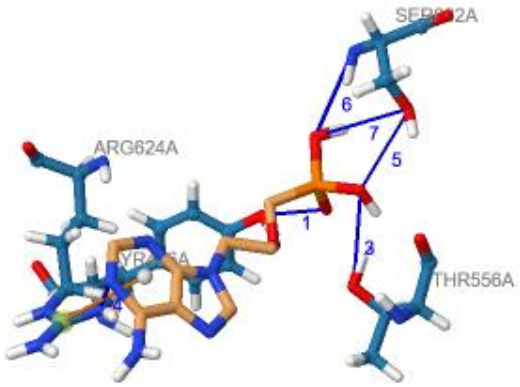
Associated content. Individual chemical evaluation of each complex.

Please note that all titles for inspected complexes follow the nomenclature as
drug name_protein_docking software

ADEFOVIR_POLYMERASE_AUTODOCKVINA



Hydrogen Bonds: 7

- Strong (<2,5 Å): 0

- Moderated: 3

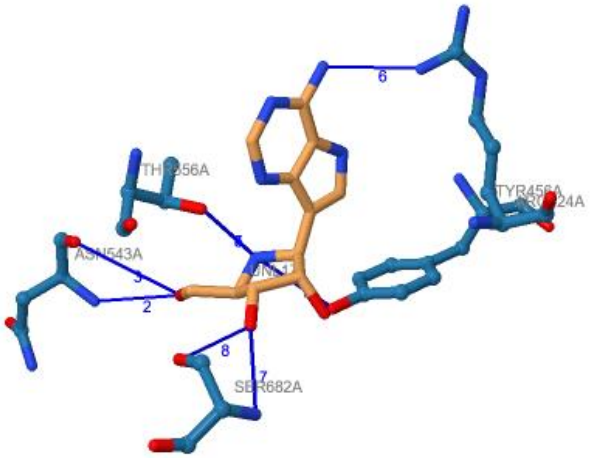
- Weak (>3,2 Å): 4

Average distance (D-A): 3,3 Å

Pi-cation interaction: 1

Hydrogen bonds are moderately intense at one end of the ligand, plus the opposite pi-cation interaction indicate favoring the stability of the complex. Spatial orientation also seems to facilitate the capture and correct orientation of the ligand.

GALIDESIVIR_POLYMERASE_PATCHDOCK



Hydrogen Bonds: 8

- Stong (<2,5 Å): 2

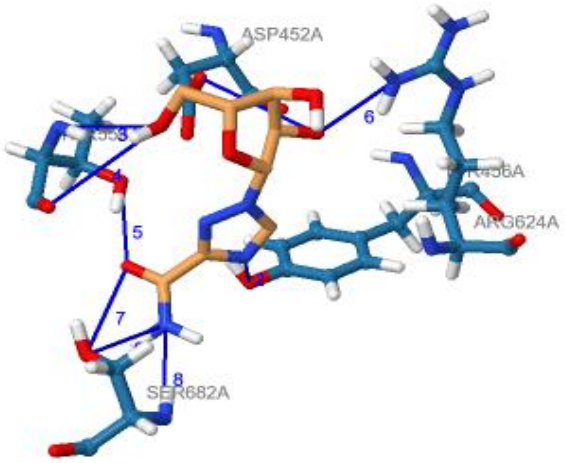
- Moderated: 1

- Weak (>3,2 Å): 5

Average Distance (D-A): 3,17 Å

Strong hydrogen bonds, mainly with SER682A and ASN543A would lead to a very stable complex.

RIBAVIRIN_POLYMERASE_AUTODOCKVINA



Hydrogen Bonds: 9

- Strong (<2,5 Å): 0

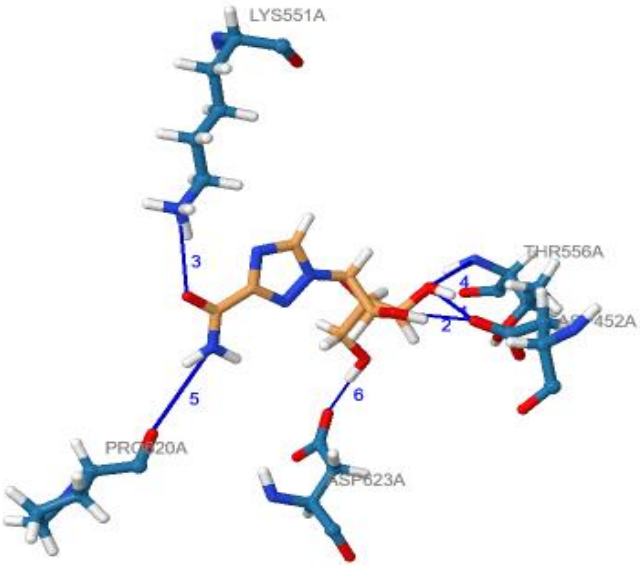
- Moderated: 5

- Weak (>3,2 Å): 4

Average Distance (D-A): 3,33 Å

Moderate strength average, multiple moderately intense H bonds close to SER682A and THR556A favor the stabilization of the complex. Relatively open structure facilitates connection.

RIBAVIRIN_POLYMERASE_DOCKTHOR



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

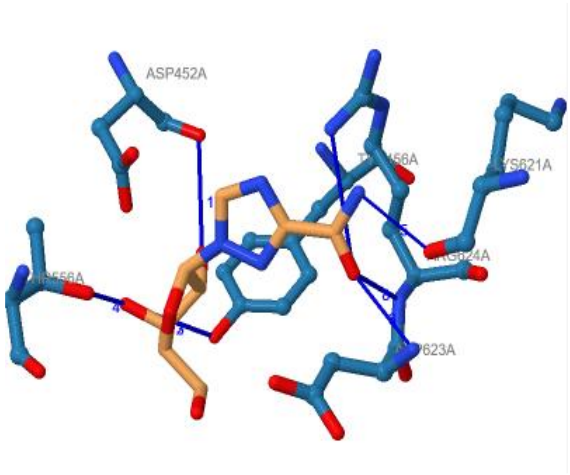
- Moderated: 5

- Weak (>3,2 Å): 1

Average Distance (D-A): 2,99 Å

Compared with AutoDock Vina, there are fewer H bonds but the most intense ones remain. Spatial conformation also seems to facilitate the connection more.

RIBAVIRIN_POLYMERASE_PATCHDOCK



Hydrogen Bonds: 8

- Strong (<2,5 Å): 1

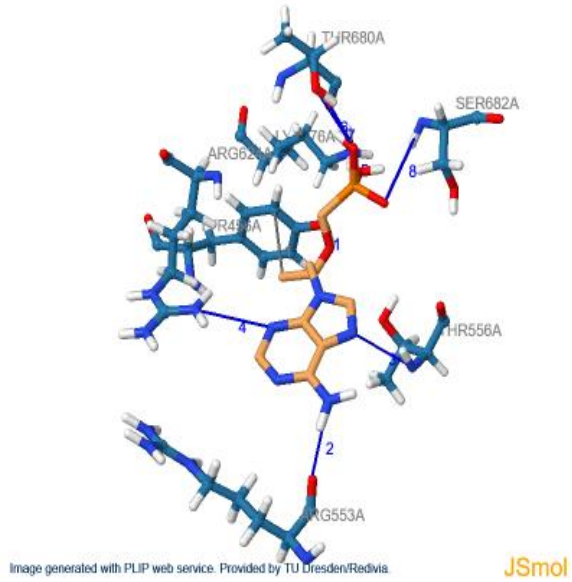
- Moderated: 3

- Weak (>3,2 Å): 4

Average Distance (D-A): 3,08 Å

Similar to AutoDock Vina, but showing some even more intense H bonds. The connection is favorable through the ASP452A-THR556A-LYS621A face.

TENOFOVIR_POLYMERASE_AUTODOCKVINA



Hydrogen Bonds: 8

- Strong (<2,5 Å):

- Moderated: 3

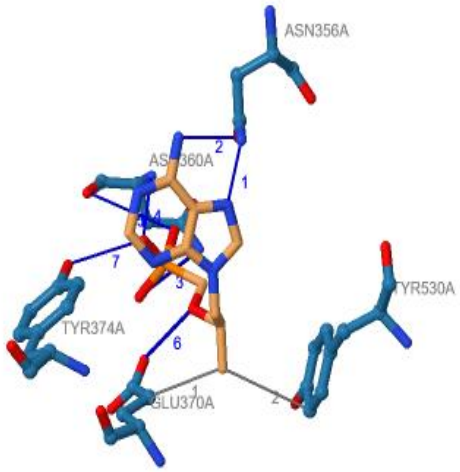
- Weak (>3,2 Å): 5

Average Distance (D-A): 3,24 Å

Hydrophobic interactions: 1 (3,96 Å)

Multiple H bonds, but of medium to low intensity. Conformation can make binding difficult, but the THR556A-ARG553A-THR680A face appears free for approach.

TENOFOVIR_POLYMERASE_PATCHDOCK



Hydrogen Bonds: 7

- Strong (<2,5 Å): 1

- Moderated: 1

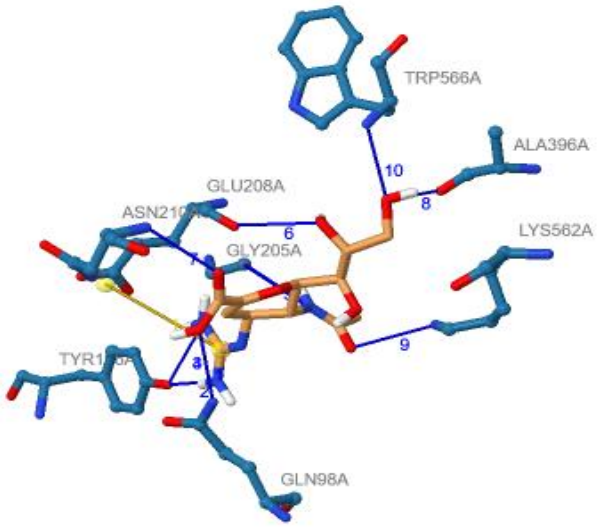
-Weak (>3,2 Å): 5

Average Distance (D-A): 3,4 Å

Hydrophobic interactions: 2 (3,33 Å; 3,69 Å)

H bonds are slightly less intense than in AutoDock Vina, even considering the greatest hydrophobic interactions. The structure only favors the connection with the entry of the ligand on the face ASN356A-TYR375A-TYR530A and with the correct orientation.

ZANAMIVIR_RBD_AUTODOCKVINA



Hydrogen Bonds: 10

- Strong (<2,5 Å): 0

- Moderated: 5

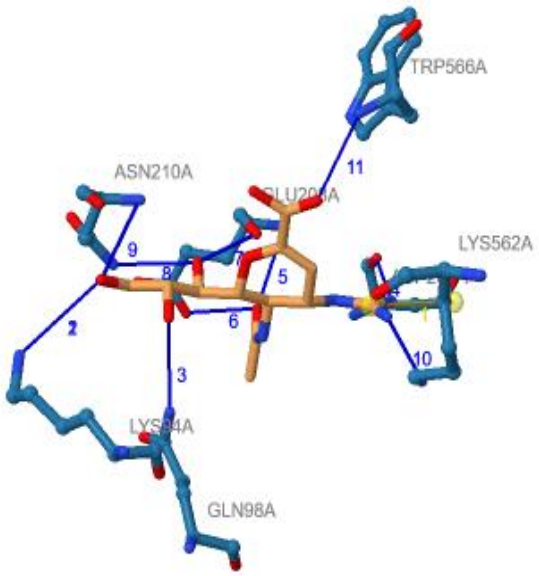
- Weak (>3,2 Å): 5

Average Distance (D-A): 2,97 Å

Saline bridge: 1

Large number of moderately intense H bonds and saline bridge suggest a stable complex. However, the positioning of amino acids makes it difficult for the ligand to enter, except perhaps if the approach is through the TRP566A-ALA396A-LYS562A-ASN210A-GLN98A face.

ZANAMIVIR_RBD_PATCHDOCK



Hydrogen Bonds: 11

- Strong (<2,5 Å): 1

- Moderated: 2

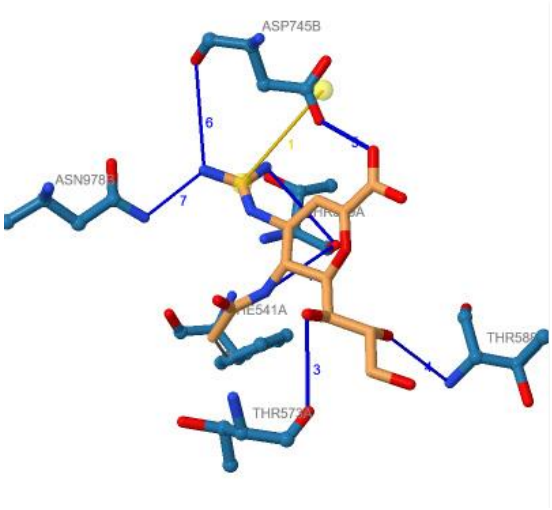
- Weak (>3,2 Å): 8

Average Distance (D-A): 3,29 Å

Saline bridge: 1

As in the case of AutoDock Vina, there are a large number of H bonds, although in general not so intense. Steric impediment also appears to be significant, the TRP566A - LYS562A- LYS94A approach, with the correct orientation of the ligand, seems to be the only viable one.

ZANAMIVIR_PROTEINSCLOSED_PACTHDOCK



Hydrogen Bonds: 7

- Strong (<2,5 Å): 0

- Moderated: 2

- Weak (>3,2 Å): 5

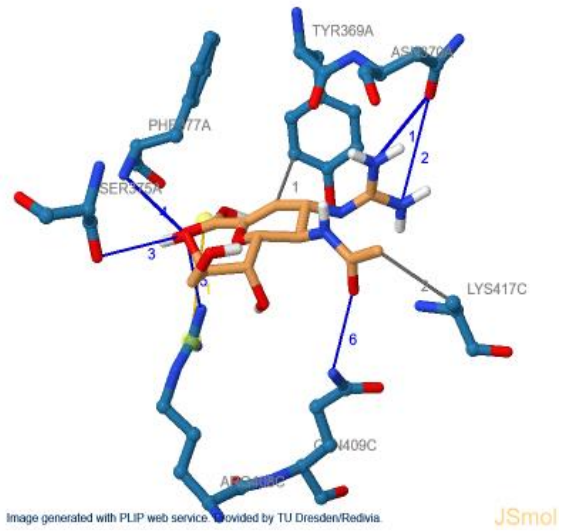
Average Distance (D-A): 3,45 Å

Saline Bridge: 1

Hydrophobic interactions: 1 (2,84 Å)

H bonds are generally weak, but 5 connections and a saline bridge between the ligand and the nearby amino acids ASN978B; ASP745B and THR549A indicate favoring complex formation by the face ASN978B- ASP745B- THR573A-THR588A if properly oriented.

ZANAMIVIR_PROTEINSOPEN_AUTODOCKVINA



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

- Moderated: 2

- Weak (>3,2 Å): 4

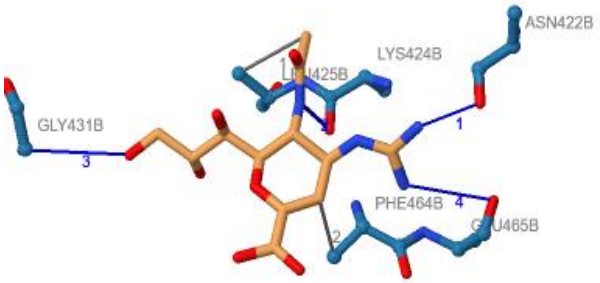
Average Distance (D-A): 3,46 Å

Saline Bridge: 1

Hydrophobic interactions: 2 (3,59 Å; 3,52 Å)

H bonds and hydrophobic interactions are well distributed, but in general less intense. Direct access to the site from the face SER375A-LYS 417C-ASN 370A (figure) it's free. Overall, the complex formation with Zanamivir seems slightly less favored than in the closed patchdock.

ZANAMIVIR_PROTEINSOPEN_PATCHDOCK



Hydrogen Bonds: 4

- Strong (<2,5 Å): 0

- Moderated: 2

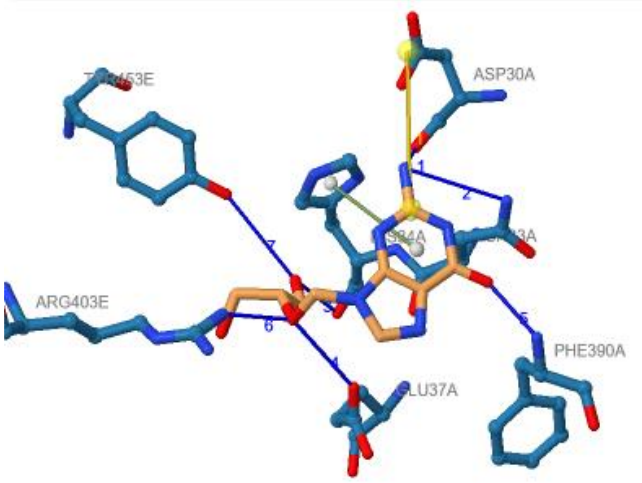
- Weak (>3,2 Å): 2

Average Distance (D-A): 3,3 Å

Hydrophobic interactions: 2 (3,41 Å; 3,17 Å)

Number of H bonds (weak) is less than in AutoDock Vina, but with greater contribution from hydrophobic interactions. The spatial distribution appears to be quite free and favorable for the capture of the ligand, although its retention may be less durable in this conformation.

GANCICLOVIR_RBD_PATCHDOCK



Hydrogen Bonds: 7

- Strong (<2,5 Å): 1

- Moderated: 1

- Weak (>3,2 Å): 5

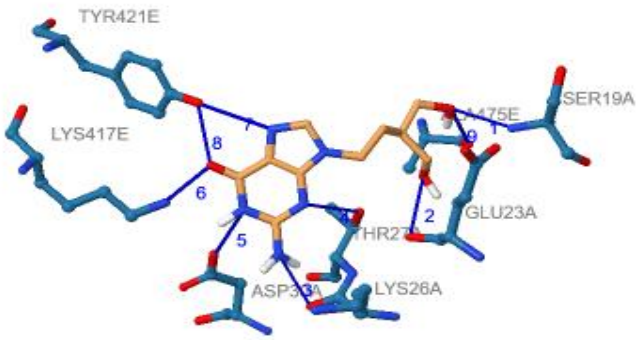
Average Distance (D-A): 3,37 Å

Pi-stack: 1

Saline Bridge: 1

Has one strong H bond, as well as pi-electron and saline interactions. Open structure facilitates connection, but there are doubts about stability.

PENCICLOVIR_RBD_AUTODOCKVINA



Hydrogen Bonds: 9

- Strong (<2,5 Å): 0

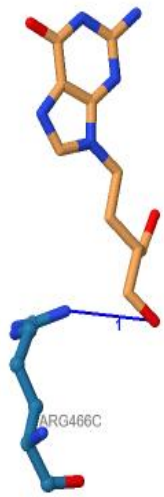
- Moderated: 7

- Weak (>3,2 Å): 2

Average Distance (D-A): 3,07 Å

The large number of moderately intense H bonds, mainly around the purine, indicates a very stable complex. Spatial orientation also seems to favor the approximation of the ligand and formation of the complex.

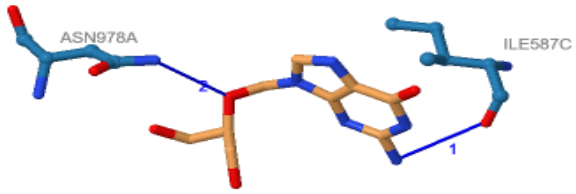
PENCICLOVIR_PROTEINSCLOSED_PATCHDOCK



Hydrogen Bonds: 1 (weak, 3,59 Å)

With only a weak H bond, it doesn't look like a good connection model.

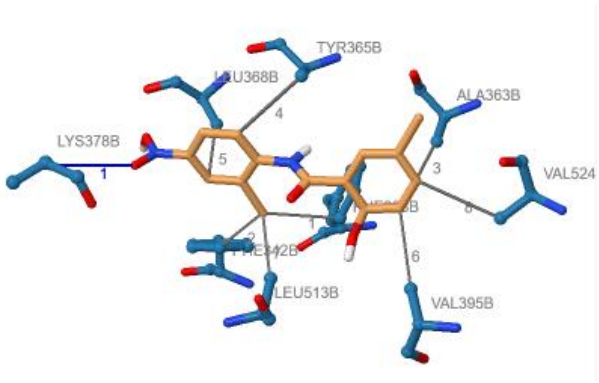
GANCICLOVIR_PROTEINSOPEN_PATCHDOCK



Hydrogen Bonds: 2 (weaks, 3,34 Å; 3,31 Å)

With only two weak H bonds, it doesn't look like a good connection model.

NICLOSAMIDE_PROTEINSOPEN_AUTODOCKVINA

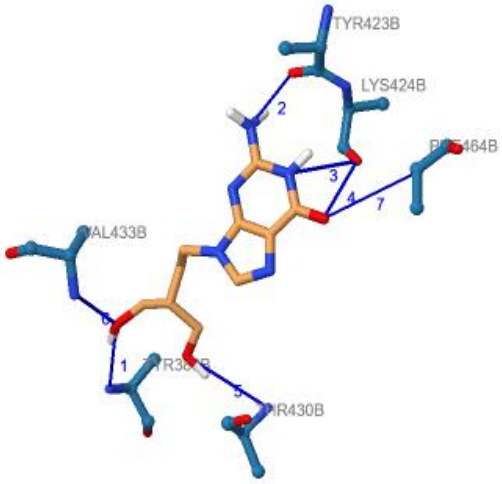


Hydrogen Bonds: 1 (weak, 3,98 Å)

Hydrophobic interactions: 8 (moderated 3,64 Å)

Model shows the ligand interacting by hydrophobicity, with only a weak H bond. It does not appear to be a very stable complex.

PENCICLOVIR_PROTEINSOPEN_AUTODOCKVINA



Hydrogen Bonds: 7

- Strong (<2,5 Å): 0

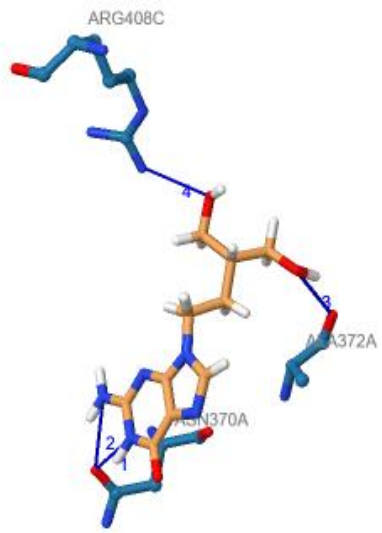
- Moderated: 2

- Weak (>3,2 Å): 5

Average Distance (D-A): 3,43 Å

There are not many strong H bonds, but the concentration of these around the purine can facilitate binding.

PENCICLOVIR_PROTEINSOPEN_DOCKTHOR



Hydrogen Bonds: 4

- Strong (<2,5 Å): 0

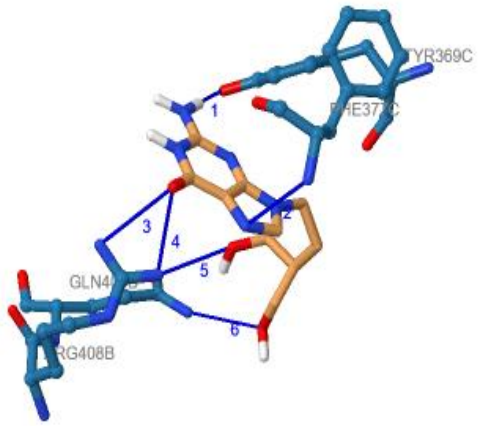
- Moderated: 3

- Weak (>3,2 Å): 1

Average Distance (D-A): 3,08 Å

Although less in quantity, the H bonds are somewhat more intense in this model, the presence at both ends of the ligand can help to form the bond.

PENCICLOVIR_PROTEINSCLOSED_AUTODOCK



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

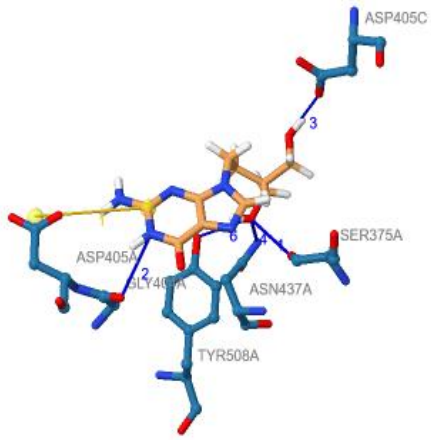
- Moderated: 3

- Weak (>3,2 Å): 3

Average Distance (D-A): 3,23 Å

Moderately strong connections. Clearance on two opposite sides should facilitate connection.

PENCICLOVIR_PROTEINSCLOSED_DOCKTHOR



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

- Moderated: 6

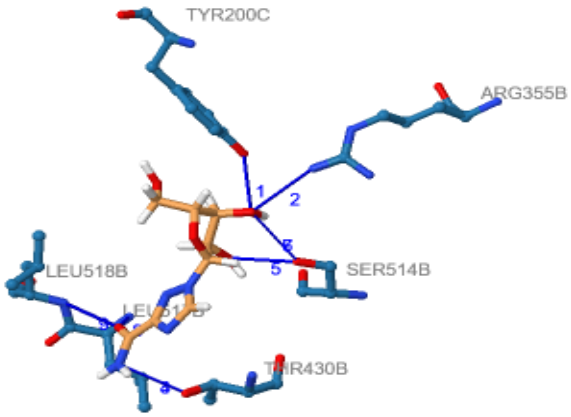
- Weak (>3,2 Å): 0

Average Distance (D-A):2,89 Å

Saline bridge: 1

A large amount of moderately intense H bonds and a saline bridge indicate great stability. The ASP405A-ASP405C face opposite the TYR508A (figure) is wide open for connection.

RIBAVIRIN_PROTEINSCLOSED_AUTODOCKVINA



Hydrogen Bonds: 9

- Strong (<2,5 Å): 0

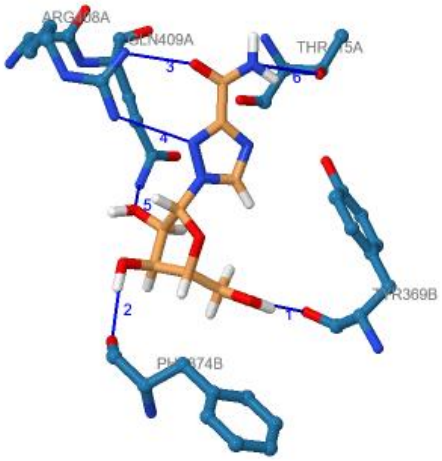
- Moderated: 7

- Weak (>3,2 Å): 2

Average Distance (D-A): 3,11 Å

Many moderately intense H bonds indicate stability. The TYR200c-ARG355B-THR430B face (figure) is open for approach.

RIBAVIRIN_PROTEINSCLOSED_DOCKTHOR



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

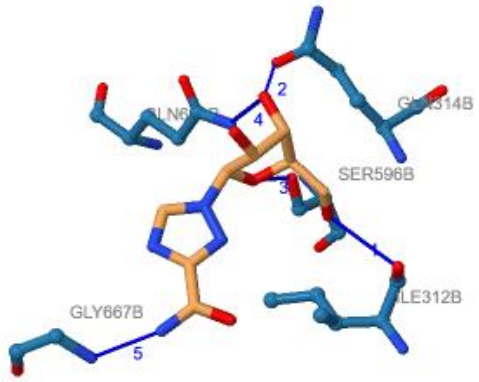
- Moderated: 4

- Weak (>3,2 Å): 2

Average Distance (D-A): 3,06 Å

Similar to the AutoDock Vina model, moderate connections and easy approach.

RIBAVIRIN_PROTEINSCLOSED_PATCHDOCK



Hydrogen Bonds: 5

- Strong (<2,5 Å): 1

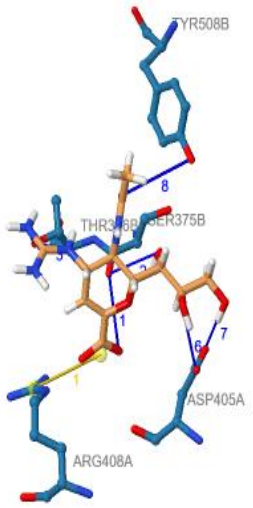
- Moderated: 2

- Weak (>3,2 Å): 2

Average Distance (D-A): 2,95 Å

Despite a stronger H bond, it is still similar to the AutoDock Vina and Dockthor models in stability and ease

ZANAMIVIR_PROTEINSCLOSED_DOCKTHOR



Hydrogen Bonds: 8

- Strong (<2,5 Å): 0

- Moderated: 2

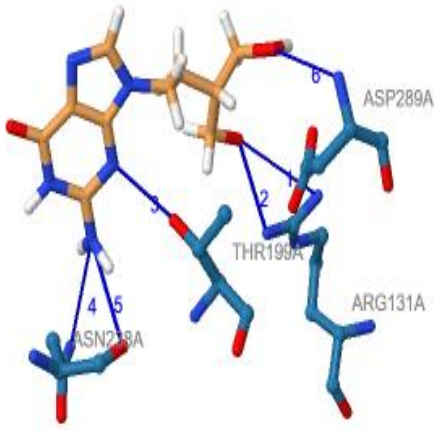
- Weak (>3,2 Å): 6

Average Distance (D-A): 3,47 Å

Saline Bridge: 1

Moderately high stability. Free approach by face ASP405A-ARG408A-TYR508B.

PENCICLOVIR_PROTEINMPRO_AUTODOCKVINA



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

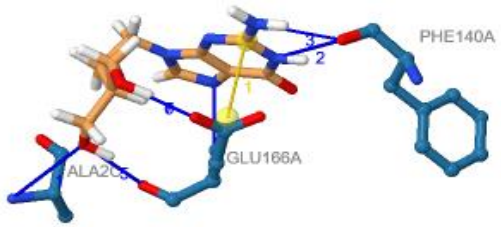
- Moderated: 2

- Weak (>3,2 Å): 4

Average Distance (D-A): 3,27 Å

Wide open and easy structure for connection, but relatively weak interactions impair stability.

PENCICLOVIR_PROTEINMPRO_DOCKTHOR



Hydrogen Bonds: 7

- Strong (<2,5 Å): 0

- Moderated: 6

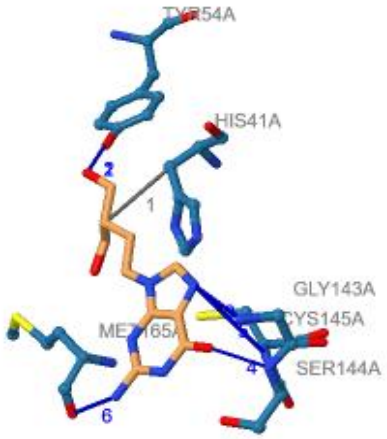
- Weak (>3,2 Å): 1

Average Distance (D-A): 2,98 Å

Saline Bridge: 1

Large number of moderately intense H bonds and saline bridge help with stability compared to AutoDock Vina model. Open structure for connection.

PENCICLOVIR_PROTEINMPRO_PATCHDOCK



Hydrogen Bonds: 6

- Strong (<2,5 Å): 1

- Moderated: 3

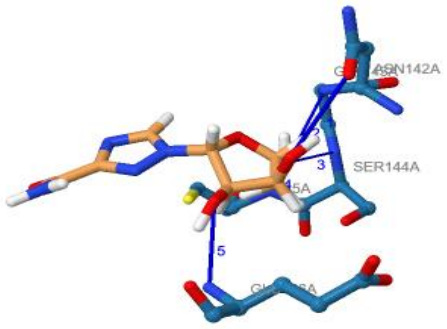
- Weak (>3,2 Å): 2

Average Distance (D-A): 3,43 Å

Hydrophobic interactions: 1 (3,93 Å)

Less interactions than Dockthor model, but some stronger. Open structure for connection on the face shown in the figure.

RIBAVIRIN_PROTEINMPRO_AUTODOCKVINA



Hydrogen Bonds: 5

- Strong (<2,5 Å): 0

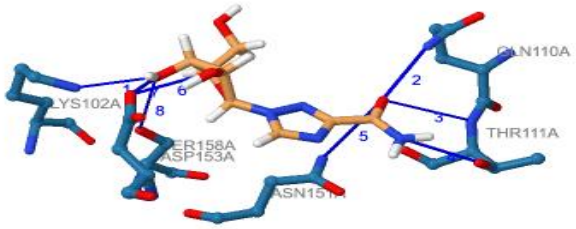
- Moderated: 2

- Weak (>3,2 Å): 3

Average Distance (D-A): 3,19 Å

Few interactions indicate low stability, despite the steric ease of binding.

RIBAVIRIN_PROTEINMPRO_DOCKTHOR



Hydrogen Bonds: 8

- Strong (<2,5 Å): 0

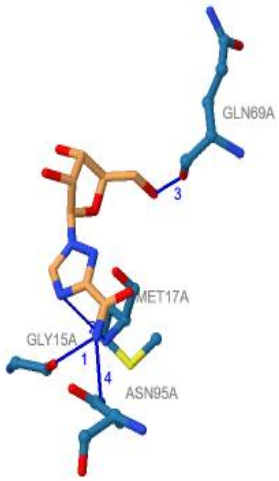
- Moderated: 3

- Weak (>3,2 Å): 5

Average Distance (D-A): 3,28 Å

Relatively more stable than the AutoDock Vina model, still maintaining an open face.

RIBAVIRIN_PROTEINMPRO_PATCHDOCK



Hydrogen Bonds: 4

- Strong (<2,5 Å): 1

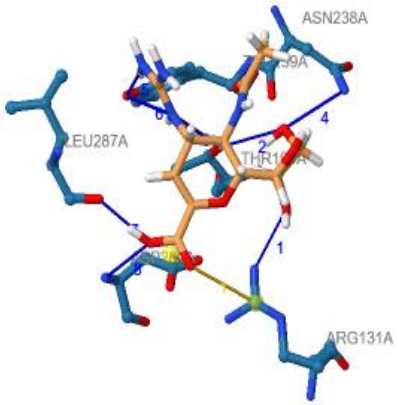
- Moderated: 2

- Weak (>3,2 Å): 1

Average Distance (D-A): 2,95 Å

Fewer interactions than the Dockthor model, but more intense. Esterically open.

ZANAMIVIR_PROTEINMPRO_AUTODOCKVINA



Hydrogen Bonds: 8

- Strong (<2,5 Å): 0

- Moderated: 4

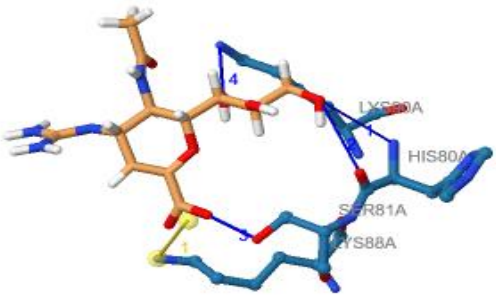
- Weak (>3,2 Å): 4

Average Distance (D-A): 3,26 Å

Saline Bridge: 1

Several moderately intense connections contribute to relative stability. Open structure for approach by one face (figure).

ZANAMIVIR_PROTEINMPRO_DOCKTHOR



Hydrogen Bonds: 4

- Strong (<2,5 Å): 1

- Moderated: 1

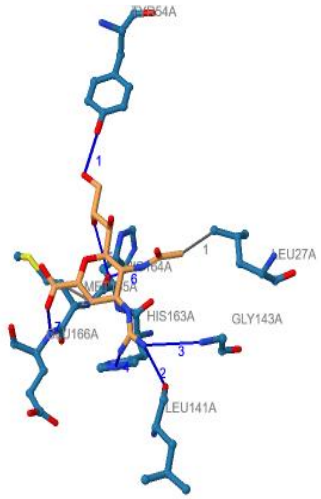
- Weak (>3,2 Å): 2

Average Distance (D-A): 3,04 Å

Saline Bridge: 1

Few but intense interactions suggest medium stability, less than that of the AutoDock Vina model, but with a more open configuration for connection.

ZANAMIVIR_PROTEINMPRO_PATCHDOCK



Hydrogen Bonds: 7

- Strong (<2,5 Å): 0

- Moderated: 4

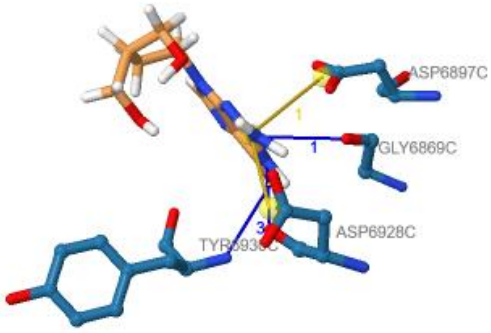
- Weak (>3,2 Å): 3

Average Distance (D-A): 3,07 Å

Hydrophobic interactions: 2 (3,26 Å; 3,53 Å)

Several moderate and hydrophobic interactions at different points in the ligand increase stability. Possible connection from the face TYR54A-LEU27A-GLY143A-LEU141A (figure)

PENCICLOVIR_NSP10_AUTODOCKVINA



Hydrogen Bonds: 3

- Strong (<2,5 Å): 0

- Moderated: 2

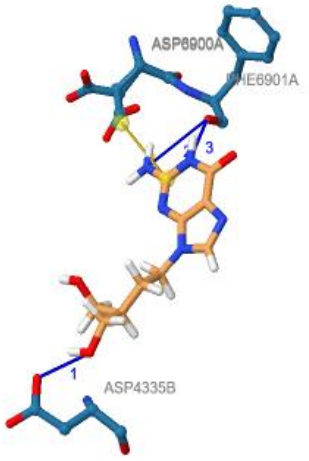
- Weak (>3,2 Å): 1

Average Distance (D-A): 3,16 Å

Saline Bridge: 2

Few interactions, just at one end of the ligand, do not indicate stability.

PENCICLOVIR_NSP10_DOCKTHOR



Hydrogen Bonds: 3

- Strong (<2,5 Å): 0

- Moderated: 2

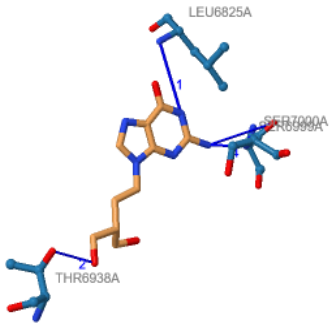
- Weak (>3,2 Å): 1

Average Distance (D-A): 3,13 Å

Saline Bridge: 1

Similar to the AutoDock Vina model, not very stable, despite interactions at both ends.

PENCICLOVIR_NSP10_PATCHDOCK



Hydrogen Bonds: 4

- Strong (<2,5 Å): 1

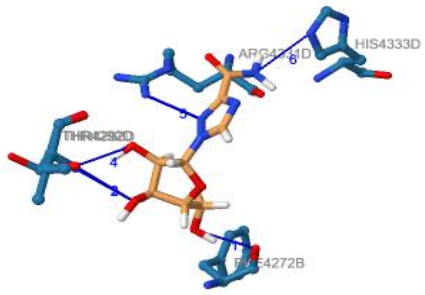
- Moderated: 1

- Weak (>3,2 Å): 2

Average Distance (D-A): 3,26 Å

Similar to the Dockthor model.

RIBAVIRIN_NSP10_AUTODOCKVINA



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

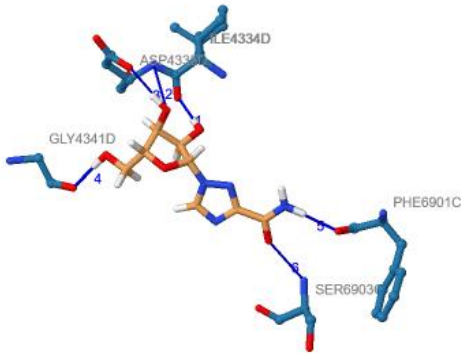
- Moderated: 4

- Weak (>3,2 Å): 2

Average Distance (D-A): 3,21 Å

Moderately intense interactions. Open structure for connection on the face of the figure.

RIBAVIRIN_NSP10_DOCKTHOR



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

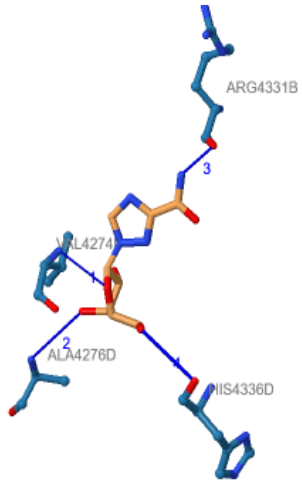
- Moderated: 4

- Weak (>3,2 Å): 2

Average Distance (D-A): 3,11 Å

Similar to the AutoDock Vina model.

RIBAVIRIN_NSP10_PATCHDOCK



Hydrogen Bonds: 4

- Strong (<2,5 Å): 0

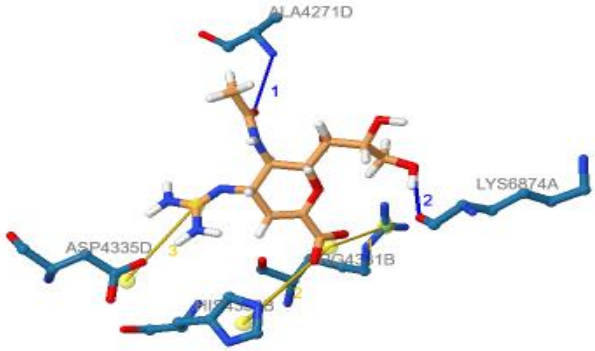
- Moderated: 2

- Weak (>3,2 Å): 2

Average Distance (D-A): 3,34 Å

Similar to AutoDock Vina and Dockthor models, but less interactions and stability.

ZANAMIVIR_NSP10_DOCKTHOR



Hydrogen Bonds: 2

- Strong (<2,5 Å): 0

- Moderated: 1

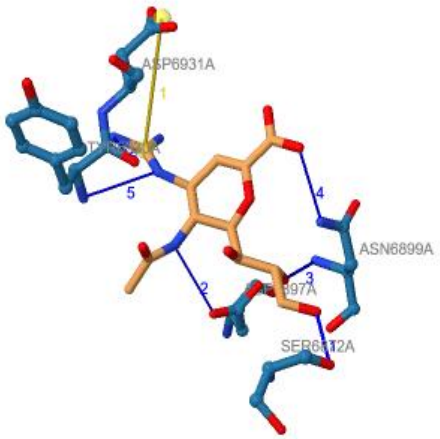
- Weak (>3,2 Å): 1

Average Distance (D-A): 3,06 Å

Saline Bridge: 3

Most interactions due to relatively distant saline bridges. Some structural difficulty to connect.

ZANAMIVIR_NSP10_PATCHDOCK



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

- Moderated: 3

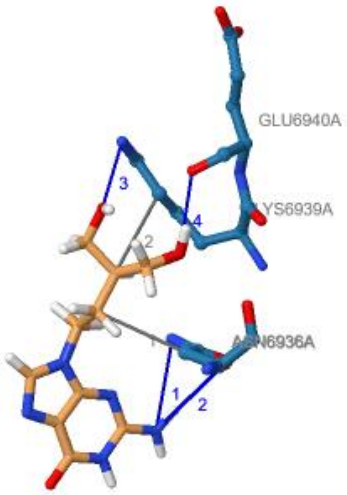
- Weak (>3,2 Å): 3

Average Distance (D-A): 3,11 Å

Saline Bridge: 1

More interactions classified as H bonds, but of strength in general not very intense. Structure offers greater steric difficulty.

PENCICLOVIR_NSP16_AUTODOCKVINA



Hydrogen Bonds: 4

- Strong (<2,5 Å): 0

- Moderated: 2

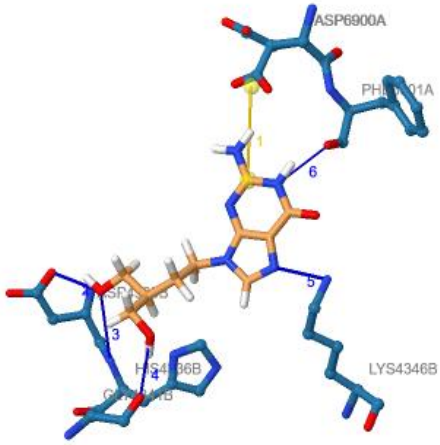
- Weak (>3,2 Å): 2

Average Distance (D-A): 3,42 Å

Hydrophobic interactions: 2 (3,59 Å; 3,94 Å)

Low intensity interactions at the ends of the ligand. Structurally free.

PENCICLOVIR_NSP16_DOCKTHOR



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

- Moderated: 5

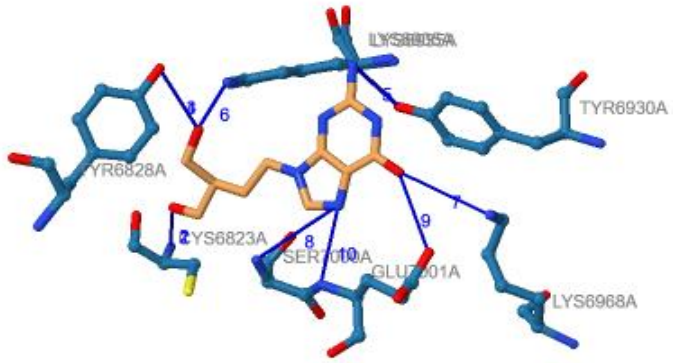
- Weak (>3,2 Å): 1

Average Distance (D-A): 3,00 Å

Saline Bridge: 1

Several moderately intense interactions at different points in the ligand. Free connection if given by the face shown in the figure.

PENCICLOVIR_NSP16_PATCHDOCK



Hydrogen Bonds: 10

- Strong (<2,5 Å): 1

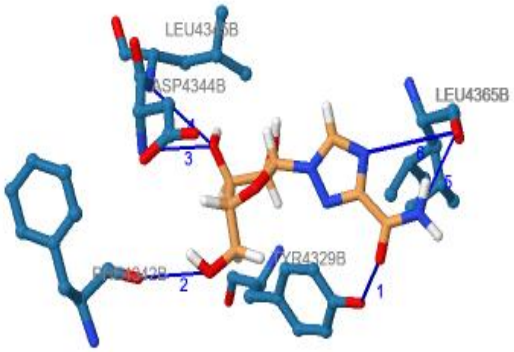
- Moderated: 4

- Weak (>3,2 Å): 5

Average Distance (D-A): 3,45 Å

There are a large number of H bonds, some strong, at different points in the ligand, indicating a great stability of complex. The connection is prevented in some directions, but possible with the correct orientation of the face and the ligand.

RIBAVIRIN_NSP16_AUTODOCKVINA



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

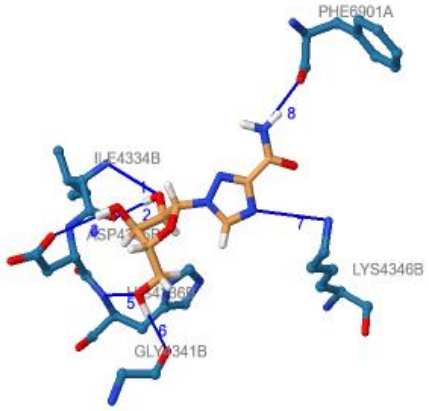
- Moderated: 4

- Weak (>3,2 Å): 2

Average Distance (D-A): 3,21 Å

Weak to moderately intense bonds at various points in the ligand. Structure makes approximation a little difficult.

RIBAVIRIN_NSP16_DOCKTHOR



Hydrogen Bonds: 8

- Strong (<2,5 Å): 0

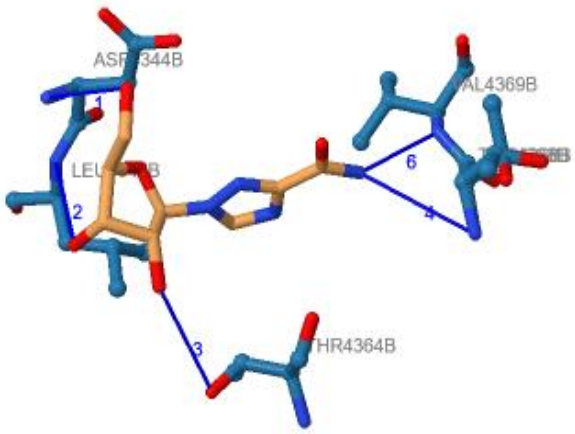
- Moderated: 3

- Weak (>3,2 Å): 5

Average Distance (D-A): 3,32 Å

Similar to the AutoDock Vina model, with a slightly more open structure.

RIBAVIRIN_NSP16_PATCHDOCK



Hydrogen Bonds: 6

- Strong (<2,5 Å): 0

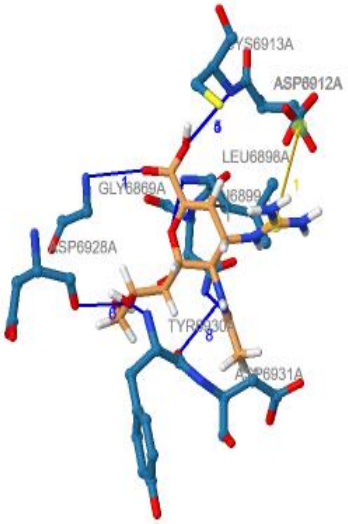
- Moderated: 2

- Weak (>3,2 Å): 4

Average Distance (D-A): 3,39 Å

Similar to the Dockthor model, but with fewer interactions.

ZANAMIVIR_NSP16_AUTODOCKVINA



Hydrogen Bonds: 8

- Strong (<2,5 Å): 0

- Moderated: 2

- Weak (>3,2 Å): 6

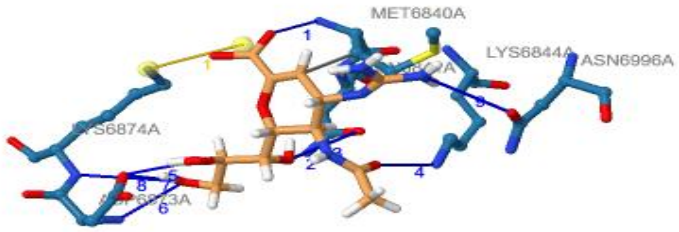
Average Distance (D-A): 3,35 Å

Hydrophobic interactions: 2 (3,79 Å; 3,48 Å)

Saline Bridge: 1

There is a great amount and diversity of interactions, but the structure makes it difficult to connect except on the face and specific orientations.

ZANAMIVIR_NSP16_DOCKTHOR



Hydrogen Bonds: 9

- Strong (<2,5 Å): 0

- Moderated: 5

- Weak (>3,2 Å): 4

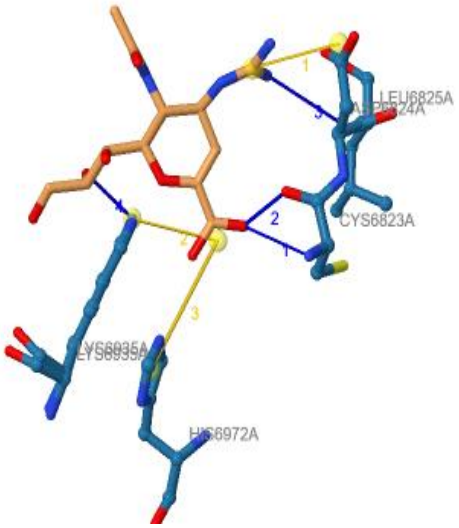
Average Distance (D-A): 3,26 Å

Hydrophobic interactions: 1 (3,37 Å)

Saline Bridge: 1

Compared to the AutoDock Vina model, there are more intense interactions and a more open structure for connection.

ZANAMIVIR_NSP16_PATCHDOCK



Hydrogen Bonds: 4

- Strong (<2,5 Å): 1

- Moderated: 1

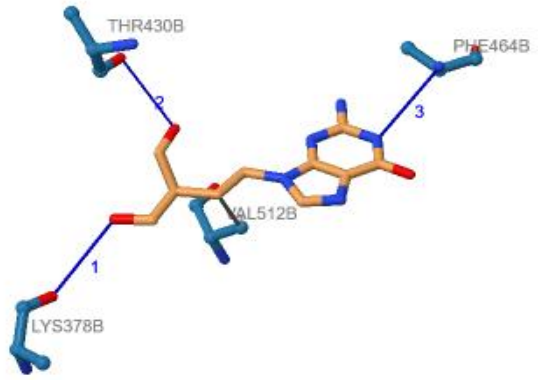
- Weak (>3,2 Å): 2

Average Distance (D-A): 3,29 Å

Saline Bridge: 3

More saline connections than H compared to the Dockthor model, but also more open structure.

PENCICLOVIR_PROTEINSOPEN_PATCHDOCK



Hydrogen Bonds: 3

- Strong (<2,5 Å): 0

- Moderated: 0

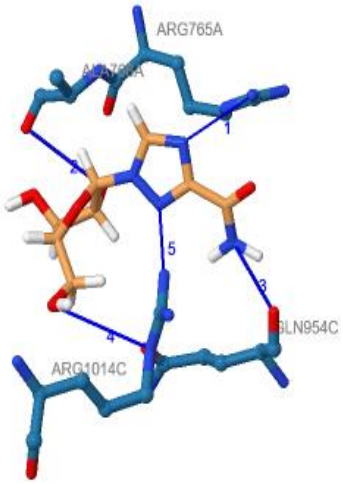
- Weak (>3,2 Å): 3

Average Distance (D-A): 3,55 Å

Hydrophobic interactions: 1 (3,94 Å)

Few interactions and low intensity do not indicate a good model.

RIBAVIRIN_PROTEINSOPEN_AUTODOCKVINA



Hydrogen Bonds: 5

- Strong (<2,5 Å):

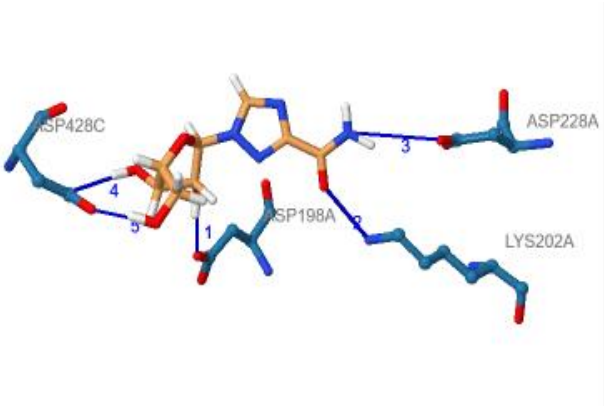
- Moderated: 1

- Weak (>3,2 Å): 4

Average Distance (D-A): 3,36 Å

Several interactions, but generally of low intensity.

RIBAVIRIN_PROTEINSOPEN_DOCKTHOR



Hydrogen Bonds: 5

- Strong (<2,5 Å):

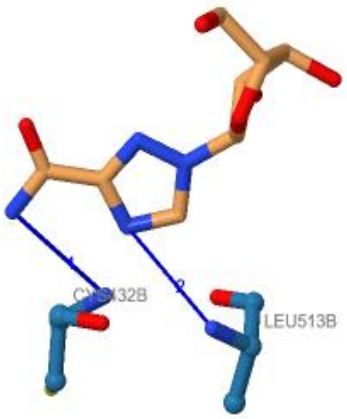
- Moderated: 4

- Weak (>3,2 Å): 1

Average Distance (D-A): 3,03 Å

More intense H bonds compared to the AutoDock Vina model. Favorable connection on one face.

RIBAVIRIN_PROTEINSOPEN_PATCHDOCK



Hydrogen Bonds: 2

- Strong (<2,5 Å): 0

- Moderated: 0

- Weak (>3,2 Å): 2

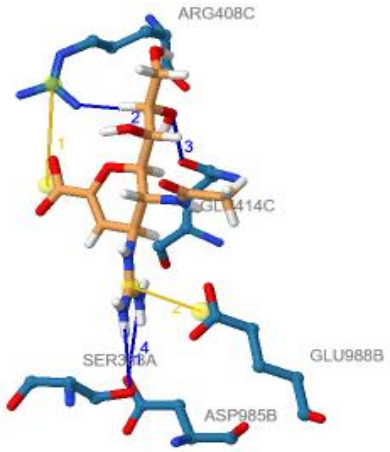
Average Distance (D-A): 3,59 Å

Only two weak interactions do not indicate a good model.

ZANAMIVIR_PROTEINSOPEN_AUTODOCKVINA

There were no interactions found in the model.

ZANAMIVIR_PROTEINSOPEN_DOCKTHOR



Hydrogen Bonds: 4

- Strong (<2,5 Å):

- Moderated: 1

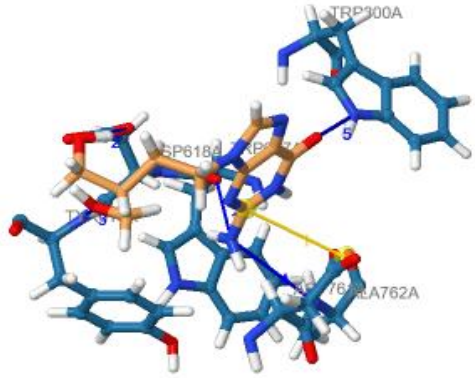
- Weak (>3,2 Å): 3

Average Distance (D-A): 3,48 Å

Saline Bridge: 2

Moderately intense interactions at the ends of the ligand. Face SER393A-ARG408C-GLU988B open for connection.

PENCICLOVIR_POLYMERASE_AUTODOCKVINA



Hydrogen Bonds: 5

- Strong (<2,5 Å):

- Moderated: 4

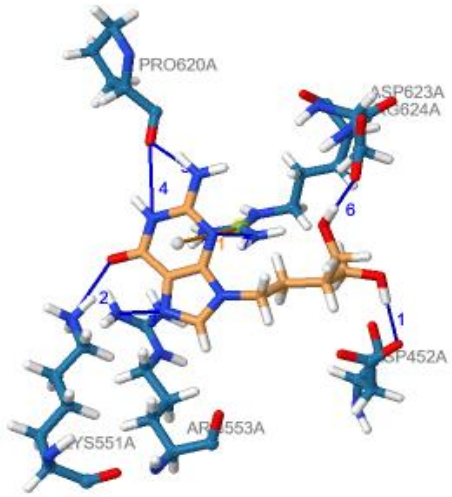
- Weak (>3,2 Å): 1

Average Distance (D-A): 3,13 Å

Saline Bridge: 1

Several moderate interactions contribute to stability. Structure is open for connection on the face shown in the figure.

PENCICLOVIR_POLYMERASE_DOCKTHOR



Hydrogen Bonds: 7

- Strong (<2,5 Å):

- Moderated: 4

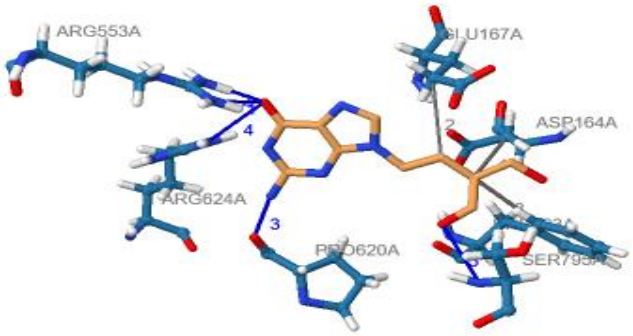
- Weak (>3,2 Å): 3

Average Distance (D-A): 3,22 Å

Pi-stacking: 1

Several interactions contribute to stability, structure makes it difficult to bond except on the face and correct ligand orientation.

PENCICLOVIR_POLYMERASE_PATCHDOCK



Hydrogen Bonds: 5

- Strong (<2,5 Å): 1

- Moderated: 2

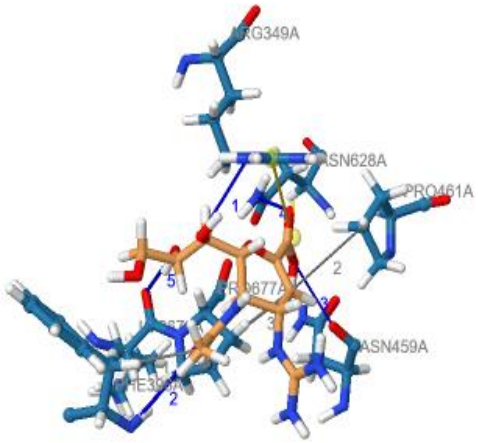
- Weak (>3,2 Å): 2

Average Distance (D-A): 2,92 Å

Hydrophobic interactions: 1 (3,79 Å; 3,69 Å; 3,30 Å)

Similar to the Dockthor model regarding the intensity of connections and structure.

ZANAMIVIR_POLYMERASE_AUTODOCKVINA



Hydrogen Bonds: 5

- Strong (<2,5 Å):

- Moderated: 1

- Weak (>3,2 Å): 4

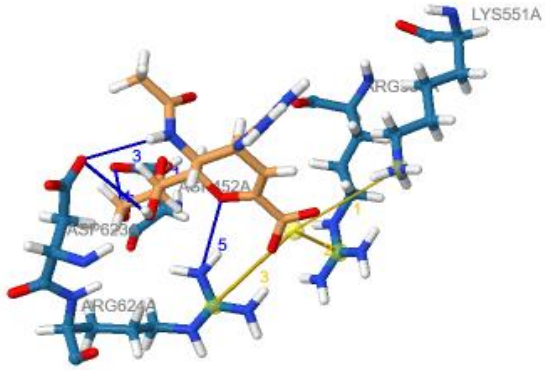
Average Distance (D-A): 3,57 Å

Hydrophobic interactions: 1 (3,59 Å; 3,73 Å; 3,75 Å)

Saline Bridge: 1

Weak H interactions are only partially offset by hydrophobic and saline interactions. Structure makes it difficult to bond except on the correct face.

ZANAMIVIR_POLYMERASE_DOCKTHOR



Hydrogen Bonds: 5

- Strong (<2,5 Å):

- Moderated: 2

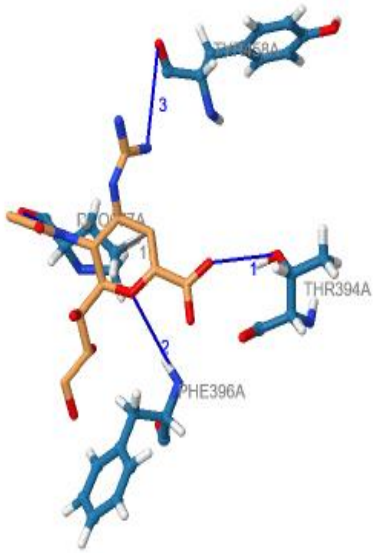
- Weak (>3,2 Å): 3

Average Distance (D-A): 3,24 Å

Saline Bridge: 3

More intense interactions than in the AutoDock Vina model, and a more open structure.

ZANAMIVIR_POLYMERASE_PATCHDOCK



Hydrogen Bonds: 4

- Strong (<2,5 Å):

- Moderated: 1

- Weak (>3,2 Å): 3

Average Distance (D-A): 3,78 Å

Hydrophobic interactions: 1 (3,39 Å)

Weaker interactions than in the Dockthor model, despite a more open structure.