**Virtual screening and molecular dynamics simulation for finding inhibitor of New Delhi metallo-β-lactamase-1**

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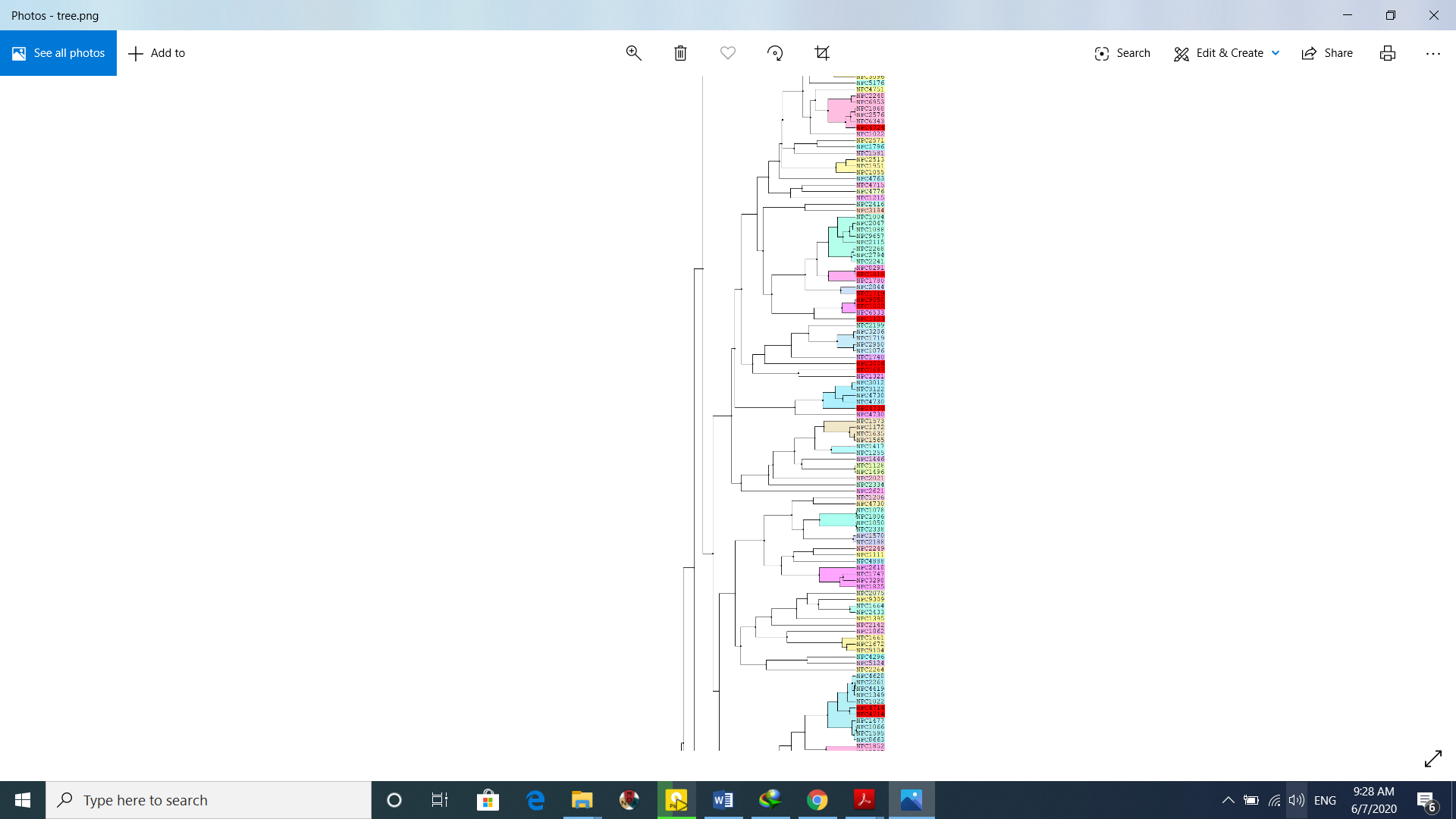


Figure Hieratical clustering of the range of the our ten final compounds

Table 1phisico-chemical properties

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Name** | **# Acceptors** | **# Donors** | **# Rot. Bonds** | **MolWt** | **cLogP** | **TPSA** | **TPSA [Ertl]** |
| NPC18185 | 12 | 10 | 13 | 578.53 | 2.46 | 3.25 | 220.76 |
| NPC98583 | 18 | 14 | 23 | 882.74 | 3.96 | 3.62 | 354.28 |
| NPC100251 | 20 | 16 | 25 | 914.73 | 3.37 | 3.95 | 394.74 |
| NPC112380 | 18 | 13 | 21 | 868.71 | 3.14 | 3.7 | 351.12 |
| NPC120633 | 9 | 8 | 12 | 680.71 | 7.58 | 2.06 | 171.07 |
| NPC171932 | 10 | 8 | 12 | 562.53 | 3.21 | 2.83 | 189.53 |
| NPC300657 | 11 | 9 | 14 | 726.69 | 7.48 | 2.54 | 213.67 |
| NPC471403 | 15 | 10 | 13 | 814.75 | 3.57 | 2.64 | 248.45 |
| NPC471404 | 16 | 11 | 14 | 830.75 | 3.27 | 2.83 | 268.68 |
| NPC472454 | 13 | 9 | 12 | 590.49 | 2.07 | 3.61 | 234.67 |
| NPC473010 | 10 | 6 | 15 | 668.74 | 6.65 | 1.87 | 166.14 |



Figure 3D alignment of the three class B1, B2 and B3 OF MBL

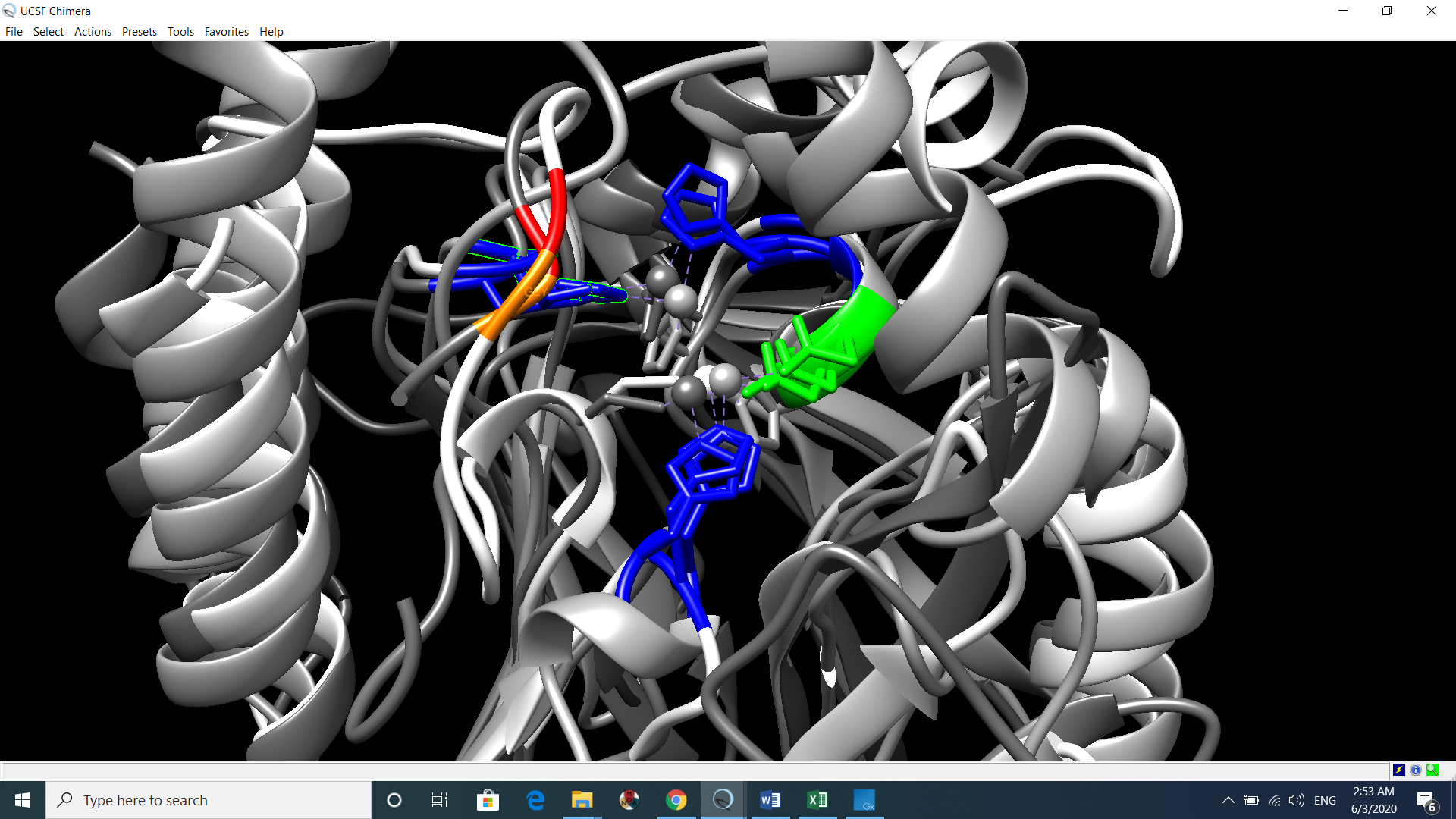


Figure Crucial residue in active site, which were conserve in the MBL. Navy blue residues are histidine. Aspartic acids had green color. Gly and Asn had orange and red color respectively

Table 2 Crucial residues which were conserve in the three class of MBL

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| NDM-1 | Ser217 | Ser251 | Asn220 | Asp124 | His250 | Lys211 | Ile35 | His189 | Gly219 | His122 |
| B1 | 1 |  | 1 | 1 | 1 |  |  | 1 | 1 | 1 |
| B2=cphA |  | SER265 | Asn233 | Asp120 | His263 | Lys224 |  | His196 | Gly232 | His118 |
| B3=BJP-1 |  |  |  | Asp105 | His242 |  |  | His177 |  | His103 |

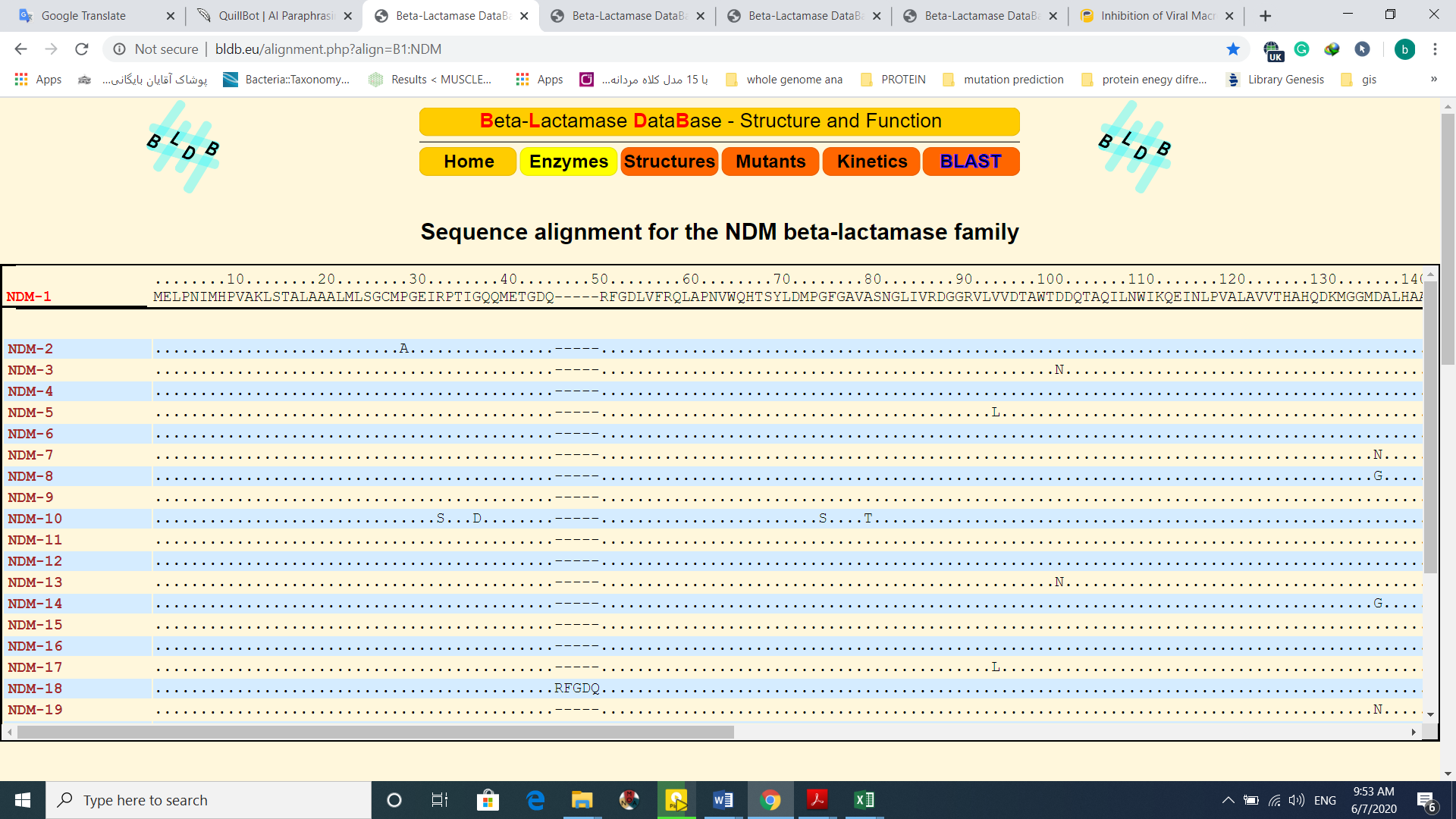


Figure Alignment of all types of the NDM

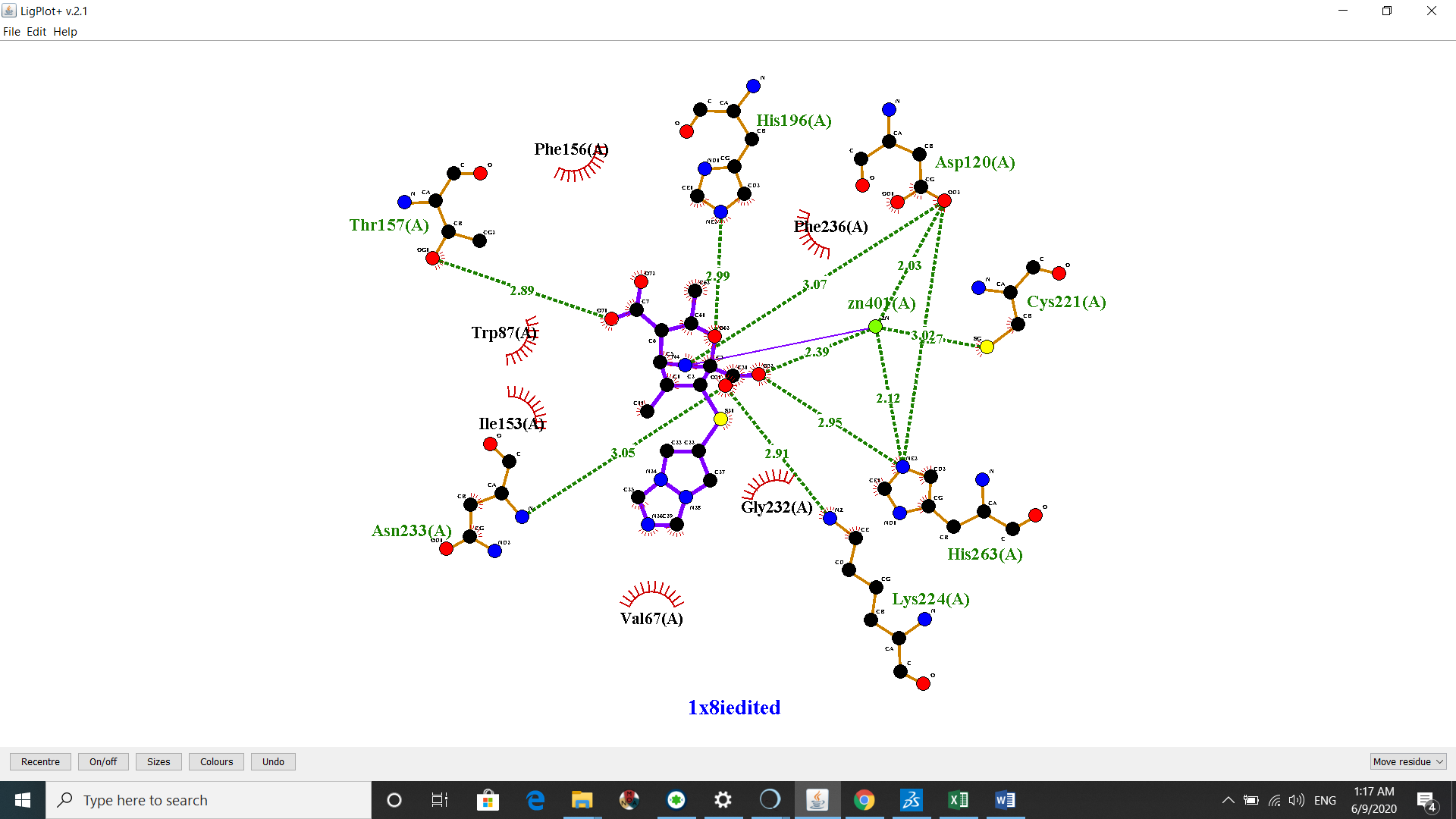


Figure cphA-biapenem (B2). Interaction among three classes of the MBLS was similar to each other. These resemblance are comparable with Figure6 for BJP(B3) and NDM-1 (B1)

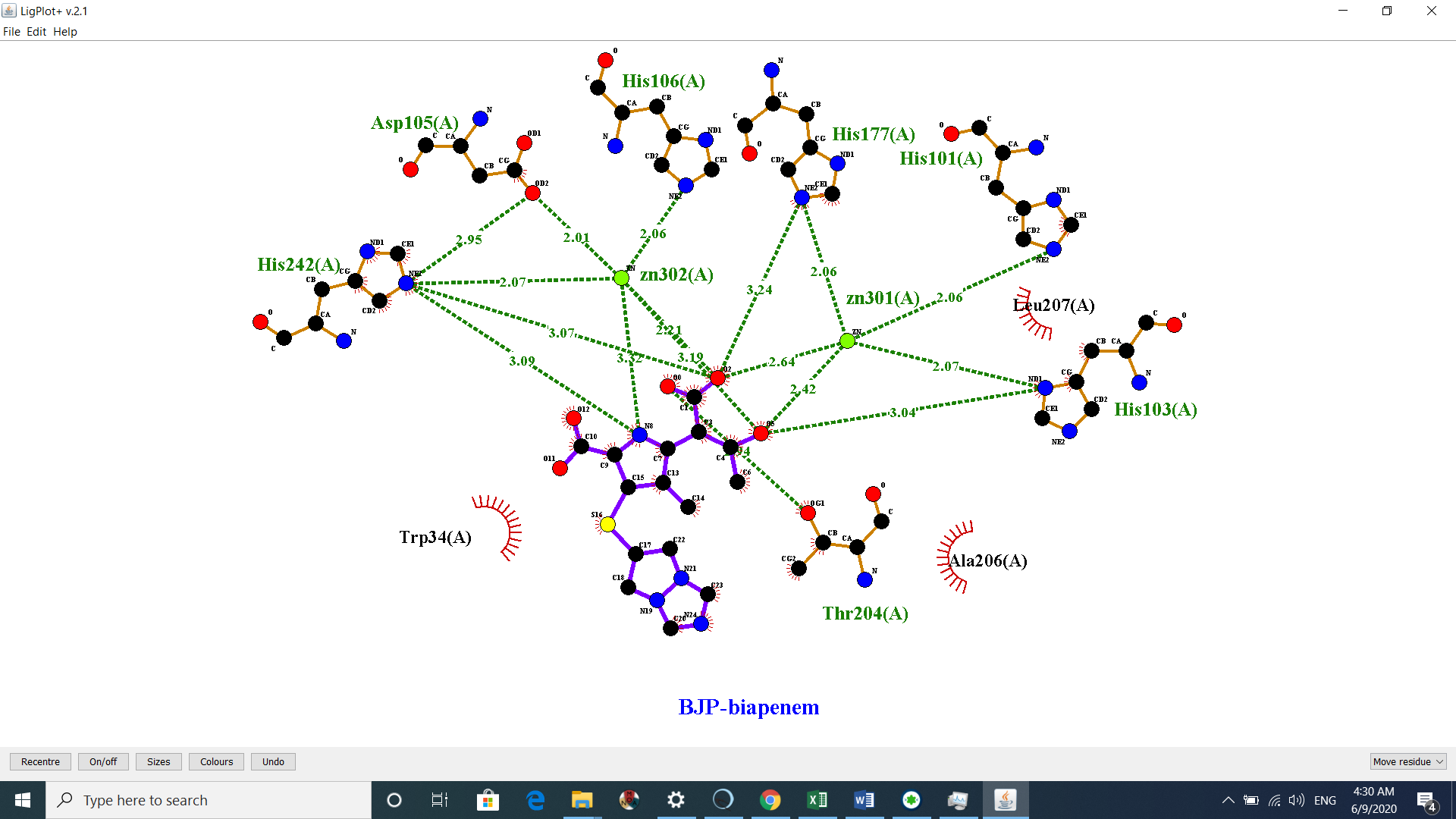


Figure BJP-biapenem

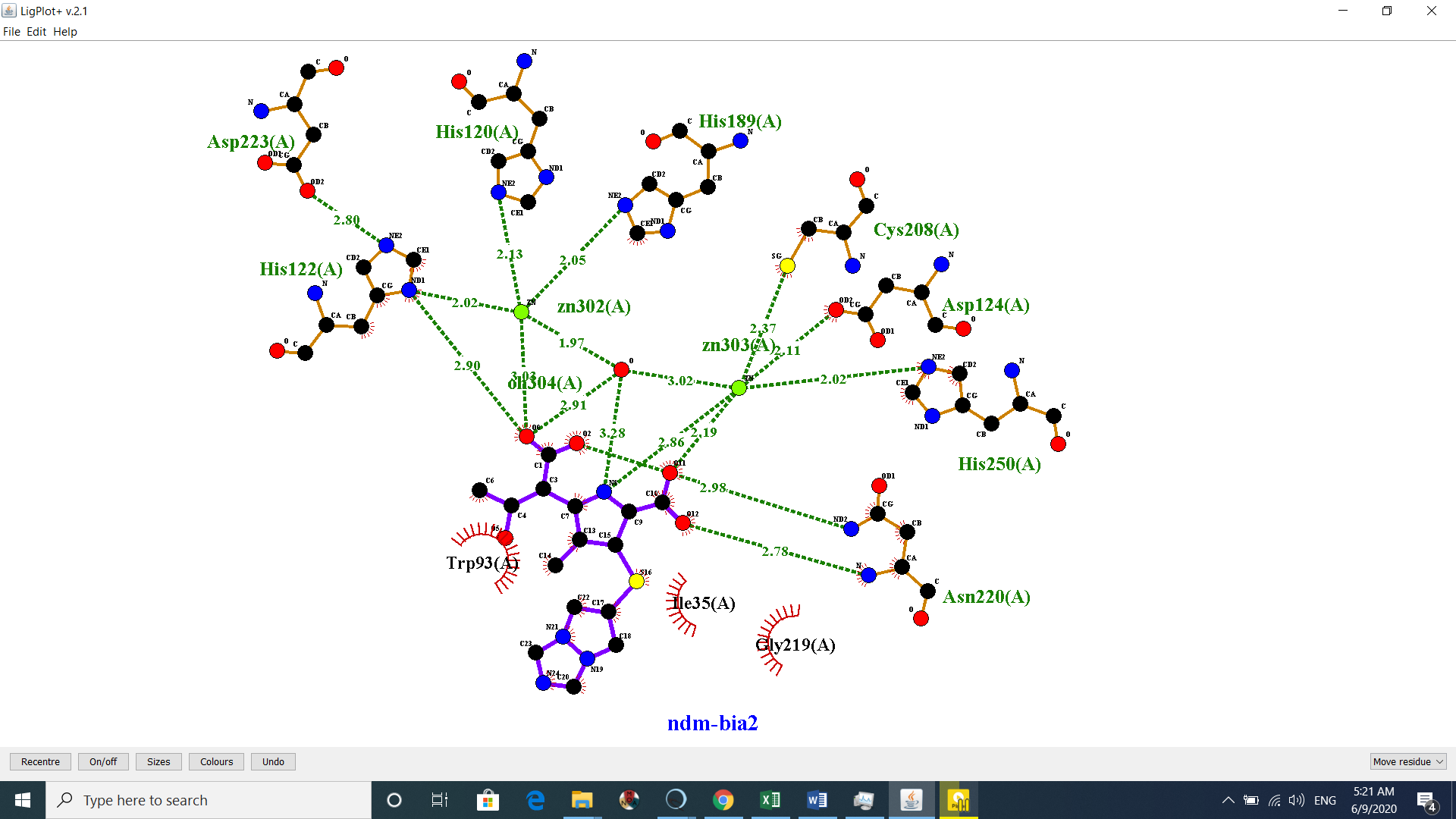


Figure NDM-biapenem

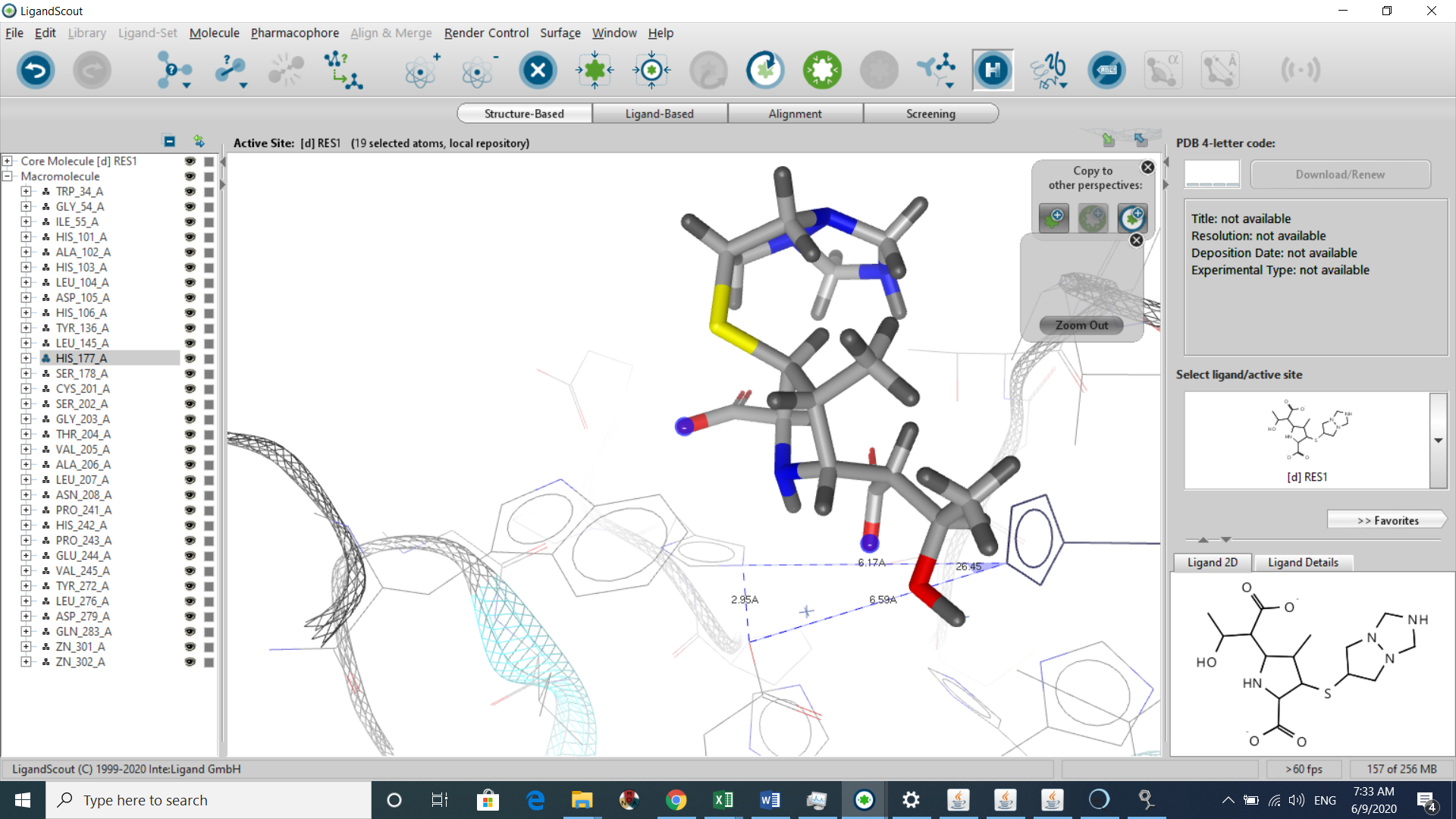
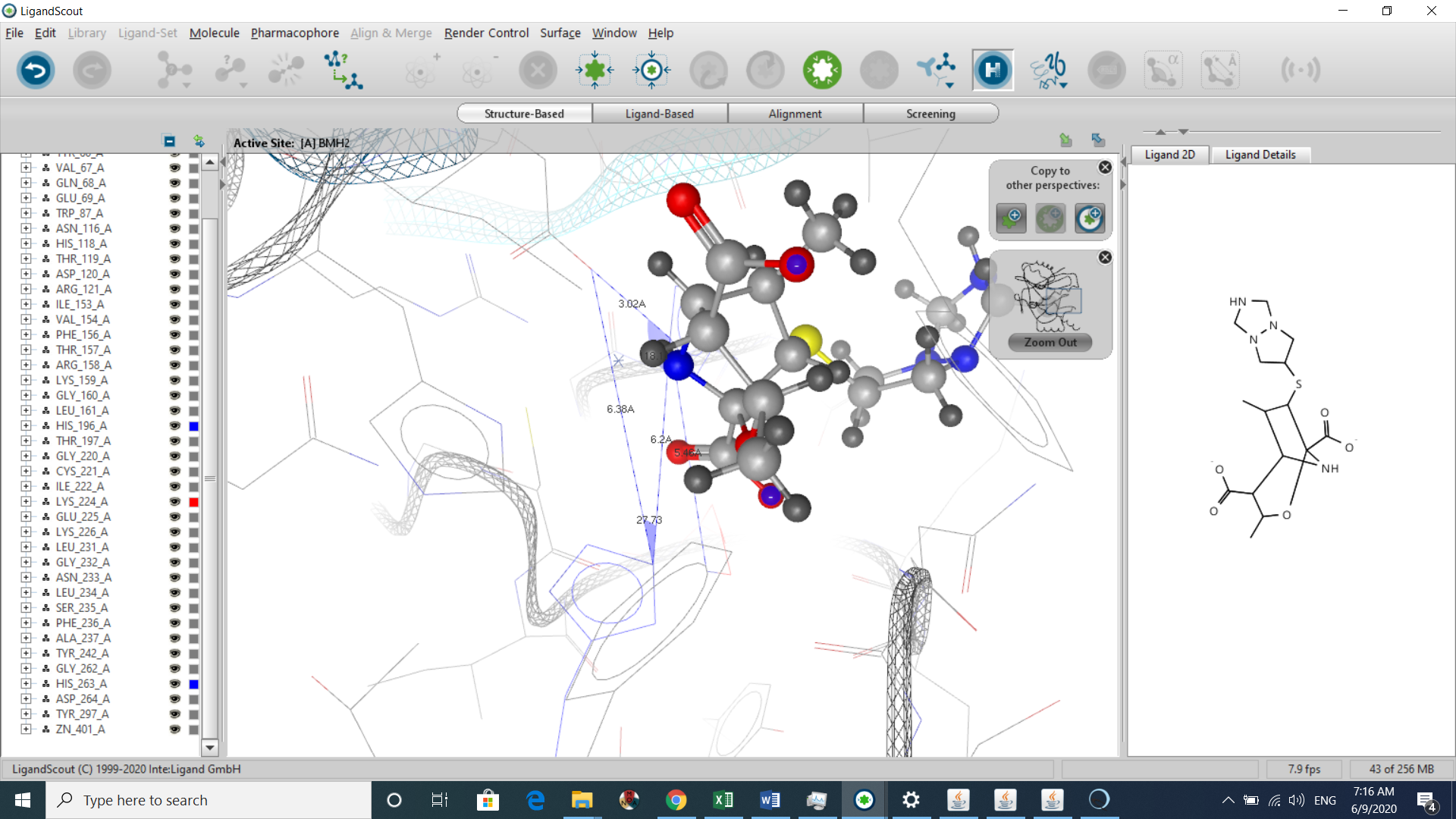
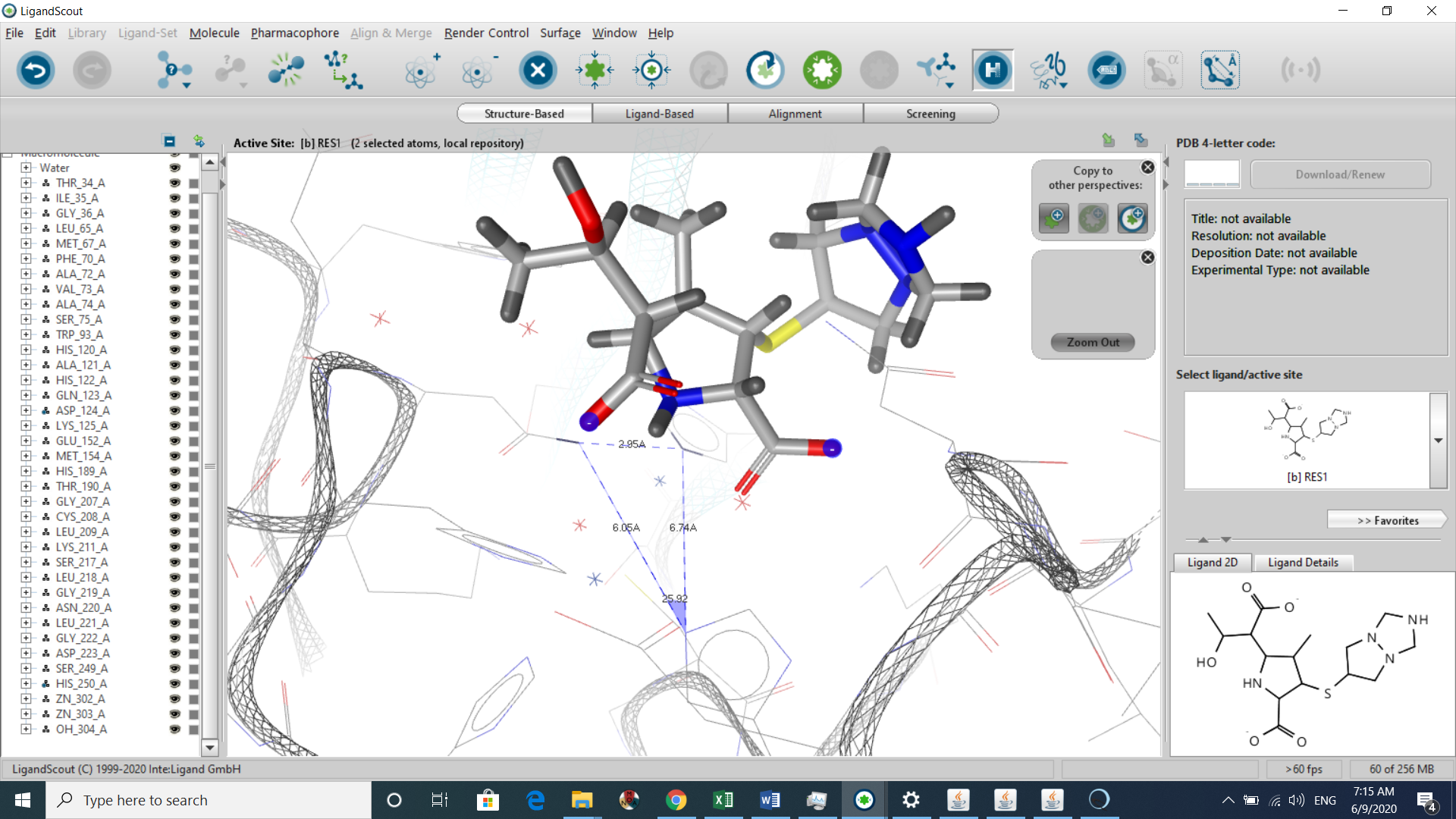


Figure Distance and angle among the three example key residue key

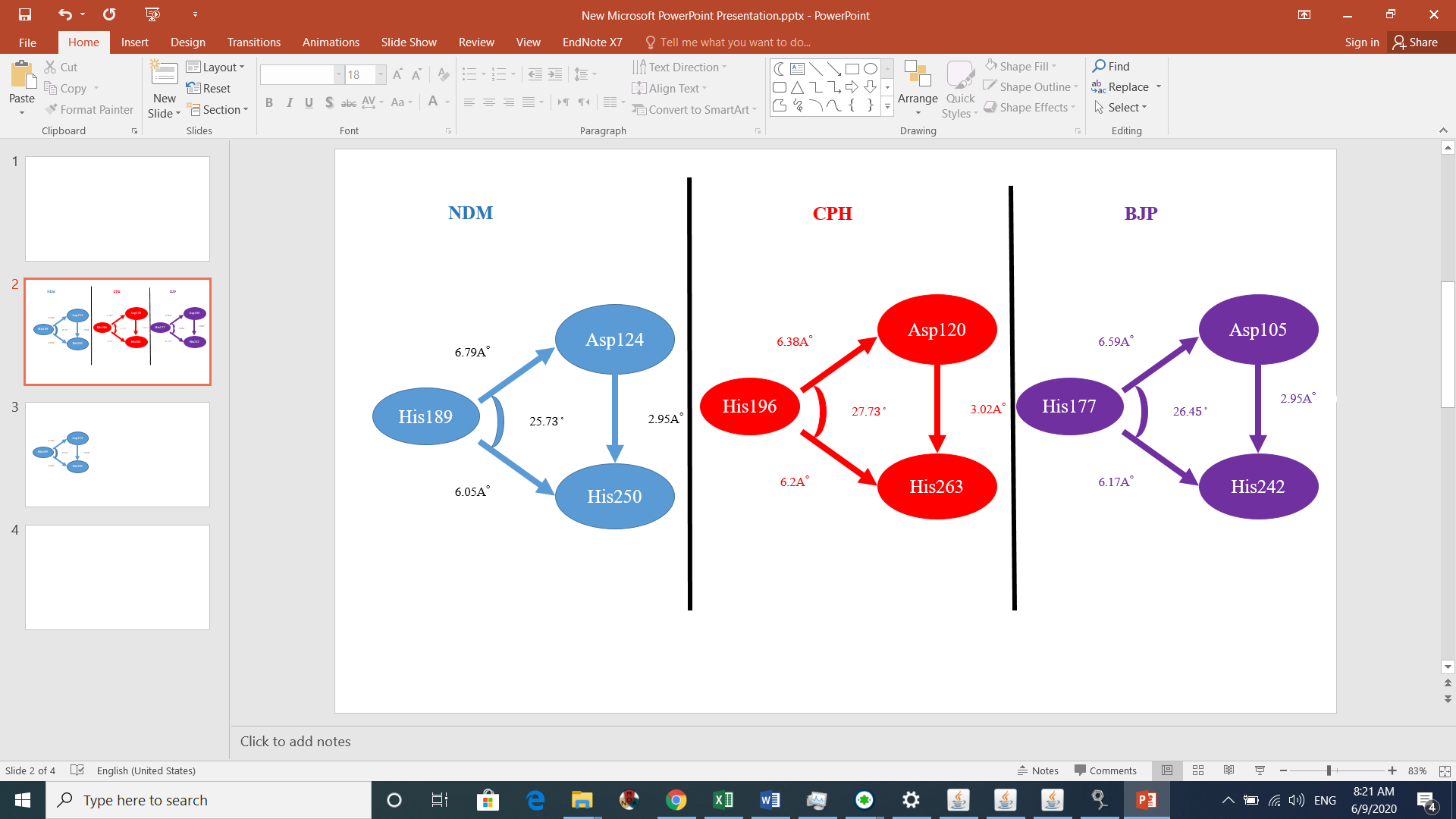


Figure Distance and angle among the three example key residue. This schematic picture showed high similarity of the coordination among analogue residue. Angels and distances between the key residue of B1, B2 and B3 classes are resemble

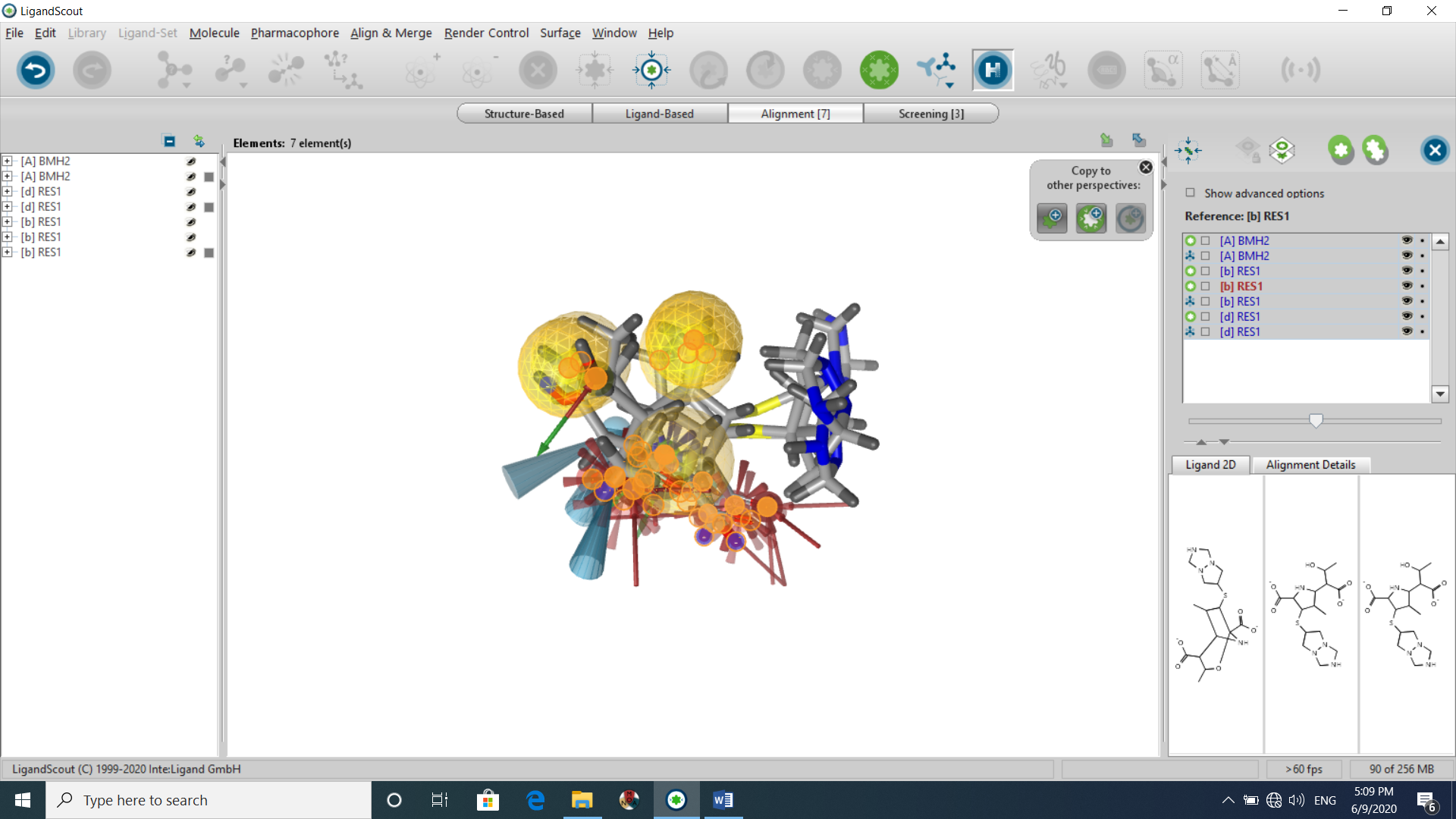


Figure Matched biapenems which docked in the NDM,BJP and cphA. pharmacophores were similar among all of them