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Structure-function relationships among selected human coronaviruses

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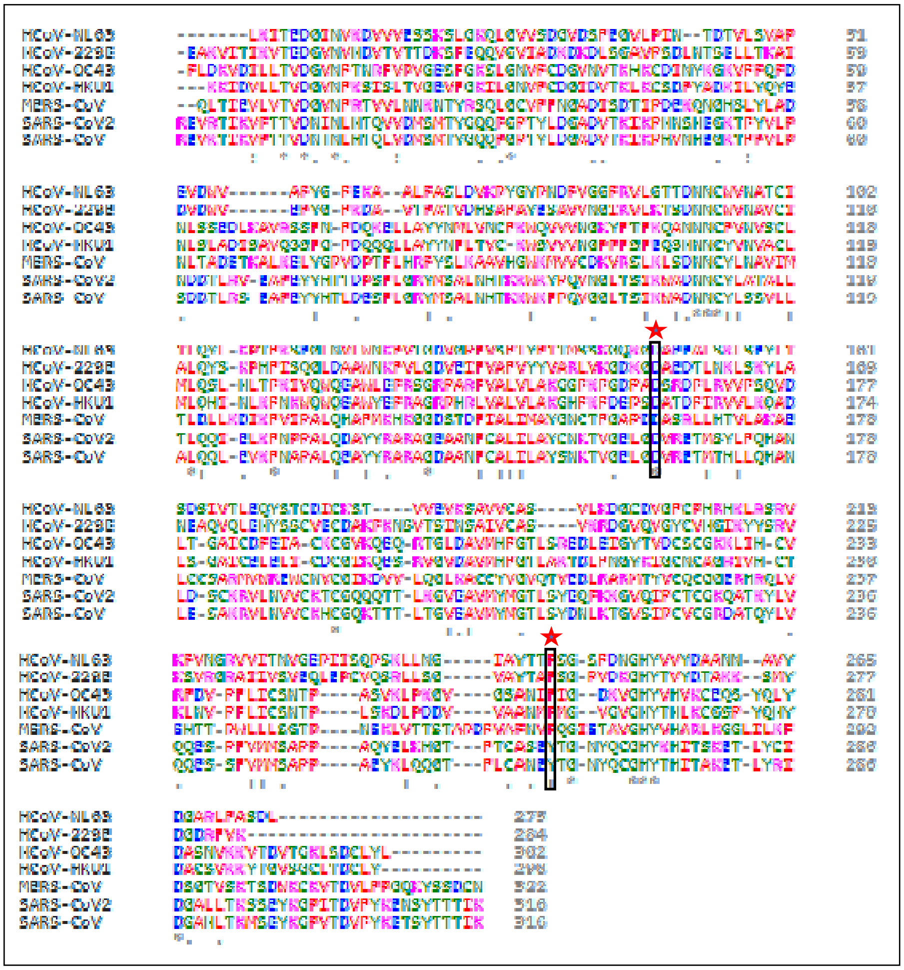
Supplementary Data



"*" Fully conserved ":" Conservation between groups of amino acids with strongly similar properties "." Conservation between groups of amino acids with weakly similar properties "*" Fully conserved ":" Conservation between groups of amino acids with strongly similar properties "." Conservation between groups of amino acids with weakly similar properties

Figure S1(a). Multiple sequence alignment of NSP3 (Pl-pro) protein of Human coronavirus OC43, Human coronavirus HKU1, Human coronavirus NL63, Human coronavirus 229E, MERS -CoV, SASR-CoV2 and SARS-CoV. The analysis was performed using Clustal Omega. The actives sites residues present in the conserved regions are highlighted in box with star marks.

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Figure S1(b). Multiple sequence alignment of NSP5 (Cl-pro) protein of Human coronavirus OC43, Human coronavirus HKU1, Human coronavirus NL63, Human coronavirus 229E, MERS -CoV, SASR-CoV2 and SARS-CoV. The analysis was performed using Clustal Omega.The actives sites residues present in the conserved regions are highlighted in box with star marks.


HCoV-NL63
HCoV-229E
HCoV-OC43
HCoV-HKU1
MERS-CoV
SARS-CoV2
SARS-CoV

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Figure S1(c). Multiple sequence alignment of NSP12 protein of Human coronavirus OC43, Human coronavirus HKU1, Human coronavirus NL63, Human coronavirus 229E, MERS -CoV, SASR-CoV2 and SARS-CoV. The analysis was performed using Clustal Omega.The actives sites residues present in the conserved regions are highlighted in box with star marks.

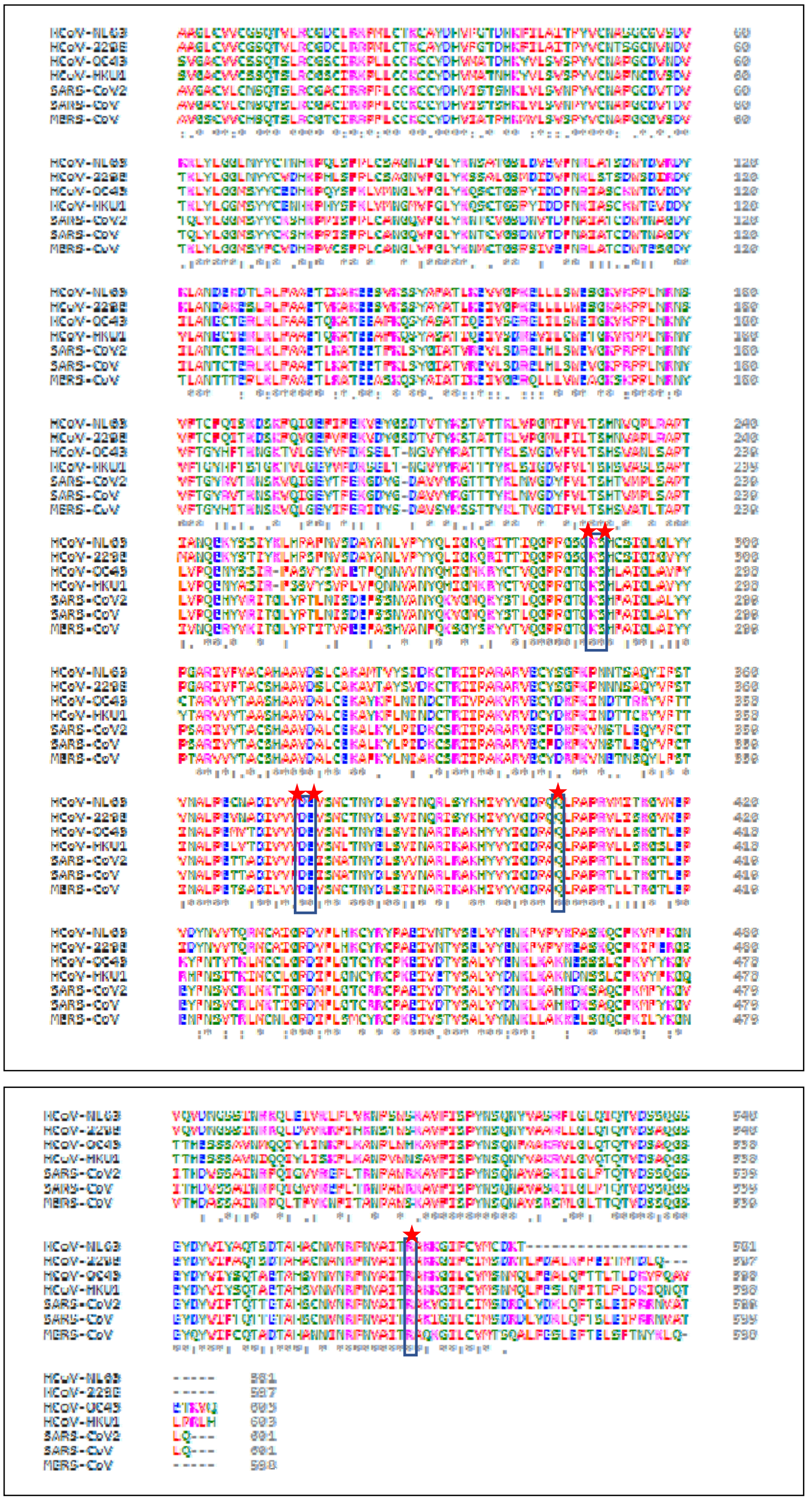

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Figure S1(d). Multiple sequence alignment of NSP13 protein of Human coronavirus OC43, Human coronavirus HKU1, Human coronavirus NL63, Human coronavirus 229E, MERS -CoV, SASR-CoV2 and SARS-CoV. The analysis was performed using Clustal Omega.The actives sites residues present in the conserved regions are highlighted in box with star marks.


HCoV-NL63
HCoV-229E
HCoV-OC43
HCoV-HKU1
MERS-CoV
SARS-CoV2
SARS-CoV

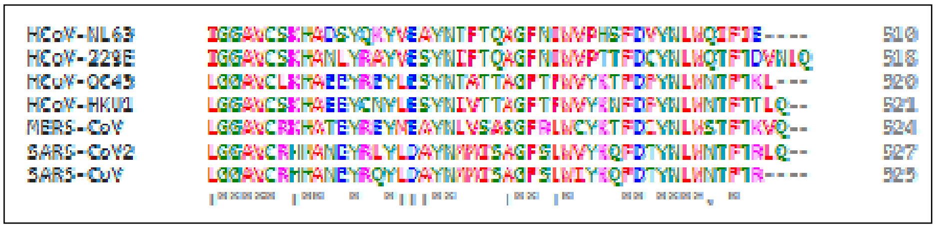

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Figure S1(e). Multiple sequence alignment of NSP14 protein of Human coronavirus OC43, Human coronavirus HKU1, Human coronavirus NL63, Human coronavirus 229E, MERS -CoV, SASR-CoV2 and SARS-CoV. The analysis was performed using Clustal Omega. The actives sites residues present in the conserved regions are highlighted in box with star marks.

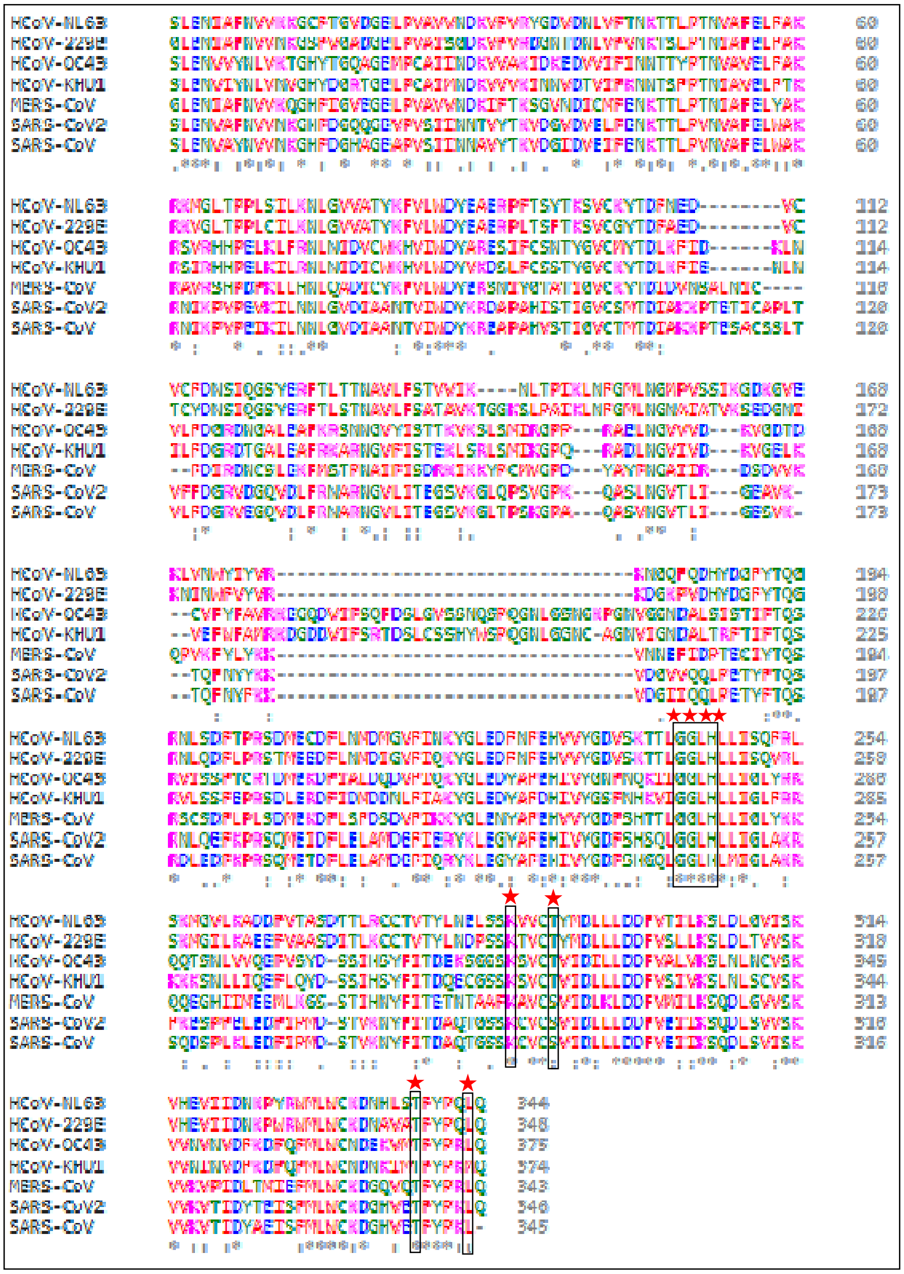

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Figure S1(f). Multiple sequence alignment of NSP15 protein of Human coronavirus OC43, Human coronavirus HKU1, Human coronavirus NL63, Human coronavirus 229E, MERS -CoV, SASR-CoV2 and SARS-CoV. The analysis was performed using Clustal Omega.The actives sites residues present in the conserved regions are highlighted in box with star marks.

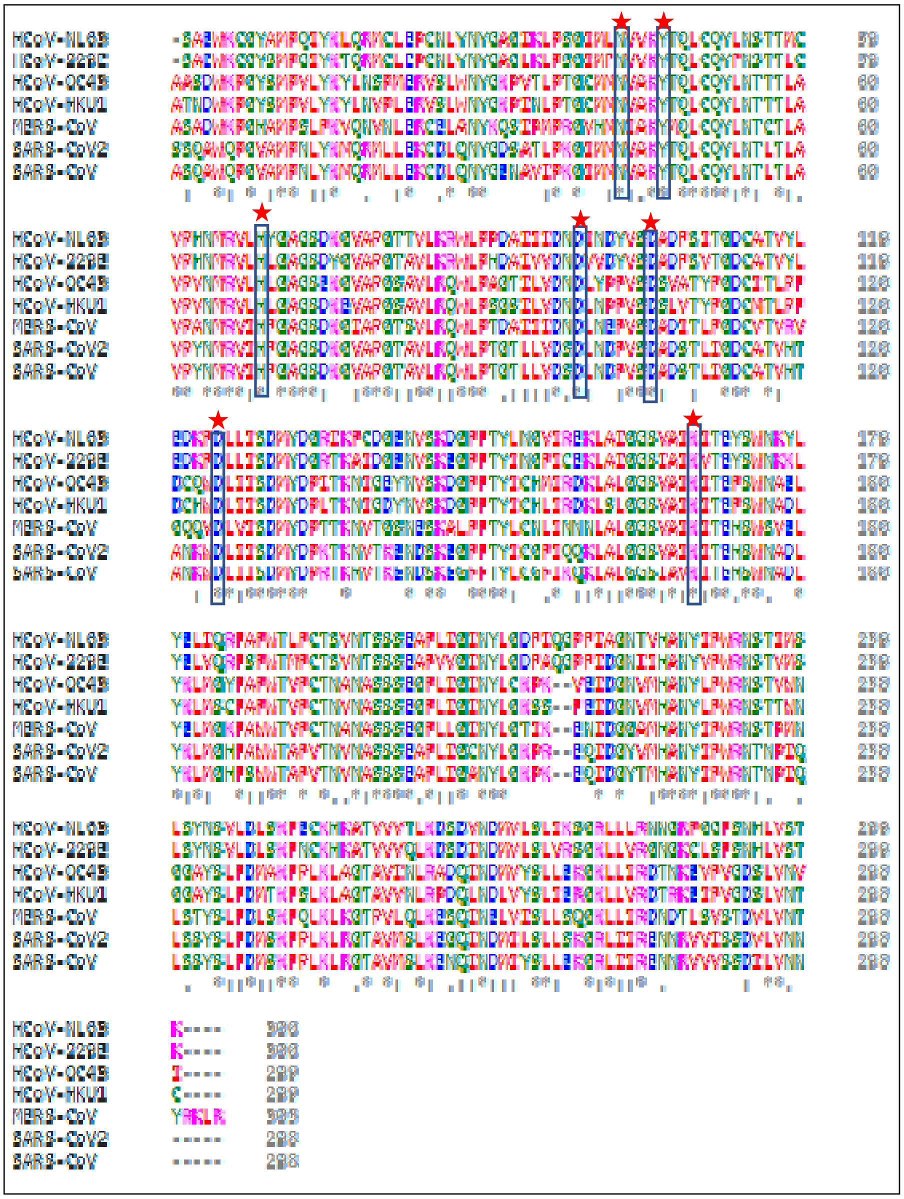

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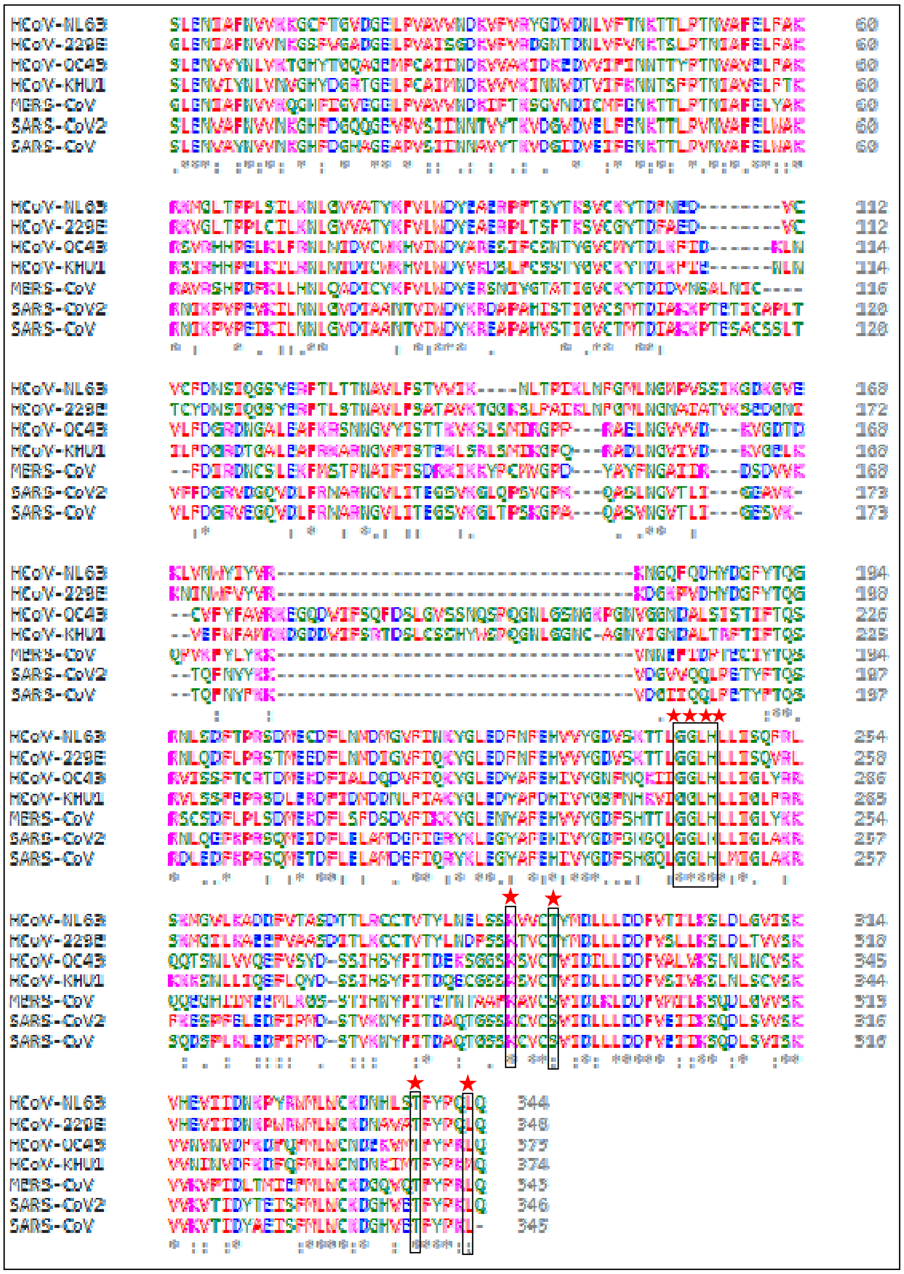
Figure S1(g). Multiple sequence alignment of NSP16 protein of Human coronavirus OC43, Human coronavirus HKU1, Human coronavirus NL63, Human coronavirus 229E, MERS -CoV, SASR-CoV2 and SARS-CoV. The analysis was performed using Clustal Omega. The actives sites residues present in the conserved regions are highlighted in box with star marks.



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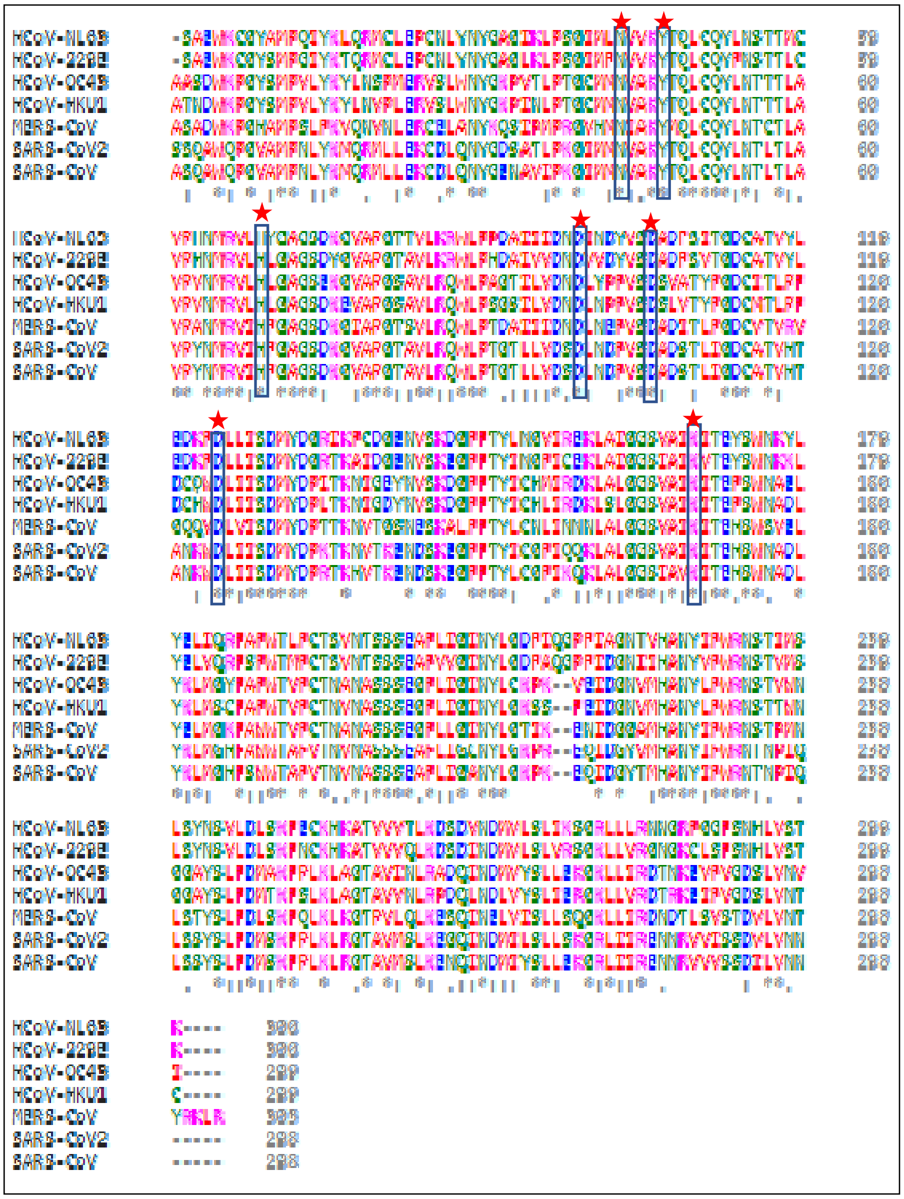

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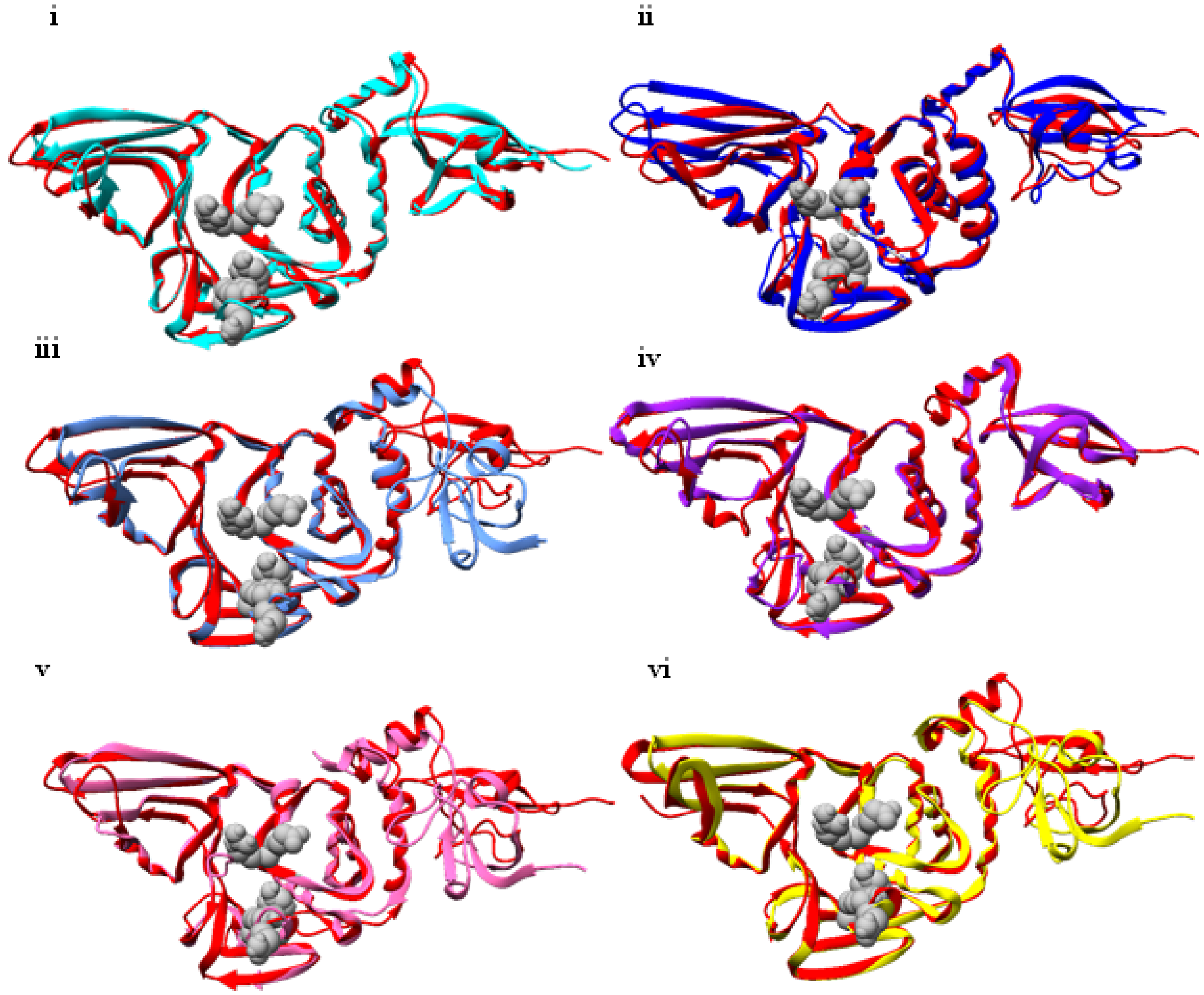


Figure S2(a). Superimposed structures of NSP3 (Pl-pro) of i) SARS-CoV2 vs SARS-CoV ii) SARS-CoV2 vs MERS-CoV iii) SARS-CoV2 vs HCoV-HKU1 iv) SARS-CoV2 vs HCoV-NL63 v) SARS-CoV2 vs HCoV-229E vi) SARS-CoV2 vs HCoV-OC43 using TM-Align and UCSF Chimera.

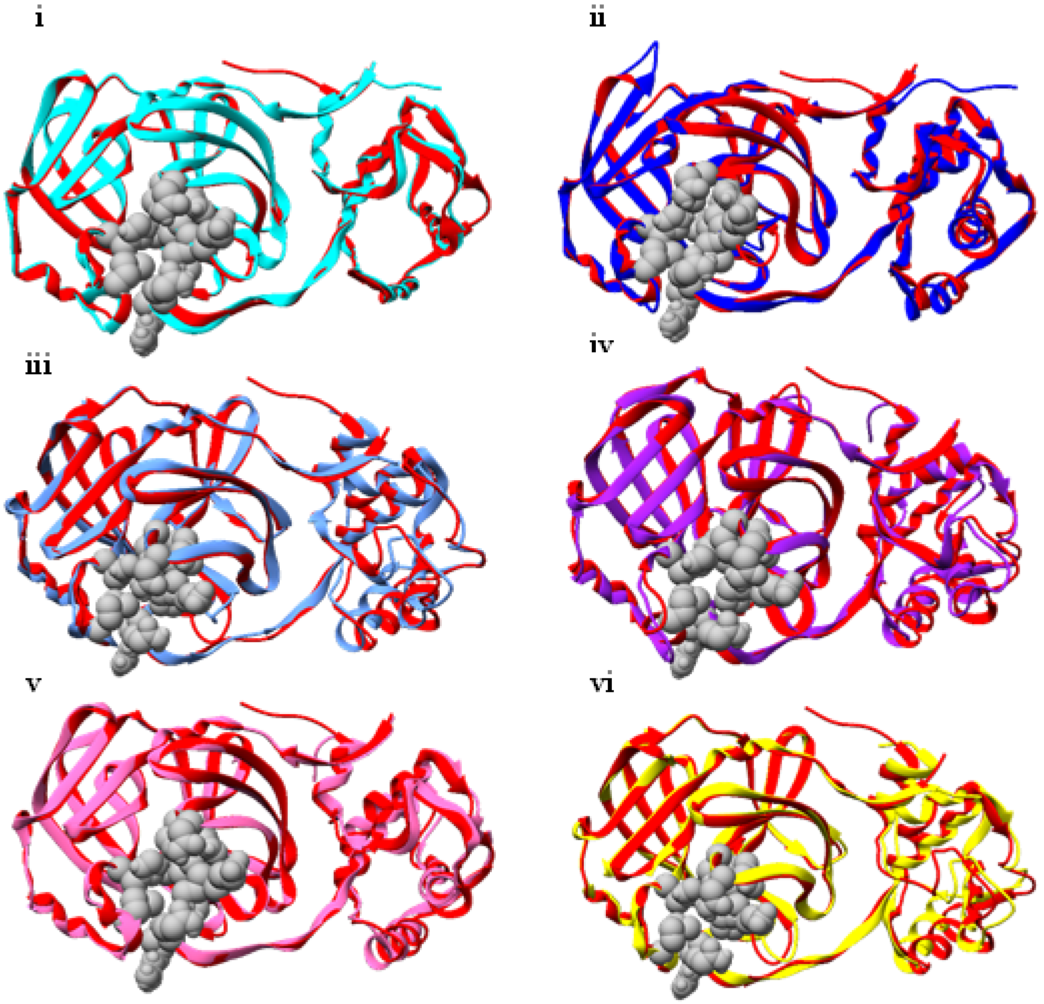


Figure S2 (b). Superimposed structures of NSP5 (3Cl-pro) of i) SARS-CoV2 vs SARS-CoV ii) SARS-CoV2 vs MERS-CoV iii) SARS-CoV2 vs HCoV-HKU1 iv) SARS-CoV2 vs HCoV-NL63 v) SARS-CoV2 vs HCoV-229E vi) SARS-CoV2 vs HCoV-OC43 using TM-Align and UCSF Chimera.

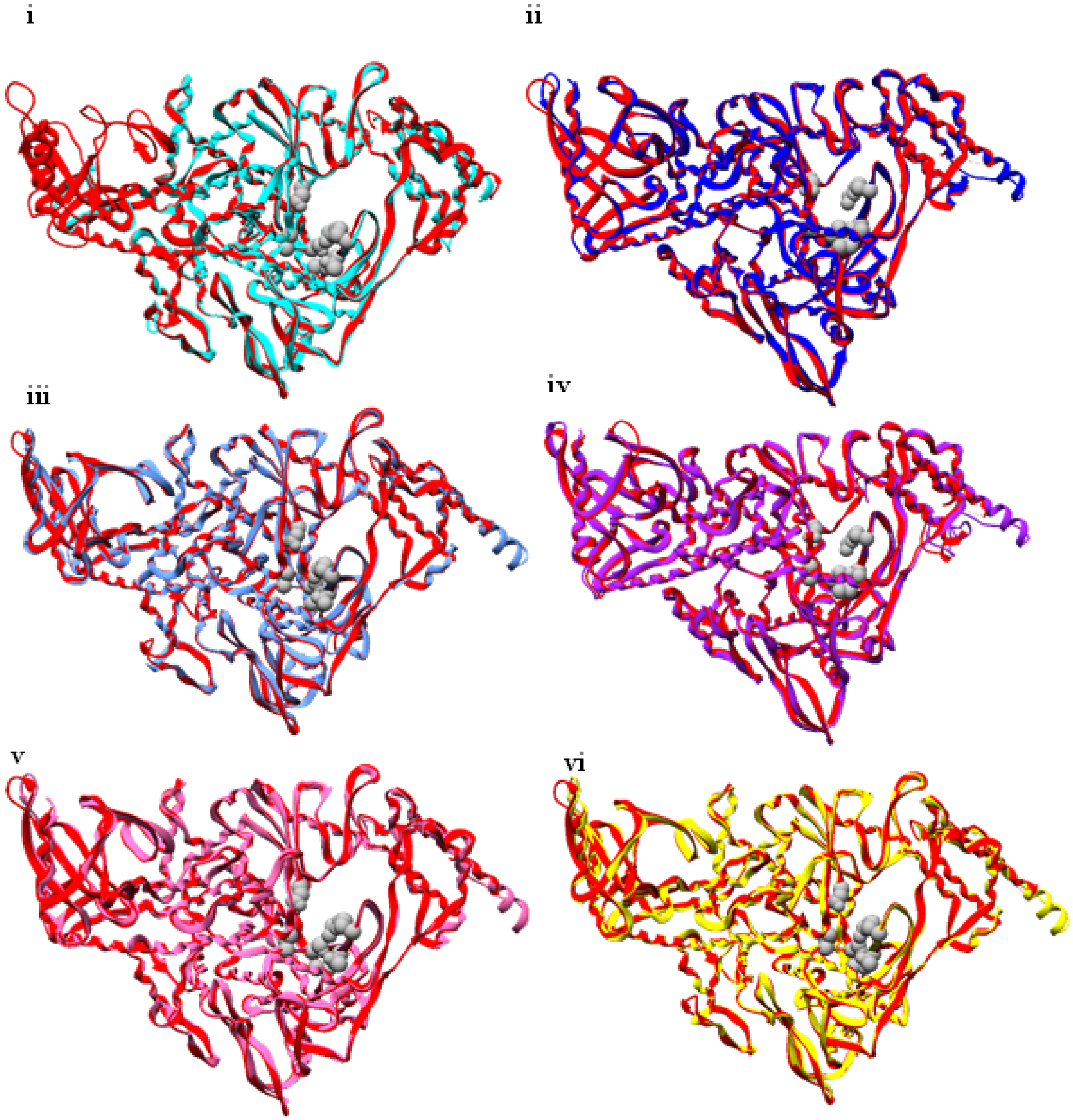


Figure S2 (c). Superimposed structures of NSP12 of i) SARS-CoV2 vs SARS-CoV ii) SARS-CoV2 vs MERS-CoV iii) SARS-CoV2 vs HCoV-HKU1 iv) SARS-CoV2 vs HCoV-NL63 v) SARS-CoV2 vs HCoV-229E vi) SARS-CoV2 vs HCoV-OC43 using TM-Align and UCSF Chimera.

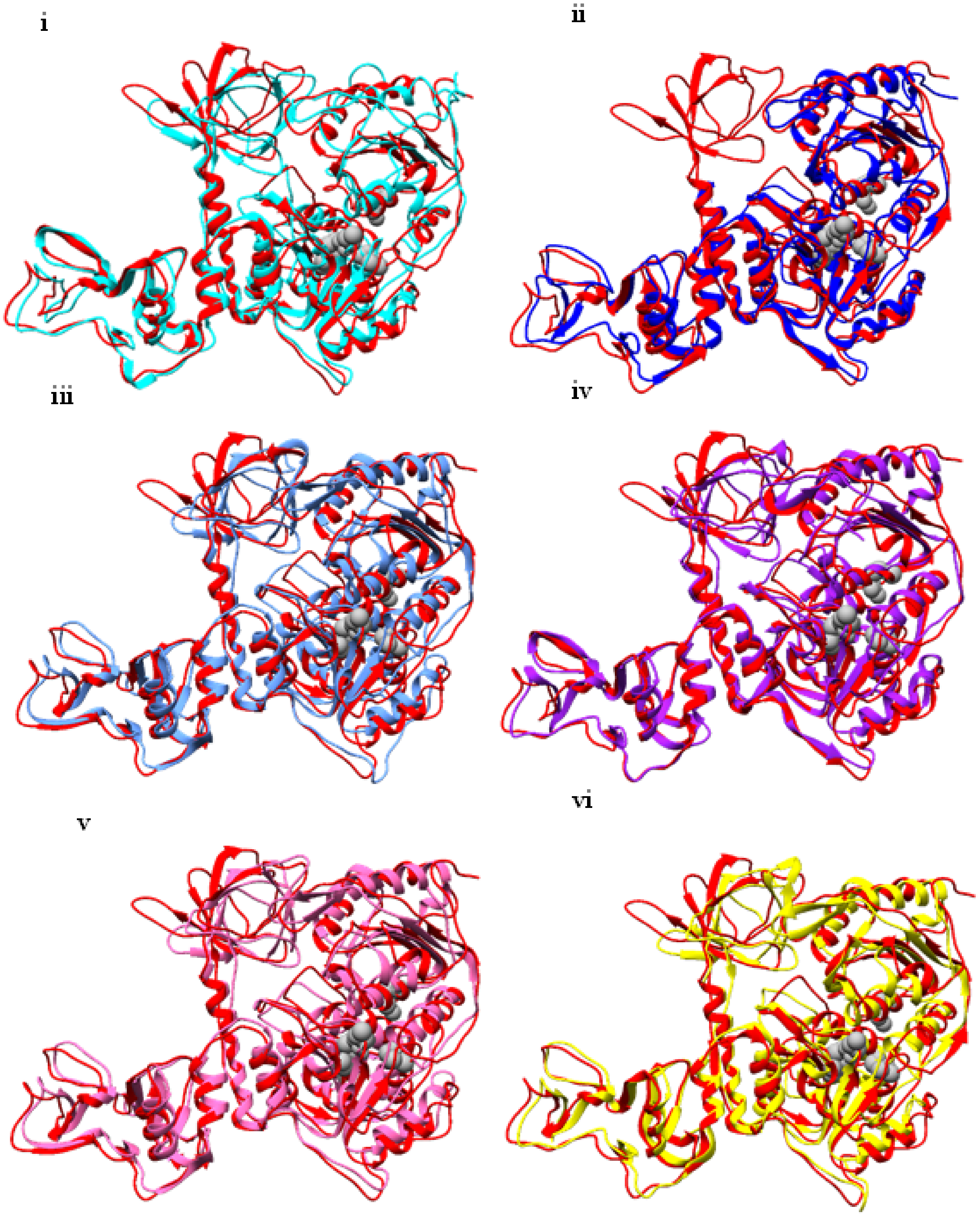


Figure S2 (d). Superimposed structures of NSP13 of i) SARS-CoV2 vs SARS-CoV ii) SARS-CoV2 vs MERS-CoV iii) SARS-CoV2 vs HCoV-HKU1 iv) SARS-CoV2 vs HCoV-NL63 v) SARS-CoV2 vs HCoV-229E vi) SARS-CoV2 vs HCoV-OC43 using TM-Align and UCSF Chimera.

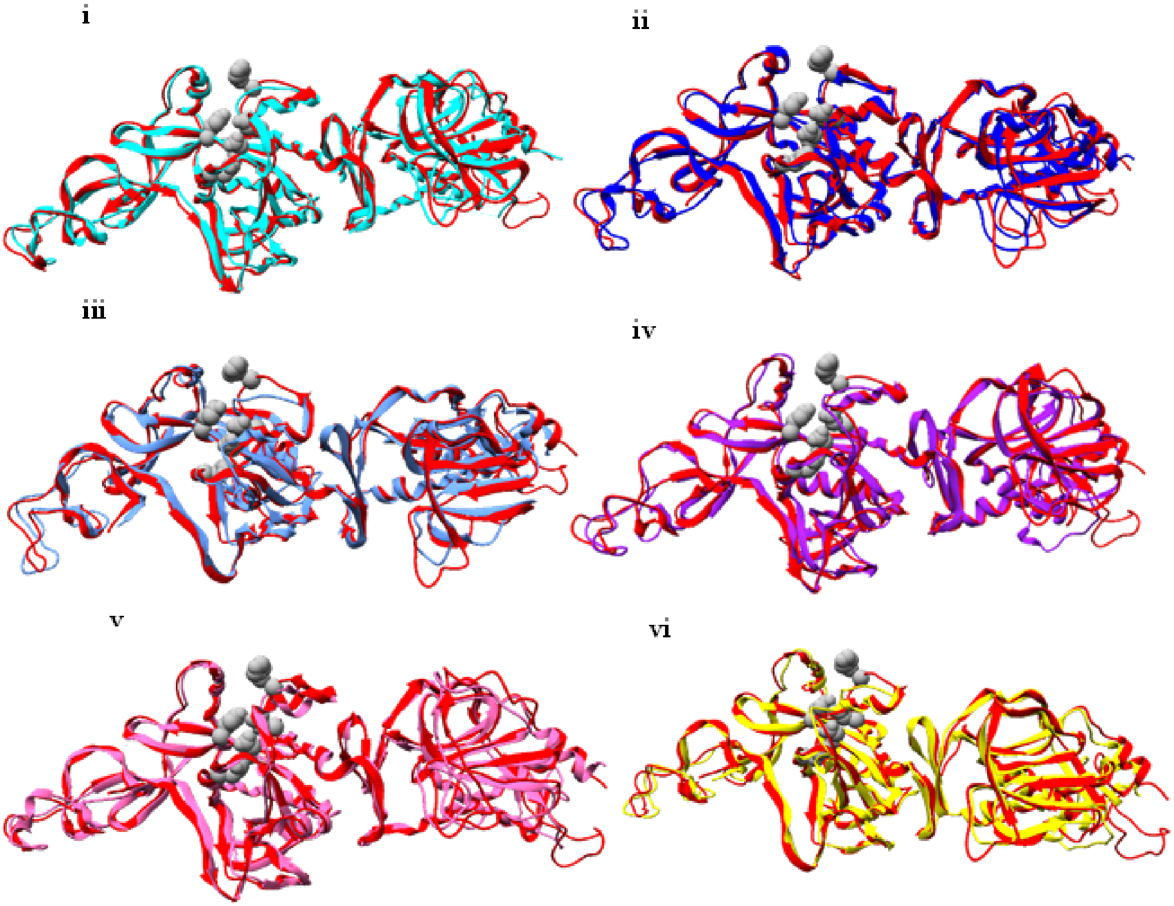


Figure S2 (e). Superimposed structures of NSP14 of i) SARS-CoV2 vs SARS-CoV ii) SARS-CoV2 vs MERS-CoV iii) SARS-CoV2 vs HCoV-HKU1 iv) SARS-CoV2 vs HCoV-NL63 v) SARS-CoV2 vs HCoV-229E vi) SARS-CoV2 vs HCoV-OC43 using TM-Align and UCSF Chimera.

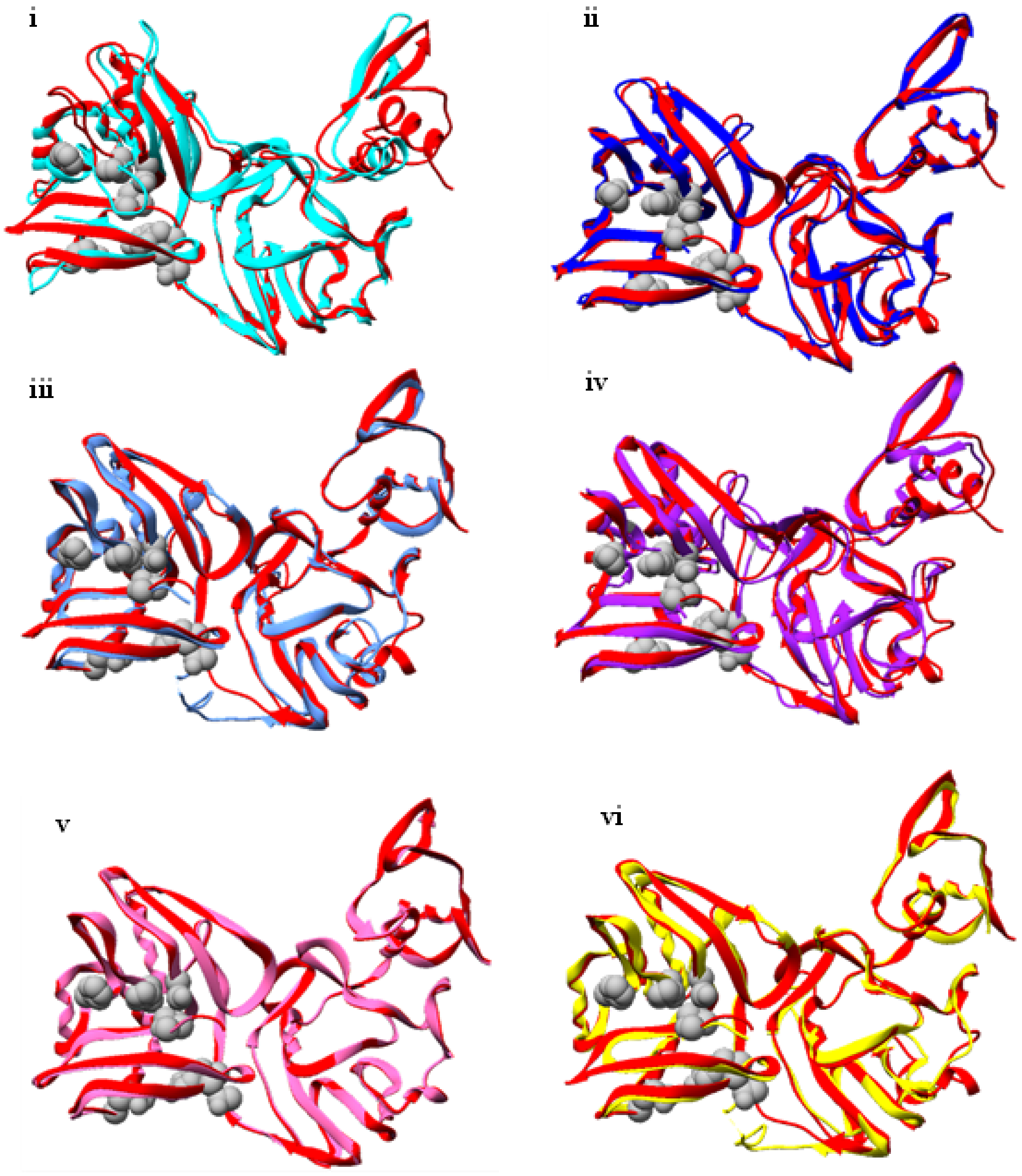


Figure S2 (f). Superimposed structures of NSP15 of i) SARS-CoV2 vs SARS-CoV ii) SARS-CoV2 vs MERS-CoV iii) SARS-CoV2 vs HCoV-HKU1 iv) SARS-CoV2 vs HCoV-NL63 v) SARS-CoV2 vs HCoV-229E vi) SARS-CoV2 vs HCoV-OC43 using TM-Align and UCSF Chimera.

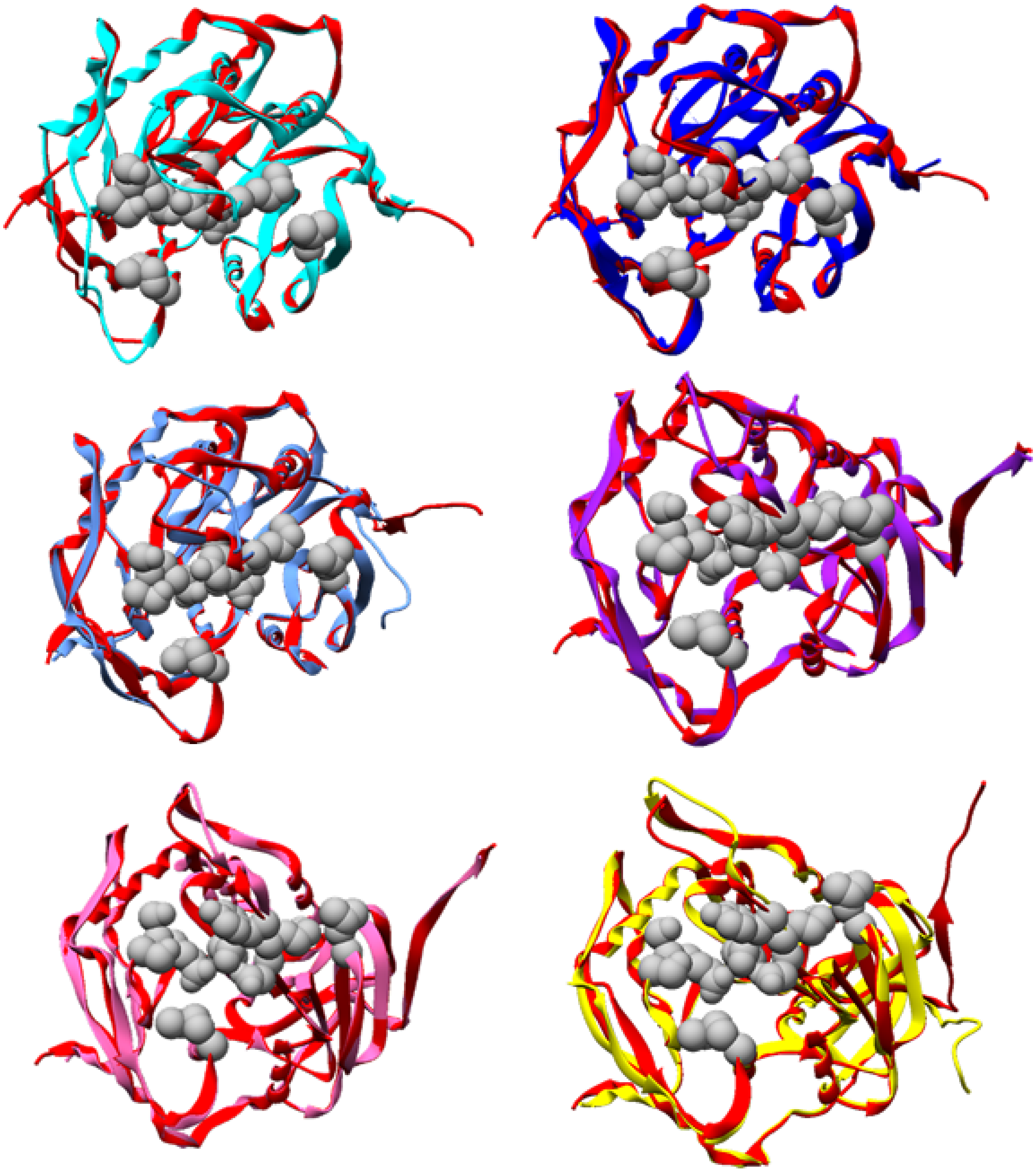


Figure S2 (g). Superimposed structures of NSP16 of i) SARS-CoV2 vs SARS-CoV ii) SARS-CoV2 vs MERS-CoV iii) SARS-CoV2 vs HCoV-HKU1 iv) SARS-CoV2 vs HCoV-NL63 v) SARS-CoV2 vs HCoV-229E vi) SARS-CoV2 vs HCoV-OC43 using TM-Align and UCSF Chimera.

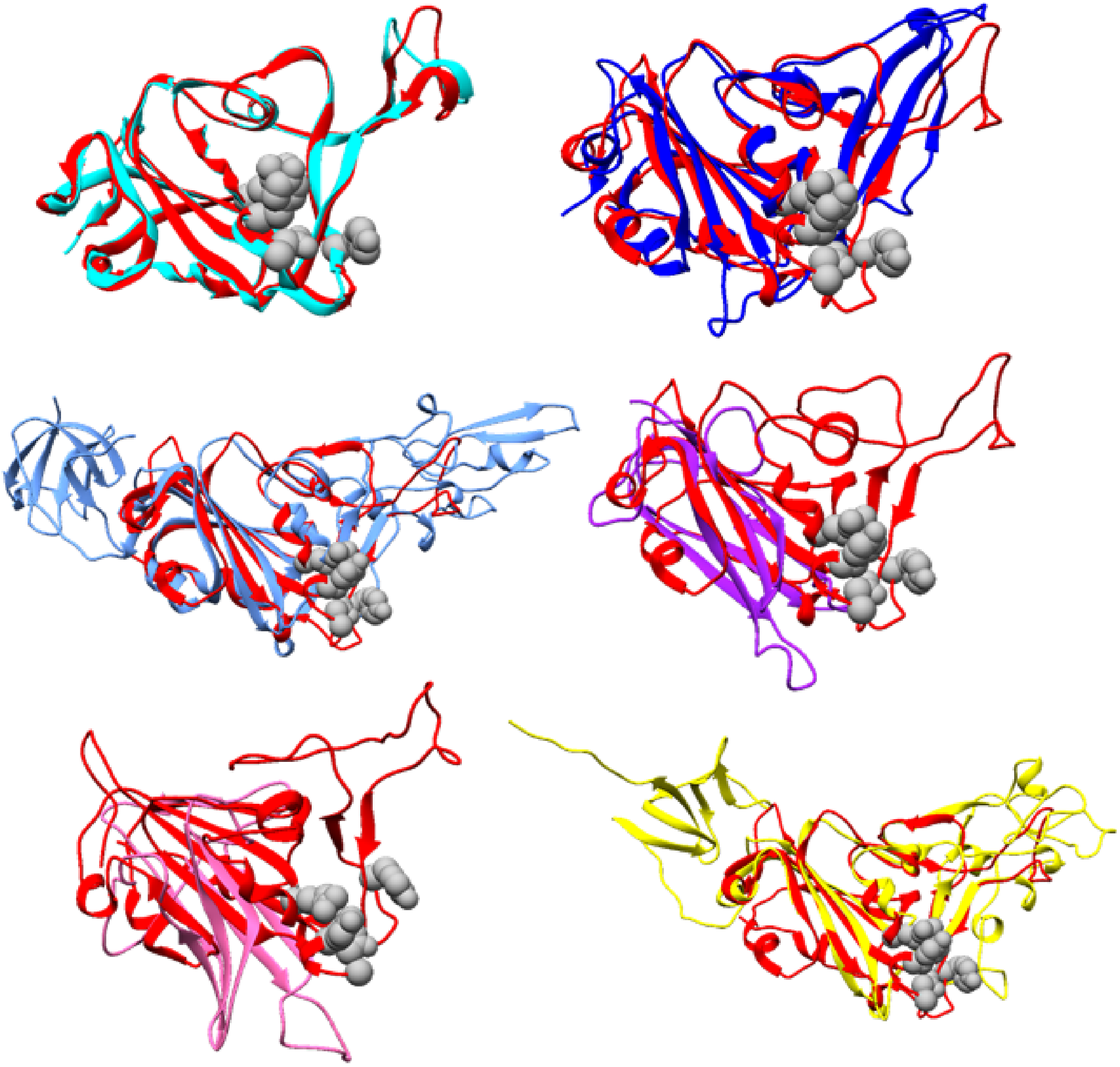


Figure S2(h). Superimposed structures of Spike RBD of i) SARS-CoV2 vs SARS-CoV ii) SARS-CoV2 vs MERS-CoV iii) SARS-CoV2 vs HCoV-HKU1 iv) SARS-CoV2 vs HCoV-NL63 v) SARS-CoV2 vs HCoV-229E vi) SARS-CoV2 vs HCoV-OC43 using TM-Align and UCSF Chimera

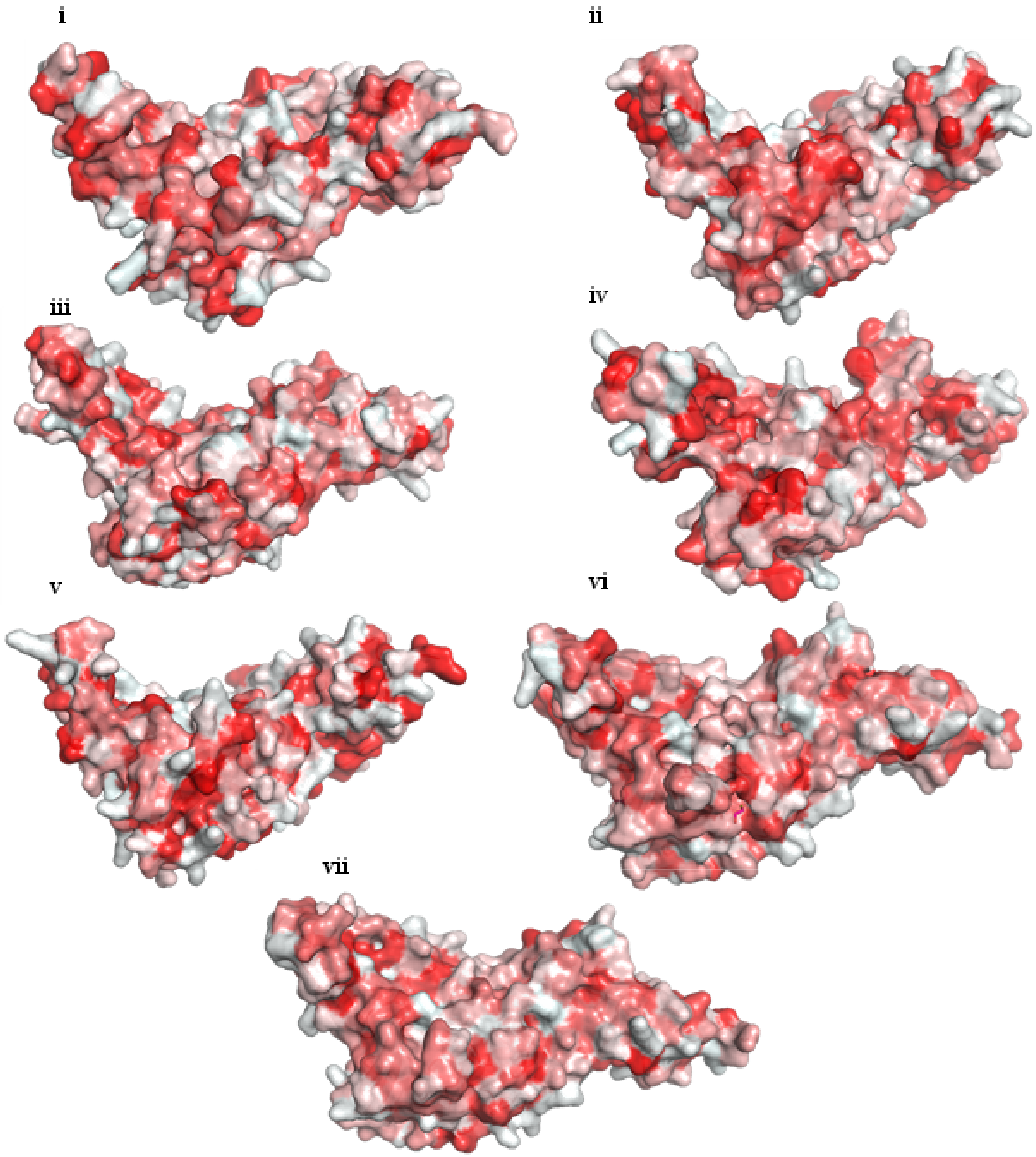


Figure S3(a). Hydrophobicity map of NSP3 protein surface of all 7 types of corona viruses (i) 229E, (ii) HKU1 (iii) MERS CoV (iv) NL63 (v) OC43 (vi)SARS CoV and (vii) SARS CoV2. Red colour regions indicate hydrophobicity and white colour regions indicate hydrophilicity.

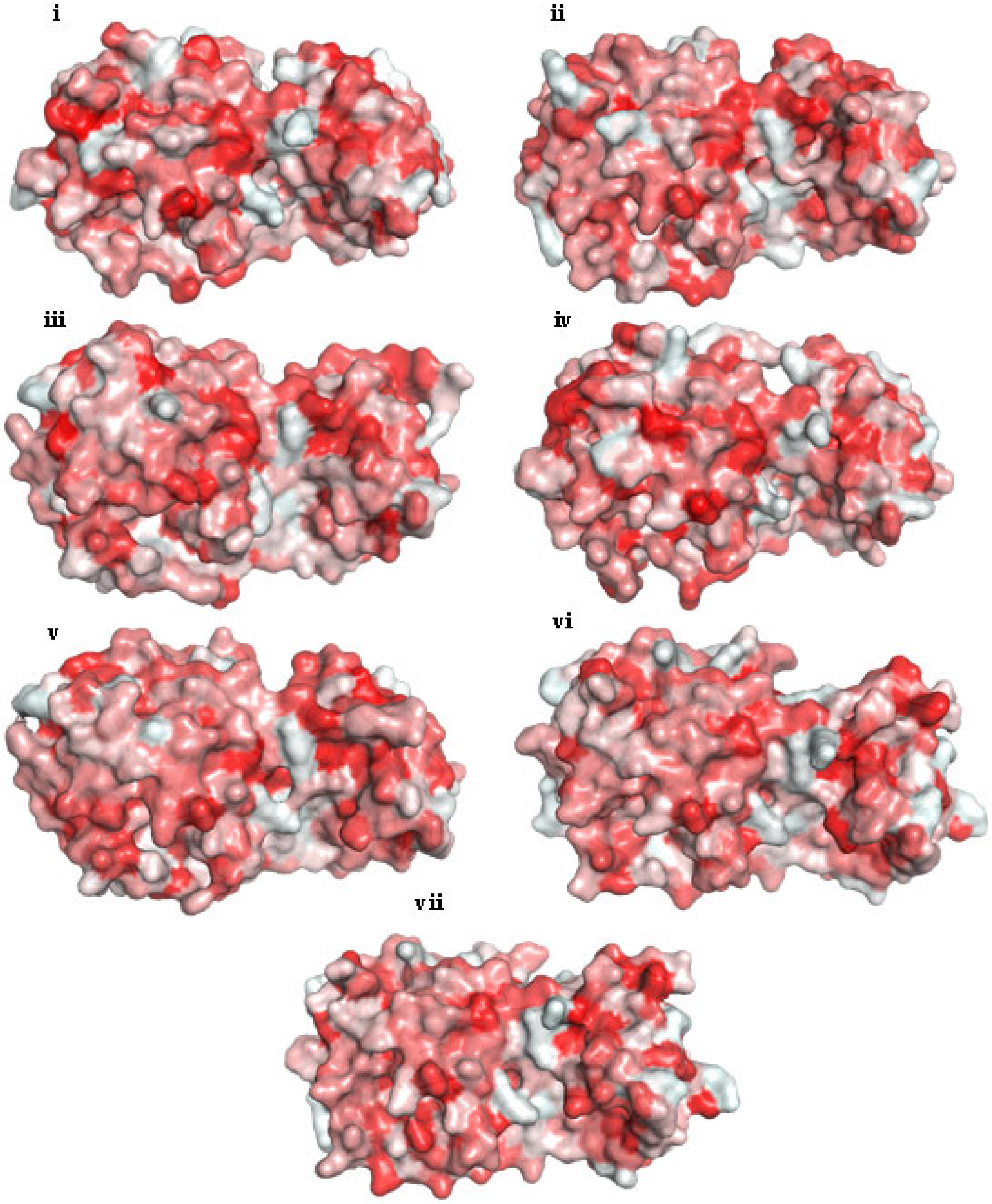


Figure S3 (b). Hydrophobicity map of NSP5 protein surface of all 7 types of corona viruses (i) 229E, (ii) HKU1 (iii) MERS CoV (iv) NL63 (v) OC43 (vi) SARS CoV and (vii) SARS CoV2. Red colour regions indicate hydrophobicity and white colour regions indicate hydrophilicity.

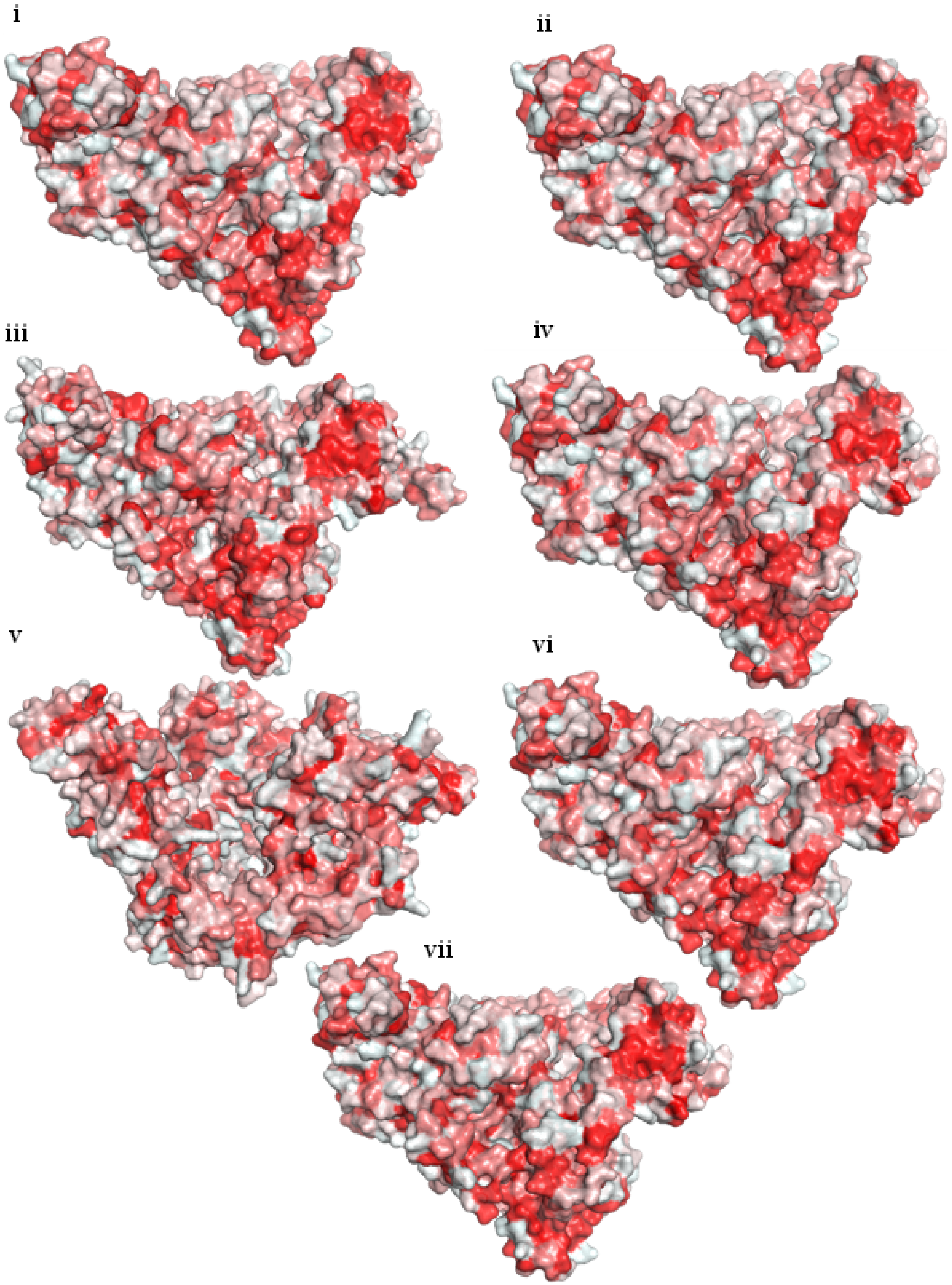


Figure S3(c). Hydrophobicity map of NSP12 protein surface of all 7 types of corona viruses (i) 229E, (ii) HKU1 (iii) MERS CoV (iv) NL63 (v) OC43 (vi) SARS CoV and (vii) SARS CoV2. Red colour regions indicate hydrophobicity and white colour regions indicate hydrophilicity

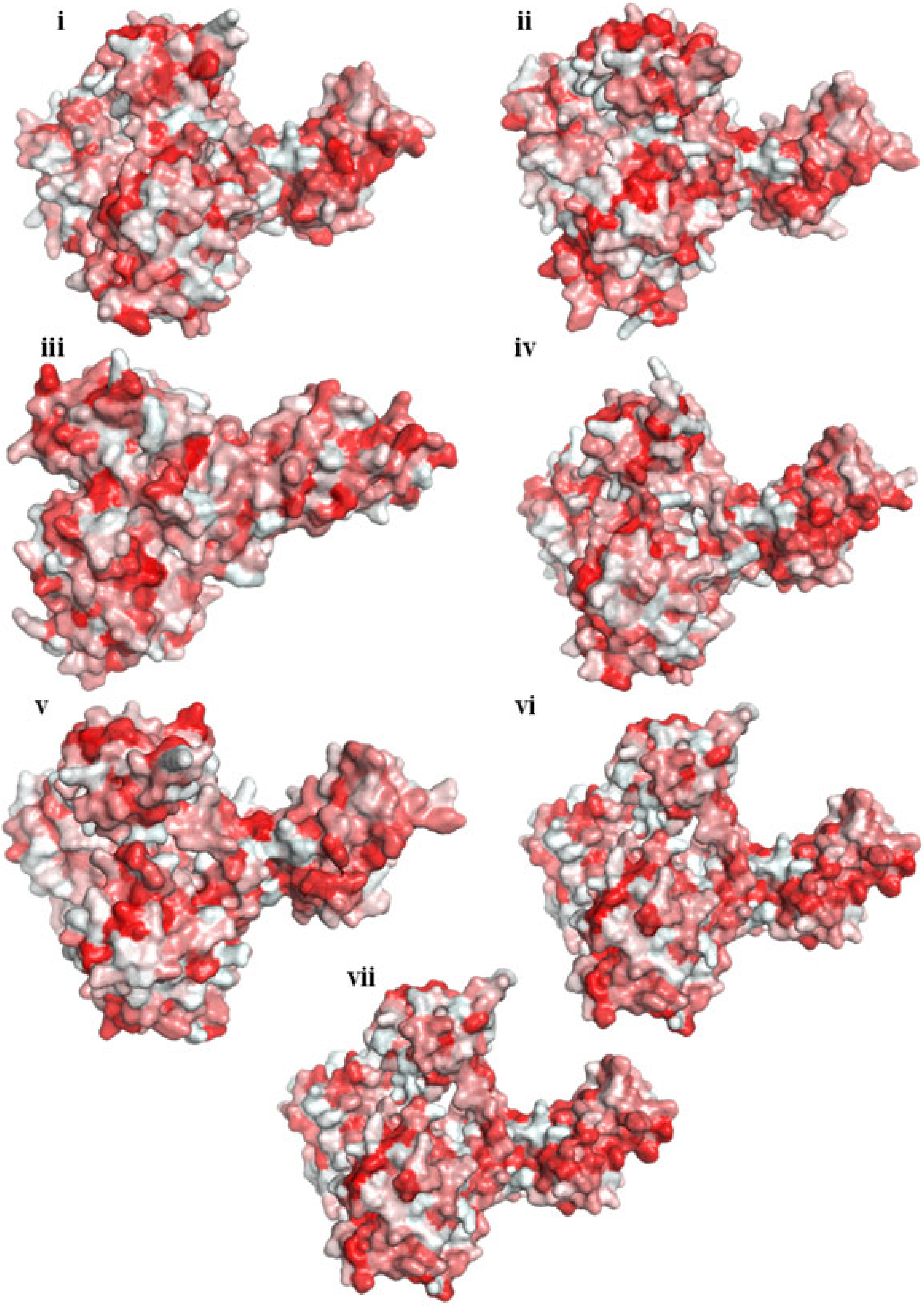


Figure S3(d). Hydrophobicity map of NSP13 protein surface of all 7 types of corona viruses (i) 229E, (ii) HKU1 (iii) MERS CoV (iv) NL63 (v) OC43 (vi) SARS CoV and (vii) SARS CoV2. Red colour regions indicate hydrophobicity and white colour regions indicate hydrophilicity

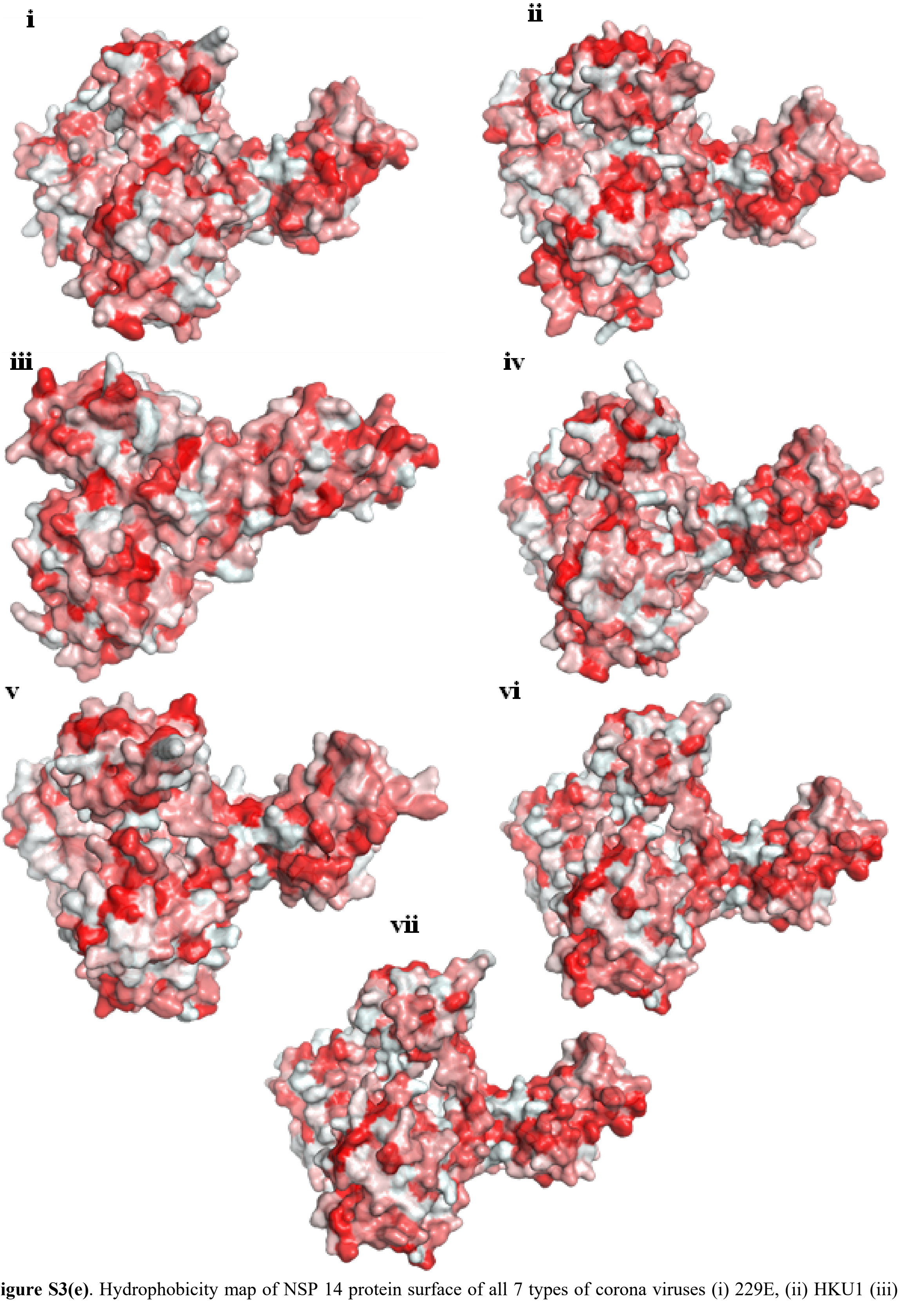


Figure S3(e). Hydrophobicity map of NSP 14 protein surface of all 7 types of corona viruses (i) 229E, (ii) HKU1 (iii) MERS CoV (iv)

NL63 (v) OC43 (vi) SARS CoV (vii) SARS CoV2. Red colour regions indicate hydrophobicity and white colour regions indicate hydrophilicity.

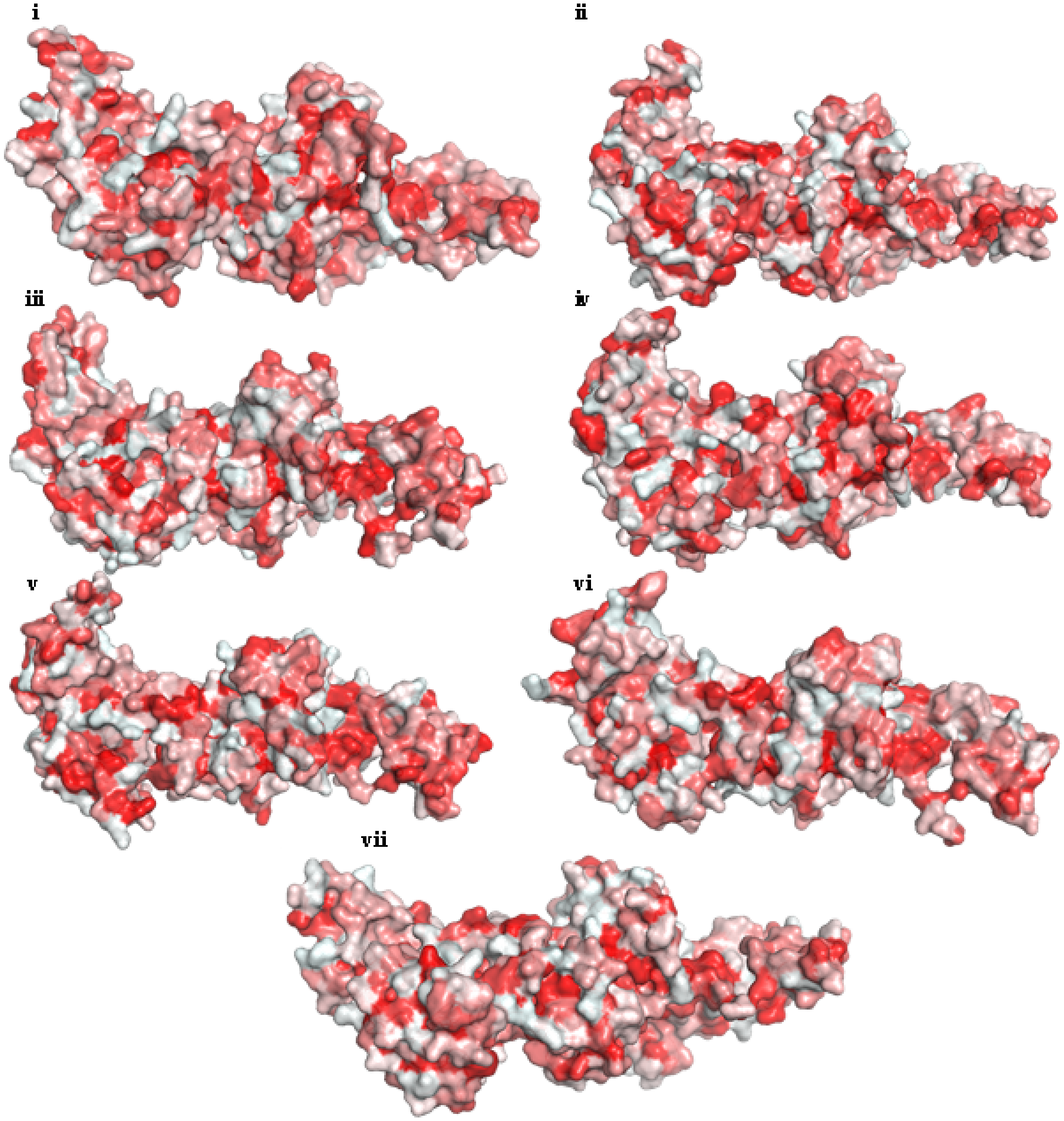


Figure S3(f). Hydrophobicity map of NSP 15 protein surface of all 7 types of corona viruses (i) 229E, (ii) HKU1 (iii) MERS CoV (iv) NL63 (v) OC43 (vi) SARS CoV and (vii) SARS CoV2. Red colour regions indicate hydrophobicity and white colour regions indicate hydrophilicity.

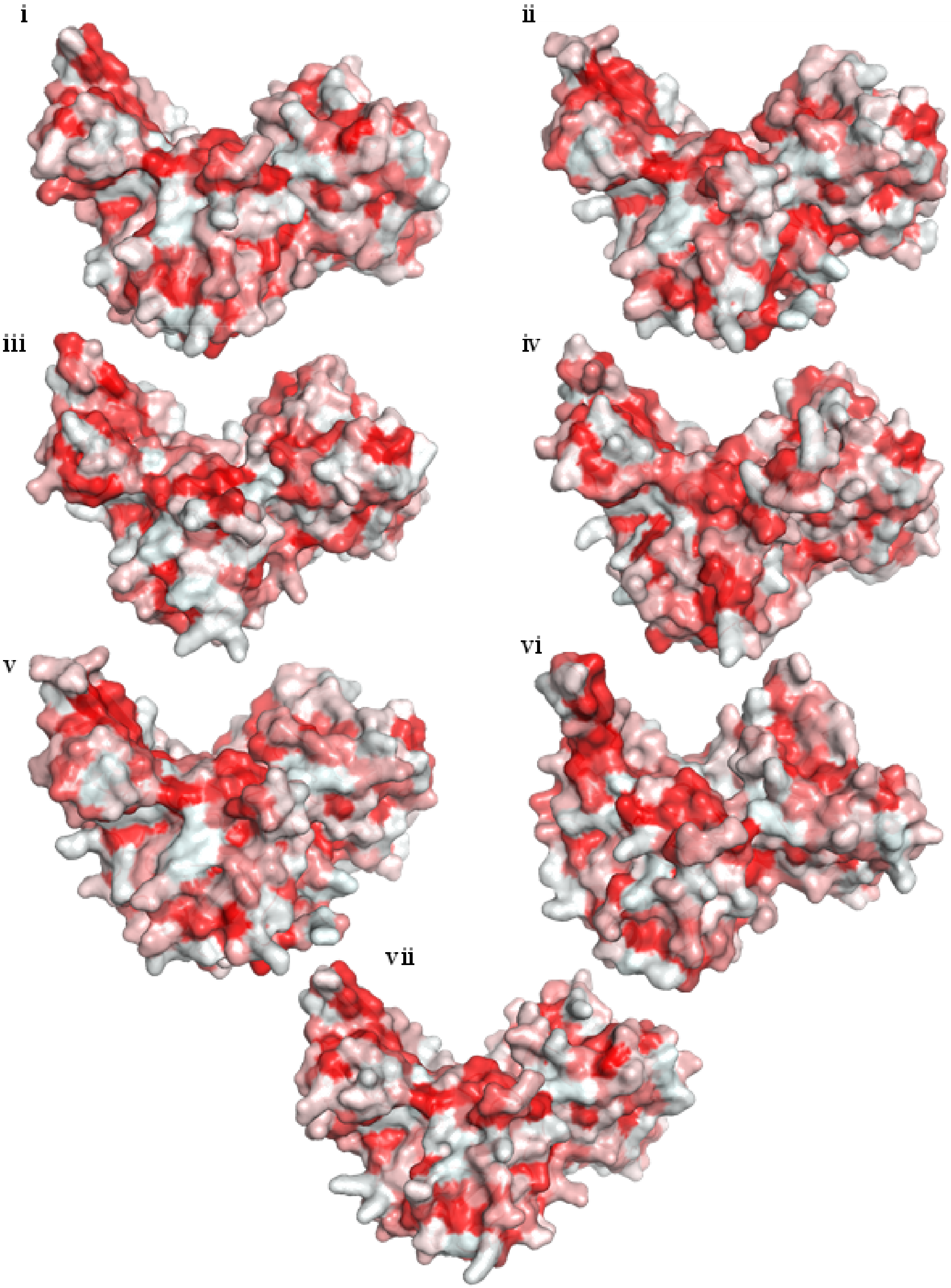


Figure S3(g). Hydrophobicity map of NSP 16 protein surface of all 7 types of corona viruses (i) 229E, (ii) HKU1 (iii) MERS CoV (iv) NL63 (v) OC43 (vi) SARS CoV and (vii) SARS CoV2. Red colour regions indicate hydrophobicity and white colour regions indicate hydrophilicity.

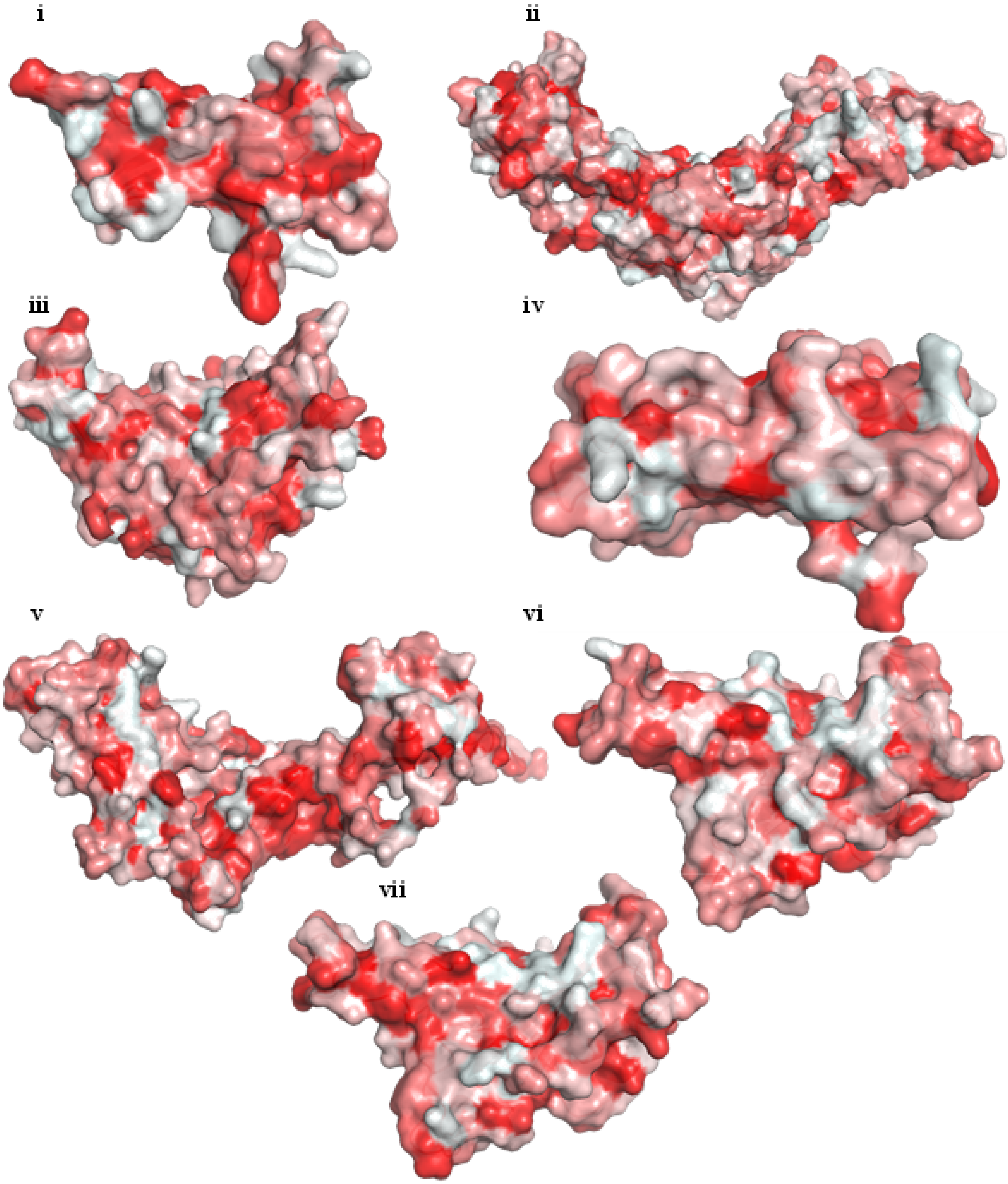
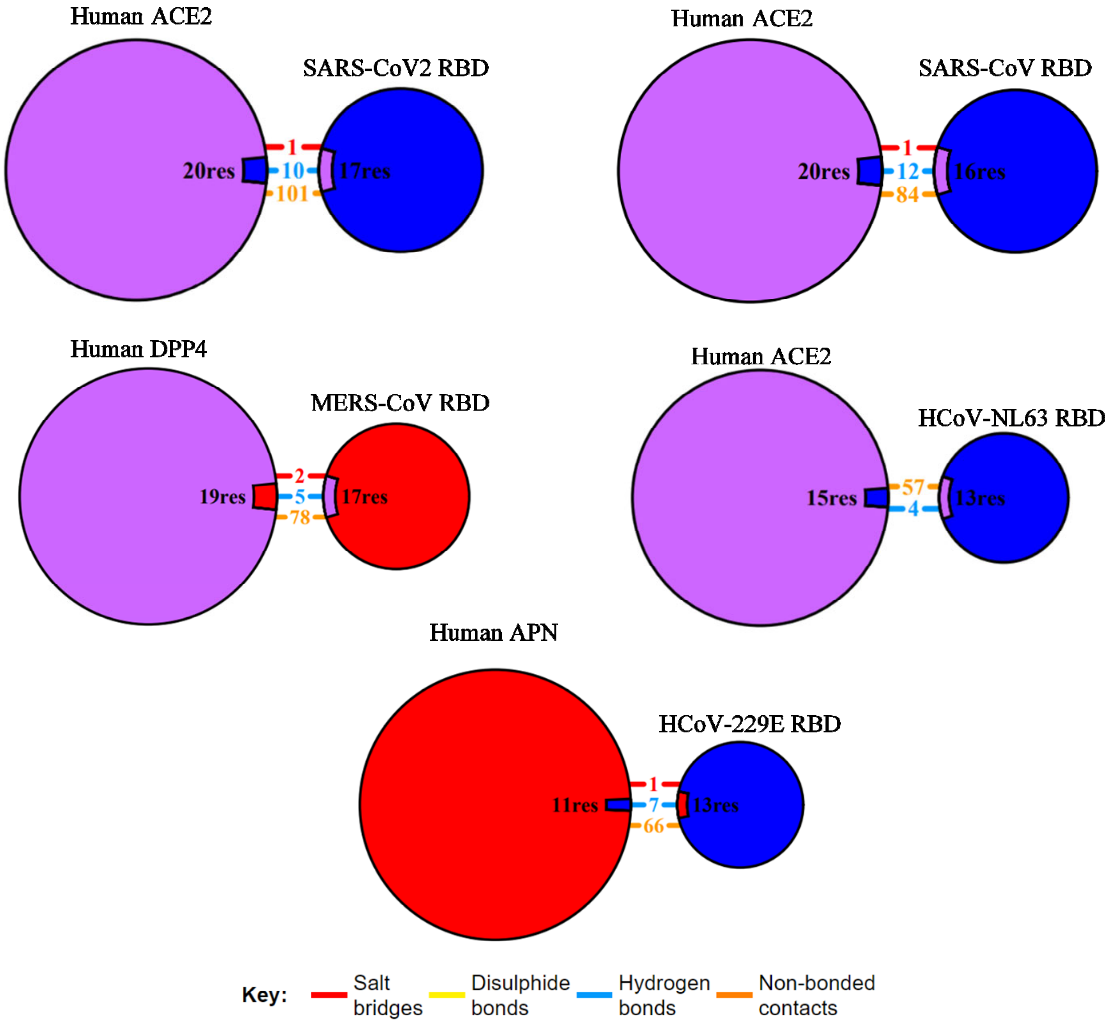


Figure S3(h): Hydrophobicity map of Spike protein surface of all 7 types of corona viruses (i) 229E, (ii) HKU1 (iii) MERS CoV (iv) NL63 (v) OC43 (vi) SARS CoV and (vii) SARS CoV2. Red colour regions indicate hydrophobicity and white colour regions indicate hydrophilicity



*ACE2 (Angiotensin-converting enzyme 2), APN (Aminopeptidase N), DPP4 (Dipeptidyl peptidase 4)

Figure S4. The protein-protein interface between the viral spike receptor binding domain and host proteins. The interactions are represented for SARS-CoV2 with ACE2, SARS-CoV with ACE2, MERS-CoV with DPP4, HCoV-NL63 with ACE2, HCoV-229E with APN. The diagrammatic representation indicates the interaction interface between the proteins such as salt bridges, hydrogen bonds and non-bonded contacts.