# **Analysis of Second Vassiliev Measure Scans for SARS-CoV-2 S Proteins**

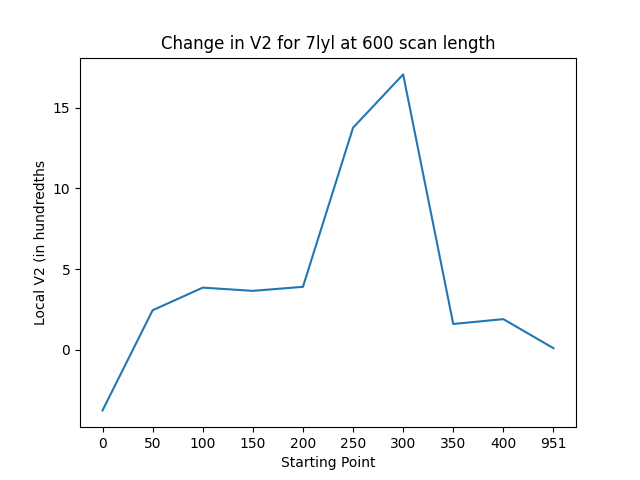
6/23/21

## Introduction

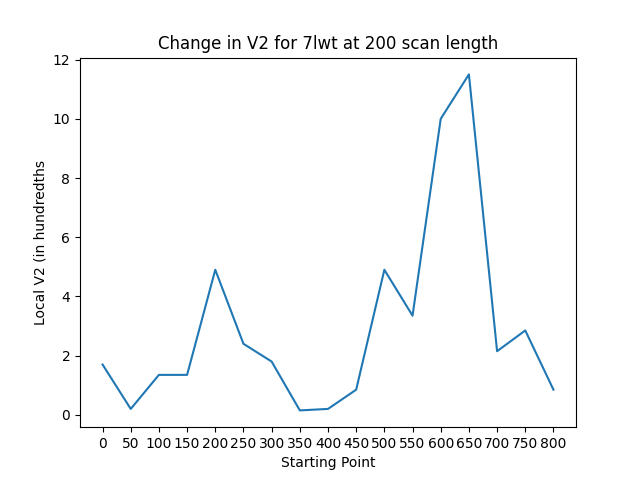
The sections following are an analysis comparing different versions of the spike proteins (S proteins) of SARS-CoV-2, its variants, and SARS-CoV from 2003. These proteins are analyzed with regards to a topological calculation called the second Vassiliev measure (V2).

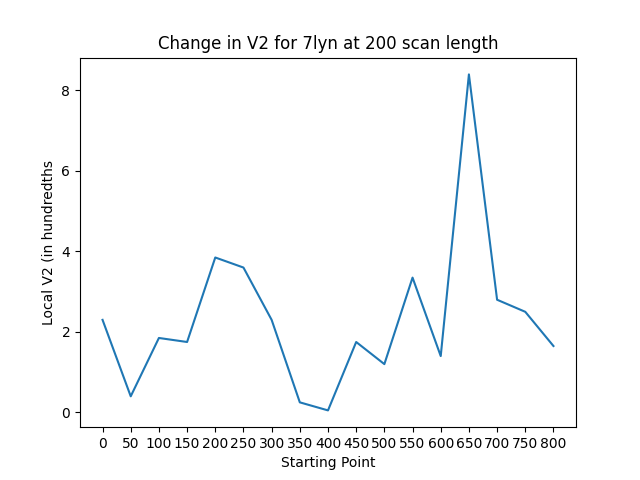
## Alpha and Beta

Both of the figures shown below display the change in V2 as the scans’ starting points increase, both figures using 600 scan lengths. These are for S proteins of the Alpha (7lws) and Beta (7lyl) variants of SARS-CoV-2, both in the RBD-down conformations. As you can see, there is an increase in V2 at the 300 starting point of each plot, which indicates the chain of the protein containing CA atoms at indices 300 to 900.



The graphs for scan lengths of 400 look similar, but with peak V2 measures at the 500 to 900 sections instead – still ending at 900, suggesting that there is a knot in the protein that becomes less of a knot after the 900-atom mark.





The graphs above are similar, except they are for the same S proteins for Alpha (7lwt) and Beta (7lyn) variants of SARS-CoV-2 but in the RBD-up conformation. Additionally, these graphs show the change in V2 across the entire proteins’ chains using scanning lengths of 200, rather than the 600 shown and 400 mentioned above. Still, in the RBD-up conformation, in 200, 400, and 600 scanning lengths, there is a peak in V2 at the section ending at around 900. In this case, however, the peak is actually from 650 to 850 – the V2 is a much smaller 0.0215 (0.028) at starting point 700 than the 0.115 (0.084) found at the peak for 7lwt (7lyn respectively). Interestingly enough, the same pattern can be found in the 200 scan-length scans of the RBD-down conformation versions of the S protein shown previously, where the peak is at atoms 650 to 850 rather than the expected 700 to 900.

## SARS-CoV-2 and 2003 SARS-CoV

While the 6zge (SARS-CoV-2 S protein) scans are still being processed, the scans for 6zgi, which is the furin-cleaved version of the S protein in closed conformation, have been processed. In this section I will compare 6zgi to 6acd, which is the RBD-up S protein for SARS-CoV from 2003.

The figures below show a familiar pattern, with 6acd’s V2 peak at 550 to 950 and 6zgi’s V2 peak at 600 to 1000. However, there is a stark difference between these proteins’ plots and those of the variants in the previous section. These plots show a reversal in sign for V2 in both proteins as the starting point progresses from 0 to 50. This is repeated in some other proteins’ scans, as with that of 7krq (a version of the S protein with a common mutation) shown as well.

