

SUPPLEMENTARY TABLE S2. EXOTIC BHB DONOR/ACCEPTOR RESIDUES OF VIRAL GLYCOPROTEINS

Bourbon Virus Glycoprotein Env Postfusion (5ZKX)

Chain A

90–94% 189/185 117/93 168/171 140/97 144/121 109/105 155/254 239/241 98/139 145/48 445/127
 95–98% 253/271 358/341 **68/57** 101/137
 99% 348/351 414/240 9/5
 100% 44/148 **103/135** 106/101 116/93 238/207 349/351

Chikugunkya Virus Glycoprotein E1–E2–E3 Prefusion (3N41)

Chain A

90–94% 18/6
 95–98%
 99%
 100% 13/10

Chain B

90–94% 58/61 245/F58 44/154 158/260 334/330 237/170 96/102 150/268 109/131 196/192 189/217 236/11 130/109
 116/123
 95–98% 31/17 27/23 16/51 55/98 75/71
 99% 240/237 99/54 280/282 98/100
 100% 23/26 72/74 74/71 88/89 92/85 118/120 166/163 185/187 200/209 283/279 300/304 F258/301

Chain F

90–94% 160/156 157/159 252/184 109/74 370/372 125/175 373/369 381/361 248/243 203/199 **85/100** 102/61 77/73
89/91 60/103
 95–98% 323/348 263/267 382/306 273/257 321/350 138/140 129/39
 99% 315/356 88/227
 100% **101/98** 151/163 161/281 258/B301 268/262

Dengue Virus Glycoprotein E-M Prefusion (3J2P)

Chain A

90–94% 405/400 390/378 382/336 242/249 263/258 187/284 **74/112** 86/82 430/427 366/363 468/463 349/339 119/66
 61/219 181/291 22/287
 95–98% 412/407 443/438 335/300 411/406 250/241 41/38 189/186 252/239 410/405 180/175 286/23 433/428 190/186
 330/327 233/220 447/441 163/139 78/75 341/377 50/136
 99% 488/482 120/89 176/179 484/479 280/277 463/458 481/476 394/374 492/487 136/132 216/212 346/343 433/429
 490/485
 100% 9/6 21/16 29/26 62/123 79/76 87/83 91/87 **104/100 106/101** 126/59 156/153 179/175 182/173 183/288 199/128
 202/204 215/211 262/257 265/261 277/272 284/25 287/184 290/19 308/325 321/369 326/307 328/305 345/342 395/
 373 396/373 398/395 400/396 401/396 404/399 408/403 413/408 415/412 416/411 420/416 421/417 434/429 434/
 428 435/430 436/431 439/434 447/443 448/444 451/9 461/456 469/464 475/472 477/473 479/475 483/479 489/484
 493/489 493/488 494/489

Chain B

90–94% 49/45 48/43 54/49 52/47
 95–98%
 99% 51/46 31/26 46/41
 100% 35/30 53/48 59/56 60/56 68/63 71/66

Dengue Virus Glycoprotein E Postfusion (1OK8)

Chain A

90–94% 284/25 161/141 298/6 392/376 382/336 334/358 245/247 363/326 303/334 119/66 202/204 354/368 **106/ 100**
 95–98% 324/310 179/175 342/345
 99% 166/168 316/319 274/276 37/293
 100% 15/18 176/179 180/175 239/234 268/264 375/393 386/383 387/383

Dhori Virus Glycoprotein G_p Postfusion (5XEB)

Chain A

90–94% 188/191 160/117 **121/157** 94/71 175/281 118/159
 95–98% 32/29 64/168
 99% 164/141
 100% 137/113

(continued)

SUPPLEMENTARY TABLE S2. (CONTINUED)

Eastern Equine Encephalitis Virus Glycoprotein E1–E2 and Capsid C-terminal Prefusion (6MX4)

Chain A

90–94% 280/5 182/184 55/52 120/48 310/382 330/345 171/168 78/75 123/178 218/203 319/303 60/103 256/251
6/1 118/113 255/251 306/316
95–98% 65/99 328/347 253/185 162/282 282/3 424/419 302/320 315/312 271/261 B337/389 322/351
99% 259/B298 84/98 257/252 201/197
100% 4/281 4/2 14/11 18/15 77/73 88/228 89/91 105/79 141/137 142/137 146/133 153/150 184/181 185/181 230/226
244/239 246/242 316/357 356/317 371/373 389/386 412/408 416/411 422/417

Chain B

90–94% 373/368 28/25 243/A58 249/246 230/227 411/408 **96/98** 33/29 77/65 381/376 201/222 319/278 42/151 180/
186 279/276 285/312 225/198 **94/100** 404/400 358/353 182/184
95–98% 234/11 25/22 73/69 104/43 282/274 315/282 14/233 180/177 337/A389
99% 195/228 **90/83** 280/276 160/157 241/237
100% 16/50 18/29 23/25 24/21 57/60 65/54 65/61 70/72 75/67 **82/78 86/87** 151/148 198/206 235/167 255/162 277/279
293/306 297/301 370/365 403/400 251/396

Chain C

90–94% 246/249 229/240 185/182 107/102 242/253 118/142 138/160 124/116 122/118 189/191 225/216
95–98% 131/174 234/236 187/193 119/121
99%
100% 133/130 143/117 157/161 161/156 162/156 215/211 230/240 235/236 240/200 251/B396

Ebola Virus Glycoprotein GP Prefusion (5JQ3)

Chain A

90–94% 186/36 100/164 115/143 71/178 160/179 266/260 43/39 477/276 173/123
95–98% 40/42 226/144 144/112 133/175 238/240 475/274 145/222
99% 237/240 192/189 101/65
100% 111/139 174/111 B511/73

Chain B

90–94% **531/527**
95–98% 599/594 622/617 555/551
99% 628/623
100% 511/A73

***Epstein–Barr Virus Glycoprotein gp350 Prefusion (2H6O)**

Chain A

90–94% 197/218 193/190 83/62 405/351 227/245 420/403 54/124 148/16 249/261 142/10 55/57 47/66 101/313 128/51
362/357 135/138 235/19 121/117 272/177 80/64 422/401 15/143 279/303
95–98% 385/388 397/394 208/204 17/145 334/389 432/428 210/202 33/30 260/257 86/112
99% 176/178 46/133 389/385 223/220
100% 44/41 58/54 73/69 74/69 98/101 194/191 195/192 209/23 234/210 243/267 277/273 314/311 339/336 355/38

Hanta Virus Glycoprotein G_c Postfusion with scFv A5 (5LJY)

Chain A

90–94% 216/224 336/411 222/239 162/164 313/310 361/398 45/19 22/44 318/315 388/368 364/366 319/314 290/287
253/250
95–98% 293/285 63/33 379/349 **95/91** 301/298 179/181 227/223 396/408
99% 46/51 50/47
100% 74/229 288/290 335/340 337/388 412/333

Hanta Virus Glycoprotein G_c Postfusion (5LJZ)

Chain A

90–94% 336/411 162/164 361/398 288/290 400/402 379/349 378/353 174/185 388/368 79/137 274/270 222/239 **127/**
113 316/17
95–98% 240/219 216/224 63/33 175/171 364/366 315/179
99% 229/236 412/333 227/223
100% 74/229 179/181 205/202 **253/118** 335/340 396/408

***Hendra Virus Glycoprotein G Receptor Bound (2VSK)**

Chain A

90–94% 453/445 490/529 232/251 226/228 409/370 481/466 190/598 535/556 463/497 572/568 410/399 291/287
465/485 293/285 375/371 359/361 480/477 269/252 371/408 528/534 496/529

(continued)

SUPPLEMENTARY TABLE S2. (CONTINUED)

95–98% 385/382 589/215 558/581 352/365 432/411 413/366 521/515 316/295 542/544 194/546 484/542 257/264
 99% 471/476 515/520 265/256 288/290 520/516 391/387
 100% 245/237 255/266 345/342 347/369 362/358 368/349 376/372 440/409 448/450 477/471 507/122 516/520 562/
 508 569/571

Chain B

90–94% 103/81 102/81 46/42 69/107
 95–98% 51/46
 99% 130/118 80/104 44/41133/167
 100% 47/50 79/143 99/95

Hendra Virus Glycoprotein F Prefusion (5EJB)

Chain A

90–94% 320/322 321/290 293/318 224/221 439/435 396/419 307/303 197/192 361/358 262/256 42/295 184/178 415/
 430 285/50 235/231 283/53 46/336 271/275 70/66 **123/120** 323/319 384/412
 95–98% 304/306 276/270 335/337 326/346 450/365 431/381 301/374 30/356 303/408
 99% 82/77
 100% 166/163 238/232 264/281 360/354 373/370 383/379 395/399 417/413 418/413 425/422 477/472

HIV Glycoprotein gp41 Prefusion (6MTJ)

Chain B

90–94% 583/578 627/622
 95–98% **532/623 543/538** 624/619
 99%
 100% **531/626**

Influenza Virus D Glycoprotein HEF Prefusion (5E64)

Chain A

90–94% 155/103 382/399 44/367 278/127 356/359 34/414 393/406 130/277 407/390 82/53 B75/402 305/155 288/210
 41/384 378/385 17/27 221/307 248/260 295/246 106/152 54/79 159/302 22/B101 403/B74
 95–98% 182/93 425/24 215/217 193/199 200/192 38/391 B25/10
 99% B18/11 69/65 72/58
 100% 12/B15 70/65 122/327 127/174 173/178 178/172 179/175 205/293 261/247 270/231 312/148 342/B77 354/357
 355/359 358/C28 374/370 382/397 404/377 358/C28

Chain B

90–94% 145/142 75/A402 A22/102 A403/74
 95–98% 48/45 **25/10**
 99% **18/A11**
 100% **16/A9** 40/29 135/138 **A12/15** A342/77

Chain C

90–94% 82/53 183/93 250/258 288/210 9/D26 295/246 72/58 305/155 155/103 205/293 41/384 130/277 215/217 179/
 175 200/192 22/D102 106/152
 95–98% 248/260 159/302 69/65 34/414 178/172 193/199 261/247 38/391 221/307 54/79 127/174
 99% 278/127 70/65
 100% 12/D15 109/50 122/327 173/178 182/93 274/270 312/148 12/D15

Chain D

90–94% C9/26
 95–98%
 99%
 100% C12/15

***Lassa Fever Virus Glycoprotein GPI Receptor Bound (4ZJF)**

Chain B

90–94% 202/214 87/231 103/225 169/218 197/191
 95–98% 216/170 156/117
 99% 162/158 211/207 99/101
 100% 199/79 97/228

Lymphatic Choriomeningitis Virus Glycoprotein GPC Prefusion (5INE)

Chain A

90–94% 311/306 **298/286** 104/106 74/379 248/244 233/166 **293/78** 368/362 166/162 69/72 391/376 382/71 161/122
 95–98% 381/385

(continued)

SUPPLEMENTARY TABLE S2. (CONTINUED)

99% 201/196 401/393 168/161

100% 73/68 96/98 105/85 162/167 208/364 210/365 249/244 **300/283** 348/343 396/398

Measles Virus Glycoprotein F Prefusion (5YXW)

Chain A

90–94% 74/B343 69/65

95–98% B280/56 53/B283 27/B359

99%

100% 102/B115 B286/49

Chain B

90–94% A47/343 230/267 307/309 444/409 241/235 232/265 274/278 326/322 188/182 398/402 **126/123**

95–98% 418/433 383/385 338/335 280/A56 187/182 363/357 235/230 53/283 27/359 338/340 310/306

99% 323/325 279/273 400/422

100% 286/49 295/291 329/349 373/370 434/384 **A102/115**

***Measles Virus Glycoprotein H Receptor Bound (3ALX)**

Chain A

90–94% 595/592 601/579 98/106 359/291 388/383 40/138 262/269 486/496 574/576 387/382 444/355 552/542 37/334
455/468 213/208 392/388 411/430 315/312 273/203

95–98% 106/45 593/590 111/41 77/66 232/220 427/414 338/319 548/544 115/111 44/107

99% 274/257 307/349 365/357 383/378 472/477 225/227 125/127 86/83 592/589 460/463 75/72 441/438

100% 54/51 104/99 117/135 204/270 214/210 215/209 229/258 287/301 293/295 313/310 357/289 463/459 464/459
478/471 482/467 493/489 494/491 499/483 518/523 588/591

MERS Virus Spike Glycoprotein Prefusion Conformation 1 (5X5C)

Chain A

90–94% 981/976 440/576 59/278 169/185 91/300 506/514 934/803 1152/778 1036/1031 493/391 302/208 329/332
256/266 148/171 400/396 273/268 280/267 325/337 297/146 824/819 1032/1027 246/178 991/987 215/210 1143/786
343/696 305/93 1037/1031 198/190 454/450 539/558 384/408 399/395 292/150

95–98% 913/908 94/96 1125/1139 522/470 907/676 301/88 320/75 54/50 127/123 108/104 185/239 76/319 113/291
133/130 674/660 508/512 939/936 1181/1178 669/664 1137/793 375/372 372/604 584/581 1035/1030 117/256 392/
490 164/154

99% 1109/1103 1131/1133 857/854 370/688 1192/1189 855/850 1042/1037 970/779 809/805

100% 131/136 175/179 179/174 180/174 187/235 195/199 214/209 337/50 354/351 375/605 376/597 389/385 408/583
470/464 519/466 551/546 552/546 599/596 609/611 651/618 670/664 741/761 759/721 765/762 773/859 798/795
799/796 808/810 870/866 986/983 987/984 1020/1016 1107/1102 1118/1114 1146/1143 1157/1203 1158/1159 1167/
1192 1173/1177

MERS Virus Spike Glycoprotein Prefusion Conformation 2 (5X5F)

Chain A

90–94% 981/976 351/346 59/278 169/185 320/75 91/300 506/514 934/803 1152/778 1036/1031 493/391 302/208 329/
332 256/266 478/426 148/171 400/396 273/268 280/267 297/146 824/819 1032/1027 246/178 522/470 991/987 215/
210 1143/786 305/93 1037/1031 198/190 113/291 407/583 454/450 539/558 384/408 399/395 292/150

95–98% 347/342 913/908 94/96 1125/1139 907/C676 80/48 301/88 54/50 127/123 108/104 185/239 133/130 674/660
508/512 939/936 1181/1178 669/664 1137/793 375/372 372/604 1035/1030 117/256 392/490 164/154

99% 1109/1103 857/854 370/688 1192/1189 855/850 1042/1037 585/438 970/C779 809/805

100% 131/136 175/179 179/174 180/174 187/235 195/199 214/209 337/50 353/348 375/605 376/597 389/385 470/464
519/466 551/546 552/546 584/439 599/596 609/611 651/618 670/664 741/761 759/721 765/762 773/B859 798/795
799/796 808/810 870/866 986/983 987/984 1020/1016 1107/1102 1118/1114 1131/1133 1146/1143 1157/1203 1158/
1159 1167/1192 1173/1177

***MERS Virus Spike Glycoprotein Receptor Bound (4L72)**

Chain A

90–94% 466/462 575/541 492/489 592/ 587 621/540 668/663 687/683 572/567 649/624 303/314 580/525 509/41 104/
117 585/552 485/489 214/197 545/625 654/628 633/629 76/72

95–98% 523/519 109/113 541/618 739/735 137/141 318/322 405/382 463/467 412/414 477/453 308/310 629/651 430/
455 153/130 456/474 355/320 520/522

99% 260/662 210/204 159/163 307/310 332/336 455/450 322/319 195/190 262/258

100% 64/67 65/67 81/85 124/127 191/194 197/170 209/203 218/222 344/340 366/370 378/381 426/422 436/441 458/
429 464/64 489/484 552/582 558/427 560/473 574/567 583/ 590 597/670 624/620 680/673 681/675

(continued)

SUPPLEMENTARY TABLE S2. (CONTINUED)

Chain B

90–94% 498/561 508/512 440/576 401/445 503/557
 95–98% 522/470 468/463 470/464
 99%
 100% 408/583 416/411 417/411 519/466 552/546 584/581

Metapneumovirus Glycoprotein F Prefusion (5WB0)

Chain F

90–94% 264/266 313/282 380/376 393/401 62/180 309/286 174/168 29/24 257/272 418/393 413/378 281/37 262/268
 338/40 314/316 214/210 284/35 407/384 39/333 30/24 434/19 175/169
 95–98% 43/275 333/329 310/320 330/332 373/383 389/385 417/393
 99% 377/379
 100% 25/29 167/51 443/26

†Metapneumovirus Glycoprotein F Postfusion (5L1X)

Chain A

90–94% 48/D433 B334/36 79/74 88/B260 B284/35
 95–98% B281/37 B279/39 30/24 66/63
 99% 25/29
 100% 36/B283 39/B333

Chain B

90–94% 334/A36 421/423 258/214 220/F208 413/378 174/168 394/417 454/451 284/A35 407/384 309/286 218/252
 373/383
 95–98% 302/366 314/316 354/349 281/A37 303/291 155/150 175/169 279/A39 213/207 251/247
 99% 252/247 372/F315 158/153
 100% 264/266 333/329 377/379 417/393 A36/283 A39/333 D372/315

***Mumps Virus Glycoprotein HN Prefusion (5B2C)**

Chain A

90–94% 323/378 385/316 259/242 179/198 483/541 409/307 315/317 518/529 197/180 211/235
 95–98% 561/573 304/325 375/326 231/214 308/321 549/553 138/217 301/297 395/295 572/562 137/189 B168/171
 99% 569/174 391/386
 100% 168/B171 221/224 250/252 283/286 310/408 406/375 411/310 417/413 455/452 462/509 468/509 542/480 548/
 143

Human Coronavirus Spike Glycoprotein Prefusion (5I08)

Chain A

90–94% 427/367 82/240 1132/1146 650/B55 272/275 1146/799 720/692 807/1139 215/199 434/431 716/718 805/802
 402/398 660/646 671/632 678/306 462/459 1114/1109 413/408 581/455 99/233 283/280 1131/1146 606/354 768/741
 137/151 263/67 463/574 262/101 1115/1109 814/942 78/256 583/585 200/214 72/40 221/48 613/318 341/437
 95–98% 1000/995 234/127 1001/996 626/319 1052/B832 1062/1058 117/114 695/717 690/680 745/736 826/822 1007/
 1002 661/665 158/18 320/623 88/26 205/100 823/820 742/B949 345/341 328/353 112/118
 99% 828/823 396/579 1138/1140 291/286 79/256 941/936
 100% 17/156 47/218 55/51 59/271 95/91 96/91 109/196 143/145 146/142 230/207 280/43 375/B1064 414/408 415/409
 416/409 449/444 586/582 600/626 605/381 621/631 651/654 728/764 739/742 767/729 817/813 827/823 927/923
 937/932 973/968 1061/1057 1116/1110

†Murine Coronavirus Spike Glycoprotein Postfusion (6B30)

Chain A

90–94% 1235/1231 750/1125 805/800 1153/1149 776/773 800/796 1176/B755 C1176/755 1143/1170 1175/1138
 95–98% 1134/1137 1165/1155 1122/754 767/1108 1085/1079 1236/1231 1121/754
 99% 1208/1203 755/1121 1110/1106
 100% 782/776 1092/1096 1107/1109 1150/1152 1159/1143 1181/757 1200/780 C1181/757 C1200/780

***Newcastle Virus Glycoprotein HN Prefusion Complexed With Thiosialoside (1USX)**

Chain A

90–94% 473/527 276/247 223/210 225/208 554/551 253/236 378/384 205/229 547/559 539/535 405/304 298/319 178/
 188 560/546 133/129 285/272 436/432 292/287 535/539 162/159 249/241 136/132
 95–98% 182/184 452/495 428/413 528/470 130/211 129/183 B217/230
 99% 456/452 555/169 540/534 368/364 408/410 215/218 550/523 505/489 294/290 275/282
 100% 456/452 555/169 540/534 368/364 408/410 215/218 550/523 505/489 294/290 275/282

(continued)

SUPPLEMENTARY TABLE S2. (CONTINUED)

***Newcastle Virus Glycoprotein HN Prefusion (3T1E)**

Chain A

90–94% 301/314 408/137 136/132 311/307 319/296 472/526 276/279 210/221 451/494 457/494 377/383 274/281
 561/543 236/251 142/475 479/482 517/500 491/501 493/499 133/129
 95–98% 549/522 284/271 474/487 190/174 305/239 185/208 524/497 402/300 504/488 399/368 404/303 535/131
 158/561
 99% 534/538 533/135 201/197 482/478
 100% 180/185 182/183 186/179 197/192 243/245 303/401 364/360 396/391 455/451 507/509 539/533 550/553
 554/549 555/B551 B555/551

Chain B

90–94% 402/300 545/527 527/469 377/383 136/132 444/423 305/239 185/208 372/315 319/296 426/441 214/217
 533/135 485/476 301/314 474/487 201/197 243/245 197/193
 95–98% 479/482 534/538 195/170 158/561 467/417 408/137 357/352 554/549 404/303
 99% 432/434 523/548 435/431 451/494 504/488 134/130 327/323
 100% 180/185 182/183 186/179 197/192 210/221 224/207 252/236 292/287 295/291 358/353 395/391 399/368
 424/443 455/451 472/526 507/509 536/131 539/533 550/553 555/A551 A555/551

Chain E

90–94% 86/81 102/97
 95–98%
 99%
 100% 89/85 98/93

Chain F

90–94%
 95–98% 93/87
 99%
 100% 86/82 100/95 104/99

†Newcastle Virus Glycoprotein F Postfusion (3MAW)

Chain A

90–94% 54/347 316/308 234/269 437/425 432/429 402/406 245/239 247/244 368/365 394/382 94/89 284/63
 95–98% 83/78 333/353 288/59 327/329 329/326
 99% 401/428 165/160 50/343 47/302 474/469 342/344 41/37
 100% 187/182 189/184 278/282 367/361 387/389

***Nipah Virus Glycoprotein G Prefusion (2VWD)**

Chain A

90–94% 297/280 359/361 226/228 307/302 235/218 212/209 311/307 222/232 357/363 213/209 385/382 484/542
 521/515 265/256 433/475 288/290 569/571 506/458
 95–98% 194/546 542/544 481/466 190/598 413/366 218/588 562/508 463/497
 99% 410/399 269/252 471/476 515/520 328/324 270/252
 100% 259/262 291/287 331/327 440/409 445/354 448/450 477/471 511/561 516/520

***Nipah Virus Glycoprotein G Receptor Bound (2VSM)**

Chain A

90–94% 297/280 307/302 359/361 545/541 385/382 235/218 445/354 357/363 481/466 451/447 269/252 288/290
 490/529 245/237 291/287 589/215 226/228 328/324 562/508 507/122
 95–98% 484/542 542/544 347/369 463/497 432/411 569/571 413/366 440/409 194/546 511/561 215/586
 99% 259/262 410/399 471/476 332/327 515/520 190/598 448/450 483/480 516/520 472/476 477/471
 100%

Chain B

90–94% 51/46 133/167 59/117 103/81 69/107 162/155 102/81 79/143 80/104 170/166
 95–98% 130/118 156/141 47/50 157/139
 99%
 100%

***Parainfluenza Type 5 Virus Glycoprotein HN Sialyllactose Soaked (1Z4X)**

Chain A

90–94% 298/300 414/440 171/173 553/160 520/516 445/492 185/159 436/415 443/411 214/197 301/297 525/463
 95–98% 362/305 466/524 552/157 309/286 461/407 358/309 351/356 505/507 269/265 533/122 424/426

(continued)

SUPPLEMENTARY TABLE S2. (CONTINUED)

99% 480/472 204/207 356/350 392/290 531/126 266/269 537/531
 100% 120/172 233/235 293/391 357/353 389/358 394/293 398/128 439/505 449/445 501/512 548/552 559/541

Pseudorabies Virus Glycoprotein B Postfusion (6ESC)

Chain A
 90–94% 239/280 681/665 198/185 223/243 248/218 249/261 258/254 379/423 214/209 219/214 461/410 216/210
 451/469 567/562 343/347 539/534 408/402 685/677 219/213 628/657 675/671 680/682 595/597 644/631
 95–98% **190/192** 303/306 435/430 312/324 460/463 647/650 417/456
 99% 688/675 215/209 474/446 298/294 241/237 619/624 161/385 403/407 **275/188**
 100% 122/124 217/211 339/353 445/439 447/443 464/459 672/674

***Puumala Virus Glycoprotein G_n (5FXU)**

Chain A
 90–94% 138/115 224/252 190/192 369/335 335/139 74/133 134/71 45/263
 95–98% 321/310 182/34 243/238 143/145
 99% 57/144 116/76 118/137
 100% 46/154 198/377 211/378 291/371 323/363 352/141

Puumala Virus Glycoprotein G_c Postfusion at pH 6.0 (5J81)

Chain A
 90–94% 1057/1059 737/795 993/1068 **772/785** 837/839 887/893 831/811 897/877 823/819
 95–98% 945/947 1036/1006 885/881 759/755 880/896 931/927 **785/771**
 99% 1021/1023 874/882 721/691 708/703
 100% 820/822 **910/776** 919/898 992/997 994/1045 1035/1010 1053/1065 1069/990

Puumala Virus Glycoprotein G_c Postfusion at pH 8.0 (5J9H)

Chain A
 90–94% 973/675 837/839 975/673 737/795 822/819 820/822 889/891 993/1068
 95–98% 931/927 887/893 1057/1059 1069/990 945/947 1036/1006 **788/744** 1053/1065 1060/1056
 99% 721/691 874/882
 100% 704/709 885/881 992/997 994/1045 1021/1023

Respiratory Sphinctial Virus Glycoprotein F Prefusion at pH 5.5 (4MMS)

Chain A
 90–94% B320/37 B475/35 B311/46 86/81 34/38 61/B193
 95–98% 51/B305 103/B241 B197/60
 99% 62/B295
 100% 48/B365 68/65

Chain B
 90–94% 265/260 267/264 324/332 320/A37 439/416 287/302 248/282 341/316 484/479 475/A35 203/198 311/A46
 479/475 A61/193 398/487 373/369 405/415
 95–98% 365/361 **D408/144** A51/305 205/199 342/352 409/411 F145/405 243/237 A103/241 408/F144 197/A60
 99% 346/348 A62/295
 100% 145/D405 294/296 421/417 445/410 A48/365

Respiratory Sphinctial Virus Glycoprotein F Prefusion at pH 9.5 (4MMR)

Chain A
 90–94% 39/33 31/B465 93/89 B370/49 51/B305 38/33 B193/58
 95–98% B314/44
 99% B466/28 81/76 34/38 84/81 98/95
 100% 48/B365 52/B305 62/B295 78/74 88/83 91/86 B306/51 B311/46

Chain B
 90–94% 338/394 A31/465 497/492 **150/146** 244/240 512/507 453/455 267/264 272/267 433/424 398/487 370/A49
 182/185 341/316 A51/305 364/361 193/A58 220/217 445/410 301/288 405/415 203/199 202/198
 95–98% 399/333 291/298 449/425 314/A44 402/399 475/A35 345/312 362/364 188/179
 99% 466/A28 308/305 346/348
 100% 173/169 297/293 306/A51 311/A46 373/369 409/411 431/426 506/501 508/503 A48/365 A52/305 A62/295

†Respiratory Sphinctial Virus Glycoprotein F Postfusion (3RRR)

Chain A
 90–94% 62/B295 90/86 34/38 51/B305 D465/54
 95–98% B308/48
 99%
 100% 39/33

(continued)

SUPPLEMENTARY TABLE S2. (CONTINUED)

Chain B

90–94% 362/364 303/286 A62/295 170/165 186/181 441/414 459/E50 436/422 465/E54 250/F238 A51/305 450/425 299/291

95–98% 348/345 439/416 449/425 308/A48 205/199 433/424 499/494 341/316 457/F307

99% 342/352 248/282 213/208 427/430 409/411 294/296 241/236 227/222 172/167 223/218 405/415 202/197 373/369 380/376 358/354

100% 219/214 226/221 460/448

Rift Valley Fever Virus Glycoprotein G_c Postfusion (6EGT)

Chain A

90–94% 893/1010 1116/1038 1113/1093 **832/817** 1026/704 747/864 1059/1075 1008/724 813/793 1017/885 802/798 909/912 1115/1091 1026/C704 972/1122 1041/1115 854/757 857/755 1076/1058 866/869 932/928 986/988 785/782 764/934 810/943 784/780

95–98% 693/729 1019/1015 **960/962** 997/993 726/723

99% 946/807 **826/820** 884/886 855/757 737/741

100% 718/1 018 780/783 788/784 821/827 899/C897 904/B900 **962/959 963/959** 994/998 1040/1045 1079/1054 1125/969 C904/900

Rubella Virus Glycoprotein E1 Postfusion (4ADI)

Chain A

90–94% 67/62 49/142 **89/139** 238/39 107/103 169/25 327/3 384/362 79/147 **123/86** 140/88 149/42 32/161 157/207 286/131

95–98% 35/351 91/97 289/279 312/307 349/411 357/389

99% 351/413 324/195 273/294

100% 16/21 22/15 110/101 172/174 180/182 188/190 248/297 282/129 C248/297

SARS Virus Spike Glycoprotein Prefusion Conformation 1 (5X58)

Chain A

90–94% 286/281 937/932 562/552 1015/1010 184/91 554/47 1039/1036 259/59 89/255 1033/1047 94/181 420/499 981/976 985/980 1047/705 68/254 658/677 239/246 261/57 702/1050 256/88 423/363 597/584 599/582 725/720 363/422 452/411 133/130 370/367 615/609 443/477 680/655 496/423 335/332 1079/1085 656/846 879/865 162/127 476/460 740/736

95–98% 235/100 932/927 350/321 636/599 461/475 43/216 565/569 116/126 240/140 1042/1038 726/721 299/585

621/280 230/104 431/425 60/258 82/231 561/552 869/866

99% 115/103 510/379 120/122 655/845 676/659 64/35 129/113 480/440 330/325 579/576 924/919 73/75 293/287 146/141

100% 51/267 223/194 226/192 379/530 392/490 398/393 454/225 507/504 526/536 530/532 635/631 674/661 754/749 765/760 **780/782 783/779** 868/862 931/927 1016/1010 1017/1011 1039/1041 1056/696 1083/1080

SARS Virus Spike Glycoprotein Prefusion Conformation 2 (5X5B)

Chain A

90–94% 120/122 859/854 657/653 696/B877 B48/551 872/868 643/676 **783/ 779** 420/499 561/552 562/552 82/231 261/57 528/525 289/284 423/363 1083/1080 363/422 268/271 452/411 1033/1047 952/B737 939/935 370/367 949/945 553/550 **778/775** 1060/692 443/477 804/799 496/423 100/234 335/332 526/536 615/612 932/927 67/33 569/564 867/862 324/349 476/460

95–98% B50/553 937/932 621/280 461/475 223/194 315/376 **780/782** 733/728 293/287 674/661 1072/1103 431/425 632/634

99% 736/731 879/865 975/970 480/440 609/604 553/561 924/919 162/127 330/325 599/582 735/731 146/141

100% 39/35 43/216 48/C551 51/267 54/264 115/103 129/113 185/199 200/184 239/246 240/140 258/86 264/276 314/376 392/490 398/393 530/532 555/556 579/576 582/303 597/584 635/631 741/738 754/749 765/760 805/800 868/862 869/866 873/868 892/887 931/927 972/966 1017/1011 1042/1038 1056/696

†SARS Virus Spike Glycoprotein Receptor Bound (2AJF)

Chain A

90–94% 207/203 107/103 42/37 97/92 461/456 55/341 536/530 393/389 263/486 216/212 156/151 352/355 348/345 366/363 564/560 344/51

95–98% 488/481 44/39 331/326 125/120 218/209 153/148 284/279 361/332 507/503 280/276 174/168

99% 341/338 563/392 293/290 560/555 40/35 210/217 603/599

100% 25/20 71/66 135/140 149/146 149/143 150/146 150/144 170/165 197/191 276/444 333/358 363/333 425/418 447/442 449/443 467/462 479/474 487/481 511/505 559/554

(continued)

SUPPLEMENTARY TABLE S2. (CONTINUED)

Chain E

90–94% 430/425 389/335 356/352 421/365 394/390
 95–98% 452/411 411/405 357/352 447/444 431/426 449/407
 99% 407/403 472/468
 100% 393/490 408/403

Semliki Forest Virus Glycoprotein E1 Postfusion (1RER)

Chain A

90–94% 321/350 53/109 31/136 160/156 157/159 181/183 21/286 10/274 261/269 327/346 366/376 128/39 370/372
104/59 47/121 20/27
 95–98% 271/36 263/267 77/73 **100/97** 274/271 167/147 217/202 **85/ 100 92/89**
 99% 28/19 315/356 308/313 33/134 24/21 314/310 255/251 316/305
 100% 45/309 **102/62** 138/140 141/137 190/187 203/199 254/250 256/251 259/340 260/256 268/262 392/389

Sindbis Virus Glycoprotein E1–E2 Prefusion (3MUU)

Chain A

90–94% 332/294 605/600 368/636 525/637 53/63 299/327 **444/460** 583/592 286/317 597/577 155/262 329/336 64/60
 510/523 424/421 13/48 612/544 563/559 621/629 314/289
 95–98% 131/108 61/52 327/338 287/275 402/485 484/403 608/603 105/92 45/35 623/627 374/370 276/286
 99% 588/585 95/102 489/399 385/381 **452/449** 437/433 40/153
 100% 20/21 54/63 98/100 100/97 101/97 263/154 280/282 290/313 300/304 322/281 324/321 337/334 380/387 432/
 429 472/410 517/514

Thogoto Virus Glycoprotein G_p Prefusion (5XEA)

Chain A

90–94% 46/221 258/260 177/173 32/412 **150/73 83/72** 116/153 184/187 120/116 132/108 202/204 156/112 160/137
 180/191
 95–98% **71/84** 176/173
 99% 174/176 **74/150** 87/68 243/222
 100% 171/258 261/257 292/186

West Nile Virus Glycoprotein E Prefusion (2HG0)

Chain A

90–94% 127/124 129/203 297/183 338/303 392/388 280/50 358/374 353/342 306/337 383/397 139/47 262/258 266/
 262 181/184 186/294 52/134 146/143 163/159 205/211
 95–98% 177/188 319/322 276/278 144/163 154/150 185/181 **106/100**
 99% 114/95 369/329 267/263 279/275 30/26
 100% 48/138 57/127 72/114 74/112 **86/82** 171/173 202/198 209/206 210/206 220/215 239/235 244/241 264/259 270/
 266 354/342 373/147 381/399 393/388 400/380

Yellow Fever Virus Glycoprotein E Prefusion (6IW4)

Chain A

90–94% **98/111** 63/123 251/61 248/231 349/368 202/198 373/391 292/175 119/66 **112/ 97** 180/286
 95–98% 352/366 347/336 265/202 302/299 148/145 364/322
 99% **106/103** 192/187 361/324 7/3
 100% 173/176 178/289 314/317

Yellow Fever Virus Glycoprotein E Postfusion (6IW1)

Chain A

90–94% 144/155 B19/11 119/66 123/62 361/324 7/32 120/89 351/366 183/166 127/197 373/391 177/172 352/366
 95–98% 19/C11 331/356 202/198 301/331 199/201 239/241 63/123
 99% 173/176 296/6 205/262
 100% 14/B16 15/18 16/C13 19/C8 163/165 165/133 221/56 314/317 347/336 B16/13 B19/8 C14/16

Zika Virus Glycoprotein E Prefusion (6CO8)

Chain A

90–94% 340/337 179/186 205/211 500/496 216/200 323/320 290/25 31/8 17/20 295/187 389/344 221/217 51/282 **114/**
95 466/461 124/62 92/117 207/209
 95–98% 384/402 443/438 333/372 309/340 335/370 322/325 185/180 361/377 238/225 138/169
 99% 376/147 452/447 28/287 471/466
 100% 50/136 **112/97** 184/180 188/294 249/252 270/265 450/445 458/453 459/453 460/457 B13/271

(continued)

SUPPLEMENTARY TABLE S2. (CONTINUED)

Chain B

90–94% 56/53 37/32

95–98%

99%

100% 13/A271

Donor/acceptor residues of BHBs in order of non-decreasing Π -values, with 7.5, 8.5, 9.5, and 9.85, respectively, corresponding to percentiles 90, 95, 99, and 100. Residues lying in generally agreed upon fusion loops are shown in bold. For 5X5C and 5X5F, the expected fusion loop is part of the structure at residues 880–900 but contains no exotic residues. Part of the fusion loop is missing from 5L1X, and the residues 100–125 presumed to lie in the fusion loop a fortiori do not appear in exotic BHBs; in 5WB0, which contains the fusion loop, there is a bond with sub-exotic Π -value 6.6, roughly the 82nd percentile, for a BHB with residues 112/109 in the fusion loop.

*A glycoprotein other than the fusion peptide that does not and is not expected to contain the fusion loop.

†The fusion loop, though part of the peptide is either missing from the the structure or disordered, and in either case a fortiori can provide no reliable exotic BHBs. For coronavirus, the putative fusion loop surrounding residues (I or L)EDLLF is controversial, disordered in 6B3O, and contains no exotic BHBs in 5I08.