File Name : fig. s1.tif

Caption : fig. s1: multiple sequence alignment of dblÎ± domains of upsb group sequences from all three plasmodium isolates with template. the most conserved residues have been highlighted with red color, while partially conserved residues pink color.

File Name : fig. s2.tif

Caption : fig. s2: multiple sequence alignment of dblÎ± domains of upsa group sequences from all three plasmodium isolates with template. the most conserved residues have been highlighted with red color, while partially conserved residues pink color.

File Name : fig. s3.tif

Caption : fig. s3: multiple sequence alignment of dblÎ± domains of upsc group sequences from all three plasmodium isolates with template. the most conserved residues have been highlighted with red color, while partially conserved residues pink color.

Table S1 Comparison of isolates Identity, Z-dope score and UPS groups

Protein Name	Identity (%)	Template	Z-dope score	UPS group
3D7_dbl1174	44	2YK0	-0.81	C
3D7_dbl1794	41	2YK0	-0.35	C
3D7_dbl1796	40	2XUOA	-0.57	C
3D7_dbl1798	44	2YKOA	-0.43	B
3D7_dbl1800	44	2XU0	-0.98	B
3D7_dbl1802	43	2XUOA	-0.48	C
3D7_dbl1806	37	2YKOA	-0.12	C
3D7_dbl1837	43	2XUOA	-0.41	B
3D7_dbl1918	44	2YKOA	-0.46	B
3D7_dbl1928	42	2YK0	-0.3	B
3D7_dbl2172	41	2YKOA	-0.37	B
3D7_dbl2602	44	2YKOA	-0.35	B
3D7_dbl2608	41	2XUOA	-0.41	B
3D7_dbl2610	39	2YKOA	-0.31	C
3D7_dbl2758	47	2YK0	-0.62	B
3D7_dbl2760	53	2XUOA	-0.87	A
3D7_dbl2762	45	2XUOA	-0.71	B
3D7_dbl2764	42	2YKOA	-0.32	B
3D7_dbl2768	26	2YKOA	-1.65	B
3D7_dbl3374	38	2XUOA	-0.66	B
3D7_dbl3377	51	2XU0	-1.12	A
3D7_dbl4106	45	2YKOA	0.04	B
3D7_dbl4675	40	2XUOA	-0.74	B
3D7_dbl4752	40	2YKOA	-0.47	B
3D7_dbl5005	51	2XU0	-1.6	A
3D7_dbl5120	49	2YK0	-0.59	A
3D7_dbl5142	38	2XUOA	-0.35	B
3D7_dbl5155	44	2XUOA	-0.65	B
3D7_dbl5159	54	2XU0	-1.09	A
3D7_dbl5331	43	2XUO	-0.18	B
3D7_dbl5343	44	2XU0	-0.92	B
3D7_dbl5387	43	2YK0	-0.14	C
3D7_dbl5391	38	2YKOA	0.18	C
3D7_dbl5393	45	2XUOA	-0.5	C
3D7_dbl5395	41	2YKOA	-0.28	B
3D7_dbl5543	41	2XU0	-0.58	C
3D7_dbl5545	43	2YKOA	-0.3	C
3D7_dbl5547	45	2XUOA	-0.62	B
3D7_dbl5551	39	2XUOA	-0.66	C
3D7_dbl5639	49	2YKOA	-0.59	B
3D7_dbl5643	39	2YK0	-0.48	B
3D7_dbl5645	41	2XUOA	-0.49	B
3D7_dbl5746	40	2XU0	-0.72	B
3D7_dbl5931	39	2YKOA	-0.43	B
3D7_dbl5933	42	2YKOA	-0.32	B
3D7_dbl5987	46	2YK0	-0.43	B
3D7_dbl6559	46	2XU0	-0.61	B

3D7_dbl6687	44	2XU0	-0.79	B
3D7_dbl6689	45	2YKOA	-0.35	B
3D7_dbl6691	38	2YKOA	-0.12	C
3D7_dbl6953	46	2XUOA	-0.66	B
3D7_dbl7176	44	2XU0	-0.82	B
3D7_dbl7212	44	2YKOA	-0.6	B
3D7_dbl7287	44	2XU0	-0.34	A
3D7_dbl7291	39	2XUOA	-0.44	B
3D7_dbl9167	41	2YKOA	-0.3	B
IGHvar01	41	2YK0	-0.55	B
IGHvar02	47	2YK0	-0.66	B
IGHvar03	41	2XU0	-0.2	B
IGHvar04	43	2XU0	-0.47	B
IGHvar05	44	2YK0	-0.54	B
IGHvar06	39	2XU0	-0.3	C
IGHvar07	44	2XU0	-0.35	B
IGHvar08	38	2YK0	-0.07	B
IGHvar09	55	2XU0	-1.27	A
IGHvar10	52	2YK0	-0.95	A
IGHvar11	51	2XU0	-0.96	B
IGHvar12	58	2XU0	-1.1	B
IGHvar13	39	2YK0	-0.34	A
IGHvar14	54	2YK0	-0.72	B
IGHvar15	46	2YK0	-0.38	B
IGHvar16	43	2YK0	-0.32	C
IGHvar17	45	2XU0	-0.67	B
IGHvar18	45	2YK0	-0.55	B
IGHvar19	46	2YK0	-0.53	B
IGHvar20	46	2YK0	-0.44	B
IGHvar21	41	2YK0	-0.3	B
IGHvar22	53	2XU0	-1.08	A
IGHvar23	50	2XU0	-0.99	A
IGHvar24	57	2XU0	-1.15	A
IGHvar26	58	2XU0	-1.11	A
IGHvar27	48	2XU0	-0.51	A
IGHvar28	45	2XU0	-0.7	C
IGHvar29	43	2YK0	-0.3	C
IGHvar30	46	2XU0	-0.72	A
IGHvar31	43	2XU0	-0.58	B
IGHvar32	54	2YK0	-1.02	A
IGHvar33	40	2YK0	-0.16	B
IGHvar34	46	2XU0	-0.74	C
IGHvar35	40	2YK0	-0.24	B
IGHvar36	45	2YK0	-0.51	C
IGHvar37	41	2YK0	-0.24	B
IGHvar38	38	2YK0	-0.28	B
IGHvar39	61	2XU0	-1.18	A
IGHvar40	46	2YK0	-0.35	B
RAJ116var01	42	2YK0	-0.29	B
RAJ116var02	51	2YK0	-0.07	A

RAJ116var03	51	2XU0	-0.89	A
RAJ116var04	43	2YK0	-0.54	B
RAJ116var05	59	2YK0	-0.96	A
RAJ116var06	42	2XU0	-0.9	B
RAJ116var07	59	2XU0	-1.22	A
RAJ116var08	44	2YK0	-0.65	B
RAJ116var09	42	2YK0	-0.63	B
RAJ116var10	45	2YK0	-0.61	B
RAJ116var12	42	2XU0	-0.55	B
RAJ116var14	43	2YK0	-0.53	B
RAJ116var15	45	2YK0	-0.44	B
RAJ116var16	63	2YK0	-1.13	A
RAJ116var17	42	2XU0	-0.12	A
RAJ116var18	43	2XU0	-0.79	B
RAJ116var19	64	2XU0	-1.22	A
RAJ116var20	42	2YK0	-0.43	B
RAJ116var21	43	2YK0	-0.41	C
RAJ116var22	42	2YK0	-0.44	B
RAJ116var24	45	2XU0	-0.66	B
RAJ116var26	41	2YK0	-0.2	B
RAJ116var27	41	2YK0	-0.4	C
RAJ116var28	41	2YK0	-0.44	C
RAJ116var29	44	2XU0	-0.56	B
RAJ116var30	44	2YK0	-0.46	B
RAJ116var31	37	2YK0	0.01	B
RAJ116var32	43	2XU0	-0.59	B
RAJ116var33	42	2YK0	-0.77	B
RAJ116var34	43	2YK0	-0.38	B
RAJ116var35	39	2XU0	-0.63	C
RAJ116var36	43	2YK0	-0.55	B
RAJ116var37	45	2XU0	-0.68	B
RAJ116var38	58	2XU0	-1.16	A
RAJ116var39	41	2YK0	-0.67	B

Table S2 Structure quality estimation analysis

Protein	**Structure Quality Estimation analysis Predicted Structure**						
	ProCheck				**G factor**	**Verify 3D**	**Errate**
	Core region	**Allowed region**	**Gener allowed region**	**Disallowed region**			
3D7_dbl7176	89.4	8.7	1.4	0.5	-0.04	89.73	73
3D7_dbl6559	88.8	9.9	0.3	1	-0.04	83.56	62.911
3D7_dbl5643	89.2	9	0.8	1	0	86.89	65.947
3D7_dbl5543	88.1	9.6	1.5	0.8	0.27	89.82	67.542
3D7_dbl5387	84.9	14.1	0.7	0.2	-0.05	80.8	64.037
3D7_dbl5120	87.7	11	1.1	0.3	0	89.43	74.121
3D7_dbl2758	89.6	9.3	0.8	0.3	-0.03	81.23	76.01
3D7_dbl3377	88	10.1	1.1	0.8	-0.07	76.73	74.67
3D7_dbl7287	84.7	12.7	1.3	1.3	-0.09	63.1	66.667
3D7_dbl6687	89.9	8.5	1.1	0.5	0.01	87.53	72.208
3D7_dbl5987	88.9	11.3	1	0.8	-0.02	81.28	68.258
3D7_dbl5746	86.8	11.1	1.1	1.1	-0.04	83.37	69.586
3D7_dbl5343	88.9	8.9	1.3	0.8	-0.04	79.8	78.827
3D7_dbl5159	90.7	8.2	0.8	0.3	0.04	86.22	87.918
3D7_dbl5005	87.6	11.6	0.6	0.3	-0.09	87	70.332
3D7_dbl1928	88.5	9.4	1.3	0.8	-0.07	75.91	62.189
3D7_dbl1800	89.9	9.3	0.8	0	0	85.09	73.75
3D7_dbl1794	87.5	10.2	1.3	1	-0.05	83.52	61.391
3D7_dbl1174	88.3	10.80	0.5	0.3	-0.04	86.67	73.48
3D7_dbl5331	84.5	12.2	2.1	1.3	-0.10	80.81	60.048
3D7_dbl1837	86.7	10.5	1.2	1.6	-0.02	78.17	59.707
3D7_dbl4752	85.8	12.4	1.3	0.5	-0.05	69.68	67.669
3D7_dbl6691	85.9	12.4	1	0.7	-0.15	83.17	57.045

3D7_dbl6689	88.5	10.2	0.3	1	-0.08	80.32	52.336
3D7_dbl9167	86.1	11.1	1.8	1	-0.14	83.1	60.563
3D7_dbl6953	87.3	10.7	0.7	1.2	-0.14	83.04	65.358
3D7_dbl7212	86.4	11	1.8	0.8	0.29	91.57	65.301
3D7_dbl4675	88.8	9.5	1.1	0.5	-0.02	83.9	77.805
3D7_dbl3374	87.7	9.4	2.1	0.8	-0.02	91.02	67.79
3D7_dbl5142	88.6	9.8	1.3	0.3	-0.24	77.55	64.03
3D7_dbl5155	85.8	12.7	1.3	0.3	-0.15	86.64	66.745
3D7_dbl5393	88.1	10.3	0.5	1	-0.06	86.53	59.907
3D7_dbl5395	84.5	11.3	3	1.3	-0.11	73.44	57.044
3D7_dbl1918	86.5	11.2	1.3	1	-0.15	91.59	55.916
3D7_dbl5545	88.6	9.4	1	1	-0.12	85.52	53.935
3D7_dbl5931	88	9	2.8	0.3	-0.08	82.07	63.42
3D7_dbl1796	87	10.7	1	1.3	-0.2	87.58	61.06
3D7_dbl1798	86.5	10.5	2.2	0.8	-0.15	92.58	64.019
3D7_dbl5639	88.8	9.1	1.6	0.5	-0.04	79.36	76.633
3D7_dbl5551	85.2	13	1	0.8	-0.25	78.72	67.15
3D7_dbl5933	86.3	12	1.5	0.2	-0.11	69.48	64.802
3D7_dbl5645	89	8.7	1.5	0.8	-0.06	79.53	61.985
3D7_dbl1802	83.8	13.2	2.3	0.8	-0.13	86.04	64.59
3D7_dbl5547	88.1	9.8	1.9	0.3	-0.12	76.6	64.304
3D7_dbl7291	89.3	8.4	1.8	0.5	-0.05	73.87	57.56
3D7_dbl2760	88.9	8.9	1.4	0.9	-0.05	88.14	75.989
3D7_dbl2172	88.1	9.6	1.3	1	-0.14	74.46	60
3D7_dbl1806	88	9.6	1.1	1.3	-0.1	66.35	61.881
3D7_dbl2608	87.3	10.3	1.6	0.8	-0.09	55.98	55.392
3D7_dbl2764	86.3	12	1.5	0.2	-0.11	69.48	64.802
3D7_dbl2610	83.1	12.9	2.2	1.7	-0.15	80.09	49.885
3D7_dbl2768	91.7	7.1	0.9	0.3	-0.02	82.7	73.368

3D7_dbl2762	87.4	9.4	2.2	1.1	-0.15	82.21	69.951
IGHvar01	84.8	12	1.8	1.5	-0.08	87.93	58.87
IGHvar02	88.5	9.9	0.3	1.4	-0.07	81.95	65.375
IGHvar03	86.4	9.3	3.3	1	-0.33	75.23	57.042
IGHvar04	87.7	10	1.5	0.8	-0.09	84.22	54.524
IGHvar05	88.5	8.8	0.8	1.9	-0.01	72.68	69.797
IGHvar06	85.6	12.3	1.5	0.5	-0.22	79.68	59.953
IGHvar07	86.9	11.1	1.8	0.3	-0.07	72.79	57.077
IGHvar09	89	9.1	0.8	1.1	-0.05	81.45	72.821
IGHvar10	89.6	8.5	1.1	0.8	-0.02	78.09	78.836
IGHvar11	88.6	10.3	0.3	0.8	0	81.47	80
IGHvar12	88.8	10.1	0.6	0.6	-0.01	81.66	81.234
IGHvar13	84.4	13.3	2.3	0.5	-0.13	77.13	53.318
IGHvar14	87.4	10.3	0.8	1.5	-0.14	74.27	55.504
IGHvar15	85.6	10.9	1.6	1.9	-0.1	86.05%	69.807
IGHvar16	87	11.3	0.5	1.2	-0.13	71.14	62.181
IGHvar17	88.8	9.3	1	1	-0.09	79.33	49.306
IGHvar18	89.9	7.9	0.5	0.5	-0.02	79.45	68.462
IGHvar19	88.5	9.2	1.5	0.8	-0.05	73.29	58.937
IGHvar20	89.1	8.6	1.6	0.8	-0.09	83.21	64.706
IGHvar21	85.2	11.1	2.9	0.8	-0.09	72.97	67.402
IGHvar22	87.4	9.7	1.7	1.1	-0.03	83.33	78.158
IGHvar23	90.5	8.4	0.8	0.3	0.01	81.45	75.897
IGHvar24	90.1	8.2	0.6	1.1	0.04	77.44	84.514
IGHvar26	91	8.8	0	0.3	0.04	80.8	81.88
IGHvar27	86.8	11	2.2	0	-0.18	75.25	68.992
IGHvar28	88.3	8.8	2.4	0.5	-0.1	72.93	76.382
IGHvar29	86.2	10.5	2	1.2	-0.11	82.92	55.399
IGHvar30	88.7	9.9	0.6	0.8	-0.09	88.49	72.296

IGHvar31	87.1	9.8	2.1	1	-0.11	85.14	66.507
IGHvar32	89.7	9.2	0.8	0.3	-0.01	80.34	81.654
IGHvar33	85.7	11.3	1.8	1.3	-0.1	74.25	72.275
IGHvar34	85.8	11.5	1.4	1.4	-0.14	67.25	70.361
IGHvar35	86.3	12.4	0.2	1	-0.05	81.76	58.255
IGHvar36	85.4	12.4	1.2	1	-0.17	87.7	57.73
IGHvar37	90.8	7.9	0.8	0.5	-0.07	75.6	65.423
IGHvar38	86.1	11.1	1.8	1	-0.08	74.37	66.43
IGHvar39	90.6	8.3	0.8	0.3	0.05	80.38	77.215
IGHvar40	87.3	10.9	1	0.8	-0.08	79.16	65.311
RAJ116var01	84.7	12.8	1	1.5	-0.13	75.29	66.509
RAJ116var02	90.2	8.5	1.4	0	-0.05	75.57	66.753
RAJ116var03	89.2	10.3	0.6	0	0.04	81.82	78.811
RAJ116var04	88.2	9.5	1	1.3	-0.08	82.39	54.436
RAJ116var05	91.8	7	0.8	0.3	-0.02	79.18	75.789
RAJ116var06	87.8	10.6	1.1	0.5	-0.05	83.21	74.129
RAJ116var07	90.2	9	0.6	0.3	-0.03	79.9	77.604
RAJ116var08	87.8	9.5	1.4	1.4	-0.07	82.13	60.66
RAJ116var09	88.1	10.3	0.5	1.6	-0.07	79.36	68.632
RAJ116var10	91.1	7.9	0.8	0.3	-0.05	76.05	59.091
RAJ116var11	86.6	11.9	0.8	0.8	-0.13	75.65	68.357
RAJ116var14	88.4	9.5	1.1	1.1	-0.07	90.39	68.357
RAJ116var15	86.8	10.6	1.3	1.3	-0.12	82.41	61.823
RAJ116var16	90.9	8.6	0.6	0	0.01	83.97	75
RAJ116var17	88.4	10.1	1.1	0.5	-0.04	76.63	77.723
RAJ116var18	89.9	9.1	0.5	0.5	0.29	86.53	72.967
RAJ116var19	91.2	7.6	0.8	0.3	0.03	90.59	86.053
RAJ116var21	85.5	11.3	2.3	1	-0.06	77.88	63.923
RAJ116var22	87.1	10.5	1.8	0.5	-0.08	77.99	66.748

RAJ116var24	86.3	10.6	2.1	1	-0.12	83.76	63.658
RAJ116var26	87.5	10.5	0.8	1.3	-0.1	80.37	68.496
RAJ116var27	87.4	11.4	1	0.2	-0.08	77.23	62.87
RAJ116var28	86.3	11.2	1.5	1	-0.09	85.35	66.042
RAJ116var29	87.1	9.9	1.3	1.6	-0.16	82.93	64.09
RAJ116var30	85.6	11	2.6	0.8	-0.1	89.25	62.679
RAJ116var31	82.5	14.2	2	1.2	-0.1	68.71	68.519
RAJ116var32	88.6	10.9	0.3	0.3	-0.05	62.71	68.983
RAJ116var33	88.1	10.6	0.8	0.5	-0.05	83.58	74.436
RAJ116var34	87.9	8.5	2.1	1.6	-0.1	85.35	53.901
RAJ116var35	86.7	10.6	1.9	0.8	-0.12	75.98	60.652
RAJ116var36	86.2	11.3	2.1	0.5	-0.08	87.87	75.238
RAJ116var37	83.5	12.5	2.4	1.6	-0.13	80.15	61.654
RAJ116var38	90.5	7.8	1.2	0.6	-0.08	89.9	83.733
RAJ116var39	88.2	9.2	1.8	0.8	-0.11	87.62	66.667

Table S3 Comparison of RMSD values in PfEMP1 and its conserved residues

Protein Name	Full Protein		CTVLARSFADIGDIVRGKDLY (MD1)		LDYVPQYLRWFEEWAEDFCR (MD2)	
	C-alpha	Main Chain	C-alpha	Main Chain	C-alpha	Main Chain
IGHvar_01	1.71	1.736	1.238	1.23	1.204	1.255
IGHdbl_02	2.477	2.493	1.971	1.967	1.433	1.393
IGHdbl_03	2.823	2.846	1.612	1.6	1.822	1.812
IGHdbl_04	2.829	2.84	1.866	1.869	1.295	1.293
IGHdbl_05	2.475	2.502	1.988	1.983	1.955	1.955
IGHdbl_06	2.526	2.556	1.137	1.106	1.882	1.876
IGHdbl_07	2.099	2.128	0.973	0.97	1.007	1.007
IGHdbl_09	2.665	2.669	2.427	2.399	2.34	2.316
IGHdbl_10	1.162	1.191	0.881	0.877	0.982	0.956
IGHdbl_11	2.853	2.865	2.47	2.442	2.24	2.223
IGHdbl_12	2.35	2.357	2.335	2.318	2.289	2.285
IGHdbl_13	2.843	2.872	2.579	2.574	2.456	2.444
IGHdbl_14	2.955	2.977	3.16	3.169	2.662	2.644
IGHdbl_15	2.302	2.326	2.274	2.267	2.197	2.191
IGHdbl_16	2.135	2.155	1.399	1.413	1.593	1.564
IGHdbl_17	2.489	2.505	2.233	2.276	1.76	1.765
IGHdbl_18	2.405	2.415	1.459	1.474	1.561	1.557
IGHdbl_19	3.082	3.085	2.424	2.418	2.487	2.472
IGHdbl_20	2.683	2.683	1.435	1.412	1.95	1.93
IGHdbl_21	2.557	2.567	2.557	2.567	2.607	2.568
IGHdbl_22	2.053	2.075	1.976	1.972	1.881	1.872

IGHdbl_23	2.96	2.971	2.946	2.924	2.87	2.858
IGHdbl_24	2.552	2.561	2.201	2.22	2.365	2.361
IGHdbl_26	2.656	2.667	2.702	2.696	2.078	2.081
IGHdbl_27	2.486	2.516	2.156	2.215	2.776	2.755
IGHdbl_28	2.603	2.608	1.999	1.99	1.157	1.169
IGHdbl_29	2.505	2.515	1.761	1.793	1.835	1.838
IGHdbl_30	1.94	1.949	1.748	1.745	1.433	1.4
IGHdbl_31	2.438	2.463	2.265	2.287	2.058	2.05
IGHdbl_32	2.524	2.538	1.25	1.247	1.537	1.53
IGHdbl_33	2.605	2.628	1.617	1.63	1.052	1.06
IGHdbl_34	2.388	2.409	1.726	1.717	1.813	1.778
IGHdbl_35	2.939	2.948	2.919	2.9	2.852	2.823
IGHdbl_36	2.896	2.919	2.945	2.981	2.379	2.355
IGHdbl_37	1.56	1.605	1.48	1.524	1.217	1.209
IGHdbl_38	1.917	1.949	0.845	0.833	1.133	1.162
IGHdbl_39	2.637	2.635	2.471	2.493	2.714	2.71
IGHdbl_40	2.371	2.384	2.721	2.715	2.952	2.965
RAJ116var01	2.76	2.779	2.64	2.642	2.662	2.672
RAJ116var02	2.693	2.705	1.769	1.744	1.768	1.742
RAJ116var03	2.591	2.596	2.268	2.266	2.551	2.526
RAJ116var04	2.694	2.712	2.539	2.535	2.651	2.635
RAJ116var05	1.963	1.966	1.564	1.559	1.544	1.524
RAJ116var06	2.055	2.074	1.903	1.907	1.598	1.597
RAJ116var07	2.48	2.479	1.566	1.553	1.829	1.849
RAJ116var08	2.739	2.759	1.656	1.661	1.456	1.446
RAJ116var09	2.294	2.313	1.799	1.778	1.333	1.314

RAJ116var10	1.871	1.875	1.583	1.591	1.454	1.45
RAJ116var12	3.377	3.392	2.606	2.591	2.445	2.424
RAJ116var14	2.757	2.805	2.881	2.916	2.503	2.515
RAJ116var15	2.631	2.626	1.022	1.822	3.265	3.25
RAJ116var16	1.949	1.976	1.937	1.984	1.087	1.085
RAJ116var17	2.595	2.59	2.372	2.397	1.583	1.615
RAJ116var18	2.5	2.526	2.015	2.0026	2.6	2.584
RAJ116var19	2.314	2.356	2.22	2.237	1.781	1.786
RAJ116var20	2.811	2.823	2.86	2.851	3.062	3.029
RAJ116var21	2.453	2.459	2.159	2.227	1.997	2.002
RAJ116var22	2.453	2.459	2.175	2.251	1.997	2.002
RAJ116var24	2.358	2.384	2.36	2.369	1.603	1.593
RAJ116var26	2.665	2.706	1.598	1.517	1.843	1.832
RAJ116var27	2.584	2.612	2.235	2.257	2.135	2.143
RAJ116var28	2.815	2.823	2.589	2.583	2.562	2.612
RAJ116var29	1.808	1.853	1.383	1.401	1.235	1.244
RAJ116var30	2.621	2.647	1.571	1.559	1.145	1.137
RAJ116var31	2.335	2.329	1.823	1.835	2.63	2.625
RAJ116var32	1.943	1.97	1.704	1.686	1.597	1.603
RAJ116var33	2.079	2.099	1.487	1.534	1.047	1.096
RAJ116var34	2.528	2.534	1.163	1.181	1.354	1.352
RAJ116var35	2.503	2.521	2.4	2.026	1.716	1.731
RAJ116var36	2.304	2.322	1.266	1.254	1.166	1.155
RAJ116var37	2.803	2.792	2.646	2.177	2.54	2.529
RAJ116var38	2.586	2.607	1.151	1.16	1.41	1.404
RAJ116var39	2.764	2.77	2.78	2.761	2.589	2.592

gi_86171174	2.759	2.775	2.738	2.716	2.662	2.639
gi_86171918	2.362	2.368	1.848	1.774	2.418	2.41
gi_86171928	1.397	1.443	0.704	0.699	0.636	0.636
gi_124504675	2.062	2.094	1.822	1.827	1.549	1.567
gi_124505155	2.538	2.548	2.428	2.486	1.821	1.827
gi_124505159	2.808	2.819	2.834	2.807	2.743	2.719
gi_124505387	2.845	2.833	2.645	2.64	2.734	2.715
gi_124505393	2.565	2.579	2.965	2.948	2.077	2.076
gi_124505395	2.939	2.955	2.564	2.569	2.721	2.708
gi_124505543	2.909	2.911	2.764	2.73	2.956	2.926
gi_124505545	2.637	2.666	2.096	2.076	2.225	2.195
gi_124505547	2.886	2.887	3.428	3.409	3.193	3.189
gi_124505551	2.639	2.683	2.656	2.72	2.728	2.718
gi_124505639	2.723	2.736	2.474	2.5	2.306	2.308
gi_124505643	1.181	1.183	0.703	0.69	0.587	0.584
gi_124505645	3.035	3.04	3.035	3.004	3.038	3.014
gi_124505931	2.491	2.499	2.162	2.187	2.534	2.533
gi_124505933	2.865	2.867	2.988	3.008	2.528	2.536
gi_124506559	2.768	2.794	2.373	2.393	1.939	1.933
gi_124507287	1.993	2.042	1.591	1.575	1.166	1.147
gi_124507291	2.214	2.24	2.209	2.225	1.64	1.631
gi_124511794	2.438	2.471	2.285	2.284	2.6	2.568
gi_124511796	2.827	2.838	2.484	2.479	2.76	2.754
gi_124511798	2.641	2.673	2.376	2.368	2.376	2.368
gi_124511800	2.514	2.527	2.836	2.872	2.647	2.624
gi_124511802	2.339	2.383	2.137	2.13	2.282	2.269

gi_124511804	2.198	2.215	1.975	1.966	1.775	1.775
gi_124511806	1.678	1.708	1.016	1.008	1.294	1.348
gi_124512172	2.392	2.422	1.939	1.941	1.295	1.286
gi_124512608	1.812	1.84	1.011	1.024	1.279	1.293
gi_124512610	2.292	2.32	1.485	1.501	2.332	2.327
gi_124512758	1.882	1.91	1.091	1.087	1.485	1.481
gi_124512760	2.17	2.175	1.798	1.784	1.669	1.677
gi_124512762	3.066	3.079	3.079	3.062	3.287	3.248
gi_124512764	2.865	2.867	2.988	3.008	2.528	2.536
gi_124775746	2.969	2.985	2.884	2.875	3.104	3.095
gi_124803374	2.696	2.719	2.591	2.577	2.774	2.752
gi_124803377	3.001	3.004	3.215	3.2	2.66	2.637
gi_124805005	2.586	2.6	2.447	2.455	2.338	2.348
gi_124805331	2.499	2.513	2.593	2.61	2.149	2.128
gi_124805343	2.575	2.588	2.846	2.827	2.503	2.482
gi_124805987	3.007	2.968	2.632	2.442	2.917	2.913
gi_124806687	2.644	2.654	2.594	2.600	1.998	2.003
gi_124806689	2.542	2.562	2.254	2.29	1.944	1.959
gi_124806691	2.466	2.488	2.488	2.458	2.913	2.978
gi_124807212	22.014	21.992	9.034	8.849	10.166	9.901
gi_258549167	22.496	22.5	7.964	7.68	7.774	7.5
gi_258596953	2.623	2.656	2.929	2.912	2.41	2.392
gi_258597176	2.873	2.871	2.535	2.54	2.645	2.644
gi_296004752	2.702	2.704	2.07	2.094	2.94	2.98
gi_296005120	2.654	2.658	1.762	1.751	1.793	1.828
gi_296005142	3.233	3.251	3.361	3.333	3.087	3.074

Table S4 Binding energies with Heparin

Protein Name	Solution No	Global Energy	Attractive VdW	Repulsive VdW	ACE
gi_86171174	4	-41.15	-34.63	25.66	-7.05
gi_86171918	7	-30.24	-21.48	2.04	-1.04
gi_86171928	9	-43.50	-26.01	16.29	-11.61
gi_124504675	1	-44.58	-28.79	7.85	-7.16
gi_124505155	5	-50.10	-28.64	19.82	-15.43
gi_124505159	2	-40.49	-31.97	33.96	-13.24
gi_124505387	6	-49.74	-23.18	2.54	-12.52
gi_124505393	9	-39.20	-22.85	4.91	-7.58
gi_124505395	1	-46.95	-26.80	9.25	-9.46
gi_124505543	1	-51.70	-24.09	9.00	-15.35
gi_124505545	1	-42.29	-29.31	16.83	-9.10
gi_124505547	7	-34.72	-25.36	38.31	-19.28
gi_124505551	2	-52.18	-25.21	7.52	-13.38
gi_124505639	9	-41.43	-24.77	4.62	-6.40
gi_124505643	10	-38.73	-25.69	10.27	-7.80
gi_124505645	4	-52.10	-32.08	14.52	-11.63
gi_124505931	1	-52.03	-23.48	1.48	-13.49
gi_124505933	6	-37.19	-17.45	3.74	-9.53
gi_124506559	7	-43.15	-32.18	6.27	-2.45
gi_124507287	5	-40.36	-29.61	12.03	-6.07
gi_124507291	6	-31.51	-23.97	17.09	-6.60
gi_124511794	5	-59.53	-34.75	9.29	-10.01
gi_124511796	3	-48.30	-31.06	20.06	-12.13
gi_124511798	9	-60.04	-24.63	9.74	-21.22
gi_124511800	5	-49.16	-22.77	4.38	-14.24
gi_124511802	1	-54.54	-26.14	7.64	-14.75
gi_124511804	3	-41.82	-25.44	5.81	-7.57
gi_124511806	9	-45.46	-21.78	5.61	-11.99
gi_124512172	4	-45.60	-23.69	7.13	-10.73
gi_124512608	7	-30.98	-21.53	8.96	-5.66
gi_124512610	9	-36.40	-25.26	11.37	-6.05
gi_124512758	2	-51.16	-25.68	5.10	-11.53
gi_124512760	3	-52.77	-27.21	16.51	-16.23
gi_124512762	2	-59.46	-25.87	7.18	-17.11
gi_124512764	6	-37.19	-17.45	3.74	-9.53
gi_124512768	2	-51.16	-25.68	5.10	-11.53
gi_124775746	4	-55.33	-25.64	3.60	-13.61
gi_124801837	5	-45.03	-27.35	7.79	-8.92
gi_124803374	1	-70.45	-34.43	18.47	-21.45
gi_124803377	8	-51.14	-22.00	11.40	-19.32
gi_124805005	5	-44.38	-24.77	10.95	-11.06
gi_124805331	10	-44.59	-23.78	10.58	-13.03
gi_124805343	7	-42.39	-24.78	12.91	-10.86
gi_124805987	10	-50.30	-22.73	4.36	-15.08
gi_124806687	8	-48.99	-22.24	5.53	-14.52
gi_124806689	2	-48.24	-24.04	9.16	-14.12

gi_124806691	5	-55.97	-26.28	14.05	-18.31
gi_124807212	4	-46.58	-20.99	11.34	-16.43
gi_258549167	1	-54.90	-28.35	14.53	-15.7
gi_258596953	2	-52.92	-27.82	10.23	-14.10
gi_258597176	1	-37.35	-26.02	8.66	-5.31
gi_296004752	10	-38.53	-21.03	5.17	-8.09
gi_296005120	9	-41.43	-24.77	4.62	-6.40
gi_296005142	8	-63.66	-24.47	4.70	-21.50
IGHvar02	3	-55.89	-30.18	14.29	-14.52
IGHvar03	9	-48.27	-28.28	12.31	-10.76
IGHvar04	2	-35.35	-33.89	31.20	-6.78
IGHvar04	9	-43.84	-24.35	4.37	-7.64
IGHvar05	2	-53.24	-30.86	7.95	-9.84
IGHvar06	1	-45.61	-25.40	13.54	-12.93
IGHvar07	10	-47.04	-22.98	4.99	-12.43
IGHvar09	6	-55.22	-35.32	28.83	-17.30
IGHvar10	3	-41.69	-23.16	3.26	-7.24
IGHvar11	10	-55.25	-27.05	5.82	-13.04
IGHvar12	8	-44.17	-25.03	7.69	-10.13
IGHvar13	6	-48.11	-31.12	16.25	-9.89
IGHvar14	7	-40.64	-25.24	5.50	-5.64
IGHvar15	7	-51.56	-25.62	6.27	-12.11
IGHvar16	2	-49.58	-26.89	9.68	-10.69
IGHvar17	3	-50.70	-27.12	11.80	-13.23
IGHvar18	7	-39.28	-26.35	14.07	-9.4
IGHvar19	3	-47.25	-26.27	9.84	-11.86
IGHvar20	8	-52.17	-24.41	8.08	-15.26
IGHvar21	8	-48.84	-30.75	12.71	-8.58
IGHvar22	9	-47.48	-30.68	23.52	-16.02
IGHvar23	4	-41.31	-26.53	9.68	-8.00
IGHvar24	9	-43.84	-24.35	4.37	-7.64
IGHvar26	6	-48.51	-26.85	11.34	-11.65
IGHvar27	8	-38.26	-26.34	20.92	-12.77
IGHvar28	2	-37.10	-24.26	4.57	-6.15
IGHvar29	3	-52.77	-24.16	10.88	-17.78
IGHvar30	5	-38.31	-20.95	7.60	-9.10
IGHvar31	2	-26.24	-16.34	2.30	-3.04
IGHvar32	10	-50.23	-26.05	9.67	-12.94
IGHvar33	8	-41.34	-20.15	7.55	-11.91
IGHvar34	6	-46.01	-26.74	11.35	-9.69
IGHvar35	3	-43.79	-23.69	5.30	-9.63
IGHvar36	8	-36.67	-22.32	13.97	-11.20
IGHvar37	8	-42.07	-28.30	7.88	-6.26
IGHvar38	4	-52.59	-24.02	5.10	-14.40
IGHvar39	2	-53.35	-30.14	13.02	-12.27
IGHvar40	8	-39.33	-24.82	11.50	-8.05
RAJ116var01	8	-48.50	-19.83	5.45	-15.75
RAJ116var02	2	-56.67	-28.22	12.89	-16.53
RAJ116var03	3	-40.41	-21.96	3.82	-7.80

RAJ116var04	10	-41.31	-26.81	12.99	-9.11
RAJ116var05	2	-57.46	-25.87	9.36	-16.96
RAJ116var06	1	-43.72	-25.88	11.35	-10.59
RAJ116var07	2	-42.89	-23.65	11.02	-12.24
RAJ116var08	2	-40.25	-21.56	9.21	-12.49
RAJ116var09	8	-47.51	-20.10	7.46	-15.73
RAJ116var10	3	-52.89	-26.39	4.67	-11.71
RAJ116var11	8	-41.36	-18.72	5.37	-13.81
RAJ116var12	1	-46.47	-24.62	10.01	-11.73
RAJ116var14	4	-51.36	-27.07	14.19	-15.1
RAJ116var15	2	-50.50	-27.44	11.55	-12.83
RAJ116var16	3	-41.30	-29.54	6.35	-3.61
RAJ116var17	1	-36.81	-22.42	6.94	-6.99
RAJ116var18	7	-61.37	-33.30	19.81	-17.65
RAJ116var19	5	-43.69	-23.79	7.49	-9.43
RAJ116var20	4	-48.73	-26.87	12.54	-13.48
RAJ116var21	4	-48.73	-26.87	12.54	-13.48
RAJ116var22	1	-44.96	-26.13	14.33	-12.94
RAJ116var24	3	-52.43	-26.55	3.81	-11.12
RAJ116var26	5	-46.59	-23.49	9.38	-12.87
RAJ116var27	2	-44.52	-28.02	4.58	-5.99
RAJ116var28	3	-52.64	-32.17	12.69	-10.19
RAJ116var29	10	-41.73	-28.88	4.86	-3.28
RAJ116var30	1	-51.01	-28.59	7.17	-10.14
RAJ116var31	7	-52.20	-29.24	8.06	-10.53
RAJ116var32	10	-37.23	-25.20	27.33	-15.42
RAJ116var33	1	-45.64	-28.04	17.43	-12.55
RAJ116var34	10	-45.82	-29.73	9.84	-6.21
RAJ116var35	4	-48.26	-31.08	18.27	-11.05
RAJ116var36	2	-48.31	-26.44	17.71	-15.30
RAJ116var37	5	-41.28	-24.07	13.00	-11.22
RAJ116var38	1	-64.61	-32.17	18.61	-20.28
RAJ116var39	4	-48.60	-31.97	25.15	-13.89

Table S5 Binding energies and their interactions with Heparin and Heparan Sulfate

Protein Name	**Binding Affinity (kcal/mol)**	**Solution No**	**Global Energy**	**Attractive VdW**	**Repulsive VdW**	**ACE**	**Interacting Residues**
	Heparin						
gi_86171174	-6.7	10	-51.96	-29.28	15.07	-13.39	Thr111,Arg115,Phe204, Arg205,Lys206,Asp208, Pro227,Thr228,Asn229, Leu230,Val233,Asp241, Ser244,Glu245,Leu365, Leu366,Asn367,Glu368
gi_124512768	-6.5	3	-51.16	-25.68	5.10	-11.53	Thr115,Tyr204,Thr216m Arg223,Pro230,Thr231, Glu378
gi_124505159	-7.4	6	-44.58	-24.54	6.36	-9.08	Arg113,Gln215,Thr216, Glu244,Tyr360,Arg374
IGHvar05	-6.9	7	-46.15	-28.22	12.80	-9.84	His99,Asp100,Glu101, His106,Lys107,Ser109, Asn110,Thr113,Ser195, Lys196,Thr197,Thr198, Arg240,Asm243,Leu366, Asn369,Lys371,Lys374, Asp375
IGHvar26	-6.7	10	-78.04	-32.98	15.47	-26.62	Asn109,Phe200,Leu363,

							Leu364,Glu366,Lys368, Tyr369
IGHvar34	-6.6	2	-45.20	-28.96	29.55	-18.24	Lys196, Ala198, Cys199, Gly200, Tyr220, Leu221, Leu228,Arg229, Glu232, Phe342,Leu346, Lys349, Tyr350,Asn358, Glu362, Glu363, Lys367
RAJ116var06	-7.2	1	-43.72	-25.88	11.35	-10.59	Thr111,Arg115,Tyr199, Phe200,Arg201,Lys202, Tyr224, Phe225, Tyr227, val228, Leu232, Asp236, Phe345,Glu348, Leu349, Lys351, Tyr353, Lys365, Glu366, Gln367, Gln370
RAJ116var19	-8.1	6	-59.83	-30.70	6.38	-13.91	Asp102,Lys103,Ser111, Thr114,Glu243,Lys250, Asn368, Asn373
RAJ116var28	-7.1	3	-52.64	-32.17	12.69	-10.19	His72,Ile146,Tyr148, Arg153, Glu150
	Heparan Sulfate						
gi_86171174							Gly108,Lys110,Thr111, Ala114,Arg115,Yr203, Arg205,Lys206,Lys207,

	-6.5	4	-35.15	-23.33	8.92	-5.30	Lys212,His213,Pro227,Thr228,Asn229,Leu230,Tyr232,Val233,Leu237,Asp241,Ser244,Glu245Phe362,Leu365,Glu368
gi_124512768	-6.4	3	-26.13	-20.01	3.03	0.03	Lys101,Gln112,Asn213,Thr115,Val116,Arg119,Phe205,Arg206,His207,Phe233,Glu244,Glu248,Leu374,Lys377,Glu378,Glu379
gi_124505159	-7.1	2	-39.00	-21.09	7.45	-9.39	Arg125,Gly126,Lys127,Arg171,Glu172,Thr340,Tyr341
IGHvar05	-6.9	6	-22.61	-20.01	7.12	0.10	Asp100,Glu101,His106,Ser109,Asn110,Cys112,Thr111,Tyr194,Ser195,Lys196,Glu232,Arg240,Glu370,Lys371,Cys373,Lys374
IGHvar26	-6.7	10	-78.04	-32.98	15.47	-26.62	Asn109,Arg116,Arg248,Leu363,Leu364,Glu366,Lys368
IGHvar34	-7.1	5	-49.17	-24.03	9.25	-13.46	Lys196,Tyr220,Lys349,

							Tyr350,Ser359
RAJ116var06	-6.0	2	-39.52	-21.04	8.89	-10.11	Tyr54,His97,Ser105, Glu241,Cys243,Arg244
RAJ116var19	-7.3	4	-32.83	-19.62	11.03	-8.26	Ser110,Ile112, Tyr200, Thr226,Asn239,Glu243, Lys364
RAJ116var28	-7.1	1	-39.68	-22.21	4.77	-6.49	Arg130,Tyr221,Asp227, Gly233,Glu267,Glu271, Lys395