

Homework 1: Domains in SARS-2 spike

Open SAR-2 spike protein in MOE. PDB id 6vsb.

Delete the NAG chains.

In the SEQ window, align the three chains. **Superpose** them.

Note that the domains do not superpose well. For each domain, select the domain residues in the MOE window (left-mouse drag), set **Superpose** to use **selected residues**, then superpose.

Answer the following questions. Paste all into a single file and save it as a PDF file.

Upload the PDF file to the Homework Server.

Domain 1: Residues 1 - 295

1.0. What is the SCOP class

1.1. How many beta sheets does it have? A beta sheet is defined as a set of beta strands that have hydrogen bonds between their backbone NH and CO groups.

1.2 How many beta strands make up each beta sheet?

1.3 What is the strand order for the sheet that have seven strands?

Domain 2. Residues 330-525 (ignore residues 444-502), the receptor binding domain (RBD).

2.1 What is the SCOP class?

2.2 What is the strand order of the 5-stranded beta sheet? (start with the lower numbered end)

2.3 Draw a TOPS diagram. Alpha helix is defined as anything that is colored red when the ribbon is colored by "structure", *except* it must be at least 4 residues long.

Domain 3. Residues 449-590, 322-331

3.1. Is this domain a beta barrel (yes/no)?

3.2 How many beta strands in the beta sheet?

3.3 What is the strand order?

3.4 Is the beta sheet (all antiparallel, all parallel, mostly antiparallel, or mostly parallel) ?

Domain 4. 590-700, 308-320

4.1 Write the strand order for each beta sheet.

Domain 5. 715-1070

5.1 What is the SCOP class of this domain

5.2 Draw a simplified contact map for residues 950-1017

5.3 Draw a simplified contact map of residues 1045-1068, 718-730