.941	-18.117
26	ASP	155	H	-21.440	73.736	-14.173
27	ASP	155	OD1	-22.091	74.399	-12.188
28	ASP	155	OD2	-21.422	73.722	-10.181
29	ASP	155	HA	-20.392	71.019	-13.552
30	ASP	155	3HB	-19.588	73.057	-12.392

31	THR	156	3HG2	-27.330	70.047	-14.586
32	THR	156	1HG	-26.633	73.452	-14.660
33	THR	156	O	-25.742	68.816	-12.816
34	THR	156	HA	-25.197	71.237	-12.373
35	GLY	157	O	-24.773	65.778	-16.143
36	GLY	157	3HA	-24.330	66.935	-13.704
37	GLY	157	2HA	-22.969	67.213	-14.817
38	LYS	158	2HE	-29.283	65.872	-13.840
39	LYS	158	2HZ	-27.419	64.375	-13.863
40	LYS	158	2HG	-27.969	67.693	-14.996
41	LYS	158	1HZ	-27.007	65.808	-14.567
42	HIE	159	N	-24.844	67.964	-18.919
43	HIE	159	H	-24.318	68.093	-18.066
44	GLY	160	O	-24.286	63.596	-18.080
45	GLY	160	3HA	-21.538	64.896	-18.143
46	GLU	162	OE1	-24.106	61.055	-10.666
47	GLU	162	OE2	-24.977	62.848	-11.662
48	GLU	162	3HB	-23.601	59.397	-12.702
49	GLU	162	3HG	-23.683	62.262	-13.668
50	VAL	163	O	-20.198	56.772	-11.980
51	LYS	164	3HZ	-23.785	58.080	-7.810
52	LYS	164	HA	-20.492	55.047	-10.197
53	VAL	25	O	-6.596	61.933	-12.418
54	VAL	25	CG1	-4.398	59.674	-10.423
55	VAL	25	3HG1	-5.063	60.407	-9.967
56	VAL	25	HB	-4.053	60.864	-12.193
57	LEU	26	HA	-8.717	62.290	-11.209
58	GLU	27	H	-8.808	63.310	-9.394
59	GLU	27	2HB	-7.686	63.163	-5.655
60	GLU	27	3HG	-7.615	65.296	-6.935
61	GLU	27	3HB	-6.945	62.319	-7.035
62	GLU	27	2HG	-6.872	64.424	-8.297
63	GLU	27	OE1	-5.512	64.920	-5.377
64	GLU	27	OE2	-4.596	64.710	-7.396
65	GLU	270	3HB	-9.787	66.859	6.311
66	GLU	270	O	-8.998	64.685	3.892
67	GLU	270	OE1	-7.992	69.325	6.500
68	GLU	270	H	-6.652	65.206	5.723
69	ILE	271	2HG2	-13.472	60.440	4.027
70	ILE	271	3HG2	-13.927	62.058	3.443
71	ILE	271	3HD1	-10.433	60.355	3.110
72	GLN	272	OE1	-18.538	63.563	5.421
73	GLN	272	2HE2	-17.496	64.940	2.802
74	GLN	272	2HG	-15.760	63.497	5.121
75	MET	273	O	-17.381	69.219	8.324
76	MET	273	3HB	-14.920	70.824	7.875
77	MET	273	2HG	-12.631	69.097	6.894
78	MET	273	3HG	-12.467	70.833	7.250
79	MET	273	1HE	-10.734	68.336	8.507
80	SER	274	3HB	-20.135	70.656	4.619
81	SER	274	HA	-19.340	69.782	6.783
82	SER	274	HG	-18.656	72.427	4.502
83	SER	274	H	-16.833	69.186	5.246
84	SER	275	HG	-24.540	68.231	4.745
85	SER	275	O	-21.302	65.126	3.373
86	SER	275	H	-21.232	68.727	5.967
87	GLY	276	3HA	-22.080	67.455	0.753

88	GLY	276	O	-19.993	67.809	-0.678
89	ASN	277	2HD2	-18.898	70.098	-0.743
90	ASN	277	OD1	-18.470	71.829	1.837
91	ASN	277	3HB	-16.384	70.083	0.779
92	ASN	277	O	-15.663	67.629	1.934
93	LEU	278	2HD1	-17.820	61.625	-0.838
94	LEU	278	3HD1	-17.544	62.868	-2.082
95	LEU	278	HG	-17.422	63.849	0.199
96	LEU	278	O	-13.931	66.648	-1.539
97	LEU	279	HG	-13.126	68.142	2.482
98	LEU	279	3HD1	-11.560	67.850	4.392
99	LEU	279	3HD2	-11.380	70.419	1.591
100	LEU	279	O	-10.104	66.596	-1.377
101	LEU	279	3HB	-10.222	68.091	1.533
102	HIE	28	HA	-12.357	65.144	-6.253
103	HIE	28	3HB	-12.447	65.763	-3.624
104	HIE	28	O	-9.852	66.827	-5.024
105	PHE	280	3HB	-8.126	64.037	1.495
106	PHE	280	HD2	-6.845	62.079	1.567
107	PHE	280	HE1	-5.215	63.005	-3.067
108	PHE	280	HE2	-5.084	60.628	0.548
109	THR	281	HA	-10.442	59.928	-0.094
110	THR	281	HB	-10.975	61.137	-2.790
111	THR	281	O	-9.155	58.162	-1.309
112	GLY	282	3HA	-7.119	57.987	-2.600
113	GLY	282	H	-7.772	60.861	-2.084
114	GLY	282	2HA	-5.923	59.299	-2.476
115	HIE	283	HE2	-3.572	63.111	-4.661
116	HIE	283	HE1	-1.284	62.103	-5.688
117	GLY	29	H	-12.273	67.077	-7.002
118	GLY	29	CA	-10.960	68.747	-6.835
119	GLY	29	3HA	-10.256	69.047	-6.059
120	GLY	29	O	-9.955	69.912	-8.658
121	ARG	3	3HG	-18.405	68.314	-15.842
122	ARG	3	NH1	-17.162	70.791	-11.909
123	ARG	3	2HH1	-17.139	71.230	-11.000
124	ARG	3	NH2	-17.043	72.879	-12.900
125	ARG	3	2HH2	-17.021	73.303	-11.984
126	SER	30	HA	-8.661	68.420	-10.292
127	SER	30	HG	-6.848	65.439	-10.994
128	CYS	31	SG	-12.741	68.470	-14.984
129	CYS	31	HG	-13.054	69.761	-15.048
130	CYS	31	H	-8.860	68.047	-12.455
131	GLN	317	3HG	-7.642	79.454	-14.936
132	GLN	317	OE1	-7.981	79.753	-12.425
133	HIE	318	HE2	-4.072	73.309	-14.486
134	VAL	32	H	-10.777	65.682	-15.606
135	VAL	32	2HG2	-7.387	63.033	-14.704
136	VAL	32	3HG2	-6.843	64.700	-15.004
137	CYS	4	H	-14.442	70.132	-18.340
138	PHE	44	O	-12.436	64.875	-15.000
139	GLU	45	3HB	-16.024	65.795	-13.177
140	GLU	45	2HG	-15.436	65.732	-10.700
141	GLU	45	OE2	-15.255	68.681	-10.563
142	LEU	46	O	-15.057	64.181	-8.200
143	LEU	46	H	-13.327	63.571	-10.799
144	ILE	47	3HG1	-20.226	63.829	-10.645

145	ILE	47	3HG2	-20.554	63.962	-7.065
146	ILE	47	3HD1	-19.336	66.087	-10.115
147	ILE	47	O	-18.220	64.069	-5.694
148	ILE	47	HA	-17.669	64.807	-7.936
149	LYS	48	2HZ	-23.913	57.986	-4.020
150	LYS	48	3HZ	-23.608	58.645	-2.539
151	LYS	48	3HD	-22.222	61.268	-3.619
152	LYS	48	3HE	-21.565	58.298	-3.724
153	LYS	48	3HB	-20.133	60.296	-5.603
154	LYS	48	2HB	-20.327	62.000	-5.129
155	LYS	48	3HG	-19.848	61.405	-2.788
156	LYS	48	HA	-17.940	61.931	-4.297
157	THR	49	O	-17.549	58.813	-1.083
158	THR	49	HA	-16.865	57.710	-4.044
159	THR	49	3HG2	-15.038	56.810	-1.626
160	THR	49	HB	-14.854	59.193	-2.320
161	ILE	5	O	-14.404	75.751	-17.406
162	GLU	50	OE2	-23.023	56.734	-0.116
163	GLU	50	3HB	-20.243	56.147	-2.596
164	GLU	50	HA	-18.693	56.754	-0.100
165	GLY	6	3HA	-13.511	77.090	-15.524
166	GLY	6	H	-11.296	75.827	-17.070
167	GLY	6	O	-11.481	77.216	-13.503
168	GLY	6	2HA	-11.984	77.920	-15.905
169	ILE	7	3HG1	-13.413	73.743	-13.008
170	ILE	7	HA	-11.171	74.945	-12.177
171	ILE	7	O	-8.909	74.330	-14.390
172	SER	8	H	-9.301	75.119	-11.385
173	SER	8	OG	-7.315	75.699	-9.731
174	SER	8	HG	-7.149	76.363	-9.057
175	SER	8	3HB	-7.741	77.106	-11.166
176	SER	8	HA	-6.969	75.712	-13.094
177	SER	8	2HB	-6.041	76.589	-11.075
178	ASN	9	2HD2	-7.580	69.077	-8.384
179	ASN	9	3HB	-7.802	70.885	-9.681
180	ASN	9	OD1	-4.763	69.748	-9.593

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**cavity\_2\_SYMTKCLPNIGVEAFRH**

Cavity point -7.780 70.462 -39.880

Volume of the Cavity = 1190

1	GLU	14	OE2	-3.011	64.136	-28.495
2	TYR	179	HH	-19.912	66.196	-30.081
3	TYR	179	HE1	-18.761	64.359	-30.791
4	LEU	295	HA	-16.474	61.887	-32.854
5	LEU	295	3HB	-15.867	62.913	-35.154
6	LEU	295	3HD2	-14.530	64.352	-33.543
7	LEU	295	1HD1	-13.397	63.569	-35.713
8	LEU	295	3HD1	-12.928	61.858	-35.863
9	MET	298	2HB	-17.293	60.886	-39.313
10	MET	298	O	-17.277	62.584	-42.359
11	MET	298	3HB	-15.964	61.517	-40.313
12	MET	298	3HG	-15.295	61.235	-37.980

13	MET	298	1HE	-13.752	62.515	-40.263
14	MET	298	3HE	-12.962	62.023	-38.746
15	MET	298	2HE	-12.630	63.626	-39.443
16	SER	299	O	-20.767	64.023	-44.661
17	SER	299	HA	-19.556	61.954	-43.650
18	SER	301	H	-20.728	68.218	-44.807
19	SER	301	HG	-21.068	70.581	-47.181
20	SER	301	HA	-17.924	68.375	-45.757
21	MET	302	O	-18.353	73.275	-45.795
22	MET	302	3HB	-15.203	73.362	-44.338
23	MET	302	2HG	-14.799	70.458	-45.110
24	MET	302	3HG	-13.536	71.708	-45.187
25	MET	302	2HE	-12.171	72.064	-41.715
26	MET	302	3HE	-11.791	71.895	-43.445
27	CYS	303	O	-17.438	76.528	-44.622
28	THR	304	3HG2	-18.199	75.679	-48.669
29	THR	304	HA	-17.970	77.604	-46.919
30	LYS	335	HA	-18.023	70.810	-38.872
31	LYS	335	3HE	-15.842	66.267	-39.717
32	LYS	335	2HD	-15.708	68.251	-42.019
33	LYS	335	3HB	-15.830	70.603	-40.098
34	LYS	335	2HE	-14.749	66.096	-41.111
35	LYS	335	3HD	-14.802	68.426	-40.497
36	ILE	336	HB	-16.237	74.370	-36.651
37	ILE	336	O	-14.292	73.888	-38.495
38	PRO	337	2HD	-16.051	76.733	-40.708
39	PRO	337	3HG	-14.840	75.784	-43.237
40	PRO	337	3HB	-12.546	75.818	-42.614
41	PHE	338	O	-9.055	74.570	-37.713
42	GLU	339	OE2	-6.656	75.094	-42.308
43	GLU	339	OE1	-4.987	74.291	-41.076
44	MET	341	SD	-3.187	78.376	-40.899
45	MET	341	3HE	-2.829	79.537	-42.973
46	LYS	345	2HE	-4.634	83.353	-44.031
47	LYS	345	O	-0.966	81.241	-44.214
48	ARG	346	O	1.272	78.037	-44.207
49	ARG	346	HA	1.263	80.380	-44.984
50	HIE	347	HA	1.785	76.624	-42.223
51	HIE	347	3HB	3.571	76.137	-40.632
52	HIE	347	2HB	3.725	77.863	-40.227
53	HIE	347	HE1	5.844	76.450	-44.872
54	VAL	348	3HG1	-1.431	73.978	-37.108
55	LEU	349	3HB	2.033	77.451	-33.907
56	LEU	349	3HD2	4.312	77.179	-35.301
57	GLY	350	O	-3.285	74.031	-34.423
58	ARG	351	HA	-4.476	72.078	-33.290
59	ARG	351	1HH2	-3.558	66.779	-28.579
60	ARG	351	2HH2	-3.515	67.015	-26.842
61	ARG	351	3HG	-4.044	71.226	-29.534
62	ARG	351	HE	-3.007	68.456	-29.981
63	ARG	351	2HH1	-2.793	68.989	-25.956
64	ARG	351	1HH1	-2.272	70.295	-27.002
65	ARG	351	3HB	-2.597	70.975	-32.188
66	ARG	351	H	-2.974	73.789	-31.324
67	LEU	352	2HD1	-10.308	72.720	-35.294
68	LEU	352	3HD1	-9.268	71.297	-35.048
69	ILE	353	O	-10.733	69.037	-27.894

70	ILE	353	2HD1	-5.292	71.676	-26.244
71	THR	354	3HG2	-15.024	71.437	-30.493
72	VAL	355	O	-14.066	67.737	-32.142
73	VAL	355	H	-11.796	68.533	-29.890
74	VAL	355	2HG1	-9.015	66.439	-31.064
75	VAL	355	3HG1	-8.995	68.012	-31.896
76	ASN	356	2HD2	-16.861	65.473	-35.049
77	ASN	356	3HB	-15.043	66.340	-34.230
78	ASN	356	HA	-13.880	68.586	-35.996
79	ASN	356	H	-12.151	68.625	-34.446
80	PRO	357	HA	-16.648	71.113	-33.306
81	PRO	357	O	-16.793	71.678	-36.515
82	PRO	357	3HB	-15.233	72.932	-32.955
83	PRO	357	2HB	-16.007	73.585	-34.419
84	ALA	36	O	-8.260	61.640	-30.743
85	ALA	36	H	-8.287	62.265	-28.423
86	ALA	36	HA	-5.912	60.638	-28.875
87	ILE	368	3HG2	-11.921	75.500	-30.700
88	LYS	37	HA	-6.462	61.650	-33.016
89	LYS	37	H	-5.732	59.802	-30.937
90	LYS	37	3HZ	-5.592	60.590	-37.544
91	LYS	37	3HE	-3.389	61.164	-36.822
92	LYS	37	3HD	-3.966	61.964	-34.512
93	LYS	37	2HE	-3.908	62.865	-36.752
94	ALA	370	3HB	-8.892	75.601	-30.601
95	GLU	371	2HB	-4.194	73.654	-26.453
96	GLU	371	3HB	-3.486	73.427	-28.070
97	GLU	371	O	-2.867	75.446	-29.663
98	GLU	371	OE1	-1.587	71.992	-26.529
99	GLU	371	2HG	-1.454	74.527	-27.441
100	PRO	373	3HB	2.458	77.546	-31.399
101	ASN	38	3HB	-10.821	59.357	-36.051
102	ASN	38	1HD2	-9.946	61.409	-38.765
103	GLY	382	2HA	-15.413	79.444	-41.650
104	GLY	382	O	-12.544	79.831	-42.864
105	VAL	383	2HG1	-14.516	78.298	-48.415
106	VAL	383	3HG2	-13.489	77.253	-45.712
107	VAL	383	3HG1	-14.016	79.998	-48.243
108	GLU	384	H	-12.198	81.002	-46.797
109	GLU	384	2HB	-10.941	82.159	-48.679
110	LYS	39	O	-11.374	62.598	-30.436
111	LYS	39	2HG	-9.843	58.361	-31.291
112	PRO	40	3HG	-16.387	62.045	-30.625
113	THR	41	H	-13.102	65.235	-28.299
114	THR	41	1HG	-10.303	67.181	-27.812

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### cavity\_3\_YPKQLNMTIDVRSFAFWGEH

Cavity point -6.013 63.925 -31.497

Volume of the Cavity = 1068

1	ASP	11	3HB	-3.412	66.075	-16.277
2	PHE	12	HZ	-6.739	73.004	-20.745
3	PHE	12	HD2	-6.053	69.246	-22.779
4	PHE	12	HE1	-4.978	72.423	-19.075
5	PHE	12	3HB	-4.075	68.025	-22.232
6	PHE	12	H	-3.374	68.016	-18.649



7	PHE	12	HD1	-3.697	70.291	-19.304
8	PHE	12	O	-2.517	65.879	-20.294
9	VAL	13	H	-5.427	65.019	-21.063
10	VAL	13	2HG1	-4.713	60.440	-19.619
11	VAL	13	3HG2	-3.149	62.878	-18.533
12	GLU	14	HA	-4.207	61.669	-24.787
13	GLU	14	3HG	-3.450	64.376	-25.490
14	GLU	14	H	-2.270	62.358	-22.620
15	GLU	14	OE2	-3.011	64.136	-28.495
16	GLU	14	O	-2.060	59.922	-23.291
17	GLU	14	3HB	-1.973	61.791	-26.219
18	PRO	144	2HB	-18.477	64.585	-26.224
19	GLY	15	3HA	-3.579	57.482	-25.703
20	GLY	15	O	-0.956	58.634	-26.788
21	VAL	16	O	-1.555	55.498	-28.727
22	VAL	16	1HG2	-0.353	54.678	-24.455
23	VAL	16	2HG2	0.768 53.324		-24.734
24	VAL	16	3HG1	1.343 53.912		-28.323
25	VAL	16	3HG2	1.383 54.994		-24.686
26	VAL	16	HA	0.910 56.536		-26.895
27	SER	17	HA	-0.834	57.450	-30.823
28	SER	17	3HB	1.186 57.521		-32.422
29	SER	17	H	1.210 56.956		-28.910
30	SER	17	HG	1.984 59.403		-31.349
31	TYR	179	HH	-19.912	66.196	-30.081
32	TYR	179	HE1	-18.761	64.359	-30.791
33	GLY	18	O	-3.697	52.603	-32.406
34	GLY	18	H	-2.099	56.110	-31.779
35	GLY	18	3HA	-1.050	53.577	-32.942
36	GLY	19	O	-4.730	54.786	-29.042
37	GLY	19	2HA	-4.039	51.804	-30.043
38	GLY	19	3HA	-3.046	52.412	-28.697
39	SER	20	O	-8.545	53.598	-26.407
40	SER	20	3HB	-8.089	52.740	-30.189
41	TRP	21	H	-5.454	53.145	-26.557
42	TRP	21	HD1	-4.421	51.208	-26.433
43	TRP	21	HE3	-4.383	51.689	-21.331
44	TRP	21	CD2	-3.466	51.330	-23.305
45	TRP	21	HE1	-1.821	50.796	-25.998
46	VAL	22	O	-6.796	55.536	-20.344
47	VAL	22	HB	-4.996	58.147	-22.543
48	ASP	23	H	-3.727	56.196	-20.322
49	ASP	23	O	-3.978	58.206	-18.221
50	ASP	23	2HB	-2.640	55.805	-18.223
51	ILE	24	HA	-5.260	59.579	-16.409
52	LEU	288	O	-8.919	53.954	-22.720
53	ARG	289	O	-12.983	53.047	-24.493
54	ARG	289	H	-11.660	52.585	-22.071
55	MET	290	CB	-11.276	55.608	-27.024
56	MET	290	3HB	-11.862	56.291	-27.638
57	MET	290	3HG	-10.479	55.517	-25.048
58	ASP	291	O	-13.923	51.540	-31.509
59	ASP	291	HA	-11.689	52.181	-30.647
60	ASP	291	H	-11.583	51.908	-27.801
61	GLN	294	3HB	-16.690	55.786	-33.572
62	LEU	295	HA	-16.474	61.887	-32.854
63	LEU	295	3HB	-15.867	62.913	-35.154

64	LEU	295	3HD2	-14.530	64.352	-33.543
65	LEU	295	1HD1	-13.397	63.569	-35.713
66	LEU	295	3HD1	-12.928	61.858	-35.863
67	MET	298	3HB	-15.964	61.517	-40.313
68	MET	298	3HG	-15.295	61.235	-37.980
69	MET	298	1HE	-13.752	62.515	-40.263
70	MET	298	3HE	-12.962	62.023	-38.746
71	MET	298	2HE	-12.630	63.626	-39.443
72	MET	302	2HE	-12.171	72.064	-41.715
73	MET	302	3HE	-11.791	71.895	-43.445
74	HIE	318	3HB	-3.286	74.521	-19.173
75	LYS	335	HA	-18.023	70.810	-38.872
76	LYS	335	3HE	-15.842	66.267	-39.717
77	LYS	335	2HD	-15.708	68.251	-42.019
78	LYS	335	3HB	-15.830	70.603	-40.098
79	LYS	335	2HE	-14.749	66.096	-41.111
80	LYS	335	3HD	-14.802	68.426	-40.497
81	ILE	336	O	-14.292	73.888	-38.495
82	PHE	338	O	-9.055	74.570	-37.713
83	GLU	339	OE1	-4.987	74.291	-41.076
84	VAL	348	3HG1	-1.431	73.978	-37.108
85	MET	35	3HE	-6.209	67.491	-24.253
86	GLY	350	O	-3.285	74.031	-34.423
87	ARG	351	HA	-4.476	72.078	-33.290
88	ARG	351	1HH2	-3.558	66.779	-28.579
89	ARG	351	2HH2	-3.515	67.015	-26.842
90	ARG	351	3HG	-4.044	71.226	-29.534
91	ARG	351	HE	-3.007	68.456	-29.981
92	ARG	351	2HH1	-2.793	68.989	-25.956
93	ARG	351	1HH1	-2.272	70.295	-27.002
94	ARG	351	3HB	-2.597	70.975	-32.188
95	ARG	351	H	-2.974	73.789	-31.324
96	LEU	352	2HD1	-10.308	72.720	-35.294
97	LEU	352	3HD1	-9.268	71.297	-35.048
98	ILE	353	O	-10.733	69.037	-27.894
99	ILE	353	3HD1	-6.315	70.391	-25.558
100	ILE	353	2HD1	-5.292	71.676	-26.244
101	THR	354	3HG2	-15.024	71.437	-30.493
102	VAL	355	O	-14.066	67.737	-32.142
103	VAL	355	H	-11.796	68.533	-29.890
104	VAL	355	2HG1	-9.015	66.439	-31.064
105	VAL	355	3HG1	-8.995	68.012	-31.896
106	ASN	356	2HD2	-16.861	65.473	-35.049
107	ASN	356	3HB	-15.043	66.340	-34.230
108	ASN	356	HA	-13.880	68.586	-35.996
109	ASN	356	H	-12.151	68.625	-34.446
110	PRO	357	HA	-16.648	71.113	-33.306
111	PRO	357	O	-16.793	71.678	-36.515
112	PRO	357	3HB	-15.233	72.932	-32.955
113	PRO	357	2HB	-16.007	73.585	-34.419
114	ALA	36	O	-8.260	61.640	-30.743
115	ALA	36	H	-8.287	62.265	-28.423
116	ALA	36	2HB	-7.134	58.494	-29.035
117	ALA	36	3HB	-7.256	59.172	-27.395
118	ALA	36	HA	-5.912	60.638	-28.875
119	ILE	368	3HG2	-11.921	75.500	-30.700
120	LYS	37	HA	-6.462	61.650	-33.016

121	LYS	37	H	-5.732	59.802	-30.937
122	LYS	37	3HZ	-5.592	60.590	-37.544
123	LYS	37	3HE	-3.389	61.164	-36.822
124	LYS	37	3HD	-3.966	61.964	-34.512
125	LYS	37	2HE	-3.908	62.865	-36.752
126	ALA	370	3HB	-8.892	75.601	-30.601
127	GLU	371	2HB	-4.194	73.654	-26.453
128	GLU	371	3HB	-3.486	73.427	-28.070
129	GLU	371	O	-2.867	75.446	-29.663
130	GLU	371	OE1	-1.587	71.992	-26.529
131	GLU	371	OE2	-1.329	73.202	-24.679
132	GLU	371	2HG	-1.454	74.527	-27.441
133	PRO	373	HA	1.767	77.498	-29.118
134	ASN	38	3HB	-10.821	59.357	-36.051
135	ASN	38	1HD2	-9.946	61.409	-38.765
136	LYS	39	3HZ	-12.676	54.711	-31.362
137	LYS	39	O	-11.374	62.598	-30.436
138	LYS	39	3HE	-10.484	55.381	-30.692
139	LYS	39	2HG	-9.843	58.361	-31.291
140	LYS	394	2HZ	0.021	76.525	-24.273
141	PRO	40	3HG	-16.387	62.045	-30.625
142	THR	41	H	-13.102	65.235	-28.299
143	THR	41	1HG	-10.303	67.181	-27.812
144	LEU	42	3HD1	-13.346	59.791	-23.054
145	LEU	42	HG	-13.574	61.608	-24.738

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**cavity\_4\_KESQDTGVIAPNLMHYWF**

Cavity point -18.476 59.321 1.702

Volume of the Cavity = 1061

1	GLU	127	OE2	-21.225	55.110	14.912
2	GLU	127	OE1	-20.000	53.651	13.767
3	GLU	127	2HB	-17.967	56.083	13.829
4	GLU	127	H	-16.946	57.800	15.160
5	LYS	129	2HE	-19.361	53.194	11.277
6	LYS	129	3HZ	-19.791	55.428	9.418
7	LYS	129	3HE	-18.630	54.812	11.411
8	LYS	129	2HG	-16.881	52.336	11.250
9	LYS	129	3HB	-15.756	52.031	9.019
10	ILE	130	3HG2	-11.520	47.552	6.787
11	ILE	130	HA	-11.295	50.235	8.254
12	VAL	131	H	-11.666	51.306	6.429
13	VAL	131	HB	-11.426	52.424	4.398
14	GLN	132	OE1	-15.223	44.603	2.892
15	GLN	132	O	-12.731	48.723	0.376
16	GLN	132	3HB	-11.807	46.196	3.495
17	PRO	133	HA	-10.584	50.077	-1.261
18	PRO	133	3HB	-8.567	49.616	-2.289
19	GLU	134	O	-14.741	46.628	-3.883
20	ASN	135	OD1	-17.554	45.527	-1.965
21	ASN	135	3HB	-17.584	47.739	-0.397
22	ASN	135	HA	-16.416	47.967	-2.566
23	ASN	135	O	-16.406	50.039	-0.387
24	ASN	135	2HD2	-15.836	45.061	0.624
25	LEU	136	1HD2	-15.268	53.670	-0.312
26	LEU	136	H	-14.761	49.794	-3.030

27	LEU	136	2HD2	-13.802	54.022	0.633
28	LEU	136	3HD2	-14.022	54.754	-0.974
29	LEU	136	3HD1	-11.469	52.039	-1.446
30	GLU	137	OE2	-22.458	52.437	-6.645
31	GLU	137	OE1	-22.315	53.718	-4.837
32	GLU	137	CB	-19.475	52.904	-4.901
33	GLU	137	3HB	-19.720	53.507	-4.026
34	GLU	137	O	-17.687	55.350	-4.563
35	TYR	138	HH	-11.238	53.496	-4.039
36	TYR	138	HE2	-11.916	56.935	-4.848
37	THR	139	1HG	-21.806	58.757	-7.160
38	THR	139	3HG2	-20.706	60.626	-9.921
39	GLU	162	OE1	-24.106	61.055	-10.666
40	GLU	162	OE2	-24.977	62.848	-11.662
41	GLU	162	3HB	-23.601	59.397	-12.702
42	VAL	163	O	-20.198	56.772	-11.980
43	LYS	164	3HE	-25.140	56.363	-8.768
44	LYS	164	3HG	-24.136	54.063	-9.438
45	LYS	164	2HE	-24.687	56.972	-10.378
46	LYS	164	2HG	-23.724	54.763	-11.022
47	LYS	164	3HZ	-23.785	58.080	-7.810
48	LYS	164	3HB	-21.816	53.406	-9.092
49	LYS	164	O	-20.196	52.275	-11.960
50	LYS	164	HA	-20.492	55.047	-10.197
51	ILE	165	3HG2	-14.868	51.811	-10.456
52	THR	166	1HG	-19.705	48.738	-6.977
53	THR	166	2HG2	-18.304	46.964	-6.383
54	THR	166	H	-17.707	49.862	-10.142
55	PRO	188	3HB	-10.266	50.383	-5.712
56	PRO	188	2HB	-9.029	50.169	-4.451
57	PRO	188	HA	-8.637	52.013	-6.477
58	PRO	188	O	-6.722	51.914	-4.718
59	THR	190	O	-4.455	54.092	-3.704
60	GLY	191	3HA	-3.816	56.186	-2.318
61	LEU	192	H	-3.725	54.618	-0.450
62	LEU	192	3HB	-3.689	55.465	2.392
63	PHE	194	HE2	-10.139	53.942	2.109
64	PHE	194	HD2	-9.436	52.004	3.517
65	PHE	194	HZ	-8.821	54.555	0.081
66	PHE	194	HE1	-6.764	53.265	-0.509
67	MET	197	2HB	-5.666	53.087	6.446
68	LEU	199	3HD2	-14.233	55.900	5.506
69	GLN	201	1HE2	-19.383	58.371	7.717
70	GLN	201	OE1	-18.196	57.062	9.478
71	GLN	201	2HE2	-18.330	59.763	7.879
72	GLN	201	3HB	-17.863	59.816	11.370
73	GLN	201	2HB	-17.076	58.268	11.759
74	GLN	201	2HG	-16.630	59.911	9.228
75	GLN	201	O	-16.578	59.877	14.163
76	MET	202	HA	-17.243	62.141	15.118
77	MET	202	O	-17.553	64.802	13.310
78	LYS	203	2HZ	-25.396	63.925	12.650
79	LYS	203	3HZ	-25.524	64.462	14.204
80	LYS	203	3HE	-23.493	63.243	13.918
81	LYS	203	3HD	-23.098	66.247	14.260
82	LYS	203	O	-19.613	62.914	10.747
83	LYS	203	2HB	-19.704	65.722	13.834

84	ASP	204	OD2	-22.559	67.515	9.642
85	ASP	204	H	-20.268	65.910	11.357
86	ASP	204	3HB	-20.182	66.911	7.886
87	ALA	206	3HB	-15.594	61.819	8.185
88	TRP	207	HE3	-11.926	62.500	11.737
89	LEU	208	3HD2	-6.962	57.129	4.026
90	LEU	208	3HB	-6.651	59.030	6.137
91	THR	269	HB	-5.379	61.084	6.157
92	GLU	27	2HB	-7.686	63.163	-5.655
93	GLU	27	3HG	-7.615	65.296	-6.935
94	GLU	270	3HB	-9.787	66.859	6.311
95	GLU	270	O	-8.998	64.685	3.892
96	GLU	270	H	-6.652	65.206	5.723
97	ILE	271	2HG2	-13.472	60.440	4.027
98	ILE	271	3HG2	-13.927	62.058	3.443
99	ILE	271	3HD1	-10.433	60.355	3.110
100	GLN	272	OE1	-18.538	63.563	5.421
101	GLN	272	2HE2	-17.496	64.940	2.802
102	GLN	272	2HG	-15.760	63.497	5.121
103	MET	273	O	-17.381	69.219	8.324
104	MET	273	HA	-15.070	68.300	8.139
105	MET	273	3HB	-14.920	70.824	7.875
106	MET	273	2HG	-12.631	69.097	6.894
107	MET	273	3HG	-12.467	70.833	7.250
108	MET	273	1HE	-10.734	68.336	8.507
109	SER	274	3HB	-20.135	70.656	4.619
110	SER	274	HA	-19.340	69.782	6.783
111	SER	274	HG	-18.656	72.427	4.502
112	SER	274	H	-16.833	69.186	5.246
113	SER	275	HG	-24.540	68.231	4.745
114	SER	275	3HB	-23.117	67.464	6.401
115	SER	275	O	-21.302	65.126	3.373
116	SER	275	H	-21.232	68.727	5.967
117	GLY	276	3HA	-22.080	67.455	0.753
118	GLY	276	O	-19.993	67.809	-0.678
119	ASN	277	2HD2	-18.898	70.098	-0.743
120	ASN	277	OD1	-18.470	71.829	1.837
121	ASN	277	3HB	-16.384	70.083	0.779
122	ASN	277	O	-15.663	67.629	1.934
123	LEU	278	2HD1	-17.820	61.625	-0.838
124	LEU	278	3HD1	-17.544	62.868	-2.082
125	LEU	278	HG	-17.422	63.849	0.199
126	LEU	278	O	-13.931	66.648	-1.539
127	LEU	279	HG	-13.126	68.142	2.482
128	LEU	279	3HD1	-11.560	67.850	4.392
129	LEU	279	3HD2	-11.380	70.419	1.591
130	LEU	279	O	-10.104	66.596	-1.377
131	LEU	279	3HB	-10.222	68.091	1.533
132	HIE	28	HA	-12.357	65.144	-6.253
133	HIE	28	3HB	-12.447	65.763	-3.624
134	HIE	28	O	-9.852	66.827	-5.024
135	PHE	280	3HB	-8.126	64.037	1.495
136	PHE	280	HD2	-6.845	62.079	1.567
137	PHE	280	HE2	-5.084	60.628	0.548
138	THR	281	HA	-10.442	59.928	-0.094
139	THR	281	HB	-10.975	61.137	-2.790
140	THR	281	O	-9.155	58.162	-1.309

141	GLY	282	3HA	-7.119	57.987	-2.600
142	GLY	282	H	-7.772	60.861	-2.084
143	GLY	282	2HA	-5.923	59.299	-2.476
144	HIE	283	O	-5.904	56.497	-7.105
145	HIE	283	H	-5.488	58.044	-4.578
146	LEU	284	1HD2	-9.905	54.175	-8.408
147	GLY	29	H	-12.273	67.077	-7.002
148	GLY	29	CA	-10.960	68.747	-6.835
149	GLY	29	3HA	-10.256	69.047	-6.059
150	GLU	45	2HG	-15.436	65.732	-10.700
151	GLU	45	OE2	-15.255	68.681	-10.563
152	LEU	46	O	-15.057	64.181	-8.200
153	LEU	46	H	-13.327	63.571	-10.799
154	ILE	47	3HG1	-20.226	63.829	-10.645
155	ILE	47	3HG2	-20.554	63.962	-7.065
156	ILE	47	3HD1	-19.336	66.087	-10.115
157	ILE	47	O	-18.220	64.069	-5.694
158	ILE	47	HA	-17.669	64.807	-7.936
159	LYS	48	2HZ	-23.913	57.986	-4.020
160	LYS	48	3HZ	-23.608	58.645	-2.539
161	LYS	48	3HD	-22.222	61.268	-3.619
162	LYS	48	3HE	-21.565	58.298	-3.724
163	LYS	48	3HB	-20.133	60.296	-5.603
164	LYS	48	2HB	-20.327	62.000	-5.129
165	LYS	48	3HG	-19.848	61.405	-2.788
166	LYS	48	HA	-17.940	61.931	-4.297
167	THR	49	O	-17.549	58.813	-1.083
168	THR	49	HA	-16.865	57.710	-4.044
169	THR	49	3HG2	-15.038	56.810	-1.626
170	THR	49	HB	-14.854	59.193	-2.320
171	GLU	50	OE1	-23.416	55.382	-1.840
172	GLU	50	OE2	-23.023	56.734	-0.116
173	GLU	50	3HG	-20.979	55.198	0.186
174	GLU	50	3HB	-20.243	56.147	-2.596
175	GLU	50	HA	-18.693	56.754	-0.100
176	ALA	51	O	-19.676	53.295	2.420
177	ALA	51	3HB	-15.789	54.067	2.206
178	LYS	52	2HZ	-24.328	52.561	-2.505
179	LYS	52	2HE	-23.718	50.364	-3.226
180	LYS	52	3HZ	-22.823	52.824	-1.883
181	LYS	52	3HD	-21.591	49.398	-2.594
182	LYS	52	2HD	-21.272	50.885	-3.518
183	LYS	52	HA	-21.325	51.646	1.250
184	LYS	52	2HB	-20.044	49.345	-0.269
185	GLN	53	2HE2	-22.810	49.793	6.988
186	GLN	53	2HB	-22.087	48.122	3.963
187	GLN	53	O	-19.688	47.995	5.336
188	PRO	54	O	-18.656	49.521	8.354
189	PRO	54	3HD	-18.845	51.747	4.449
190	PRO	54	3HG	-17.024	52.776	5.509
191	ALA	55	3HB	-16.439	45.561	8.720
192	ALA	55	H	-16.112	47.886	7.511
193	THR	56	1HG	-19.773	50.800	13.299
194	THR	56	H	-18.142	48.380	11.543
195	THR	56	HB	-18.455	48.977	13.936

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