

Structural basis for the neutralization of MERS-CoV by a human monoclonal antibody MERS-27

Xiaojuan Yu^{1, *}, Senyan Zhang^{1, *}, Liwei Jiang^{2, *}, Ye Cui¹, Dongxia Li³, Dongli Wang¹,
Nianshuang Wang¹, Lili Fu², Xuanlin Shi², Ziqiang Li³, Linqi Zhang^{2, #}, Xinquan Wang^{1, 4, #}

¹Ministry of Education Key Laboratory of Protein Science, Center for Structural Biology, School of Life Sciences, Collaborative Innovation Center for Biotherapy, Tsinghua University, Beijing, China

²Comprehensive AIDS Research Center, Collaborative Innovation Center for Diagnosis and Treatment of Infectious Diseases, School of Medicine, Tsinghua University, Beijing, China

³Beijing VDJBio Co., Ltd, Suite B311, 5 Kaituo Road, Zhongguancun BioMedical Garden, Haidian District, Beijing, China

⁴Collaborative Innovation Center for Biotherapy, State Key Laboratory of Biotherapy and Cancer Center, West China Hospital, West China Medical School, Sichuan University, Chengdu, China

*Equal contribution

#Corresponding authors

Xinquan Wang: xinquanwang@mail.tsinghua.edu.cn

Linqi Zhang: zhanglinqi@mail.tsinghua.edu.cn

Figure S1. Gel filtration profiles and SDS-PAGE gels of purified MERS-CoV RBD, MERS-27 Fab, and the RBD-Fab complex.

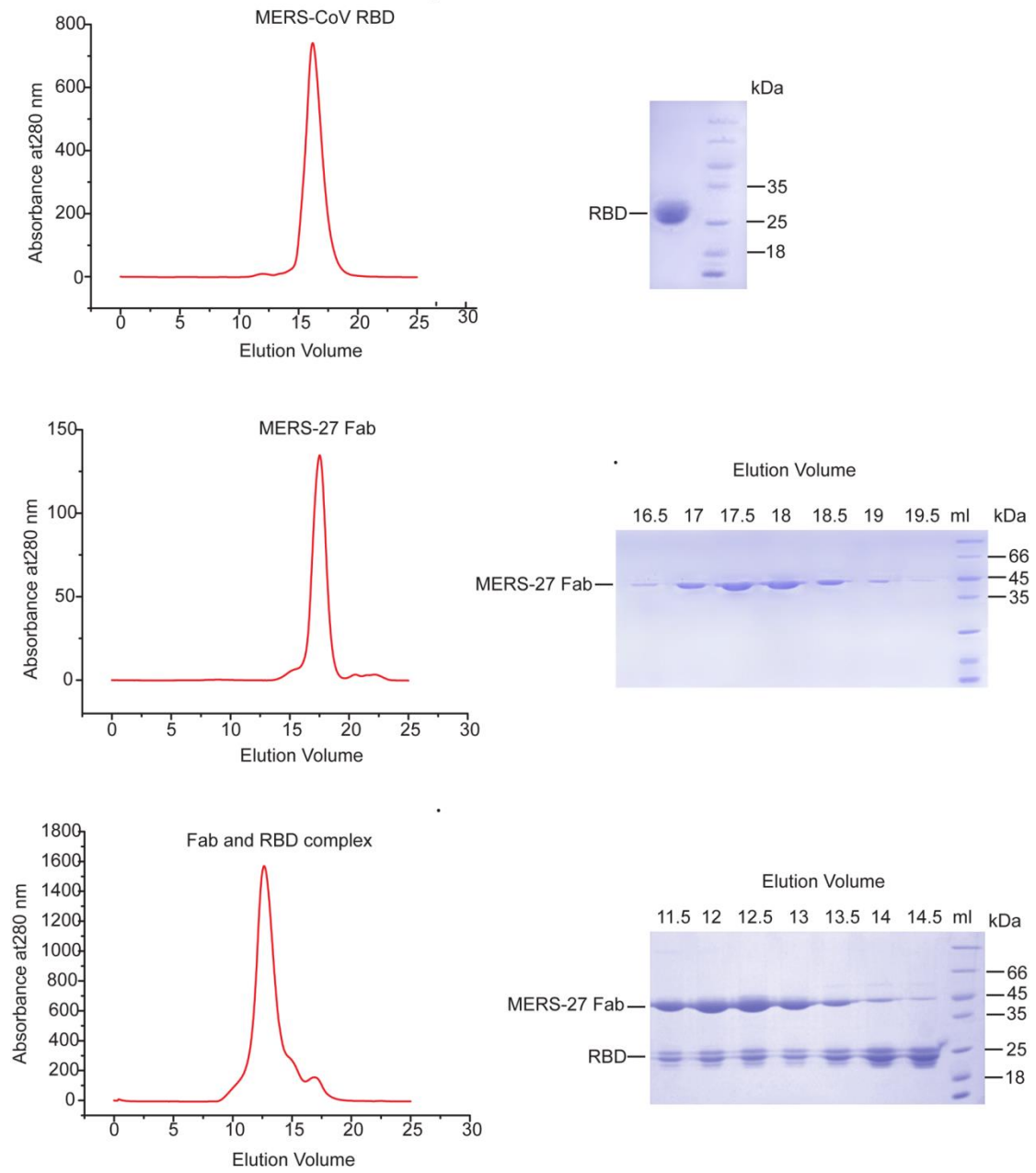


Figure S2. Stereo view of the two complexes of MERS-CoV RBD with MERS-27 Fab in the crystallographic asymmetric unit.

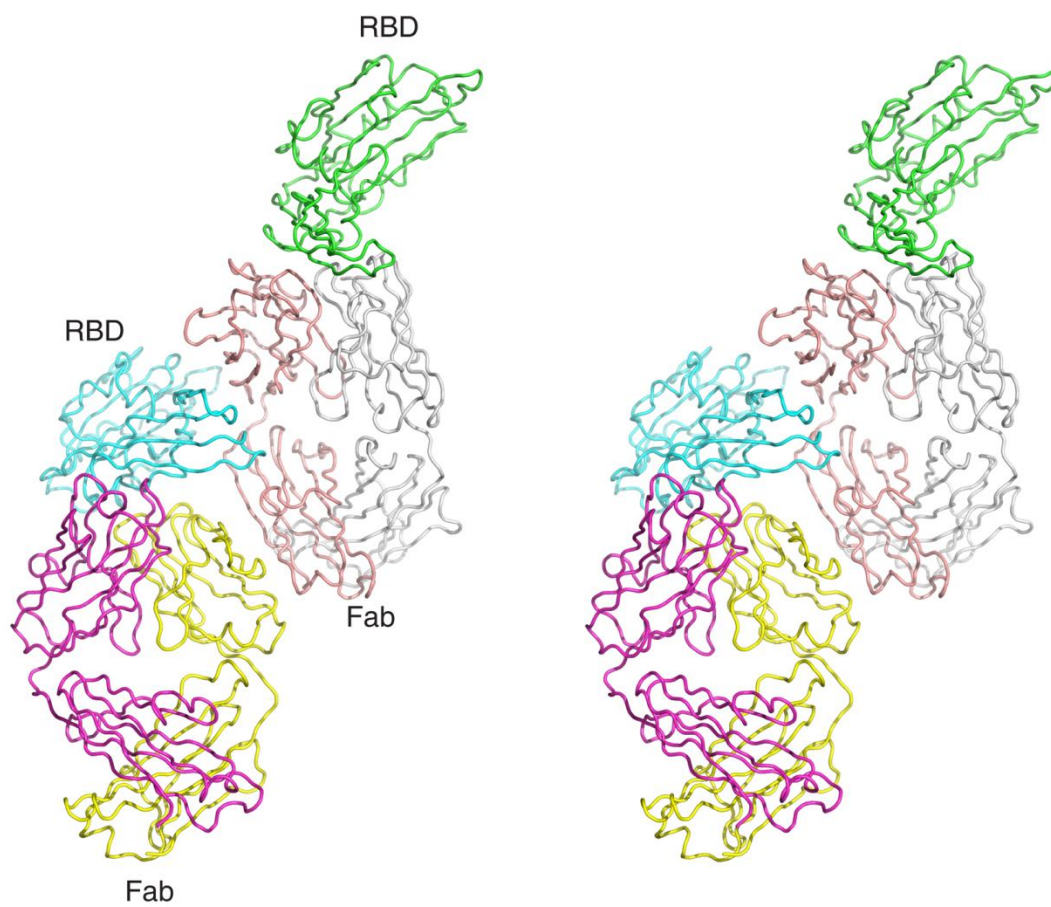


Figure S3. Structural superimposition of RBD in unbound (blue), DPP4-bound (orange), and MERS-27-bound (green) states.

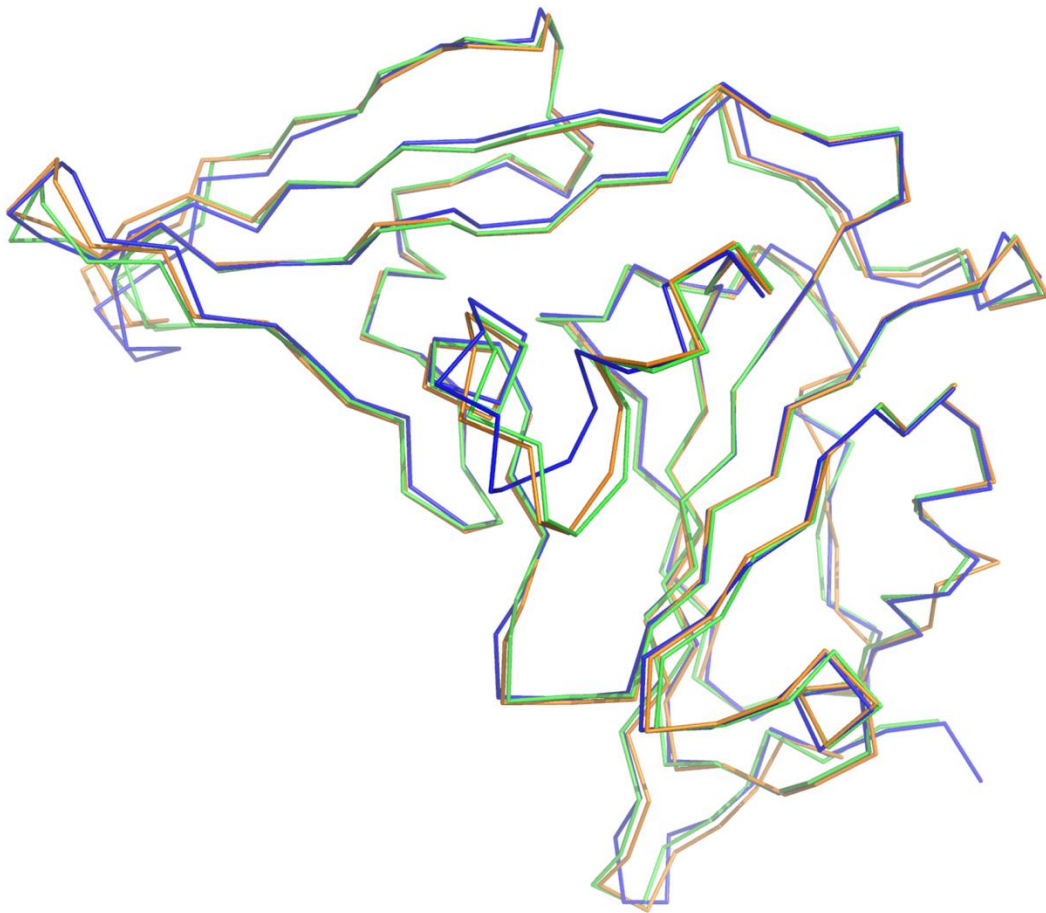


Figure S4. The MERS-CoV RBD residue Asp539 forms a hydrogen bond with Tyr33 of heavy chain upon MERS-27 binding (A). This RBD residue forms a salt bridge with Lys267 upon receptor DPP4 binding (B).

