Fig. 6: Atomic B-factors from VDR X-ray structure (PDB code: 1DB1)

This plot represents the average atomic B-factors for the VDR/1,25D x-ray construct (PDB code: 1DB1). The B-factors plotted here represent the average B-factor for atoms composing the R-group of a given residue. A low B-factor indicates the R-group shows less molecular heterogeneity and thus shows a more defined electron density. The average B-factor for all residues in the structure is ~ 24 Å². The black dotted lines indicate loops that connect the helices and β-sheet. The gap observed between H2 and H3 represents the deleted loop region. R274 and S237 are the most static residues in the structure and are labeled. Importantly these two residues form hydrogen bonds (H-bonds) with the 1α-OH group in the G-pocket (Fig. 2F) and the 3β-OH group in the A-pocket (Fig. 2D).