Supplementary Materials

Figure 1. Stereoview of metal-binding site of the metal-dependent HAD superfamily members. (A) phosphonatase-Mg(II)-tungstate complex (pdb:1FEZ) (*1*), (B) phosphoserine phosphatase-Mg(II)-BeF_3^- complex (pdb: 1J97) (*2*), (C) β-phosphoglucomutase-glucose-1,6-bisphosphate intermediate complex (pdb:1O03) (*3*), (D) deoxy-D-Mannose- octulosonate 8- phosphate phosphatase-Co(II)-sulfate complex (pdb:1K1E) (*4*), (E) human mitochondrial deoxyribonucleotidase-Mg(II)-phosphate complex (pdb: 1MH9) (*5*), (F) lipid phosphatase domain of the bifunctional phosphatase/epoxide hydrolase (pdb:1CQZ) (*6*), (G) phosphatase domain of bifunctional T4 polynucleotide kinase/phosphatase (pdb: 1LTQ) (*7*), (H) P domain of membrane bound ATP dependent Ca(II) pump (pdb: 1EUL) (*8*). Color Scheme: Mg(II) and the backbone of loop 4 in all the structures are colored green, the nucleophilic Asp is red and the residue two amino-acid residues downstream is magenta, the inner-sphere Mg(II) ligand, which binds metal ion directly, is colored blue while the outer sphere ligand that interacts through a water bridge is cyan. The active site ligand (substrate or inhibitors) are colored gray, the Mg(II) water ligands are color light blue. Other Mg(II) ligands not belonging to the above and the third carboxylate residues in loop 4 are colored gold. In the cases of F, G, H, no metal ions are observed in X-ray structures, but the dependence on Mg(II) was confirmed previously by biochemical analysis.

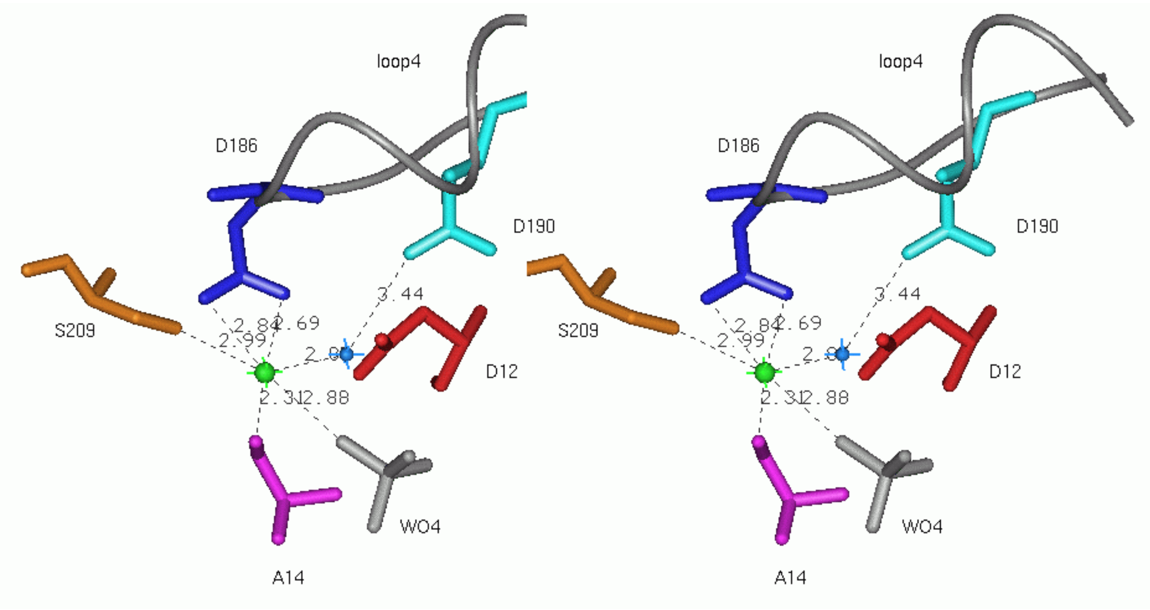

Figure 1A

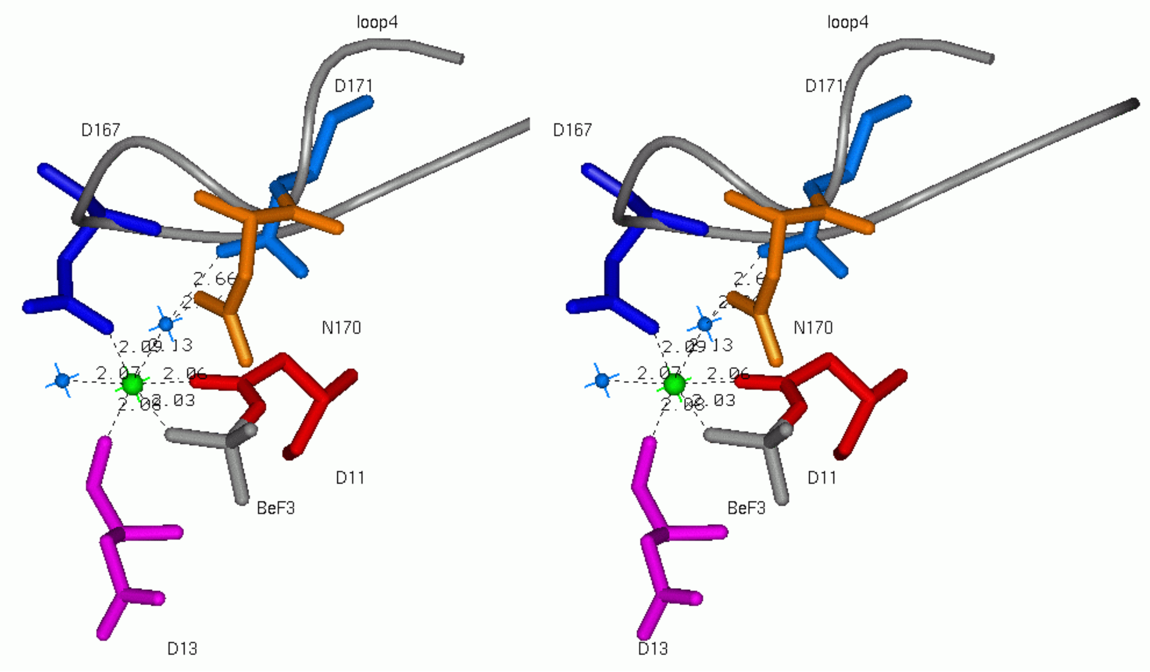

Figure 1B

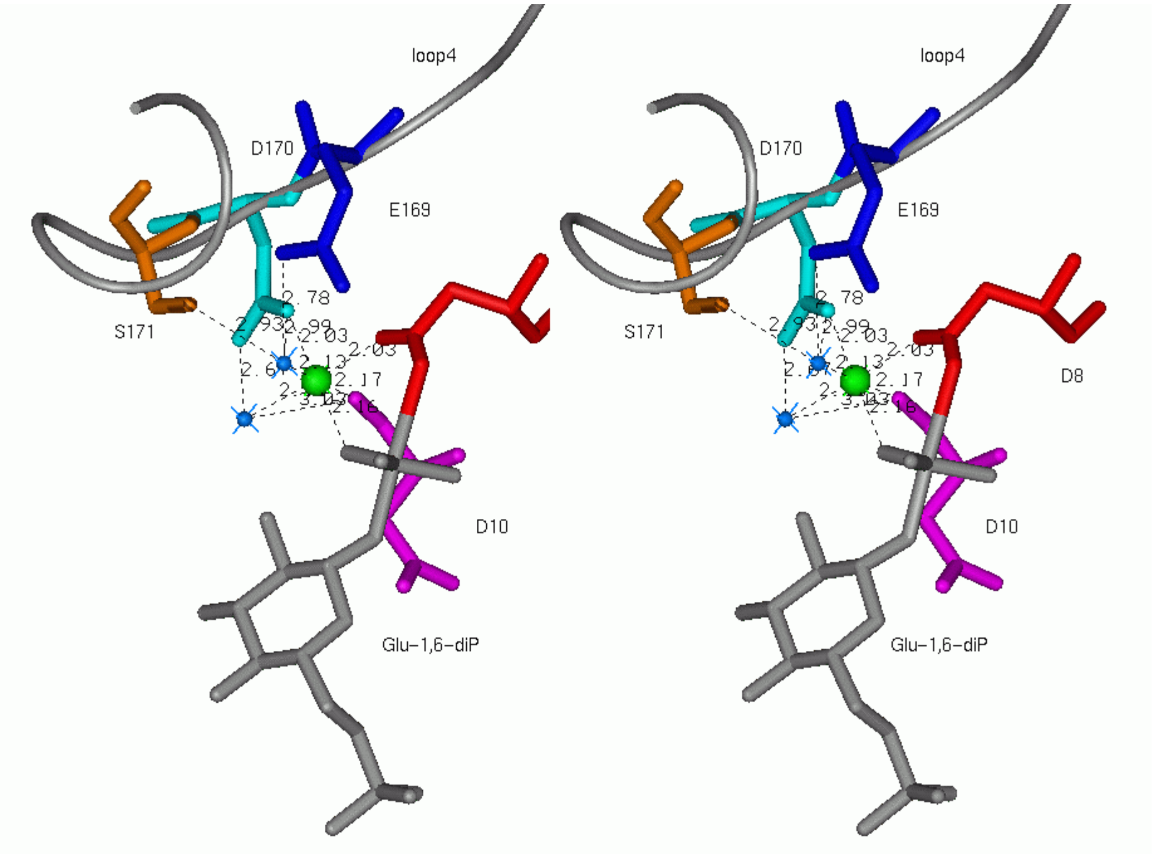
loop4
D170
E169
S171
D8
D10
Glu-1,6-diP
2.78
2.93
2.99
2.03
2.03
2.13
2.17
2.67
3.03
2.16

Figure 1C

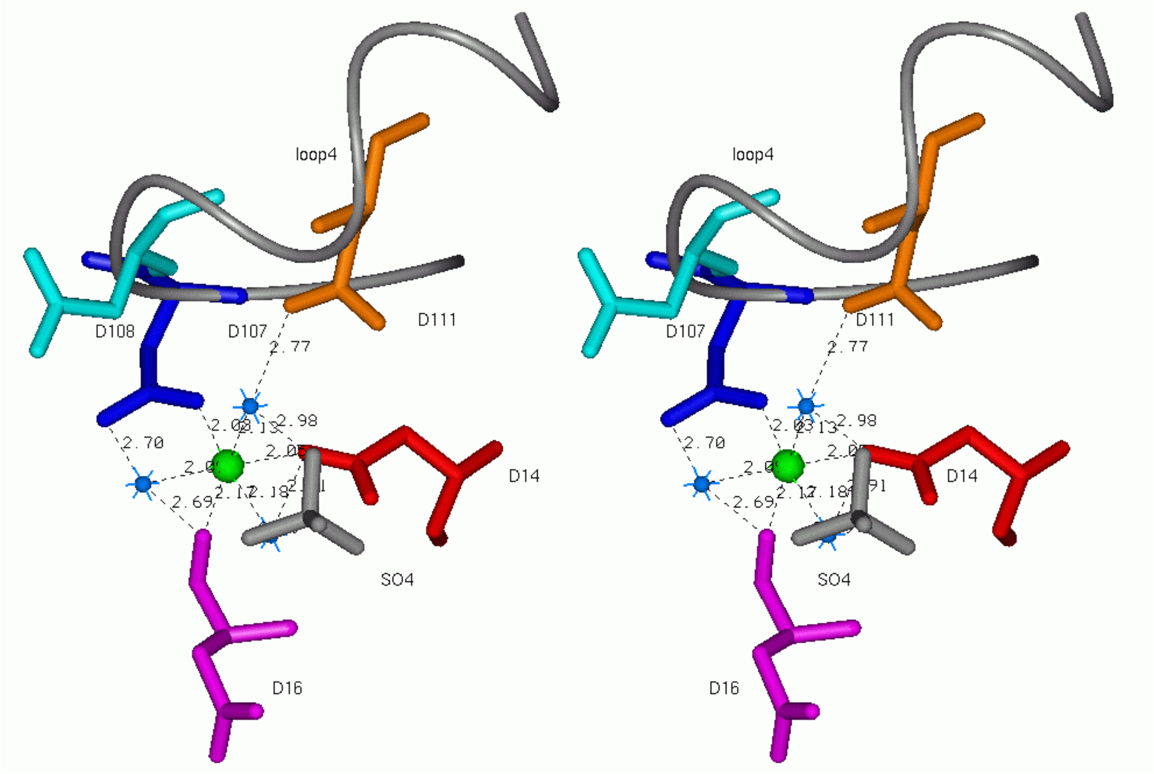
loop4
D108
D107
D111
2.77
2.98
2.03
2.13
2.70
2.05
2.17
2.18
2.69
D14
SO4
D16
loop4
D107
D111
2.77
2.98
2.70
2.69
2.91
D14
SO4
D16

Figure 1D

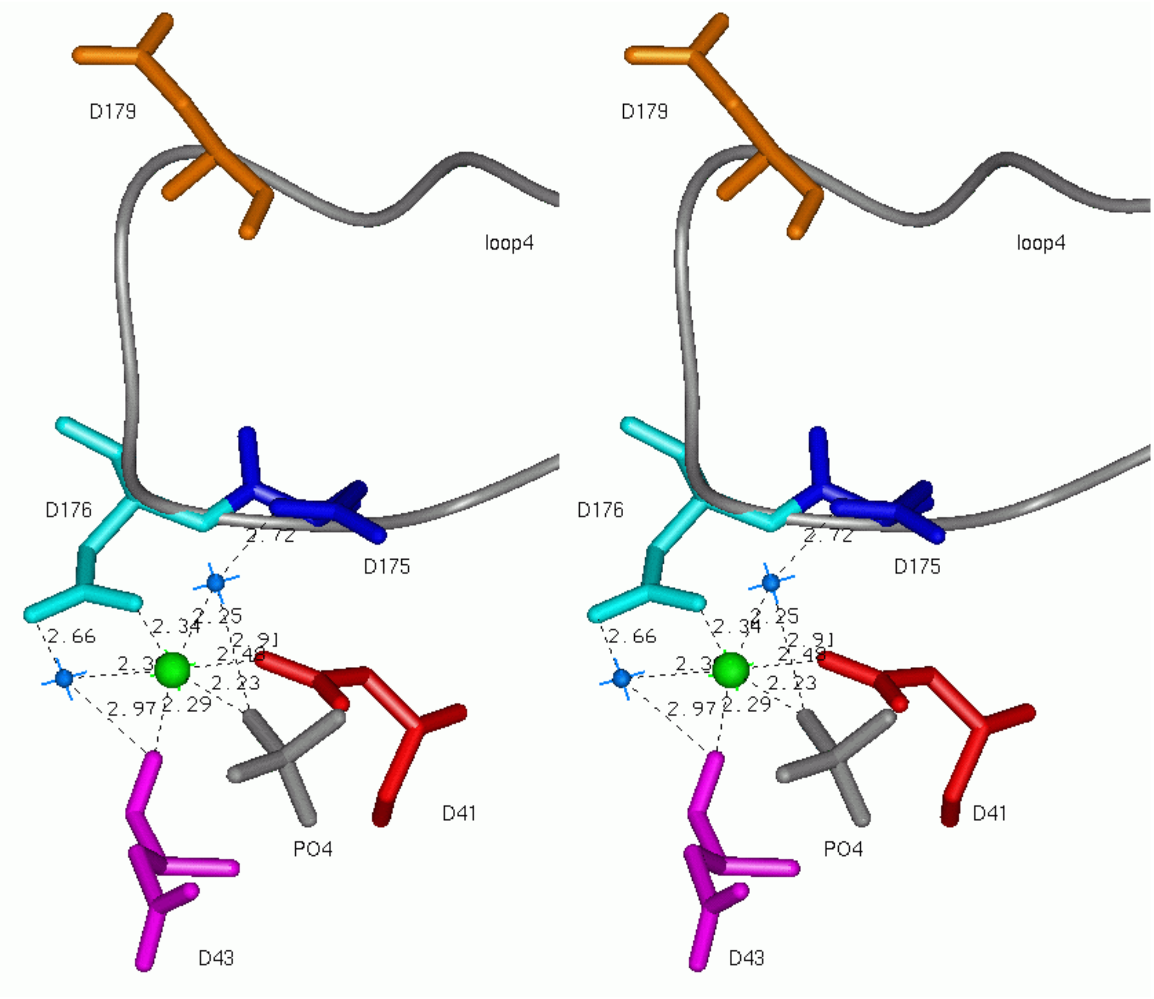
D179
loop4
D176
D175
2.72
2.25
2.34
2.66
2.91
2.48
2.3
2.23
2.97
2.29
D41
PO4
D43

Figure 1E

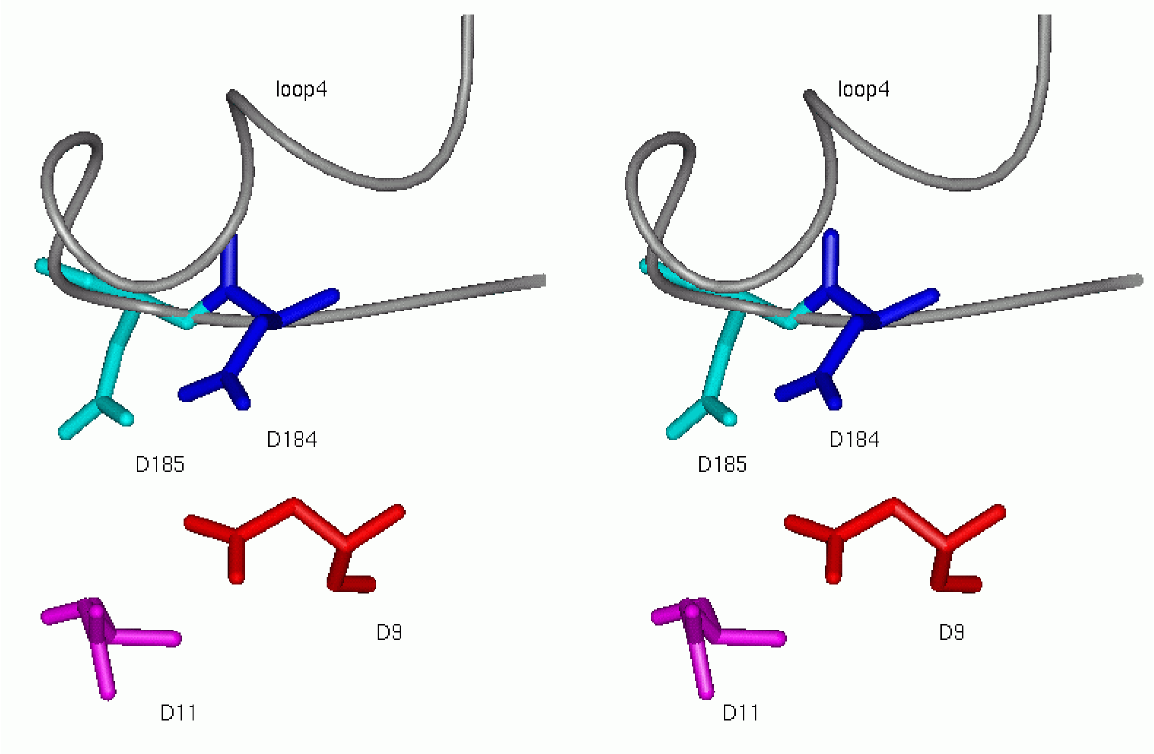

Figure 1F

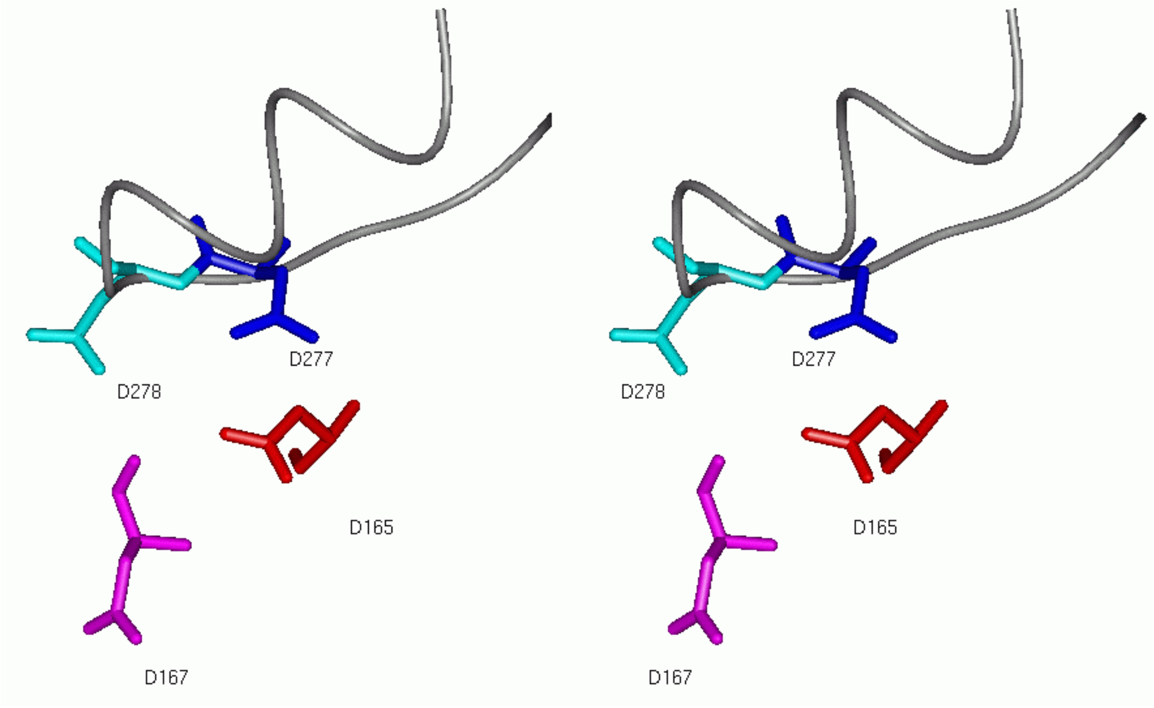

Figure 1G

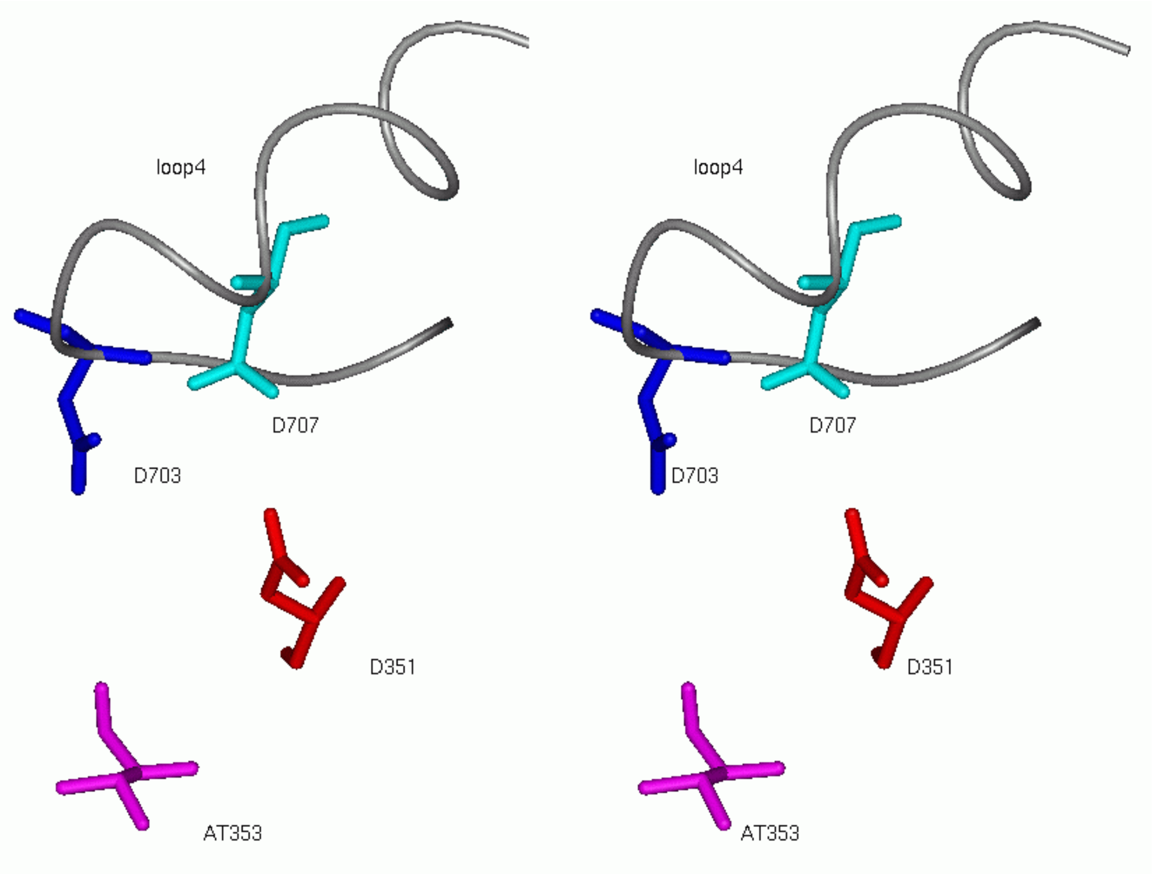

Figure 1H

References

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