

ORIGINAL RESEARCH ARTICLE

Omicron variants of SARS CoV-2 indicate how small molecules can interfere with spike glycoprotein trimerization

Supplementary materials

Table S1. Shannon's entropy values per residue.

Position	Refseq	log Shannon index $\times 10^6$	7WZ1			
			Shannon index	Chain A	Chain B	Chain C
1	M	2.324872476	0.000102254	-	-	-
2	F	4.306246974	0.000741616	-	-	-
3	V	7.2666661	0.014317691	-	-	-
4	F	2.515666346	0.000123749	-	-	-
5	L	8.022047183	0.030474096	-	-	-
6	V	5.135662651	0.001699769	-	-	-
7	L	2.694935395	0.000148046	-	-	-
8	L	4.258423926	0.000706985	-	-	-
9	P	5.203559533	0.001819186	-	-	-
10	L	2.76924674	0.000159466	-	-	-
11	V	4.171423049	0.000648076	-	-	-
12	S	5.868178015	0.003536041	-	-	-
13	S	7.290713623	0.014666169	-	-	-
14	Q	5.311477874	0.002026495	-	-	-
15	C	3.7845506	0.000440159	-	-	-
16	V	4.787415979	0.001199909	-	-	-
17	N	3.987341708	0.000539114	-	-	-
18	L	7.364707082	0.015792528	-	-	-
19	T	10.08947495	0.240881416	-	-	-
20	T	7.276494838	0.01445911	-	-	-
21	R	5.548867334	0.002569464	-	-	-
22	T	5.955076824	0.003857065	-	-	-
23	Q	5.647588907	0.002836068	-	-	-
24	L	6.355573558	0.005756924	L	-	L
25	P	6.578343582	0.007193468	P	-	P
26	P	7.957308659	0.028563751	P	P	P
27	A	9.67135051	0.158567493	A	A	A
28	Y	5.085046088	0.001615874	Y	Y	Y
29	T	5.802371376	0.003310838	T	T	T
30	N	4.659955747	0.001056314	N	N	N
31	S	4.514099362	0.000912953	S	S	S
32	F	4.922337716	0.001373233	F	F	F
33	T	5.001891794	0.001486942	T	T	T

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
34	R	4.49012317	0.000891324	R	R	R
35	G	4.83626709	0.001259981	G	G	G
36	V	4.966994531	0.001435947	V	V	V
37	Y	5.312483886	0.002028535	Y	Y	Y
38	Y	5.369335051	0.0021472	Y	Y	Y
39	P	5.370251665	0.002149169	P	P	P
40	D	5.606140195	0.00272092	D	D	D
41	K	5.572155109	0.002630003	K	K	K
42	V	5.588874895	0.002674346	V	V	V
43	F	5.614776854	0.002744521	F	F	F
44	R	5.63136617	0.002790431	R	R	R
45	S	5.693698035	0.002969899	S	S	S
46	S	5.582084739	0.002656248	S	S	S
47	V	5.688445482	0.00295434	V	V	V
48	L	5.65251046	0.002850061	L	L	L
49	H	6.307387833	0.0054861	H	H	H
50	S	5.705596183	0.003005446	S	S	S
51	T	5.669720178	0.002899534	T	T	T
52	Q	6.568655852	0.007124116	Q	Q	Q
53	D	6.365047526	0.005811724	D	D	D
54	L	6.53029378	0.006855996	L	L	L
55	F	6.229573599	0.00507539	F	F	F
56	L	6.255792123	0.005210219	L	L	L
57	P	6.228304768	0.005068954	P	P	P
58	F	6.264594559	0.005256284	F	F	F
59	F	6.345428932	0.005698818	F	F	F
60	S	6.313701266	0.005520846	S	S	S
61	N	6.445896875	0.006301116	N	N	N
62	V	6.32798546	0.005600273	V	V	V
63	T	6.151053013	0.004692112	T	T	T
64	W	6.459804015	0.006389358	W	W	W
65	F	6.380284264	0.005900954	F	F	F
66	H	6.396995611	0.006000396	H	H	H
67	A	9.473808015	0.130143518	V	V	V
68	I	7.177439535	0.013095509	I	I	I
69	H	7.936007114	0.027961734	-	-	-
70	V	9.334080288	0.113172149	-	-	-
71	S	6.129749268	0.00459321	-	-	-
72	G	6.207976904	0.004966954	-	-	-
73	T	5.886963567	0.003603096	-	-	-

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
74	N	6.017101247	0.004103873	-	-	-
75	G	6.537388134	0.006904808	-	-	-
76	T	7.75417684	0.023312895	-	-	-
77	K	6.847627157	0.009416439	-	-	-
78	R	5.912651565	0.003696851	-	R	-
79	F	5.664609675	0.002884754	-	F	F
80	D	7.243952664	0.013996153	D	D	D
81	N	7.504321448	0.018158727	N	N	N
82	P	7.523708716	0.01851421	P	P	P
83	V	7.585483459	0.019693985	V	V	V
84	L	7.546187291	0.018935096	L	L	L
85	P	7.585252263	0.019689433	P	P	P
86	F	7.610445949	0.020191783	F	F	F
87	N	7.572809914	0.019445968	N	N	N
88	D	7.593511982	0.019852735	D	D	D
89	G	7.502420595	0.018124243	G	G	G
90	V	7.577043206	0.019528463	V	V	V
91	Y	7.553202648	0.019068399	Y	Y	Y
92	F	7.574990297	0.019488414	F	F	F
93	A	7.583492859	0.019654821	A	A	A
94	S	7.639678674	0.020790756	S	S	S
95	T	9.635671367	0.153009679	I	I	I
96	E	5.721587032	0.003053892	E	E	E
97	K	6.25729451	0.005218053	K	K	K
98	S	6.66645682	0.007856071	S	S	S
99	N	5.646061866	0.002831741	N	N	N
100	I	5.71485283	0.003033396	I	I	I
101	I	5.671599723	0.002904989	I	I	I
102	R	5.970564896	0.003917269	R	R	R
103	G	5.559959937	0.002598124	G	G	G
104	W	5.552654987	0.002579214	W	W	W
105	I	5.706174928	0.003007186	I	I	I
106	F	5.706491351	0.003008138	F	F	F
107	G	5.742065071	0.003117074	G	G	G
108	T	5.774818256	0.003220859	T	T	T
109	T	8.176109032	0.035549953	T	T	T
110	L	6.430982835	0.006207838	L	L	L
111	D	6.53901206	0.00691603	D	D	D
112	S	8.456329456	0.047047572	S	S	S
113	K	7.287830673	0.014623948	K	K	K

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
114	T	7.219035166	0.013651713	T	T	T
115	Q	7.32780785	0.015220416	Q	Q	Q
116	S	7.303301835	0.014851957	S	S	S
117	L	7.389903894	0.016195505	L	L	L
118	L	7.414049223	0.01659131	L	L	L
119	I	7.283556671	0.014561579	I	I	I
120	V	7.295336388	0.014734125	V	V	V
121	N	7.343129969	0.015455421	N	N	N
122	N	7.280753166	0.014520813	N	N	N
123	A	7.301045004	0.014818477	A	A	A
124	T	7.293581265	0.014708287	T	T	T
125	N	7.277283972	0.014470524	N	N	N
126	V	7.213121352	0.013571217	V	V	V
127	V	7.28318387	0.014556151	V	V	V
128	I	7.281931874	0.014537939	I	I	I
129	K	7.111503708	0.012259897	K	K	K
130	V	6.718791112	0.008278162	V	V	V
131	C	6.650733045	0.00773351	C	C	C
132	E	6.513667925	0.006742952	E	E	E
133	F	6.426233426	0.006178424	F	F	F
134	Q	6.560339656	0.007065116	Q	Q	Q
135	F	6.555692118	0.007032357	F	F	F
136	C	6.550120428	0.006993284	C	C	C
137	N	6.456983056	0.00637136	N	N	N
138	D	7.822425995	0.024959532	D	D	D
139	P	6.727656627	0.008351878	P	P	P
140	F	6.706542624	0.008177385	F	F	F
141	L	6.816831954	0.009130877	L	L	L
142	G	9.628752166	0.151954629	-	-	-
143	V	7.708250685	0.022266437	-	-	-
144	Y	7.367277199	0.015833169	-	-	-
145	Y	8.118438585	0.033557769	-	-	-
146	H	8.543237328	0.051319312	-	-	-
147	K	8.603320068	0.05449723	-	-	-
148	N	8.416251423	0.045199284	-	-	-
149	N	6.540570527	0.006926817	-	-	-
150	K	6.332473233	0.005625462	-	-	-
151	S	6.67428318	0.007917797	-	-	-
152	W	8.069399931	0.031951839	-	-	-
153	M	7.137845244	0.012587132	-	-	-

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
154	E	6.664173389	0.007838153	-	-	-
155	S	6.63908871	0.007643981	-	-	-
156	E	8.638013662	0.056421115	E	E	E
157	F	8.091339466	0.032660594	F	F	F
158	R	9.485350512	0.131654403	R	R	R
159	V	8.235946027	0.037742087	V	V	V
160	Y	8.209260717	0.036748247	Y	Y	Y
161	S	8.181067759	0.035726674	S	S	S
162	S	5.951773901	0.003844347	S	S	S
163	A	5.98180025	0.003961529	A	A	A
164	N	7.030956156	0.011311116	N	N	N
165	N	5.775924211	0.003224423	N	N	N
166	C	7.57799684	0.019547094	C	C	C
167	T	7.576269888	0.019513367	T	T	T
168	F	7.530483432	0.018640064	F	F	F
169	E	7.524973886	0.018537648	E	E	E
170	Y	7.543948066	0.018892743	Y	Y	Y
171	V	7.547093306	0.018952259	V	V	V
172	S	7.532320345	0.018674336	S	S	S
173	Q	7.628905916	0.020567985	Q	Q	Q
174	P	7.572577302	0.019441445	P	P	P
175	F	7.541388753	0.018844452	F	F	F
176	L	7.644583284	0.020892978	L	L	L
177	M	7.648010055	0.020964696	M	M	M
178	D	7.669455342	0.021419145	-	-	-
179	L	7.53984032	0.018815296	-	-	-
180	E	7.570079011	0.019392935	-	-	-
181	G	6.673043606	0.007907988	Q	Q	Q
182	K	6.039877934	0.004198418	G	G	G
183	Q	6.382383164	0.005913353	N	N	N
184	G	5.960753705	0.003879024	F	F	F
185	N	6.034796053	0.004177136	K	K	K
186	F	5.843066298	0.003448351	N	N	N
187	K	5.648928712	0.002839871	L	L	L
188	N	5.491404724	0.002425978	R	R	R
189	L	5.214665706	0.001839503	E	E	E
190	R	7.279232366	0.014498746	F	F	F
191	E	5.051889892	0.001563176	V	V	V
192	F	5.14775406	0.001720447	F	F	F
193	V	5.36800496	0.002144346	K	K	K

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
194	F	5.185213953	0.001786117	N	N	N
195	K	5.073003015	0.00159653	I	I	I
196	N	5.000505307	0.001484882	D	D	D
197	I	5.166955741	0.001753801	G	G	G
198	D	5.25917188	0.001923222	Y	Y	Y
199	G	5.019989321	0.001514097	F	F	F
200	Y	4.977553033	0.001451188	K	K	K
201	F	4.646927003	0.001042641	I	I	I
202	K	4.643039809	0.001038596	Y	Y	Y
203	I	4.550313112	0.00094662	S	S	S
204	Y	5.147559179	0.001720111	K	K	K
205	S	5.14006877	0.001707275	H	H	H
206	K	4.990857816	0.001470625	T	T	T
207	H	5.29724377	0.001997854	P	P	P
208	T	5.598157345	0.002699286	I	I	I
209	P	5.879710532	0.003577057	I	I	I
210	I	7.113081002	0.01227925	V	V	V
211	N	9.406439352	0.121664732	R	R	R
212	L	9.322628863	0.111883559	E	E	E
213	V	9.672689104	0.158779892	P	P	P
214	R	7.909822378	0.027239066	E	E	E
215	D	8.765582926	0.064097973	D	D	D
216	L	6.251711648	0.005189002	L	L	L
217	P	5.919274903	0.003721418	P	P	P
218	Q	5.911541163	0.003692748	Q	Q	Q
219	G	5.772021716	0.003211864	G	G	G
220	F	5.651015526	0.002845803	F	F	F
221	S	6.168167472	0.004773106	S	S	S
222	A	7.432533034	0.016900832	A	A	A
223	L	5.577892339	0.002645135	L	L	L
224	E	5.664905327	0.002885607	E	E	E
225	P	5.520215716	0.002496889	P	P	P
226	L	5.632370952	0.002793236	L	L	L
227	V	5.763872462	0.003185796	V	V	V
228	D	5.72266926	0.003057199	D	D	D
229	L	5.965789961	0.003898609	L	L	L
230	P	5.878101673	0.003571306	P	P	P
231	I	5.888237986	0.00360769	I	I	I
232	G	5.735489936	0.003096646	G	G	G
233	I	5.724362636	0.00306238	I	I	I

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
234	N	5.68208854	0.002935619	N	N	N
235	I	5.86892326	0.003538678	I	I	I
236	T	5.831402315	0.003408363	T	T	T
237	R	5.884062044	0.003592656	R	R	R
238	F	5.564569507	0.002610128	F	F	F
239	Q	5.647824861	0.002836738	Q	Q	Q
240	T	5.941626073	0.003805532	T	T	T
241	L	5.586656597	0.00266842	L	L	L
242	L	5.836869466	0.003427048	L	L	L
243	A	5.957848724	0.003867772	A	A	A
244	L	4.78990515	0.0012029	L	-	L
245	H	7.532039306	0.018669088	H	-	H
246	R	7.373836002	0.015937356	R	-	R
247	S	7.443459698	0.017086514	S	-	S
248	Y	7.544019827	0.018894099	-	-	-
249	L	7.358536351	0.015695376	-	-	-
250	T	7.38502055	0.016116609	-	-	-
251	P	7.548569234	0.018980252	-	-	-
252	G	7.389621547	0.016190932	-	-	-
253	D	8.120940313	0.033641826	-	-	-
254	S	7.469146847	0.017531104	-	-	-
255	S	7.705932848	0.022214887	-	-	-
256	S	7.540987459	0.018836892	-	-	-
257	G	8.581426596	0.053317063	-	-	-
258	W	8.513504397	0.0498159	-	-	-
259	T	8.482796577	0.048309411	-	-	-
260	A	7.657010033	0.021154229	-	-	-
261	G	7.711645846	0.022342164	G	-	G
262	A	7.744505708	0.02308852	A	A	A
263	A	7.632612487	0.020644363	A	A	A
264	A	7.673987648	0.021516444	A	A	A
265	Y	7.538071188	0.018782038	Y	Y	Y
266	Y	7.624918673	0.020486139	Y	Y	Y
267	V	8.531495183	0.050720238	V	V	V
268	G	7.584811183	0.01968075	G	G	G
269	Y	7.603801433	0.020058064	Y	Y	Y
270	L	7.546853122	0.018947707	L	L	L
271	Q	6.680342148	0.007965916	Q	Q	Q
272	P	6.673886106	0.007914654	P	P	P
273	R	6.566262758	0.007107088	R	R	R

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
274	T	6.506732331	0.006696347	T	T	T
275	F	6.424718635	0.006169072	F	F	F
276	L	6.414041202	0.006103553	L	L	L
277	L	6.348281084	0.005715095	L	L	L
278	K	6.391567325	0.005967912	K	K	K
279	Y	6.355541731	0.005756741	Y	Y	Y
280	N	6.41048819	0.006081905	N	N	N
281	E	6.577058994	0.007184233	E	E	E
282	N	6.591395578	0.007287973	N	N	N
283	G	6.660407116	0.007808688	G	G	G
284	T	6.755249741	0.008585541	T	T	T
285	I	6.776797369	0.008772547	I	I	I
286	T	6.775007022	0.008756855	T	T	T
287	D	6.827607555	0.0092298	D	D	D
288	A	6.4298139	0.006200585	A	A	A
289	V	6.989079997	0.010847231	V	V	V
290	D	6.357100847	0.005765724	D	D	D
291	C	6.556401599	0.007037348	C	C	C
292	A	6.55293752	0.007013012	A	A	A
293	L	6.546857998	0.006970506	L	L	L
294	D	6.370679929	0.005844551	D	D	D
295	P	6.382360177	0.005913217	P	P	P
296	L	6.350227378	0.005726229	L	L	L
297	S	6.185698372	0.004857521	S	S	S
298	E	6.394246219	0.005983921	E	E	E
299	T	6.531475394	0.006864102	T	T	T
300	K	6.546657875	0.006969111	K	K	K
301	C	6.68441404	0.007998419	C	C	C
302	T	6.674167819	0.007916884	T	T	T
303	L	6.65201105	0.0077434	L	L	L
304	K	6.535553042	0.006892148	K	K	K
305	S	6.549264149	0.006987298	S	S	S
306	F	6.463993667	0.006416184	F	F	F
307	T	6.542812612	0.006942365	T	T	T
308	V	6.47366088	0.006478511	V	V	V
309	E	6.402358905	0.006032664	E	E	E
310	K	6.385005033	0.005928877	K	K	K
311	G	6.37933312	0.005895344	G	G	G
312	I	6.552880987	0.007012616	I	I	I
313	Y	6.571368371	0.007143467	Y	Y	Y

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
314	Q	6.559766812	0.00706107	Q	Q	Q
315	T	6.487524086	0.006568949	T	T	T
316	S	6.443549584	0.006286342	S	S	S
317	N	6.502879444	0.006670596	N	N	N
318	F	6.567642881	0.007116903	F	F	F
319	R	6.93953009	0.01032285	R	R	R
320	V	6.940165143	0.010329408	V	V	V
321	Q	6.491006065	0.006591862	Q	Q	Q
322	P	6.264492757	0.005255749	P	P	P
323	T	6.494593285	0.006615551	T	T	T
324	E	6.343815501	0.005689631	E	E	E
325	S	6.302649135	0.005460165	S	S	S
326	I	6.293844467	0.005412301	I	I	I
327	V	6.4891686	0.006579761	V	V	V
328	R	4.203680179	0.000669322	R	R	R
329	F	4.207232349	0.000671704	F	F	F
330	P	4.856193317	0.00128534	P	P	P
331	N	4.229488102	0.000686821	N	N	N
332	I	4.218501253	0.000679316	I	I	I
333	T	4.23722857	0.000692158	T	T	T
334	N	4.343622555	0.000769859	N	N	N
335	L	4.477501106	0.000880145	L	L	L
336	C	4.273212619	0.000717518	C	C	C
337	P	4.521155309	0.000919418	P	P	P
338	F	4.717422028	0.001118795	F	F	F
339	G	9.71209493	0.165161659	D	D	D
340	E	5.194891483	0.001803486	E	E	E
341	V	4.917092574	0.001366049	V	V	V
342	F	4.970518258	0.001441015	F	F	F
343	N	5.139352777	0.001706053	N	N	N
344	A	5.470938235	0.002376831	A	A	A
345	T	5.15531855	0.00173351	T	T	T
346	R	9.651025548	0.155377146	R	R	R
347	F	4.964404383	0.001432232	F	F	F
348	A	5.431661523	0.002285286	A	A	A
349	S	5.004212291	0.001490396	S	S	S
350	V	4.511162241	0.000910276	V	V	V
351	Y	4.752625483	0.001158881	Y	Y	Y
352	A	4.870091897	0.001303329	A	A	A
353	W	5.068622904	0.001589553	W	W	W

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
354	N	5.220376531	0.001850038	N	N	N
355	R	5.63256199	0.00279377	R	R	R
356	K	6.653148263	0.007752211	K	K	K
357	R	5.787845651	0.003263093	R	R	R
358	I	5.688821082	0.00295545	I	I	I
359	S	5.796113402	0.003290183	S	S	S
360	N	5.742612375	0.003118781	N	N	N
361	C	5.932235309	0.003769963	C	C	C
362	V	5.9017298	0.003656695	V	V	V
363	A	5.868271669	0.003536372	A	A	A
364	D	5.368430968	0.00214526	D	D	D
365	Y	5.451357283	0.002330743	Y	Y	Y
366	S	5.549561122	0.002571247	S	S	S
367	V	5.991922018	0.00400183	V	V	V
368	L	6.088731794	0.00440862	L	L	L
369	Y	5.923122843	0.003735765	Y	Y	Y
370	N	6.392895567	0.005975844	N	N	N
371	S	10.13690325	0.252581273	L	L	L
372	A	6.464650773	0.006420401	A	A	A
373	S	9.689561392	0.1614816	P	P	P
374	F	6.454340716	0.006354546	F	F	F
375	S	9.696137585	0.162547034	F	F	F
376	T	9.6864882	0.160986098	T	T	T
377	F	6.307765089	0.00548817	F	F	F
378	K	6.066104101	0.004309983	K	K	K
379	C	5.838177098	0.003431532	C	C	C
380	Y	5.760627128	0.003175474	Y	Y	Y
381	G	5.563671741	0.002607786	G	G	G
382	V	5.739540968	0.003109217	V	V	V
383	S	5.332797968	0.002070164	S	S	S
384	P	5.558086675	0.002593262	P	P	P
385	T	5.70093876	0.002991481	T	T	T
386	K	5.202220626	0.001816752	K	K	K
387	L	5.275986327	0.001955833	L	L	L
388	N	5.228732976	0.001865563	N	N	N
389	D	5.306924634	0.002017289	D	D	D
390	L	5.236095115	0.001879348	L	L	L
391	C	5.182340493	0.001780992	C	C	C
392	F	5.198058551	0.001809207	F	F	F
393	T	5.109584428	0.001656015	T	T	T

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
394	N	5.301155817	0.002005685	N	N	N
395	V	5.17237597	0.001763333	V	V	V
396	Y	5.255854532	0.001916852	Y	Y	Y
397	A	5.305801384	0.002015024	A	A	A
398	D	5.219966593	0.00184928	D	D	D
399	S	5.148883658	0.001722391	S	S	S
400	F	5.206678435	0.001824869	F	F	F
401	V	5.207589421	0.001826532	V	V	V
402	I	5.239490314	0.00188574	I	I	I
403	R	5.25807264	0.001921109	R	R	R
404	G	5.202670612	0.00181757	G	G	G
405	D	9.654140888	0.155861953	D	D	D
406	E	5.42403291	0.002267919	E	E	E
407	V	5.67459564	0.002913705	V	V	V
408	R	9.660911431	0.156920804	R	R	R
409	Q	5.927042108	0.003750435	Q	Q	Q
410	I	7.05949555	0.011638579	I	I	I
411	A	7.213654139	0.01357845	A	A	A
412	P	7.146204292	0.01269279	P	P	P
413	G	7.234555546	0.013865245	G	G	G
414	Q	7.315545477	0.015034917	Q	Q	Q
415	T	7.301849018	0.014830396	T	T	T
416	G	7.418434683	0.01666423	G	G	G
417	K	9.837468183	0.187222546	N	N	N
418	I	7.463715895	0.017436151	I	I	I
419	A	7.489283245	0.017887695	A	A	A
420	D	7.450655843	0.017209915	D	D	D
421	Y	7.274212569	0.014426148	Y	Y	Y
422	N	7.223402234	0.013711461	N	N	N
423	Y	7.187504826	0.013227985	Y	Y	Y
424	K	7.204113969	0.013449525	K	K	K
425	L	7.24933535	0.014071693	L	L	L
426	P	7.243416575	0.013988651	P	P	P
427	D	7.491808457	0.017932923	D	D	D
428	D	7.248223131	0.014056051	D	D	D
429	F	7.227458664	0.013767193	F	F	F
430	T	7.250625315	0.014089856	T	T	T
431	G	7.232756676	0.013840326	G	G	G
432	C	7.541539082	0.018847285	C	C	C
433	V	7.578308363	0.019553185	V	V	V

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
434	I	7.530728125	0.018644626	I	I	I
435	A	7.505670801	0.018183246	A	A	A
436	W	7.485500333	0.017820155	W	W	W
437	N	7.455081575	0.01728625	N	N	N
438	S	6.56600062	0.007105225	S	S	S
439	N	7.17453193	0.013057488	N	N	N
440	N	9.762477071	0.173696042	K	K	K
441	L	7.158552466	0.012850494	L	L	L
442	D	7.156685325	0.012826523	D	D	D
443	S	7.092051879	0.012023724	S	S	S
444	K	8.775749207	0.064752935	K	K	K
445	V	7.348995171	0.015546336	V	V	V
446	G	9.451253125	0.127241002	S	S	S
447	G	6.845189579	0.009393513	G	G	G
448	N	6.74406519	0.008490051	N	N	N
449	Y	6.823428467	0.009191308	Y	Y	Y
450	N	7.243997517	0.01399678	N	N	N
451	Y	6.904989918	0.009972385	Y	Y	Y
452	L	9.988118435	0.217663055	L	L	L
453	Y	6.738649553	0.008444196	Y	Y	Y
454	R	6.744291365	0.008491971	R	R	R
455	L	6.808899076	0.00905873	L	L	L
456	F	6.791212489	0.00889992	F	F	F
457	R	6.87761675	0.009703111	R	R	R
458	K	6.907942419	0.010001872	K	K	K
459	S	6.882618712	0.009751767	S	S	S
460	N	8.680373489	0.058862446	N	N	N
461	L	6.576977554	0.007183648	L	L	L
462	K	6.629739792	0.007572851	K	K	K
463	P	6.127015009	0.004580668	P	P	P
464	F	5.91891557	0.003720081	F	F	F
465	E	5.967580177	0.003905594	E	E	E
466	R	5.983058593	0.003966517	R	R	R
467	D	5.907361818	0.003677347	D	D	D
468	I	5.930867627	0.00376481	I	I	I
469	S	5.878235898	0.003571786	S	S	S
470	T	6.184872857	0.004853513	T	T	T
471	E	6.331885707	0.005622158	E	E	E
472	I	5.783987757	0.003250528	I	I	I
473	Y	5.735956652	0.003098092	Y	Y	Y

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
474	Q	5.99129705	0.00399933	Q	Q	Q
475	A	6.446596995	0.006305529	A	A	A
476	G	6.64270204	0.007671651	G	G	G
477	S	9.696570828	0.162617471	N	N	N
478	T	9.470759702	0.129747404	K	K	K
479	P	6.745967064	0.008506213	P	P	P
480	C	6.534514385	0.006884994	C	C	C
481	N	6.508358792	0.006707247	N	N	N
482	G	6.437602049	0.006249065	G	G	G
483	V	6.552677321	0.007011188	V	V	V
484	E	9.822608664	0.184461077	A	A	A
485	G	6.45379205	0.006351061	G	G	G
486	F	9.535755575	0.138460542	F	F	F
487	N	6.291859557	0.005401568	N	N	N
488	C	6.222059875	0.005037398	C	C	C
489	Y	6.415903671	0.006114931	Y	Y	Y
490	F	7.176948637	0.013089082	F	F	F
491	P	6.476977931	0.006500036	P	P	P
492	L	6.48542739	0.006555191	L	L	L
493	Q	9.661216449	0.156968675	R	R	R
494	S	6.962078547	0.010558259	S	S	S
495	Y	6.469047234	0.00644869	Y	Y	Y
496	G	9.550673912	0.140541627	S	S	S
497	F	7.845226684	0.025535164	F	F	F
498	Q	9.791981585	0.178897211	R	R	R
499	P	7.871044592	0.026203013	P	P	P
500	T	7.871547432	0.026216192	T	T	T
501	N	9.72915682	0.168003806	Y	Y	Y
502	G	7.8511992	0.02568813	G	G	G
503	V	7.878272854	0.026393101	V	V	V
504	G	7.860003192	0.025915286	G	G	G
505	Y	9.78825135	0.178231125	H	H	H
506	Q	7.756035031	0.023356255	Q	Q	Q
507	P	7.718367585	0.022492848	P	P	P
508	Y	7.69462534	0.021965107	Y	Y	Y
509	R	7.401312499	0.016381331	R	R	R
510	V	5.911576152	0.003692878	V	V	V
511	V	5.943825196	0.00381391	V	V	V
512	V	6.074453687	0.00434612	V	V	V
513	L	6.160929352	0.004738683	L	L	L

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
514	S	6.224397848	0.005049189	S	S	S
515	F	6.162878462	0.004747928	F	F	F
516	E	6.240447041	0.005130878	E	E	E
517	L	6.261005041	0.005237451	L	L	L
518	L	6.209015429	0.004972115	L	L	L
519	H	6.213105059	0.00499249	H	H	H
520	A	6.537512504	0.006905667	A	A	A
521	P	6.533947584	0.006881092	P	P	P
522	A	6.827236776	0.009226378	A	A	A
523	T	6.499153614	0.006645789	T	T	T
524	V	6.417649247	0.006125614	V	V	V
525	C	6.450653488	0.006331159	C	C	C
526	G	6.482644264	0.006536972	G	G	G
527	P	6.512986597	0.006738359	P	P	P
528	K	6.534084374	0.006882034	K	K	K
529	K	4.274669281	0.000718564	K	K	K
530	S	3.549029	0.000347795	S	S	S
531	T	2.548321027	0.000127856	T	T	T
532	N	3.424495475	0.000307071	N	N	N
533	L	2.38823444	0.000108942	L	L	L
534	V	3.078150026	0.000217182	V	V	V
535	K	2.145575546	8.55×10^{-5}	K	K	K
536	N	2.551065195	0.000128208	N	N	N
537	K	1.981458193	7.25×10^{-5}	K	K	K
538	C	1.74223594	5.71×10^{-5}	C	C	C
539	V	2.300889941	9.98×10^{-5}	V	V	V
540	N	3.06561708	0.000214477	N	N	N
541	F	1.983003765	7.26×10^{-5}	F	F	F
542	N	1.921942814	6.83×10^{-5}	N	N	N
543	F	2.566589096	0.000130213	F	F	F
544	N	2.408344688	0.000111155	N	N	N
545	G	2.368310363	0.000106793	G	G	G
546	L	2.891439669	0.000180192	L	L	L
547	T	9.429792341	0.124539403	K	K	K
548	G	2.286686033	9.84×10^{-5}	G	G	G
549	T	3.376477434	0.000292675	T	T	T
550	G	2.039168316	7.68×10^{-5}	G	G	G
551	V	3.583342333	0.000359936	V	V	V
552	L	4.181285045	0.000654499	L	L	L
553	T	3.878911454	0.000483715	T	T	T

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
554	E	4.589515298	0.000984467	E	E	E
555	S	2.498109761	0.000121595	S	S	S
556	N	4.160454954	0.000641007	N	N	N
557	K	2.445802062	0.000115398	K	K	K
558	K	4.881126033	0.00131779	K	K	K
559	F	2.348351563	0.000104683	F	F	F
560	L	2.738643302	0.00015466	L	L	L
561	P	3.887719297	0.000487995	P	P	P
562	F	2.930293651	0.000187331	F	F	F
563	Q	2.725633938	0.000152661	Q	Q	Q
564	Q	3.031705008	0.000207326	Q	Q	Q
565	F	3.790488365	0.00044278	F	F	F
566	G	3.067056075	0.000214786	G	G	G
567	R	3.442917748	0.000312781	R	R	R
568	D	3.567747428	0.000354367	D	D	D
569	I	3.961783467	0.00052551	I	I	I
570	A	8.77387015	0.064631374	A	A	A
571	D	2.687034692	0.000146881	D	D	D
572	T	5.837363716	0.003428742	T	T	T
573	T	4.833673751	0.001256718	T	T	T
574	D	5.021726588	0.00151673	D	D	D
575	A	4.057445498	0.000578264	A	A	A
576	V	3.239909712	0.000255314	V	V	V
577	R	3.052420601	0.000211665	R	R	R
578	D	1.950347987	7.03×10^{-5}	D	D	D
579	P	2.348089855	0.000104656	P	P	P
580	Q	3.536803438	0.000343569	Q	Q	Q
581	T	2.293772808	9.91×10^{-5}	T	T	T
582	L	2.824705612	0.00016856	L	L	L
583	E	5.496073536	0.00243733	E	E	E
584	I	4.114287578	0.000612086	I	I	I
585	L	4.016455297	0.00055504	L	L	L
586	D	3.072797234	0.000216022	D	D	D
587	I	2.853071471	0.00017341	I	I	I
588	T	3.829659707	0.000460469	T	T	T
589	P	2.960710634	0.000193117	P	P	P
590	C	2.725633938	0.000152661	C	C	C
591	S	3.203662628	0.000246225	S	S	S
592	F	3.070671231	0.000215564	F	F	F
593	G	2.910655278	0.000183688	G	G	G

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
594	G	3.297714451	0.000270507	G	G	G
595	V	3.256631753	0.000259619	V	V	V
596	S	3.124580653	0.000227504	S	S	S
597	V	2.907001514	0.000183018	V	V	V
598	I	3.568935888	0.000354788	I	I	I
599	T	3.080157954	0.000217618	T	T	T
600	P	3.072326138	0.000215921	P	P	P
601	G	2.8388086	0.000170954	G	G	G
602	T	2.698347271	0.000148552	T	T	T
603	N	3.576081808	0.000357333	N	N	N
604	T	4.819434243	0.00123895	T	T	T
605	S	2.91995928	0.000185405	S	S	S
606	N	3.571546974	0.000355716	N	N	N
607	Q	4.382663003	0.000800509	Q	Q	Q
608	V	4.046168579	0.00057178	V	V	V
609	A	2.122261628	8.35×10^{-5}	A	A	A
610	V	2.254072171	9.53×10^{-5}	V	V	V
611	L	2.596651873	0.000134187	L	L	L
612	Y	2.585271286	0.000132669	Y	Y	Y
613	Q	6.1103404	0.00450492	Q	Q	Q
614	D	6.695558458	0.008088055	G	G	G
615	V	4.221382128	0.000681276	V	V	V
616	N	4.26761976	0.000713516	N	N	N
617	C	1.473605251	4.36×10^{-5}	C	C	C
618	T	4.187193691	0.000658378	T	T	T
619	E	5.683610335	0.00294009	E	E	E
620	V	2.271049199	9.69×10^{-5}	V	V	V
621	P	4.377170358	0.000796124	-	-	-
622	V	5.128306262	0.001687311	-	-	-
623	A	4.833084939	0.001255978	-	-	-
624	I	3.686287632	0.000398965	-	-	-
625	H	3.888461767	0.000488357	-	-	-
626	A	4.453162085	0.000858981	-	-	-
627	D	4.081901407	0.00059258	-	-	-
628	Q	5.107309026	0.001652251	-	-	-
629	L	3.012845024	0.000203452	-	-	-
630	T	3.441484356	0.000312333	-	-	-
631	P	4.462471737	0.000867015	-	-	-
632	T	4.664494423	0.001061119	-	-	-
633	W	3.662557165	0.000389608	-	-	-

Table S1. (Continued).

Position	Refseq	log Shannon index $\times 10^6$	7WZ1			
			Shannon index	Chain A	Chain B	Chain C
634	R	3.819603269	0.000455861	-	-	-
635	V	3.643375767	0.000382206	-	-	-
636	Y	3.208064324	0.000247312	-	-	-
637	S	3.165407504	0.000236984	-	-	-
638	T	3.765720371	0.000431948	-	-	-
639	G	3.407121006	0.000301782	-	-	-
640	S	5.345272811	0.002096151	-	-	-
641	N	4.284214637	0.000725455	N	N	N
642	V	4.343174393	0.000769514	V	V	V
643	F	4.608843045	0.00100368	F	F	F
644	Q	2.477844173	0.000119155	Q	Q	Q
645	T	2.722785075	0.000152227	T	T	T
646	R	4.167279723	0.000645396	R	R	R
647	A	4.607441871	0.001002274	A	A	A
648	G	2.991834569	0.000199222	G	G	G
649	C	2.851132116	0.000173074	C	C	C
650	L	2.852167336	0.000173253	L	L	L
651	I	3.875484906	0.000482061	I	I	I
652	G	2.972390966	0.000195386	G	G	G
653	A	5.196925257	0.001807157	A	A	A
654	E	5.05675764	0.001570804	E	E	E
655	H	9.646630168	0.154695703	Y	Y	Y
656	V	3.326864544	0.000278509	V	V	V
657	N	3.627518158	0.000376193	N	N	N
658	N	7.547255431	0.018955332	N	N	N
659	S	3.629355358	0.000376885	S	S	S
660	Y	3.878419604	0.000483477	Y	Y	Y
661	E	5.17566212	0.001769137	E	E	E
662	C	2.971468929	0.000195206	C	C	C
663	D	3.096850903	0.000221282	D	D	D
664	I	3.170818804	0.00023827	I	I	I
665	P	3.166731927	0.000237298	P	P	P
666	I	5.804349816	0.003317394	I	I	I
667	G	4.495346258	0.000895992	G	G	G
668	A	3.31560057	0.000275389	A	A	A
669	G	2.815564473	0.000167026	G	G	G
670	I	4.71280122	0.001113637	I	I	I
671	C	2.940050681	0.000189168	C	C	C
672	A	4.372715772	0.000792586	A	A	A
673	S	4.197084587	0.000664922	S	S	S

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
674	Y	3.644673773	0.000382703	Y	Y	Y
675	Q	6.317984981	0.005544546	Q	Q	Q
676	T	4.613857919	0.001008726	T	T	T
677	Q	7.153725125	0.01278861	-	-	-
678	T	5.688968092	0.002955884	-	-	-
679	N	9.679748284	0.159904714	-	-	-
680	S	6.280743528	0.005341857	-	-	-
681	P	9.880195377	0.195395399	-	-	-
682	R	5.416631181	0.002251195	-	-	-
683	R	4.653256014	0.001049261	-	-	-
684	A	6.094077359	0.004432249	-	-	-
685	R	5.441795722	0.002308564	-	-	-
686	S	4.785420951	0.001197518	-	-	-
687	V	4.899941184	0.001342819	-	-	-
688	A	6.333193389	0.005629514	-	-	-
689	S	5.065526565	0.001584639	S	S	S
690	Q	5.059500811	0.001575119	Q	Q	Q
691	S	5.296301916	0.001995973	S	S	S
692	I	4.65930479	0.001055627	I	I	I
693	I	4.519865528	0.000918232	I	I	I
694	A	5.070782724	0.00159299	A	A	A
695	Y	4.50940825	0.00090868	Y	Y	Y
696	T	4.477350188	0.000880012	T	T	T
697	M	8.117251506	0.033517957	M	M	M
698	S	8.129584174	0.033933882	S	S	S
699	L	8.10506905	0.033112103	L	L	L
700	G	8.103510945	0.033060551	G	G	G
701	A	8.568392388	0.052626627	A	A	A
702	E	4.509011592	0.00090832	E	E	E
703	N	8.854185821	0.070036437	N	N	N
704	S	9.158696064	0.09496666	S	S	S
705	V	4.289399379	0.000729227	V	V	V
706	A	6.50002727	0.006651598	A	A	A
707	Y	4.084665468	0.000594221	Y	Y	Y
708	S	4.121220266	0.000616344	S	S	S
709	N	4.41859747	0.000829798	N	N	N
710	N	4.150318677	0.000634542	N	N	N
711	S	3.932427495	0.000510307	S	S	S
712	I	4.877746499	0.001313344	I	I	I
713	A	4.73002919	0.001132989	A	A	A

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
714	I	4.865940277	0.001297929	I	I	I
715	P	4.731718345	0.001134904	P	P	P
716	T	8.775205586	0.064717743	T	T	T
717	N	3.60688855	0.000368512	N	N	N
718	F	3.432237233	0.000309458	F	F	F
719	T	4.908443802	0.001354285	T	T	T
720	I	4.071680099	0.000586554	I	I	I
721	S	4.531135891	0.00092864	S	S	S
722	V	4.506575739	0.00090611	V	V	V
723	T	5.648576688	0.002838871	T	T	T
724	T	4.375710614	0.000794963	T	T	T
725	E	3.916282348	0.000502134	E	E	E
726	I	4.12857671	0.000620895	I	I	I
727	L	3.828258526	0.000459824	L	L	L
728	P	3.963750072	0.000526544	P	P	P
729	V	4.281231895	0.000723295	V	V	V
730	S	5.171841201	0.00176239	S	S	S
731	M	4.899927073	0.0013428	M	M	M
732	T	7.004884064	0.011020023	T	T	T
733	K	4.347258734	0.000772664	K	K	K
734	T	4.359956205	0.000782537	T	T	T
735	S	4.793876861	0.001207687	S	S	S
736	V	4.497711622	0.000898114	V	V	V
737	D	4.18299081	0.000655616	D	D	D
738	C	4.07404218	0.000587941	C	C	C
739	T	4.891879289	0.001332037	T	T	T
740	M	4.92717346	0.001379889	M	M	M
741	Y	3.677431269	0.000395447	Y	Y	Y
742	I	3.743754122	0.000422563	I	I	I
743	C	3.919089311	0.000503546	C	C	C
744	G	4.141110506	0.000628726	G	G	G
745	D	4.323219825	0.000754311	D	D	D
746	S	3.962530611	0.000525902	S	S	S
747	T	5.316164755	0.002036015	T	T	T
748	E	4.162988233	0.000642633	E	E	E
749	C	3.968871328	0.000529248	C	C	C
750	S	4.078635389	0.000590648	S	S	S
751	N	4.115085286	0.000612574	N	N	N
752	L	4.79319637	0.001206865	L	L	L
753	L	3.549681121	0.000348022	L	L	L

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
754	L	4.39222778	0.000808203	L	L	L
755	Q	3.831403921	0.000461273	Q	Q	Q
756	Y	4.09214286	0.00059868	Y	Y	Y
757	G	4.040321342	0.000568446	G	G	G
758	S	4.147123869	0.000632518	S	S	S
759	F	3.962530611	0.000525902	F	F	F
760	C	4.190029714	0.000660248	C	C	C
761	T	4.549911318	0.00094624	T	T	T
762	Q	4.410355437	0.000822987	Q	Q	Q
763	L	4.514025656	0.000912886	L	L	L
764	N	9.666762334	0.157841624	K	K	K
765	R	5.229732932	0.001867429	R	R	R
766	A	4.341185174	0.000767985	A	A	A
767	L	4.184684934	0.000656728	L	L	L
768	T	4.184270092	0.000656456	T	T	T
769	G	5.638280919	0.002809793	G	G	G
770	I	3.860888867	0.000475076	I	I	I
771	A	4.877024624	0.001312396	A	A	A
772	V	4.066121944	0.000583303	V	V	V
773	E	3.238182293	0.000254874	E	E	E
774	Q	3.148859796	0.000233095	Q	Q	Q
775	D	3.166070158	0.000237141	D	D	D
776	K	3.240988392	0.00025559	K	K	K
777	N	3.166526606	0.000237249	N	N	N
778	T	4.249017158	0.000700365	T	T	T
779	Q	4.805079056	0.001221291	Q	Q	Q
780	E	5.396391339	0.002206089	E	E	E
781	V	4.134105053	0.000624337	V	V	V
782	F	4.074060274	0.000587952	F	F	F
783	A	4.589067216	0.000984026	A	A	A
784	Q	4.445527155	0.000852448	Q	Q	Q
785	V	4.472012861	0.000875327	V	V	V
786	K	4.320450458	0.000752225	K	K	K
787	Q	4.642525984	0.001038062	Q	Q	Q
788	I	4.312075384	0.000745951	I	I	I
789	Y	4.296952183	0.000734755	Y	Y	Y
790	K	4.29428697	0.000732799	K	K	K
791	T	5.48272134	0.002405003	T	T	T
792	P	4.217188868	0.000678425	P	P	P
793	P	4.578061342	0.000973255	P	P	P

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
794	I	3.970867215	0.000530305	I	I	I
795	K	4.096682006	0.000601404	K	K	K
796	D	9.657214213	0.156341705	Y	Y	Y
797	F	3.826383091	0.000458962	F	F	F
798	G	4.725322061	0.001127668	G	G	G
799	G	3.495799834	0.000329767	G	G	G
800	F	3.060186326	0.000213315	F	F	F
801	N	4.062386788	0.000581128	N	N	N
802	F	2.908321306	0.00018326	F	F	F
803	S	3.26639477	0.000262167	S	S	S
804	Q	3.81559588	0.000454038	Q	Q	Q
805	I	3.850071136	0.000469964	I	I	I
806	L	5.242280082	0.001891008	L	L	L
807	P	5.397728673	0.002209041	P	P	P
808	D	5.334304031	0.002073284	D	D	D
809	P	6.417472274	0.00612453	P	P	P
810	S	5.177629146	0.00177262	S	S	S
811	K	5.068310903	0.001589057	K	K	K
812	P	6.075387004	0.004350178	P	P	P
813	S	5.348049006	0.002101978	S	S	S
814	K	5.437426248	0.002298498	K	K	K
815	R	5.427877704	0.002276656	R	R	R
816	S	5.390399442	0.00219291	S	S	S
817	F	5.397321173	0.002208141	P	P	P
818	I	5.515306103	0.00248466	I	I	I
819	E	4.975947898	0.001448861	E	E	E
820	D	5.075505671	0.001600531	D	D	D
821	L	4.913304288	0.001360883	L	L	L
822	L	5.042480204	0.001548536	L	L	L
823	F	4.61055906	0.001005403	F	F	F
824	N	4.73156226	0.001134727	N	N	N
825	K	4.613021282	0.001007882	K	K	K
826	V	4.751084314	0.001157097	V	V	V
827	T	4.726778214	0.001129311	T	T	T
828	L	4.637351744	0.001032705	-	-	-
829	A	4.902807378	0.001346673	-	-	-
830	D	4.621439124	0.001016402	-	-	-
831	A	4.820830669	0.001240681	-	-	-
832	G	3.61568096	0.000371767	-	-	-
833	F	3.144139068	0.000231997	-	-	-

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
834	I	5.214861714	0.001839864	-	-	-
835	K	3.464143959	0.000319491	-	-	-
836	Q	4.3838345	0.000801448	-	-	-
837	Y	3.691848405	0.000401189	-	-	-
838	G	3.735995312	0.000419297	-	-	-
839	D	4.178144224	0.000652447	-	-	-
840	C	2.929335285	0.000187152	-	-	-
841	L	3.927766446	0.000507934	-	-	-
842	G	4.197411529	0.000665139	-	-	-
843	D	4.259167766	0.000707511	-	-	-
844	I	4.073541271	0.000587647	-	-	-
845	A	5.691877776	0.002964498	-	-	-
846	A	4.91942162	0.001369234	-	-	-
847	R	3.563467423	0.000352853	R	R	R
848	D	2.595307495	0.000134007	D	D	D
849	L	3.18171246	0.00024088	L	L	L
850	I	4.061690892	0.000580724	I	I	I
851	C	3.809964671	0.000451488	C	C	C
852	A	4.389881876	0.000806309	A	A	A
853	Q	3.68069758	0.000396741	Q	Q	Q
854	K	4.207870931	0.000672133	K	K	K
855	F	3.686628792	0.000399101	F	F	F
856	N	9.415833204	0.122813018	K	K	K
857	G	3.836068584	0.000463429	G	G	G
858	L	4.659063675	0.001055372	L	L	L
859	T	6.800226149	0.008980504	T	T	T
860	V	3.741241921	0.000421503	V	V	V
861	L	2.930841196	0.000187434	L	L	L
862	P	3.414906882	0.000304141	P	P	P
863	P	3.252687279	0.000258597	P	P	P
864	L	3.269481331	0.000262977	L	L	L
865	L	7.230056494	0.013803005	L	L	L
866	T	3.231007908	0.000253051	T	T	T
867	D	3.794735463	0.000444665	D	D	D
868	E	3.636342026	0.000379528	E	E	E
869	M	3.635138364	0.000379071	M	M	M
870	I	4.36409029	0.000785779	I	I	I
871	A	4.539748584	0.000936672	A	A	A
872	Q	3.306341525	0.000272851	Q	Q	Q
873	Y	3.320958281	0.000276869	Y	Y	Y

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
874	T	3.607097664	0.000368589	T	T	T
875	S	3.299563975	0.000271008	S	S	S
876	A	3.40919366	0.000302409	A	A	A
877	L	3.222907046	0.00025101	L	L	L
878	L	3.261277223	0.000260828	L	L	L
879	A	6.191774386	0.004887125	A	A	A
880	G	3.290264601	0.0002685	G	G	G
881	T	3.505369279	0.000332937	T	T	T
882	I	3.905853039	0.000496925	I	I	I
883	T	5.086087885	0.001617558	T	T	T
884	S	4.300380898	0.000737279	S	S	S
885	G	3.529585377	0.000341098	G	G	G
886	W	3.838319802	0.000464474	W	W	W
887	T	3.276906337	0.000264937	T	T	T
888	F	4.931031122	0.001385223	F	F	F
889	G	2.840721776	0.000171281	G	G	G
890	A	3.418136555	0.000305125	A	A	A
891	G	2.92121314	0.000185638	G	G	G
892	A	4.655087542	0.001051184	P	P	P
893	A	3.6621391	0.000389446	A	A	A
894	L	2.596344854	0.000134146	L	L	L
895	Q	2.840721776	0.000171281	Q	Q	Q
896	I	3.136425346	0.000230214	I	I	I
897	P	2.463053125	0.000117406	P	P	P
898	F	2.580339251	0.000132016	F	F	F
899	A	4.694476865	0.001093416	P	P	P
900	M	3.22004944	0.000250294	M	M	M
901	Q	2.8388086	0.000170954	Q	Q	Q
902	M	3.152343018	0.000233908	M	M	M
903	A	3.481507259	0.000325087	A	A	A
904	Y	3.312566506	0.000274555	Y	Y	Y
905	R	4.122141953	0.000616912	R	R	R
906	F	3.260666951	0.000260669	F	F	F
907	N	3.353181981	0.000285936	N	N	N
908	G	3.238793663	0.000255029	G	G	G
909	I	3.800167071	0.000447087	I	I	I
910	G	3.132111277	0.000229223	G	G	G
911	V	3.440791259	0.000312116	V	V	V
912	T	3.270976514	0.00026337	T	T	T
913	Q	3.449509539	0.000314849	Q	Q	Q

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
914	N	3.334768505	0.000280719	N	N	N
915	V	3.463648983	0.000319333	V	V	V
916	L	3.238182293	0.000254874	L	L	L
917	Y	3.481017714	0.000324928	Y	Y	Y
918	E	3.633240393	0.000378352	E	E	E
919	N	3.305644111	0.000272661	N	N	N
920	Q	3.339872156	0.000282155	Q	Q	Q
921	K	3.278013096	0.00026523	K	K	K
922	L	4.465802302	0.000869908	L	L	L
923	I	3.353978694	0.000286164	I	I	I
924	A	3.994828438	0.000543165	A	A	A
925	N	4.15098718	0.000634967	N	N	N
926	Q	3.583349926	0.000359939	Q	Q	Q
927	F	2.951108623	0.000191271	F	F	F
928	N	2.891488016	0.000180201	N	N	N
929	S	4.771737474	0.001181243	S	S	S
930	A	3.56875805	0.000354725	A	A	A
931	I	3.758580673	0.000428875	I	I	I
932	G	4.45736791	0.000862602	G	G	G
933	K	3.408625609	0.000302237	K	K	K
934	I	4.05311787	0.000575767	I	I	I
935	Q	3.254957193	0.000259185	Q	Q	Q
936	D	5.861434673	0.003512277	D	D	D
937	S	3.678999811	0.000396068	S	S	S
938	L	5.232232014	0.001872102	L	L	L
939	S	7.106731886	0.012201534	S	S	S
940	S	6.880923861	0.009735253	S	S	S
941	T	6.842617234	0.009369381	T	T	T
942	A	5.947807793	0.00382913	P	P	P
943	S	4.454223732	0.000859894	S	S	S
944	A	3.683455292	0.000397836	A	A	A
945	L	3.705749983	0.000406805	L	L	L
946	G	4.732991428	0.00113635	G	G	G
947	K	3.958187328	0.000523623	K	K	K
948	L	3.679502667	0.000396267	L	L	L
949	Q	3.94324317	0.000515856	Q	Q	Q
950	D	9.357297692	0.115830453	D	D	D
951	V	3.696819016	0.000403188	V	V	V
952	V	3.82774071	0.000459586	V	V	V
953	N	3.124529096	0.000227492	N	N	N

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
954	Q	9.655461481	0.15606792	H	H	H
955	N	3.283295155	0.000266635	N	N	N
956	A	3.313164281	0.000274719	A	A	A
957	Q	6.474877586	0.006486398	Q	Q	Q
958	A	3.612320005	0.000370519	A	A	A
959	L	3.276539791	0.00026484	L	L	L
960	N	3.587611864	0.000361476	N	N	N
961	T	4.582669606	0.000977751	T	T	T
962	L	3.373734814	0.000291873	L	L	L
963	V	2.888783044	0.000179714	V	V	V
964	K	3.811417951	0.000452145	K	K	K
965	Q	2.515151631	0.000123685	Q	Q	Q
966	L	2.444297116	0.000115224	L	L	L
967	S	3.261742402	0.00026095	S	S	S
968	S	3.325905573	0.000278242	S	S	S
969	N	9.651548825	0.155458473	K	K	K
970	F	2.387931841	0.000108909	F	F	F
971	G	2.408892216	0.000111216	G	G	G
972	A	2.349409552	0.000104794	A	A	A
973	I	2.308617188	0.000100605	I	I	I
974	S	2.195828236	8.99×10^{-5}	S	S	S
975	S	2.388780138	0.000109002	S	S	S
976	V	2.64186624	0.000140394	V	V	V
977	L	1.951346494	7.04×10^{-5}	L	L	L
978	N	4.400165398	0.000814643	N	N	N
979	D	2.589571885	0.000133241	D	D	D
980	I	2.286686033	9.84×10^{-5}	I	I	I
981	L	9.411994674	0.1223425	F	F	F
982	S	8.76140408	0.063830676	S	S	S
983	R	4.545048984	0.00094165	R	R	R
984	L	4.529596431	0.000927211	L	L	L
985	D	4.528274311	0.000925986	D	D	D
986	K	4.618064709	0.001012978	P	P	P
987	V	3.26237679	0.000261115	P	P	P
988	E	2.347036652	0.000104545	E	E	E
989	A	2.148502468	8.57×10^{-5}	A	A	A
990	E	3.091117383	0.000220016	E	E	E
991	V	2.170698259	8.76×10^{-5}	V	V	V
992	Q	2.239518914	9.39×10^{-5}	Q	Q	Q
993	I	2.574056792	0.000131189	I	I	I

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
994	D	2.121120669	8.34×10^{-5}	D	D	D
995	R	2.219157163	9.20×10^{-5}	R	R	R
996	L	2.194744746	8.98×10^{-5}	L	L	L
997	I	2.562688148	0.000129706	I	I	I
998	T	2.617005614	0.000136947	T	T	T
999	G	2.839848741	0.000171132	G	G	G
1000	R	2.595307495	0.000134007	R	R	R
1001	L	2.549397848	0.000127994	L	L	L
1002	Q	2.870935579	0.000176535	Q	Q	Q
1003	S	3.069239019	0.000215255	S	S	S
1004	L	2.480830895	0.000119512	L	L	L
1005	Q	3.129906772	0.000228718	Q	Q	Q
1006	T	3.984059295	0.000537347	T	T	T
1007	Y	2.462610059	0.000117354	Y	Y	Y
1008	V	2.547937939	0.000127807	V	V	V
1009	T	4.476957615	0.000879666	T	T	T
1010	Q	2.935972786	0.000188398	Q	Q	Q
1011	Q	2.862823358	0.000175109	Q	Q	Q
1012	L	2.802185538	0.000164806	L	L	L
1013	I	2.768547403	0.000159355	I	I	I
1014	R	3.717203108	0.000411491	R	R	R
1015	A	2.550164478	0.000128092	A	A	A
1016	A	3.785344678	0.000440509	A	A	A
1017	E	2.411520269	0.000111509	E	E	E
1018	I	2.777990771	0.000160867	I	I	I
1019	R	2.349917204	0.000104847	R	R	R
1020	A	6.586975866	0.007255833	A	A	A
1021	S	3.10878829	0.000223939	S	S	S
1022	A	2.742225828	0.000155215	A	A	A
1023	N	3.233078651	0.000253576	N	N	N
1024	L	2.971236163	0.00019516	L	L	L
1025	A	3.972533418	0.000531189	A	A	A
1026	A	3.701678472	0.000405153	A	A	A
1027	T	7.152043804	0.012767126	T	T	T
1028	K	2.426614132	0.000113205	K	K	K
1029	M	2.669304436	0.000144299	M	M	M
1030	S	2.61256363	0.00013634	S	S	S
1031	E	2.463053125	0.000117406	E	E	E
1032	C	2.684395293	0.000146493	C	C	C
1033	V	2.987183417	0.000198298	V	V	V

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
1034	L	2.899693113	0.000181686	L	L	L
1035	G	2.698729718	0.000148608	G	G	G
1036	Q	2.497423023	0.000121511	Q	Q	Q
1037	S	2.952136814	0.000191468	S	S	S
1038	K	2.480600535	0.000119484	K	K	K
1039	R	2.148502468	8.57×10^{-5}	R	R	R
1040	V	3.85487012	0.000472225	V	V	V
1041	D	3.31418649	0.000275	D	D	D
1042	F	2.388780138	0.000109002	F	F	F
1043	C	2.349917204	0.000104847	C	C	C
1044	G	2.463053125	0.000117406	G	G	G
1045	K	4.019019076	0.000556465	K	K	K
1046	G	2.95238783	0.000191516	G	G	G
1047	Y	3.912778149	0.000500378	Y	Y	Y
1048	H	3.051081244	0.000211382	H	H	H
1049	L	3.904311913	0.000496159	L	L	L
1050	M	3.867054656	0.000478014	M	M	M
1051	S	2.498109761	0.000121595	S	S	S
1052	F	3.281989295	0.000266287	F	F	F
1053	P	2.42736234	0.00011329	P	P	P
1054	Q	2.17054282	8.76×10^{-5}	Q	Q	Q
1055	S	2.383885561	0.00010847	S	S	S
1056	A	2.349140482	0.000104766	A	A	A
1057	P	2.041248108	7.70×10^{-5}	P	P	P
1058	H	3.931559061	0.000509864	H	H	H
1059	G	2.094899037	8.12×10^{-5}	G	G	G
1060	V	2.714554427	0.000150979	V	V	V
1061	V	2.455981002	0.000116579	V	V	V
1062	F	2.807305729	0.000165652	F	F	F
1063	L	4.355985499	0.000779436	L	L	L
1064	H	1.781407909	5.94×10^{-5}	H	H	H
1065	V	3.543387061	0.000345839	V	V	V
1066	T	2.813574565	0.000166694	T	T	T
1067	Y	2.374844441	0.000107493	Y	Y	Y
1068	V	3.754947659	0.00042732	V	V	V
1069	P	3.166232734	0.00023718	P	P	P
1070	A	5.294709519	0.001992797	A	A	A
1071	Q	4.522013814	0.000920207	Q	Q	Q
1072	E	4.577545251	0.000972753	E	E	E
1073	K	5.530194545	0.00252193	K	K	K

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
1074	N	5.625675497	0.002774596	N	N	N
1075	F	3.077457086	0.000217031	F	F	F
1076	T	3.503319461	0.000332256	T	T	T
1077	T	2.636917917	0.000139701	T	T	T
1078	A	5.64562139	0.002830494	A	A	A
1079	P	4.281920482	0.000723793	P	P	P
1080	A	2.017882584	7.52×10^{-5}	A	A	A
1081	I	4.264504962	0.000711297	I	I	I
1082	C	1.47476977	4.37×10^{-5}	C	C	C
1083	H	3.867370052	0.000478165	H	H	H
1084	D	5.125575115	0.001682709	D	D	D
1085	G	4.778294126	0.001189013	G	G	G
1086	K	3.353939714	0.000286152	K	K	K
1087	A	4.55454769	0.000950637	A	A	A
1088	H	3.108241385	0.000223816	H	H	H
1089	F	2.338874915	0.000103696	F	F	F
1090	P	2.457618167	0.00011677	P	P	P
1091	R	4.758598899	0.001165825	R	R	R
1092	E	3.853166949	0.000471421	E	E	E
1093	G	2.040117571	7.69×10^{-5}	G	G	G
1094	V	3.206378052	0.000246895	V	V	V
1095	F	2.482834943	0.000119752	F	F	F
1096	V	3.531124089	0.000341623	V	V	V
1097	S	2.331258215	0.000102909	S	S	S
1098	N	2.087632837	8.07×10^{-5}	N	N	N
1099	G	3.881348581	0.000484896	G	G	G
1100	T	2.871971655	0.000176718	T	T	T
1101	H	5.713935531	0.003030614	H	H	H
1102	W	3.046721266	0.000210462	W	W	W
1103	F	3.003309112	0.000201521	F	F	F
1104	V	6.616828317	0.007475703	V	V	V
1105	T	1.304306908	3.69×10^{-5}	T	T	T
1106	Q	1.773939422	5.89×10^{-5}	Q	Q	Q
1107	R	3.461449645	0.000318631	R	R	R
1108	N	2.242589225	9.42×10^{-5}	N	N	N
1109	F	3.216991766	0.000249529	F	F	F
1110	Y	2.488752055	0.000120462	Y	Y	Y
1111	E	4.360007635	0.000782577	E	E	E
1112	P	3.631717341	0.000377776	P	P	P
1113	Q	4.475144551	0.000878073	Q	Q	Q

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
1114	I	4.530038573	0.000927621	I	I	I
1115	I	3.488726732	0.000327442	I	I	I
1116	T	4.388445155	0.000805151	T	T	T
1117	T	5.589301654	0.002675487	T	T	T
1118	D	8.769157026	0.064327475	D	D	D
1119	N	2.520126286	0.000124302	N	N	N
1120	T	3.910980684	0.000499479	T	T	T
1121	F	4.282599881	0.000724285	F	F	F
1122	V	5.329824809	0.002064018	V	V	V
1123	S	4.202151962	0.0006683	S	S	S
1124	G	5.512377512	0.002477394	G	G	G
1125	N	3.640151042	0.000380976	N	N	N
1126	C	2.407841424	0.0001111	C	C	C
1127	D	3.987935401	0.000539434	D	D	D
1128	V	3.469930627	0.000321345	V	V	V
1129	V	3.594517974	0.000363982	V	V	V
1130	I	4.051632789	0.000574913	I	I	I
1131	G	3.134513588	0.000229775	G	G	G
1132	I	4.039646386	0.000568063	I	I	I
1133	V	4.492252539	0.000893224	V	V	V
1134	N	3.199251525	0.000245142	N	N	N
1135	N	3.217358761	0.000249621	N	N	N
1136	T	3.715858542	0.000410939	T	T	T
1137	V	3.456722201	0.000317129	V	V	V
1138	Y	2.953958914	0.000191817	Y	Y	Y
1139	D	4.912591073	0.001359913	D	D	D
1140	P	4.893474013	0.001334163	P	P	P
1141	L	3.791150794	0.000443074	L	L	L
1142	Q	3.172738722	0.000238728	Q	Q	Q
1143	P	4.89234374	0.001332655	P	P	P
1144	E	4.290859894	0.000730292	E	E	E
1145	L	2.319124564	0.000101668	L	L	L
1146	D	4.96410247	0.0014318	D	D	D
1147	S	4.978130333	0.001452026	S	S	S
1148	F	2.121298749	8.34×10^{-5}	-	-	-
1149	K	3.226794425	0.000251988	-	-	-
1150	E	4.36748433	0.00078845	-	-	-
1151	E	3.386700477	0.000295682	-	-	-
1152	L	1.88615616	6.59×10^{-5}	-	-	-
1153	D	4.914467311	0.001362467	-	-	-

Table S1. (Continued).

Position	Refseq	log Shannon index $\times 10^6$	7WZ1			
			Shannon index	Chain A	Chain B	Chain C
1154	K	2.853072266	0.00017341	-	-	-
1155	Y	3.375372736	0.000292352	-	-	-
1156	F	2.354687437	0.000105348	-	-	-
1157	K	3.033728388	0.000207745	-	-	-
1158	N	2.504986732	0.000122434	-	-	-
1159	H	3.760465002	0.000429684	-	-	-
1160	T	2.721910522	0.000152094	-	-	-
1161	S	2.973362524	0.000195576	-	-	-
1162	P	6.305378327	0.005475087	-	-	-
1163	D	5.118650753	0.001671097	-	-	-
1164	V	4.977269807	0.001450778	-	-	-
1165	D	4.030227604	0.000562737	-	-	-
1166	L	2.897160873	0.000181226	-	-	-
1167	G	5.398594909	0.002210955	-	-	-
1168	D	4.709519448	0.001109988	-	-	-
1169	I	4.264724134	0.000711453	-	-	-
1170	S	4.740998771	0.001145486	-	-	-
1171	G	4.287828195	0.000728082	-	-	-
1172	I	3.828615759	0.000459988	-	-	-
1173	N	3.897513492	0.000492798	-	-	-
1174	A	4.362467417	0.000784505	-	-	-
1175	S	3.812489925	0.00045263	-	-	-
1176	V	7.251572356	0.014103206	-	-	-
1177	V	4.813565431	0.0012317	-	-	-
1178	N	4.09141911	0.000598247	-	-	-
1179	I	3.873473148	0.000481092	-	-	-
1180	Q	4.166991546	0.000645211	-	-	-
1181	K	4.382917253	0.000800713	-	-	-
1182	E	4.463936145	0.000868286	-	-	-
1183	I	4.104738907	0.000606269	-	-	-
1184	D	4.692091843	0.001090811	-	-	-
1185	R	4.464664382	0.000868919	-	-	-
1186	L	3.720430375	0.000412822	-	-	-
1187	N	4.245414559	0.000697847	-	-	-
1188	E	3.600995192	0.000366347	-	-	-
1189	V	3.490694433	0.000328087	-	-	-
1190	A	2.611317636	0.00013617	-	-	-
1191	K	7.470739994	0.017559056	-	-	-
1192	N	3.59074276	0.00036261	-	-	-
1193	L	1.952392499	7.05×10^{-5}	-	-	-

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
1194	N	2.252404673	9.51×10^{-5}	-	-	-
1195	E	4.111996044	0.000610685	-	-	-
1196	S	2.571730541	0.000130885	-	-	-
1197	L	2.978014751	0.000196488	-	-	-
1198	I	3.467377575	0.000320526	-	-	-
1199	D	5.331073601	0.002066597	-	-	-
1200	L	3.842045535	0.000466207	-	-	-
1201	Q	5.076553549	0.001602209	-	-	-
1202	E	5.20352909	0.001819131	-	-	-
1203	L	4.003679102	0.000547994	-	-	-
1204	G	2.545581038	0.000127506	-	-	-
1205	K	4.074209243	0.00058804	-	-	-
1206	Y	2.980197556	0.000196917	-	-	-
1207	E	4.323515879	0.000754534	-	-	-
1208	Q	4.761829243	0.001169597	-	-	-
1209	Y	2.864194817	0.000175349	-	-	-
1210	I	3.587934989	0.000361593	-	-	-
1211	K	2.597929764	0.000134359	-	-	-
1212	W	2.627011571	0.000138324	-	-	-
1213	P	3.276372179	0.000264795	-	-	-
1214	W	3.277954012	0.000265215	-	-	-
1215	Y	3.197798966	0.000244786	-	-	-
1216	I	3.990964448	0.00054107	-	-	-
1217	W	2.937132767	0.000188617	-	-	-
1218	L	2.826691846	0.000168895	-	-	-
1219	G	5.923043975	0.003735471	-	-	-
1220	F	2.845085842	0.00017203	-	-	-
1221	I	4.332540668	0.000761375	-	-	-
1222	A	3.499879702	0.000331115	-	-	-
1223	G	3.769914752	0.000433764	-	-	-
1224	L	4.169110616	0.000646579	-	-	-
1225	I	4.620289623	0.001015234	-	-	-
1226	A	3.776238914	0.000436516	-	-	-
1227	I	4.279556015	0.000722084	-	-	-
1228	V	5.704927064	0.003003436	-	-	-
1229	M	5.539321804	0.002545053	-	-	-
1230	V	4.479927145	0.000882282	-	-	-
1231	T	4.433821709	0.000842528	-	-	-
1232	I	4.031488725	0.000563447	-	-	-
1233	M	4.443275438	0.000850531	-	-	-

Table S1. (Continued).

7WZ1						
Position	Refseq	log Shannon index $\times 10^6$	Shannon index	Chain A	Chain B	Chain C
1234	L	3.880003778	0.000484244	-	-	-
1235	C	4.86573255	0.00129766	-	-	-
1236	C	4.568657954	0.000964146	-	-	-
1237	M	5.544452364	0.002558144	-	-	-
1238	T	5.01597974	0.001508038	-	-	-
1239	S	5.253070023	0.001911522	-	-	-
1240	C	5.165201183	0.001750727	-	-	-
1241	C	5.164434248	0.001749385	-	-	-
1242	S	5.327174667	0.002058555	-	-	-
1243	C	5.702099418	0.002994955	-	-	-
1244	L	5.301492259	0.00200636	-	-	-
1245	K	5.254540424	0.001914335	-	-	-
1246	G	5.237663453	0.001882298	-	-	-
1247	C	5.553301632	0.002580883	-	-	-
1248	C	4.966678045	0.001435492	-	-	-
1249	S	5.437344887	0.002298311	-	-	-
1250	C	5.116283534	0.001667146	-	-	-
1251	G	5.215977599	0.001841918	-	-	-
1252	S	5.538529317	0.002543037	-	-	-
1253	C	4.704252564	0.001104157	-	-	-
1254	C	4.641199487	0.001036686	-	-	-
1255	K	4.603899452	0.00099873	-	-	-
1256	F	3.653733679	0.000386186	-	-	-
1257	D	4.00267681	0.000547445	-	-	-
1258	E	4.746480091	0.001151782	-	-	-
1259	D	4.97549566	0.001448206	-	-	-
1260	D	5.645852553	0.002831148	-	-	-
1261	S	4.54986055	0.000946192	-	-	-
1262	E	4.346030327	0.000771715	-	-	-
1263	P	6.038369105	0.004192088	-	-	-
1264	V	6.851520509	0.009453172	-	-	-
1265	L	5.556983428	0.002590402	-	-	-
1266	K	4.602840119	0.000997673	-	-	-
1267	G	4.592683895	0.000987591	-	-	-
1268	V	3.936509265	0.000512394	-	-	-
1269	K	3.393470298	0.000297691	-	-	-
1270	L	3.426917053	0.000307816	-	-	-
1271	H	1.542513541	4.68×10^{-5}	-	-	-
1272	Y	2.194113236	8.97×10^{-5}	-	-	-
1273	T	3.654493955	0.00038648	-	-	-

Table S2. PISA identified residues in the major contact patch of the A-B PPI from the 7WZ1 structure ASA and BSA are, respectively, solvent-accessible, and buried surface areas in Å²; ΔⁱG is the solvation energy effect in kcal/mol; values in parenthesis refer to the buried area percentage. Red cells highlight residues contributing to the formation of a pocket defined by EPOS-BP in the contact patch.

Residue in contact	ASA	BSA*	ΔⁱG
A: VAL785	18.20	2.09 (20)	-0.02
A: LYS786	103.37	18.69 (20)	0.02
A: GLN787	116.42	55.12 (50)	-0.46
A: ILE788	76.55	59.46 (80)	0.58
A: TYR789	54.57	39.86 (80)	0.63
A: LYS790	155.55	82.03 (60)	-0.79
A: PRO792	52.77	37.67 (80)	0.60
A: ILE794	67.39	0.74 (10)	-0.01
A: TYR796	178.17	36.24 (30)	0.16
A: PHE797	21.19	18.72 (90)	0.30
A: GLY798	21.34	4.39 (30)	-0.02
A: GLY880	1.18	0.17 (20)	0.00
A: ILE882	4.29	2.61 (70)	-0.01
A: THR883	44.81	44.03 (100)	0.27
A: SER884	4.61	2.51 (60)	0.04
A: TRP886	89.48	21.66 (30)	0.19
A: THR887	31.74	9.38 (30)	0.15
A: GLY889	42.54	21.73 (60)	-0.12
A: ALA890	100.77	90.43 (90)	0.65
A: GLY891	38.89	11.02 (30)	0.17
A: PRO892	102.10	61.99 (70)	0.99
A: ALA893	46.34	24.05 (60)	0.16
A: LEU894	98.31	85.62 (90)	1.37
A: GLN895	171.44	153.05 (90)	-0.59
A: ILE896	37.66	22.90 (70)	0.17
A: PRO897	79.13	74.63 (100)	1.19
A: PHE898	9.73	9.57 (100)	0.01
A: MET900	76.55	71.38 (100)	1.72
B: LEU699	172.88	149.54 (90)	1.79
B: GLY700	49.13	15.00 (40)	0.21
B: ALA701	103.40	45.98 (50)	0.09
B: GLU702	167.63	49.61 (30)	0.22
B: ASN703	128.72	83.23 (70)	-0.06
B: SER704	100.43	23.43 (30)	0.37
B: VAL705	135.92	119.57 (90)	1.31
B: ALA706	88.93	18.45 (30)	-0.02
B: TYR707	201.54	166.46 (90)	1.41
B: SER708	51.64	7.61 (20)	-0.09
B: ASN709	149.39	34.78 (30)	-0.40
B: SER711	50.61	38.28 (80)	-0.09
B: ILE712	49.88	42.57 (90)	0.67
B: ALA713	60.18	53.51 (90)	0.40

Table S3. Hydrogen bonds between protomer A and B in the same contact patch.

A: PHE43 [N]	3.18	B: PHE565 [O]
A: LYS856 [NZ]	2.61	B: THR572 [OG1]
A: GLY283 [O]	3.89	B: GLN563 [NE2]
A: LYS41 [O]	3.26	B: GLN564 [N]
A: LYS41 [O]	3.54	B: PHE565 [N]
A: PHE43 [O]	3.08	B: ARG567 [N]

Table S4. Best 10 potential trimer disruptors of the spike glycoprotein.

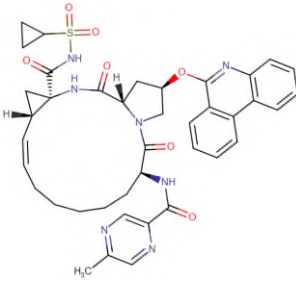
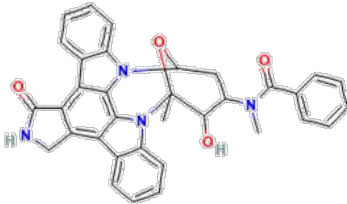
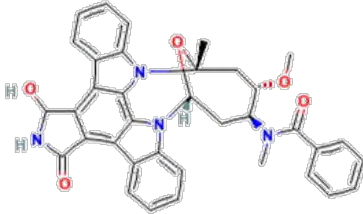
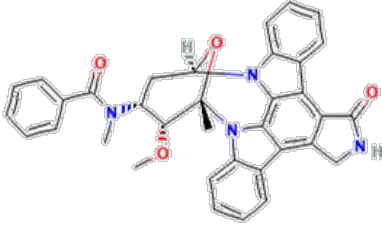
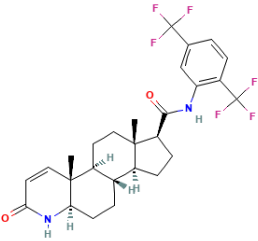

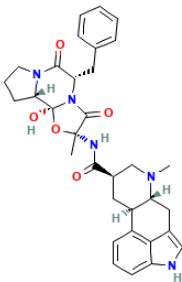
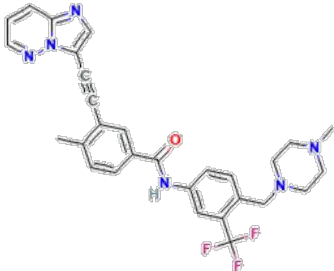
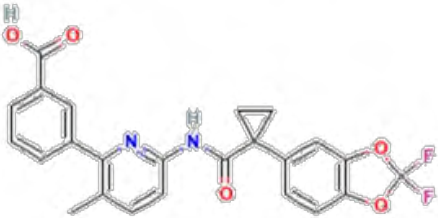
Best candidate-ligand ranking	Compound	2D structure
1	Paritaprevir	
2	O-desmethyl midostaurin	
3	CGP52421	
4	Midostaurin	
5	Dutasteride	

Table S4. (Continued).

Best candidate-ligand ranking	Compound	2D structure
6	Bendroflumethiazide	
7	Dihydroergotamine	
8	Ponatinib	
9	Lumacaftor	
10	Clofazimine	