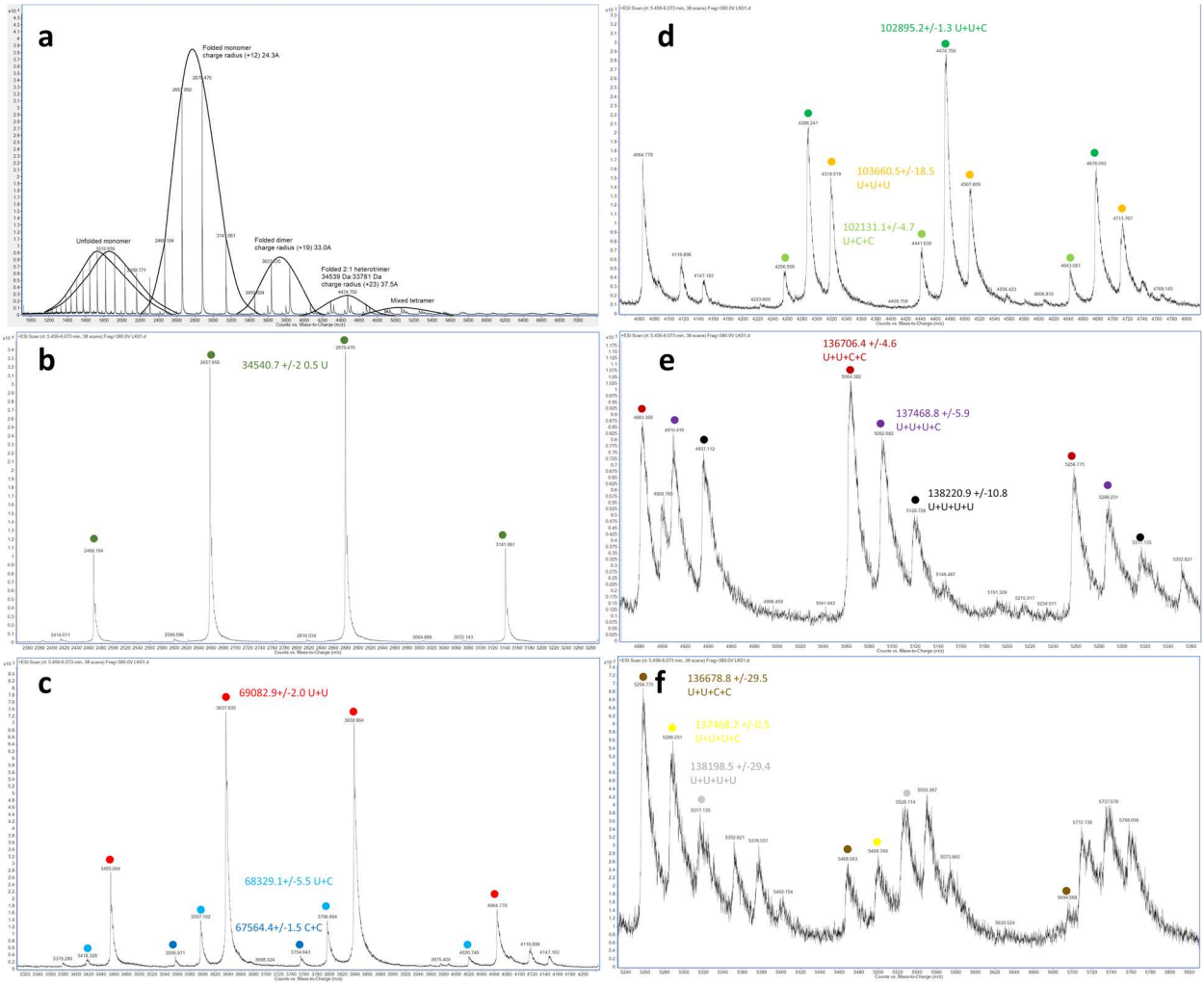
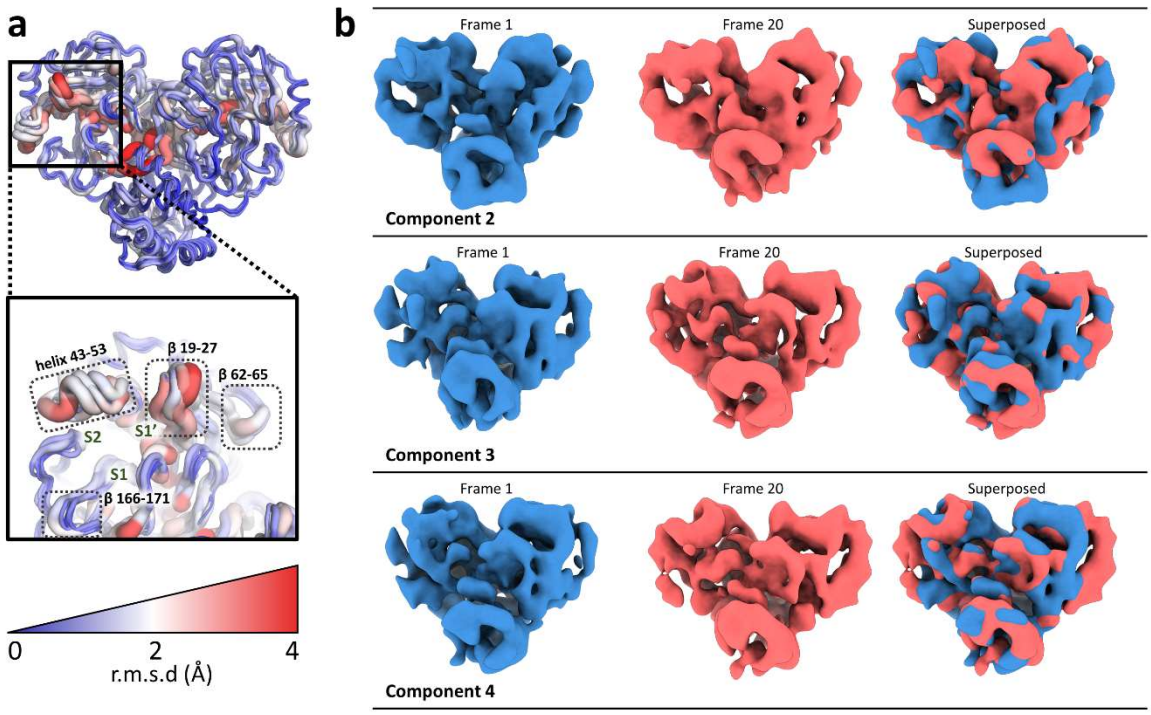
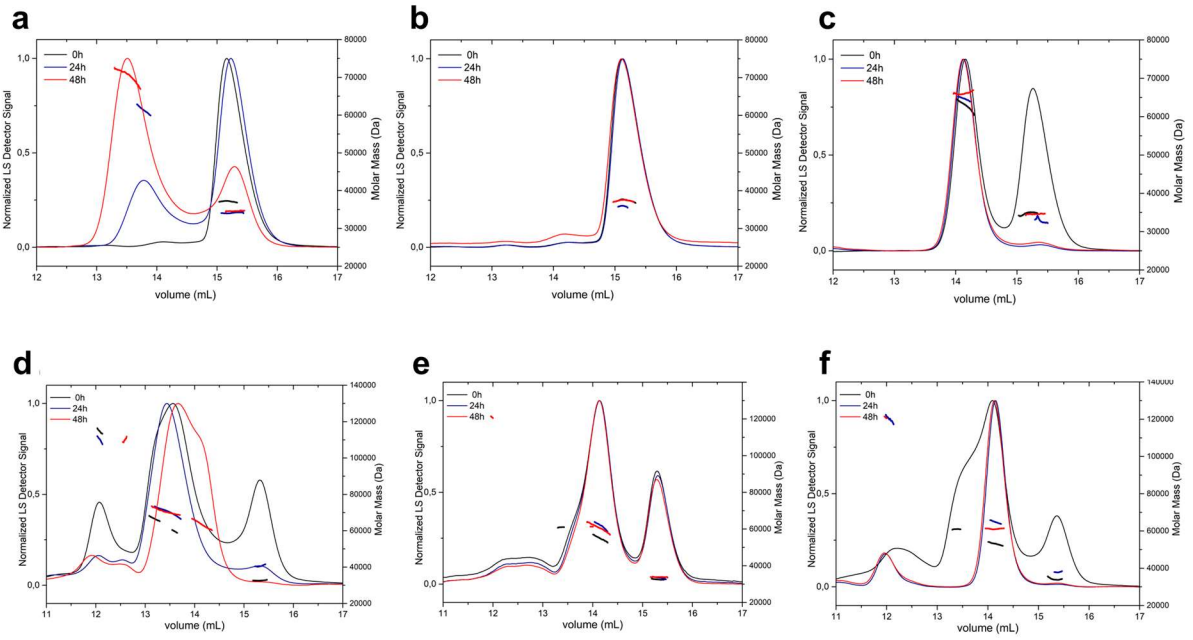
Supplementary Material Information



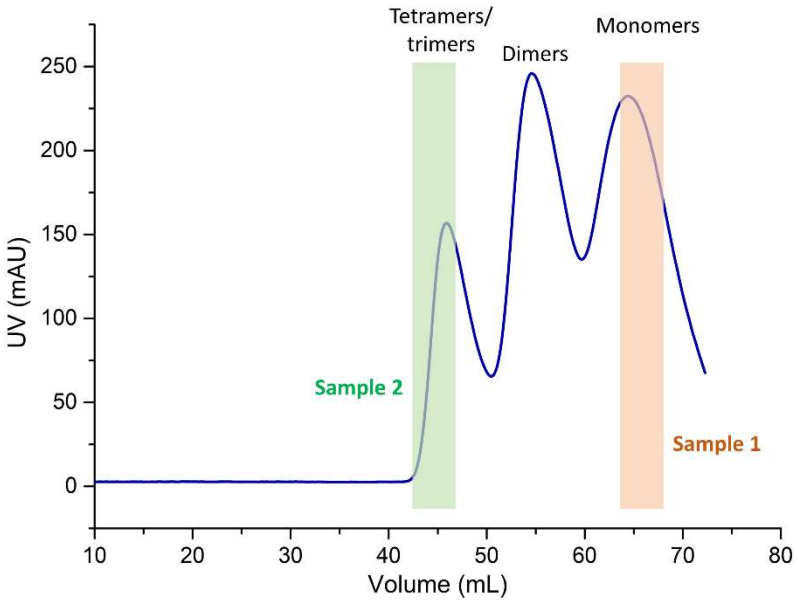
Supplementary Figure 1. Native mass spectroscopy of SARS-CoV-2 M^{pro} C145S data analysis. a. Complete profile from the sample 2, showing distinct oligomeric states. b. Analysis of primary peak containing folded monomers. c. Analysis of peaks containing folded dimers, showing that oligomers can be formed by all combinatory possibilities uncleaved (U) and cleaved (C) particles. d. Analysis of peaks containing folded trimers, showing that oligomers can be formed by all combinatory possibilities U and particles. e and f Analysis of peaks containing folded tetramers, showing that oligomers can be formed by all combinatory possibilities U and C particles.



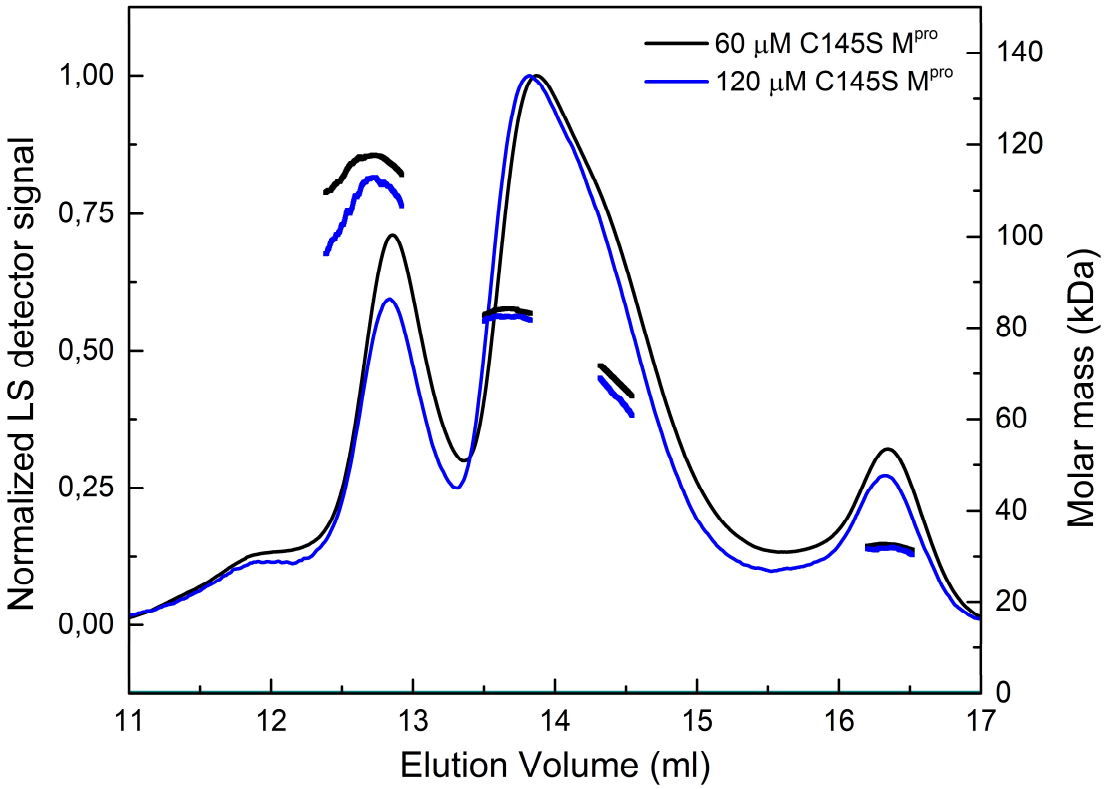
Supplementary Figure 2. 3DVA of SARS-CoV-2 M^{pro} C145S. a. Aligned models of M^{pro} that were morphed in distinct frames of 3DVA models, colored according to its r.m.s.d. The square box is highlighting the active site loops were we observed the largest r.m.s.d values. b. 3DVA maps of components 2, 3 and 4 showing first (blue), last (red) and superposed maps.



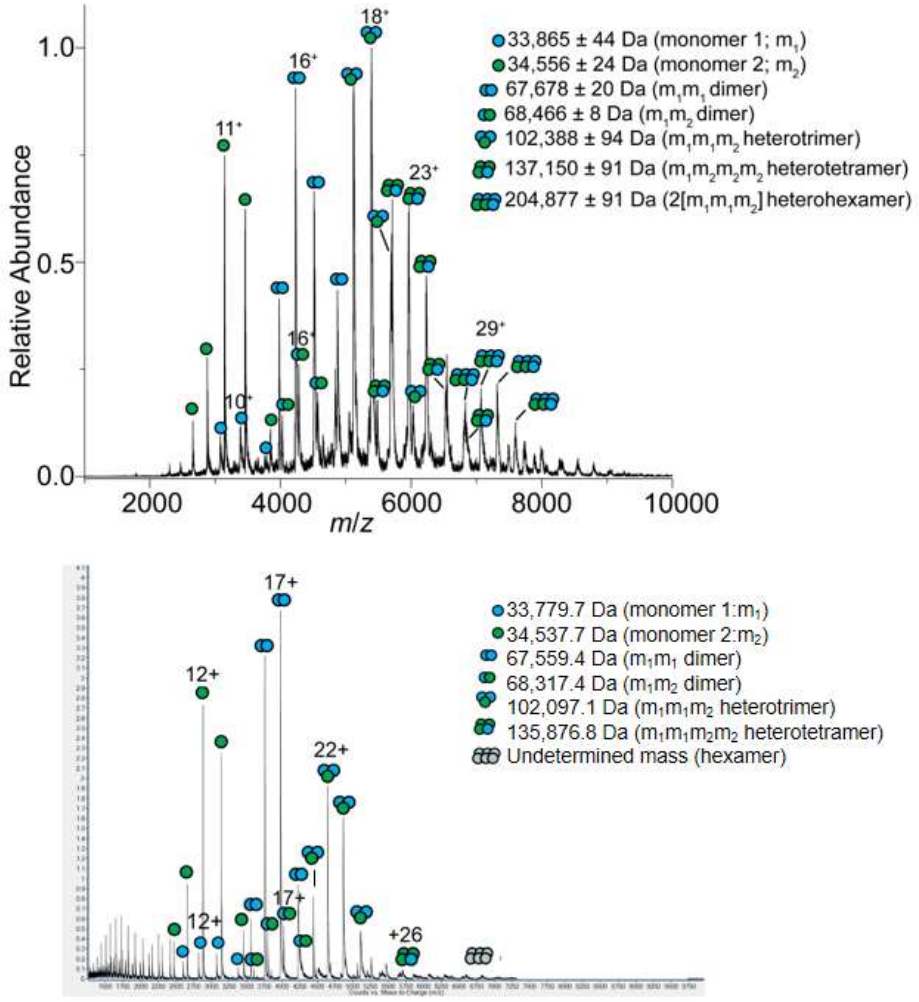
Supplementary Figure 3. SEC elution profiles of monomeric peak of C145S M^{pro}. a. SEC-MALS elution profiles of C145S M^{pro} monomers after 0h (black), 24h (blue) and 48h (red) incubation. b. SEC-MALS elution profiles of C145S M^{pro} monomers in presence of MAT-POS-e194df51-1 after 0h (black), 24h (blue) and 48h (red) incubation. c. SEC-MALS elution profiles of C145S M^{pro} monomers in presence of Nirmatrelvir after 0h (black), 24h (blue) and 48h (red) incubation. d. SEC-MALS elution profiles of C145S M^{pro} tetramers after 0h (black), 24h (blue) and 48h (red) incubation. e. SEC-MALS elution profiles of C145S M^{pro} tetramers in presence of MAT-POS-e194df51-1 after 0h (black), 24h (blue) and 48h (red) incubation. f. SEC-MALS elution profiles of C145S M^{pro} tetramers in presence of Nirmatrelvir after 0h (black), 24h (blue) and 48h (red) incubation. In SEC-MAL graphs, curves correspond to the change in the normalized scattered light intensity at 90° (lines) and calculated molar mass of the corresponding peak (dots) are given for each peak. Due the limits of resolution, trimers and tetramers were treated as tetramers. Graphs were plotted from individual SEC-MALS experiments (n=1), compared with multiple concentration controls.



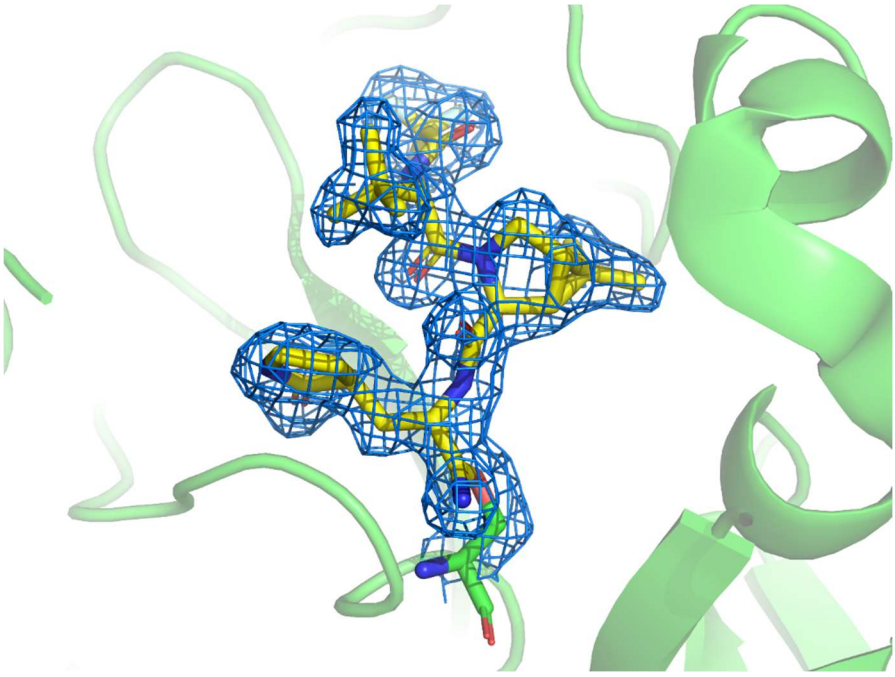
Supplementary Figure 4. Final size exclusion chromatography from SARS-CoV-2 M^{pro} C145S purification. Graph shows overlapping peaks of multiple oligomeric states. Colored areas demark fractions used for composing sample 1 (orange area) and sample 2 (green area). SDS-page shows sample 1 (left) and sample 2 (right), with molecular marker. Graphs were plotted of individual a size exclusion chromatography from SARS-CoV-2 experiment exemplary. Original SDS-page is available in Source data.



Supplementary Figure 5. SEC-MALS calibration showing two injections concentration of sample 2. In black, we see the injection of sample 2 at 60 μM, while in blue we see the injection of sample 2 at 120 μM. Graphs were plotted from individual SEC-MALS experiments in two concentrations.



Supplementary Figure 6. Native mass spectrometry analysis of M^{pro} C145S tetrameric sample in two different instruments. At the top, native mass spectrometry using Orbitrap Q-Exactive UHMR instrument. At bottom, the data from main Figure 1, collected in the Agilent 1100 HPLC system, and plotted in the same style for comparison. Monomer peaks corresponding to the light and heavy forms of M^{pro} are labelled with blue and green circles, respectively. Molecular weights are green - 33,865 ± 44 Da; blue - 34,556 ± 24 Da. Homo- and hetero-oligomer peaks are labelled according to this color scheme, with the number of each colored circle corresponding to the oligomer assignment. Graphs were plotted from individual Native mass spectrometry experiments.



Supplementary Figure 7. C145S bound to Nirmatrelvir. Figure show electron-density from Nirmatrelvir bound to C145S M^{pro}. Electron density is represented as blue mesh and was calculated from 2Fo-Fc map with 1.0 σ. Nirmatrelvir (yellow) and S145 residue are show as sticks and M^{pro} as green cartoon. Maps and models are available in PDB under code 8EYJ.

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COVID Moonshot Consortium

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