

Supplementary File-S2(a) [Accessibility free energies ΔG in kcal/mol]

Seq	PBP3	PBP3_F533L	PBP3_T91A
56	1.146015	1.146015	1.146015
57	1.716206	1.716206	1.716206
58	1.340219	1.340219	1.340219
59	1.324414	1.324414	1.324414
60	1.512021	1.512021	1.512021
61	1.621169	1.621169	1.621169
62	6.569576	6.569576	6.569576
63	1.47127	1.47127	1.47127
64	3.294618	3.294618	3.294618
65	-1.935692	-1.935692	-1.935692
66	0.797952	0.797952	0.797952
67	3.139911	3.139911	3.139911
68	1.599801	1.599801	1.599801
69	-1.63535	-1.63535	-1.63535
70	0.188971	0.188971	0.188971
71	-0.658459	-0.658459	-0.658459
72	0.227551	0.227551	0.227551
73	-1.310418	-1.310418	-1.310418
74	-1.095262	-1.095262	-1.095262
75	1.002632	1.002632	1.002632
76	0.269702	0.269702	0.269702
77	-0.646463	-0.646463	-0.646463
78	-0.581359	-0.581359	-0.581359
79	-0.992194	-0.992194	-0.992194
80	0.580093	0.580093	0.580093
81	-0.33668	-0.33668	-0.33668
82	-2.129507	-2.129507	-2.129507
83	-0.676509	-0.676509	-0.676509
84	0.843365	0.843365	0.843365
85	3.618154	3.618154	3.618154
86	1.966527	1.966527	2.042191
87	-1.378761	-1.378761	-1.287061
88	6.558066	6.558066	6.698696
89	-0.758175	-0.758175	-1.201564
90	0.748845	0.748845	0.841143
91	-1.196393	-1.196393	0.961953
92	-0.398562	-0.398562	-0.080888
93	-1.332576	-1.332576	-0.907355
94	-3.520883	-3.520883	-3.329582
95	-1.384777	-1.384777	-1.024014
96	-3.804405	-3.804405	-3.513698
97	-1.562408	-1.562408	-1.562408
98	-3.545879	-3.545879	-3.545879
99	-4.111554	-4.111554	-4.111554

Seq	PBP3	PBP3_F533L	PBP3_T91A
100	-2.699846	-2.699846	-2.699846
101	-1.198091	-1.198091	-1.198091
102	-0.255124	-0.255124	-0.255124
103	-1.581173	-1.581173	-1.581173
104	-0.481768	-0.481768	-0.481768
105	0.719215	0.719215	0.719215
106	-0.250965	-0.250965	-0.250965
107	-0.101203	-0.101203	-0.101203
108	-1.064347	-1.064347	-1.064347
109	0.564026	0.564026	0.564026
110	-2.668821	-2.668821	-2.668821
111	-0.297453	-0.297453	-0.297453
112	-1.653277	-1.653277	-1.653277
113	-1.329807	-1.329807	-1.329807
114	-3.298323	-3.298323	-3.298323
115	-1.778936	-1.778936	-1.778936
116	-2.037228	-2.037228	-2.037228
117	0.61381	0.61381	0.61381
118	-0.068265	-0.068265	-0.068265
119	-1.873526	-1.873526	-1.873526
120	-1.279149	-1.279149	-1.279149
121	-0.377388	-0.377388	-0.377388
122	2.447488	2.447488	2.447488
123	-0.342765	-0.342765	-0.342765
124	0.505863	0.505863	0.505863
125	-2.314736	-2.314736	-2.314736
126	0.115716	0.115716	0.115716
127	-0.350948	-0.350948	-0.350948
128	-0.149962	-0.149962	-0.149962
129	-1.82766	-1.82766	-1.82766
130	-1.815132	-1.815132	-1.815132
131	-0.652074	-0.652074	-0.652074
132	-3.553808	-3.553808	-3.553808
133	-1.360522	-1.360522	-1.360522
134	-0.375949	-0.375949	-0.375949
135	-2.459231	-2.459231	-2.459231
136	-0.425335	-0.425335	-0.425335
137	-1.723825	-1.723825	-1.723825
138	1.767483	1.767483	1.767483
139	2.518415	2.518415	2.518415
140	1.048134	1.048134	1.048134
141	-0.777431	-0.777431	-0.777431
142	-0.406945	-0.406945	-0.406945
143	-0.085438	-0.085438	-0.085438

Contd..S2(a)

Seq	PBP3	PBP3_F533L	PBP3_T91A
144	0.615646	0.615646	0.615646
145	-0.543595	-0.543595	-0.543595
146	-1.502745	-1.502745	-1.502745
147	-0.989522	-0.989522	-0.989522
148	-0.683402	-0.683402	-0.683402
149	-0.804952	-0.804952	-0.804952
150	3.178347	3.178347	3.178347
151	-2.697971	-2.697971	-2.697971
152	0.329607	0.329607	0.329607
153	6.957231	6.957231	6.957231
154	3.961131	3.961131	3.961131
155	0.87634	0.87634	0.87634
156	-0.108906	-0.108906	-0.108906
157	1.200491	1.200491	1.200491
158	1.308977	1.308977	1.308977
159	-0.627359	-0.627359	-0.627359
160	-1.006519	-1.006519	-1.006519
161	-3.381737	-3.381737	-3.381737
162	-2.764305	-2.764305	-2.764305
163	-0.015619	-0.015619	-0.015619
164	-2.831617	-2.831617	-2.831617
165	-1.472949	-1.472949	-1.472949
166	-0.70914	-0.70914	-0.70914
167	-1.075932	-1.075932	-1.075932
168	1.030558	1.030558	1.030558
169	0.434393	0.434393	0.434393
170	4.27245	4.27245	4.27245
171	-0.082357	-0.082357	-0.082357
172	2.238255	2.238255	2.238255
173	-0.128867	-0.128867	-0.128867
174	0.478106	0.478106	0.478106
175	-0.637161	-0.637161	-0.637161
176	1.748066	1.748066	1.748066
177	0.085963	0.085963	0.085963
178	-1.490125	-1.490125	-1.490125
179	5.245556	5.245556	5.245556
180	1.29731	1.29731	1.29731
181	1.104374	1.104374	1.104374
182	-0.158033	-0.158033	-0.158033
183	1.008807	1.008807	1.008807
184	-0.70399	-0.70399	-0.70399
185	2.339601	2.339601	2.339601
186	-2.115039	-2.115039	-2.115039

Seq	PBP3	PBP3_F533L	PBP3_T91A
187	1.418287	1.418287	1.418287
188	0.866048	0.866048	0.866048
189	1.452258	1.452258	1.452258
190	-0.22447	-0.22447	-0.22447
191	2.109095	2.109095	2.109095
192	-0.097566	-0.097566	-0.097566
193	0.279921	0.279921	0.279921
194	-0.592112	-0.592112	-0.592112
195	0.202253	0.202253	0.202253
196	1.62728	1.62728	1.62728
197	-0.643363	-0.643363	-0.643363
198	1.274366	1.274366	1.274366
199	-0.103001	-0.103001	-0.103001
200	-1.281396	-1.281396	-1.281396
201	0.386452	0.386452	0.386452
202	-0.165578	-0.165578	-0.165578
203	1.3148	1.3148	1.3148
204	-1.178535	-1.178535	-1.178535
205	-0.923406	-0.923406	-0.923406
206	-0.396189	-0.396189	-0.396189
207	1.711319	1.711319	1.711319
208	-0.737927	-0.737927	-0.737927
209	1.170201	1.170201	1.170201
210	-0.471486	-0.471486	-0.471486
211	-0.69264	-0.69264	-0.69264
212	-1.497769	-1.497769	-1.497769
213	-0.143726	-0.143726	-0.143726
214	-1.675431	-1.675431	-1.675431
215	-0.944399	-0.944399	-0.944399
216	0.222303	0.222303	0.222303
217	-0.90953	-0.90953	-0.90953
218	0.554246	0.554246	0.554246
219	-2.707878	-2.707878	-2.707878
220	0.345665	0.345665	0.345665
221	-2.288329	-2.288329	-2.288329
222	0.071353	0.071353	0.071353
223	-1.436886	-1.436886	-1.436886
224	0.410045	0.410045	0.410045
225	-1.201619	-1.201619	-1.201619
226	-0.87412	-0.87412	-0.87412
227	-1.175383	-1.175383	-1.175383
228	3.180235	3.180235	3.180235
229	2.384323	2.384323	2.384323

Contd..S2(a)

Seq	PBP3	PBP3_F533L	PBP3_T91A
230	0.879668	0.879668	0.879668
231	-1.154434	-1.154434	-1.154434
232	2.15144	2.15144	2.15144
233	-0.733153	-0.733153	-0.733153
234	4.886321	4.886321	4.886321
235	-2.503847	-2.503847	-2.503847
236	-1.293792	-1.293792	-1.293792
237	-1.153525	-1.153525	-1.153525
238	-0.743952	-0.743952	-0.743952
239	-2.822037	-2.822037	-2.822037
240	2.606012	2.606012	2.606012
241	-2.595512	-2.595512	-2.595512
242	0.97941	0.97941	0.97941
243	1.122141	1.122141	1.122141
244	-0.111074	-0.111074	-0.111074
245	-1.511627	-1.511627	-1.511627
246	-0.426553	-0.426553	-0.426553
247	-0.692555	-0.692555	-0.692555
248	-0.530614	-0.530614	-0.530614
249	-2.423796	-2.423796	-2.423796
250	-2.821062	-2.821062	-2.821062
251	-2.768331	-2.768331	-2.768331
252	-2.533674	-2.533674	-2.533674
253	1.032361	1.032361	1.032361
254	-0.872555	-0.872555	-0.872555
255	-1.357931	-1.357931	-1.357931
256	0.472757	0.472757	0.472757
257	-0.193366	-0.193366	-0.193366
258	4.586996	4.586996	4.586996
259	-1.688269	-1.688269	-1.688269
260	-1.355921	-1.355921	-1.355921
261	0.00438	0.00438	0.00438
262	0.014057	0.014057	0.014057
263	2.139411	2.139411	2.139411
264	3.037076	3.037076	3.037076
265	5.479735	5.479735	5.479735
266	1.382675	1.382675	1.382675
267	2.087853	2.087853	2.087853
268	0.158721	0.158721	0.158721
269	0.155931	0.155931	0.155931
270	2.643744	2.643744	2.643744
271	0.026482	0.026482	0.026482
272	0.05379	0.05379	0.05379

Seq	PBP3	PBP3_F533L	PBP3_T91A
273	-0.647569	-0.647569	-0.647569
274	-0.620969	-0.620969	-0.620969
275	-0.096391	-0.096391	-0.096391
276	2.513663	2.513663	2.513663
277	0.506281	0.506281	0.506281
278	-0.311796	-0.311796	-0.311796
279	1.569131	1.569131	1.569131
280	0.545548	0.545548	0.545548
281	1.498359	1.498359	1.498359
282	-0.289106	-0.289106	-0.289106
283	1.793152	1.793152	1.793152
284	5.661725	5.661725	5.661725
285	-0.492214	-0.492214	-0.492214
286	-0.879741	-0.879741	-0.879741
287	1.778866	1.778866	1.778866
288	2.614555	2.614555	2.614555
289	0.603159	0.603159	0.603159
290	-0.806063	-0.806063	-0.806063
291	0.780793	0.780793	0.780793
292	3.92196	3.92196	3.92196
293	3.131318	3.131318	3.131318
294	1.446403	1.446403	1.446403
295	2.934024	2.934024	2.934024
296	0.245799	0.245799	0.245799
297	7.617965	7.617965	7.617965
298	1.89391	1.89391	1.89391
299	0.196593	0.196593	0.196593
300	1.607726	1.607726	1.607726
301	0.152953	0.152953	0.152953
302	2.160479	2.160479	2.160479
303	-0.724818	-0.724818	-0.724818
304	-1.564191	-1.564191	-1.564191
305	-0.511441	-0.511441	-0.511441
306	0.655138	0.655138	0.655138
307	0.321759	0.321759	0.321759
308	-0.311426	-0.311426	-0.311426
309	-0.859236	-0.859236	-0.859236
310	-1.375047	-1.375047	-1.375047
311	0.596056	0.596056	0.596056
312	0.447164	0.447164	0.447164
313	-1.218968	-1.218968	-1.218968
314	0.227607	0.227607	0.227607
315	1.556229	1.556229	1.556229

Contd..S2(a)

Seq	PBP3	PBP3_F533L	PBP3_T91A
316	-0.805993	-0.805993	-0.805993
317	-0.676387	-0.676387	-0.676387
318	-0.607369	-0.607369	-0.607369
319	1.508134	1.508134	1.508134
320	-0.887369	-0.887369	-0.887369
321	1.185467	1.185467	1.185467
322	-0.182701	-0.182701	-0.182701
323	0.248877	0.248877	0.248877
324	-0.250225	-0.250225	-0.250225
325	-0.718274	-0.718274	-0.718274
326	1.607007	1.607007	1.607007
327	0.30874	0.30874	0.30874
328	3.559537	3.559537	3.559537
329	0.679834	0.679834	0.679834
330	-0.341679	-0.341679	-0.341679
331	0.736044	0.736044	0.736044
332	4.049217	4.049217	4.049217
333	4.990831	4.990831	4.990831
334	0.301048	0.301048	0.301048
335	-0.957947	-0.957947	-0.957947
336	-0.082666	-0.082666	-0.082666
337	0.162684	0.162684	0.162684
338	-1.006248	-1.006248	-1.006248
339	-0.527314	-0.527314	-0.527314
340	-1.191261	-1.191261	-1.191261
341	-1.187295	-1.187295	-1.187295
342	-1.549111	-1.549111	-1.549111
343	0.067536	0.067536	0.067536
344	0.558927	0.558927	0.558927
345	-1.158663	-1.158663	-1.158663
346	-2.528185	-2.528185	-2.528185
347	0.957653	0.957653	0.957653
348	0.56852	0.56852	0.56852
349	0.293274	0.293274	0.293274
350	1.094544	1.094544	1.094544
351	1.260048	1.260048	1.260048
352	0.406687	0.406687	0.406687
353	-0.101257	-0.101257	-0.101257
354	-1.193022	-1.193022	-1.193022
355	-0.117257	-0.117257	-0.117257
356	-0.347727	-0.347727	-0.347727
357	-2.137066	-2.137066	-2.137066
358	-2.510598	-2.510598	-2.510598
359	1.507468	1.507468	1.507468
360	-0.784075	-0.784075	-0.784075

Seq	PBP3	PBP3_F533L	PBP3_T91A
361	-1.069532	-1.069532	-1.069532
362	-0.679258	-0.679258	-0.679258
363	-1.086067	-1.086067	-1.086067
364	-2.435195	-2.435195	-2.435195
365	-1.868043	-1.868043	-1.868043
366	-3.266651	-3.266651	-3.266651
367	-1.156552	-1.156552	-1.156552
368	-2.467118	-2.467118	-2.467118
369	-3.174608	-3.174608	-3.174608
370	-2.456599	-2.456599	-2.456599
371	-0.58609	-0.58609	-0.58609
372	-0.420455	-0.420455	-0.420455
373	-1.28516	-1.28516	-1.28516
374	0.151724	0.151724	0.151724
375	-0.615136	-0.615136	-0.615136
376	0.182398	0.182398	0.182398
377	-0.304179	-0.304179	-0.304179
378	-1.008216	-1.008216	-1.008216
379	0.339773	0.339773	0.339773
380	-0.592071	-0.592071	-0.592071
381	-0.664641	-0.664641	-0.664641
382	-0.232741	-0.232741	-0.232741
383	0.279281	0.279281	0.279281
384	1.152472	1.152472	1.152472
385	0.526899	0.526899	0.526899
386	1.572394	1.572394	1.572394
387	-0.788948	-0.788948	-0.788948
388	1.867535	1.867535	1.867535
389	0.316342	0.316342	0.316342
390	-1.605623	-1.605623	-1.605623
391	-2.903499	-2.903499	-2.903499
392	-1.204608	-1.204608	-1.204608
393	-3.142532	-3.142532	-3.142532
394	-2.027052	-2.027052	-2.027052
395	-1.914615	-1.914615	-1.914615
396	-2.668718	-2.668718	-2.668718
397	-3.399643	-3.399643	-3.399643
398	-0.441653	-0.441653	-0.441653
399	-1.805489	-1.805489	-1.805489
400	0.143966	0.143966	0.143966
401	-0.749825	-0.749825	-0.749825
402	0.896839	0.896839	0.896839
403	-2.074774	-2.074774	-2.074774

Contd..S2(a)

Seq	PBP3	PBP3_F533L	PBP3_T91A
404	0.090013	0.090013	0.090013
405	-1.92079	-1.92079	-1.92079
406	-1.930926	-1.930926	-1.930926
407	0.049875	0.049875	0.049875
408	-1.189591	-1.189591	-1.189591
409	0.513652	0.513652	0.513652
410	-0.557077	-0.557077	-0.557077
411	-1.952406	-1.952406	-1.952406
412	-0.378954	-0.378954	-0.378954
413	-2.18193	-2.18193	-2.18193
414	-0.11184	-0.11184	-0.11184
415	-2.915825	-2.915825	-2.915825
416	-2.081966	-2.081966	-2.081966
417	1.781197	1.781197	1.781197
418	-2.69853	-2.69853	-2.69853
419	-2.545034	-2.545034	-2.545034
420	-1.311591	-1.311591	-1.311591
421	-2.621297	-2.621297	-2.621297
422	-1.181392	-1.181392	-1.181392
423	-2.405888	-2.405888	-2.405888
424	-2.591359	-2.591359	-2.591359
425	-2.99758	-2.99758	-2.99758
426	-1.517152	-1.517152	-1.517152
427	0.943461	0.943461	0.943461
428	-0.697895	-0.697895	-0.697895
429	0.790198	0.790198	0.790198
430	0.180727	0.180727	0.180727
431	0.609929	0.609929	0.609929
432	-1.216734	-1.216734	-1.216734
433	-0.052423	-0.052423	-0.052423
434	0.219124	0.219124	0.219124
435	0.089651	0.089651	0.089651
436	-1.181593	-1.181593	-1.181593
437	0.021755	0.021755	0.021755
438	-0.505735	-0.505735	-0.505735
439	-0.031025	-0.031025	-0.031025
440	-0.12972	-0.12972	-0.12972
441	-0.351736	-0.351736	-0.351736
442	1.750052	1.750052	1.750052
443	0.095691	0.095691	0.095691
444	-3.227591	-3.227591	-3.227591
445	-0.387515	-0.387515	-0.387515
446	3.308236	3.308236	3.308236

Seq	PBP3	PBP3_F533L	PBP3_T91A
447	-0.449353	-0.449353	-0.449353
448	-2.098842	-2.098842	-2.098842
449	-2.334728	-2.334728	-2.334728
450	-0.8619	-0.8619	-0.8619
451	-0.586824	-0.586824	-0.586824
452	-3.734679	-3.734679	-3.734679
453	-1.984767	-1.984767	-1.984767
454	-1.609936	-1.609936	-1.609936
455	-1.001107	-1.001107	-1.001107
456	-1.628775	-1.628775	-1.628775
457	-3.103479	-3.103479	-3.103479
458	1.312983	1.312983	1.312983
459	-0.010876	-0.010876	-0.010876
460	-1.220271	-1.220271	-1.220271
461	-2.616652	-2.616652	-2.616652
462	1.576136	1.576136	1.576136
463	-0.875806	-0.875806	-0.875806
464	-3.216551	-3.216551	-3.216551
465	-3.324631	-3.324631	-3.324631
466	-1.627107	-1.627107	-1.627107
467	0.706597	0.706597	0.706597
468	-1.732436	-1.732436	-1.732436
469	-1.260171	-1.260171	-1.260171
470	-0.157124	-0.157124	-0.157124
471	-0.083875	-0.083875	-0.083875
472	5.05142	5.05142	5.05142
473	-1.107564	-1.107564	-1.107564
474	-1.21756	-1.21756	-1.21756
475	0.033039	0.033039	0.033039
476	-1.523049	-1.523049	-1.523049
477	-1.042726	-1.042726	-1.042726
478	-0.39086	-0.39086	-0.39086
479	0.283079	0.283079	0.283079
480	-0.096559	-0.096559	-0.096559
481	-0.984676	-0.984676	-0.984676
482	-0.857818	-0.857818	-0.857818
483	-0.115338	-0.115338	-0.115338
484	7.300702	7.300702	7.300702
485	1.018792	1.018792	1.018792
486	1.766307	1.766307	1.766307
487	1.046336	1.046336	1.046336
488	0.113636	0.113636	0.113636
489	1.303297	1.303297	1.303297

Contd..S2(a)

Seq	PBP3	PBP3_F533L	PBP3_T91A
490	1.238167	1.238167	1.238167
491	2.424333	2.424333	2.424333
492	0.391737	0.391737	0.391737
493	3.123603	3.123603	3.123603
494	0.739914	0.739914	0.739914
495	1.240828	1.240828	1.240828
496	-0.455113	-0.455113	-0.455113
497	1.069904	1.069904	1.069904
498	3.467078	3.467078	3.467078
499	1.331245	1.331245	1.331245
500	0.030314	0.030314	0.030314
501	0.182503	0.182503	0.182503
502	0.97899	0.97899	0.97899
503	0.026745	0.026745	0.026745
504	4.333886	4.333886	4.333886
505	-0.181729	-0.181729	-0.181729
506	-2.167836	-2.167836	-2.167836
507	-1.271299	-1.271299	-1.271299
508	-0.323322	-0.323322	-0.323322
509	0.203887	0.203887	0.203887
510	-1.418102	-1.418102	-1.418102
511	-1.472374	-1.472374	-1.472374
512	2.376419	2.376419	2.376419
513	0.226353	0.226353	0.226353
514	0.004115	0.004115	0.004115
515	-0.595485	-0.595485	-0.595485
516	-0.137127	-0.137127	-0.137127
517	-1.150107	-1.150107	-1.150107
518	-2.788643	-2.788643	-2.788643
519	-3.264735	-3.264735	-3.264735
520	-3.839326	-3.839326	-3.839326
521	-3.78019	-3.78019	-3.78019
522	-3.505256	-3.505256	-3.505256
523	-3.630981	-3.630981	-3.630981
524	-3.863052	-3.863052	-3.863052
525	-0.637721	-0.637721	-0.637721
526	0.291718	0.291718	0.291718
527	0.129421	0.129421	0.129421
528	0.159589	0.159589	0.159589
529	-0.686152	-0.686152	-0.686152
530	1.619334	1.619334	1.619334
531	1.403496	1.403496	1.403496
532	3.285823	3.285823	3.285823

Seq	PBP3	PBP3_F533L	PBP3_T91A
533	3.291267	3.291267	3.291267
534	2.206395	2.206395	2.206395
535	1.182654	1.182654	1.182654
536	3.202104	3.202104	3.202104
537	-0.566603	-0.566603	-0.566603
538	1.748898	1.748898	1.748898
539	-1.652708	-1.652708	-1.652708
540	0.063749	0.063749	0.063749
541	-0.196846	-0.196846	-0.196846
542	-1.978598	-1.978598	-1.978598
543	0.024499	0.024499	0.024499
544	-1.2039	-1.2039	-1.2039
545	-1.985596	-1.985596	-1.985596
546	-2.095456	-2.095456	-2.095456
547	0.108554	0.108554	0.108554
548	0.619723	0.619723	0.619723
549	-2.481637	-2.481637	-2.481637
550	-2.29336	-2.29336	-2.29336
551	-1.113306	-1.113306	-1.113306
552	0.573552	0.573552	0.573552
553	-0.380251	-0.380251	-0.380251
554	-2.666222	-2.666222	-2.666222
555	-1.915395	-1.915395	-1.915395
556	-0.188605	-0.188605	-0.188605
557	-1.126937	-1.126937	-1.126937
558	-0.305977	-0.305977	-0.305977
559	-1.005388	-1.005388	-1.005388

Supplementary File-S2(b) [Torsion free energies ΔG in kcal/mol]

Seq	PBP3	PBP3_F533L	PBP3_T91A
56	0	0	0
57	0.293422	0.293422	0.293422
58	-0.363504	-0.363504	-0.363504
59	-1.511173	-1.511173	-1.511173
60	2.670865	2.670865	2.670865
61	1.895884	1.895884	1.895884
62	1.896064	1.896064	1.896064
63	3.291504	3.291504	3.291504
64	-1.192135	-1.192135	-1.192135
65	-4.43541	-4.43541	-4.43541
66	-3.788794	-3.788794	-3.788794
67	-2.302059	-2.302059	-2.302059
68	-2.038004	-2.038004	-2.038004
69	-6.90691	-6.90691	-6.90691
70	-14.654777	-14.654777	-14.654777
71	-5.782951	-5.782951	-5.782951
72	-8.036805	-8.036805	-8.036805
73	-2.297054	-2.297054	-2.297054
74	-4.251518	-4.251518	-4.251518
75	-4.543692	-4.543692	-4.543692
76	-3.522141	-3.522141	-3.522141
77	-4.113986	-4.113986	-4.113986
78	-5.869324	-5.869324	-5.869324
79	-1.226989	-1.226989	-1.226989
80	-2.001995	-2.001995	-2.001995
81	-2.652523	-2.652523	-2.652523
82	-2.324404	-2.324404	-2.324404
83	-0.910238	-0.910238	-0.910238
84	0.977952	0.977952	0.365006
85	0.718284	0.718284	0.011662
86	-1.06717	-1.06717	-2.567581
87	-1.984073	-1.984073	-3.749864
88	-0.326941	-0.326941	-2.532076
89	-0.097581	-0.097581	-2.57094
90	3.972488	3.972488	4.174168
91	2.887499	2.887499	-2.588532
92	2.449255	2.449255	1.043638
93	-1.269727	-1.269727	-2.719347
94	-1.418181	-1.418181	-2.781344
95	-2.592655	-2.592655	-3.656937
96	0.221952	0.221952	-0.376806
97	-3.388958	-3.388958	-3.830377
98	-3.908378	-3.908378	-4.35536
99	-4.584574	-4.584574	-4.584574
100	-4.759912	-4.759912	-4.759912

Seq	PBP3	PBP3_F533L	PBP3_T91A
101	-4.67148	-4.671482	-4.671482
102	-3.20269	-3.202692	-3.202692
103	-4.52698	-4.526982	-4.526982
104	-11.6257	-11.625707	-11.625707
105	-0.34264	-0.342639	-0.342639
106	-4.1216	-4.121598	-4.121598
107	-1.18078	-1.180784	-1.180784
108	-2.318	-2.317998	-2.317998
109	-1.96046	-1.960457	-1.960457
110	-2.22419	-2.224193	-2.224193
111	-3.13857	-3.138567	-3.138567
112	-1.37159	-1.371585	-1.371585
113	-2.21567	-2.215668	-2.215668
114	-2.45868	-2.458676	-2.458676
115	-2.33142	-2.331419	-2.331419
116	-0.69211	-0.692109	-0.692109
117	-0.3877	-0.387696	-0.387696
118	-1.86776	-1.867758	-1.867758
119	4.906344	4.906344	4.906344
120	-0.74995	-0.749946	-0.749946
121	2.153675	2.153675	2.153675
122	0.922636	0.922636	0.922636
123	-1.09051	-1.09051	-1.09051
124	3.901777	3.901777	3.901777
125	2.56028	2.56028	2.56028
126	-1.14288	-1.142882	-1.142882
127	0.107442	0.107442	0.107442
128	-9.23084	-9.230836	-9.230836
129	-2.41169	-2.411686	-2.411686
130	-4.94912	-4.949117	-4.949117
131	2.117627	2.117627	2.117627
132	1.49562	1.49562	1.49562
133	2.558592	2.558592	2.558592
134	2.715425	2.715425	2.715425
135	2.62029	2.62029	2.62029
136	3.663977	3.663977	3.663977
137	1.151655	1.151655	1.151655
138	0.010352	0.010352	0.010352
139	4.20195	4.20195	4.20195
140	0.750547	0.750547	0.750547
141	0.810096	0.810096	0.810096
142	-1.78142	-1.781419	-1.781419
143	-3.70382	-3.703818	-3.703818
144	-8.46071	-8.460706	-8.460706
145	-2.3592	-2.359201	-2.359201

Cond..S2(b)

Seq	PBP3	PBP3_F533L	PBP3_T91A
146	-2.035673	-2.035673	-2.035673
147	-1.509545	-1.509545	-1.509545
148	-0.905661	-0.905661	-0.905661
149	1.114384	1.114384	1.114384
150	0.819273	0.819273	0.819273
151	-0.124719	-0.124719	-0.124719
152	0.313314	0.313314	0.313314
153	2.859043	2.859043	2.859043
154	0.260916	0.260916	0.260916
155	-1.696911	-1.696911	-1.696911
156	1.844979	1.844979	1.844979
157	-1.615697	-1.615697	-1.615697
158	-9.867667	-9.867667	-9.867667
159	1.820998	1.820998	1.820998
160	1.093559	1.093559	1.093559
161	5.846147	5.846147	5.846147
162	-0.379422	-0.379422	-0.379422
163	1.117725	1.117725	1.117725
164	1.285606	1.285606	1.285606
165	3.510038	3.510038	3.510038
166	-8.840515	-8.840515	-8.840515
167	-3.55226	-3.55226	-3.55226
168	-3.707263	-3.707263	-3.707263
169	-2.905668	-2.905668	-2.905668
170	0.685353	0.685353	0.685353
171	-0.3516	-0.3516	-0.3516
172	-2.322189	-2.322189	-2.322189
173	1.955721	1.955721	1.955721
174	1.23737	1.23737	1.23737
175	0.169139	0.169139	0.169139
176	3.401731	3.401731	3.401731
177	-5.085718	-5.085718	-5.085718
178	0.474609	0.474609	0.474609
179	-0.022751	-0.022751	-0.022751
180	-0.457985	-0.457985	-0.457985
181	-0.369638	-0.369638	-0.369638
182	1.403092	1.403092	1.403092
183	-1.679268	-1.679268	-1.679268
184	-2.091709	-2.091709	-2.091709
185	-1.827616	-1.827616	-1.827616
186	0.206541	0.206541	0.206541
187	1.303492	1.303492	1.303492
188	-5.409125	-5.409125	-5.409125

Seq	PBP3	PBP3_F533L	PBP3_T91A
189	-2.57005	-2.570052	-2.570052
190	-4.93566	-4.935656	-4.935656
191	3.643422	3.643422	3.643422
192	2.491628	2.491628	2.491628
193	2.241669	2.241669	2.241669
194	0.77705	0.77705	0.77705
195	-0.02926	-0.029257	-0.029257
196	2.524508	2.524508	2.524508
197	4.516665	4.516665	4.516665
198	2.755667	2.755667	2.755667
199	5.89523	5.89523	5.89523
200	2.517799	2.517799	2.517799
201	5.240226	5.240226	5.240226
202	5.942558	5.942558	5.942558
203	-0.09588	-0.095882	-0.095882
204	2.679395	2.679395	2.679395
205	0.571573	0.571573	0.571573
206	2.646434	2.646434	2.646434
207	2.971515	2.971515	2.971515
208	0.753103	0.753103	0.753103
209	2.033332	2.033332	2.033332
210	3.024214	3.024214	3.024214
211	0.809024	0.809024	0.809024
212	2.554152	2.554152	2.554152
213	0.759236	0.759236	0.759236
214	2.223676	2.223676	2.223676
215	-3.7665	-3.766496	-3.766496
216	5.252286	5.252286	5.252286
217	2.75106	2.75106	2.75106
218	2.34301	2.34301	2.34301
219	2.217469	2.217469	2.217469
220	2.788354	2.788354	2.788354
221	4.214491	4.214491	4.214491
222	3.99573	3.99573	3.99573
223	6.579286	6.579286	6.579286
224	4.582259	4.582259	4.582259
225	-1.1968	-1.196803	-1.196803
226	-1.82666	-1.826663	-1.826663
227	-2.14137	-2.141367	-2.141367
228	-2.8175	-2.817503	-2.817503
229	-2.88992	-2.889924	-2.889924
230	-3.41444	-3.414436	-3.414436
231	-3.81383	-3.813829	-3.813829

Cond..S2(b)

Seq	PBP3	PBP3_F533L	PBP3_T91A
232	-4.311802	-4.311802	-4.311802
233	-5.454129	-5.454129	-5.454129
234	-5.183018	-5.183018	-5.183018
235	-4.893414	-4.893414	-4.893414
236	-5.602176	-5.602176	-5.602176
237	-5.26886	-5.26886	-5.26886
238	-5.810773	-5.810773	-5.810773
239	-5.070414	-5.070414	-5.070414
240	-5.661705	-5.661705	-5.661705
241	-5.264555	-5.264555	-5.264555
242	-7.019568	-7.019568	-7.019568
243	-13.41582	-13.41582	-13.41582
244	-5.330567	-5.330567	-5.330567
245	-3.092288	-3.092288	-3.092288
246	0.096389	0.096389	0.096389
247	-11.739236	-11.739236	-11.739236
248	-2.470833	-2.470833	-2.470833
249	-2.949042	-2.949042	-2.949042
250	-5.232189	-5.232189	-5.232189
251	-4.354406	-4.354406	-4.354406
252	-4.444844	-4.444844	-4.444844
253	-3.561208	-3.561208	-3.561208
254	-0.739397	-0.739397	-0.739397
255	-0.333182	-0.333182	-0.333182
256	-3.267319	-3.267319	-3.267319
257	-9.890112	-9.890112	-9.890112
258	0.509672	0.509672	0.509672
259	0.766979	0.766979	0.766979
260	-1.119051	-1.119051	-1.119051
261	-0.350461	-0.350461	-0.350461
262	-1.275016	-1.275016	-1.275016
263	-0.379856	-0.379856	-0.379856
264	0.679911	0.679911	0.679911
265	-0.579445	-0.579445	-0.579445
266	-12.407563	-12.407563	-12.407563
267	-1.185687	-1.185687	-1.185687
268	-2.137327	-2.137327	-2.137327
269	-3.806262	-3.806262	-3.806262
270	-1.702411	-1.702411	-1.702411
271	-4.785132	-4.785132	-4.785132
272	1.585843	1.585843	1.585843
273	-1.657536	-1.657536	-1.657536
274	-0.792509	-0.792509	-0.792509
275	2.118265	2.118265	2.118265
276	2.616799	2.616799	2.616799

Seq	PBP3	PBP3_F533L	PBP3_T91A
277	1.020737	1.020737	1.020737
278	-0.98232	-0.982321	-0.982321
279	-2.44158	-2.441581	-2.441581
280	-0.80196	-0.801956	-0.801956
281	2.462283	2.462283	2.462283
282	3.781559	3.781559	3.781559
283	2.462508	2.462508	2.462508
284	-0.96896	-0.968964	-0.968964
285	-0.16933	-0.16933	-0.16933
286	1.260928	1.260928	1.260928
287	4.361692	4.361692	4.361692
288	-0.97534	-0.975339	-0.975339
289	-1.72376	-1.723761	-1.723761
290	-1.11329	-1.11329	-1.11329
291	-1.92721	-1.927209	-1.927209
292	-2.11893	-2.118933	-2.118933
293	-8.72058	-8.720575	-8.720575
294	-3.70009	-3.700088	-3.700088
295	-2.70791	-2.70791	-2.70791
296	0.961832	0.961832	0.961832
297	3.198919	3.198919	3.198919
298	0.490721	0.490721	0.490721
299	-0.23917	-0.239168	-0.239168
300	0.277592	0.277592	0.277592
301	-1.46489	-1.464887	-1.464887
302	-1.30919	-1.309185	-1.309185
303	-1.9984	-1.998395	-1.998395
304	-2.54552	-2.54552	-2.54552
305	-3.08271	-3.082712	-3.082712
306	-2.11833	-2.118331	-2.118331
307	-6.23819	-6.238187	-6.238187
308	-11.1001	-11.100111	-11.100111
309	-3.06216	-3.062164	-3.062164
310	-2.1751	-2.175097	-2.175097
311	-3.5607	-3.560699	-3.560699
312	1.584089	1.584089	1.584089
313	-5.55219	-5.552193	-5.552193
314	-3.64056	-3.640561	-3.640561
315	-4.39468	-4.394675	-4.394675
316	-5.08202	-5.082019	-5.082019
317	-3.8169	-3.816897	-3.816897
318	-1.22982	-1.229816	-1.229816
319	-3.09318	-3.093184	-3.093184
320	-15.3593	-15.359327	-15.359327
321	-9.70906	-9.709064	-9.709064

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Seq	PBP3	PBP3_F533L	PBP3_T91A
322	-2.759783	-2.759783	-2.759783
323	-2.109875	-2.109875	-2.109875
324	-1.983749	-1.983749	-1.983749
325	-1.380488	-1.380488	-1.380488
326	-11.900695	-11.900695	-11.900695
327	0.813435	0.813435	0.813435
328	0.486736	0.486736	0.486736
329	-3.231621	-3.231621	-3.231621
330	1.188286	1.188286	1.188286
331	-2.11436	-2.11436	-2.11436
332	-0.982747	-0.982747	-0.982747
333	1.008296	1.008296	1.008296
334	1.406461	1.406461	1.406461
335	-0.82566	-0.82566	-0.82566
336	-1.188459	-1.188459	-1.188459
337	2.939057	2.939057	2.939057
338	1.009133	1.009133	1.009133
339	3.334102	3.334102	3.334102
340	2.399111	2.399111	2.399111
341	0.878936	0.878936	0.878936
342	2.069689	2.069689	2.069689
343	3.77411	3.77411	3.77411
344	4.823307	4.823307	4.823307
345	3.444824	3.444824	3.444824
346	4.574886	4.574886	4.574886
347	4.009524	4.009524	4.009524
348	4.031747	4.031747	4.031747
349	9.282671	9.282671	9.282671
350	3.222213	3.222213	3.222213
351	5.392809	5.392809	5.392809
352	4.684128	4.684128	4.684128
353	6.136354	6.136354	6.136354
354	4.387161	4.387161	4.387161
355	3.091518	3.091518	3.091518
356	1.867105	1.867105	1.867105
357	1.675908	1.675908	1.675908
358	1.561283	1.561283	1.561283
359	1.89144	1.89144	1.89144
360	1.90202	1.90202	1.90202
361	0.016626	0.016626	0.016626
362	-8.439427	-8.439427	-8.439427
363	2.052365	2.052365	2.052365
364	0.72034	0.72034	0.72034

Seq	PBP3	PBP3_F533L	PBP3_T91A
365	1.45429	1.45429	1.45429
366	1.145696	1.145696	1.145696
367	0.224886	0.224886	0.224886
368	0.292527	0.292527	0.292527
369	-1.19871	-1.19871	-1.19871
370	-0.78644	-0.786442	-0.786442
371	-0.79275	-0.792753	-0.792753
372	-0.2289	-0.228901	-0.228901
373	-0.44514	-0.44514	-0.44514
374	-6.80813	-6.808131	-6.808131
375	-1.5988	-1.598798	-1.598798
376	-7.69988	-7.699876	-7.699876
377	-1.46045	-1.460448	-1.460448
378	-4.43613	-4.436129	-4.436129
379	-7.06657	-7.066569	-7.066569
380	-8.72066	-8.720664	-8.720664
381	0.242308	0.242308	0.242308
382	-8.78412	-8.784117	-8.784117
383	-5.99909	-5.999093	-5.999093
384	-7.43025	-7.430249	-7.430249
385	-10.7939	-10.793929	-10.793929
386	-3.20305	-3.203048	-3.203048
387	-2.71726	-2.717264	-2.717264
388	0.13843	0.13843	0.13843
389	-11.5609	-11.560867	-11.560867
390	-1.50574	-1.505742	-1.505742
391	-2.81379	-2.813793	-2.813793
392	-4.31327	-4.313272	-4.313272
393	1.988842	1.988842	1.988842
394	-4.30965	-4.309649	-4.309649
395	0	0	0
396	-0.70935	-0.709351	-0.709351
397	-0.97311	-0.973113	-0.973113
398	-4.45834	-4.458343	-4.458343
399	-1.43258	-1.432584	-1.432584
400	-1.20831	-1.208314	-1.208314
401	-1.98701	-1.987009	-1.987009
402	-1.02444	-1.024442	-1.024442
403	-1.25895	-1.258948	-1.258948
404	-1.26372	-1.263719	-1.263719
405	-1.99668	-1.996684	-1.996684
406	-2.43517	-2.435165	-2.435165
407	-3.13814	-3.138138	-3.138138

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Seq	PBP3	PBP3_F533L	PBP3_T91A
408	-6.653034	-6.653034	-6.653034
409	-2.254355	-2.254355	-2.254355
410	4.586899	4.586899	4.586899
411	-2.289442	-2.289442	-2.289442
412	-1.249961	-1.249961	-1.249961
413	-0.827016	-0.827016	-0.827016
414	-0.597214	-0.597214	-0.597214
415	-2.953864	-2.953864	-2.953864
416	-3.031334	-3.031334	-3.031334
417	-2.382327	-2.382327	-2.382327
418	-3.74248	-3.74248	-3.74248
419	-4.595704	-4.595704	-4.595704
420	-4.313155	-4.313155	-4.313155
421	-5.080159	-5.080159	-5.080159
422	-5.448838	-5.448838	-5.448838
423	-5.485667	-5.485667	-5.485667
424	-5.429442	-5.429442	-5.429442
425	-4.648523	-4.648523	-4.648523
426	-4.962823	-4.962823	-4.962823
427	-6.796395	-6.796395	-6.796395
428	-7.698918	-7.698918	-7.698918
429	-14.024528	-14.024528	-14.024528
430	-2.61543	-2.61543	-2.61543
431	-4.674855	-4.674855	-4.674855
432	-1.221134	-1.221134	-1.221134
433	-5.952161	-5.952161	-5.952161
434	-0.449807	-0.449807	-0.449807
435	-1.134358	-1.134358	-1.134358
436	-1.336641	-1.336641	-1.336641
437	-1.060848	-1.060848	-1.060848
438	-0.498417	-0.498417	-0.498417
439	-0.945531	-0.945531	-0.945531
440	3.114027	3.114027	3.114027
441	-0.299822	-0.299822	-0.299822
442	-2.006474	-2.006474	-2.006474
443	-3.506724	-3.506724	-3.506724
444	-1.026674	-1.026674	-1.026674
445	4.032765	4.032765	4.032765
446	-0.861708	-0.861708	-0.861708
447	-0.351764	-0.351764	-0.351764
448	4.755366	4.755366	4.755366
449	-4.238696	-4.238696	-4.238696
450	-4.314508	-4.314508	-4.314508

Seq	PBP3	PBP3_F533L	PBP3_T91A
451	1.478508	1.478508	1.478508
452	2.303762	2.303762	2.303762
453	2.525182	2.525182	2.525182
454	1.589902	1.589902	1.589902
455	1.678883	1.678883	1.678883
456	0.626251	0.626251	0.626251
457	0.352052	0.352052	0.352052
458	1.692463	1.692463	1.692463
459	1.886061	1.886061	1.886061
460	1.106451	1.106451	1.106451
461	-0.42247	-0.422471	-0.422471
462	-0.022	-0.021997	-0.021997
463	0.851027	0.851027	0.851027
464	0.385104	0.385104	0.385104
465	-0.52478	-0.524777	-0.524777
466	-0.09252	-0.092524	-0.092524
467	3.442893	3.442893	3.442893
468	2.630651	2.630651	2.630651
469	2.699681	2.699681	2.699681
470	5.325842	5.325842	5.325842
471	-1.15804	-1.158036	-1.158036
472	2.386218	2.386218	2.386218
473	3.590479	3.590479	3.590479
474	1.91777	1.91777	1.91777
475	2.455356	2.455356	2.455356
476	-2.1303	-2.1303	-2.1303
477	-3.77526	-3.775264	-3.775264
478	-6.47322	-6.47322	-6.47322
479	-1.05531	-1.055305	-1.055305
480	-0.15195	-0.151952	-0.151952
481	-0.10035	-0.100346	-0.100346
482	1.422817	1.422817	1.422817
483	-6.76726	-6.767256	-6.767256
484	0.630942	0.630942	0.630942
485	-2.20765	-2.207646	-2.207646
486	5.41982	5.41982	5.41982
487	0.985268	0.985268	0.985268
488	1.587181	1.587181	1.587181
489	-0.1183	-0.1183	-0.1183
490	-1.84251	-1.842513	-1.842513
491	-2.1209	-2.120899	-2.120899
492	-1.64748	-1.647476	-1.647476
493	3.144405	3.144405	3.144405

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Seq	PBP3	PBP3_F533L	PBP3_T91A
494	2.471418	2.471418	2.471418
495	4.425303	4.425303	4.425303
496	0.369261	0.369261	0.369261
497	-3.33652	-3.33652	-3.33652
498	1.328067	1.328067	1.328067
499	2.567255	2.567255	2.567255
500	2.986002	2.986002	2.986002
501	4.643614	4.643614	4.643614
502	3.37398	3.37398	3.37398
503	4.332665	4.332665	4.332665
504	2.197811	2.197811	2.197811
505	1.592576	1.592576	1.592576
506	1.879388	1.879388	1.879388
507	1.253092	1.253092	1.253092
508	2.359178	2.359178	2.359178
509	4.215202	4.215202	4.215202
510	0.593611	0.593611	0.593611
511	-0.147788	-0.147788	-0.147788
512	-12.324711	-12.324711	-12.324711
513	0.431754	0.431754	0.431754
514	0.770053	0.770053	0.770053
515	0.870125	0.870125	0.870125
516	-3.931735	-3.931735	-3.931735
517	-1.466974	-1.466974	-1.466974
518	-1.17249	-1.17249	-1.17249
519	-0.819483	-0.819483	-0.819483
520	-2.195812	-2.195812	-2.195812
521	-4.14349	-4.14349	-4.14349
522	-4.978156	-4.978156	-4.978156
523	-4.839555	-4.839555	-4.839555
524	-3.086738	-3.086738	-3.086738
525	-1.21939	-1.21939	-1.21939
526	-0.747572	-0.747572	-0.747572
527	-4.753793	-4.753793	-4.753793
528	-1.21534	-1.21534	-1.21534
529	-2.780533	-2.780533	-2.780533
530	-1.061781	-1.061781	-1.061781
531	4.129931	4.129931	4.129931
532	-1.568366	-1.568366	-1.568366
533	0.46921	0.46921	0.46921
534	-6.955464	-6.955464	-6.955464
535	9.108323	9.108323	9.108323
536	8.081997	8.081997	8.081997
537	7.869197	7.869197	7.869197

Seq	PBP3	PBP3_F533L	PBP3_T91A
538	8.916662	8.916662	8.916662
539	7.576942	7.576942	7.576942
540	4.902357	4.902357	4.902357
541	4.795178	4.795178	4.795178
542	4.683833	4.683833	4.683833
543	3.082038	3.082038	3.082038
544	1.291142	1.291142	1.291142
545	0.261338	0.261338	0.261338
546	-0.62743	-0.627425	-0.627425
547	-1.00015	-1.000154	-1.000154
548	-0.23629	-0.236289	-0.236289
549	-2.85228	-2.852277	-2.852277
550	-4.49535	-4.495346	-4.495346
551	-4.65822	-4.658216	-4.658216
552	-3.17919	-3.179193	-3.179193
553	-5.26263	-5.262632	-5.262632
554	-8.47992	-8.479922	-8.479922
555	-3.56506	-3.565063	-3.565063
556	-7.5424	-7.542395	-7.542395
557	-4.69544	-4.695438	-4.695438
558	-3.90235	-3.902352	-3.902352
559	0	0	0