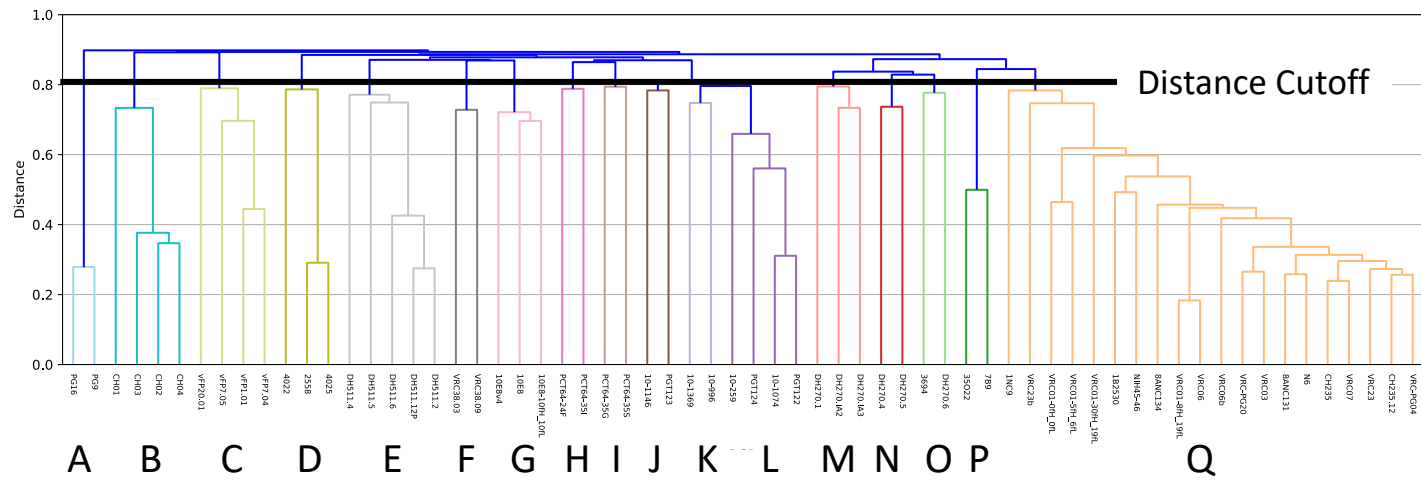


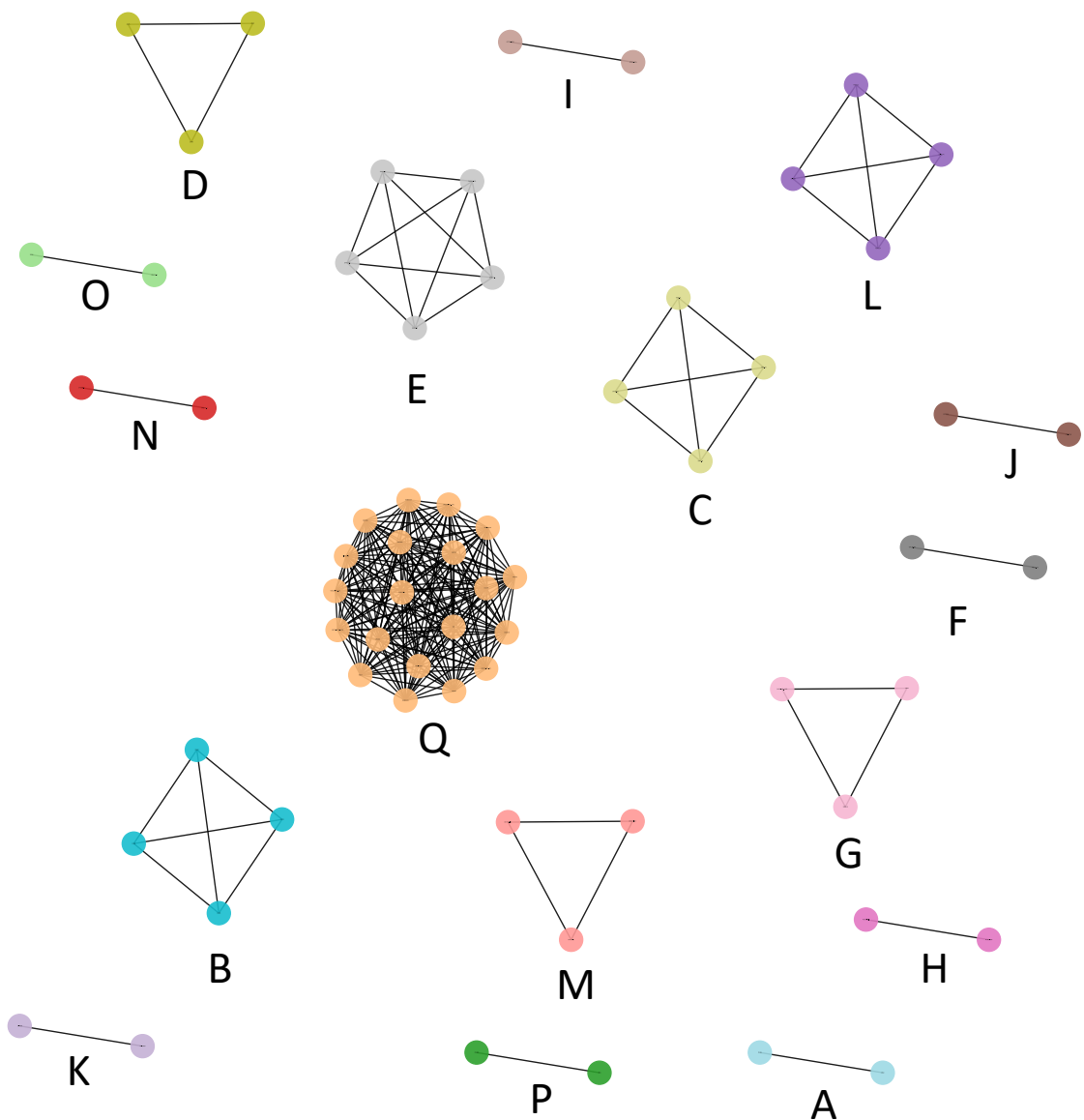
Clusters	Total number of PDBs	PDBs code
1	27	3se8HL,3se9HL,4j6rHL,4jb9HL,4jdtHL,4jpvHL,4jpwHL,4lsuHL,4olzHL,4rx4AD,4s1qHL,4s1rHL,4s1sHL,4xmpHL,4xnyHL,4xnzHL,4xvtHL,4ydiHL,4ydIBC,4yflHL,5cd5CD,5f96HL,5f9oHL,5f9wBC,5fecAB,5i9qBC,5te7HL
2	4	1deeFE,1xf5BA,1yntBA,4ioiBA
3	4	5u3jHL,5u3IHL,5u3nHL,5u3oHL
4	3	1ahwBA,1jpsHL,1uj3BA
5	3	1yy9DC,3b2uCD,5sx5HL
6	3	2b1hHL,3mlrHL,3mlwHL
7	3	3baeHL,3iflHL,3ifoAB
8	3	4tvpHL,5cezHL,5t3zHL
9	2	1a2yBA,1bvkBA
10	2	1eo8HL,1qfuHL
11	2	1frgHL,1ifhHL
12	2	1ggiHL,4jo1IM
13	2	1kc5HL,1kcsHL
14	2	1p2cBA,1yqvHL
15	2	1sy6HL,1xiwHG
16	2	1tziBA,4zffHL
17	2	2aepHL,2aeqHL
18	2	2eizBA,3d9aHL
19	2	2i9IHG,4u6hAB
20	2	2oslHL,3bkyHL
21	2	2xraHL,3ma9HL
22	2	3bn9DC,3so3CB
23	2	3effDC,3psBA
24	2	3eyfBA,4hhaBA
25	2	3gbnHL,4fqihHL
26	2	3l5wHL,3l5xHL
27	2	3u2sAB,4dgoHL
28	2	3ujiHL,3ujjHL
29	2	4al8HL,4bz1HL
30	2	4edwHL,4edxBA
31	2	4hxxAB,5ugyHL
32	2	4hlzGH,4py8IJ
33	2	4hs6HL,4hs8HL
34	2	4jpkHL,5iesHL
35	2	4jznIP,4z0xBA
36	2	4kvnHL,5k9oAB
37	2	4lqfHL,4lu5IM
38	2	4ojfHL,4onfHL
39	2	4r8wHL,5kaqQR
40	2	4ut6HL,5lcvHL
41	2	4utaHL,5h37KL
42	2	4y5vGH,4y5yAB
43	2	4ydvHL,5drzBA
44	2	4zs6CD,5do2HL
45	2	5d1qBA,5d1xBA
46	2	5esvHL,5eszAB
47	2	5f3bAB,5f3hAB
48	2	5fgbCA,5fgcEB
49	2	5jw3HL,5k9kHL
50	2	5kveHL,5kvfHL
51	2	5tljDC,5tlkHG
52	2	5vicHL,5vigAB

Suppl Table 1.

# Tree representation of hierarchical clusters

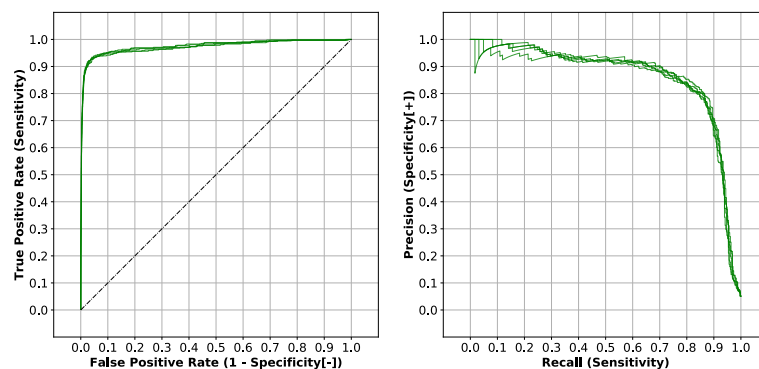


# Network representation of clusters

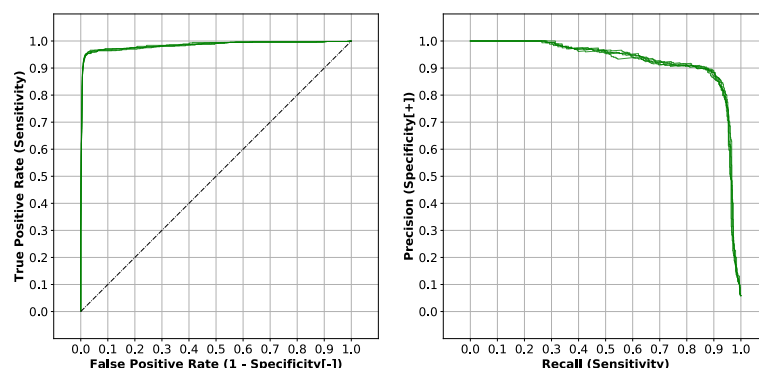


**Suppl Fig. 1. Relationship between hierarchical clusters and networks.** The Tree was sliced at a cutoff distance (0.796) and clusters were displayed as networks with edge-lengths proportional to their node distance.

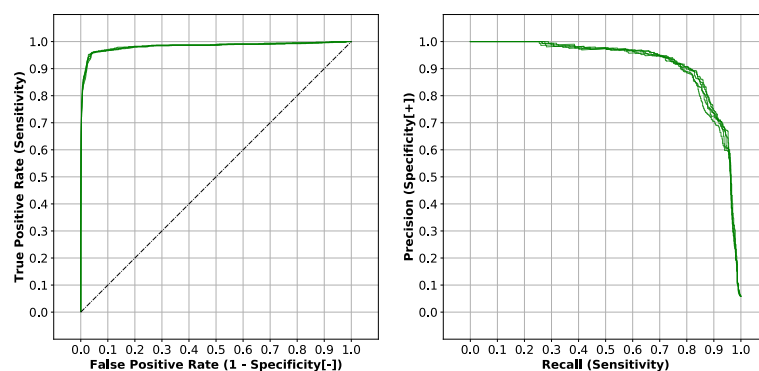
**A**



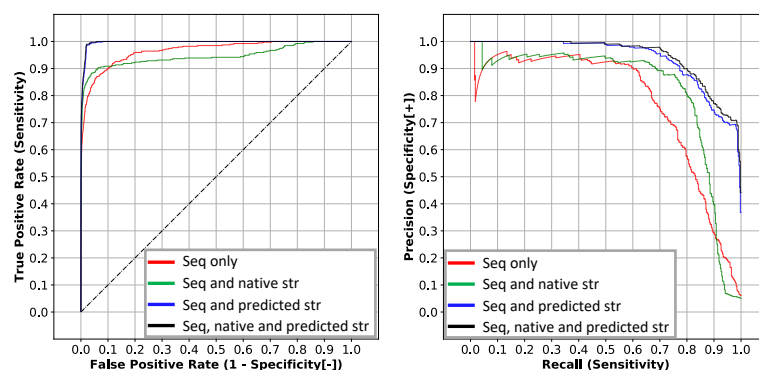
**B**



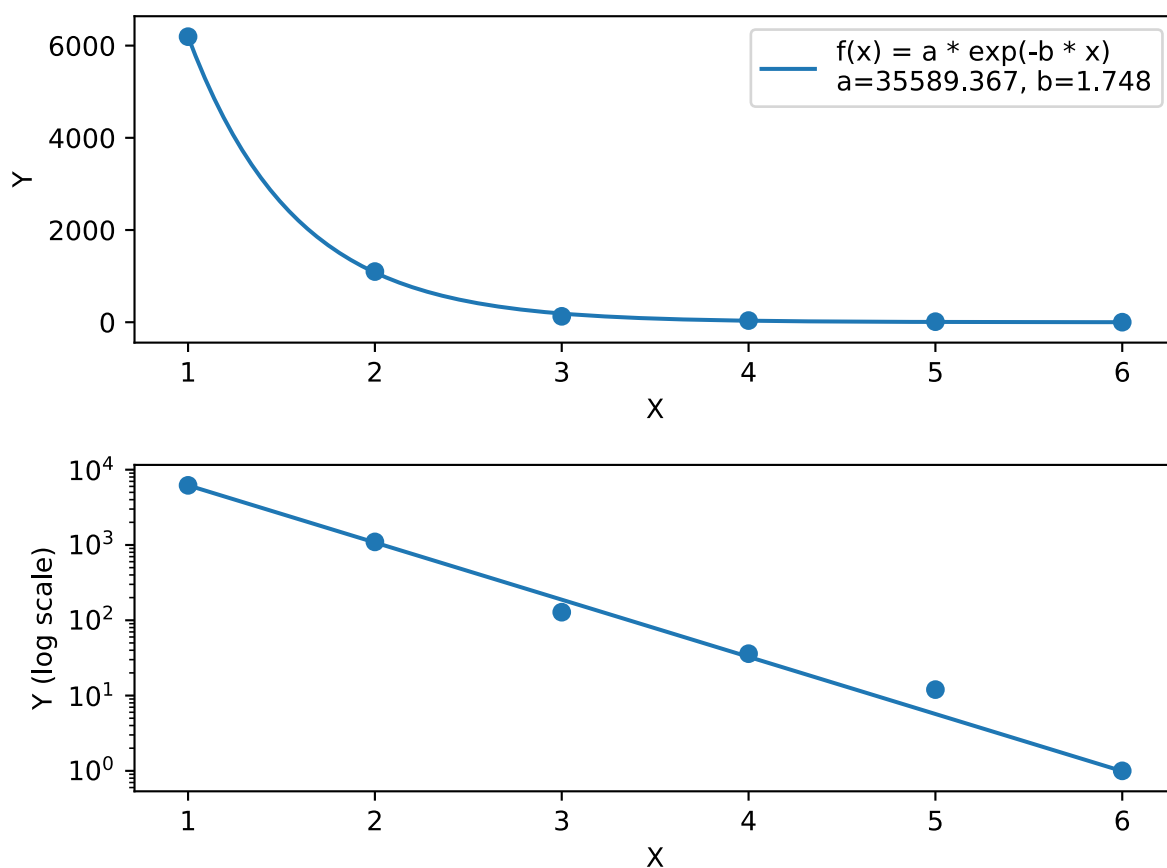
**C**



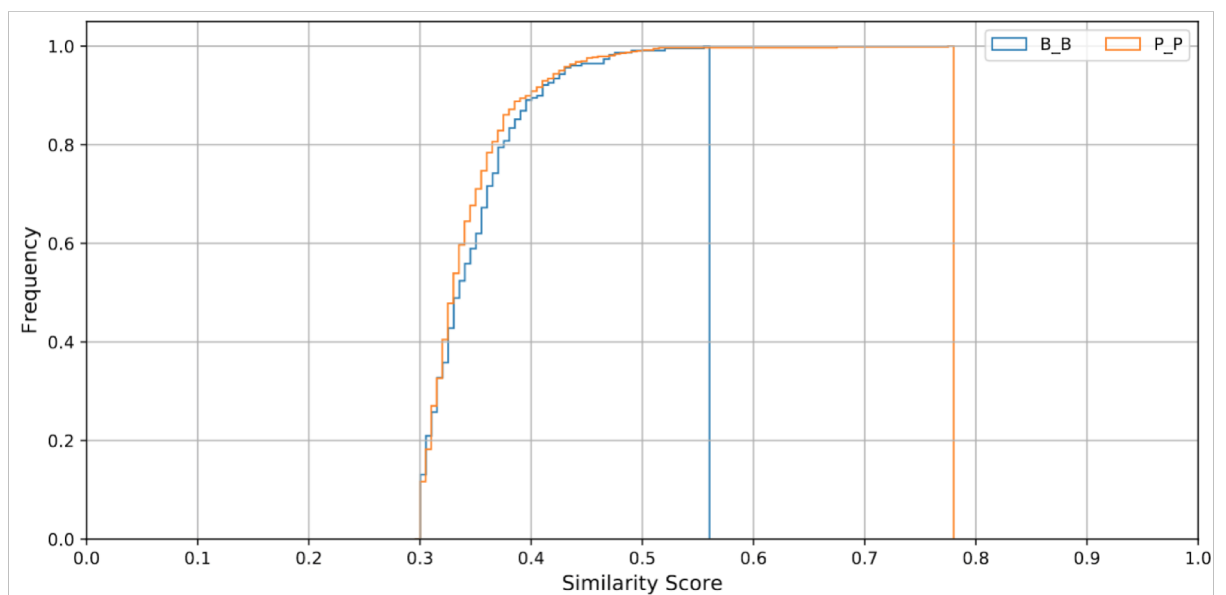
**D**



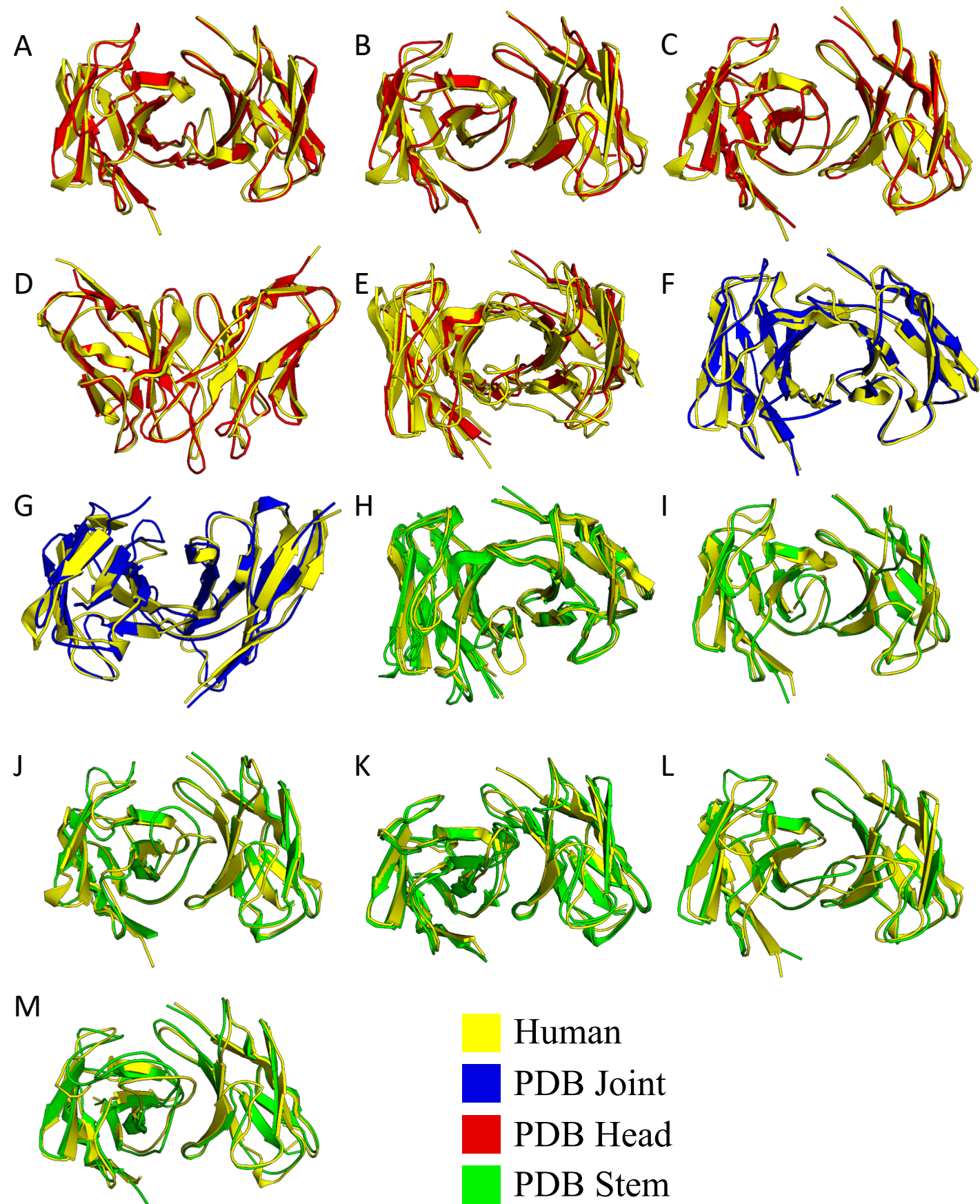
**Suppl Fig. 2. Comparison of SVM models.** The ROC and Precision-Recall curves for 5-fold cross-validation using sequence only (A), sequence and native structure (B) and sequence and predicted structures (C). The various SVMs, were also tested using Repertoire Builder models built with a template sequence identity blacklist of 80% (D).



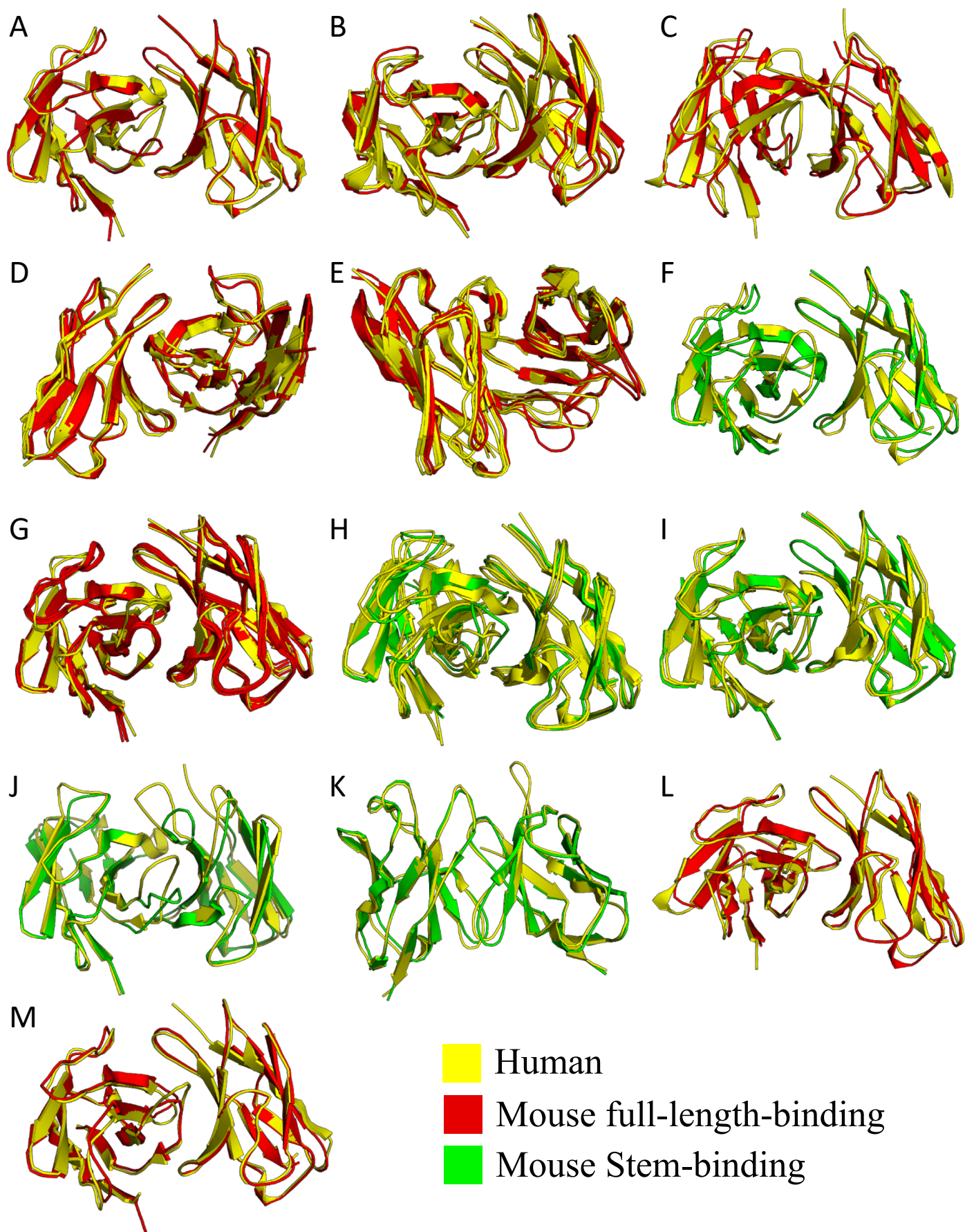
**Suppl Fig. 3. Human BCR cluster size dependence.** The best fit for distribution (Y) of cluster size (X) for the human BCR data was obtained by an exponential function.



**Suppl Fig. 4. Cumulative distribution of human BCR similarity scores.** The plot shows cumulative distributions for BCR similarity scores of pairs of plasmablasts (P\_P) and pairs of B cells (B\_B). Vertical lines indicate the maximum similarity observed.



**Suppl Fig. 5. Visualization of structures of clusters containing human and known anti-HA PDB entries.** The label of each illustration corresponds with the label of the cluster in Fig.5. The structures of PDB entries were characterized by their HA-binding modes as head (red), joint (blue) or stem (green). The structures of human BCRs were colored yellow.



**Suppl Fig. 6. Visualization of structures of clusters composed of human and mouse BCRs obtained post flu vaccination.** The label of each illustration is consistent with the cluster label in Fig.6. The structures of human, mouse stem-binding and mouse full-length-binding BCRs were showed as yellow, red and green, respectively.