

## BAB V

### KESIMPULAN DAN SARAN

#### A. Kesimpulan

1. Nilai afinitas dari senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin terhadap DHFR bakteri lebih tinggi dibandingkan DHFR sel mamalia dilihat dari  $\Delta G$  *binding*.
2. Pola interaksi lima belas senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin terhadap enzim DHFR bakteri menunjukkan ikatan hidrogen dengan asam amino Asp31A dan DHFR sel mamalia menunjukkan ikatan hidrogen dengan asam amino Glu30A dan Val115A. Gugus fungsi senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin yang mempunyai pola interaksi yang baik adalah struktur nomer 1, 2, 7, 8, 11, 14, dan 15 dari DHFR bakteri (trimetoprim) sedangkan struktur 1, 2, 7, 8, 9, 10, 14 dan 15 dari DHFR sel mamalia (metotreksat).

#### B. Saran

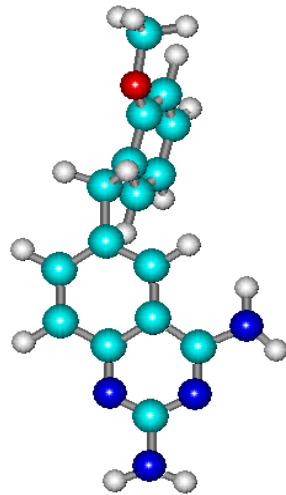
Perlu dilakukan penelitian lebih lanjut tentang adsorpsi, distribusi, metabolisme, ekskresi dengan profil farmakokinetik yang baik secara eksperimental tentang senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin terhadap DHFR bakteri dan DHFR sel mamalia.

## DAFTAR PUSTAKA

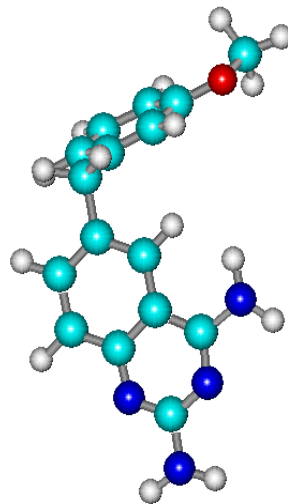
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Lampiran 1. Hasil optimasi geometri struktur 3 dimensi dari 15 senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin menggunakan metode Mekanika Molekuler (MM+) dengan *software* HyperChem Release 7.0

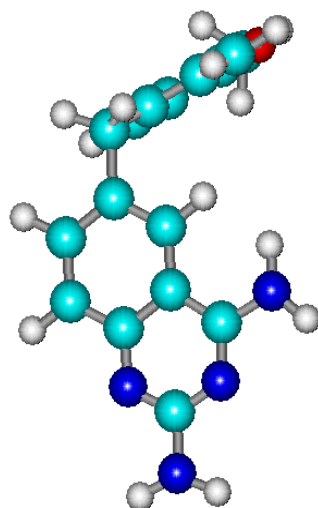
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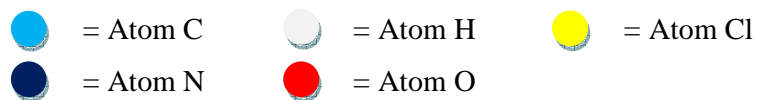
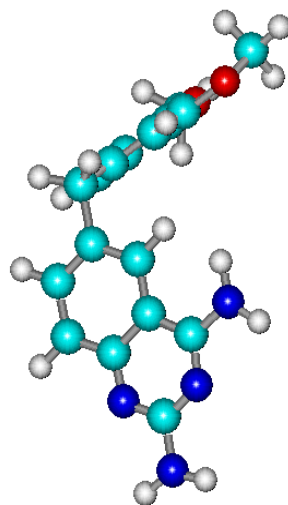
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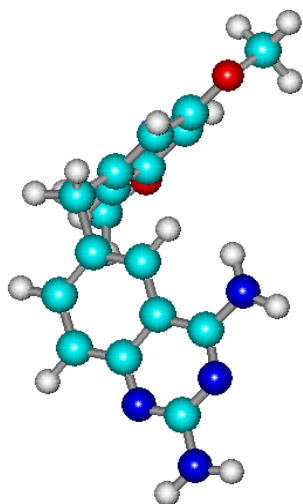
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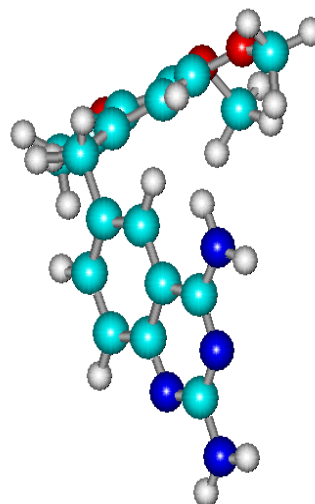
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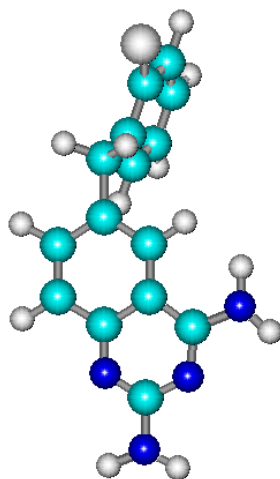
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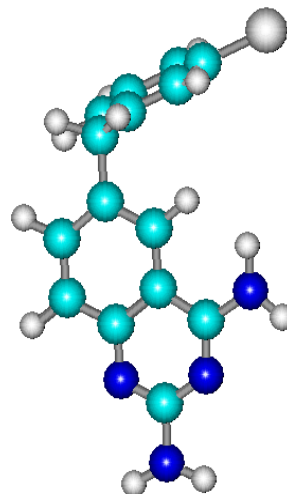
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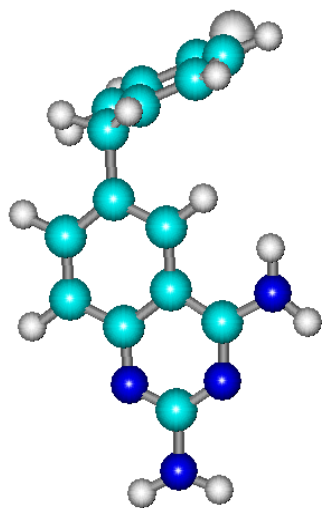
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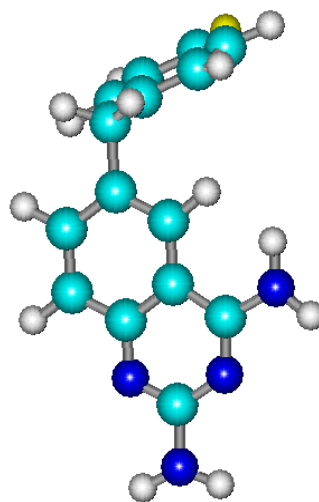
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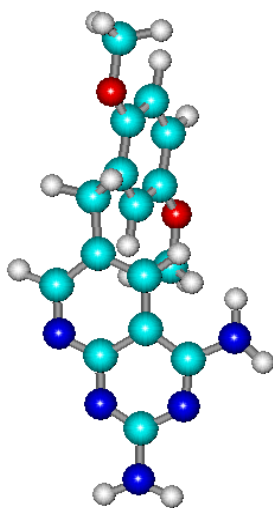
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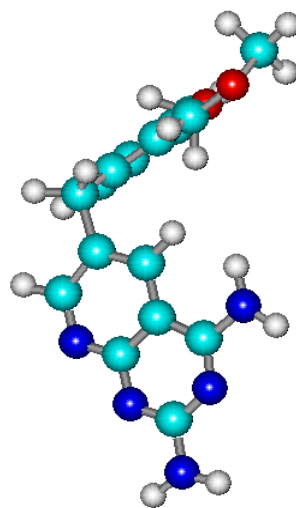
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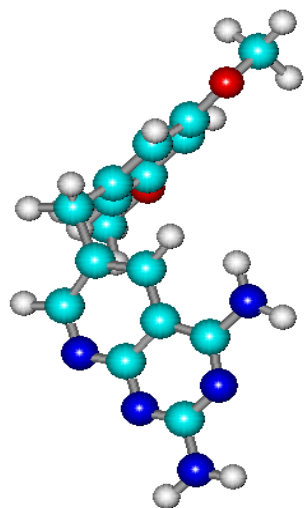
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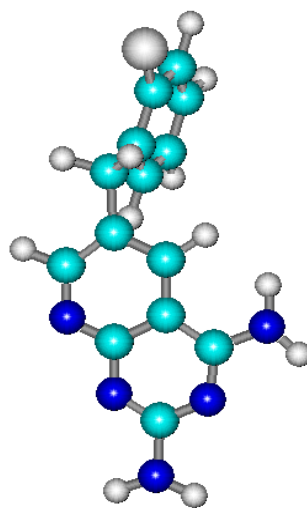
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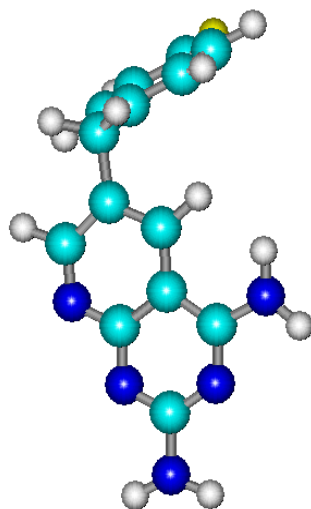
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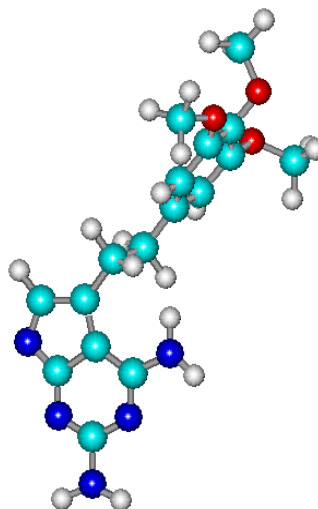
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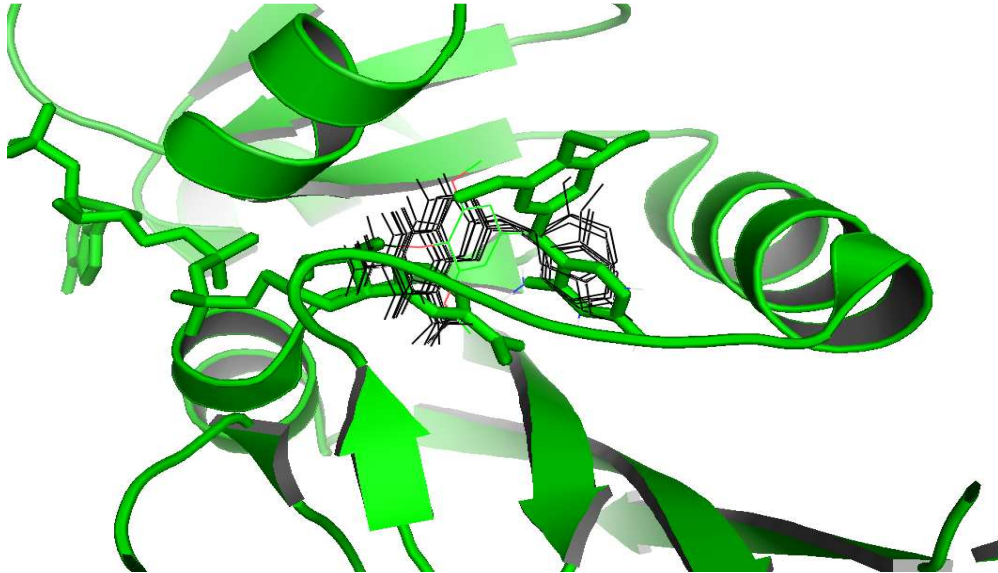
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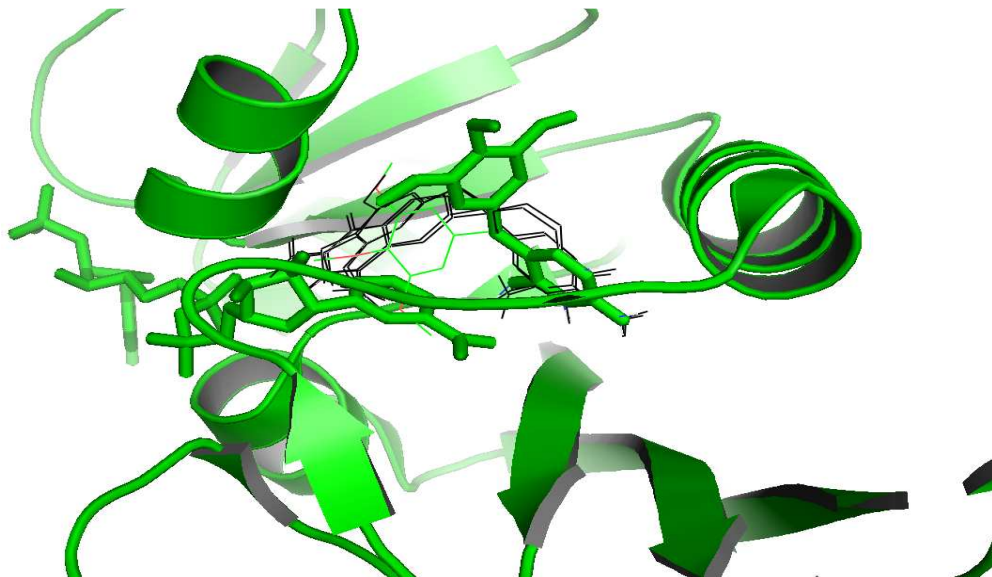
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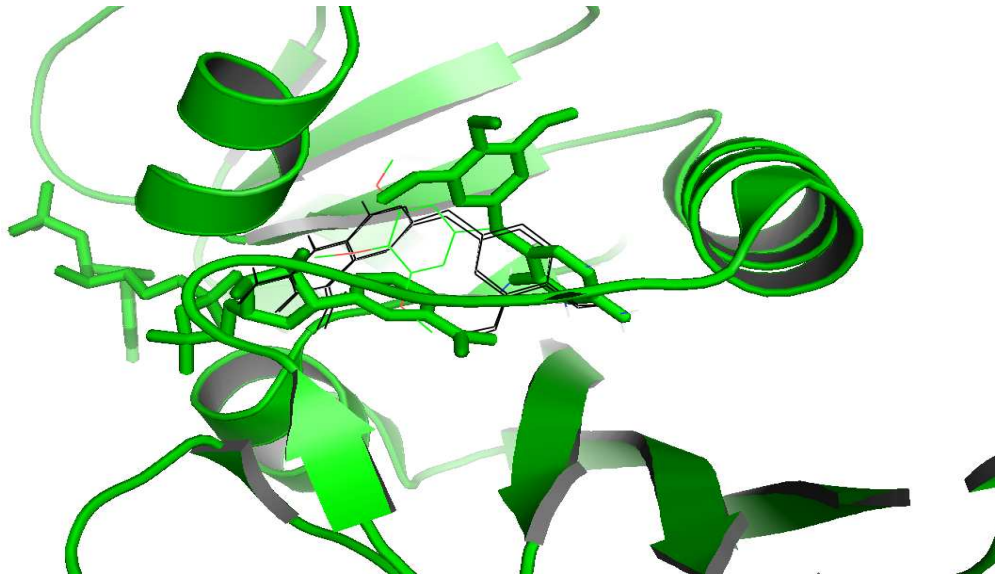
Lampiran 2. Pola interaksi dari 15 senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin pada DHFR bakteri.



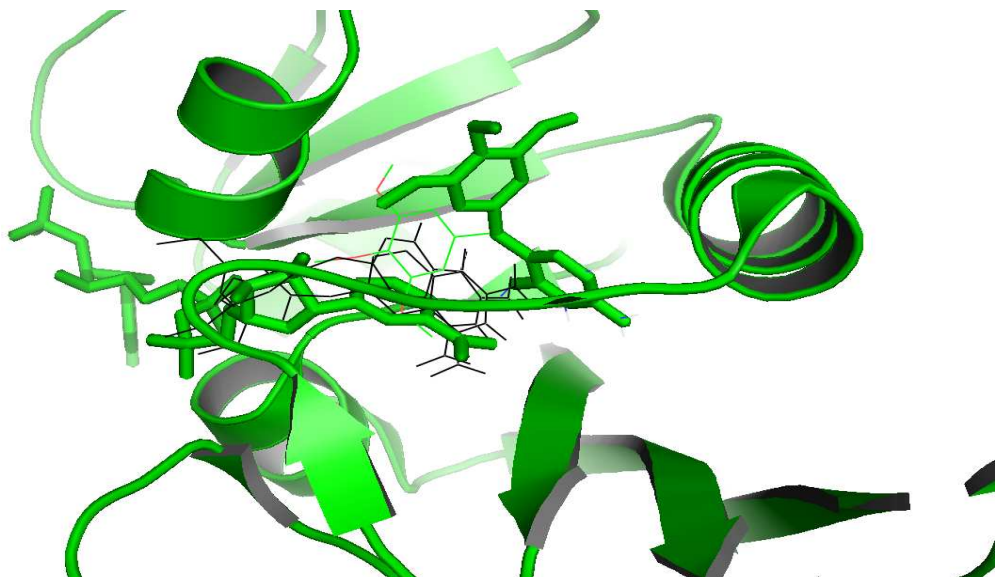
*Overlay struktur nomer 1, 2, 7, 8, 11, 14, dan 15 pada gambar di atas trimetoprim (hijau) senyawa turunan (hitam)*



*Overlay struktur nomer 3, 6, 9, dan 10 pada gambar di atas trimetoprim (hijau) senyawa turunan (hitam)*

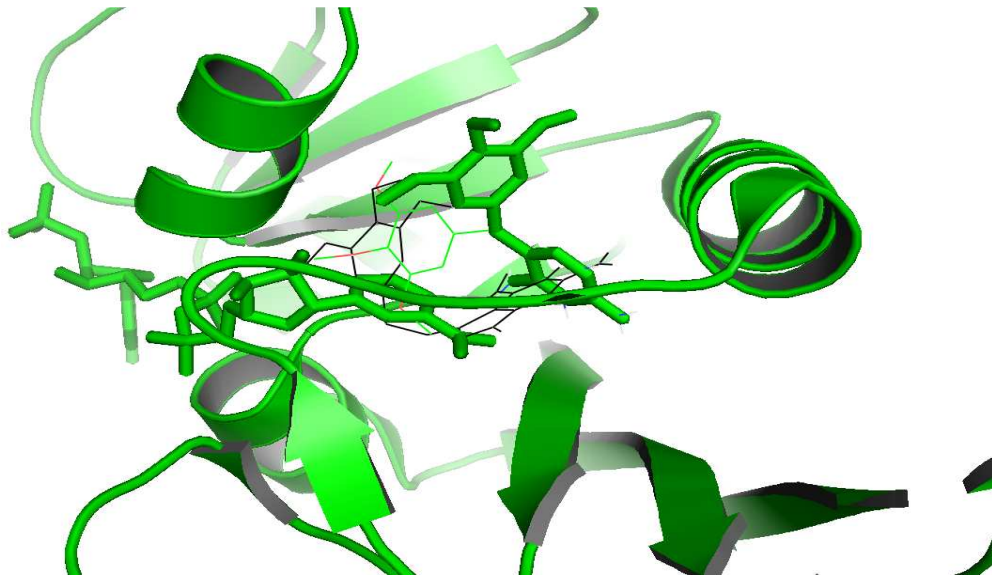


*Overlay struktur nomer 4 dan 12 pada gambar di atas trimetoprim (hijau) senyawa turunan (hitam)*



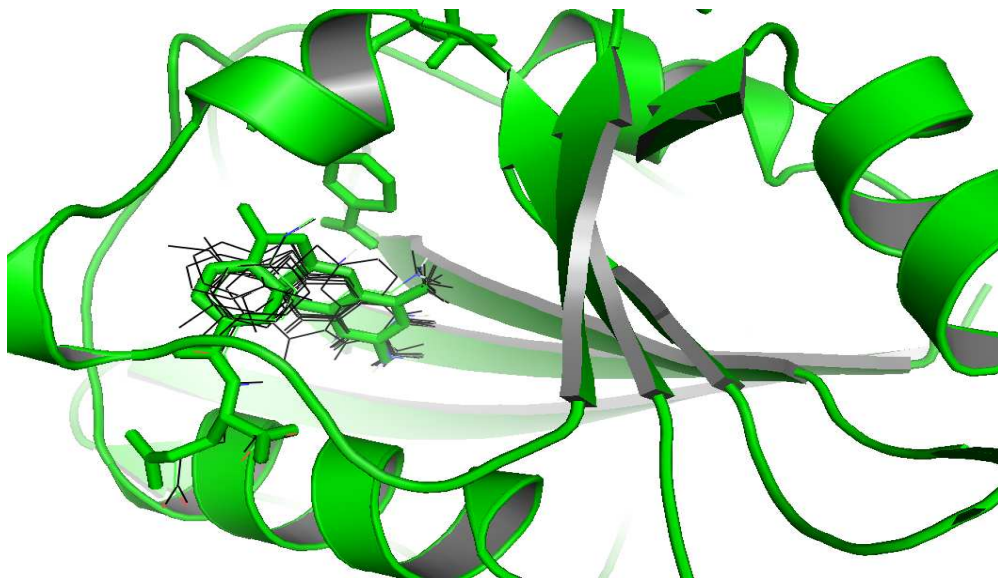


*Overlay* struktur nomer 5 dan 13 pada gambar di atas trimetoprim (hijau) senyawa turunan (hitam)

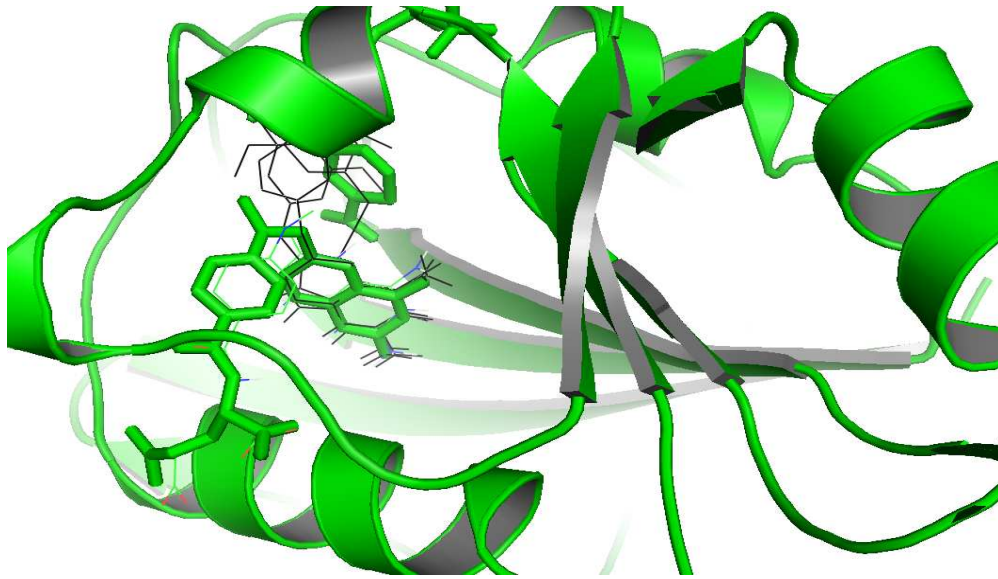


Struktur nomer 15 pada gambar di atas trimetoprim (hijau) senyawa turunan (hitam)

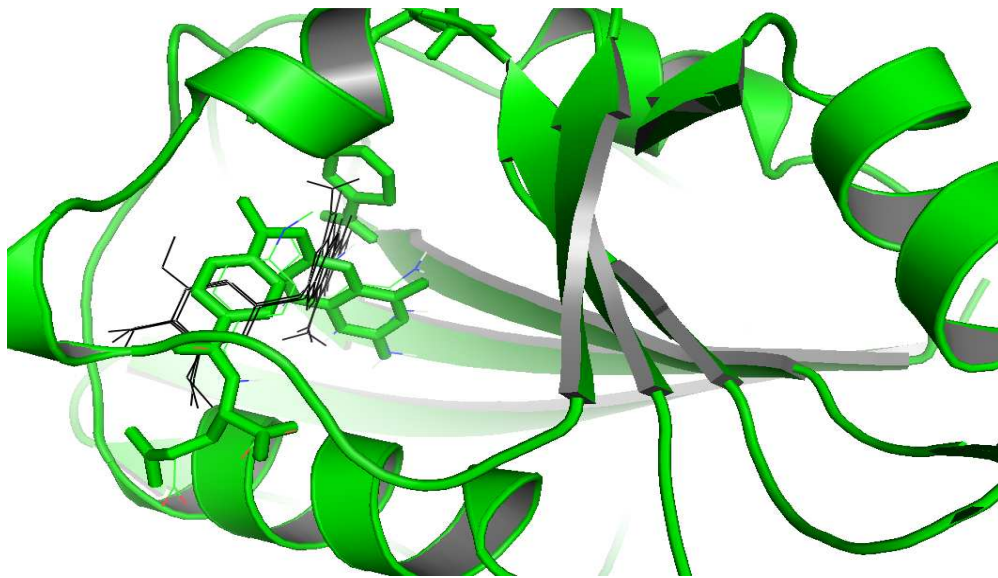
Lampiran 3. Pola interaksi dari 15 senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin pada DHFR sel mamalia.



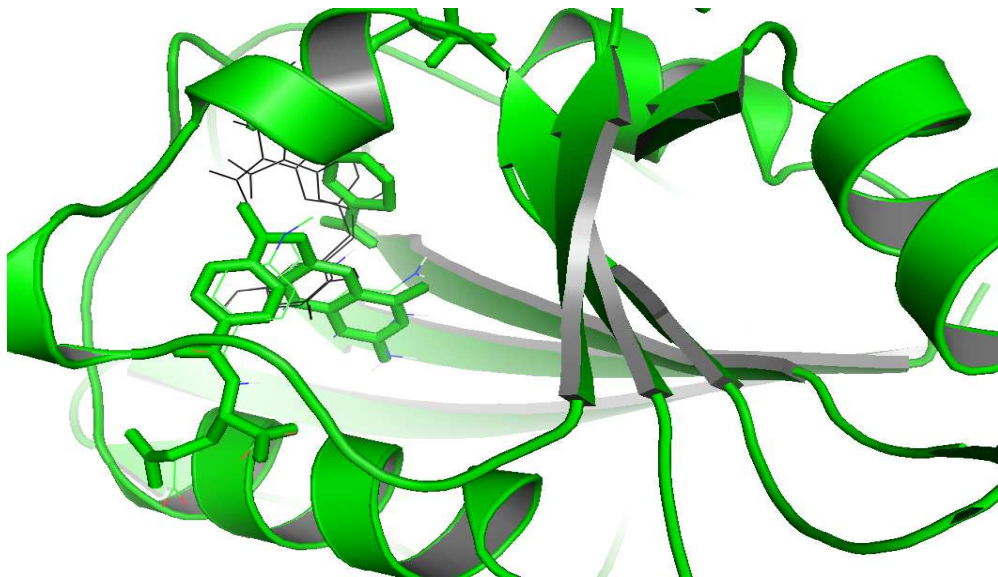
*Overlay* struktur nomer 1, 2, 7, 8, 9, 10, 14, 15 pada gambar di atas metotreksat (hijau) senyawa turunan (hitam)



*Overlay struktur nomer 4, 13, dan 15 pada gambar di atas metotreksat (hijau) senyawa turunan (hitam)*



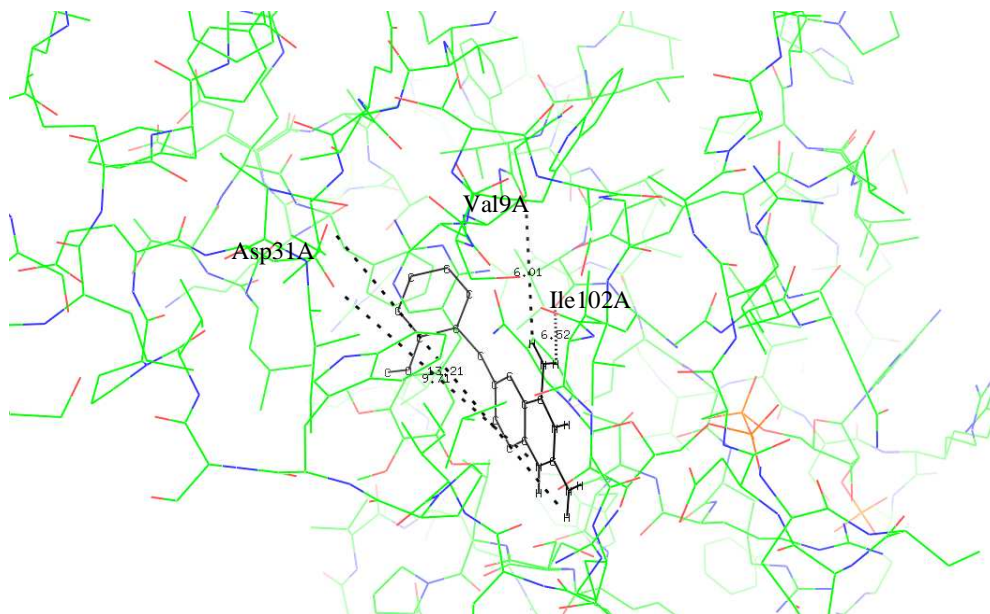
*Overlay struktur nomer 3, 6, dan 12 pada gambar di atas metotreksat (hijau) senyawa turunan (hitam)*



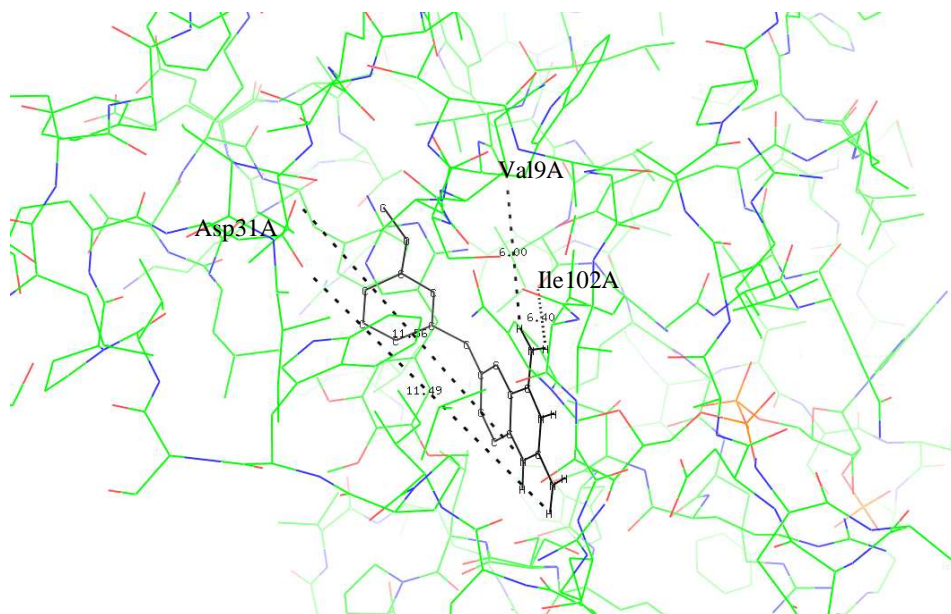
Overlay struktur nomer 5 dan 11 pada gambar di atas metotreksat (hijau) senyawa turunan (hitam)

Lampiran 4 Jarak ikatan hidrogen dengan senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin pada DHFR bakteri

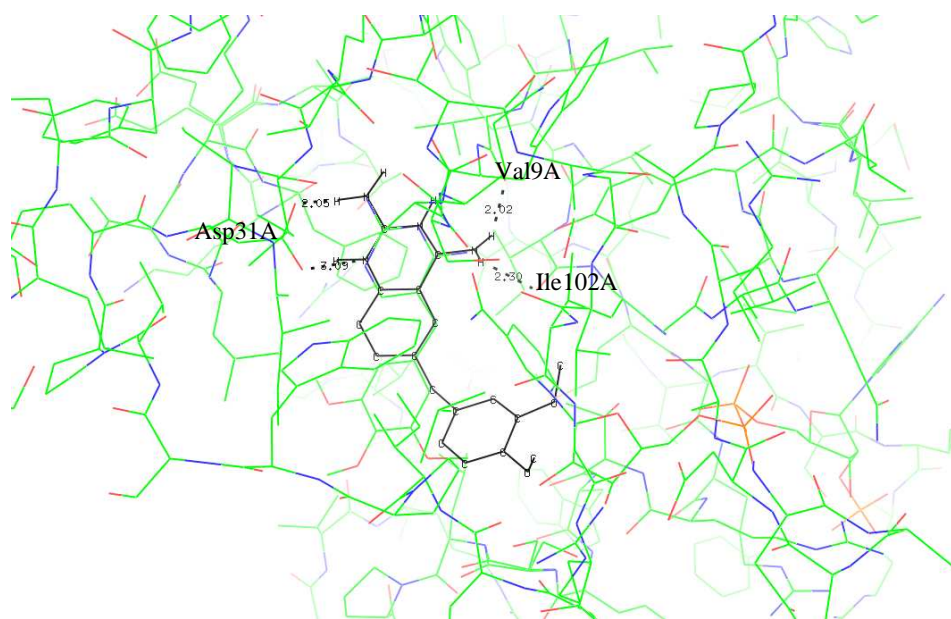
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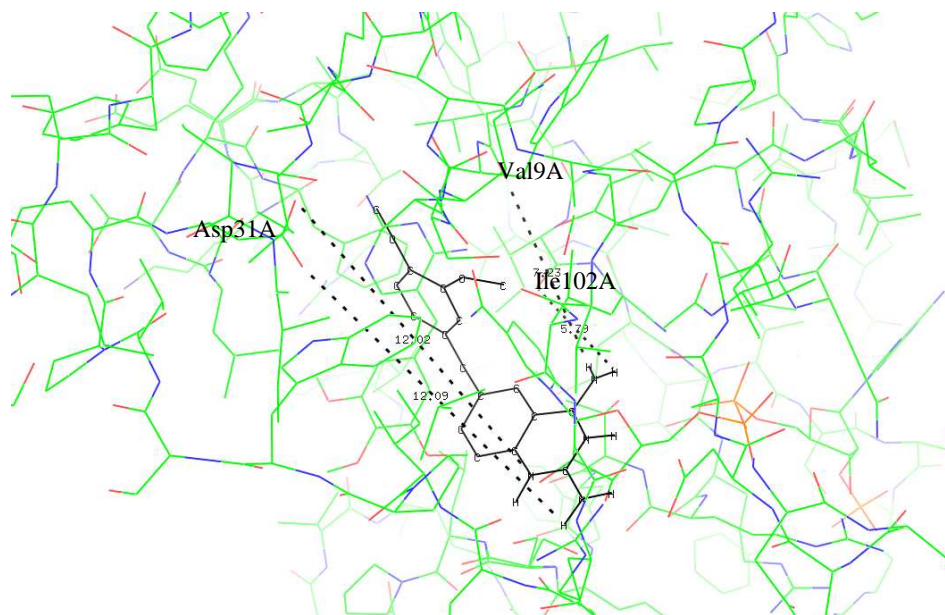
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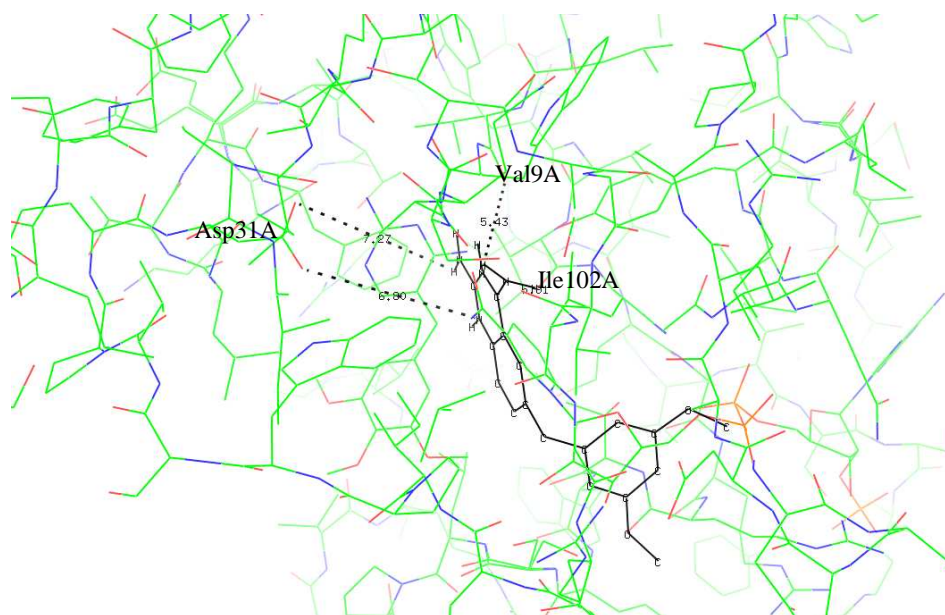
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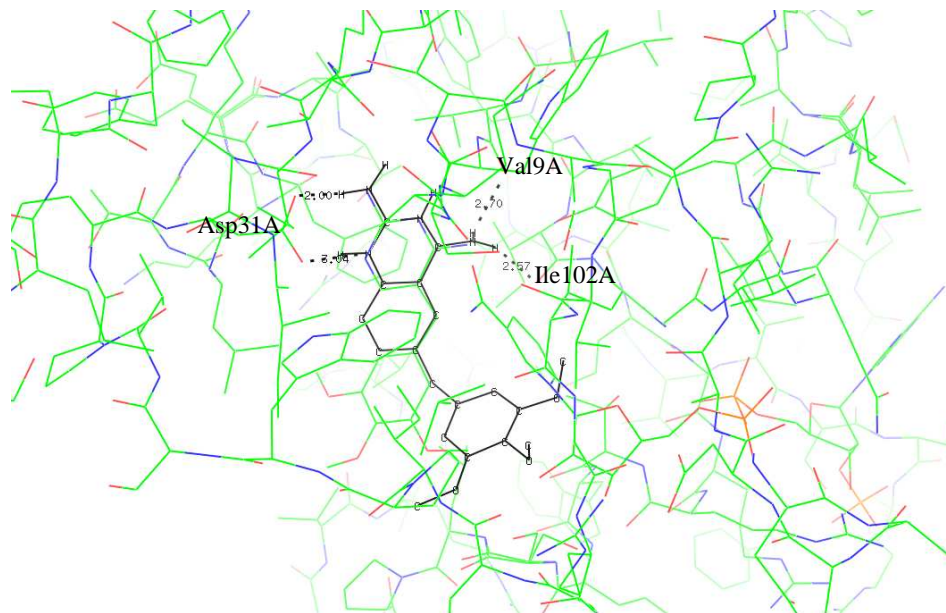
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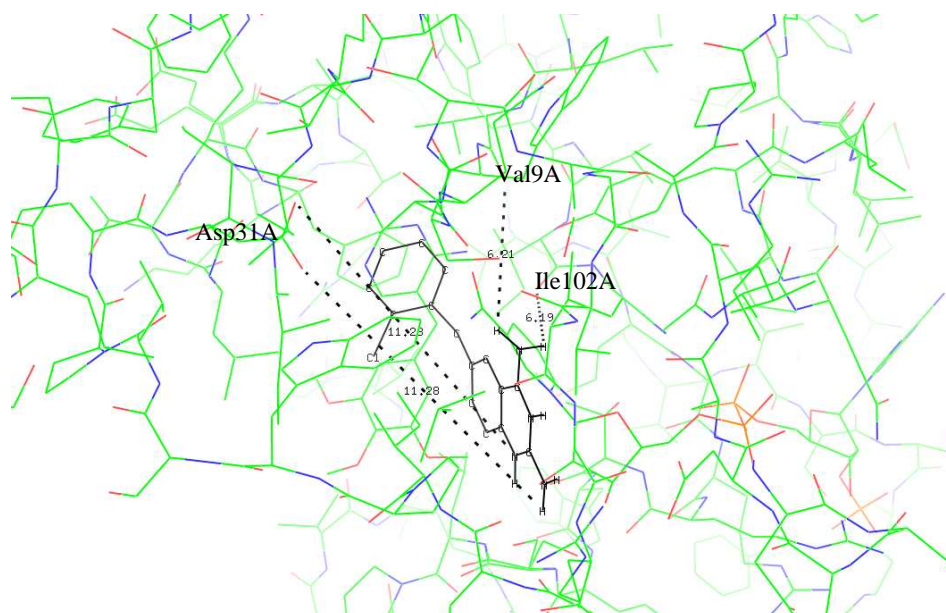
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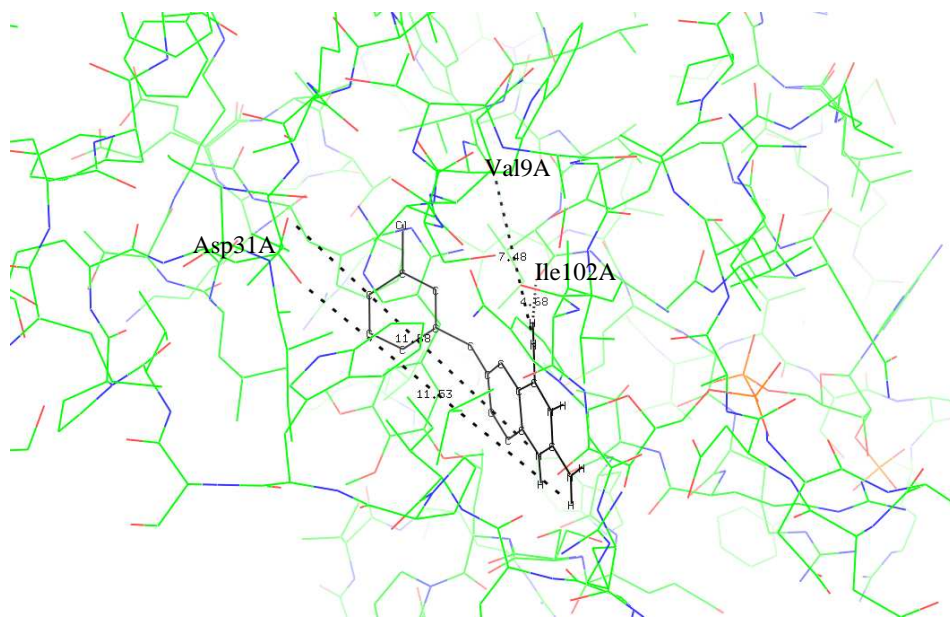
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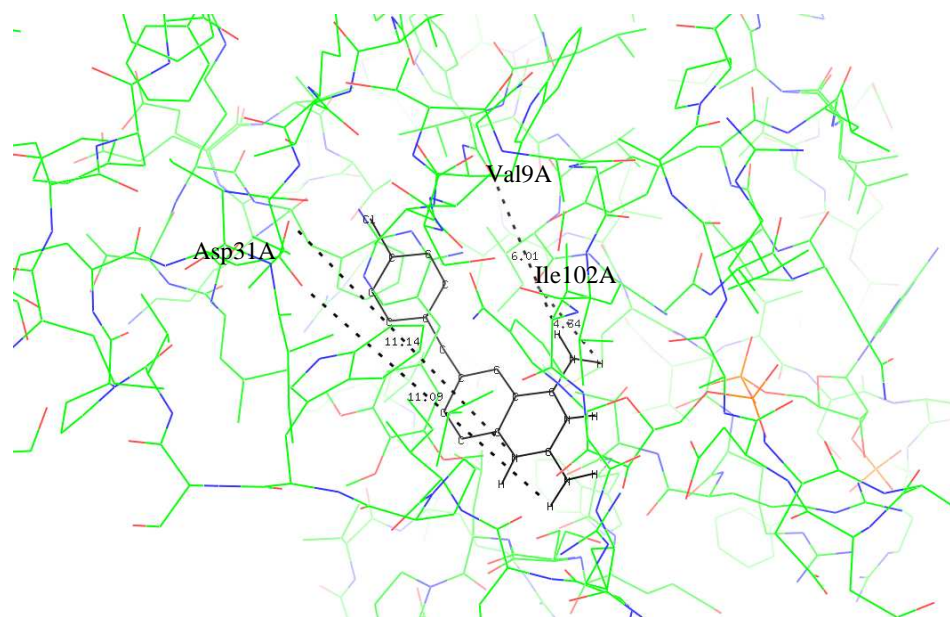
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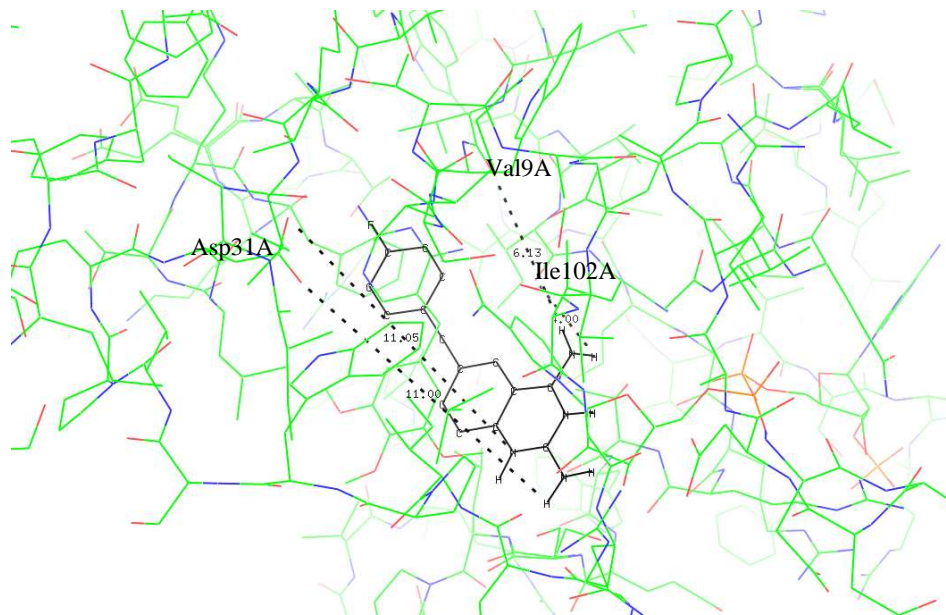
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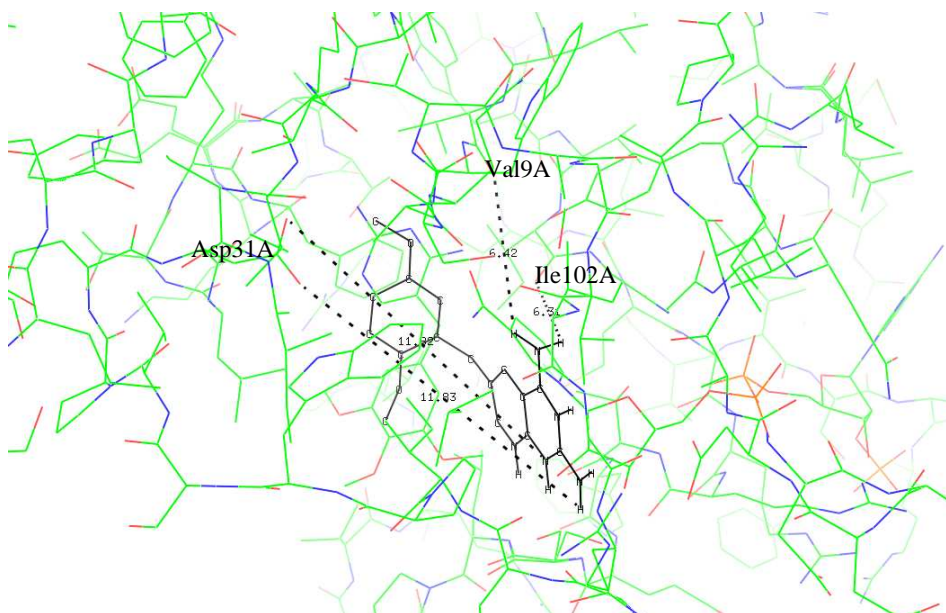
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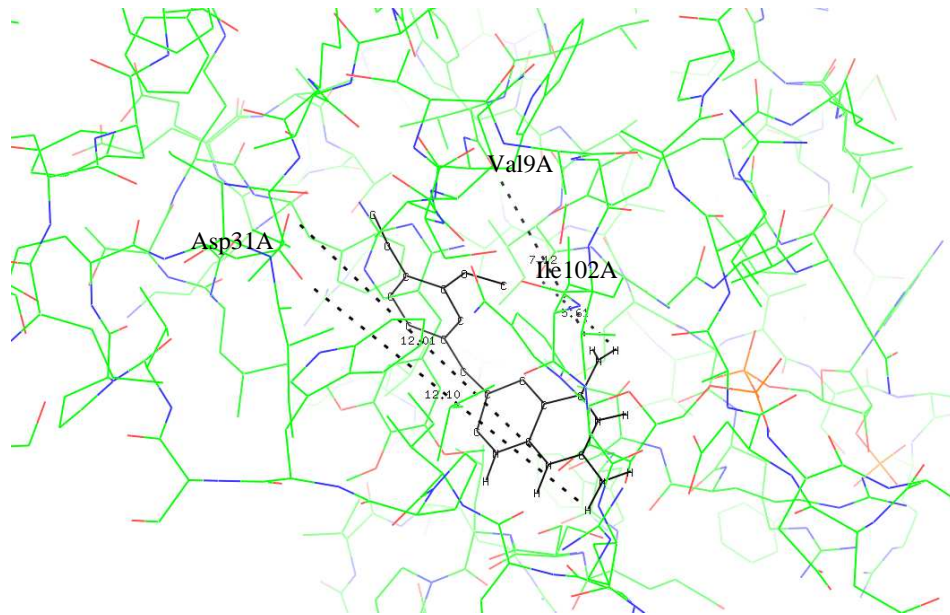


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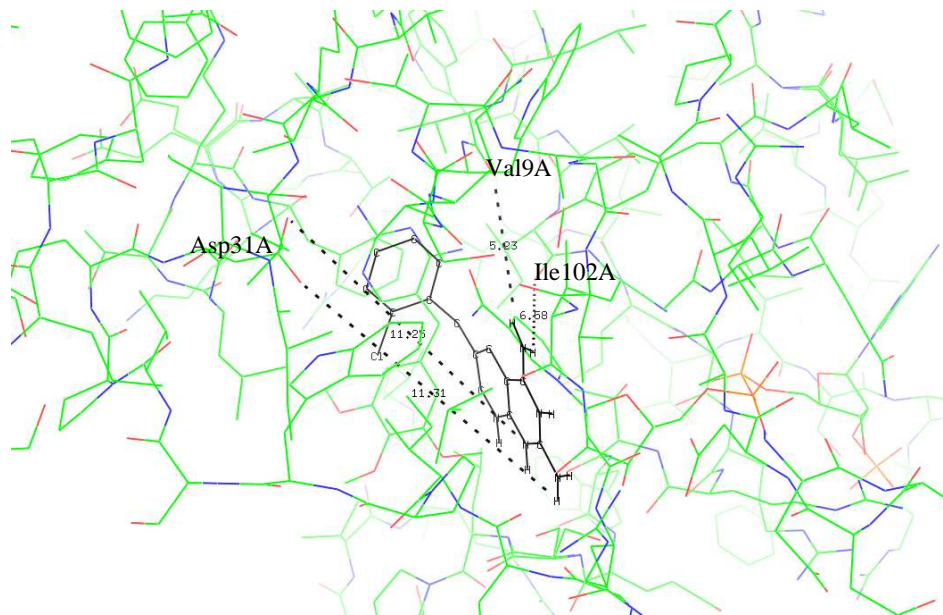
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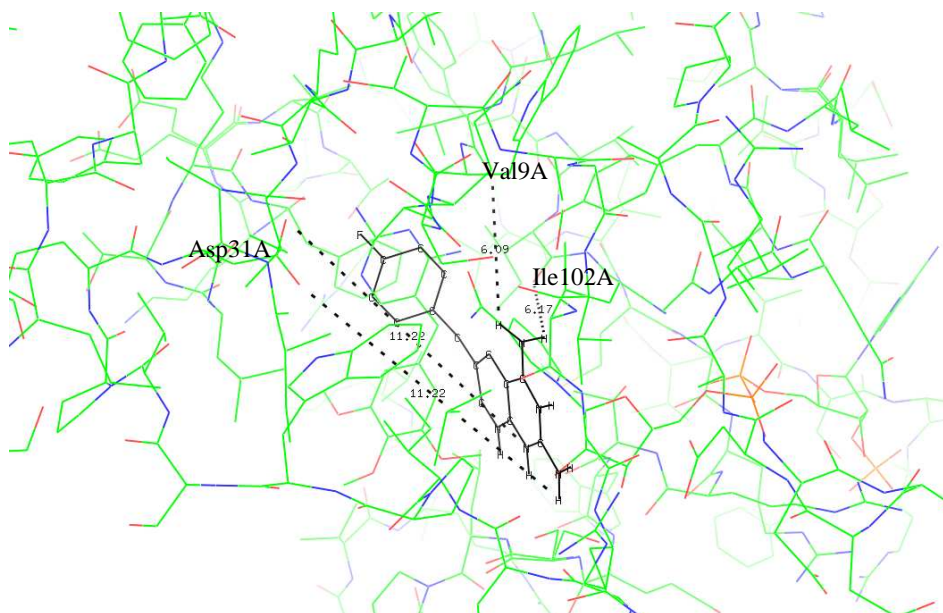
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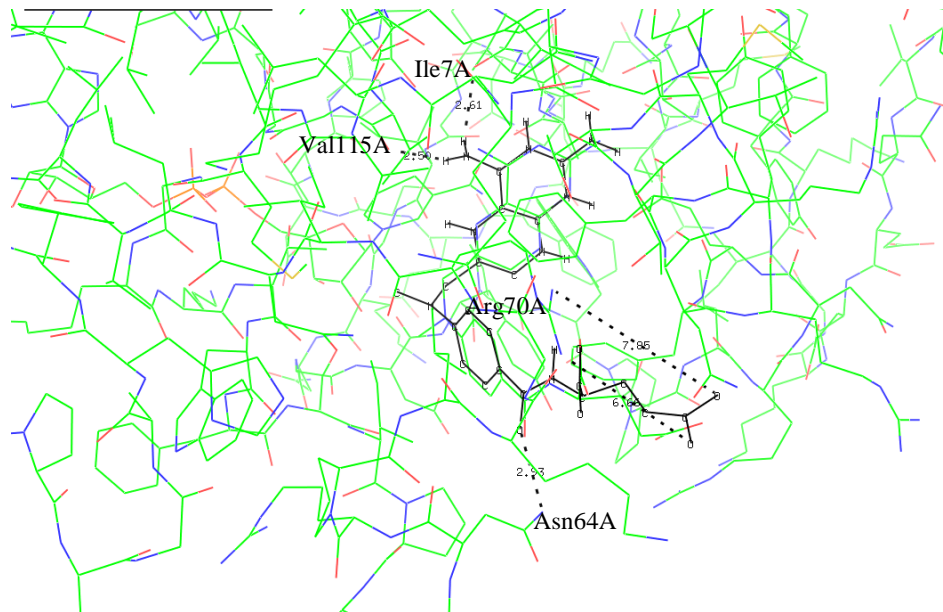


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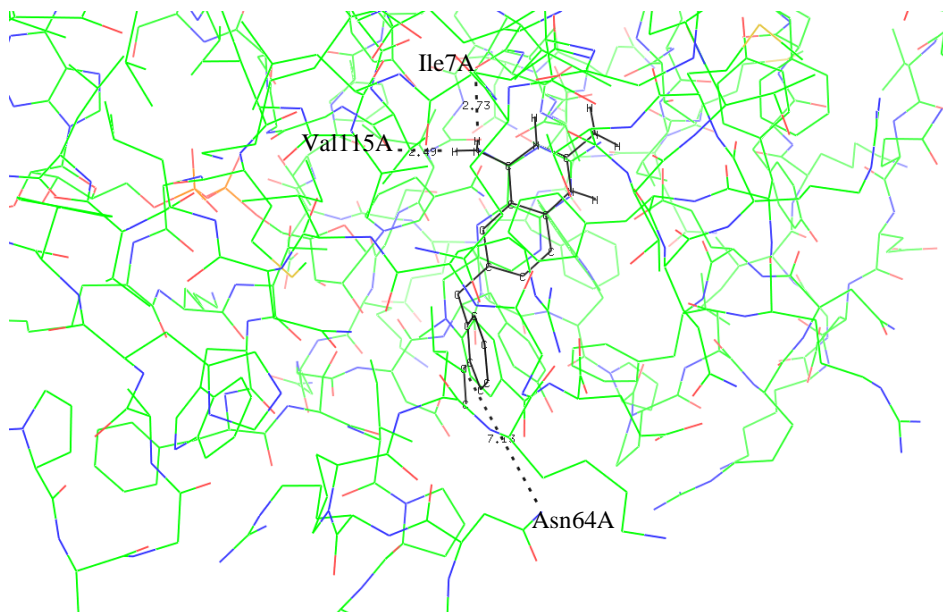


Lampiran 5 Jarak ikatan hidrogen dengan senyawa turunan 2,4-diaminopirido[2,3-d] pirimidin pada DHFR sel mamalia

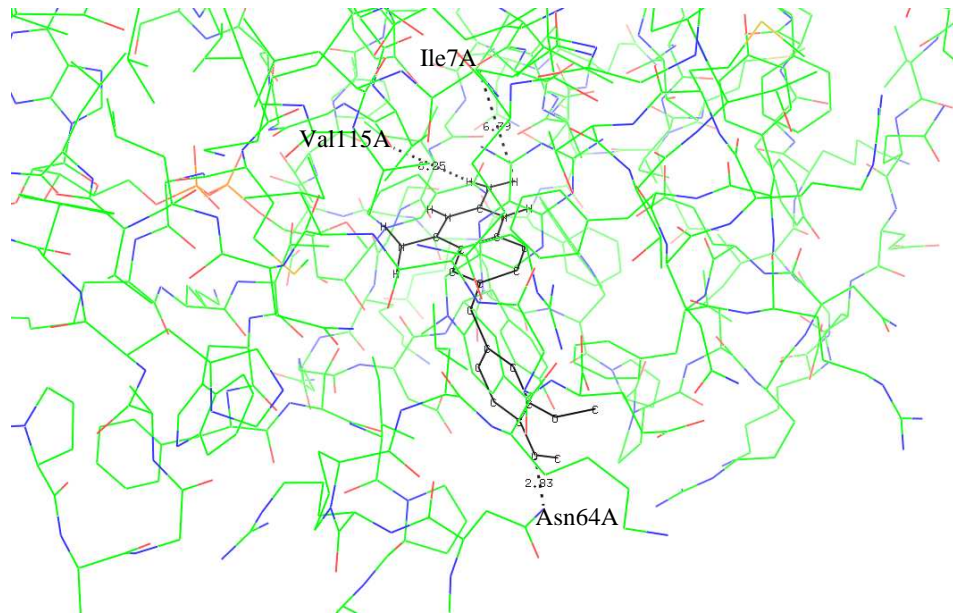
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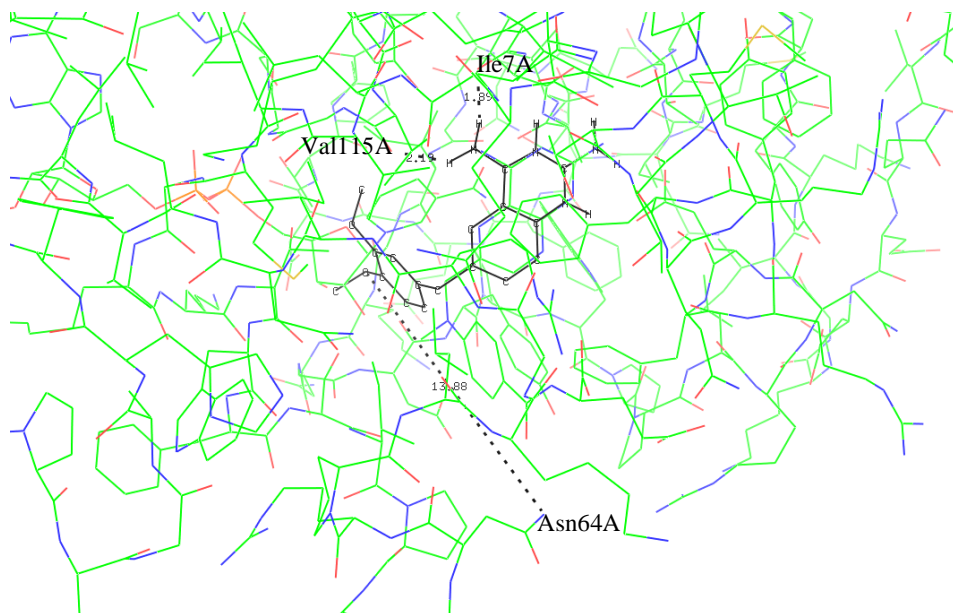
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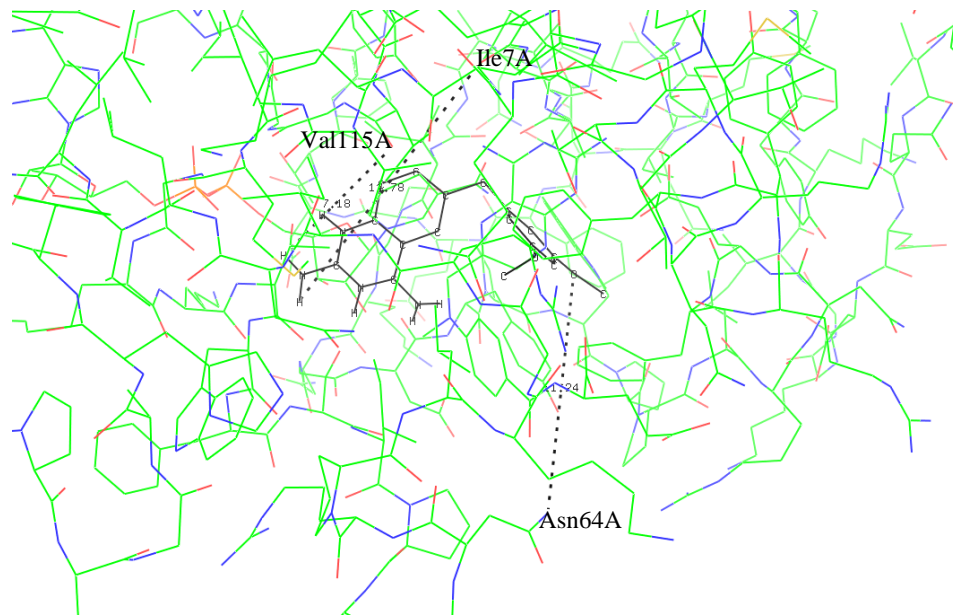
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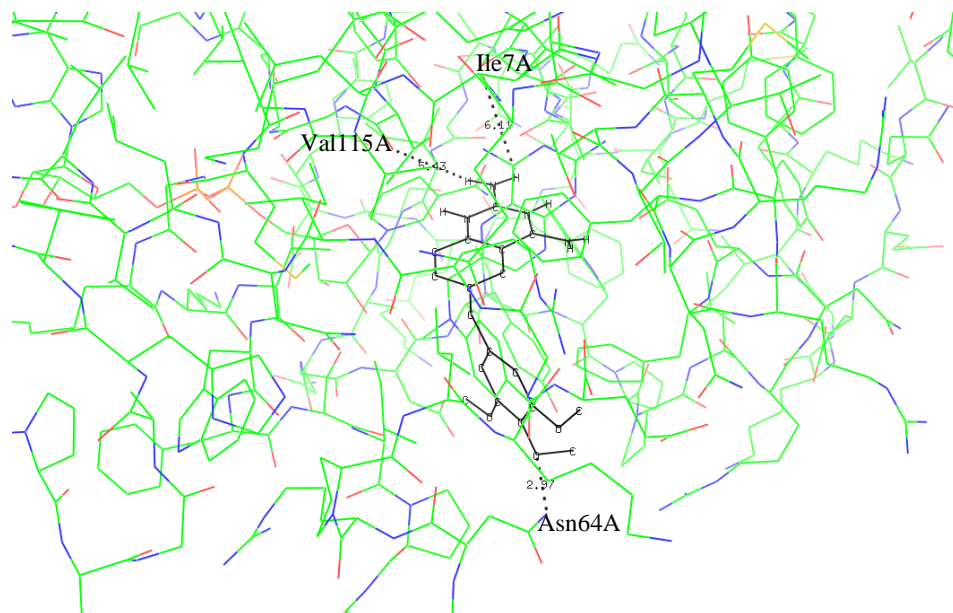
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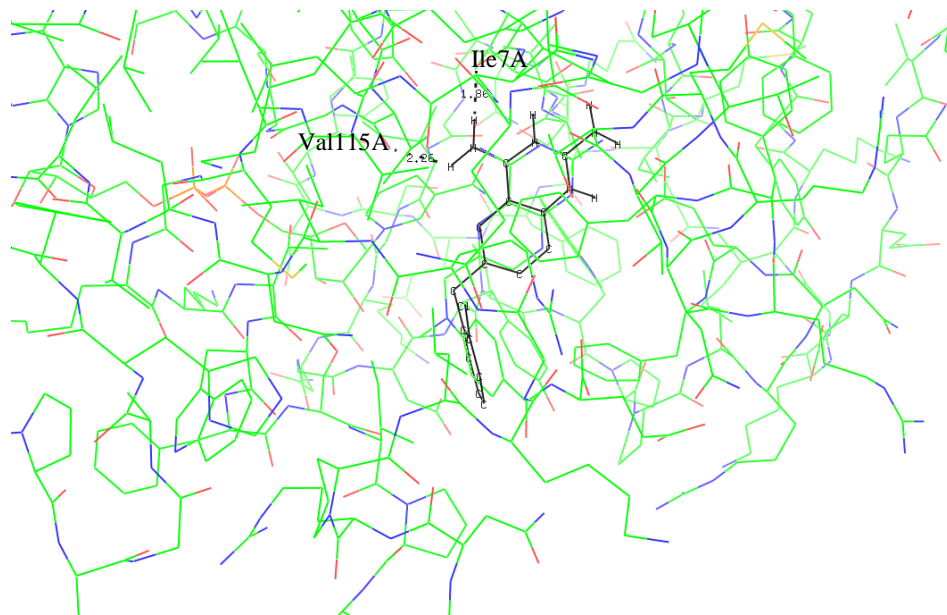
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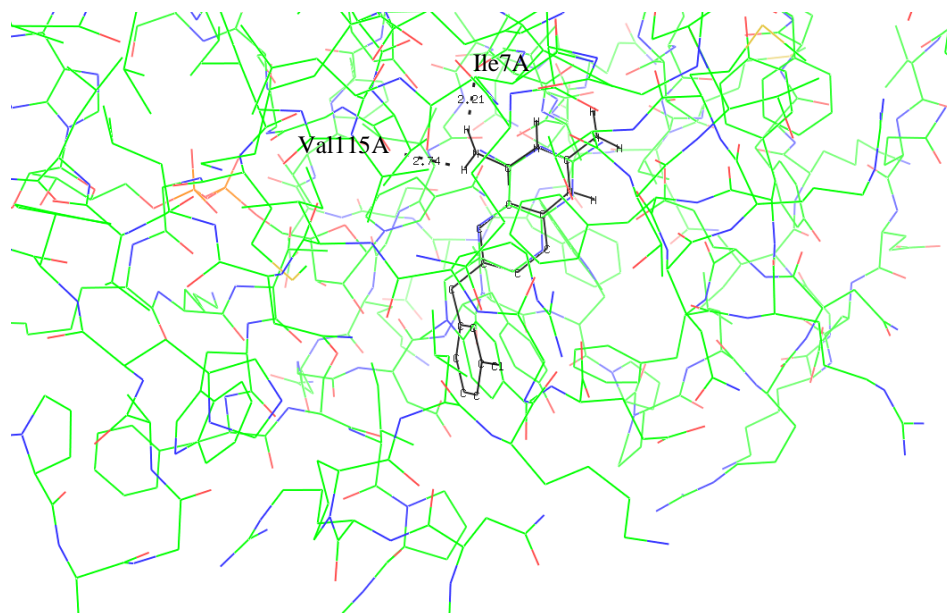
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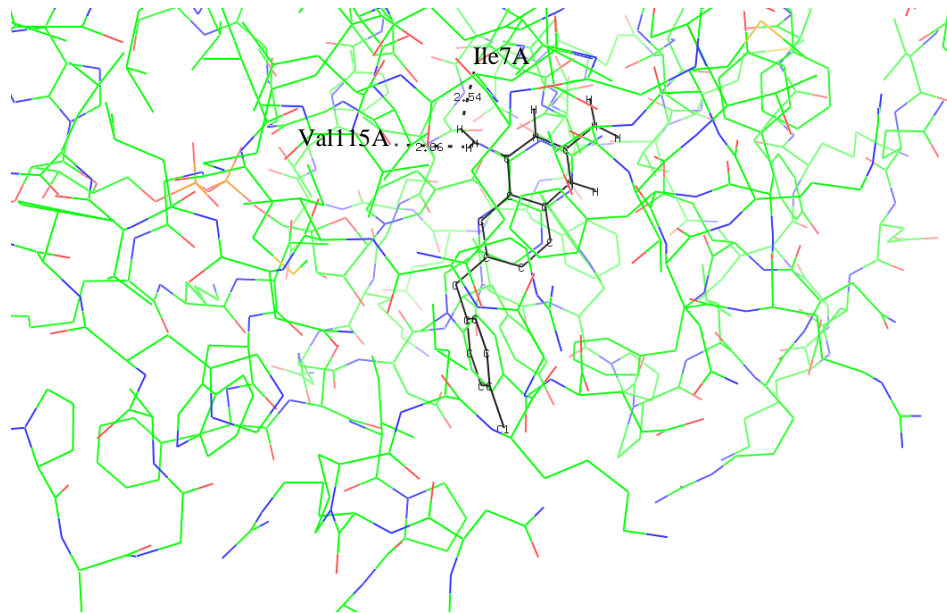
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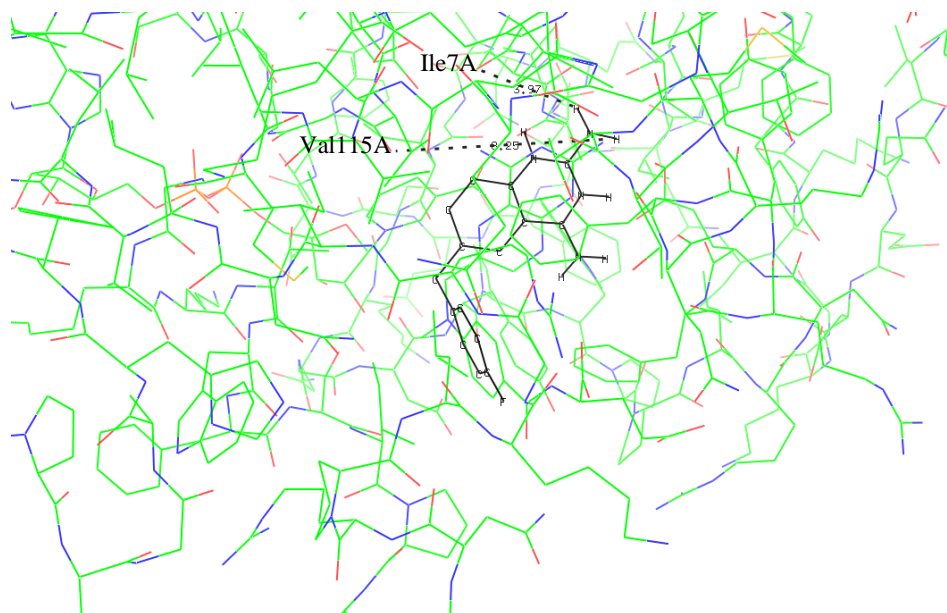
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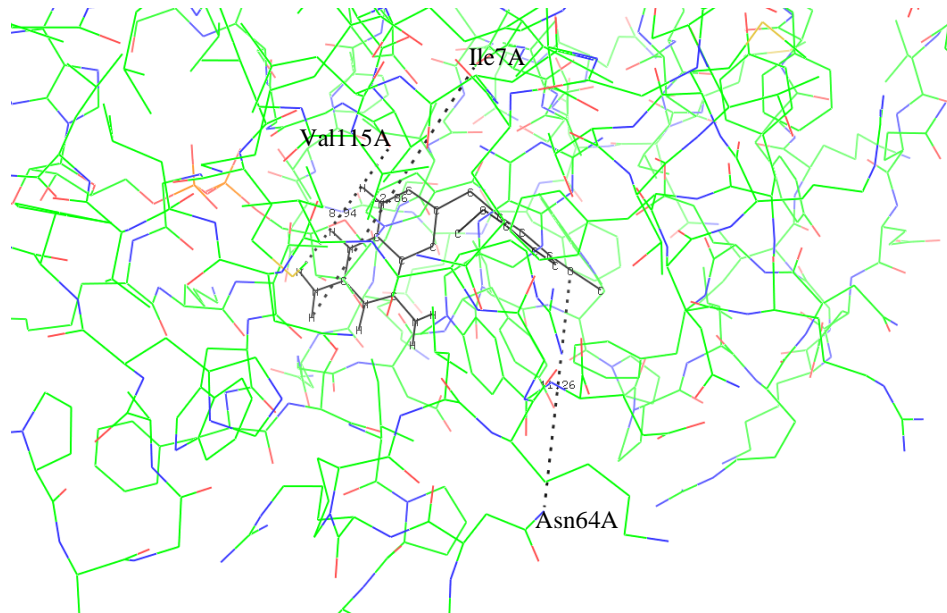
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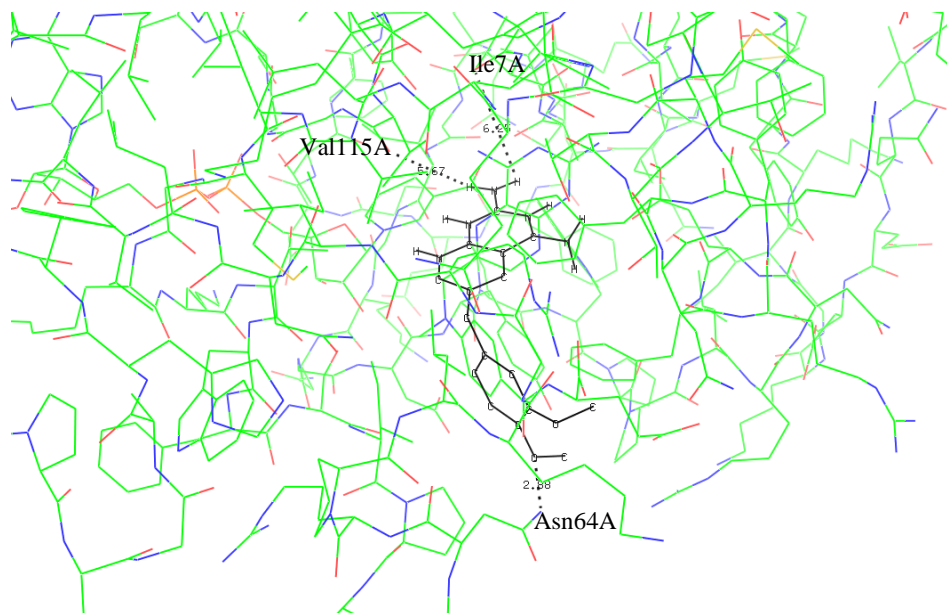
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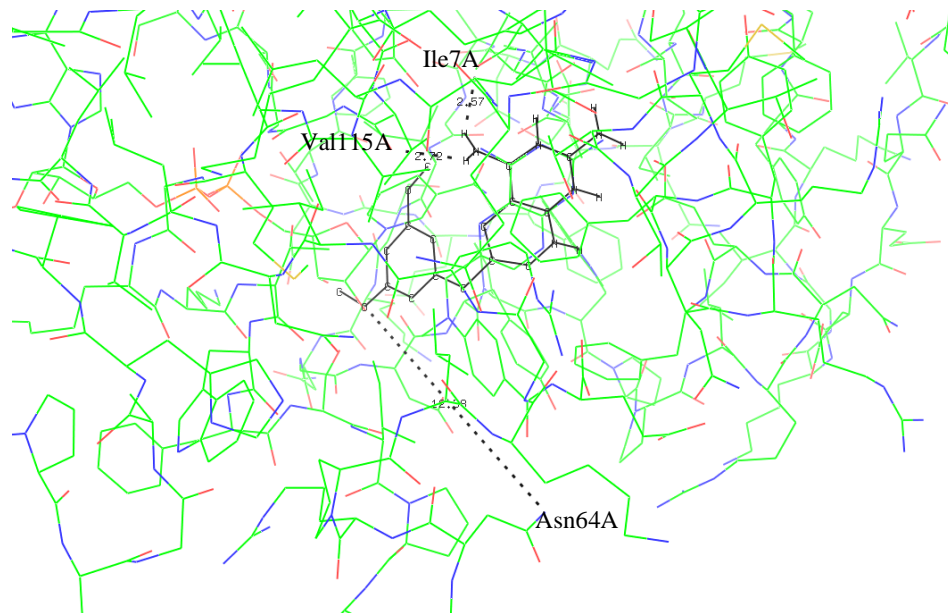


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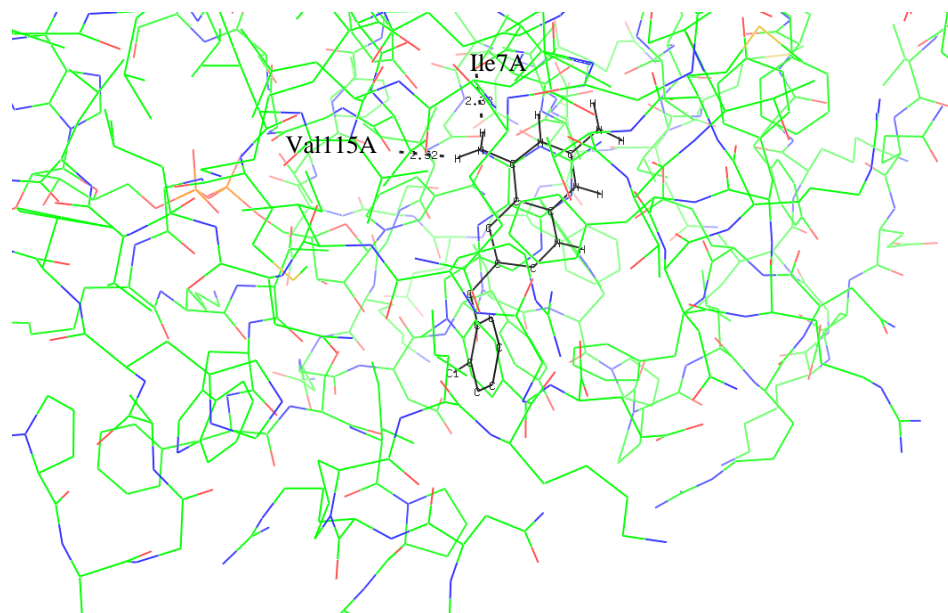




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