Exploring the Transmembrane Allostery in MexB: DB08385 Variant as Promising Inhibitor like Candidate Against *Pseudomonas aeruginosa* Antibiotic Resistance – A Computational Study

Abhishek Bera[a], Shreya Mukherjee[a], Niladri Patra[a]*

Email: npatra2@iitism.ac.in

[a]Department of Chemistry & Chemical Biology, Indian Institute of Technology (ISM) Dhanbad, Dhanbad-826004, India

Supporting Information

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Table. S1. Top ten scoring molecules obtained from DrugRep ligand-based pharmacophore search using BDM88855 as reference molecule.

DrugBank ID	Name	Similarity score	M.W (g/mol)	ALogP	HBD	HBA	RB	Remarks
DB08385	4-(Quinolin-3-ylmethyl)piperidine-1-Carboxylic Acid	0.350	270.33	2.841	1	3	3	Related to PF 750, FAAH inhibitor, Perfect fit for MexB TM groove
DB14202	2-(Morpholinothio)benzothiazole	0.324	252.4	2.399	0	4	2	Standardized Chemical Allergen
DB02428	Quinoline-2-carboxylic acid	0.318	173.17	2.074	1	3	1	Endogenous metabolite, too small for MexB TM pocket
DB13823	Pipemidic acid	0.287	303.32	-2.335	2	8	3	pyridopyrimidine

								antibiotic derivative
DB13437	Medazepam	0.280	270.75	4.139	0	2	1	Anxiolytic, anticonvulsant, and sedative
DB04690	Camptothecine	0.278	348.4	1.746	1	5	1	An EC 5.99.1.2 (DNA topoisomerase) inhibitor
DB09197	Mepiprazole	0.276	304.82	3.25	1	3	4	A minor tranquilizer
DB13611	Chlormidazole	0.275	256.73	4.06	0	1	2	Antifungals
DB04582	(R)-Imazaquin	0.270	311.33	2.652	2	5	3	Herbicide
DB06852	(S)-3-(1H-benzo[d]imidazol-2-yl)-6-chloro-4-(quinuclidin-3-ylamino)quinolin-2(1H)-one	0.266	419.9	3.089	3	4	3	potent inhibitor of Chk1

Figure. S1. Comparison of the average RMSD fluctuation of the transmembrane @CA atoms of (a) MexB L protomer and MexB L protomer (trio); (b) DB08385, Variant 1 and Variant 2 bound MexB systems.

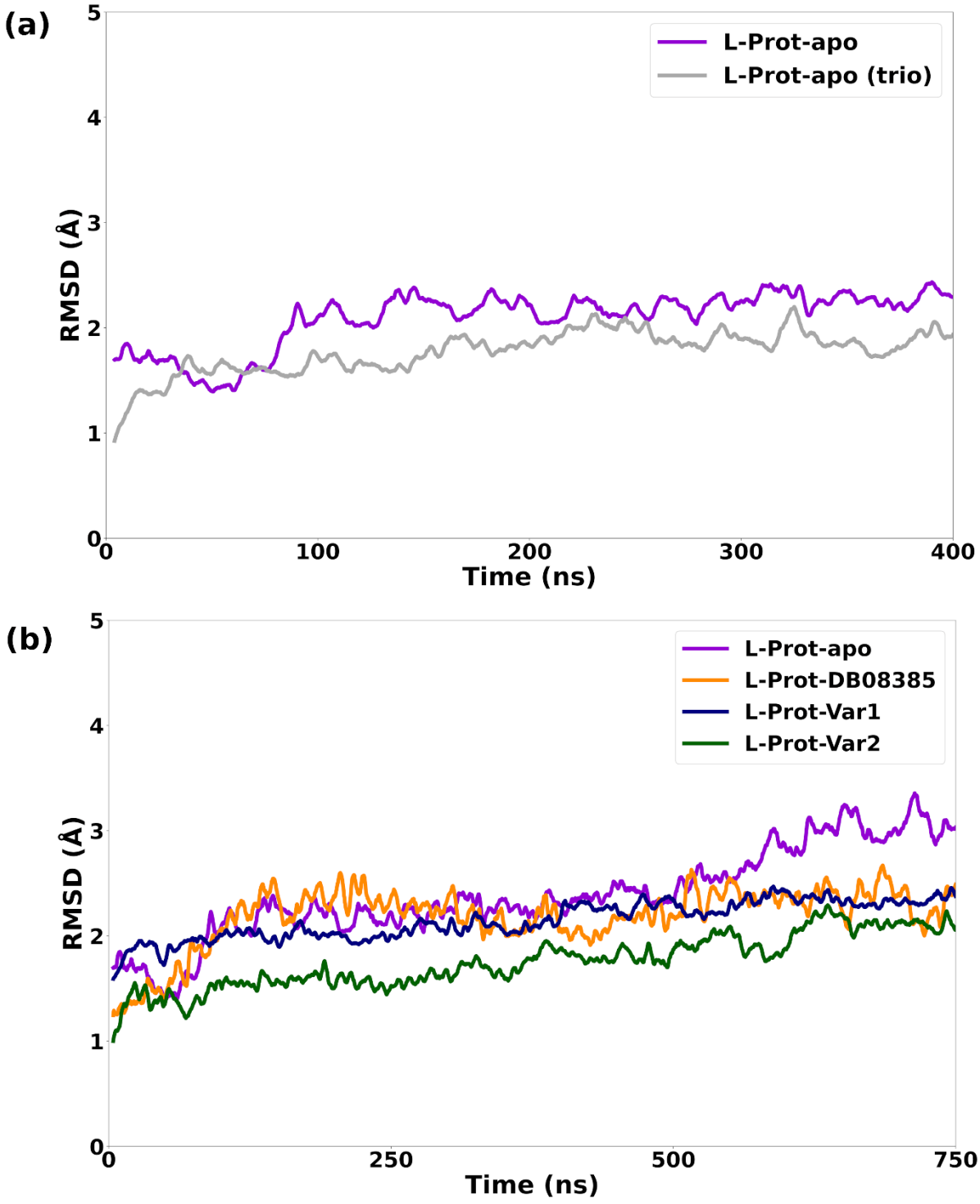
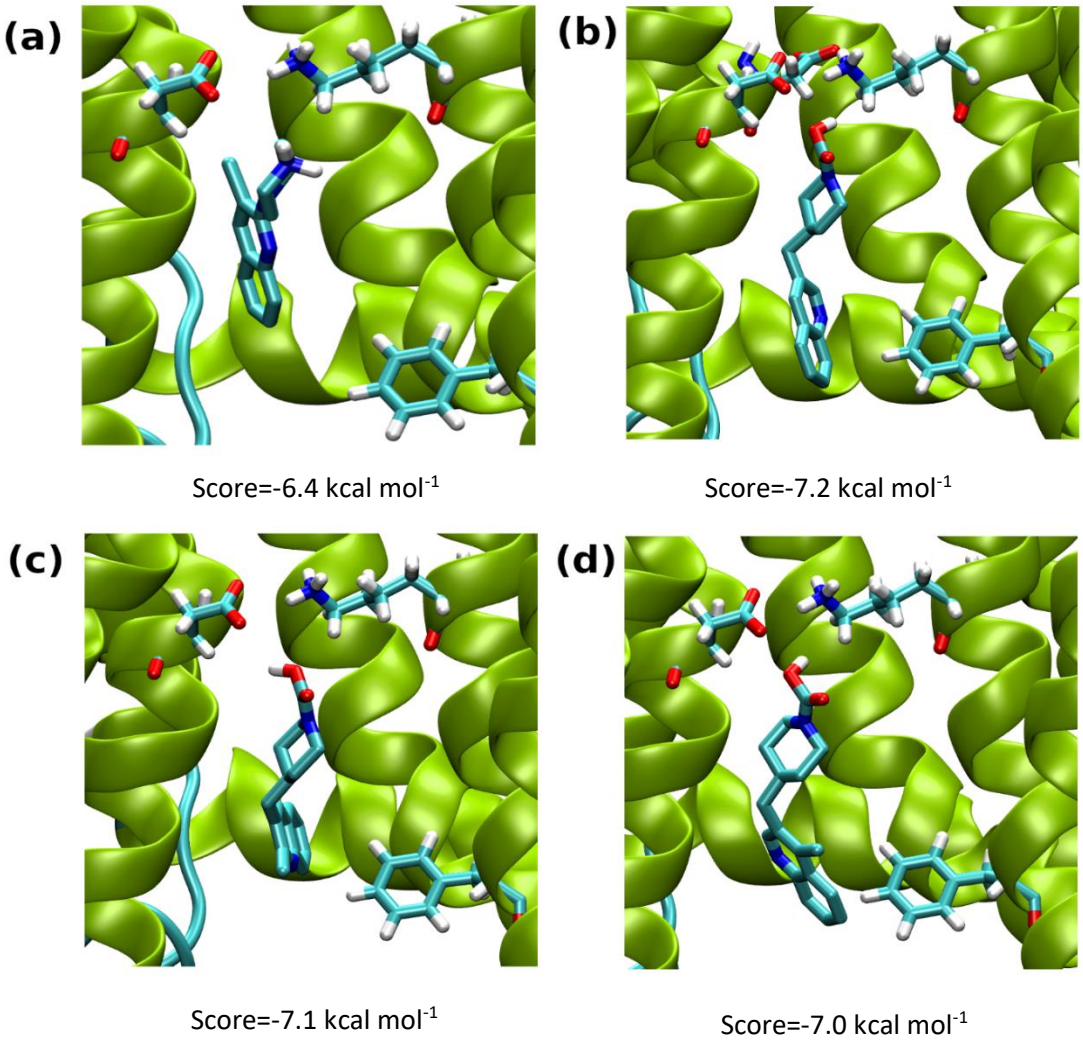


Figure. S2. Selected suitable flexible docking poses of (a) BDM88855, (b) DB08385, (c) 2-Cl DB08385 or Variant 1 and (d)-Cl DB08385 or Variant 2 used as initial structure for MD simulation along with their respective vina scores.



Flexible docking in Vina

Flexible residues – ASP408, VAL411, LYS939, LEU943, PHE947

center_x = -2.701, center_y = -4.592, center_z = -6.100

size_x = 12, size_y = 10, size_z = 18

exhaustiveness = 25

spacing = 1.0

Figure. S3. Center-of-mass distance between (a) DB08385 (deprot), (c) 2-Cl DB08385 (deprot) and (d)-Cl DB08385 (deprot) and ASP407-ASP408-LYS939 triad of MexB transmembrane site during unbiased MD simulation.

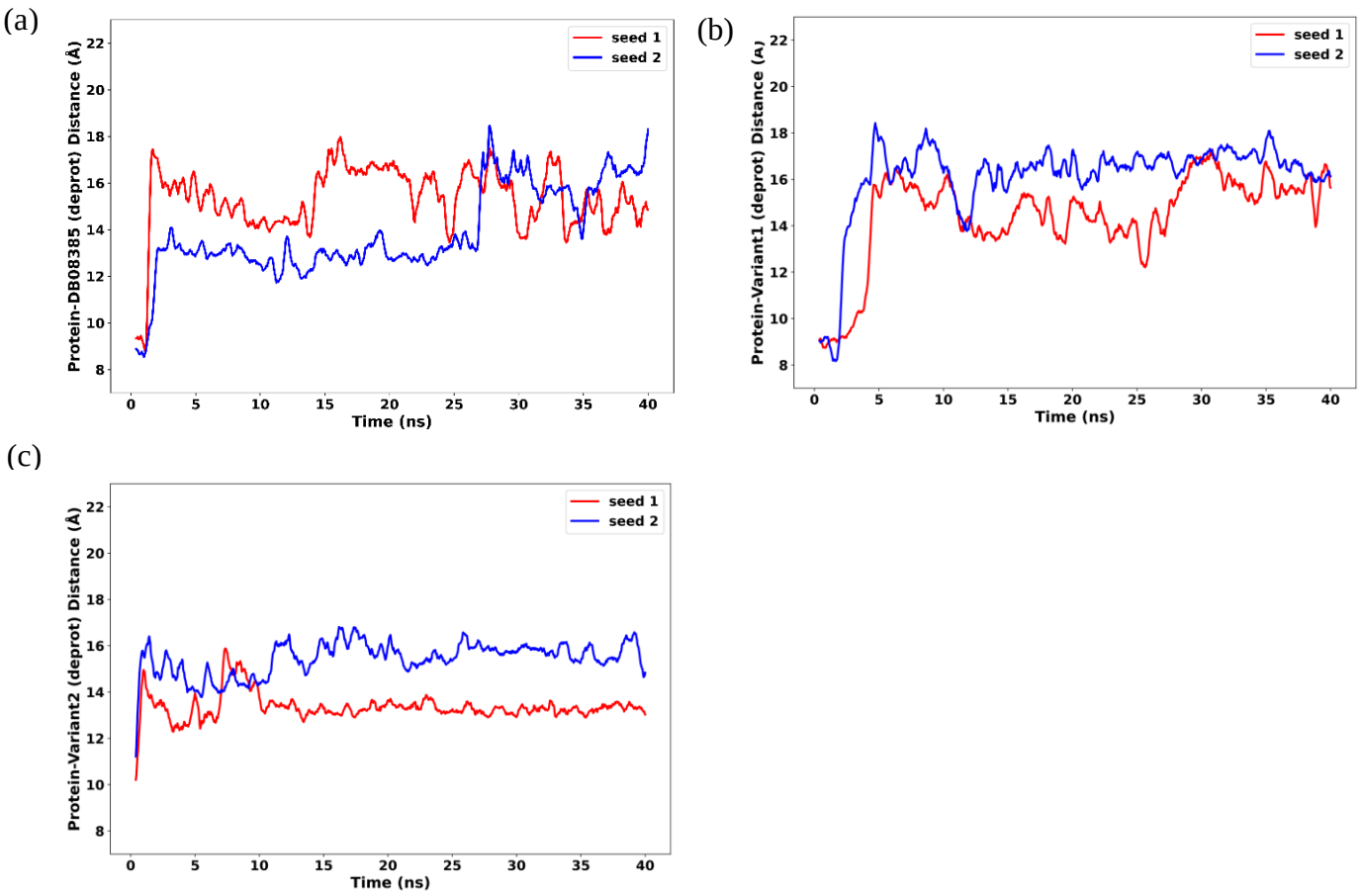


Figure. S4. Transmembrane pocket volume for apo and different ligand bound MexB systems.

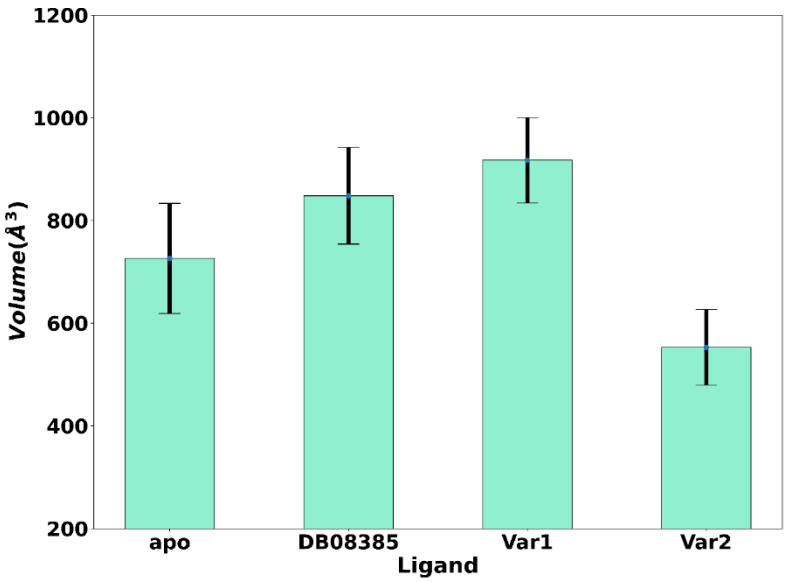


Figure. S5. Graphical representation of equilibrium ligand positions obtained from MD trajectories - (a) DB08385 (Conf 1), (b) DB08385 (Conf 2), (c) Variant 1 and (d) Variant 2 (before detachment from binding site) inside the TM cavity

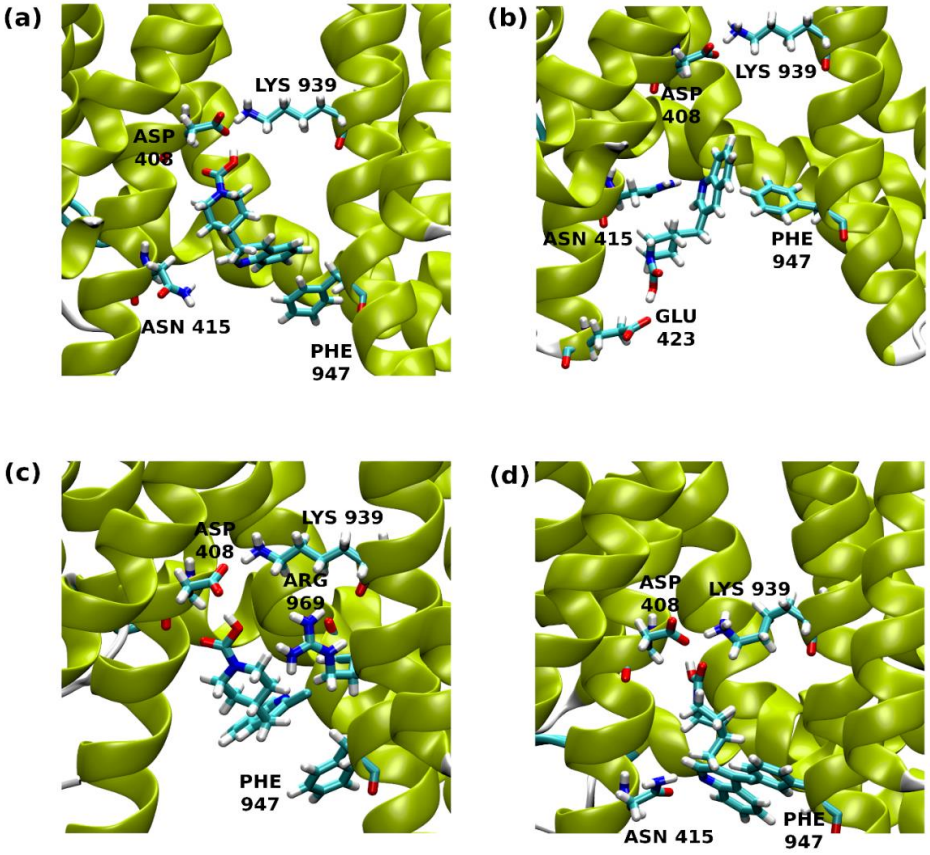


Figure. S6. Radius of Gyration of TM4 and TM10 for the apo and ligand bound MexB systems.

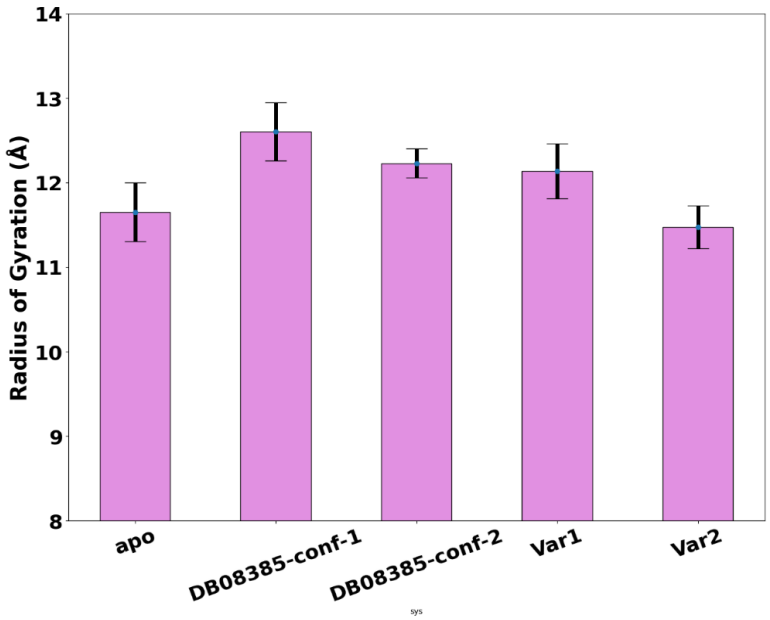


Figure. S7. Bar plot showing occupancies for the three hydrogen bond interactions, e.g., ASP408-LYS939, ASP407-LYS939 and ASP407-ARG969 in apo, DB08385, Variant 1 and Variant 2 bound MexB systems.

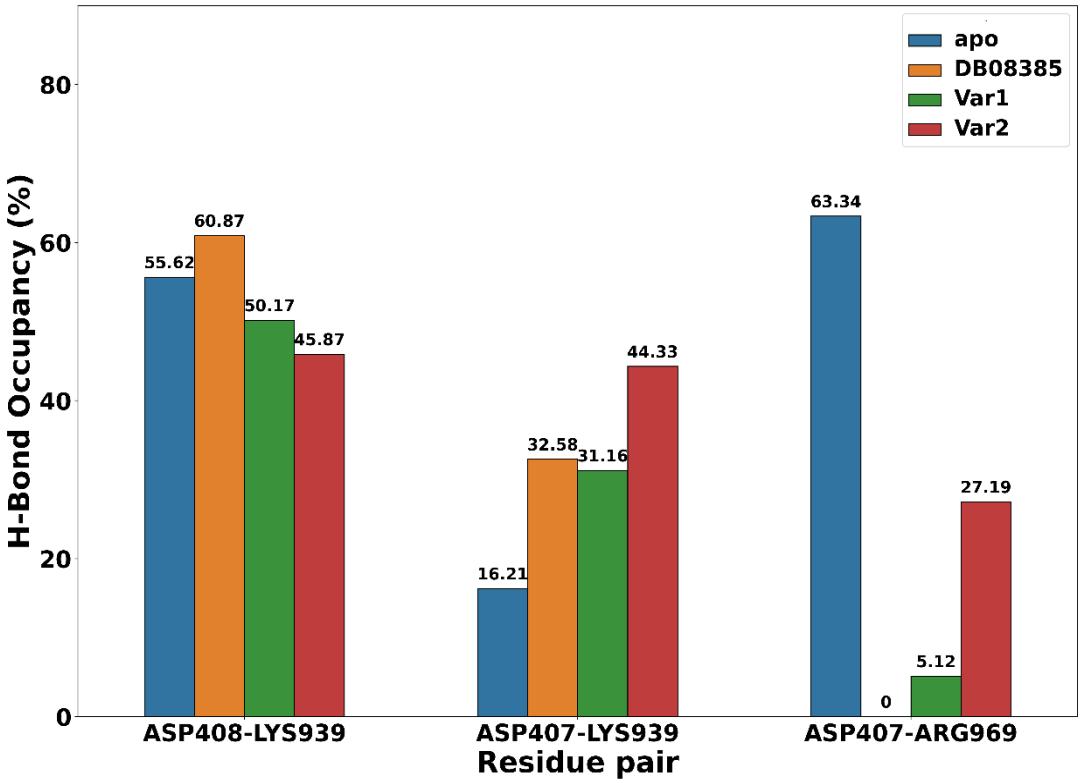


Figure. S3. Probability distribution plots showing adequate overlapping between consecutive sampling windows for (a) DB08385 (Conf 1), and (b) Variant 1 bound MexB systems.

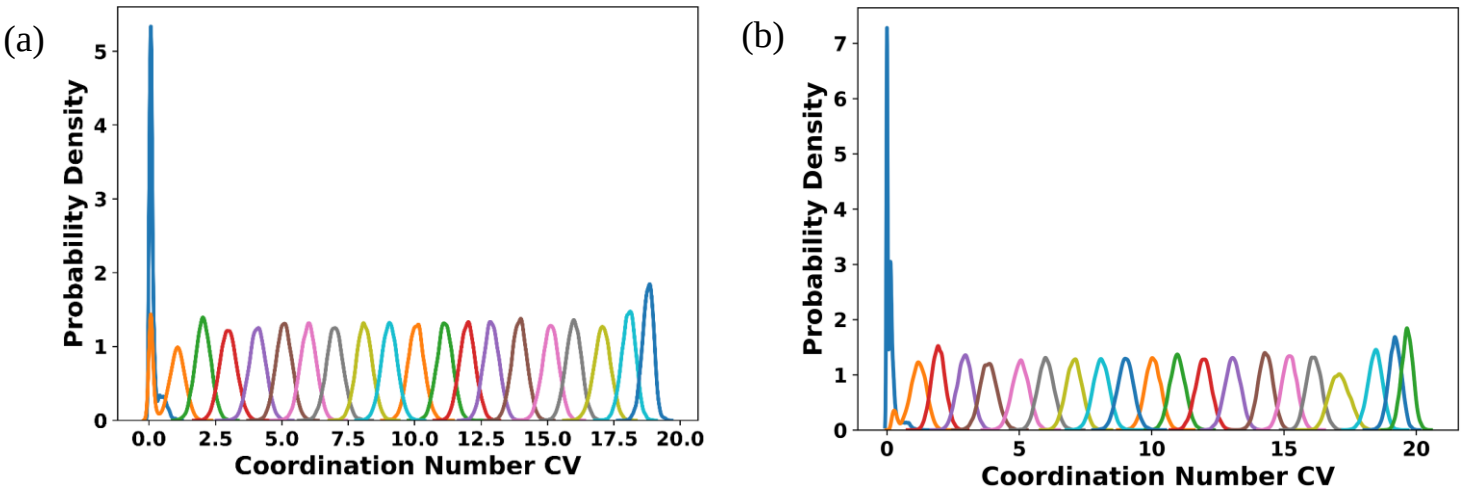


Figure. S4. Dynamic Cross Correlation Matrices for (a) apo, (b) DB08385 (Conf1), (c) DB08385 (Conf2), (d) Variant 1 (Var1), and (e) Variant 2 (Var2) bound MexB systems.

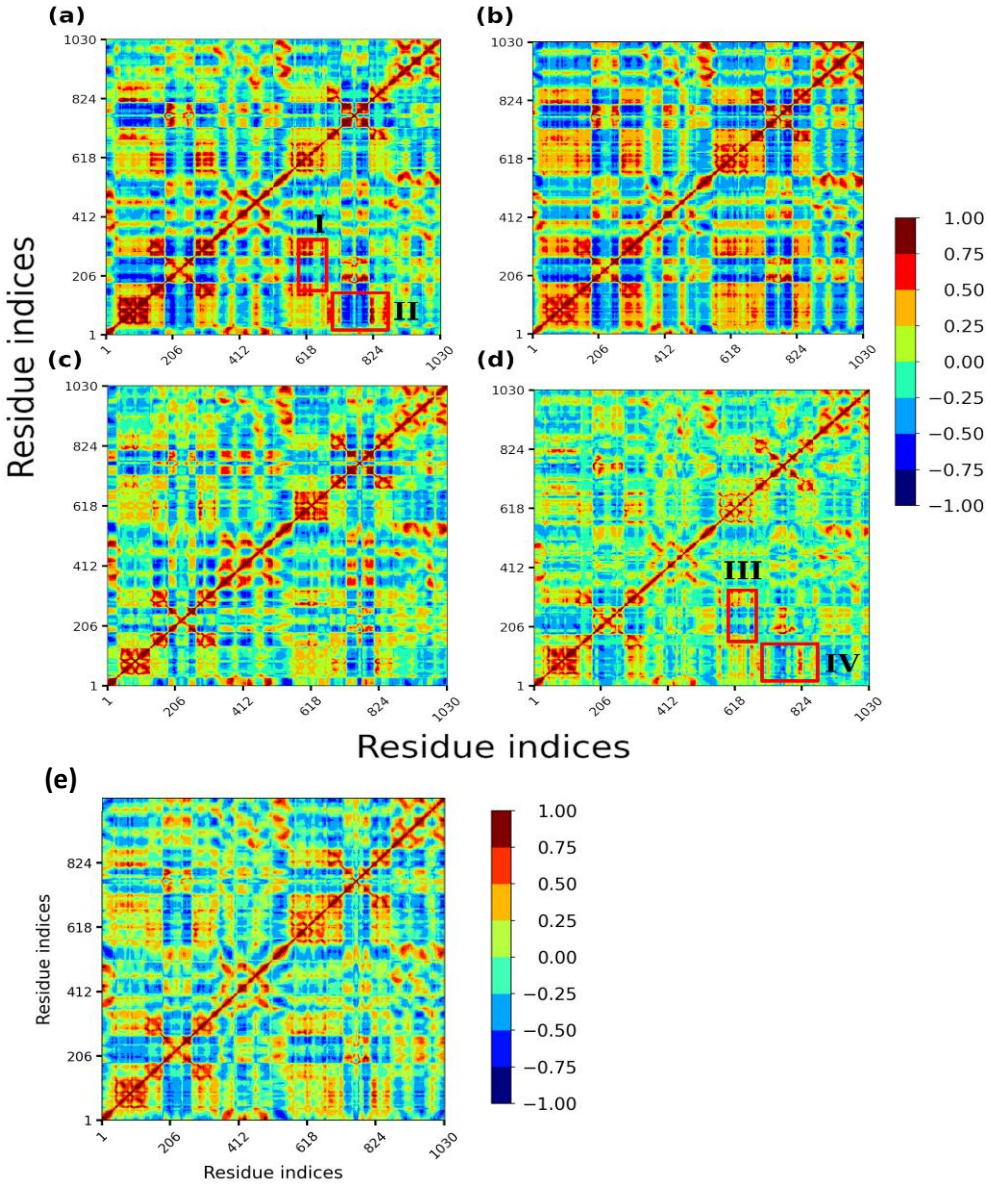


Figure. S5. Variation in eigenvector centralities for apo and Variant 1 bound MexB L protomer. Blue dots indicate important nodes in protein communication network where more intensity of the blue color signifying more central nodes among them.

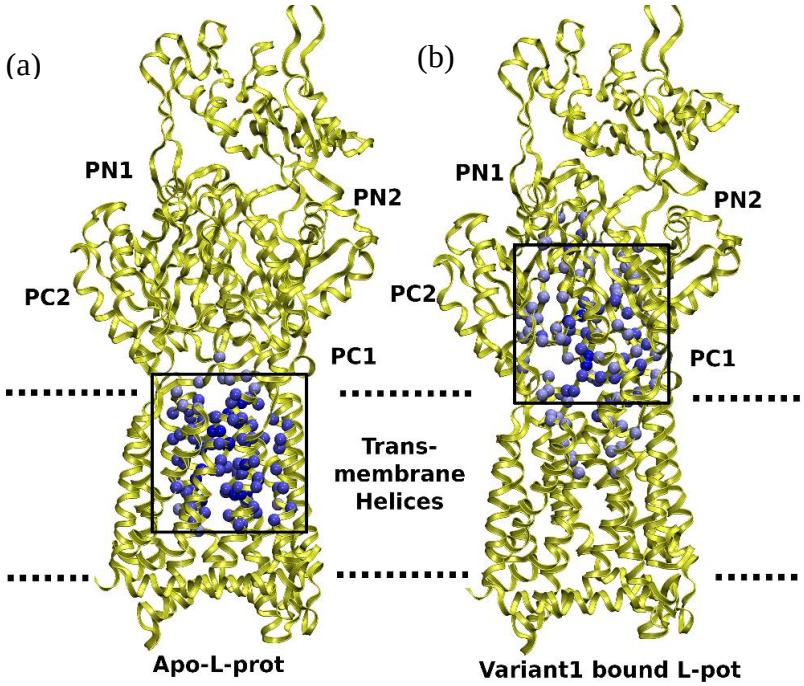


Table. S2. Eigenvector centralities for apo, DB08385 (Conf 1 and 2), Variant1 bound MexB L protomer along with their respective deviations from apo structure.

Residue	Apo	DB08385 (Conf1)	DB08385 (Conf2)	Variant1	DB08385 (Conf 1)-Apo	DB08385 (Conf 2)-Apo	Variant1-Apo
1	0.027	0.021	0.023	0.017	-0.006	-0.004	-0.010
2	0.030	0.023	0.026	0.012	-0.008	-0.004	-0.018
3	0.024	0.016	0.019	0.014	-0.008	-0.005	-0.010
4	0.020	0.014	0.015	0.011	-0.007	-0.005	-0.009
5	0.025	0.017	0.019	0.014	-0.008	-0.006	-0.012
6	0.024	0.017	0.018	0.013	-0.008	-0.007	-0.012
7	0.017	0.012	0.012	0.009	-0.005	-0.005	-0.008
8	0.018	0.013	0.014	0.010	-0.005	-0.004	-0.008
9	0.022	0.016	0.017	0.012	-0.006	-0.005	-0.010

10	0.020	0.015	0.015	0.011	-0.005	-0.005	-0.009
11	0.021	0.015	0.015	0.012	-0.007	-0.006	-0.010
12	0.029	0.020	0.022	0.017	-0.009	-0.007	-0.012
13	0.030	0.023	0.023	0.017	-0.008	-0.007	-0.013
14	0.023	0.018	0.019	0.015	-0.005	-0.004	-0.008
15	0.028	0.021	0.023	0.018	-0.008	-0.005	-0.010
16	0.034	0.028	0.030	0.023	-0.005	-0.004	-0.011
17	0.026	0.025	0.025	0.020	-0.001	-0.001	-0.006
18	0.027	0.023	0.023	0.020	-0.004	-0.004	-0.007
19	0.037	0.030	0.033	0.024	-0.007	-0.005	-0.013
20	0.029	0.033	0.034	0.025	0.004	0.006	-0.004
21	0.027	0.028	0.028	0.021	0.001	0.001	-0.006
22	0.038	0.031	0.032	0.025	-0.008	-0.006	-0.014
23	0.044	0.038	0.040	0.029	-0.006	-0.004	-0.015
24	0.033	0.035	0.037	0.027	0.002	0.004	-0.006
25	0.038	0.031	0.033	0.024	-0.007	-0.005	-0.014
26	0.049	0.038	0.042	0.033	-0.010	-0.007	-0.016
27	0.048	0.042	0.041	0.036	-0.006	-0.007	-0.012
28	0.041	0.037	0.031	0.033	-0.004	-0.010	-0.008
29	0.044	0.038	0.038	0.034	-0.006	-0.006	-0.011
30	0.048	0.044	0.043	0.039	-0.003	-0.005	-0.009
31	0.047	0.045	0.037	0.046	-0.001	-0.009	-0.001
32	0.049	0.048	0.035	0.045	-0.001	-0.014	-0.004
33	0.049	0.052	0.036	0.051	0.004	-0.013	0.002
34	0.054	0.055	0.039	0.058	0.001	-0.015	0.004
35	0.055	0.058	0.043	0.057	0.003	-0.012	0.002
36	0.054	0.059	0.053	0.053	0.005	-0.001	-0.001
37	0.049	0.058	0.050	0.055	0.009	0.001	0.006
38	0.046	0.056	0.040	0.052	0.010	-0.006	0.006
39	0.042	0.053	0.029	0.058	0.011	-0.014	0.016
40	0.036	0.047	0.025	0.052	0.011	-0.011	0.016
41	0.032	0.043	0.030	0.046	0.011	-0.002	0.014
42	0.026	0.039	0.032	0.048	0.013	0.006	0.023

43	0.020	0.032	0.032	0.044	0.012	0.012	0.023
44	0.019	0.034	0.032	0.047	0.015	0.013	0.028
45	0.014	0.028	0.029	0.041	0.014	0.015	0.027
46	0.015	0.031	0.023	0.044	0.016	0.007	0.029
47	0.013	0.031	0.024	0.041	0.017	0.011	0.027
48	0.013	0.033	0.018	0.041	0.021	0.005	0.029
49	0.011	0.027	0.018	0.033	0.016	0.007	0.022
50	0.010	0.023	0.015	0.033	0.013	0.005	0.023
51	0.012	0.020	0.014	0.030	0.009	0.003	0.018
52	0.009	0.021	0.014	0.034	0.011	0.005	0.024
53	0.010	0.020	0.020	0.028	0.010	0.010	0.018
54	0.011	0.027	0.023	0.036	0.016	0.012	0.025
55	0.009	0.025	0.023	0.027	0.016	0.014	0.017
56	0.008	0.022	0.022	0.025	0.014	0.014	0.017
57	0.010	0.029	0.023	0.025	0.019	0.013	0.015
58	0.010	0.028	0.025	0.034	0.018	0.016	0.024
59	0.008	0.022	0.023	0.029	0.014	0.016	0.021
60	0.007	0.021	0.023	0.027	0.014	0.016	0.020
61	0.009	0.025	0.026	0.032	0.016	0.017	0.023
62	0.010	0.027	0.027	0.033	0.018	0.017	0.023
63	0.008	0.022	0.023	0.029	0.014	0.015	0.021
64	0.007	0.018	0.020	0.023	0.011	0.014	0.017
65	0.008	0.020	0.023	0.027	0.012	0.015	0.019
66	0.009	0.021	0.023	0.028	0.013	0.014	0.019
67	0.006	0.016	0.017	0.022	0.010	0.010	0.015
68	0.006	0.014	0.016	0.020	0.008	0.010	0.014
69	0.009	0.018	0.020	0.025	0.009	0.011	0.016
70	0.009	0.016	0.017	0.023	0.008	0.009	0.014
71	0.007	0.016	0.015	0.021	0.008	0.008	0.014
72	0.009	0.018	0.020	0.023	0.009	0.010	0.014
73	0.012	0.020	0.020	0.026	0.008	0.008	0.014
74	0.017	0.026	0.024	0.034	0.009	0.006	0.016
75	0.014	0.025	0.025	0.034	0.011	0.010	0.019

76	0.019	0.030	0.027	0.041	0.011	0.008	0.022
77	0.017	0.030	0.028	0.042	0.012	0.011	0.025
78	0.014	0.028	0.029	0.040	0.014	0.015	0.026
79	0.015	0.030	0.028	0.044	0.015	0.013	0.028
80	0.015	0.030	0.028	0.045	0.015	0.013	0.030
81	0.015	0.032	0.033	0.048	0.017	0.018	0.033
82	0.014	0.030	0.032	0.046	0.016	0.018	0.032
83	0.014	0.034	0.036	0.049	0.020	0.022	0.035
84	0.012	0.034	0.032	0.046	0.022	0.020	0.034
85	0.013	0.035	0.033	0.046	0.022	0.019	0.032
86	0.014	0.035	0.023	0.043	0.021	0.009	0.029
87	0.015	0.036	0.026	0.045	0.021	0.011	0.031
88	0.014	0.031	0.024	0.045	0.017	0.011	0.031
89	0.016	0.033	0.024	0.046	0.017	0.008	0.030
90	0.015	0.029	0.029	0.040	0.014	0.014	0.026
91	0.018	0.033	0.030	0.045	0.015	0.012	0.027
92	0.017	0.030	0.033	0.041	0.013	0.016	0.024
93	0.021	0.034	0.035	0.047	0.012	0.014	0.026
94	0.022	0.032	0.034	0.045	0.010	0.012	0.023
95	0.025	0.036	0.031	0.043	0.011	0.006	0.018
96	0.035	0.042	0.024	0.042	0.007	-0.011	0.007
97	0.038	0.037	0.029	0.032	-0.001	-0.008	-0.005
98	0.026	0.034	0.029	0.037	0.008	0.003	0.011
99	0.026	0.030	0.026	0.037	0.004	0.001	0.011
100	0.027	0.033	0.028	0.040	0.006	0.001	0.014
101	0.023	0.029	0.024	0.034	0.005	0.000	0.010
102	0.017	0.021	0.020	0.028	0.004	0.004	0.012
103	0.017	0.025	0.023	0.034	0.007	0.006	0.016
104	0.017	0.025	0.023	0.033	0.008	0.007	0.017
105	0.013	0.020	0.021	0.028	0.007	0.009	0.015
106	0.010	0.017	0.019	0.024	0.007	0.009	0.014
107	0.011	0.019	0.023	0.025	0.009	0.012	0.015
108	0.010	0.019	0.022	0.025	0.009	0.012	0.015

109	0.006	0.013	0.016	0.018	0.007	0.009	0.012
110	0.006	0.014	0.018	0.019	0.008	0.011	0.013
111	0.008	0.018	0.022	0.024	0.010	0.014	0.016
112	0.006	0.015	0.018	0.020	0.009	0.011	0.013
113	0.004	0.010	0.014	0.015	0.006	0.010	0.011
114	0.006	0.016	0.019	0.021	0.010	0.013	0.016
115	0.007	0.018	0.019	0.022	0.011	0.012	0.015
116	0.004	0.013	0.015	0.016	0.009	0.011	0.012
117	0.004	0.013	0.016	0.018	0.009	0.012	0.014
118	0.007	0.018	0.022	0.024	0.011	0.016	0.018
119	0.007	0.017	0.019	0.024	0.010	0.012	0.018
120	0.007	0.016	0.018	0.022	0.008	0.011	0.015
121	0.008	0.016	0.016	0.025	0.007	0.008	0.017
122	0.010	0.023	0.021	0.030	0.013	0.011	0.020
123	0.009	0.020	0.020	0.027	0.011	0.011	0.018
124	0.009	0.017	0.014	0.026	0.008	0.005	0.017
125	0.013	0.023	0.015	0.032	0.011	0.002	0.019
126	0.014	0.026	0.018	0.032	0.012	0.004	0.018
127	0.013	0.026	0.025	0.035	0.014	0.012	0.023
128	0.015	0.031	0.027	0.040	0.016	0.011	0.024
129	0.014	0.026	0.029	0.038	0.012	0.015	0.025
130	0.017	0.032	0.033	0.043	0.015	0.016	0.026
131	0.022	0.035	0.040	0.044	0.014	0.018	0.022
132	0.026	0.041	0.043	0.046	0.015	0.017	0.020
133	0.033	0.049	0.055	0.057	0.015	0.022	0.024
134	0.036	0.052	0.055	0.061	0.016	0.019	0.025
135	0.034	0.051	0.046	0.063	0.017	0.011	0.029
136	0.029	0.048	0.037	0.056	0.019	0.007	0.026
137	0.032	0.046	0.035	0.055	0.014	0.003	0.023
138	0.027	0.040	0.028	0.049	0.013	0.002	0.022
139	0.021	0.036	0.026	0.044	0.015	0.006	0.023
140	0.018	0.031	0.025	0.037	0.013	0.007	0.019
141	0.015	0.029	0.024	0.034	0.015	0.009	0.019

142	0.012	0.022	0.021	0.028	0.010	0.009	0.016
143	0.010	0.020	0.020	0.026	0.011	0.010	0.016
144	0.008	0.016	0.017	0.022	0.009	0.009	0.014
145	0.007	0.015	0.015	0.021	0.008	0.008	0.014
146	0.005	0.012	0.013	0.017	0.007	0.008	0.012
147	0.006	0.014	0.015	0.019	0.008	0.009	0.013
148	0.005	0.013	0.015	0.018	0.007	0.010	0.012
149	0.007	0.016	0.017	0.021	0.009	0.010	0.014
150	0.008	0.018	0.018	0.024	0.010	0.010	0.017
151	0.011	0.023	0.023	0.029	0.012	0.012	0.018
152	0.010	0.023	0.022	0.028	0.012	0.012	0.018
153	0.008	0.019	0.018	0.023	0.010	0.010	0.015
154	0.010	0.021	0.021	0.027	0.012	0.011	0.017
155	0.012	0.024	0.025	0.028	0.013	0.013	0.017
156	0.009	0.020	0.022	0.024	0.011	0.012	0.015
157	0.009	0.019	0.020	0.025	0.010	0.011	0.015
158	0.012	0.024	0.025	0.030	0.012	0.013	0.018
159	0.012	0.026	0.027	0.030	0.013	0.015	0.017
160	0.010	0.020	0.022	0.025	0.010	0.012	0.016
161	0.009	0.019	0.020	0.024	0.009	0.010	0.014
162	0.013	0.024	0.024	0.029	0.011	0.011	0.016
163	0.016	0.029	0.031	0.033	0.013	0.015	0.017
164	0.014	0.026	0.027	0.031	0.012	0.013	0.018
165	0.014	0.025	0.025	0.027	0.010	0.011	0.013
166	0.019	0.030	0.030	0.031	0.011	0.011	0.012
167	0.020	0.033	0.030	0.036	0.013	0.010	0.015
168	0.018	0.028	0.026	0.032	0.010	0.008	0.015
169	0.021	0.030	0.029	0.030	0.009	0.008	0.009
170	0.022	0.030	0.031	0.031	0.008	0.009	0.009
171	0.026	0.036	0.038	0.040	0.010	0.012	0.014
172	0.023	0.037	0.038	0.043	0.013	0.014	0.020
173	0.024	0.040	0.036	0.048	0.015	0.011	0.024
174	0.020	0.039	0.039	0.051	0.019	0.019	0.031

175	0.018	0.039	0.039	0.051	0.021	0.021	0.033
176	0.018	0.040	0.040	0.051	0.022	0.022	0.033
177	0.016	0.037	0.037	0.049	0.021	0.021	0.033
178	0.017	0.038	0.036	0.044	0.021	0.019	0.027
179	0.018	0.034	0.030	0.035	0.016	0.012	0.017
180	0.015	0.032	0.032	0.021	0.017	0.017	0.006
181	0.012	0.031	0.028	0.027	0.019	0.017	0.016
182	0.009	0.026	0.023	0.026	0.017	0.014	0.018
183	0.009	0.023	0.021	0.026	0.014	0.012	0.017
184	0.007	0.013	0.016	0.017	0.006	0.009	0.010
185	0.007	0.017	0.011	0.018	0.010	0.003	0.011
186	0.005	0.015	0.017	0.015	0.010	0.012	0.010
187	0.005	0.013	0.018	0.015	0.008	0.013	0.010
188	0.004	0.010	0.014	0.012	0.006	0.011	0.009
189	0.003	0.008	0.012	0.011	0.005	0.009	0.008
190	0.003	0.008	0.011	0.010	0.005	0.008	0.007
191	0.002	0.005	0.007	0.006	0.003	0.006	0.005
192	0.002	0.004	0.007	0.006	0.003	0.005	0.004
193	0.002	0.005	0.008	0.006	0.003	0.006	0.005
194	0.001	0.004	0.006	0.005	0.003	0.005	0.004
195	0.001	0.003	0.005	0.004	0.002	0.004	0.003
196	0.001	0.002	0.005	0.003	0.002	0.004	0.003
197	0.001	0.003	0.005	0.004	0.002	0.005	0.003
198	0.001	0.004	0.007	0.006	0.003	0.005	0.005
199	0.002	0.006	0.009	0.009	0.004	0.008	0.007
200	0.002	0.008	0.013	0.012	0.006	0.010	0.010
201	0.002	0.007	0.012	0.011	0.005	0.010	0.009
202	0.001	0.005	0.009	0.007	0.004	0.008	0.006
203	0.002	0.007	0.011	0.009	0.005	0.009	0.007
204	0.002	0.009	0.014	0.012	0.006	0.011	0.009
205	0.002	0.007	0.011	0.009	0.005	0.009	0.007
206	0.002	0.006	0.009	0.007	0.004	0.008	0.005
207	0.002	0.008	0.010	0.009	0.006	0.008	0.007

208	0.002	0.008	0.013	0.010	0.006	0.011	0.007
209	0.002	0.006	0.009	0.006	0.004	0.007	0.005
210	0.002	0.006	0.007	0.006	0.004	0.005	0.004
211	0.003	0.009	0.011	0.008	0.006	0.008	0.006
212	0.002	0.008	0.011	0.009	0.006	0.008	0.006
213	0.003	0.008	0.010	0.008	0.006	0.007	0.006
214	0.002	0.006	0.007	0.006	0.004	0.004	0.004
215	0.002	0.005	0.004	0.005	0.003	0.003	0.003
216	0.001	0.003	0.003	0.003	0.002	0.002	0.002
217	0.001	0.002	0.002	0.003	0.001	0.001	0.002
218	0.001	0.001	0.002	0.002	0.001	0.002	0.001
219	0.000	0.001	0.001	0.001	0.001	0.001	0.001
220	0.000	0.001	0.001	0.001	0.000	0.001	0.001
221	0.000	0.001	0.000	0.001	0.000	0.000	0.001
222	0.000	0.001	0.000	0.001	0.000	0.000	0.001
223	0.000	0.000	0.000	0.000	0.000	0.000	0.000
224	0.000	0.000	0.000	0.000	0.000	0.000	0.000
225	0.000	0.000	0.000	0.000	0.000	0.000	0.000
226	0.000	0.000	0.000	0.000	0.000	0.000	0.000
227	0.000	0.000	0.000	0.000	0.000	0.000	0.000
228	0.000	0.000	0.000	0.000	0.000	0.000	0.000
229	0.000	0.000	0.000	0.000	0.000	0.000	0.000
230	0.000	0.000	0.000	0.000	0.000	0.000	0.000
231	0.000	0.001	0.001	0.001	0.000	0.001	0.001
232	0.000	0.000	0.001	0.001	0.000	0.001	0.001
233	0.001	0.001	0.002	0.002	0.000	0.001	0.001
234	0.001	0.002	0.003	0.002	0.001	0.002	0.001
235	0.001	0.002	0.003	0.004	0.001	0.002	0.002
236	0.001	0.002	0.004	0.004	0.001	0.003	0.003
237	0.002	0.001	0.004	0.005	-0.001	0.003	0.004
238	0.002	0.001	0.005	0.007	-0.001	0.003	0.004
239	0.003	0.001	0.009	0.009	-0.002	0.006	0.006
240	0.003	0.003	0.007	0.009	-0.001	0.004	0.006

241	0.005	0.001	0.010	0.011	-0.004	0.005	0.006
242	0.005	0.003	0.012	0.011	-0.002	0.008	0.006
243	0.004	0.004	0.015	0.011	0.000	0.010	0.007
244	0.003	0.005	0.010	0.007	0.002	0.007	0.005
245	0.003	0.006	0.010	0.007	0.003	0.007	0.004
246	0.003	0.008	0.009	0.008	0.005	0.006	0.005
247	0.002	0.008	0.009	0.007	0.005	0.007	0.005
248	0.002	0.005	0.007	0.005	0.004	0.005	0.003
249	0.002	0.006	0.008	0.006	0.004	0.007	0.004
250	0.001	0.004	0.007	0.005	0.003	0.006	0.003
251	0.001	0.004	0.007	0.005	0.003	0.006	0.004
252	0.001	0.003	0.006	0.005	0.002	0.004	0.004
253	0.001	0.002	0.005	0.005	0.001	0.004	0.004
254	0.001	0.002	0.004	0.005	0.001	0.003	0.004
255	0.001	0.002	0.004	0.003	0.001	0.003	0.003
256	0.000	0.001	0.002	0.003	0.001	0.002	0.002
257	0.000	0.002	0.003	0.003	0.001	0.002	0.003
258	0.001	0.002	0.004	0.003	0.001	0.003	0.003
259	0.001	0.002	0.005	0.004	0.002	0.004	0.003
260	0.001	0.003	0.005	0.004	0.002	0.004	0.003
261	0.001	0.004	0.006	0.004	0.002	0.005	0.003
262	0.002	0.005	0.008	0.006	0.004	0.006	0.004
263	0.002	0.006	0.008	0.006	0.004	0.006	0.004
264	0.002	0.004	0.006	0.005	0.003	0.005	0.003
265	0.002	0.006	0.008	0.007	0.004	0.006	0.005
266	0.003	0.008	0.011	0.010	0.005	0.008	0.007
267	0.003	0.010	0.013	0.012	0.007	0.010	0.008
268	0.004	0.012	0.015	0.012	0.009	0.012	0.009
269	0.004	0.014	0.016	0.015	0.010	0.012	0.010
270	0.006	0.017	0.018	0.018	0.011	0.012	0.012
271	0.009	0.022	0.021	0.024	0.013	0.012	0.015
272	0.012	0.028	0.025	0.031	0.016	0.013	0.019
273	0.011	0.029	0.028	0.034	0.017	0.017	0.023

274	0.014	0.032	0.035	0.038	0.018	0.020	0.023
275	0.014	0.030	0.033	0.036	0.016	0.018	0.022
276	0.017	0.039	0.037	0.040	0.022	0.020	0.023
277	0.015	0.037	0.036	0.045	0.021	0.021	0.030
278	0.014	0.034	0.030	0.036	0.019	0.016	0.022
279	0.013	0.031	0.028	0.037	0.018	0.015	0.023
280	0.011	0.025	0.025	0.032	0.014	0.014	0.020
281	0.012	0.023	0.022	0.028	0.012	0.010	0.017
282	0.011	0.021	0.020	0.025	0.010	0.009	0.014
283	0.009	0.020	0.020	0.026	0.010	0.010	0.017
284	0.008	0.018	0.019	0.024	0.010	0.011	0.016
285	0.009	0.021	0.021	0.028	0.012	0.012	0.019
286	0.011	0.023	0.023	0.030	0.013	0.013	0.020
287	0.012	0.027	0.024	0.034	0.015	0.012	0.021
288	0.016	0.032	0.027	0.040	0.016	0.011	0.025
289	0.018	0.035	0.028	0.046	0.017	0.010	0.028
290	0.020	0.039	0.027	0.048	0.019	0.007	0.028
291	0.022	0.040	0.035	0.048	0.018	0.013	0.026
292	0.025	0.044	0.044	0.051	0.018	0.019	0.025
293	0.029	0.043	0.045	0.047	0.015	0.017	0.018
294	0.026	0.039	0.042	0.043	0.013	0.015	0.017
295	0.030	0.043	0.045	0.047	0.013	0.014	0.017
296	0.033	0.040	0.036	0.044	0.006	0.003	0.010
297	0.034	0.039	0.037	0.044	0.006	0.003	0.010
298	0.038	0.041	0.037	0.044	0.003	0.000	0.006
299	0.038	0.044	0.036	0.049	0.005	-0.002	0.011
300	0.038	0.041	0.032	0.044	0.003	-0.006	0.005
301	0.033	0.036	0.033	0.036	0.003	0.000	0.003
302	0.028	0.035	0.033	0.039	0.008	0.005	0.011
303	0.028	0.037	0.032	0.042	0.009	0.004	0.014
304	0.027	0.032	0.031	0.033	0.006	0.004	0.006
305	0.023	0.030	0.028	0.030	0.006	0.005	0.006
306	0.021	0.031	0.027	0.033	0.010	0.006	0.012

307	0.020	0.027	0.025	0.029	0.007	0.005	0.009
308	0.018	0.023	0.023	0.025	0.005	0.005	0.007
309	0.016	0.023	0.021	0.028	0.007	0.005	0.012
310	0.015	0.023	0.021	0.026	0.008	0.006	0.012
311	0.013	0.020	0.019	0.022	0.007	0.007	0.010
312	0.010	0.015	0.015	0.018	0.005	0.005	0.008
313	0.009	0.016	0.016	0.020	0.007	0.007	0.011
314	0.009	0.017	0.016	0.020	0.008	0.007	0.011
315	0.006	0.012	0.012	0.014	0.006	0.006	0.008
316	0.006	0.012	0.012	0.013	0.006	0.006	0.007
317	0.007	0.015	0.014	0.016	0.008	0.007	0.009
318	0.006	0.013	0.012	0.014	0.007	0.007	0.008
319	0.005	0.012	0.012	0.013	0.007	0.007	0.008
320	0.005	0.012	0.014	0.014	0.007	0.009	0.009
321	0.007	0.015	0.015	0.018	0.008	0.008	0.011
322	0.009	0.017	0.018	0.019	0.008	0.009	0.010
323	0.012	0.021	0.020	0.024	0.009	0.008	0.012
324	0.015	0.025	0.023	0.028	0.010	0.008	0.013
325	0.019	0.029	0.026	0.033	0.011	0.007	0.014
326	0.020	0.032	0.029	0.035	0.011	0.009	0.015
327	0.025	0.038	0.035	0.042	0.013	0.010	0.017
328	0.029	0.041	0.031	0.048	0.011	0.001	0.018
329	0.039	0.049	0.030	0.060	0.010	-0.009	0.021
330	0.037	0.046	0.036	0.060	0.008	-0.002	0.022
331	0.037	0.045	0.029	0.054	0.008	-0.007	0.017
332	0.045	0.053	0.020	0.058	0.008	-0.025	0.013
333	0.047	0.054	0.018	0.059	0.007	-0.029	0.012
334	0.043	0.047	0.021	0.054	0.004	-0.022	0.011
335	0.044	0.049	0.020	0.053	0.005	-0.025	0.009
336	0.053	0.058	0.029	0.058	0.006	-0.024	0.005
337	0.053	0.055	0.017	0.048	0.003	-0.035	-0.005
338	0.048	0.049	0.041	0.040	0.002	-0.006	-0.008
339	0.049	0.050	0.042	0.044	0.001	-0.007	-0.005

340	0.060	0.054	0.042	0.044	-0.006	-0.018	-0.016
341	0.055	0.051	0.046	0.039	-0.004	-0.009	-0.016
342	0.050	0.046	0.046	0.039	-0.004	-0.005	-0.012
343	0.056	0.048	0.046	0.044	-0.008	-0.011	-0.013
344	0.061	0.038	0.043	0.044	-0.022	-0.018	-0.017
345	0.048	0.042	0.042	0.040	-0.006	-0.007	-0.008
346	0.051	0.043	0.042	0.038	-0.008	-0.009	-0.013
347	0.060	0.049	0.047	0.042	-0.011	-0.013	-0.018
348	0.030	0.043	0.045	0.040	0.013	0.015	0.009
349	0.051	0.042	0.041	0.036	-0.010	-0.010	-0.015
350	0.056	0.041	0.043	0.036	-0.015	-0.013	-0.020
351	0.049	0.045	0.048	0.038	-0.004	-0.001	-0.011
352	0.058	0.040	0.040	0.032	-0.018	-0.018	-0.026
353	0.049	0.033	0.039	0.028	-0.016	-0.010	-0.021
354	0.055	0.035	0.043	0.029	-0.021	-0.012	-0.027
355	0.052	0.037	0.044	0.030	-0.014	-0.008	-0.022
356	0.041	0.031	0.035	0.022	-0.010	-0.006	-0.019
357	0.039	0.029	0.035	0.021	-0.010	-0.004	-0.018
358	0.043	0.030	0.037	0.022	-0.013	-0.006	-0.021
359	0.039	0.030	0.037	0.023	-0.009	-0.001	-0.016
360	0.034	0.025	0.027	0.017	-0.009	-0.007	-0.017
361	0.035	0.026	0.027	0.017	-0.010	-0.008	-0.018
362	0.032	0.026	0.027	0.017	-0.007	-0.006	-0.016
363	0.032	0.022	0.025	0.017	-0.010	-0.007	-0.015
364	0.038	0.026	0.031	0.020	-0.012	-0.007	-0.017
365	0.043	0.030	0.036	0.023	-0.013	-0.007	-0.020
366	0.043	0.031	0.034	0.022	-0.012	-0.008	-0.021
367	0.043	0.030	0.034	0.023	-0.012	-0.008	-0.020
368	0.053	0.024	0.042	0.028	-0.029	-0.011	-0.025
369	0.052	0.034	0.040	0.028	-0.018	-0.012	-0.024
370	0.048	0.039	0.039	0.026	-0.009	-0.009	-0.022
371	0.054	0.039	0.044	0.028	-0.015	-0.011	-0.026
372	0.059	0.043	0.046	0.034	-0.016	-0.013	-0.025

373	0.051	0.040	0.040	0.029	-0.010	-0.010	-0.022
374	0.044	0.037	0.039	0.027	-0.006	-0.004	-0.016
375	0.050	0.042	0.049	0.034	-0.008	-0.002	-0.016
376	0.036	0.046	0.050	0.037	0.011	0.015	0.001
377	0.040	0.041	0.044	0.032	0.001	0.004	-0.009
378	0.049	0.041	0.043	0.030	-0.008	-0.006	-0.019
379	0.061	0.047	0.051	0.036	-0.014	-0.010	-0.025
380	0.060	0.047	0.052	0.038	-0.014	-0.009	-0.022
381	0.053	0.040	0.044	0.033	-0.014	-0.010	-0.021
382	0.055	0.042	0.047	0.034	-0.014	-0.008	-0.021
383	0.058	0.050	0.043	0.039	-0.008	-0.015	-0.019
384	0.049	0.044	0.046	0.035	-0.005	-0.004	-0.014
385	0.046	0.040	0.041	0.031	-0.006	-0.005	-0.015
386	0.050	0.045	0.039	0.034	-0.004	-0.011	-0.015
387	0.049	0.046	0.037	0.038	-0.003	-0.012	-0.011
388	0.053	0.050	0.034	0.041	-0.003	-0.019	-0.012
389	0.055	0.052	0.024	0.047	-0.003	-0.031	-0.008
390	0.064	0.052	0.046	0.048	-0.012	-0.018	-0.016
391	0.063	0.056	0.039	0.054	-0.007	-0.024	-0.009
392	0.068	0.058	0.031	0.060	-0.009	-0.036	-0.008
393	0.068	0.062	0.043	0.057	-0.007	-0.025	-0.011
394	0.071	0.058	0.064	0.051	-0.013	-0.007	-0.020
395	0.057	0.055	0.063	0.054	-0.001	0.007	-0.003
396	0.026	0.059	0.053	0.019	0.033	0.027	-0.007
397	0.041	0.060	0.055	0.011	0.019	0.014	-0.030
398	0.030	0.056	0.053	0.022	0.026	0.023	-0.008
399	0.050	0.055	0.053	0.023	0.006	0.003	-0.027
400	0.055	0.050	0.049	0.014	-0.005	-0.006	-0.041
401	0.064	0.041	0.047	0.010	-0.023	-0.016	-0.054
402	0.069	0.050	0.049	0.020	-0.019	-0.020	-0.049
403	0.070	0.049	0.050	0.018	-0.021	-0.019	-0.051
404	0.072	0.008	0.050	0.013	-0.064	-0.022	-0.059
405	0.063	0.023	0.047	0.026	-0.040	-0.016	-0.036

406	0.060	0.023	0.049	0.041	-0.036	-0.010	-0.019
407	0.063	0.030	0.050	0.038	-0.034	-0.014	-0.025
408	0.056	0.038	0.045	0.039	-0.018	-0.012	-0.017
409	0.050	0.036	0.045	0.033	-0.014	-0.005	-0.017
410	0.050	0.031	0.048	0.030	-0.019	-0.002	-0.020
411	0.051	0.034	0.047	0.029	-0.016	-0.003	-0.021
412	0.043	0.034	0.040	0.027	-0.009	-0.003	-0.016
413	0.041	0.032	0.037	0.024	-0.010	-0.004	-0.017
414	0.040	0.028	0.036	0.025	-0.012	-0.004	-0.015
415	0.038	0.028	0.033	0.023	-0.010	-0.006	-0.015
416	0.032	0.023	0.028	0.019	-0.009	-0.004	-0.013
417	0.032	0.023	0.027	0.019	-0.009	-0.005	-0.014
418	0.033	0.022	0.028	0.018	-0.011	-0.005	-0.015
419	0.027	0.018	0.020	0.015	-0.009	-0.007	-0.012
420	0.025	0.017	0.019	0.013	-0.008	-0.006	-0.011
421	0.025	0.016	0.019	0.012	-0.009	-0.006	-0.013
422	0.023	0.014	0.017	0.010	-0.009	-0.006	-0.013
423	0.018	0.012	0.015	0.009	-0.007	-0.004	-0.010
424	0.017	0.011	0.013	0.009	-0.005	-0.003	-0.008
425	0.018	0.013	0.014	0.010	-0.005	-0.004	-0.008
426	0.018	0.013	0.014	0.010	-0.005	-0.003	-0.008
427	0.022	0.016	0.018	0.012	-0.006	-0.004	-0.010
428	0.021	0.015	0.017	0.012	-0.006	-0.005	-0.010
429	0.019	0.013	0.015	0.011	-0.006	-0.004	-0.008
430	0.023	0.016	0.020	0.014	-0.007	-0.003	-0.009
431	0.027	0.020	0.024	0.015	-0.007	-0.004	-0.012
432	0.023	0.016	0.020	0.013	-0.007	-0.003	-0.010
433	0.024	0.017	0.022	0.015	-0.007	-0.002	-0.009
434	0.032	0.024	0.030	0.020	-0.008	-0.001	-0.011
435	0.032	0.018	0.030	0.020	-0.014	-0.003	-0.012
436	0.030	0.011	0.024	0.019	-0.019	-0.006	-0.011
437	0.037	0.022	0.023	0.007	-0.015	-0.014	-0.029
438	0.042	0.030	0.029	0.028	-0.012	-0.013	-0.014

439	0.043	0.029	0.033	0.022	-0.014	-0.010	-0.021
440	0.042	0.032	0.028	0.022	-0.010	-0.013	-0.020
441	0.048	0.034	0.014	0.025	-0.014	-0.034	-0.023
442	0.052	0.026	0.019	0.032	-0.027	-0.033	-0.020
443	0.051	0.041	0.032	0.029	-0.010	-0.019	-0.022
444	0.051	0.040	0.029	0.030	-0.012	-0.023	-0.022
445	0.055	0.044	0.020	0.033	-0.011	-0.035	-0.022
446	0.056	0.038	0.029	0.032	-0.018	-0.027	-0.024
447	0.055	0.045	0.048	0.030	-0.011	-0.007	-0.025
448	0.054	0.046	0.041	0.031	-0.008	-0.013	-0.023
449	0.061	0.038	0.033	0.036	-0.023	-0.028	-0.025
450	0.059	0.037	0.048	0.034	-0.023	-0.011	-0.025
451	0.053	0.046	0.050	0.032	-0.007	-0.003	-0.021
452	0.056	0.046	0.050	0.034	-0.010	-0.007	-0.022
453	0.060	0.044	0.046	0.038	-0.016	-0.014	-0.023
454	0.055	0.043	0.046	0.035	-0.012	-0.010	-0.021
455	0.051	0.045	0.046	0.032	-0.006	-0.005	-0.019
456	0.058	0.045	0.045	0.040	-0.013	-0.013	-0.018
457	0.054	0.050	0.044	0.041	-0.003	-0.009	-0.012
458	0.047	0.048	0.043	0.038	0.001	-0.003	-0.009
459	0.047	0.049	0.042	0.041	0.002	-0.005	-0.006
460	0.042	0.037	0.036	0.042	-0.005	-0.006	0.001
461	0.043	0.047	0.048	0.046	0.004	0.005	0.003
462	0.048	0.056	0.053	0.049	0.008	0.005	0.001
463	0.054	0.058	0.055	0.046	0.004	0.001	-0.008
464	0.051	0.050	0.054	0.045	0.000	0.004	-0.006
465	0.051	0.056	0.056	0.047	0.005	0.005	-0.004
466	0.060	0.060	0.061	0.049	0.000	0.001	-0.010
467	0.060	0.056	0.056	0.047	-0.004	-0.004	-0.013
468	0.054	0.051	0.053	0.045	-0.003	0.000	-0.009
469	0.060	0.058	0.048	0.046	-0.002	-0.011	-0.014
470	0.068	0.060	0.040	0.045	-0.008	-0.028	-0.023
471	0.062	0.048	0.053	0.041	-0.014	-0.009	-0.021

472	0.060	0.053	0.058	0.041	-0.006	-0.001	-0.019
473	0.066	0.053	0.056	0.043	-0.012	-0.009	-0.023
474	0.065	0.038	0.039	0.044	-0.027	-0.026	-0.021
475	0.061	0.041	0.057	0.037	-0.020	-0.004	-0.024
476	0.058	0.049	0.054	0.034	-0.009	-0.005	-0.024
477	0.058	0.045	0.056	0.040	-0.013	-0.002	-0.018
478	0.057	0.021	0.051	0.039	-0.036	-0.007	-0.019
479	0.055	0.044	0.051	0.032	-0.011	-0.004	-0.023
480	0.050	0.041	0.049	0.030	-0.008	-0.001	-0.019
481	0.055	0.029	0.050	0.036	-0.026	-0.005	-0.018
482	0.050	0.034	0.048	0.031	-0.016	-0.003	-0.019
483	0.048	0.032	0.042	0.025	-0.016	-0.006	-0.023
484	0.049	0.033	0.043	0.026	-0.016	-0.006	-0.024
485	0.045	0.025	0.040	0.030	-0.021	-0.006	-0.015
486	0.040	0.025	0.038	0.025	-0.015	-0.002	-0.015
487	0.039	0.023	0.030	0.021	-0.015	-0.008	-0.018
488	0.038	0.028	0.030	0.020	-0.009	-0.007	-0.017
489	0.039	0.034	0.035	0.023	-0.006	-0.005	-0.017
490	0.033	0.026	0.029	0.019	-0.007	-0.004	-0.014
491	0.029	0.022	0.023	0.015	-0.006	-0.006	-0.014
492	0.030	0.023	0.024	0.016	-0.007	-0.006	-0.014
493	0.030	0.023	0.025	0.017	-0.007	-0.006	-0.013
494	0.025	0.019	0.019	0.013	-0.006	-0.006	-0.012
495	0.023	0.017	0.017	0.012	-0.006	-0.006	-0.011
496	0.026	0.019	0.019	0.013	-0.007	-0.007	-0.012
497	0.025	0.019	0.019	0.014	-0.006	-0.006	-0.011
498	0.020	0.016	0.016	0.012	-0.004	-0.004	-0.008
499	0.021	0.016	0.017	0.013	-0.005	-0.004	-0.008
500	0.022	0.013	0.015	0.012	-0.009	-0.007	-0.010
501	0.017	0.010	0.013	0.009	-0.006	-0.004	-0.008
502	0.015	0.009	0.013	0.009	-0.006	-0.002	-0.006
503	0.018	0.011	0.016	0.011	-0.007	-0.002	-0.007
504	0.025	0.012	0.020	0.014	-0.012	-0.005	-0.011

505	0.024	0.013	0.019	0.012	-0.011	-0.004	-0.012
506	0.030	0.012	0.026	0.000	-0.018	-0.004	-0.030
507	0.027	0.011	0.021	0.001	-0.016	-0.006	-0.027
508	0.015	0.011	0.018	0.013	-0.004	0.003	-0.002
509	0.015	0.010	0.017	0.012	-0.005	0.003	-0.003
510	0.024	0.014	0.020	0.012	-0.011	-0.004	-0.012
511	0.025	0.016	0.020	0.013	-0.009	-0.005	-0.012
512	0.024	0.014	0.020	0.013	-0.010	-0.004	-0.011
513	0.026	0.016	0.024	0.013	-0.011	-0.003	-0.013
514	0.021	0.012	0.018	0.009	-0.009	-0.003	-0.012
515	0.021	0.011	0.017	0.009	-0.010	-0.005	-0.012
516	0.028	0.018	0.024	0.014	-0.010	-0.004	-0.015
517	0.030	0.019	0.025	0.014	-0.011	-0.006	-0.016
518	0.022	0.014	0.020	0.011	-0.008	-0.002	-0.011
519	0.023	0.017	0.024	0.012	-0.007	0.000	-0.012
520	0.031	0.022	0.029	0.016	-0.009	-0.002	-0.016
521	0.028	0.019	0.025	0.013	-0.009	-0.003	-0.015
522	0.021	0.014	0.020	0.010	-0.006	-0.001	-0.010
523	0.025	0.019	0.026	0.012	-0.006	0.001	-0.013
524	0.030	0.021	0.030	0.015	-0.010	0.000	-0.016
525	0.022	0.015	0.021	0.010	-0.008	-0.001	-0.012
526	0.021	0.015	0.020	0.010	-0.006	0.000	-0.011
527	0.028	0.019	0.027	0.013	-0.009	-0.001	-0.015
528	0.024	0.016	0.026	0.012	-0.009	0.001	-0.012
529	0.019	0.012	0.018	0.008	-0.007	-0.001	-0.010
530	0.022	0.014	0.021	0.010	-0.007	-0.001	-0.012
531	0.026	0.017	0.026	0.012	-0.009	0.000	-0.014
532	0.019	0.012	0.019	0.009	-0.008	0.000	-0.011
533	0.015	0.010	0.015	0.007	-0.005	0.001	-0.008
534	0.019	0.014	0.019	0.009	-0.005	0.000	-0.010
535	0.017	0.011	0.018	0.008	-0.005	0.001	-0.009
536	0.011	0.007	0.013	0.005	-0.004	0.002	-0.006
537	0.011	0.008	0.013	0.005	-0.004	0.001	-0.006

538	0.015	0.011	0.015	0.007	-0.004	0.001	-0.008
539	0.014	0.009	0.015	0.006	-0.005	0.001	-0.007
540	0.014	0.009	0.016	0.007	-0.005	0.002	-0.007
541	0.020	0.013	0.019	0.009	-0.008	-0.001	-0.011
542	0.021	0.014	0.020	0.009	-0.007	-0.001	-0.011
543	0.020	0.013	0.020	0.010	-0.007	0.000	-0.011
544	0.023	0.014	0.022	0.011	-0.009	-0.002	-0.012
545	0.027	0.017	0.024	0.012	-0.009	-0.003	-0.014
546	0.024	0.017	0.023	0.012	-0.007	-0.001	-0.012
547	0.026	0.017	0.024	0.012	-0.009	-0.002	-0.013
548	0.033	0.022	0.030	0.016	-0.010	-0.003	-0.016
549	0.031	0.025	0.032	0.017	-0.007	0.001	-0.014
550	0.029	0.022	0.029	0.016	-0.007	0.001	-0.013
551	0.033	0.024	0.032	0.018	-0.009	-0.001	-0.015
552	0.038	0.030	0.038	0.024	-0.009	0.000	-0.014
553	0.035	0.027	0.037	0.023	-0.008	0.001	-0.013
554	0.033	0.025	0.033	0.021	-0.007	0.001	-0.012
555	0.038	0.033	0.039	0.027	-0.004	0.001	-0.011
556	0.043	0.034	0.043	0.032	-0.009	0.001	-0.011
557	0.038	0.030	0.037	0.029	-0.008	0.000	-0.008
558	0.039	0.035	0.040	0.031	-0.004	0.001	-0.008
559	0.041	0.041	0.047	0.035	0.000	0.006	-0.006
560	0.049	0.044	0.025	0.041	-0.005	-0.024	-0.008
561	0.051	0.047	0.055	0.043	-0.004	0.004	-0.008
562	0.053	0.054	0.041	0.053	0.001	-0.011	0.000
563	0.050	0.057	0.027	0.054	0.007	-0.023	0.004
564	0.055	0.061	0.017	0.060	0.006	-0.038	0.005
565	0.053	0.061	0.021	0.062	0.009	-0.032	0.009
566	0.049	0.061	0.054	0.062	0.011	0.005	0.013
567	0.048	0.061	0.055	0.063	0.013	0.007	0.015
568	0.040	0.055	0.049	0.053	0.015	0.009	0.013
569	0.039	0.053	0.051	0.056	0.014	0.012	0.018
570	0.033	0.046	0.029	0.047	0.013	-0.004	0.015

571	0.029	0.043	0.044	0.049	0.014	0.015	0.020
572	0.028	0.041	0.048	0.047	0.013	0.020	0.019
573	0.025	0.040	0.047	0.045	0.015	0.022	0.020
574	0.021	0.035	0.039	0.041	0.014	0.018	0.020
575	0.020	0.036	0.040	0.042	0.016	0.020	0.022
576	0.017	0.032	0.035	0.039	0.015	0.019	0.022
577	0.015	0.031	0.035	0.040	0.016	0.020	0.025
578	0.014	0.026	0.030	0.034	0.012	0.017	0.020
579	0.013	0.024	0.027	0.029	0.011	0.014	0.016
580	0.013	0.026	0.030	0.034	0.014	0.017	0.021
581	0.013	0.021	0.015	0.035	0.008	0.002	0.022
582	0.016	0.024	0.020	0.036	0.008	0.003	0.020
583	0.015	0.018	0.022	0.037	0.002	0.007	0.022
584	0.015	0.023	0.032	0.032	0.007	0.016	0.017
585	0.013	0.022	0.025	0.032	0.009	0.013	0.019
586	0.011	0.021	0.024	0.027	0.010	0.013	0.017
587	0.013	0.026	0.030	0.036	0.013	0.017	0.024
588	0.013	0.024	0.025	0.031	0.011	0.013	0.018
589	0.010	0.018	0.021	0.025	0.009	0.011	0.015
590	0.011	0.021	0.024	0.028	0.011	0.013	0.017
591	0.013	0.025	0.027	0.031	0.012	0.014	0.018
592	0.011	0.021	0.022	0.027	0.010	0.011	0.017
593	0.008	0.017	0.018	0.023	0.008	0.009	0.015
594	0.012	0.023	0.022	0.028	0.011	0.011	0.017
595	0.012	0.023	0.022	0.028	0.010	0.009	0.016
596	0.009	0.017	0.017	0.023	0.009	0.008	0.014
597	0.009	0.017	0.017	0.023	0.008	0.007	0.014
598	0.013	0.023	0.022	0.028	0.010	0.009	0.015
599	0.012	0.022	0.020	0.027	0.011	0.009	0.016
600	0.008	0.018	0.015	0.022	0.009	0.007	0.013
601	0.009	0.017	0.017	0.021	0.008	0.008	0.012
602	0.016	0.023	0.021	0.028	0.007	0.005	0.012
603	0.014	0.026	0.022	0.026	0.012	0.008	0.013

604	0.016	0.024	0.021	0.024	0.008	0.005	0.008
605	0.021	0.031	0.028	0.032	0.010	0.007	0.012
606	0.018	0.028	0.027	0.031	0.010	0.009	0.013
607	0.016	0.027	0.026	0.030	0.011	0.010	0.015
608	0.015	0.025	0.024	0.028	0.010	0.010	0.013
609	0.014	0.026	0.026	0.031	0.012	0.012	0.016
610	0.015	0.029	0.028	0.034	0.014	0.013	0.019
611	0.015	0.030	0.030	0.037	0.015	0.015	0.022
612	0.015	0.033	0.034	0.040	0.018	0.018	0.025
613	0.014	0.033	0.035	0.040	0.018	0.021	0.026
614	0.015	0.035	0.038	0.045	0.020	0.023	0.029
615	0.018	0.041	0.040	0.048	0.023	0.022	0.030
616	0.024	0.046	0.043	0.051	0.022	0.018	0.027
617	0.031	0.049	0.034	0.050	0.017	0.003	0.019
618	0.025	0.045	0.025	0.054	0.021	0.000	0.029
619	0.023	0.044	0.026	0.057	0.021	0.003	0.034
620	0.023	0.040	0.034	0.055	0.017	0.011	0.032
621	0.015	0.036	0.034	0.047	0.021	0.019	0.032
622	0.014	0.028	0.035	0.039	0.014	0.021	0.025
623	0.017	0.033	0.035	0.040	0.016	0.017	0.023
624	0.016	0.033	0.040	0.042	0.017	0.024	0.026
625	0.017	0.036	0.038	0.044	0.018	0.021	0.027
626	0.019	0.037	0.038	0.043	0.019	0.019	0.024
627	0.018	0.035	0.035	0.040	0.017	0.017	0.022
628	0.020	0.035	0.037	0.041	0.015	0.017	0.021
629	0.022	0.035	0.037	0.042	0.013	0.015	0.020
630	0.023	0.035	0.037	0.040	0.012	0.014	0.017
631	0.024	0.035	0.035	0.039	0.011	0.011	0.016
632	0.022	0.033	0.029	0.034	0.011	0.007	0.012
633	0.027	0.038	0.025	0.037	0.011	-0.002	0.010
634	0.033	0.043	0.020	0.039	0.010	-0.013	0.006
635	0.028	0.031	0.020	0.033	0.004	-0.008	0.005
636	0.020	0.028	0.022	0.029	0.008	0.001	0.009

637	0.023	0.033	0.028	0.032	0.009	0.005	0.008
638	0.025	0.032	0.030	0.030	0.007	0.005	0.005
639	0.028	0.031	0.031	0.029	0.003	0.003	0.001
640	0.034	0.041	0.036	0.037	0.007	0.002	0.004
641	0.026	0.028	0.029	0.035	0.002	0.003	0.009
642	0.025	0.037	0.030	0.039	0.012	0.004	0.014
643	0.030	0.040	0.041	0.043	0.010	0.010	0.013
644	0.031	0.041	0.044	0.046	0.010	0.013	0.015
645	0.032	0.045	0.045	0.049	0.012	0.013	0.016
646	0.026	0.034	0.035	0.037	0.009	0.010	0.011
647	0.022	0.032	0.032	0.035	0.009	0.010	0.013
648	0.025	0.036	0.039	0.040	0.011	0.014	0.016
649	0.022	0.031	0.032	0.033	0.010	0.011	0.012
650	0.019	0.027	0.027	0.032	0.008	0.008	0.013
651	0.017	0.027	0.028	0.032	0.010	0.011	0.015
652	0.018	0.029	0.033	0.034	0.011	0.015	0.016
653	0.015	0.023	0.026	0.031	0.008	0.011	0.016
654	0.012	0.021	0.023	0.031	0.009	0.011	0.018
655	0.013	0.022	0.025	0.031	0.009	0.012	0.018
656	0.018	0.027	0.030	0.036	0.009	0.012	0.017
657	0.014	0.019	0.022	0.029	0.005	0.008	0.014
658	0.013	0.018	0.022	0.028	0.005	0.009	0.015
659	0.012	0.018	0.020	0.024	0.005	0.008	0.012
660	0.012	0.018	0.023	0.027	0.006	0.011	0.015
661	0.013	0.024	0.027	0.032	0.010	0.014	0.019
662	0.015	0.027	0.030	0.033	0.011	0.015	0.018
663	0.016	0.030	0.031	0.034	0.014	0.015	0.018
664	0.019	0.034	0.037	0.036	0.014	0.017	0.017
665	0.024	0.037	0.043	0.041	0.013	0.018	0.017
666	0.029	0.043	0.047	0.043	0.014	0.019	0.014
667	0.033	0.048	0.052	0.048	0.015	0.019	0.016
668	0.037	0.054	0.029	0.055	0.018	-0.008	0.019
669	0.038	0.059	0.035	0.059	0.020	-0.003	0.021

670	0.055	0.063	0.046	0.069	0.008	-0.008	0.015
671	0.053	0.061	0.034	0.066	0.008	-0.018	0.013
672	0.045	0.057	0.030	0.068	0.011	-0.015	0.023
673	0.042	0.054	0.035	0.063	0.012	-0.008	0.021
674	0.047	0.051	0.017	0.065	0.004	-0.031	0.018
675	0.046	0.048	0.001	0.065	0.002	-0.045	0.019
676	0.039	0.062	0.023	0.070	0.023	-0.016	0.031
677	0.040	0.061	0.023	0.062	0.021	-0.017	0.022
678	0.038	0.062	0.041	0.051	0.024	0.003	0.013
679	0.035	0.057	0.044	0.050	0.022	0.009	0.015
680	0.032	0.050	0.042	0.050	0.018	0.010	0.018
681	0.026	0.044	0.032	0.048	0.018	0.006	0.022
682	0.022	0.039	0.032	0.041	0.017	0.010	0.019
683	0.016	0.031	0.029	0.043	0.015	0.013	0.027
684	0.012	0.025	0.024	0.033	0.013	0.011	0.021
685	0.010	0.022	0.019	0.029	0.012	0.008	0.019
686	0.007	0.016	0.016	0.022	0.009	0.009	0.015
687	0.006	0.016	0.015	0.021	0.009	0.009	0.014
688	0.004	0.011	0.013	0.015	0.007	0.009	0.011
689	0.005	0.012	0.014	0.017	0.008	0.009	0.012
690	0.005	0.012	0.014	0.016	0.007	0.009	0.011
691	0.006	0.014	0.017	0.020	0.008	0.011	0.015
692	0.007	0.016	0.021	0.025	0.009	0.014	0.018
693	0.007	0.015	0.018	0.022	0.008	0.011	0.015
694	0.006	0.014	0.016	0.020	0.007	0.009	0.013
695	0.008	0.018	0.020	0.025	0.009	0.011	0.017
696	0.009	0.019	0.021	0.026	0.009	0.011	0.017
697	0.008	0.015	0.017	0.021	0.007	0.009	0.013
698	0.009	0.016	0.018	0.023	0.007	0.009	0.014
699	0.012	0.020	0.022	0.028	0.009	0.010	0.016
700	0.011	0.018	0.020	0.025	0.008	0.010	0.015
701	0.009	0.015	0.016	0.020	0.006	0.008	0.011
702	0.011	0.018	0.020	0.025	0.007	0.008	0.014

703	0.014	0.024	0.025	0.030	0.009	0.010	0.016
704	0.011	0.017	0.019	0.023	0.006	0.008	0.012
705	0.010	0.014	0.016	0.020	0.005	0.006	0.010
706	0.015	0.021	0.022	0.028	0.006	0.008	0.014
707	0.014	0.021	0.022	0.027	0.007	0.007	0.013
708	0.012	0.016	0.017	0.023	0.004	0.005	0.011
709	0.016	0.019	0.020	0.025	0.003	0.004	0.009
710	0.018	0.023	0.023	0.027	0.005	0.005	0.009
711	0.024	0.029	0.026	0.029	0.004	0.002	0.005
712	0.026	0.032	0.031	0.034	0.006	0.004	0.007
713	0.026	0.034	0.034	0.038	0.008	0.008	0.013
714	0.024	0.034	0.035	0.042	0.010	0.011	0.018
715	0.021	0.032	0.035	0.041	0.011	0.014	0.019
716	0.019	0.033	0.035	0.041	0.014	0.016	0.022
717	0.018	0.033	0.036	0.044	0.016	0.018	0.026
718	0.021	0.042	0.039	0.051	0.020	0.018	0.029
719	0.021	0.037	0.034	0.046	0.016	0.013	0.025
720	0.019	0.032	0.037	0.048	0.013	0.018	0.029
721	0.017	0.026	0.033	0.041	0.009	0.015	0.023
722	0.013	0.020	0.026	0.035	0.007	0.013	0.022
723	0.012	0.023	0.026	0.033	0.010	0.014	0.021
724	0.010	0.020	0.023	0.026	0.010	0.013	0.016
725	0.010	0.021	0.020	0.027	0.011	0.010	0.017
726	0.007	0.015	0.014	0.023	0.008	0.007	0.016
727	0.007	0.016	0.019	0.021	0.009	0.012	0.014
728	0.004	0.014	0.016	0.017	0.009	0.011	0.013
729	0.003	0.010	0.012	0.013	0.007	0.009	0.010
730	0.002	0.008	0.011	0.011	0.006	0.008	0.009
731	0.001	0.006	0.007	0.008	0.005	0.006	0.006
732	0.001	0.006	0.007	0.008	0.005	0.006	0.007
733	0.001	0.003	0.004	0.004	0.003	0.003	0.004
734	0.001	0.003	0.004	0.004	0.002	0.003	0.003
735	0.001	0.004	0.005	0.006	0.003	0.005	0.005

736	0.001	0.003	0.005	0.005	0.003	0.004	0.004
737	0.000	0.002	0.002	0.002	0.001	0.002	0.002
738	0.001	0.002	0.003	0.003	0.002	0.003	0.003
739	0.001	0.003	0.004	0.004	0.002	0.003	0.003
740	0.001	0.004	0.006	0.006	0.003	0.005	0.005
741	0.001	0.005	0.006	0.007	0.004	0.005	0.006
742	0.002	0.007	0.008	0.010	0.005	0.007	0.009
743	0.002	0.008	0.010	0.012	0.006	0.008	0.010
744	0.002	0.007	0.010	0.011	0.005	0.008	0.009
745	0.002	0.008	0.011	0.012	0.006	0.009	0.010
746	0.003	0.011	0.014	0.016	0.008	0.011	0.013
747	0.003	0.010	0.013	0.014	0.007	0.011	0.011
748	0.003	0.009	0.013	0.014	0.006	0.010	0.011
749	0.004	0.012	0.017	0.018	0.009	0.013	0.014
750	0.005	0.015	0.020	0.020	0.010	0.015	0.015
751	0.004	0.014	0.019	0.018	0.010	0.014	0.014
752	0.004	0.014	0.017	0.018	0.009	0.013	0.014
753	0.007	0.016	0.019	0.021	0.009	0.012	0.015
754	0.012	0.020	0.023	0.024	0.007	0.011	0.012
755	0.008	0.021	0.021	0.021	0.012	0.012	0.013
756	0.006	0.017	0.024	0.020	0.011	0.018	0.014
757	0.006	0.017	0.024	0.021	0.011	0.018	0.015
758	0.005	0.013	0.019	0.017	0.008	0.014	0.013
759	0.005	0.013	0.018	0.017	0.008	0.013	0.012
760	0.006	0.014	0.019	0.018	0.008	0.013	0.012
761	0.006	0.014	0.017	0.016	0.008	0.012	0.010
762	0.005	0.014	0.016	0.015	0.009	0.012	0.010
763	0.005	0.010	0.014	0.016	0.004	0.008	0.011
764	0.006	0.011	0.012	0.015	0.005	0.006	0.008
765	0.008	0.013	0.014	0.014	0.005	0.006	0.006
766	0.008	0.017	0.018	0.018	0.009	0.010	0.010
767	0.009	0.019	0.021	0.020	0.010	0.012	0.011
768	0.008	0.021	0.023	0.023	0.013	0.015	0.014

769	0.008	0.019	0.025	0.022	0.011	0.018	0.015
770	0.006	0.017	0.021	0.018	0.011	0.015	0.012
771	0.007	0.019	0.021	0.020	0.012	0.014	0.012
772	0.005	0.015	0.022	0.016	0.010	0.018	0.012
773	0.005	0.015	0.021	0.017	0.010	0.016	0.012
774	0.004	0.012	0.018	0.016	0.008	0.013	0.012
775	0.005	0.013	0.018	0.017	0.008	0.013	0.012
776	0.007	0.015	0.020	0.021	0.008	0.014	0.014
777	0.005	0.013	0.017	0.018	0.007	0.011	0.012
778	0.005	0.012	0.017	0.017	0.007	0.012	0.012
779	0.006	0.014	0.017	0.020	0.008	0.011	0.014
780	0.007	0.015	0.019	0.021	0.008	0.012	0.015
781	0.005	0.012	0.015	0.017	0.007	0.010	0.012
782	0.004	0.011	0.014	0.014	0.007	0.009	0.010
783	0.003	0.008	0.011	0.011	0.005	0.008	0.008
784	0.004	0.010	0.013	0.013	0.006	0.010	0.009
785	0.003	0.010	0.013	0.014	0.007	0.010	0.010
786	0.002	0.007	0.010	0.009	0.005	0.007	0.007
787	0.002	0.007	0.010	0.009	0.005	0.007	0.006
788	0.002	0.007	0.011	0.010	0.005	0.008	0.008
789	0.002	0.006	0.009	0.009	0.004	0.007	0.007
790	0.001	0.006	0.008	0.009	0.004	0.007	0.007
791	0.001	0.004	0.006	0.007	0.003	0.005	0.005
792	0.001	0.003	0.004	0.004	0.002	0.004	0.004
793	0.001	0.002	0.004	0.004	0.002	0.003	0.003
794	0.000	0.002	0.003	0.003	0.001	0.002	0.003
795	0.001	0.002	0.004	0.004	0.001	0.003	0.003
796	0.001	0.002	0.003	0.003	0.001	0.003	0.003
797	0.001	0.002	0.005	0.004	0.002	0.004	0.003
798	0.001	0.003	0.005	0.005	0.002	0.004	0.004
799	0.001	0.005	0.007	0.007	0.003	0.006	0.005
800	0.002	0.006	0.009	0.009	0.005	0.007	0.007
801	0.002	0.006	0.008	0.008	0.004	0.006	0.006

802	0.001	0.003	0.005	0.005	0.002	0.004	0.004
803	0.001	0.004	0.006	0.006	0.003	0.005	0.005
804	0.002	0.007	0.009	0.010	0.005	0.007	0.008
805	0.002	0.007	0.009	0.010	0.005	0.007	0.008
806	0.004	0.011	0.012	0.014	0.008	0.008	0.010
807	0.004	0.011	0.011	0.017	0.007	0.007	0.012
808	0.006	0.014	0.012	0.012	0.008	0.006	0.006
809	0.008	0.015	0.019	0.012	0.007	0.011	0.004
810	0.010	0.016	0.021	0.017	0.007	0.011	0.007
811	0.011	0.021	0.025	0.025	0.010	0.014	0.014
812	0.015	0.025	0.029	0.040	0.010	0.014	0.025
813	0.013	0.034	0.033	0.043	0.021	0.020	0.030
814	0.014	0.034	0.035	0.046	0.020	0.021	0.032
815	0.012	0.028	0.031	0.042	0.016	0.020	0.030
816	0.013	0.027	0.031	0.041	0.015	0.019	0.028
817	0.011	0.024	0.024	0.035	0.013	0.013	0.025
818	0.013	0.026	0.025	0.037	0.013	0.012	0.024
819	0.011	0.025	0.023	0.033	0.014	0.012	0.021
820	0.009	0.022	0.022	0.032	0.013	0.013	0.023
821	0.008	0.020	0.019	0.030	0.011	0.010	0.022
822	0.009	0.021	0.022	0.034	0.012	0.012	0.025
823	0.011	0.024	0.026	0.036	0.013	0.015	0.025
824	0.014	0.029	0.031	0.041	0.015	0.017	0.027
825	0.019	0.034	0.034	0.044	0.015	0.016	0.025
826	0.020	0.035	0.036	0.043	0.014	0.016	0.022
827	0.026	0.042	0.042	0.051	0.016	0.016	0.026
828	0.028	0.041	0.042	0.048	0.014	0.014	0.020
829	0.035	0.045	0.042	0.046	0.010	0.007	0.011
830	0.036	0.042	0.038	0.041	0.006	0.002	0.006
831	0.030	0.035	0.033	0.036	0.006	0.003	0.007
832	0.036	0.042	0.034	0.040	0.006	-0.003	0.004
833	0.033	0.041	0.032	0.039	0.008	-0.002	0.006
834	0.015	0.036	0.032	0.038	0.021	0.017	0.023

835	0.009	0.042	0.036	0.047	0.033	0.026	0.038
836	0.013	0.046	0.038	0.052	0.033	0.026	0.039
837	0.012	0.038	0.034	0.047	0.026	0.022	0.035
838	0.013	0.031	0.031	0.041	0.018	0.018	0.027
839	0.021	0.037	0.033	0.038	0.015	0.012	0.017
840	0.025	0.035	0.032	0.042	0.010	0.007	0.017
841	0.021	0.028	0.025	0.033	0.007	0.004	0.012
842	0.020	0.026	0.024	0.029	0.006	0.004	0.009
843	0.020	0.027	0.026	0.031	0.007	0.006	0.011
844	0.017	0.025	0.021	0.029	0.008	0.003	0.011
845	0.014	0.019	0.018	0.022	0.006	0.004	0.009
846	0.013	0.019	0.019	0.024	0.006	0.006	0.011
847	0.012	0.020	0.017	0.024	0.008	0.005	0.012
848	0.007	0.011	0.012	0.014	0.004	0.004	0.007
849	0.006	0.010	0.010	0.012	0.003	0.004	0.006
850	0.008	0.013	0.014	0.017	0.005	0.007	0.009
851	0.006	0.012	0.013	0.016	0.006	0.007	0.010
852	0.005	0.010	0.013	0.013	0.005	0.008	0.008
853	0.005	0.012	0.013	0.015	0.006	0.008	0.010
854	0.007	0.015	0.014	0.019	0.008	0.007	0.012
855	0.010	0.019	0.016	0.023	0.010	0.006	0.013
856	0.013	0.026	0.019	0.030	0.013	0.006	0.017
857	0.015	0.028	0.022	0.036	0.013	0.007	0.022
858	0.021	0.036	0.025	0.041	0.015	0.004	0.020
859	0.025	0.040	0.027	0.048	0.015	0.002	0.023
860	0.031	0.049	0.027	0.054	0.018	-0.003	0.023
861	0.040	0.055	0.035	0.056	0.015	-0.005	0.016
862	0.035	0.046	0.036	0.051	0.012	0.002	0.017
863	0.028	0.043	0.034	0.045	0.015	0.006	0.016
864	0.039	0.051	0.042	0.046	0.012	0.002	0.007
865	0.043	0.050	0.037	0.051	0.007	-0.007	0.008
866	0.036	0.028	0.029	0.043	-0.008	-0.007	0.007
867	0.036	0.030	0.032	0.041	-0.006	-0.003	0.005

868	0.044	0.016	0.033	0.044	-0.028	-0.011	-0.001
869	0.049	0.015	0.018	0.046	-0.034	-0.032	-0.003
870	0.053	0.052	0.036	0.044	-0.001	-0.017	-0.009
871	0.046	0.049	0.047	0.038	0.003	0.002	-0.007
872	0.050	0.049	0.045	0.044	-0.001	-0.005	-0.006
873	0.042	0.041	0.036	0.034	-0.001	-0.006	-0.008
874	0.040	0.040	0.037	0.031	0.000	-0.003	-0.009
875	0.045	0.044	0.044	0.034	-0.001	-0.001	-0.011
876	0.046	0.043	0.044	0.035	-0.003	-0.002	-0.011
877	0.038	0.036	0.038	0.026	-0.002	0.000	-0.012
878	0.039	0.035	0.041	0.025	-0.003	0.003	-0.013
879	0.046	0.040	0.045	0.031	-0.006	-0.001	-0.016
880	0.042	0.037	0.045	0.026	-0.006	0.002	-0.017
881	0.036	0.032	0.039	0.021	-0.004	0.003	-0.015
882	0.040	0.034	0.045	0.023	-0.006	0.004	-0.017
883	0.045	0.037	0.045	0.025	-0.008	-0.001	-0.021
884	0.036	0.030	0.041	0.020	-0.005	0.005	-0.016
885	0.033	0.028	0.039	0.017	-0.005	0.006	-0.016
886	0.040	0.032	0.045	0.020	-0.008	0.005	-0.020
887	0.038	0.029	0.045	0.020	-0.009	0.006	-0.018
888	0.028	0.022	0.035	0.015	-0.006	0.007	-0.013
889	0.029	0.023	0.034	0.015	-0.006	0.005	-0.014
890	0.037	0.028	0.039	0.019	-0.009	0.002	-0.018
891	0.031	0.023	0.034	0.017	-0.009	0.003	-0.015
892	0.024	0.016	0.028	0.012	-0.007	0.005	-0.011
893	0.022	0.015	0.025	0.011	-0.007	0.003	-0.010
894	0.024	0.017	0.026	0.012	-0.007	0.002	-0.012
895	0.023	0.016	0.025	0.012	-0.007	0.002	-0.012
896	0.026	0.019	0.026	0.014	-0.007	0.000	-0.012
897	0.031	0.025	0.037	0.017	-0.006	0.006	-0.015
898	0.030	0.023	0.034	0.015	-0.007	0.005	-0.015
899	0.032	0.024	0.035	0.016	-0.008	0.003	-0.016
900	0.041	0.032	0.040	0.021	-0.009	0.000	-0.020

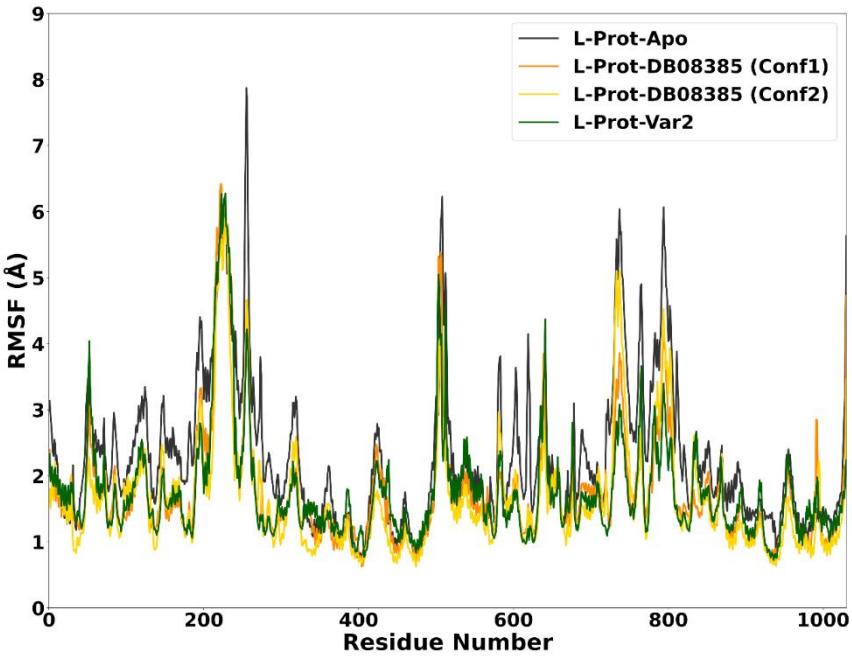
901	0.037	0.029	0.041	0.021	-0.008	0.004	-0.016
902	0.034	0.027	0.038	0.019	-0.007	0.004	-0.015
903	0.040	0.032	0.043	0.023	-0.008	0.003	-0.017
904	0.042	0.034	0.044	0.026	-0.008	0.002	-0.016
905	0.038	0.029	0.038	0.023	-0.009	0.000	-0.015
906	0.044	0.031	0.040	0.024	-0.013	-0.004	-0.020
907	0.056	0.037	0.046	0.031	-0.019	-0.010	-0.025
908	0.050	0.038	0.047	0.032	-0.012	-0.003	-0.018
909	0.044	0.034	0.042	0.028	-0.010	-0.002	-0.017
910	0.048	0.037	0.046	0.031	-0.011	-0.002	-0.018
911	0.047	0.044	0.050	0.038	-0.004	0.003	-0.010
912	0.049	0.041	0.046	0.034	-0.009	-0.003	-0.015
913	0.040	0.036	0.043	0.031	-0.004	0.003	-0.009
914	0.039	0.040	0.047	0.036	0.001	0.008	-0.003
915	0.040	0.044	0.051	0.042	0.005	0.011	0.003
916	0.034	0.039	0.045	0.037	0.005	0.011	0.003
917	0.033	0.033	0.040	0.032	0.000	0.007	-0.001
918	0.044	0.039	0.043	0.039	-0.006	-0.001	-0.005
919	0.034	0.042	0.045	0.045	0.008	0.011	0.011
920	0.054	0.047	0.049	0.050	-0.007	-0.005	-0.004
921	0.055	0.049	0.051	0.049	-0.006	-0.004	-0.006
922	0.056	0.051	0.055	0.046	-0.006	-0.001	-0.011
923	0.061	0.055	0.058	0.050	-0.006	-0.003	-0.011
924	0.062	0.058	0.059	0.052	-0.003	-0.002	-0.010
925	0.062	0.061	0.048	0.041	-0.001	-0.014	-0.021
926	0.064	0.057	0.053	0.046	-0.007	-0.011	-0.018
927	0.058	0.055	0.046	0.046	-0.003	-0.013	-0.012
928	0.061	0.057	0.041	0.049	-0.004	-0.020	-0.012
929	0.068	0.052	0.053	0.048	-0.016	-0.015	-0.020
930	0.063	0.050	0.055	0.042	-0.013	-0.008	-0.022
931	0.057	0.048	0.054	0.040	-0.010	-0.003	-0.017
932	0.066	0.050	0.055	0.043	-0.017	-0.012	-0.023
933	0.065	0.045	0.054	0.040	-0.020	-0.011	-0.025

934	0.054	0.042	0.053	0.034	-0.012	-0.001	-0.020
935	0.059	0.045	0.048	0.039	-0.014	-0.011	-0.021
936	0.068	0.045	0.054	0.041	-0.024	-0.015	-0.027
937	0.055	0.040	0.052	0.032	-0.015	-0.004	-0.023
938	0.050	0.040	0.050	0.031	-0.010	0.000	-0.019
939	0.058	0.043	0.042	0.038	-0.015	-0.016	-0.020
940	0.055	0.040	0.052	0.032	-0.015	-0.003	-0.023
941	0.048	0.035	0.048	0.026	-0.013	0.000	-0.022
942	0.044	0.034	0.033	0.026	-0.010	-0.011	-0.018
943	0.044	0.036	0.033	0.029	-0.008	-0.010	-0.015
944	0.039	0.029	0.043	0.023	-0.010	0.004	-0.016
945	0.036	0.026	0.031	0.020	-0.011	-0.006	-0.016
946	0.037	0.025	0.022	0.021	-0.012	-0.015	-0.016
947	0.034	0.024	0.020	0.015	-0.010	-0.014	-0.019
948	0.029	0.021	0.024	0.017	-0.009	-0.005	-0.013
949	0.027	0.018	0.019	0.015	-0.009	-0.009	-0.012
950	0.029	0.019	0.013	0.014	-0.010	-0.016	-0.015
951	0.023	0.015	0.014	0.010	-0.008	-0.009	-0.013
952	0.018	0.012	0.015	0.010	-0.006	-0.003	-0.008
953	0.017	0.011	0.012	0.009	-0.006	-0.005	-0.009
954	0.015	0.010	0.009	0.007	-0.005	-0.006	-0.008
955	0.011	0.008	0.010	0.006	-0.003	-0.001	-0.005
956	0.014	0.010	0.014	0.008	-0.003	0.000	-0.006
957	0.014	0.010	0.015	0.008	-0.004	0.001	-0.006
958	0.018	0.011	0.017	0.009	-0.006	-0.001	-0.008
959	0.016	0.011	0.018	0.009	-0.005	0.002	-0.007
960	0.015	0.011	0.016	0.009	-0.004	0.001	-0.006
961	0.020	0.014	0.019	0.012	-0.006	-0.001	-0.008
962	0.023	0.016	0.025	0.014	-0.007	0.002	-0.009
963	0.022	0.015	0.026	0.013	-0.007	0.004	-0.009
964	0.024	0.017	0.026	0.015	-0.007	0.002	-0.009
965	0.029	0.021	0.031	0.019	-0.008	0.002	-0.011
966	0.031	0.023	0.037	0.018	-0.008	0.006	-0.012

967	0.030	0.022	0.035	0.017	-0.008	0.005	-0.013
968	0.033	0.023	0.037	0.020	-0.009	0.004	-0.013
969	0.038	0.028	0.044	0.023	-0.010	0.005	-0.016
970	0.042	0.029	0.040	0.021	-0.013	-0.001	-0.021
971	0.042	0.030	0.042	0.021	-0.011	0.001	-0.020
972	0.046	0.033	0.047	0.026	-0.013	0.001	-0.020
973	0.049	0.036	0.048	0.027	-0.012	-0.001	-0.021
974	0.053	0.037	0.048	0.026	-0.016	-0.005	-0.027
975	0.052	0.039	0.047	0.028	-0.013	-0.005	-0.025
976	0.061	0.043	0.051	0.034	-0.018	-0.010	-0.027
977	0.058	0.044	0.053	0.033	-0.014	-0.006	-0.026
978	0.052	0.043	0.051	0.031	-0.010	-0.002	-0.021
979	0.058	0.051	0.052	0.036	-0.007	-0.005	-0.021
980	0.067	0.054	0.049	0.043	-0.012	-0.017	-0.024
981	0.061	0.049	0.052	0.042	-0.013	-0.009	-0.020
982	0.056	0.048	0.051	0.044	-0.009	-0.005	-0.013
983	0.064	0.051	0.048	0.046	-0.013	-0.016	-0.018
984	0.068	0.052	0.049	0.050	-0.016	-0.019	-0.018
985	0.057	0.047	0.051	0.045	-0.010	-0.007	-0.012
986	0.052	0.048	0.048	0.046	-0.004	-0.004	-0.006
987	0.061	0.046	0.048	0.050	-0.015	-0.013	-0.011
988	0.060	0.052	0.053	0.052	-0.008	-0.007	-0.008
989	0.047	0.048	0.048	0.044	0.001	0.000	-0.003
990	0.050	0.049	0.052	0.049	-0.001	0.001	-0.001
991	0.049	0.051	0.046	0.047	0.001	-0.004	-0.003
992	0.048	0.052	0.038	0.021	0.004	-0.010	-0.027
993	0.053	0.057	0.052	0.012	0.004	0.000	-0.041
994	0.055	0.058	0.020	0.021	0.003	-0.035	-0.034
995	0.054	0.053	0.050	0.039	-0.001	-0.004	-0.014
996	0.058	0.053	0.059	0.031	-0.005	0.002	-0.027
997	0.062	0.059	0.050	0.020	-0.002	-0.011	-0.042
998	0.060	0.053	0.056	0.022	-0.007	-0.004	-0.038
999	0.058	0.053	0.057	0.037	-0.005	-0.001	-0.022

1000	0.064	0.057	0.060	0.016	-0.007	-0.004	-0.048
1001	0.067	0.044	0.058	0.016	-0.023	-0.009	-0.051
1002	0.068	0.051	0.055	0.017	-0.017	-0.014	-0.051
1003	0.058	0.048	0.053	0.023	-0.010	-0.005	-0.035
1004	0.038	0.045	0.054	0.051	0.006	0.015	0.012
1005	0.034	0.046	0.053	0.048	0.013	0.019	0.014
1006	0.056	0.045	0.050	0.041	-0.012	-0.007	-0.015
1007	0.043	0.043	0.048	0.037	-0.001	0.005	-0.006
1008	0.045	0.042	0.048	0.036	-0.003	0.004	-0.009
1009	0.053	0.040	0.048	0.035	-0.013	-0.005	-0.018
1010	0.053	0.038	0.046	0.030	-0.016	-0.008	-0.024
1011	0.046	0.034	0.042	0.027	-0.012	-0.004	-0.019
1012	0.046	0.035	0.046	0.028	-0.010	0.000	-0.018
1013	0.053	0.037	0.048	0.028	-0.016	-0.005	-0.025
1014	0.046	0.031	0.042	0.025	-0.014	-0.004	-0.021
1015	0.045	0.027	0.036	0.022	-0.017	-0.008	-0.023
1016	0.043	0.029	0.041	0.023	-0.014	-0.002	-0.021
1017	0.041	0.028	0.039	0.021	-0.013	-0.002	-0.020
1018	0.032	0.022	0.032	0.016	-0.010	-0.001	-0.016
1019	0.031	0.022	0.030	0.016	-0.009	-0.001	-0.015
1020	0.036	0.026	0.038	0.019	-0.010	0.002	-0.016
1021	0.029	0.019	0.030	0.015	-0.010	0.001	-0.013
1022	0.024	0.016	0.024	0.012	-0.008	0.000	-0.012
1023	0.029	0.019	0.028	0.013	-0.010	-0.001	-0.016
1024	0.026	0.017	0.025	0.014	-0.008	0.000	-0.012
1025	0.022	0.013	0.021	0.010	-0.008	-0.001	-0.012
1026	0.024	0.014	0.020	0.010	-0.011	-0.004	-0.014
1027	0.007	0.013	0.019	0.010	0.007	0.013	0.003
1028	0.006	0.013	0.018	0.009	0.007	0.012	0.003
1029	0.003	0.012	0.019	0.008	0.009	0.016	0.005
1030	0.004	0.013	0.017	0.010	0.009	0.013	0.007

Figure. S11. Line plot showing comparative root mean squared fluctuation values for apo and ligand bound MexB L protomer excluding Variant 1.



Section. S1. gmx_MMPBSA input parameters

input file generated by gmx_MMPBSA (v1.6.3)

Be careful with the variables you modify; some can have severe consequences on the results you obtain.

General namelist variables

&general

sys_name = "mmpbsa1" # System name

startframe = 1 # First frame to analyze

endframe = 500 # Last frame to analyze

interval = 10 # Number of frames between adjacent frames analyzed

PBRadii = 7 # Define PBRadii to build amber topology from GROMACS files

temperature = 310 # Temperature

```
  verbose          = 1                    # How many energy terms to print in the final output
  interaction_entropy= 1
  ie_segment= 25
/
# (AMBER) Possion-Boltzmann namelist variables
&pb
  ipb              = 1                    # Dielectric model for PB
  inp              = 2                    # Nonpolar solvation method
  sander_apbs      = 0                    # Use sander.APBS?
  indi             = 2.0                  # Internal dielectric constant
  exdi             = 80.0                 # External dielectric constant
  istrng           = 0.150                # Ionic strength (M)
  radiopt          = 0                    # Use optimized radii?
  fillratio        = 1.25                 # Ratio between the longest dimension of the rectangular finite-difference grid and that of the solute
  memopt           = 3
  solvopt          = 2
  emem             = 4.0
  mctrdz           = 7.0
  mthick           = 40.0
  poretype         = 1
  sasopt           = 0
  bcopt            = 10
  nfocus           = 1
  linit            = 1000
  eneopt           = 1
  cutfd            = 7.0
```

```
  cutnb              = 99.0
  maxarcdot          = 15000
  npbverb            = 1
/
```