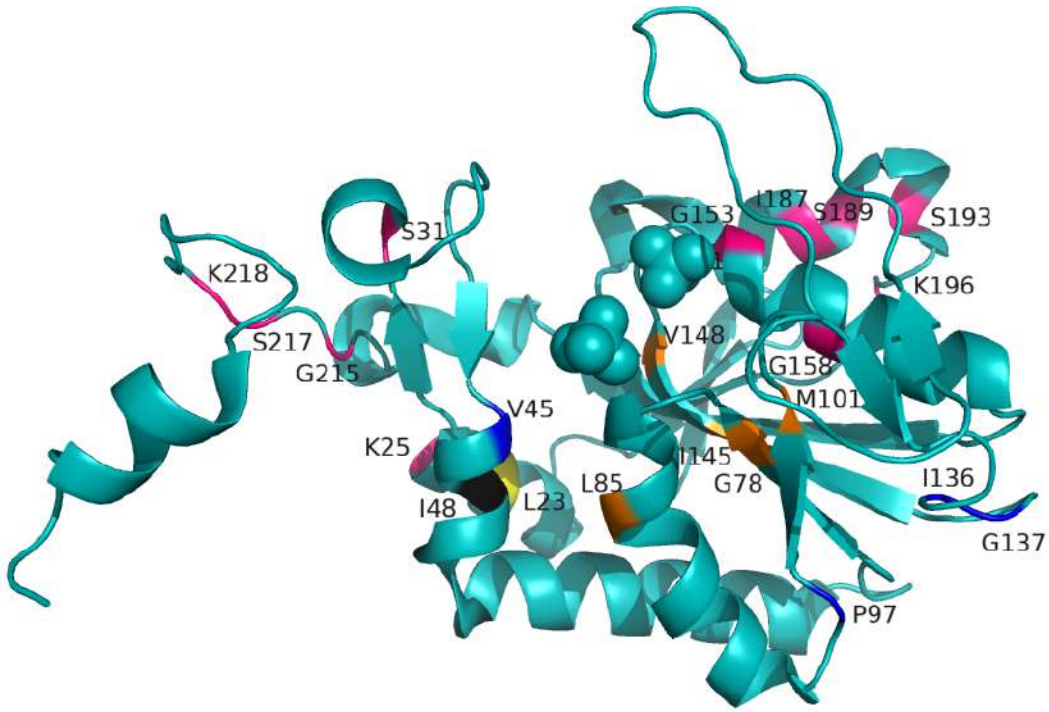
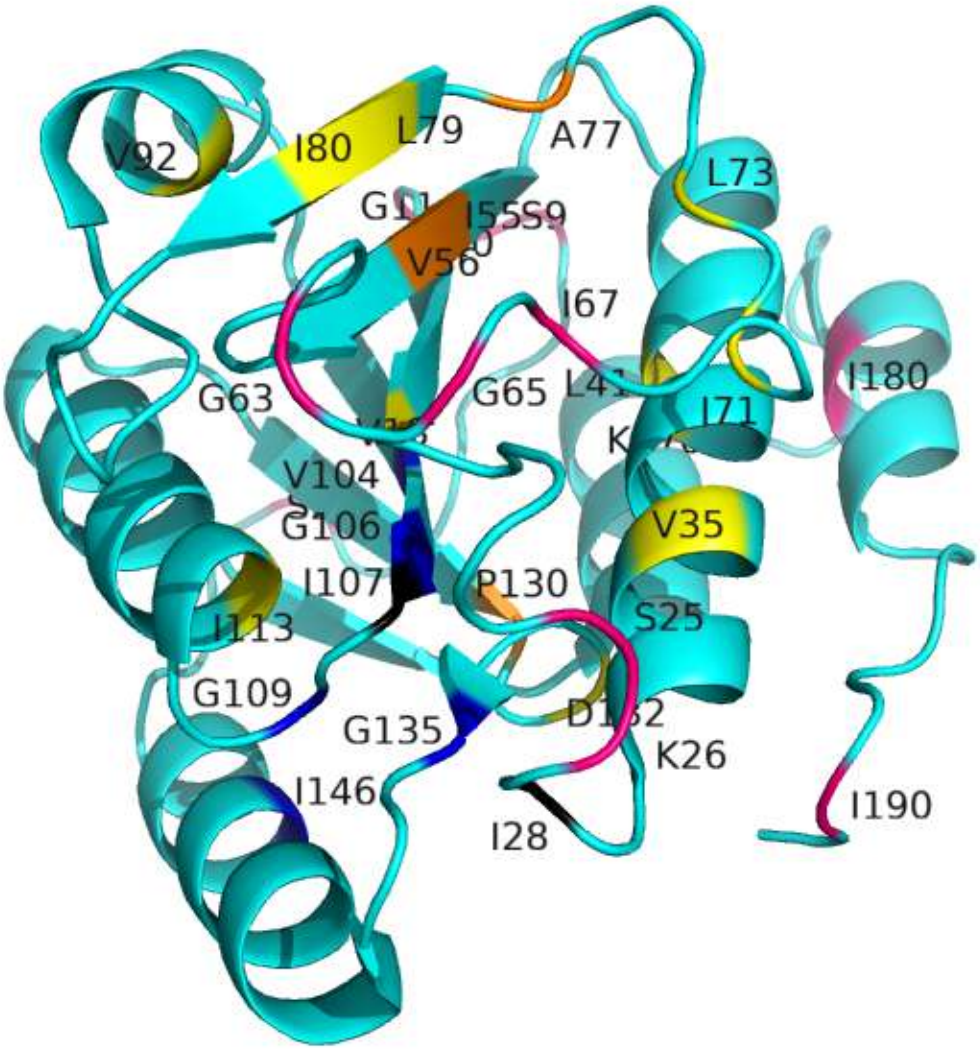
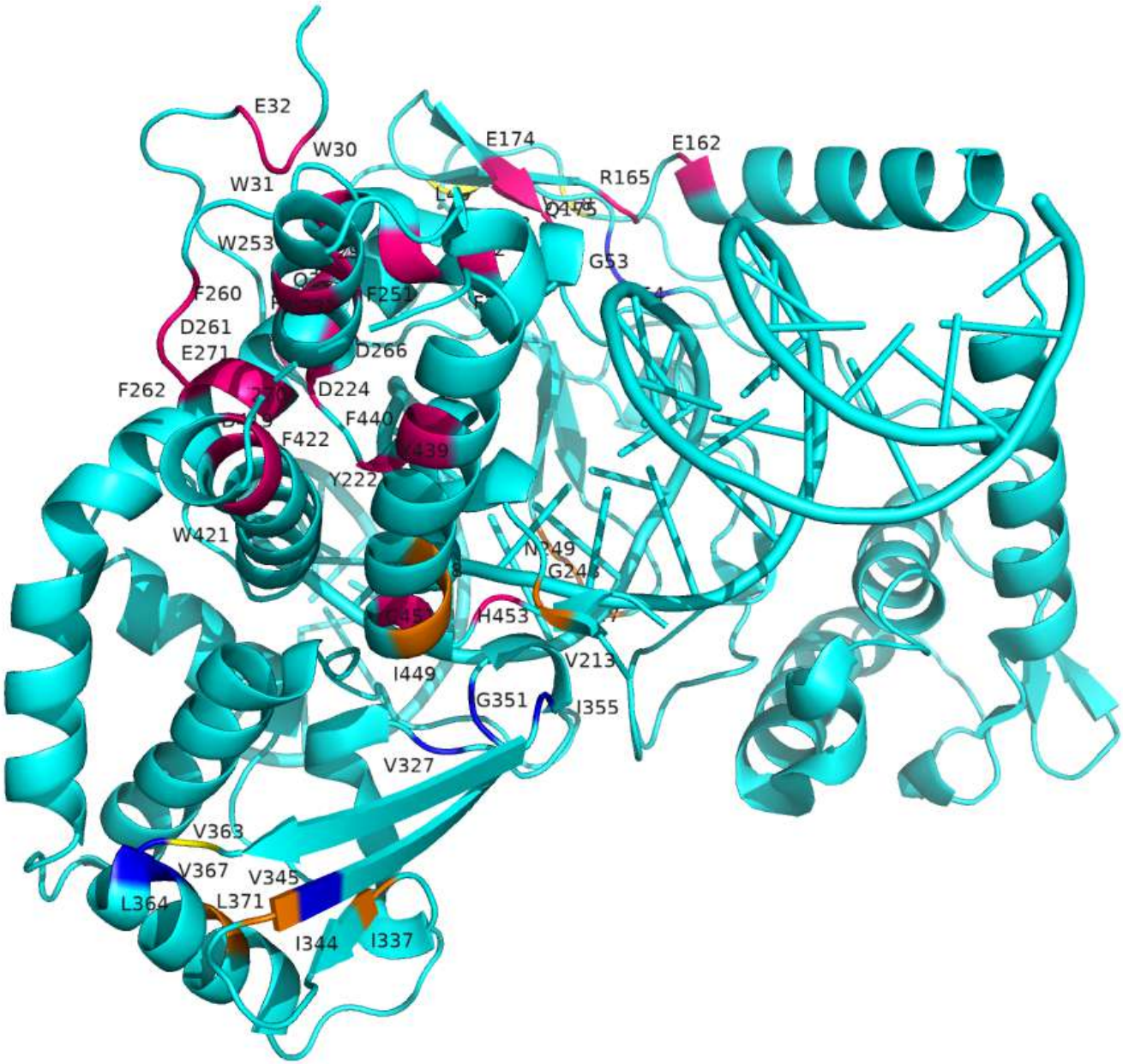


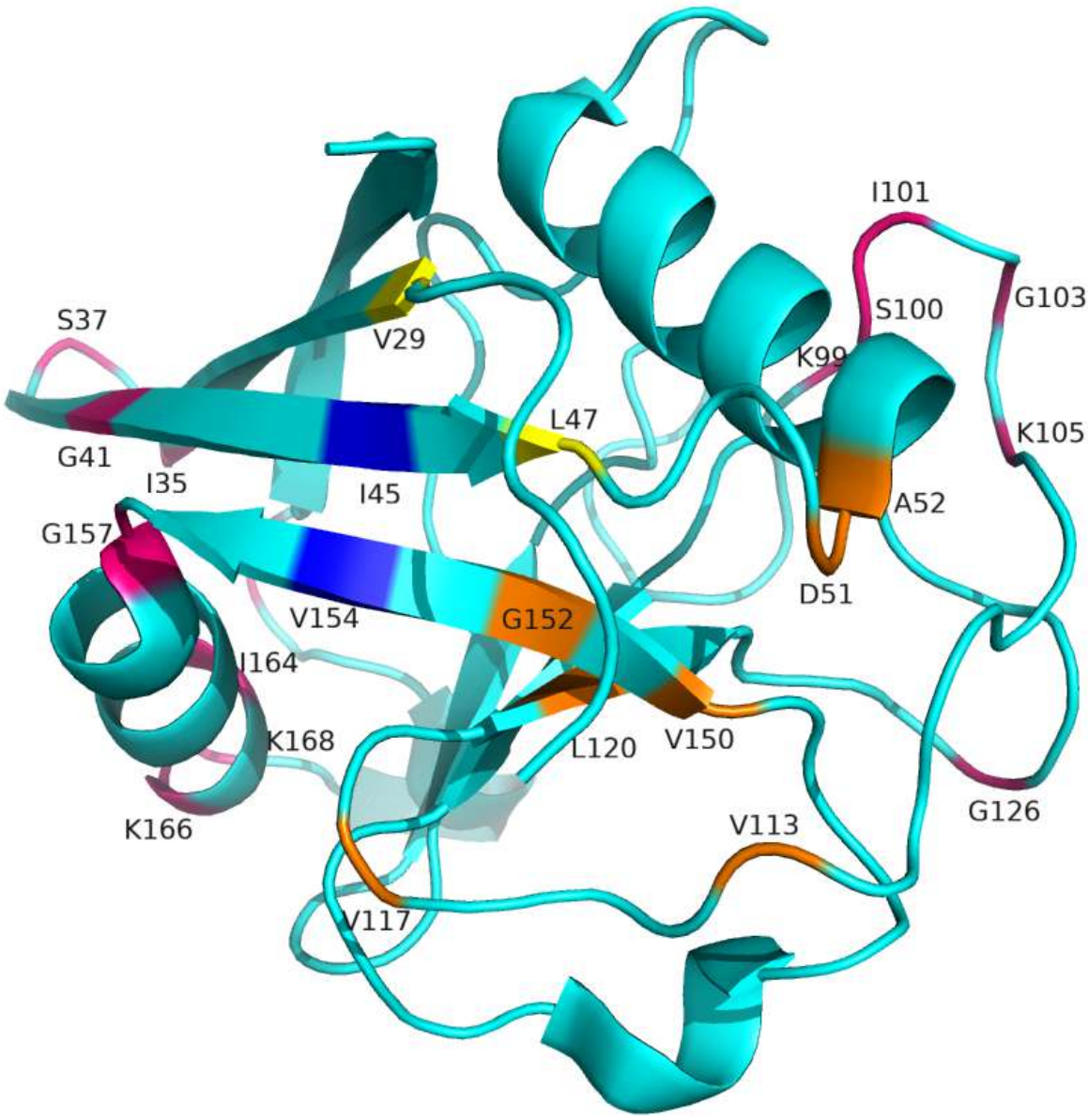
Supplementary Figure 1. Active site residues & drug binding motifs of 1QCD. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



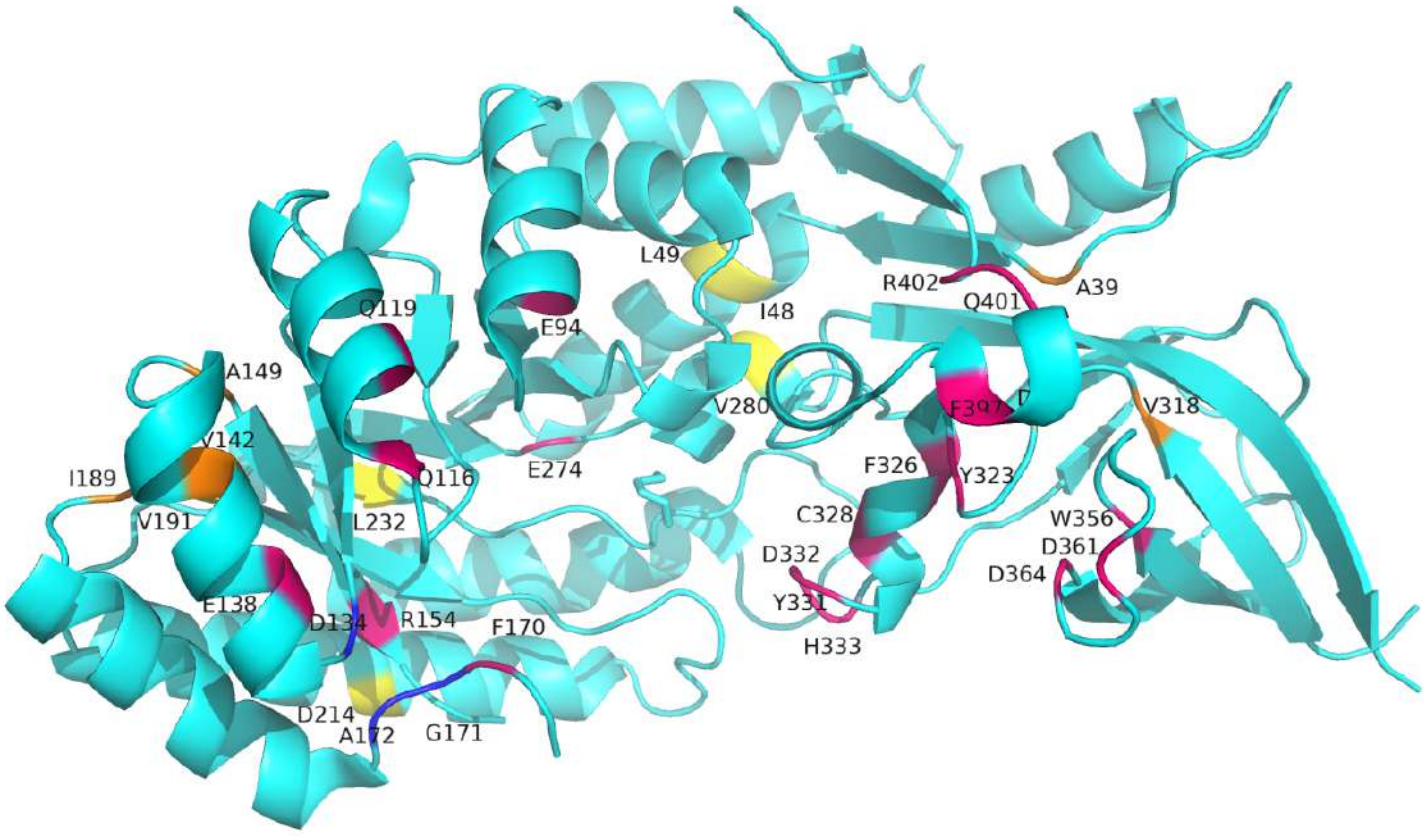
Supplementary Figure 2. Active site residues & drug binding motifs of 1X9G. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue



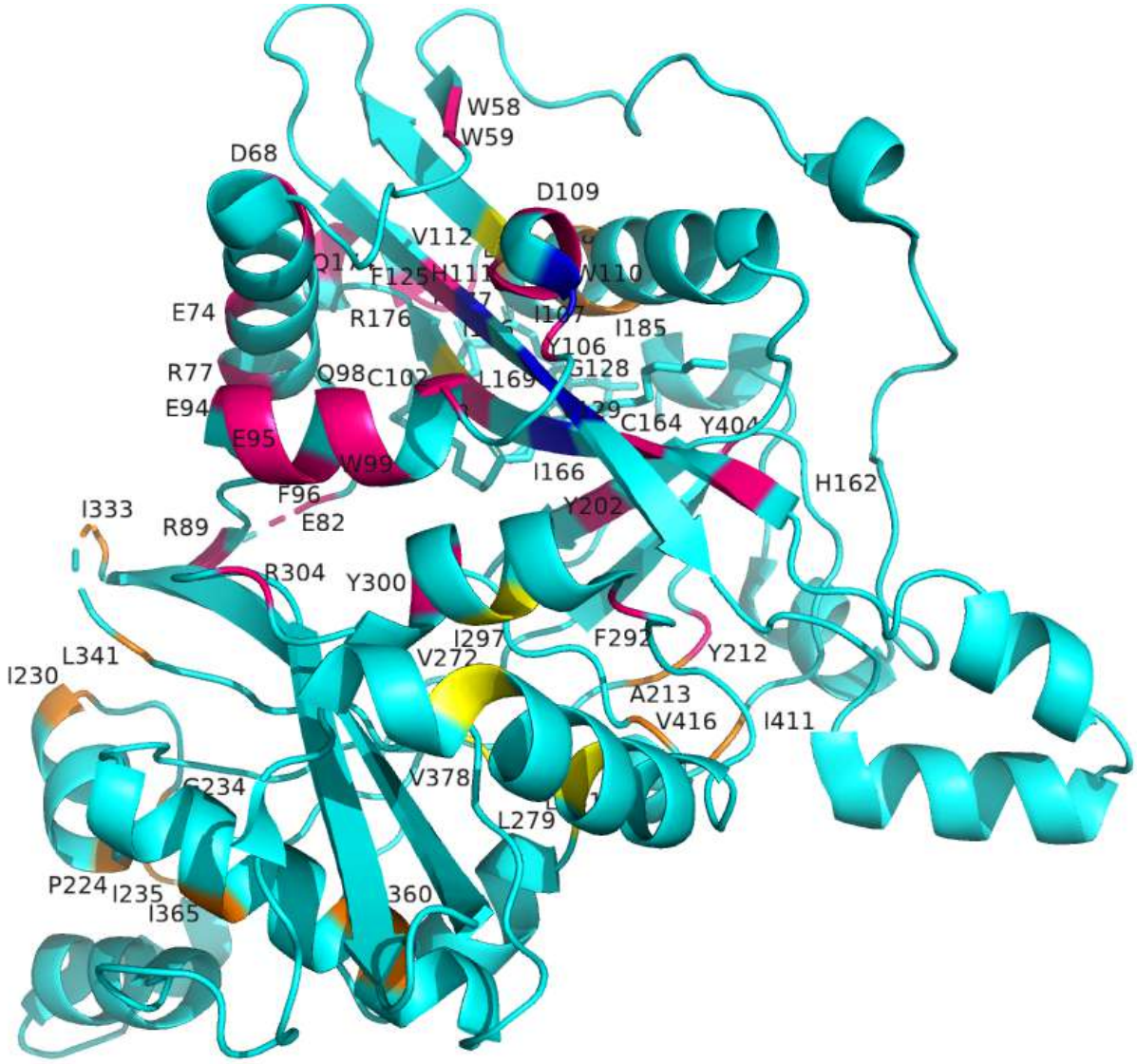
Supplementary Figure 3. Active site residues & drug binding motifs of 2B9S. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



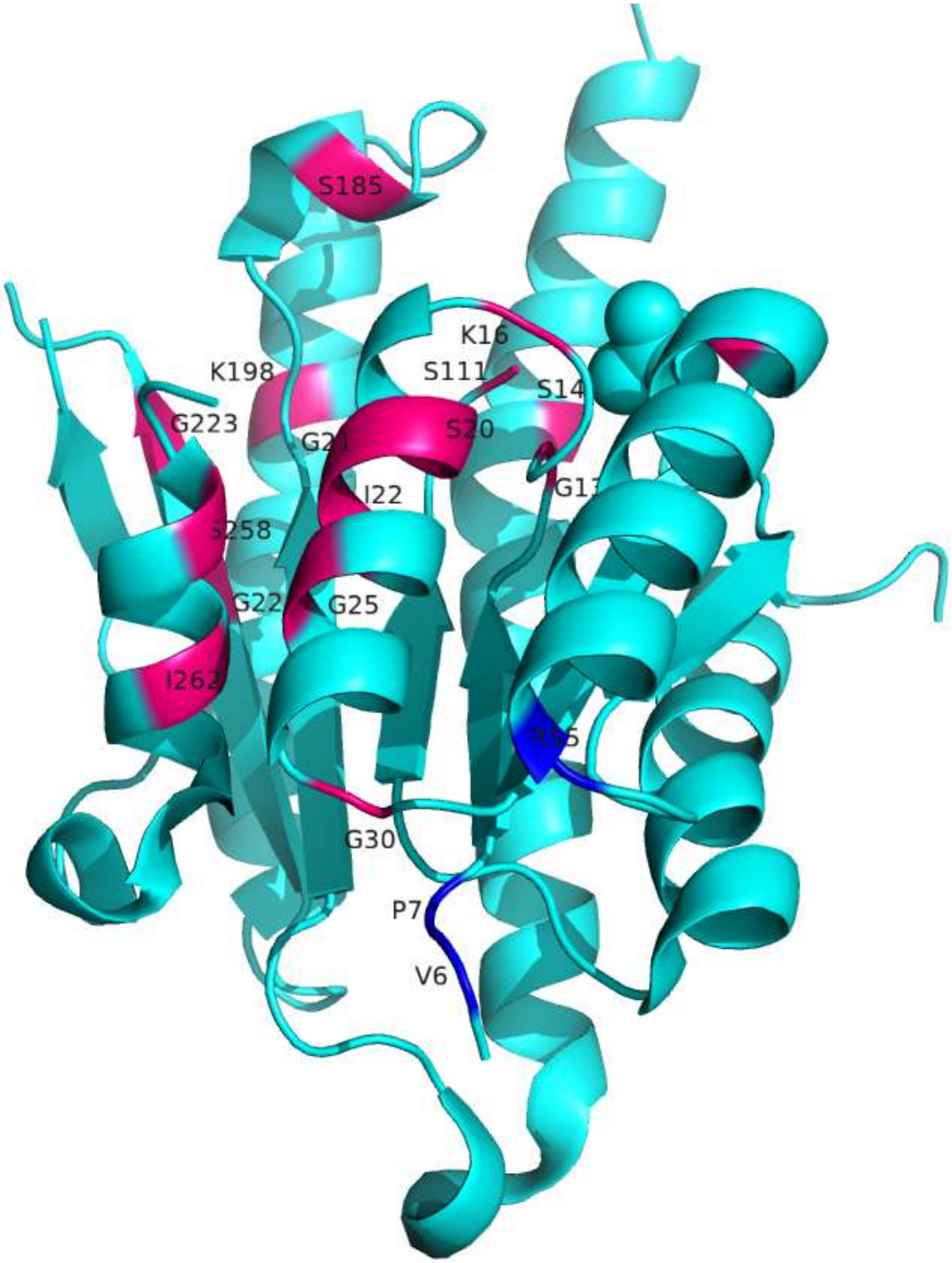
Supplementary Figure 4. Active site residues & drug binding motifs of 2HAQ. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



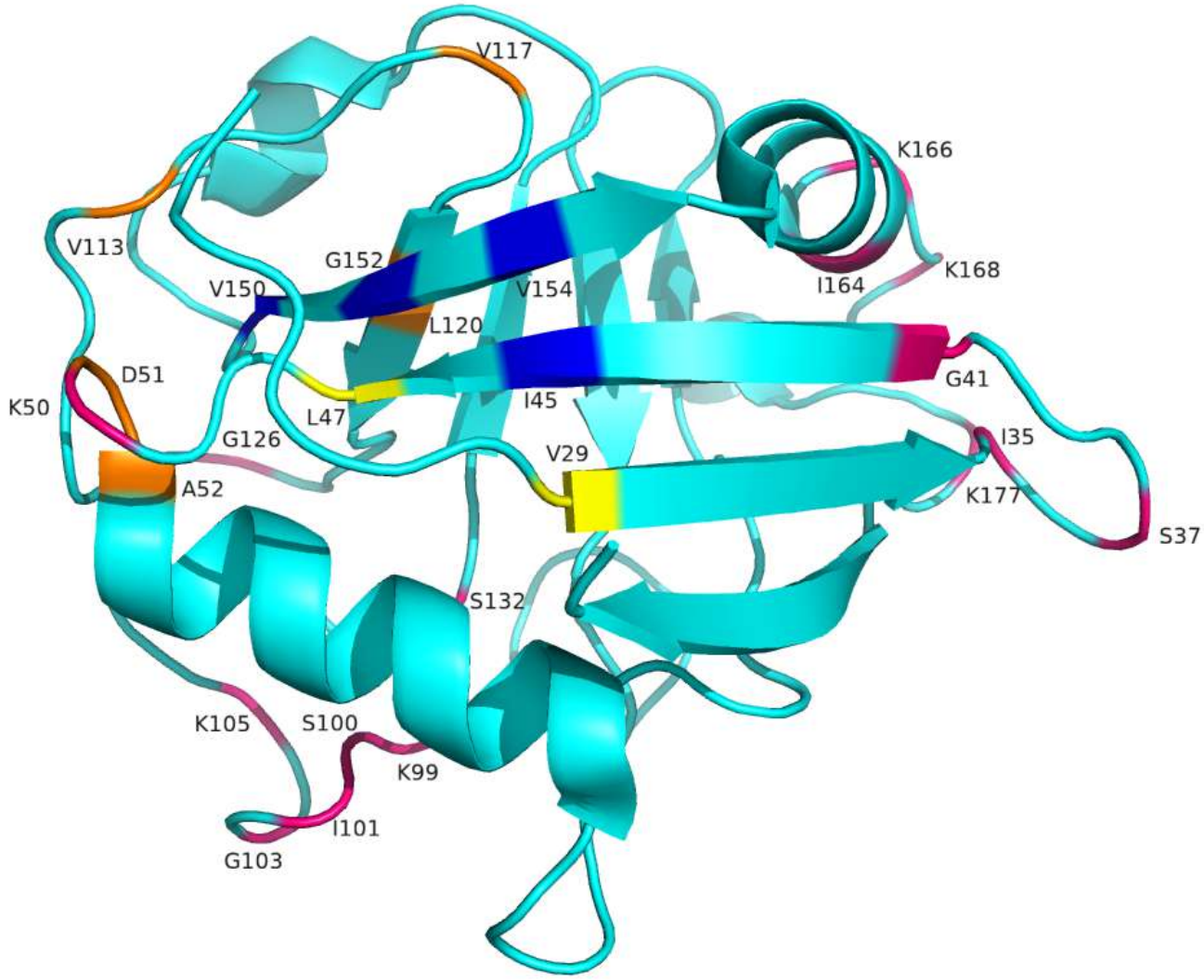
Supplementary Figure 5. Active site residues & drug binding motifs of 2ON3. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



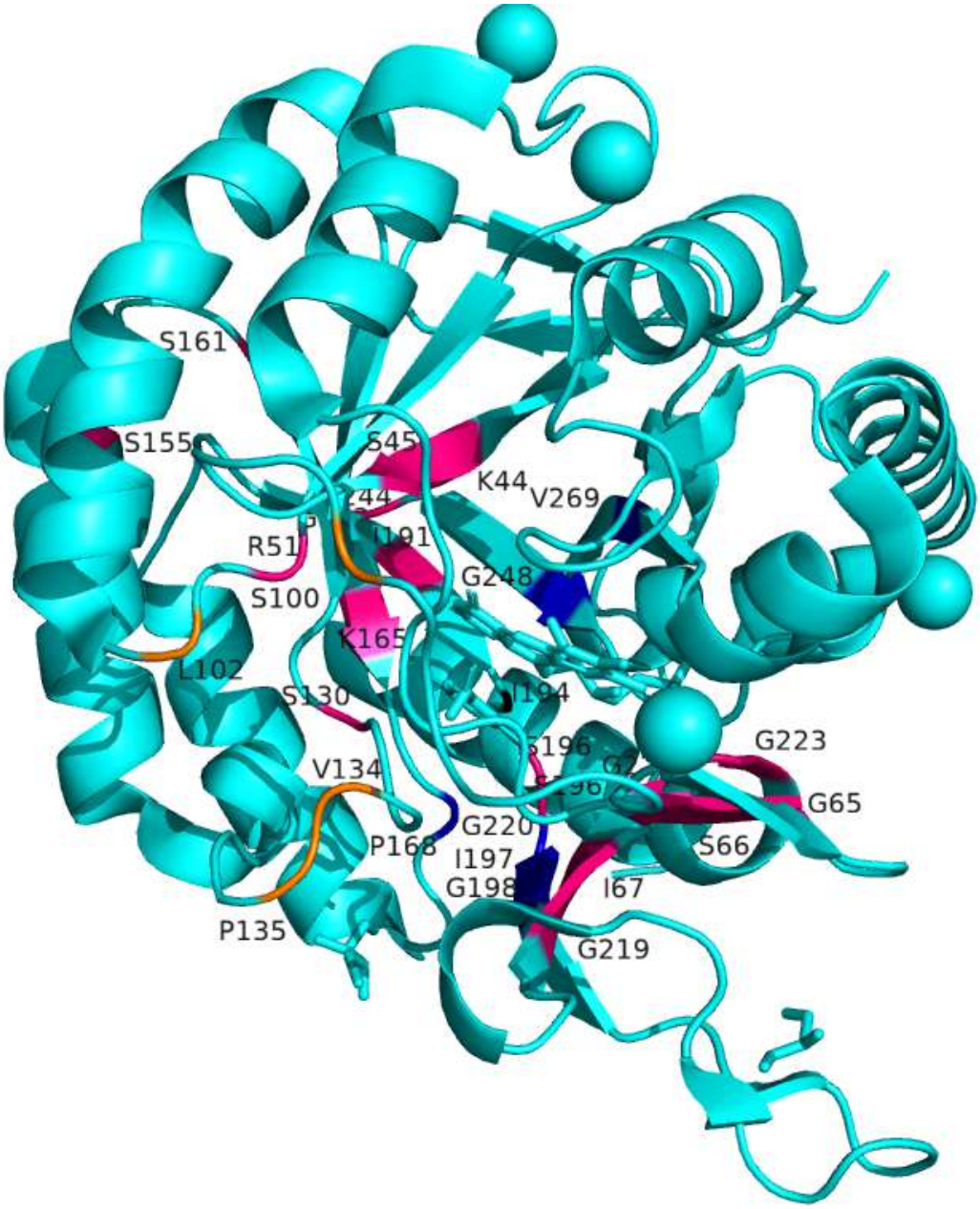
Supplementary Figure 6. Active site residues & drug binding motifs of 2WUU. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



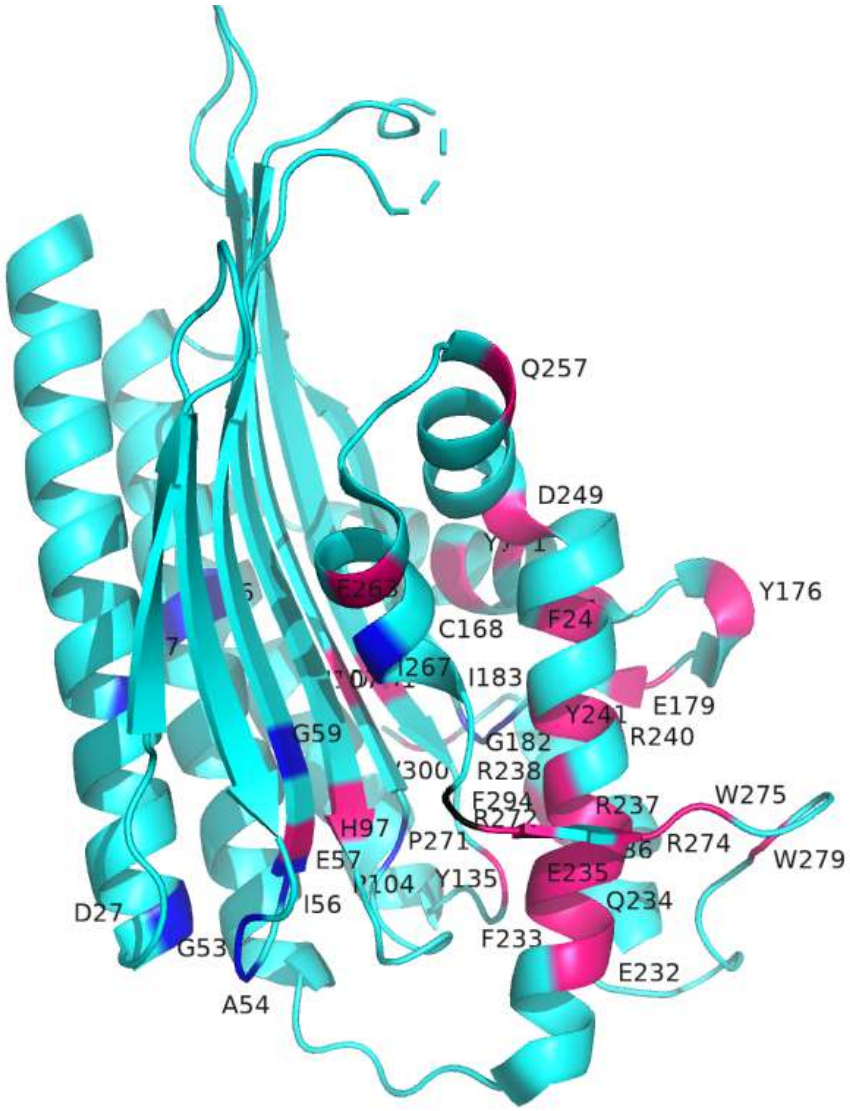
Supplementary Figure 7. Active site residues & drug binding motifs of 2XOX. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



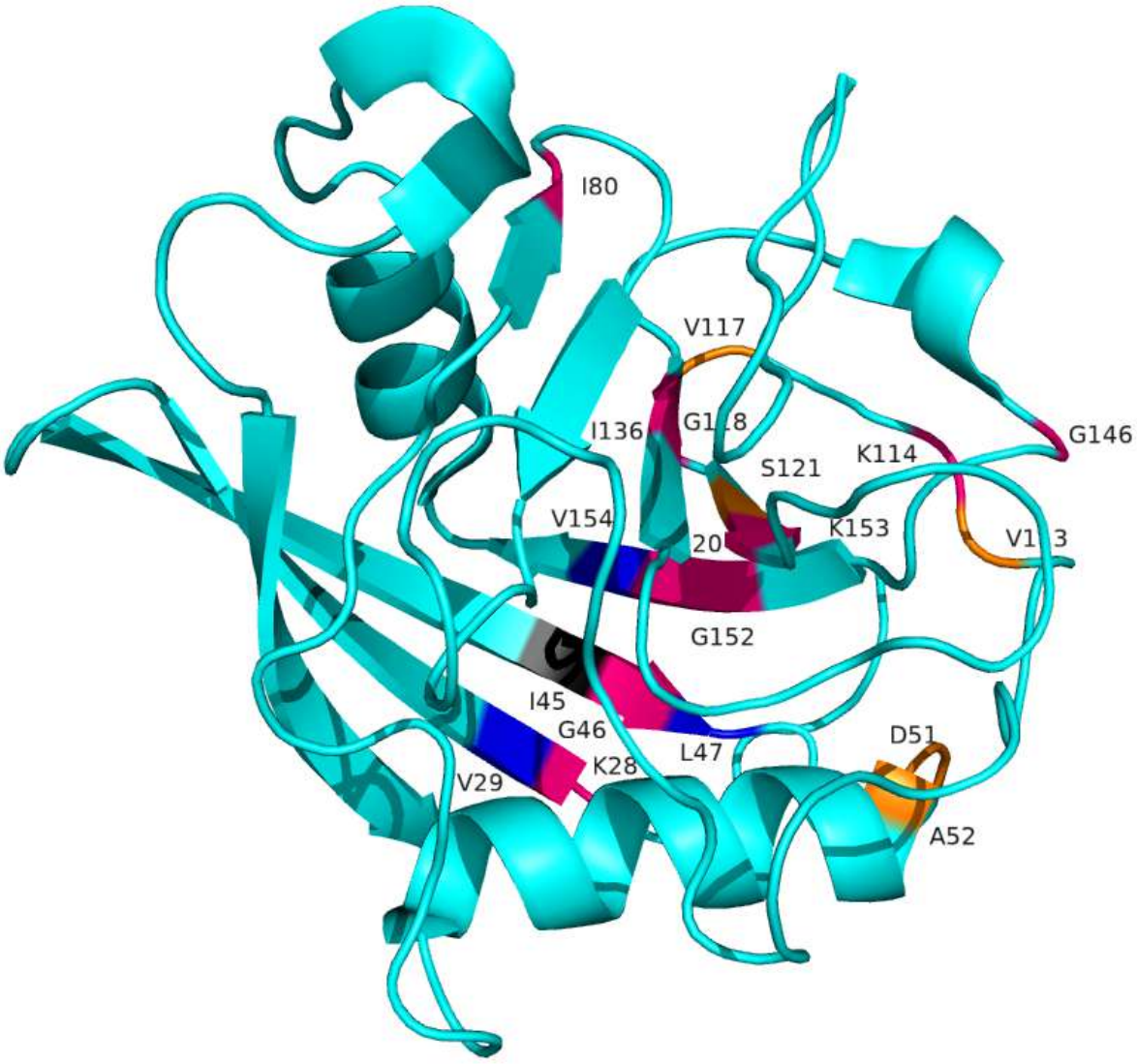
Supplementary Figure 8. Active site residues & drug binding motifs of 3BT8. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



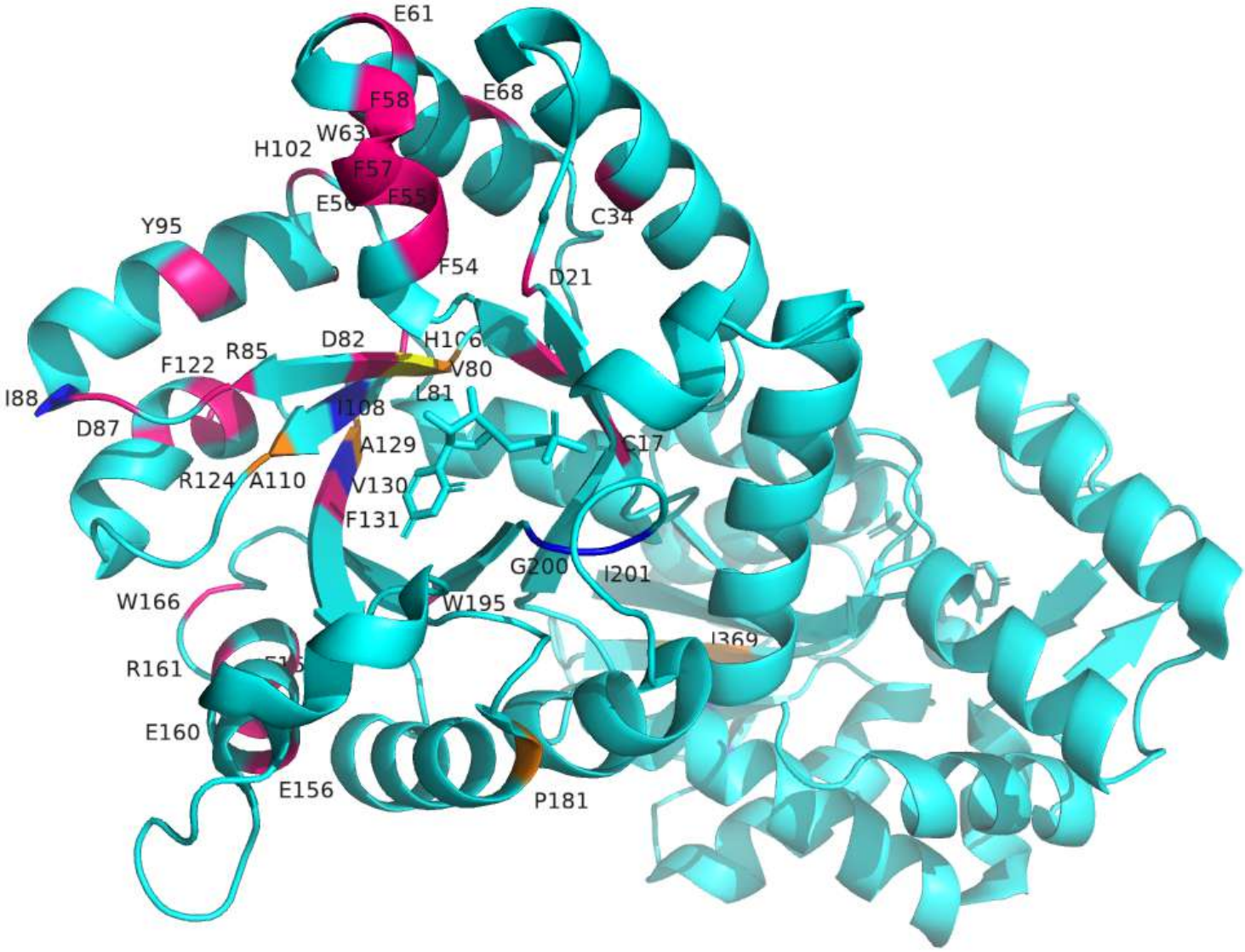
Supplementary Figure 9. Active site residues & drug binding motifs of 3C61. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



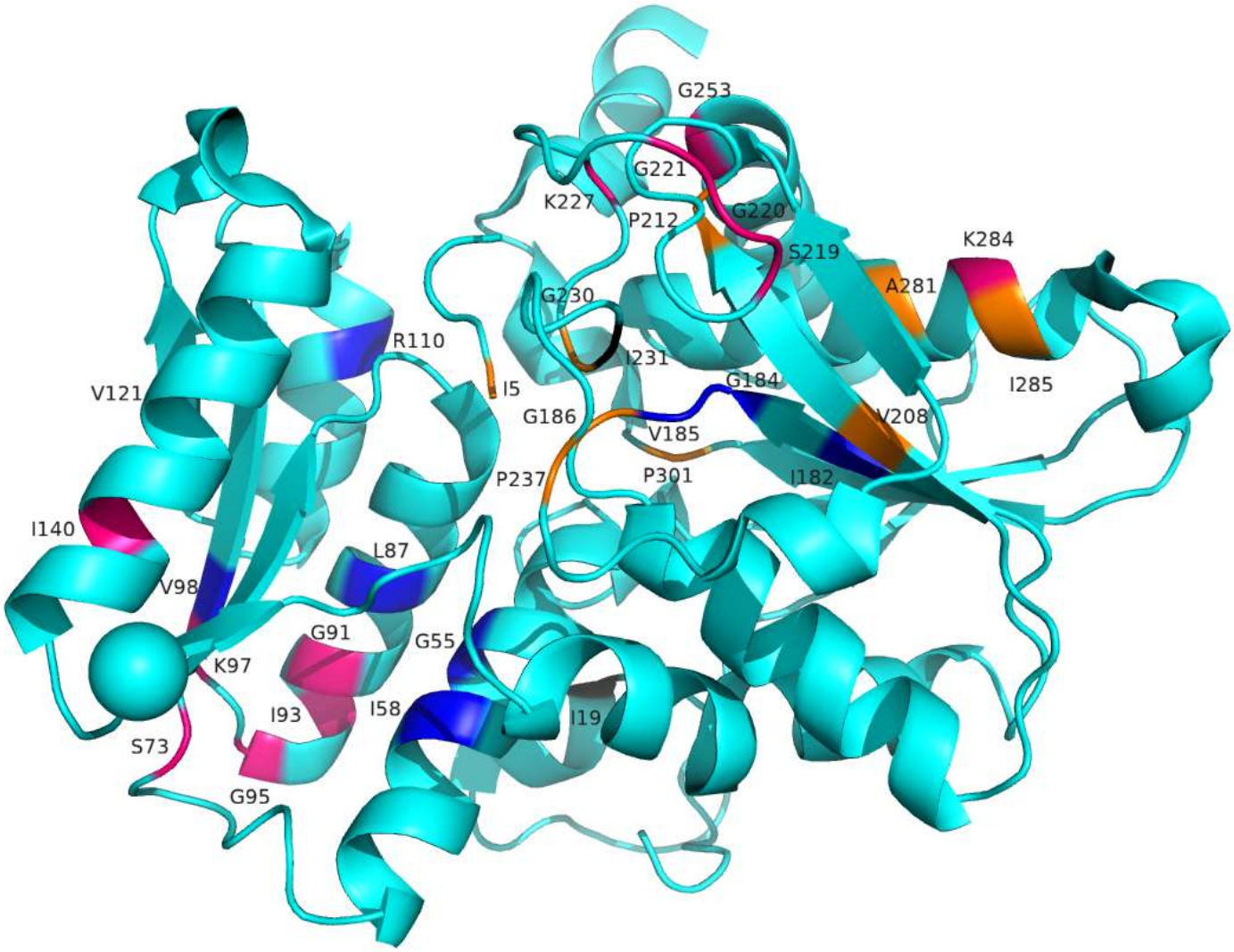
Supplementary Figure 10. Active site residues & drug binding motifs of 3EJO. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



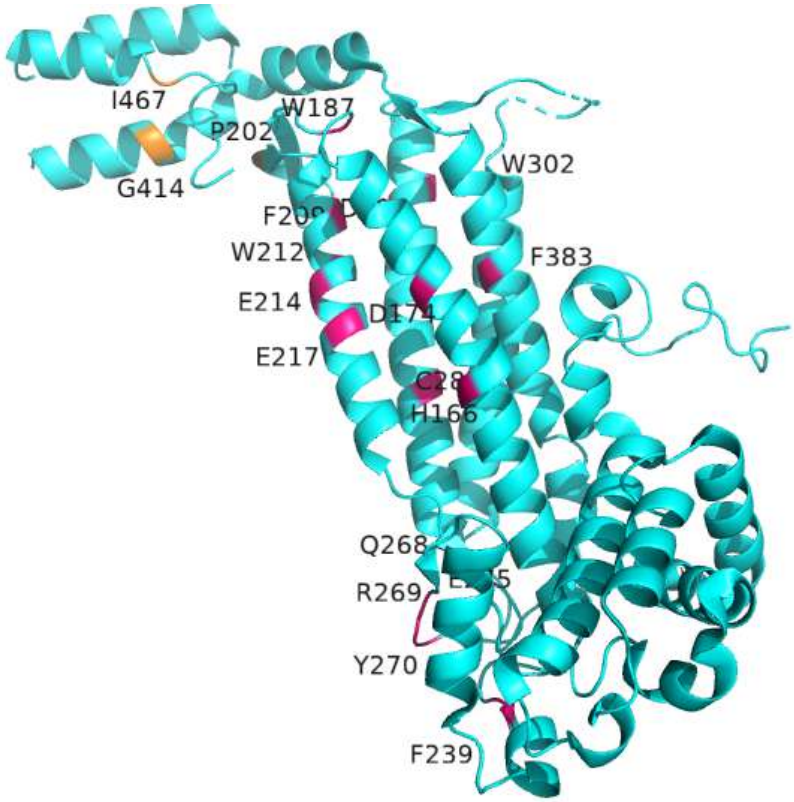
Supplementary Figure 11. Active site residues & drug binding motifs of 3EOV. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



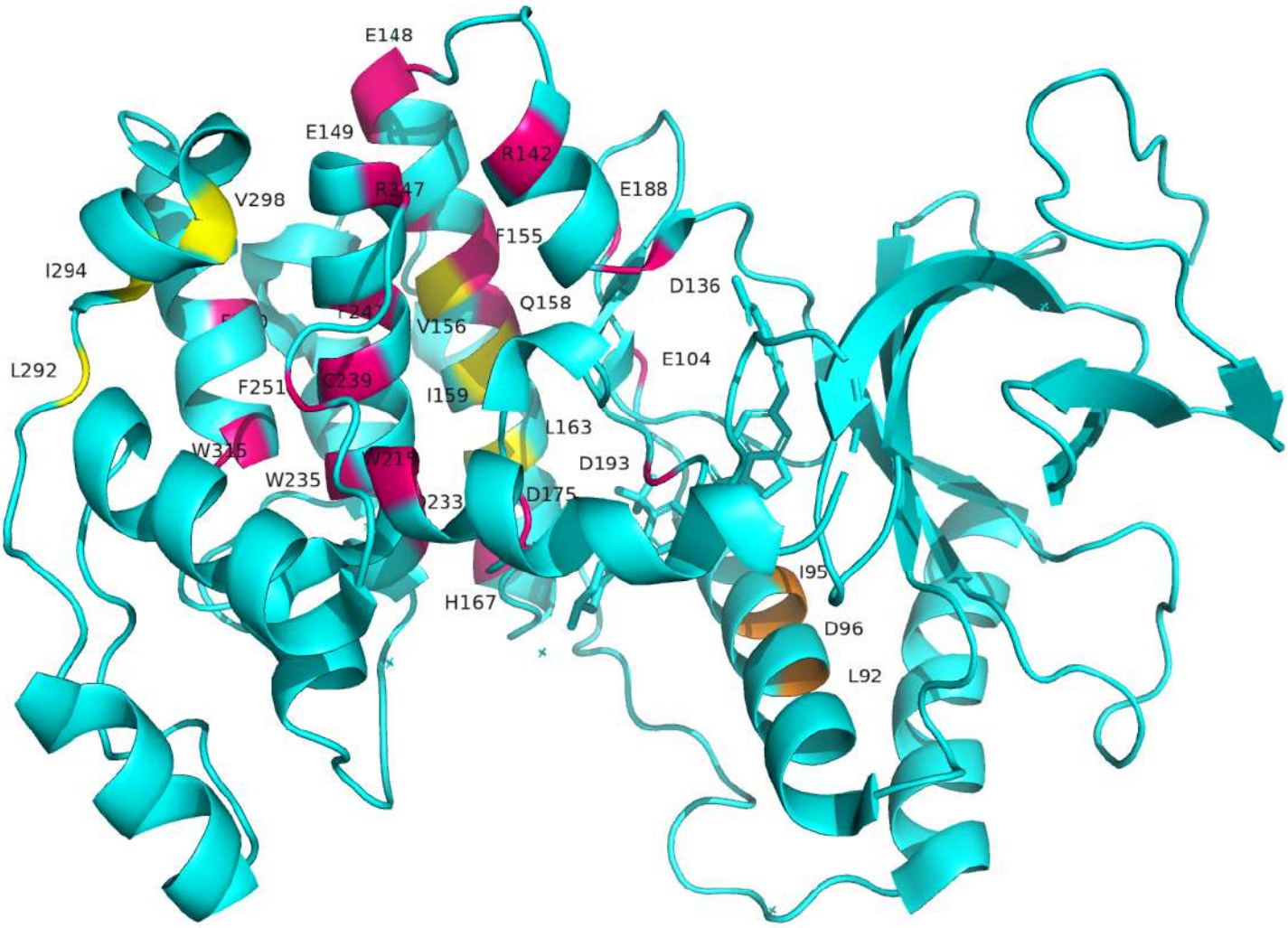
Supplementary Figure 12. Active site residues & drug binding motifs of 3QW4. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



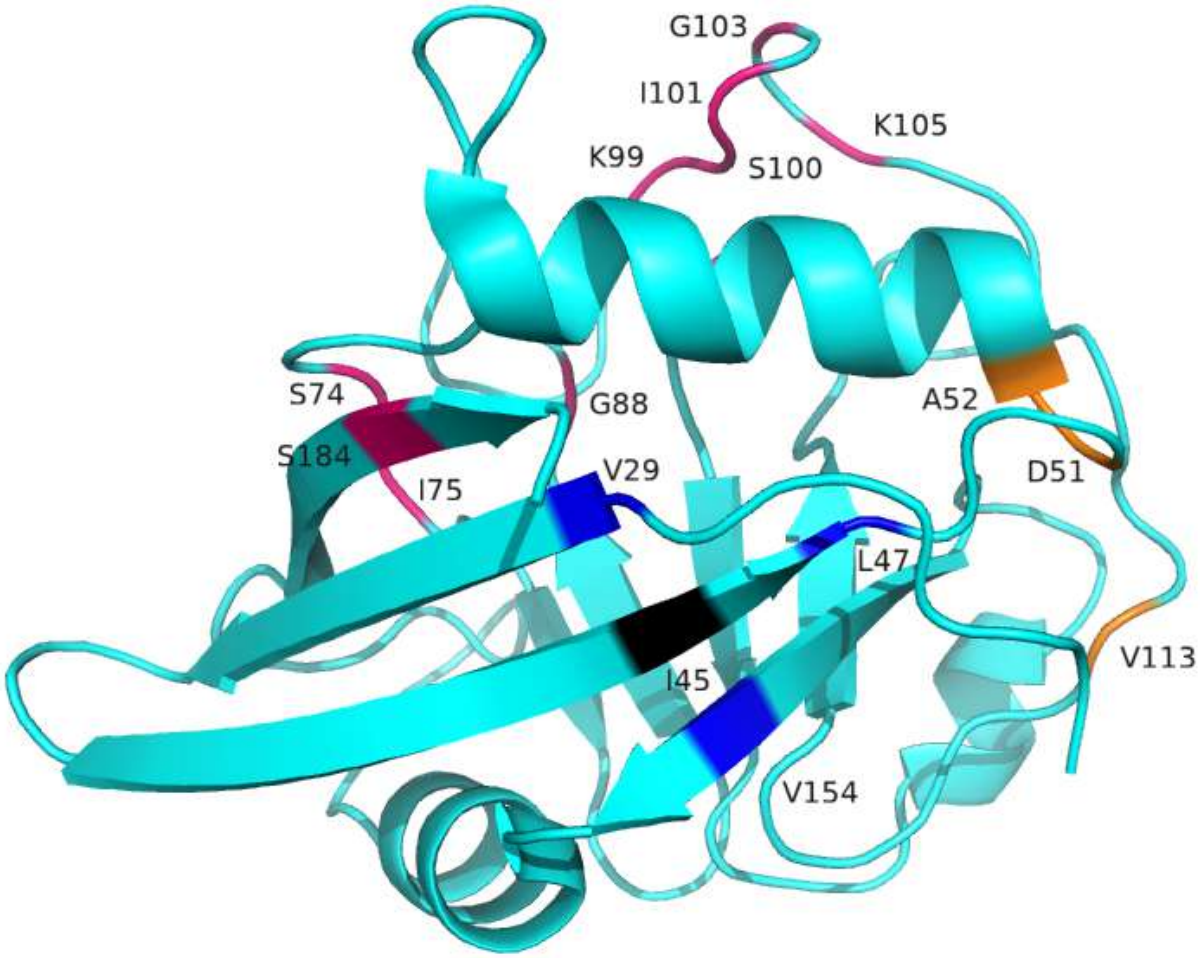
Supplementary Figure 13. Active site residues & drug binding motifs of 3TBH. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



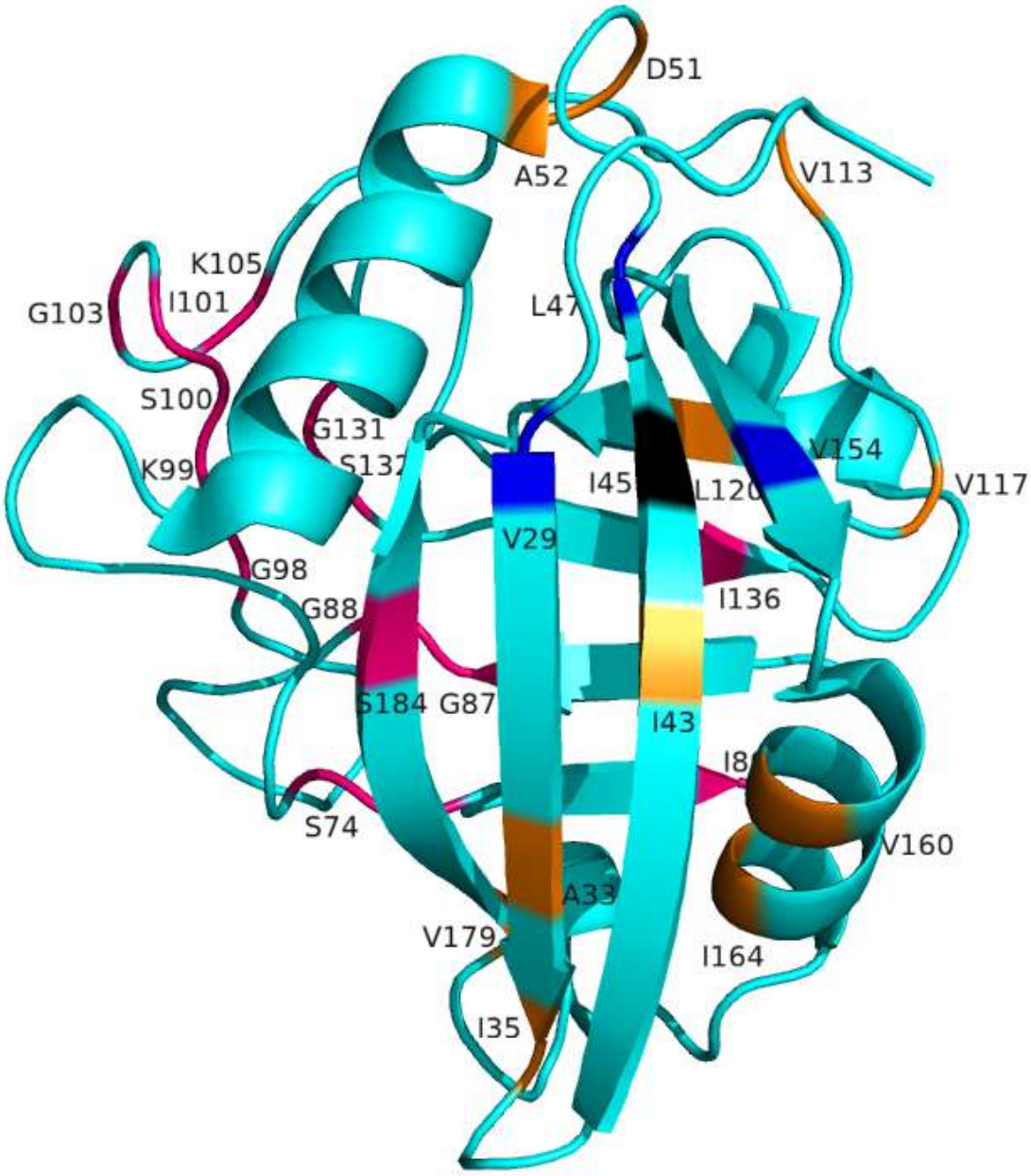
Supplementary Figure 14. Active site residues & drug binding motifs of 4MX2. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



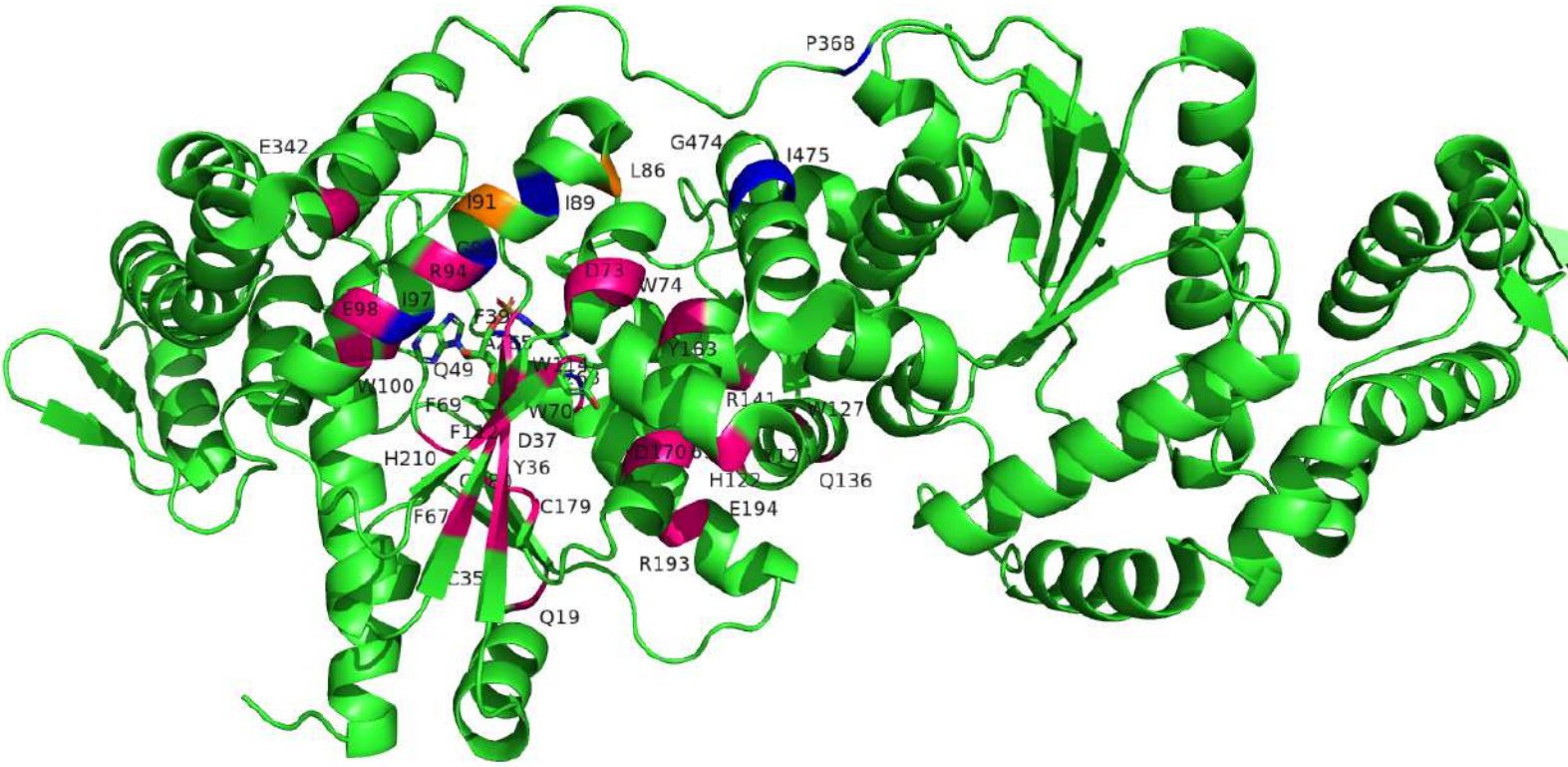
Supplementary Figure 15. Active site residues & drug binding motifs of 4O2Z. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



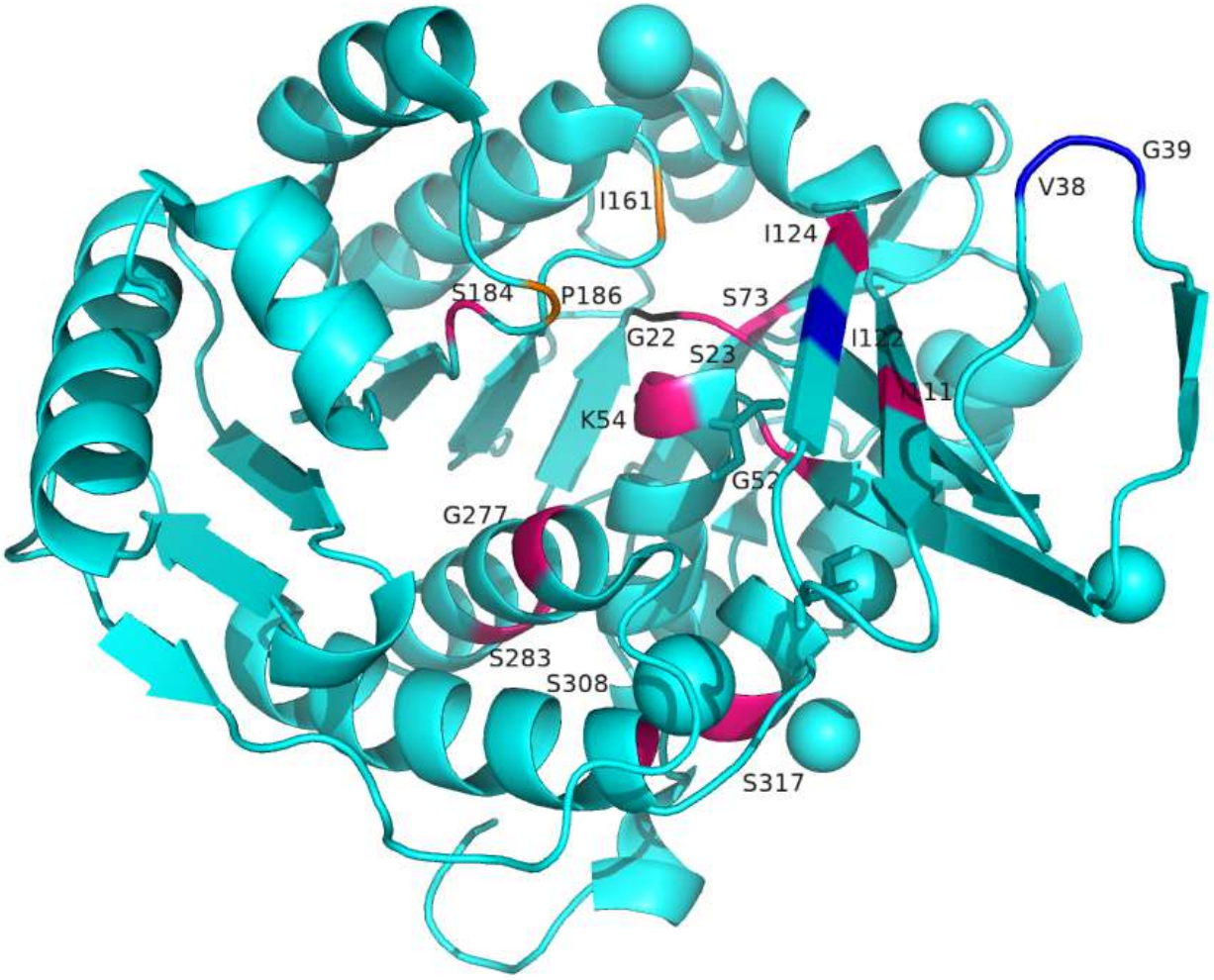
Supplementary Figure 16. Active site residues & drug binding motifs of 4S1E. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



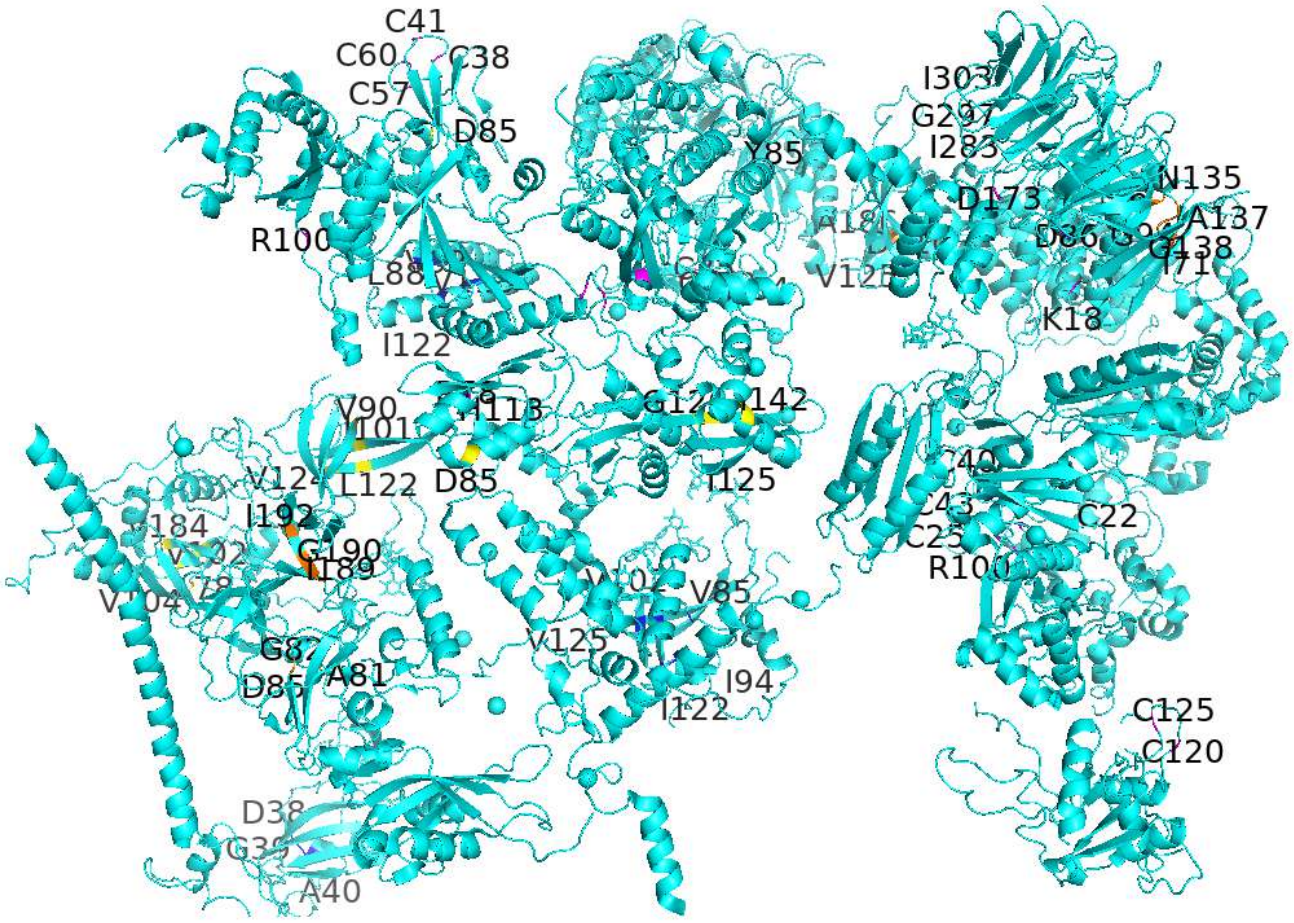
Supplementary Figure 17. Active site residues & drug binding motifs of 4S1J. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



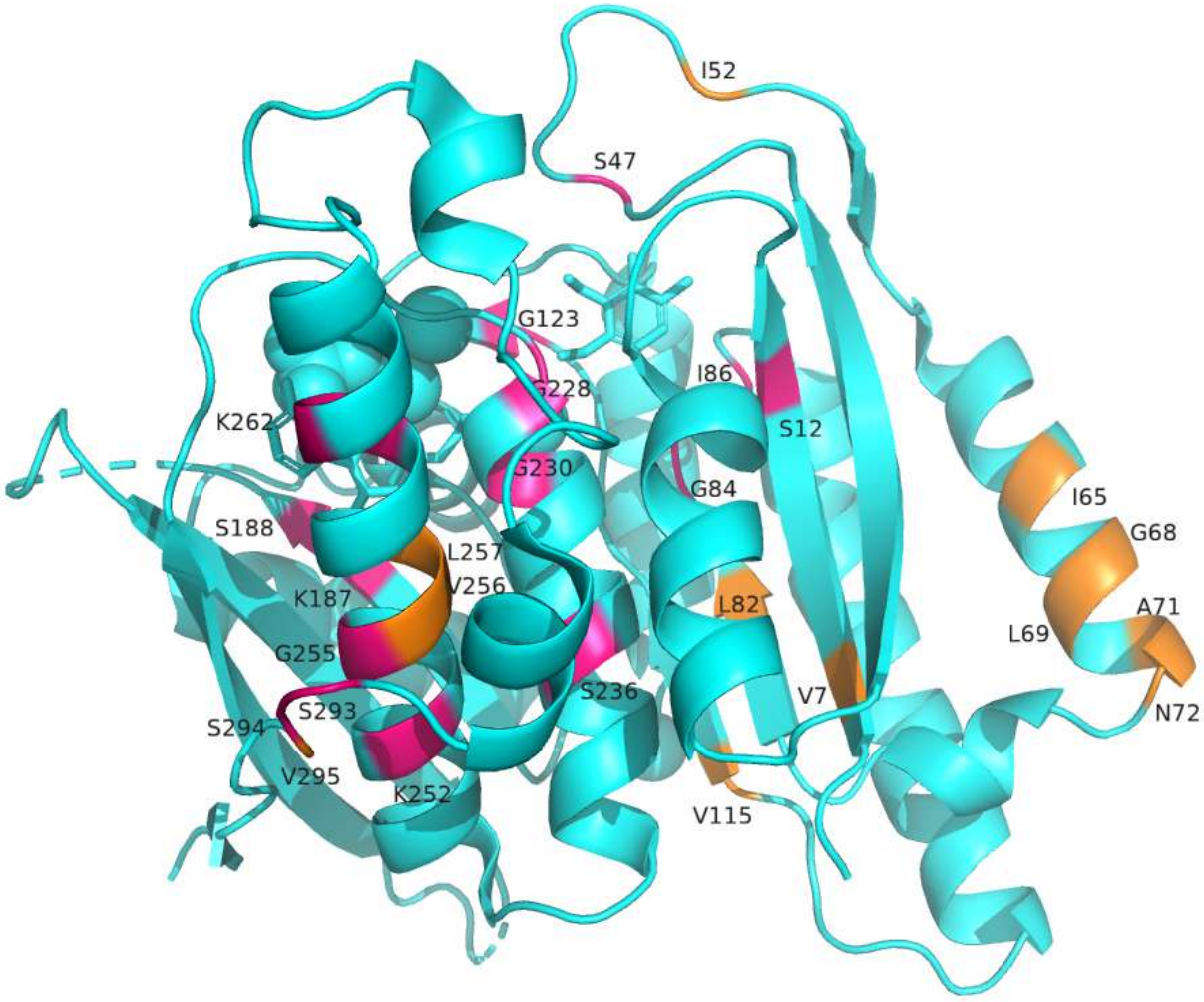
Supplementary Figure 18. Active site residues & drug binding motifs of 5USF. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



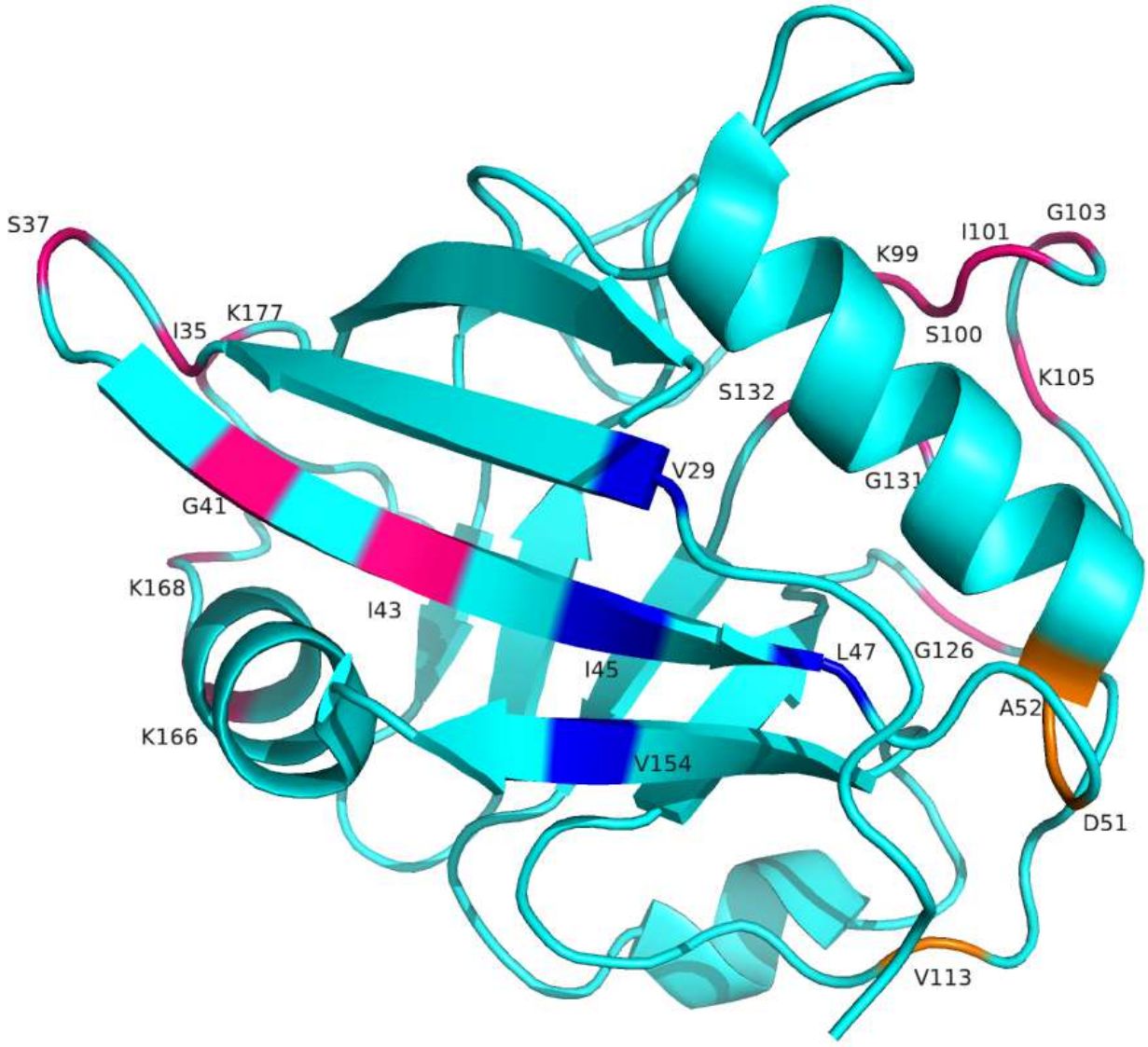
Supplementary Figure 19. Active site residues & drug binding motifs of 5ZWY. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



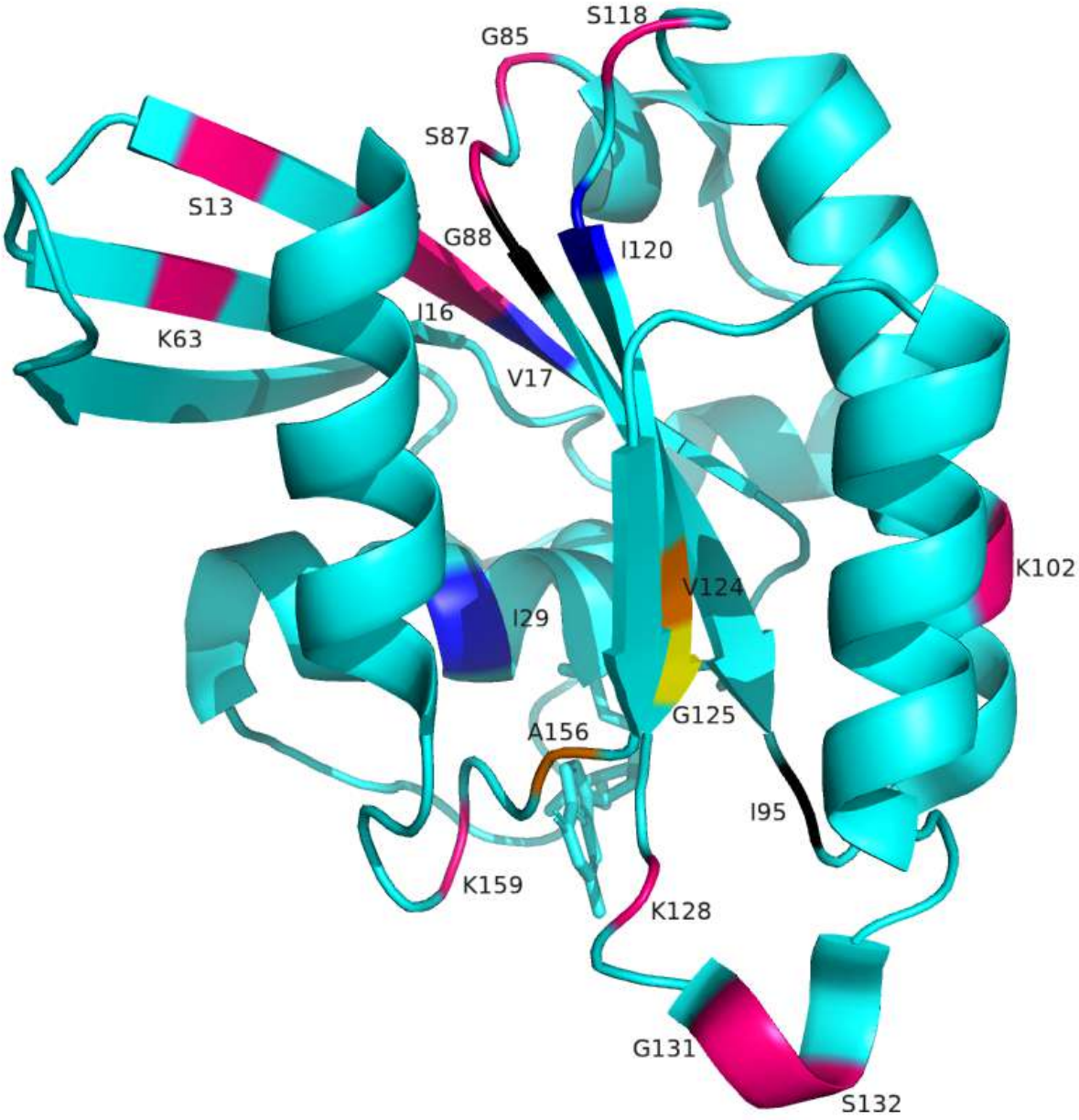
Supplementary Figure 20. Active site residues & drug binding motifs of 6AZ1. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



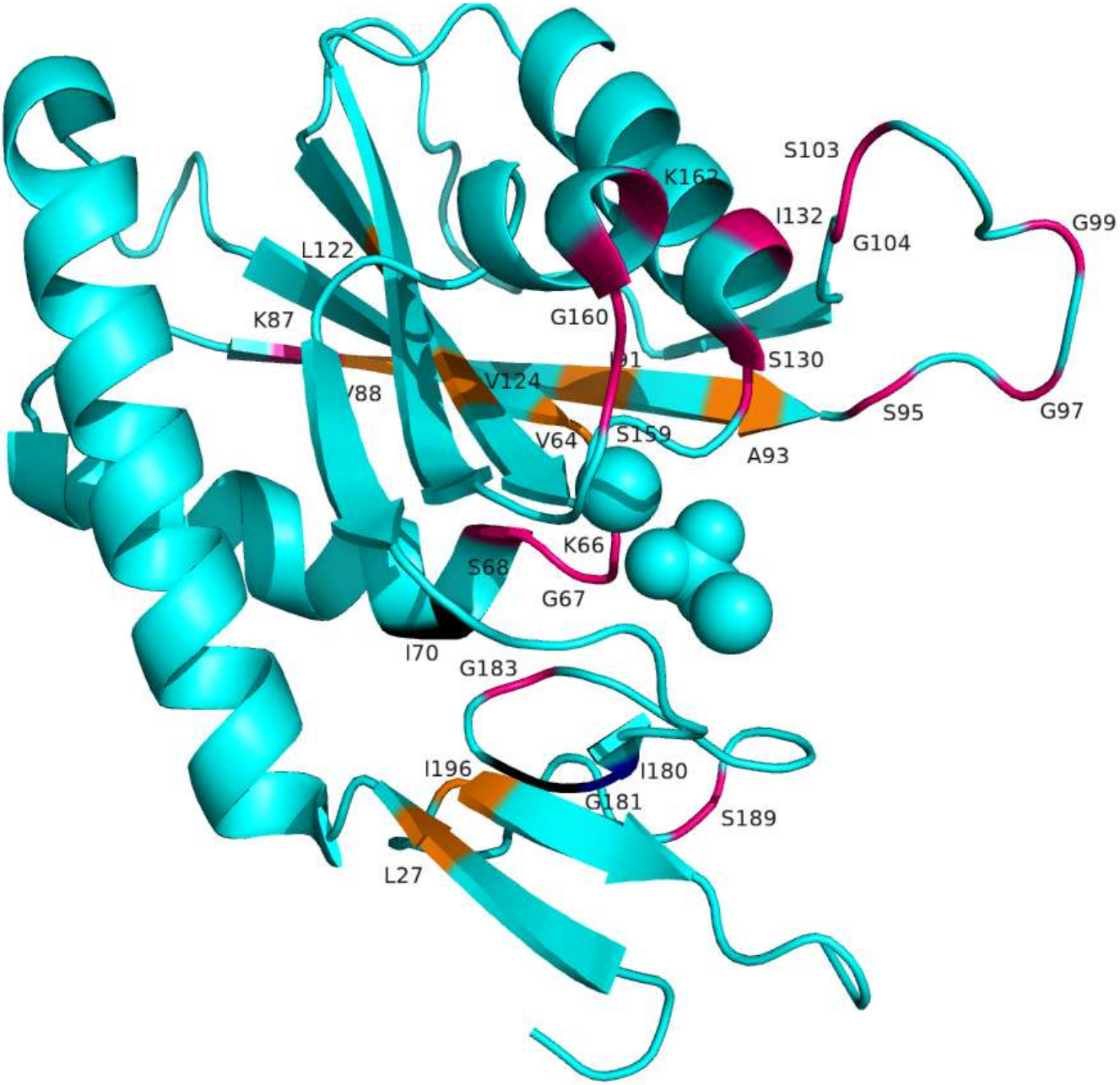
Supplementary Figure 21. Active site residues & drug binding motifs of 6K90. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



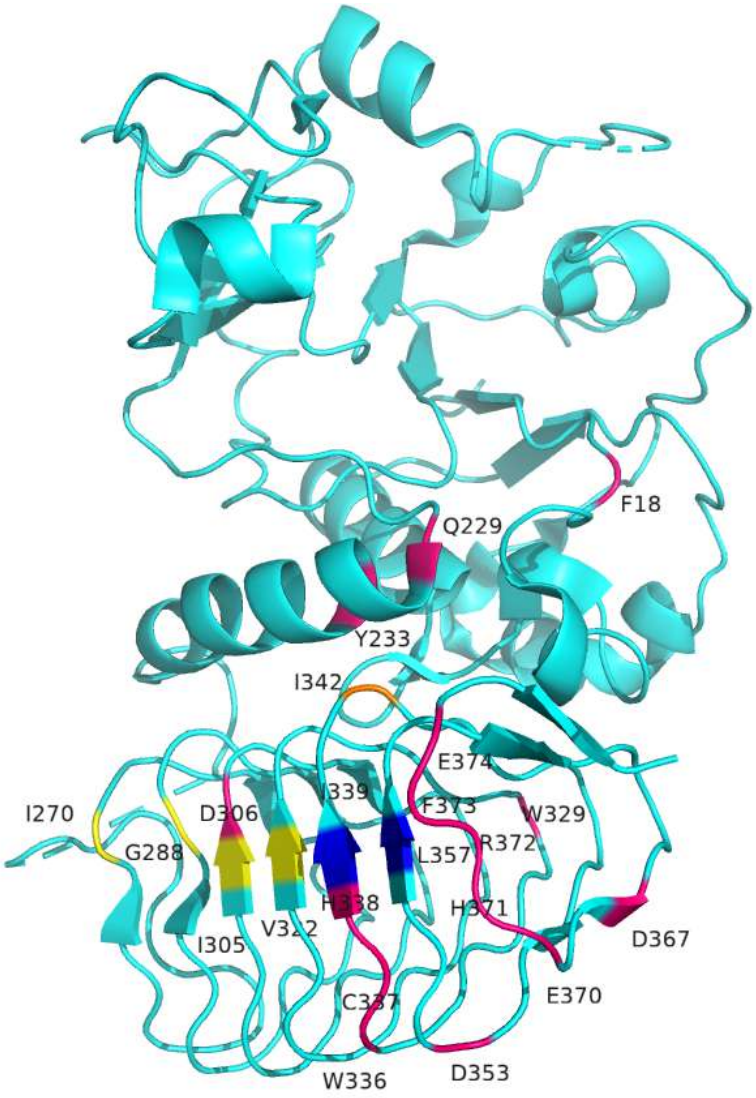
Supplementary Figure 22. Active site residues & drug binding motifs of 6L2B. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



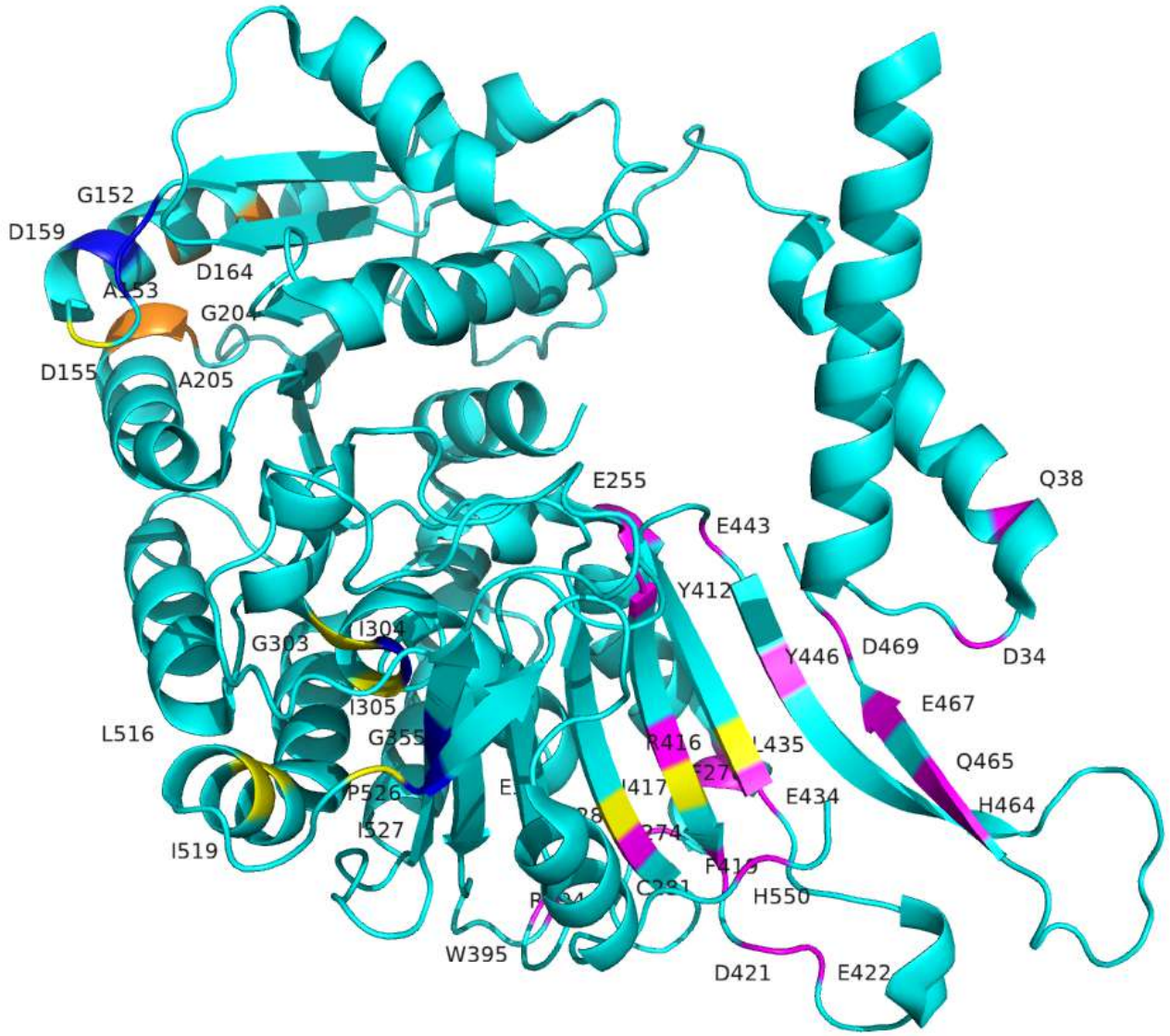
Supplementary Figure 23. Active site residues & drug binding motifs of 6L6O. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



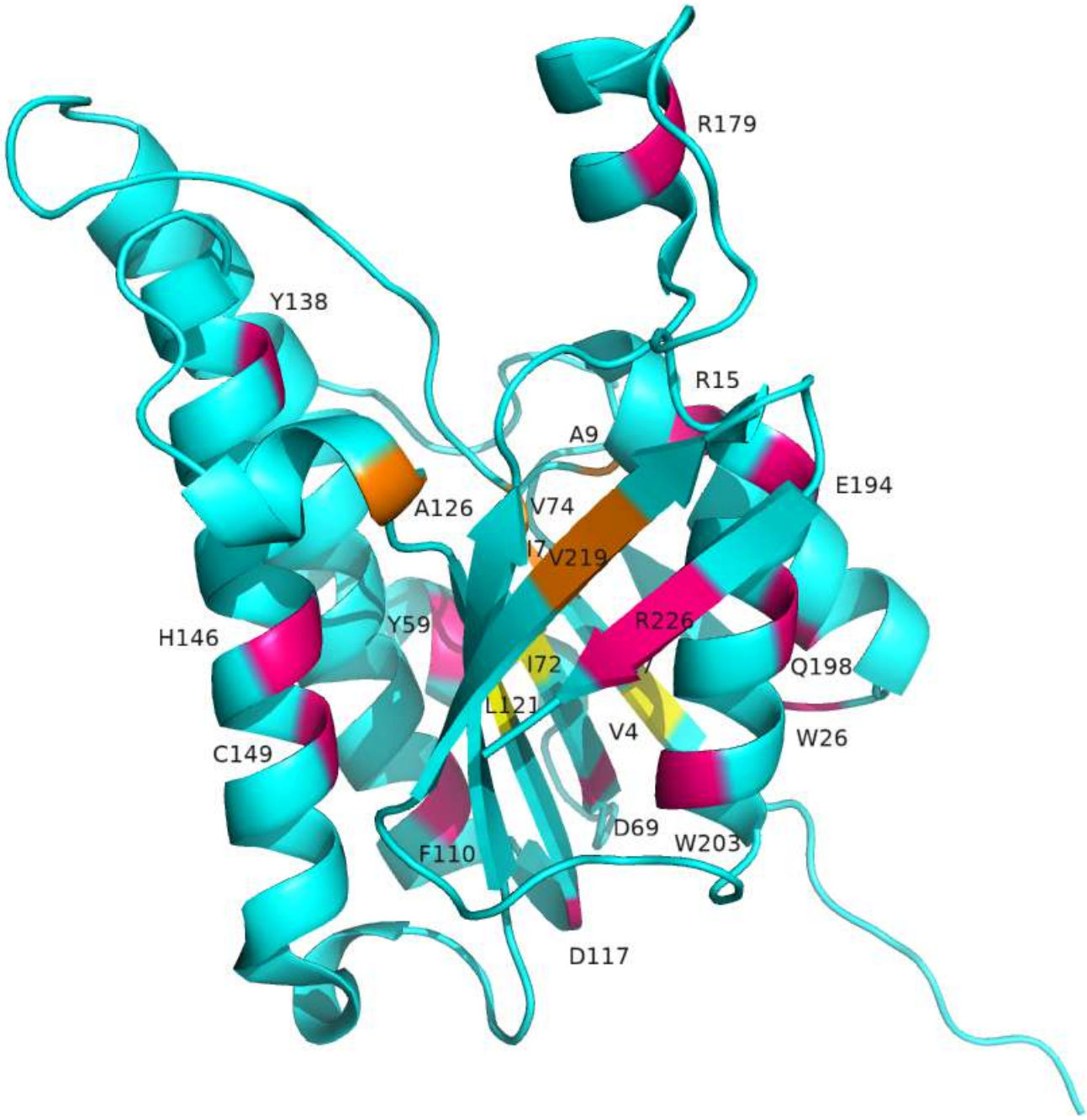
Supplementary Figure 24. Active site residues & drug binding motifs of 7CMJ. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



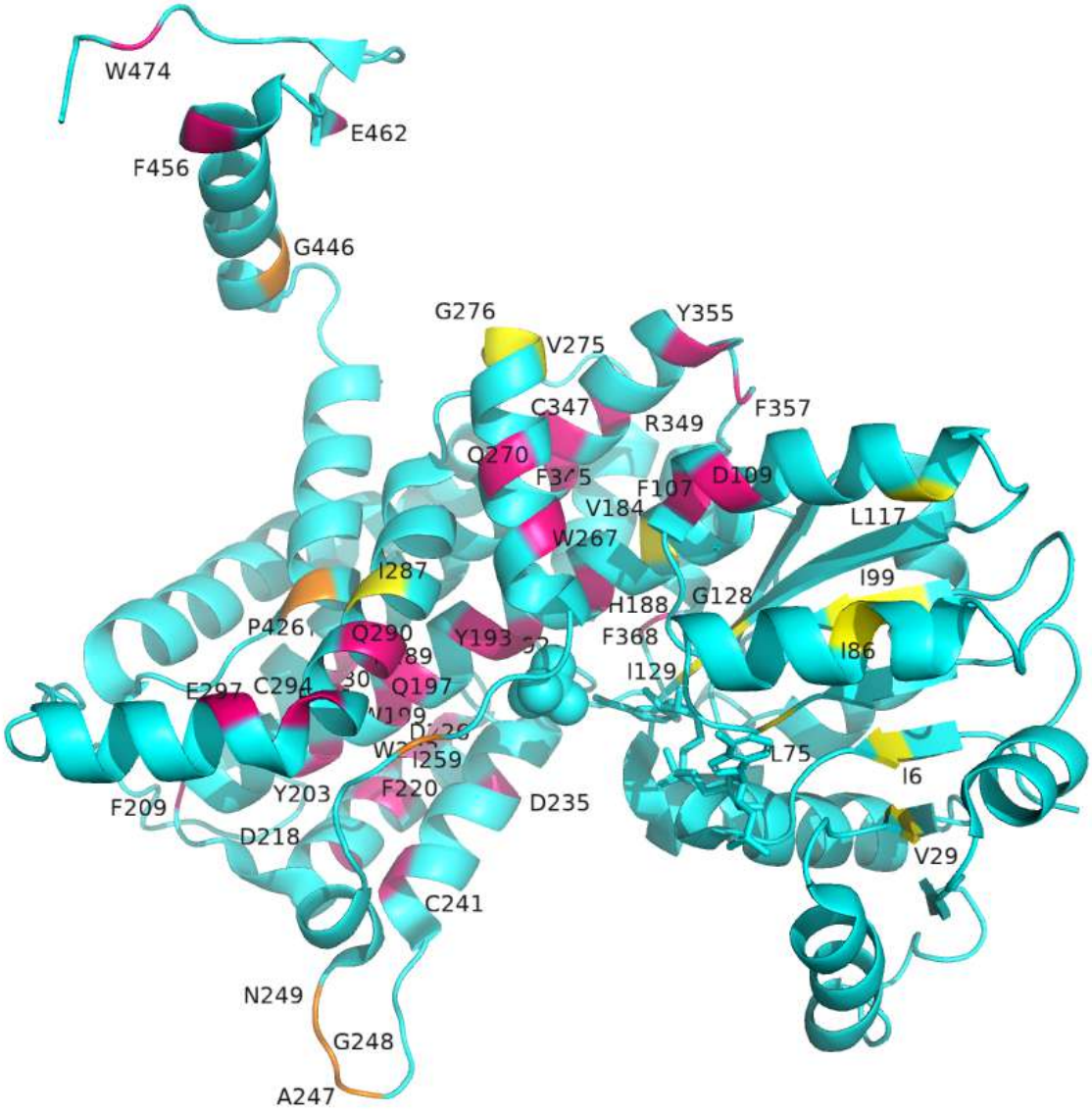
Supplementary Figure 25. Active site residues & drug binding motifs of 7WHR. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



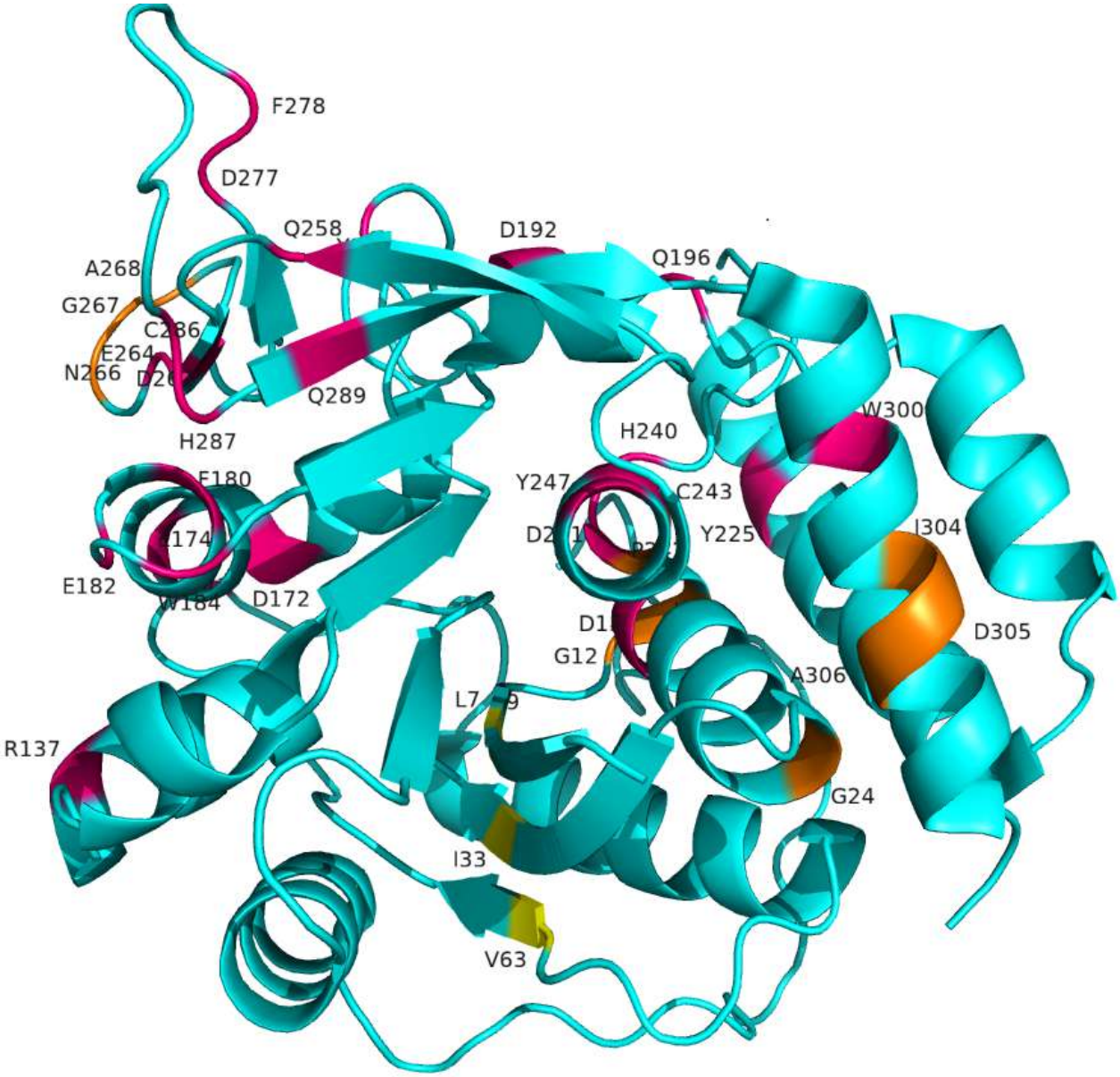
Supplementary Figure 26. Active site residues & drug binding motifs of 7ZHV. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



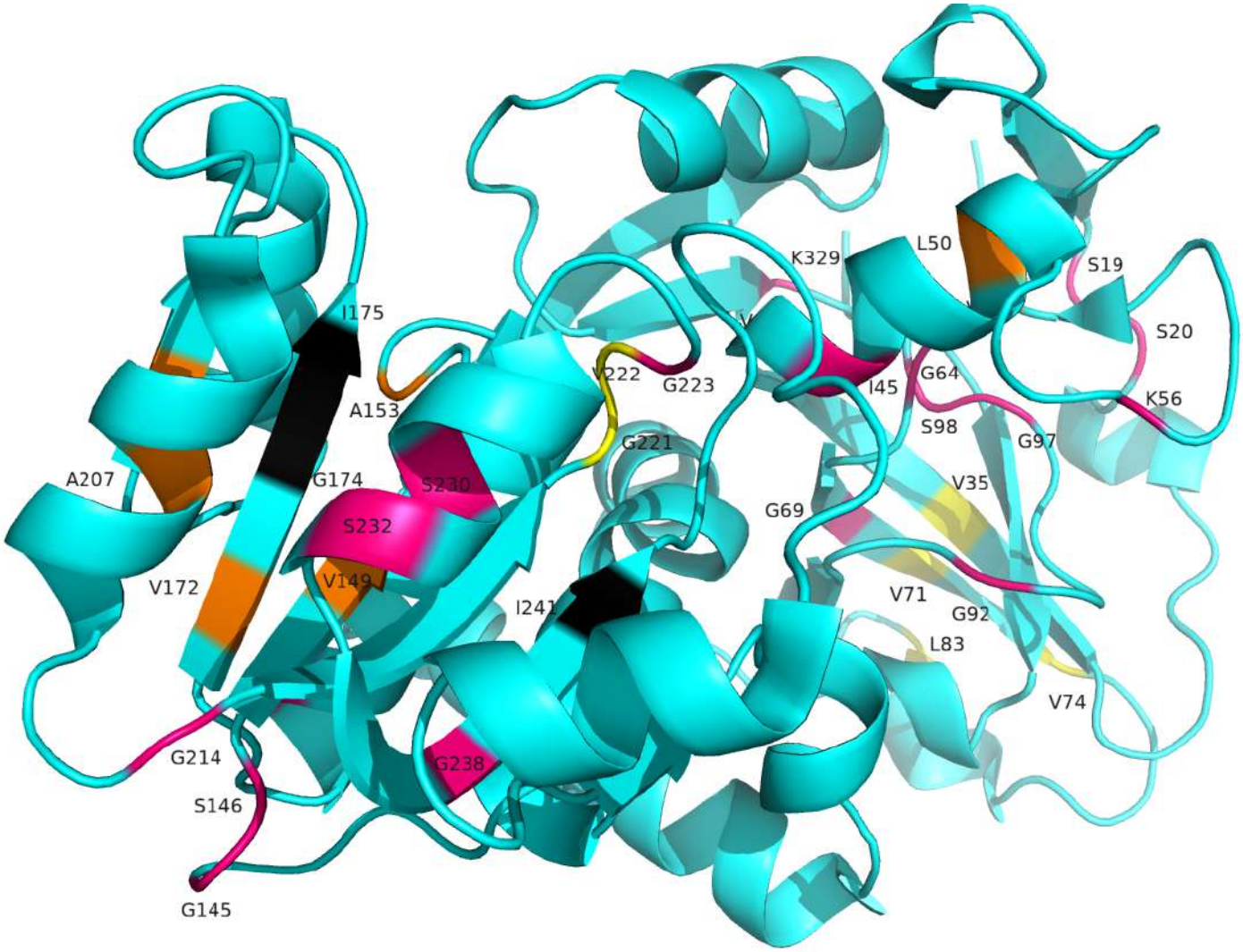
Supplementary Figure 27. Active site residues & drug binding motifs of 8B5U. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



Supplementary Figure 28. Active site residues & drug binding motifs of 8C79. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



Supplementary Figure 29. Active site residues & drug binding motifs of 8CTM. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.



Supplementary Figure 30. Active site residues & drug binding motifs of 8J6E. Enzyme showing drug binding motifs of Amprenavir (478-Yellow), and Darunavir (017-Orange) in close association with active site residues (Pink). Blue represents common binding residue of 478 and 017. Black represents common drug binding and active site residue.

Supplementary Tables

Supplementary Table 1. Possible binding sites of 1QCD against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Tipranavir	HIV-1 PROTEASE	0.97 A	3	208 ALA 207 ASP 206 ASP	R
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.20 A	3	166 ASP 74 THR 73 PRO	R
Darunavir	HIV-1 PROTEASE	1.05 A	3	137 GLY 136 ILE 97 PRO	L
	FIV PROTEASE	0.55 A	3	101 MET 78 GLY 145 ILE	R
	ASPARTYL PROTEASE	0.92 A	3	85 LEU 148 VAL 45 VAL	L
Amprenavir	PROTEASE	0.97 A	3	137 GLY 136 ILE 97 PRO	L
	PROTEASE	1.12 A	3	23 LEU 45 VAL 48 ILE	R

Supplementary Tables

Supplementary Table 2. Possible binding sites of 1X9G against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	PROTEIN (PROTEASE)	1.08 A	3	146 ILE 109 GLY 107 ILE	R
	HIV-II PROTEASE	0.82 A	3	104 VAL 106 GLY 107 ILE	L
	PROTEASE RETROPEPSIN;PRO TEASE RETROPEPSIN	1.15 A	3	90 PRO 89 VAL 80 ILE	L
	PROTEASE RETROPEPSIN	1.14 A	3	113 ILE 135 GLY 28 ILE	R
Ritonavir	POL POLYPROTEIN	1.01 A	3	146 ILE 109 GLY 107 ILE	R
	PROTEASE;PROTEA SE	0.92 A	3	146 ILE 135 GLY 107 ILE	R
	GAG-POL POLYPROTEIN;GAG -POL POLYPROTEIN	0.97 A	3	113 ILE 135 GLY 28 ILE	R
Darunavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.93 A	3	146 ILE 109 GLY 107 ILE	R
	PROTEASE (RETROPEPSIN);PR OTEASE (RETROPEPSIN)	1.01 A	3	146 ILE 135 GLY 107 ILE	R
	PROTEASE	1.18 A	4	146 ILE 109 GLY 107 ILE 130 PRO	R
	PROTEASE	1.38 A	4	146 ILE 135 GLY 107 ILE 130 PRO	L
	PROTEASE;PROTEA SE	0.59 A	3	104 VAL 106 GLY 107 ILE	R
	FIV PROTEASE;FIV PROTEASE	1.04 A	3	77 ALA 55 ILE 56 VAL	L
Ribavirin	RNA POLYMERASE	0.93 A	3	13 THR 52 THR 51 ASN	L
Saquinavir	PROTEASE E35D-SQV	0.82 A	3	146 ILE 135 GLY 107 ILE	R
	PROTEASE E35D-SQV;PROTEASE E35D-SQV	1.17 A	3	113 ILE 135 GLY 28 ILE	L
	PROTEASE	0.92 A	3	146 ILE 109 GLY 107 ILE	L
Amprenavir	HIV-1 PROTEASE	1.17 A	3	132 ASP	L

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				41 LEU 18 VAL	
	PROTEASE	0.83 A	3	79 LEU 92 VAL 80 ILE	L
	PROTEASE;PROTEASE	1.02 A	3	146 ILE 109 GLY 107 ILE	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.14 A	3	113 ILE 135 GLY 28 ILE	R
	PROTEASE	0.46 A	3	104 VAL 106 GLY 107 ILE	R
	PROTEASE	1.20 A	3	73 LEU 35 VAL 71 ILE	L
	PROTEASE;PROTEASE	0.81 A	3	146 ILE 135 GLY 107 ILE	R
Lopinavir	PROTEASE	0.90 A	3	146 ILE 109 GLY 107 ILE	R
	PROTEASE	1.17 A	3	113 ILE 135 GLY 28 ILE	L
Atazanavir	PROTEASE;PROTEASE	1.01 A	3	146 ILE 109 GLY 107 ILE	R
	PROTEASE;PROTEASE	1.10 A	3	90 PRO 89 VAL 80 ILE	L
	PROTEASE;PROTEASE	0.94 A	3	179 ARG 49 PRO 48 VAL	L
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.07 A	3	146 ILE 109 GLY 107 ILE	R
Tipranavir	HIV-1 PROTEASE	1.05 A	3	172 ALA 171 ASP 174 ASP	L
	HIV-1 PROTEASE	1.06 A	3	146 ILE 109 GLY 107 ILE	R

Supplementary Tables

Supplementary Table 3. Possible binding sites of 2B9S against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	1.00 A	3	A 29 ASP - A 233 ASP A 81 PRO - A 219 PRO A 82 VAL - A 218 VAL	R
	HIV-II PROTEASE;HIV-II PROTEASE	0.64 A	3	B 47 VAL - A 327 VAL B 49 GLY - A 351 GLY B 50 ILE - A 355 ILE	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.09 A	3	A 81 PRO - B 238 PRO A 82 VAL - B 237 VAL A 84 ILE - B 242 ILE	L
Darunavir	POL POLYPROTEIN	0.95 A	3	B 147 ILE - A 212 ILE B 149 GLY - A 53 GLY B 150 VAL - A 54 VAL	L
	PROTEASE	0.84 A	3	B 123 LEU - A 371 LEU B 132 ILE - A 344 ILE B 182 ILE - A 337 ILE	L
	PROTEASE (RETROPEPSIN);PROTEASE (RETROPEPSIN)	0.81 A	3	A 25 ASN - A 249 ASN A 27 GLY - A 248 GLY A 28 ALA - A 247 ALA	L
	PROTEASE	0.64 A	3	B 147 VAL - A 327 VAL B 149 GLY - A 351 GLY B 150 ILE - A 355 ILE	R
	FIV PROTEASE;FIV PROTEASE	1.10 A	3	B 33 ALA - A 448 ALA B 35 ILE - A 449 ILE B 37 VAL - B 213 VAL	L
	ASPARTYL PROTEASE	1.09 A	3	B 23 LEU - A 364 LEU B 32 VAL - A 345 VAL B 82 VAL - A 367 VAL	L
Saquinavir	HIV-1 PROTEASE	1.21 A	3	A 32 VAL - A 230 VAL A 81 PRO - A 221 PRO A 84 ILE - A 210 ILE	R
	PROTEASE	0.85 A	3	A 8 ARG - A 310 ARG A 32 VAL - A 447 VAL A 80 THR - A 417 THR	R
	PROTEASE E35D-SQV;PROTEASE E35D-SQV	0.92 A	3	B 8 ARG - A 301 ARG B 23 LEU - A 388 LEU B 25 ASN - A 389 ASN	L
	PROTEASE	1.17 A	3	A 9 ARG - A 44 ARG A 33 VAL - A 261 VAL A 81 THR - A 237 THR	L
Lopinavir	PROTEASE;PROTEASE	1.24 A	3	A 32 VAL - A 230 VAL A 81 PRO - A 221 PRO A 84 ILE - A 210 ILE	R
Tipranavir	PROTEASE;PROTEASE	0.83 A	3	B 47 ILE - A 355 ILE B 49 GLY - A 351 GLY B 50 VAL - A 327 VAL	L
	PROTEASE	1.11 A	3	A 47 ILE - A 212 ILE A 49 GLY - A 53 GLY A 50 VAL - A 54 VAL	L
Amprenavir	PROTEASE;PROTEASE	1.04 A	3	A 23 LEU - A 49 LEU A 32 VAL - A 218 VAL A 84 ILE - A 212 ILE	L
	PROTEASE;PROTEASE	1.11 A	3	A 47 ILE - A 212 ILE A 49 GLY - A 53 GLY A 50 VAL - A 54 VAL	L
	PROTEASE	0.81 A	3	B 147 ILE - A 355 ILE B 149 GLY - A 351 GLY B 150 VAL - A 327 VAL	L
	PROTEASE;PROTEASE	1.14 A	4	B 123 LEU - A 364 LEU	L

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				B 132 VAL - A 345 VAL B 182 VAL - A 367 VAL B 184 VAL - A 363 VAL	
Atazanavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.84 A	3	B 47 ILE - A 355 ILE B 49 GLY - A 351 GLY B 50 VAL - A 327 VAL	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.17 A	3	B 47 ILE - A 212 ILE B 49 GLY - A 53 GLY B 50 VAL - A 54 VAL	R
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.77 A	3	A1123 ARG - A 410 ARG A1157 ALA - A 414 ALA A1159 SER - B 218 SER	R
	NS3 PROTEASE, NS4A PROTEIN	1.12 A	3	A1123 ARG - A 301 ARG A1157 ALA - A 299 ALA A1159 SER - A 293 SER	L

Supplementary Tables

Supplementary Table 4. Possible binding sites of 2HAQ against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	HIV-II PROTEASE;HIV-II PROTEASE	1.28 A	3	B 47 VAL - A 150 VAL B 49 GLY - A 152 GLY B 50 ILE - A 45 ILE	R
Saquinavir	PROTEASE	0.70 A	3	A 8 ARG - A 78 ARG A 32 VAL - A 161 VAL A 80 THR - A 138 THR	L
Amprenavir	PROTEASE	0.84 A	3	B 23 LEU - A 47 LEU B 32 VAL - A 154 VAL B 84 ILE - A 45 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.33 A	4	A 23 LEU - A 47 LEU A 32 VAL - A 154 VAL A 82 VAL - A 29 VAL A 84 ILE - A 45 ILE	L
Darunavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.98 A	3	A 23 LEU - A 120 LEU A 32 VAL - A 117 VAL A 82 VAL - A 154 VAL	L
	PROTEASE	1.25 A	3	B 147 VAL - A 150 VAL B 149 GLY - A 152 GLY B 150 ILE - A 45 ILE	L
	HIV-1 PROTEASE	1.05 A	3	B 128 ALA - A 52 ALA B 130 ASP - A 51 ASP B 132 VAL - A 113 VAL	R

Supplementary Tables

Supplementary Table 5. Possible binding sites of 2KVK against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	PROTEASE RETROPEPSIN	0.59 A	3	B 147 ILE - A 3 ILE B 149 GLY - A 35 GLY B 150 ILE - A 31 ILE	R
Ritonavir	POL POLYPROTEIN;POL POLYPROTEIN	0.58 A	3	A 47 ILE - A 3 ILE A 49 GLY - A 35 GLY A 50 ILE - A 31 ILE	R
Darunavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.72 A	3	B 47 ILE - A 3 ILE B 49 GLY - A 35 GLY B 50 ILE - A 31 ILE	R
	FIV PROTEASE;FIV PROTEASE	0.74 A	3	B 33 ALA - A 105 ALA B 35 ILE - A 38 ILE B 37 VAL - A 6 VAL	L
	PROTEASE	0.94 A	3	B 123 LEU - A 124 LEU B 132 ILE - A 87 ILE B 182 ILE - A 84 ILE	R
	PROTEASE (RETROPEPSIN);PROTEASE (RETROPEPSIN)	1.23 A	3	A 47 ILE - A 38 ILE A 49 GLY - A 35 GLY A 50 ILE - A 3 ILE	L
Simeprevir	GENOME POLYPROTEIN	0.92 A	3	A 136 LYS - A 36 LYS A 137 GLY - A 35 GLY A 139 SER - A 4 SER	L
Saquinavir	PROTEASE;PROTEASE	0.91 A	3	B 8 ARG - A 20 ARG B 23 LEU - A 81 LEU B 25 ASP - A 68 ASP	L
	PROTEASE E35D-SQV;PROTEASE E35D-SQV	0.72 A	3	B 47 ILE - A 3 ILE B 49 GLY - A 35 GLY B 50 ILE - A 31 ILE	L
	PROTEASE	1.21 A	3	B 147 ILE - A 38 ILE B 149 GLY - A 35 GLY B 150 ILE - A 3 ILE	L
Amprenavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.75 A	3	A 47 ILE - A 3 ILE A 49 GLY - A 35 GLY A 50 ILE - A 31 ILE	R
	PROTEASE	1.14 A	3	B 23 LEU - A 19 LEU B 32 VAL - A 12 VAL B 84 ILE - A 16 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.49 A	3	A 47 ILE - A 38 ILE A 49 GLY - A 35 GLY A 50 ILE - A 3 ILE	R
	PROTEASE;PROTEASE	1.10 A	3	A 23 LEU - A 19 LEU A 32 VAL - A 109 VAL A 84 ILE - A 16 ILE	L
Lopinavir	PROTEASE	1.08 A	3	A 47 ILE - A 38 ILE A 49 GLY - A 35 GLY A 50 ILE - A 3 ILE	L
	PROTEASE	0.66 A	3	B 47 ILE - A 3 ILE B 49 GLY - A 35 GLY B 50 ILE - A 31 ILE	R
	HIV-1 PROTEASE	1.16 A	3	A 48 GLY - A 32 GLY A 49 GLY - A 35 GLY A 50 ILE - A 3 ILE	L
Atazanavir	HIV-1 PROTEASE	0.75 A	3	B 47 ILE - A 3 ILE B 49 GLY - A 35 GLY B 50 ILE - A 31 ILE	R
	PROTEASE;PROTEASE	1.27 A	3	A 47 ILE - A 38 ILE A 49 GLY - A 35 GLY A 50 ILE - A 3 ILE	L
Nelfinavir	PROTEASE	0.76 A	3	A 47 ILE - A 3 ILE	R

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	RETROPEPSIN;PROTEASE RETROPEPSIN			A 49 GLY - A 35 GLY A 50 ILE - A 31 ILE	
	PROTEASE RETROPEPSIN	1.45 A	3	B 47 ILE - A 38 ILE B 49 GLY - A 35 GLY B 50 ILE - A 3 ILE	L
Tipranavir	HIV-1 PROTEASE	0.60 A	3	A 47 ILE - A 3 ILE A 49 GLY - A 35 GLY A 50 ILE - A 31 ILE	L
	HIV-1 PROTEASE	1.43 A	3	A 47 ILE - A 38 ILE A 49 GLY - A 35 GLY A 50 ILE - A 3 ILE	L
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.96 A	3	A1123 ARG - A 137 ARG A1157 ALA - A 74 ALA A1159 SER - A 76 SER	R

Supplementary Tables

Supplementary Table 6. Possible binding sites of 2ON3 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.34 A	3	A 47 ILE - B 234 ILE A 48 GLY - B 235 GLY A 49 GLY - B 236 GLY	L
	PROTEIN (PROTEASE);PROTEIN (PROTEASE)	0.90 A	3	A 8 ARG - A 270 ARG A 23 LEU - A 231 LEU A 25 ASP - A 233 ASP	R
Darunavir	FIV PROTEASE;FIV PROTEASE	0.81 A	3	B 33 ALA - B 149 ALA B 35 ILE - B 189 ILE B 37 VAL - B 142 VAL	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.69 A	3	B 125 ASP - B 134 ASP B 127 GLY - B 171 GLY B 128 ALA - B 172 ALA	R
	HIV-1 PROTEASE	0.84 A	3	B 128 ALA - B 39 ALA B 130 ASP - B 320 ASP B 132 VAL - B 318 VAL	R
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.71 A	3	B 25 ASP - B 134 ASP B 27 GLY - B 171 GLY B 28 ALA - B 172 ALA	R
Amprenavir	PROTEASE;PROTEASE	0.68 A	3	A 25 ASP - B 134 ASP A 27 GLY - B 171 GLY A 28 ALA - B 172 ALA	R
	PROTEASE;PROTEASE	0.55 A	3	A 23 LEU - B 49 LEU A 32 VAL - B 280 VAL A 84 ILE - B 48 ILE	R
	HIV-1 PROTEASE	0.81 A	3	B 129 ASP - B 214 ASP B 176 LEU - B 232 LEU B 182 VAL - B 191 VAL	L
Saquinavir	PROTEASE;PROTEASE	0.70 A	3	B 25 ASP - B 134 ASP B 27 GLY - B 171 GLY B 28 ALA - B 172 ALA	R
Tipranavir	HIV-1 PROTEASE	0.62 A	3	B 25 ASP - B 134 ASP B 27 GLY - B 171 GLY B 28 ALA - B 172 ALA	R

Supplementary Tables

Supplementary Table 7. Possible binding sites of 2WUU against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Ritonavir	POL POLYPROTEIN;POL POLYPROTEIN	0.60 A	3	A 47 ILE - A 107 ILE A 49 GLY - A 128 GLY A 50 ILE - A 166 ILE	R
Darunavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.80 A	3	A 49 GLY - A 234 GLY A 50 ILE - A 235 ILE A 81 PRO - A 224 PRO	L
	POL POLYPROTEIN	0.86 A	3	B 147 ILE - A 126 ILE B 149 GLY - A 128 GLY B 150 VAL - A 129 VAL	R
	FIV PROTEASE;FIV PROTEASE	0.84 A	3	B 33 ALA - A 213 ALA B 35 ILE - A 411 ILE B 37 VAL - A 416 VAL	R
	PROTEASE;PROTEASE	0.74 A	3	A 47 ILE - A 107 ILE A 49 GLY - A 128 GLY A 50 ILE - A 166 ILE	R
	PROTEASE	0.89 A	3	B 123 LEU - A 359 LEU B 132 ILE - A 365 ILE B 182 ILE - A 360 ILE	R
	PROTEASE	0.81 A	3	B 123 LEU - A 341 LEU B 132 ILE - A 333 ILE B 182 ILE - A 230 ILE	R
	PROTEASE	0.80 A	3	B 123 LEU - A 180 LEU B 132 ILE - A 185 ILE B 182 ILE - A 183 ILE	L
Indinavir	PROTEASE RETROPEPSIN	1.06 A	3	B 132 VAL - A 197 VAL B 181 PRO - A 130 PRO B 184 ILE - A 163 ILE	L
	PROTEASE RETROPEPSIN	0.59 A	3	B 147 ILE - A 107 ILE B 149 GLY - A 128 GLY B 150 ILE - A 166 ILE	R
Saquinavir	PROTEASE;PROTEASE	0.74 A	3	A 47 ILE - A 107 ILE A 49 GLY - A 128 GLY A 50 ILE - A 166 ILE	R
	HIV-1 PROTEASE	1.26 A	4	A 23 LEU - A 133 LEU A 81 PRO - A 130 PRO A 82 VAL - A 131 VAL A 84 ILE - A 163 ILE	R
Amprenavir	PROTEASE;PROTEASE	0.79 A	3	A 47 ILE - A 107 ILE A 49 GLY - A 128 GLY A 50 ILE - A 166 ILE	R
	PROTEASE	0.92 A	3	B 147 ILE - A 126 ILE B 149 GLY - A 128 GLY B 150 VAL - A 129 VAL	L
	PROTEASE;PROTEASE	0.80 A	3	A 23 LEU - A 169 LEU A 32 VAL - A 112 VAL A 84 ILE - A 126 ILE	R
	PROTEASE	1.03 A	3	B 23 LEU - A 279 LEU B 32 VAL - A 272 VAL B 84 ILE - A 297 ILE	R
	PROTEASE	1.01 A	3	B 23 LEU - A 381 LEU B 32 VAL - A 378 VAL B 84 ILE - A 380 ILE	L
Lopinavir	PROTEASE;PROTEASE	0.71 A	3	B 47 ILE - A 107 ILE B 49 GLY - A 128 GLY B 50 ILE - A 166 ILE	R
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.76 A	3	A 47 ILE - A 107 ILE A 49 GLY - A 128 GLY A 50 ILE - A 166 ILE	R

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Atazanavir	HIV-1 PROTEASE	0.66 A	3	B 47 ILE - A 107 ILE B 49 GLY - A 128 GLY B 50 ILE - A 166 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.98 A	3	B 47 ILE - A 126 ILE B 49 GLY - A 128 GLY B 50 VAL - A 129 VAL	R
Tipranavir	PROTEASE	1.04 A	3	A 47 ILE - A 126 ILE A 49 GLY - A 128 GLY A 50 VAL - A 129 VAL	L
	HIV-1 PROTEASE	0.71 A	3	A 47 ILE - A 107 ILE A 49 GLY - A 128 GLY A 50 ILE - A 166 ILE	L

Supplementary Tables

Supplementary Table 8. Possible binding sites of 2XOX against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Lopinavir	PROTEASE	0.66 A	3	B 8 ARG - A 55 ARG B 81 PRO - A 7 PRO B 82 VAL - A 6 VAL	R
Indinavir	PROTEASE RETROPEPSIN	0.74 A	3	B 108 ARG - A 55 ARG B 181 PRO - A 7 PRO B 182 VAL - A 6 VAL	R
Saquinavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.75 A	3	B 8 ARG - B 55 ARG B 81 PRO - B 7 PRO B 82 VAL - B 6 VAL	R
Darunavir	WILD-TYPE HIV-1 PROTEASE DIMER;WILD-TYPE HIV-1 PROTEASE DIMER	0.77 A	3	A 8 ARG - A 55 ARG A 81 PRO - A 7 PRO A 82 VAL - A 6 VAL	R
Atazanavir	PROTEASE;PROTEASE	0.90 A	3	B 8 ARG - A 55 ARG B 81 PRO - A 7 PRO B 82 VAL - A 6 VAL	R
Ritonavir	PROTEASE	0.83 A	3	A 8 ARG - A 55 ARG A 81 PRO - A 7 PRO A 82 VAL - A 6 VAL	R

Supplementary Tables

Supplementary Table 9. Possible binding sites of 3BT8 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Ribavirin	RNA POLYMERASE	1.02 A	3	A 308 THR - A 56 THR A 309 THR - A 55 THR A 312 ASN - A 58 ASN	L
Indinavir	HIV-II PROTEASE;HIV-II PROTEASE	1.18 A	3	B 47 VAL - A 150 VAL B 49 GLY - A 152 GLY B 50 ILE - A 45 ILE	R
Saquinavir	PROTEASE	0.78 A	3	A 8 ARG - A 78 ARG A 32 VAL - A 161 VAL A 80 THR - A 138 THR	L
Darunavir	PROTEASE	1.15 A	3	B 147 VAL - A 150 VAL B 149 GLY - A 152 GLY B 150 ILE - A 45 ILE	L
	HIV-1 PROTEASE	1.01 A	3	B 128 ALA - A 52 ALA B 130 ASP - A 51 ASP B 132 VAL - A 113 VAL	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.93 A	3	A 23 LEU - A 120 LEU A 32 VAL - A 117 VAL A 82 VAL - A 154 VAL	L
Amprenavir	PROTEASE	0.83 A	3	B 23 LEU - A 47 LEU B 32 VAL - A 154 VAL B 84 ILE - A 45 ILE	R
	PROTEASE	1.24 A	3	B 147 VAL - A 150 VAL B 149 GLY - A 152 GLY B 150 ILE - A 45 ILE	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.31 A	4	A 23 LEU - A 47 LEU A 32 VAL - A 154 VAL A 82 VAL - A 29 VAL A 84 ILE - A 45 ILE	L

Supplementary Tables

Supplementary Table 10. Possible binding sites of 3C61 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Darunavir	POL POLYPROTEIN	0.71 A	3	B 147 ILE - B 194 ILE B 149 GLY - B 248 GLY B 150 VAL - B 269 VAL	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.96 A	4	B 8 ARG - D 51 ARG B 23 LEU - D 102 LEU B 81 PRO - D 135 PRO B 82 VAL - D 134 VAL	L
	HIV-1 PROTEASE	0.70 A	3	B 49 GLY - A 198 GLY B 50 ILE - A 197 ILE B 81 PRO - B 168 PRO	L
Saquinavir	HIV-1 PROTEASE;HIV-1 PROTEASE	1.16 A	4	B 8 ARG - C 51 ARG B 23 LEU - C 102 LEU B 81 PRO - C 135 PRO B 82 VAL - C 134 VAL	L
	HIV-1 PROTEASE	0.79 A	3	A 47 ILE - D 124 ILE A 49 GLY - D 163 GLY A 50 VAL - D 164 VAL	R
	HIV-1 PROTEASE	0.71 A	3	A 47 ILE - B 194 ILE A 49 GLY - B 248 GLY A 50 VAL - B 269 VAL	L
Tipranavir	PROTEASE	0.63 A	3	A 47 ILE - B 194 ILE A 49 GLY - B 248 GLY A 50 VAL - B 269 VAL	L
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.31 A	4	A 23 LEU - C 8 LEU A 32 VAL - C 123 VAL A 81 PRO - C 94 PRO A 84 ILE - C 124 ILE	R
Lopinavir	HIV-1 PROTEASE	0.79 A	3	A 48 GLY - D 307 GLY A 49 GLY - D 265 GLY A 50 ILE - D 246 ILE	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.67 A	3	A 8 ARG - C 51 ARG A 81 PRO - C 135 PRO A 82 VAL - C 134 VAL	R
Amprenavir	PROTEASE	0.80 A	3	B 149 GLY - B 198 GLY B 150 ILE - B 197 ILE B 181 PRO - A 168 PRO	L
	PROTEASE;PROTEASE	0.60 A	3	A 47 ILE - B 194 ILE A 49 GLY - B 248 GLY A 50 VAL - B 269 VAL	L
Atazanavir	HIV-1 PROTEASE	0.74 A	3	A 47 ILE - D 124 ILE A 49 GLY - D 163 GLY A 50 VAL - D 164 VAL	R

Supplementary Tables

Supplementary Table 11. Possible binding sites of 3EJO against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.34 A	3	A 47 ILE - A 183 ILE A 48 GLY - A 184 GLY A 49 GLY - A 185 GLY	L
	POL POLYPROTEIN;POL POLYPROTEIN	0.84 A	3	A 47 ILE - B 56 ILE A 48 GLY - B 59 GLY A 49 GLY - B 60 GLY	L
	POL POLYPROTEIN	0.77 A	3	B 47 ILE - B 267 ILE B 49 GLY - B 59 GLY B 50 ILE - B 56 ILE	R
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.25 A	4	A 47 ILE - A 267 ILE A 48 GLY - A 60 GLY A 49 GLY - A 59 GLY A 50 ILE - A 56 ILE	R
Ritonavir	POL POLYPROTEIN	0.67 A	3	B 47 ILE - B 267 ILE B 49 GLY - B 59 GLY B 50 ILE - B 56 ILE	L
Darunavir	POL POLYPROTEIN	0.53 A	3	B 147 ILE - A 19 ILE B 149 GLY - A 207 GLY B 150 VAL - A 206 VAL	R
	HIV-1 PROTEASE	0.78 A	3	A 47 ILE - B 267 ILE A 49 GLY - B 59 GLY A 50 ILE - B 56 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.76 A	3	B 125 ASP - B 27 ASP B 127 GLY - B 53 GLY B 128 ALA - B 54 ALA	R
	HIV-1 PROTEASE	0.66 A	3	B 49 GLY - A 182 GLY B 50 ILE - A 183 ILE B 81 PRO - A 104 PRO	L
	HIV-1 PROTEASE	0.89 A	3	B 49 GLY - A 53 GLY B 50 ILE - A 56 ILE B 81 PRO - A 271 PRO	R
Saquinavir	PROTEASE;PROTEASE	0.72 A	3	B 25 ASP - B 27 ASP B 27 GLY - B 53 GLY B 28 ALA - B 54 ALA	R
	PROTEASE;PROTEASE	0.64 A	3	B 147 ILE - B 267 ILE B 149 GLY - B 59 GLY B 150 ILE - B 56 ILE	R
	HIV-1 PROTEASE	0.73 A	3	A 47 ILE - B 19 ILE A 49 GLY - B 207 GLY A 50 VAL - B 206 VAL	R
	HIV-1 PROTEASE	1.20 A	4	A 47 ILE - A 267 ILE A 48 GLY - A 60 GLY A 49 GLY - A 59 GLY A 50 ILE - A 56 ILE	R
Amprenavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.70 A	3	A 47 ILE - B 267 ILE A 49 GLY - B 59 GLY A 50 ILE - B 56 ILE	R
	PROTEASE;PROTEASE	0.78 A	3	A 25 ASP - B 27 ASP A 27 GLY - B 53 GLY A 28 ALA - B 54 ALA	R
	PROTEASE	0.70 A	3	B 149 GLY - A 182 GLY B 150 ILE - A 183 ILE B 181 PRO - A 104 PRO	R
	PROTEASE;PROTEASE	0.63 A	3	A 47 ILE - B 19 ILE A 49 GLY - B 207 GLY A 50 VAL - B 206 VAL	R
Lopinavir	PROTEASE	0.69 A	3	B 47 ILE - B 267 ILE B 49 GLY - B 59 GLY	L

Supplementary Tables

				B 50 ILE - B 56 ILE	
	HIV-1 PROTEASE	0.92 A	3	A 48 GLY - B 259 GLY A 49 GLY - B 260 GLY A 50 ILE - B 265 ILE	R
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.70 A	3	A 47 ILE - B 267 ILE A 49 GLY - B 59 GLY A 50 ILE - B 56 ILE	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.74 A	3	B 25 ASP - B 27 ASP B 27 GLY - B 53 GLY B 28 ALA - B 54 ALA	R
Atazanavir	HIV-1 PROTEASE	0.83 A	3	B 47 ILE - A 267 ILE B 49 GLY - A 59 GLY B 50 ILE - A 56 ILE	L
	HIV-1 PROTEASE	0.83 A	3	A 47 ILE - B 19 ILE A 49 GLY - B 207 GLY A 50 VAL - B 206 VAL	R
Tipranavir	PROTEASE	0.61 A	3	A 47 ILE - B 19 ILE A 49 GLY - B 207 GLY A 50 VAL - B 206 VAL	R
	PROTEASE	0.94 A	3	A 47 ILE - A 211 ILE A 49 GLY - A 207 GLY A 50 VAL - A 206 VAL	R
	HIV-1 PROTEASE	0.59 A	3	A 47 ILE - B 267 ILE A 49 GLY - B 59 GLY A 50 ILE - B 56 ILE	L
	HIV-1 PROTEASE	0.75 A	3	B 25 ASP - B 27 ASP B 27 GLY - B 53 GLY B 28 ALA - B 54 ALA	R
	HIV-1 PROTEASE	0.90 A	3	B 25 ASP - A 159 ASP B 27 GLY - A 157 GLY B 28 ALA - A 158 ALA	R

Supplementary Tables

Supplementary Table 12. Possible binding sites of 3EOV against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Darunavir	GAG-POL POLYPROTEIN	1.38 A	4	B 123 LEU - B 47 LEU B 132 VAL - B 154 VAL B 182 VAL - B 29 VAL B 184 ILE - B 45 ILE	L
	HIV-1 PROTEASE	0.86 A	3	B 128 ALA - A 52 ALA B 130 ASP - A 51 ASP B 132 VAL - A 113 VAL	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.97 A	3	A 23 LEU - A 47 LEU A 32 VAL - A 154 VAL A 82 VAL - A 29 VAL	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.96 A	3	A 23 LEU - B 120 LEU A 32 VAL - B 117 VAL A 82 VAL - B 154 VAL	L
Ribavirin	RNA POLYMERASE	0.98 A	3	A 308 THR - B 56 THR A 309 THR - B 55 THR A 312 ASN - B 58 ASN	L
Saquinavir	PROTEASE;PROTEASE	0.56 A	3	A 8 ARG - A 78 ARG A 32 VAL - A 161 VAL A 80 THR - A 138 THR	L
Amprenavir	HIV-1 PROTEASE;HIV-1 PROTEASE	1.31 A	4	A 23 LEU - B 47 LEU A 32 VAL - B 154 VAL A 82 VAL - B 29 VAL A 84 ILE - B 45 ILE	L
	PROTEASE	0.84 A	3	B 23 LEU - B 47 LEU B 32 VAL - B 154 VAL B 84 ILE - B 45 ILE	R
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.87 A	3	C1041 GLN - B 133 GLN C1058 GLY - B 97 GLY C1137 GLY - B 131 GLY	R

Supplementary Tables

Supplementary Table 13. Possible binding sites of 3JCS against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.68 A	3	A 47 ILE - A 169 ILE A 48 GLY - A 131 GLY A 49 GLY - A 172 GLY	L
	POL POLYPROTEIN;POL POLYPROTEIN	0.73 A	3	A 47 ILE - m 54 ILE A 48 GLY - m 53 GLY A 49 GLY - m 66 GLY	L
	PROTEASE RETROPEPSIN	0.64 A	3	B 132 VAL - W 53 VAL B 181 PRO - W 98 PRO B 184 ILE - W 103 ILE	L
	PROTEASE RETROPEPSIN	0.64 A	3	B 147 ILE - c 99 ILE B 149 GLY - c 101 GLY B 150 ILE - c 102 ILE	L
Ritonavir	POL POLYPROTEIN;POL POLYPROTEIN	0.68 A	3	A 47 ILE - c 99 ILE A 49 GLY - c 101 GLY A 50 ILE - c 102 ILE	L
	PROTEASE	0.63 A	3	A 47 ILE - N 134 ILE A 49 GLY - N 132 GLY A 50 ILE - N 131 ILE	R
Darunavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.66 A	3	A 47 ILE - A 169 ILE A 49 GLY - A 167 GLY A 50 ILE - A 166 ILE	L
	PROTEASE (RETROPEPSIN);PROTEASE (RETROPEPSIN)	0.61 A	3	A 47 ILE - c 99 ILE A 49 GLY - c 101 GLY A 50 ILE - c 102 ILE	L
	POL POLYPROTEIN	0.84 A	4	B 123 LEU - Y 43 LEU B 181 PRO - Y 82 PRO B 182 VAL - Y 11 VAL B 184 ILE - Y 25 ILE	R
	GAG-POL POLYPROTEIN	1.49 A	4	B 123 LEU - G 271 LEU B 132 VAL - G 217 VAL B 182 VAL - G 237 VAL B 184 ILE - G 179 ILE	R
	GAG-POL POLYPROTEIN	1.45 A	4	B 123 LEU - H 29 LEU B 132 VAL - H 137 VAL B 182 VAL - H 53 VAL B 184 ILE - H 27 ILE	L
	GAG-POL POLYPROTEIN	0.90 A	4	B 123 LEU - M 116 LEU B 132 VAL - M 61 VAL B 182 VAL - M 135 VAL B 184 ILE - M 133 ILE	R
	HIV-1 PROTEASE	0.67 A	3	A 47 ILE - N 134 ILE A 49 GLY - N 132 GLY A 50 ILE - N 131 ILE	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.55 A	3	A 23 LEU - Z 11 LEU A 32 VAL - C 136 VAL A 82 VAL - C 244 VAL	L
Simeprevir	GENOME POLYPROTEIN	0.53 A	3	A 57 HIS - C 141 HIS A 58 GLY - C 140 GLY A 81 ASP - C 178 ASP	R
Ribavirin	RNA POLYMERASE	0.56 A	3	A 308 THR - E 72 THR A 309 THR - E 71 THR A 312 ASN - E 70 ASN	R
Saquinavir	PROTEIN (PROTEASE)	0.58 A	3	B 247 ILE - N 134 ILE B 249 GLY - N 132 GLY B 250 ILE - N 131 ILE	L
	HIV-1 PROTEASE	0.72 A	3	A 32 VAL - W 53 VAL A 81 PRO - W 98 PRO	L

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				A 84 ILE - W 103 ILE	
	PROTEASE;PROTEASE	0.60 A	3	A 47 ILE - c 99 ILE A 49 GLY - c 101 GLY A 50 ILE - c 102 ILE	L
	PROTEASE	0.54 A	3	A 80 THR - B 95 THR A 81 PRO - B 96 PRO A 82 VAL - B 97 VAL	R
	PROTEASE	0.96 A	4	A 24 LEU - Y 43 LEU A 82 PRO - Y 82 PRO A 83 VAL - Y 11 VAL A 85 ILE - Y 25 ILE	R
Lopinavir	HIV-1 PROTEASE	0.66 A	3	A 48 GLY - h 80 GLY A 49 GLY - h 81 GLY A 50 ILE - h 43 ILE	L
	HIV-1 PROTEASE	0.70 A	3	A 48 GLY - m 67 GLY A 49 GLY - m 53 GLY A 50 ILE - m 54 ILE	L
	PROTEASE	0.69 A	3	A 47 ILE - B 312 ILE A 49 GLY - B 291 GLY A 50 ILE - B 290 ILE	L
	PROTEASE	0.70 A	3	A 47 ILE - c 99 ILE A 49 GLY - c 101 GLY A 50 ILE - c 102 ILE	L
	PROTEASE	0.69 A	3	A 47 ILE - A 169 ILE A 49 GLY - A 167 GLY A 50 ILE - A 166 ILE	L
	PROTEASE;PROTEASE	0.56 A	3	A 32 VAL - W 53 VAL A 81 PRO - W 98 PRO A 84 ILE - W 103 ILE	L
	PROTEASE;PROTEASE	0.62 A	3	B 47 ILE - N 134 ILE B 49 GLY - N 132 GLY B 50 ILE - N 131 ILE	L
Nelfinavir	ASPARTYLPROTEASE	0.65 A	3	A 80 THR - B 95 THR A 81 PRO - B 96 PRO A 82 VAL - B 97 VAL	R
	PROTEASE RETROPEPSIN	0.63 A	3	A 47 ILE - N 134 ILE A 49 GLY - N 132 GLY A 50 ILE - N 131 ILE	R
Atazanavir	PROTEASE;PROTEASE	0.62 A	3	A 47 ILE - c 99 ILE A 49 GLY - c 101 GLY A 50 ILE - c 102 ILE	L
	PROTEASE	1.13 A	4	B 47 ILE - B 89 ILE B 48 VAL - B 90 VAL B 49 GLY - B 91 GLY B 50 ILE - B 102 ILE	L
	PROTEASE;PROTEASE	0.63 A	3	B 47 ILE - N 134 ILE B 49 GLY - N 132 GLY B 50 ILE - N 131 ILE	R
Tipranavir	HIV-1 PROTEASE	0.72 A	3	B 47 ILE - N 134 ILE B 49 GLY - N 132 GLY B 50 ILE - N 131 ILE	L
	PROTEASE	0.63 A	3	A 47 ILE - K 73 ILE A 49 GLY - K 83 GLY A 50 VAL - K 84 VAL	R
Amprenavir	PROTEASE	0.72 A	3	B 149 GLY - A 131 GLY B 150 ILE - A 169 ILE B 181 PRO - A 151 PRO	L
	PROTEASE;PROTEASE	0.70 A	3	A 47 ILE - A 169 ILE A 49 GLY - A 167 GLY A 50 ILE - A 166 ILE	L
	PROTEASE;PROTEASE	0.62 A	3	A 23 LEU - V 85 LEU A 32 VAL - V 113 VAL A 84 ILE - V 127 ILE	L
	PROTEASE	0.62 A	3	B 23 LEU - M 116 LEU B 32 VAL - M 61 VAL B 84 ILE - M 133 ILE	R
	PROTEASE;PROTEASE	1.17 A	4	A 23 LEU - M 116 LEU	L

				A 32 VAL - M 152 VAL A 82 VAL - M 135 VAL A 84 ILE - M 151 ILE	
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.37 A	4	A 23 LEU - H 29 LEU A 32 VAL - H 137 VAL A 82 VAL - H 53 VAL A 84 ILE - H 27 ILE	L
	PROTEASE;PROTEASE	0.66 A	3	A 47 ILE - c 99 ILE A 49 GLY - c 101 GLY A 50 ILE - c 102 ILE	L
	PROTEASE;PROTEASE	1.22 A	4	B 123 LEU - e 145 LEU B 132 VAL - e 142 VAL B 182 VAL - e 168 VAL B 184 VAL - e 144 VAL	R
	PROTEASE	1.43 A	4	B 23 LEU - a 32 LEU B 32 ILE - a 55 ILE B 82 ILE - a 48 ILE B 84 ILE - a 51 ILE	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.90 A	4	A 23 LEU - M 116 LEU A 32 VAL - M 61 VAL A 82 VAL - M 135 VAL A 84 ILE - M 133 ILE	R
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.52 A	3	A1132 ILE - H 25 ILE A1136 LYS - H 49 LYS A1137 GLY - H 48 GLY	R
	NS3 PROTEASE, NS4A PROTEIN	0.64 A	3	A1132 ILE - L 43 ILE A1136 LYS - L 47 LYS A1137 GLY - P 163 GLY	R

Supplementary Tables

Supplementary Table 14. Possible binding sites of 3QW4 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.83 A	3	A 47 ILE - B 201 ILE A 48 GLY - B 202 GLY A 49 GLY - B 205 GLY	R
	POL POLYPROTEIN;POL POLYPROTEIN	0.74 A	3	A 47 ILE - B 201 ILE A 48 GLY - B 206 GLY A 49 GLY - B 205 GLY	R
Atazanavir	HIV-1 PROTEASE	0.82 A	3	B 47 ILE - B 88 ILE B 49 GLY - C 200 GLY B 50 ILE - C 201 ILE	R
Saquinavir	PROTEASE;PROTEASE	0.72 A	3	B 147 ILE - B 88 ILE B 149 GLY - C 200 GLY B 150 ILE - C 201 ILE	L
	PROTEASE;PROTEASE	1.01 A	4	B 108 ARG - C 403 ARG B 123 LEU - C 373 LEU B 125 ASP - C 372 ASP B 128 ALA - C 325 ALA	R
	PROTEASE;PROTEASE	1.31 A	4	B 108 ARG - C 403 ARG B 123 LEU - C 373 LEU B 125 ASP - C 372 ASP B 128 ALA - C 326 ALA	L
Lopinavir	HIV-1 PROTEASE	1.47 A	4	A 32 VAL - B 227 VAL A 81 PRO - B 199 PRO A 82 VAL - B 198 VAL A 84 ILE - B 201 ILE	L
Darunavir	ASPARTYL PROTEASE;ASPARTYL PROTEASE	0.86 A	3	A 47 ILE - B 88 ILE A 49 GLY - C 200 GLY A 50 ILE - C 201 ILE	R
	PROTEASE	0.89 A	3	B 123 LEU - B 341 LEU B 132 ILE - B 369 ILE B 182 ILE - B 319 ILE	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.71 A	3	A 49 GLY - C 200 GLY A 50 ILE - C 201 ILE A 81 PRO - C 181 PRO	L
	FIV PROTEASE;FIV PROTEASE	0.81 A	3	B 33 ALA - C 129 ALA B 35 ILE - C 108 ILE B 37 VAL - C 80 VAL	R

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	FIV PROTEASE;FIV PROTEASE	0.90 A	3	B 33 ALA - C 110 ALA B 35 ILE - C 108 ILE B 37 VAL - C 130 VAL	L
Amprenavir	PROTEASE;PROTEASE	0.73 A	3	A 23 LEU - B 341 LEU A 32 VAL - B 368 VAL A 84 ILE - B 319 ILE	R
	PROTEASE;PROTEASE	0.51 A	3	A 23 LEU - B 81 LEU A 32 VAL - B 130 VAL A 84 ILE - B 108 ILE	L
	PROTEASE;PROTEASE	0.88 A	3	A 47 ILE - B 88 ILE A 49 GLY - C 200 GLY A 50 ILE - C 201 ILE	L
Ritonavir	PROTEASE;PROTEASE	0.74 A	3	B 47 ILE - B 88 ILE B 49 GLY - C 200 GLY B 50 ILE - C 201 ILE	L

Supplementary Tables

Supplementary Table 15. Possible binding sites of 3TBH against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.86 A	3	A 47 ILE - A 231 ILE A 48 GLY - A 186 GLY A 49 GLY - A 188 GLY	L
	POL POLYPROTEIN;POL POLYPROTEIN	0.54 A	3	A 47 ILE - B 5 ILE A 48 GLY - B 4 GLY A 49 GLY - B 2 GLY	R
	POL POLYPROTEIN;POL POLYPROTEIN	0.95 A	3	A 47 ILE - B 5 ILE A 48 GLY - B 4 GLY A 49 GLY - A 81 GLY	L
	POL POLYPROTEIN	0.82 A	3	B 47 ILE - A 19 ILE B 49 GLY - A 55 GLY B 50 ILE - A 58 ILE	R
	HIV-II PROTEASE;HIV-II PROTEASE	0.71 A	3	B 47 VAL - A 98 VAL B 49 GLY - A 91 GLY B 50 ILE - A 93 ILE	R
	PROTEASE RETROPEPSIN	0.76 A	3	B 147 ILE - A 182 ILE B 149 GLY - A 184 GLY B 150 ILE - A 231 ILE	L
Darunavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.87 A	3	A 49 GLY - A 186 GLY A 50 ILE - B 5 ILE A 81 PRO - A 212 PRO	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.90 A	3	A 49 GLY - A 186 GLY A 50 ILE - A 231 ILE A 81 PRO - A 301 PRO	L
	POL POLYPROTEIN	0.87 A	3	B 147 ILE - A 182 ILE B 149 GLY - A 184 GLY B 150 VAL - A 185 VAL	L
	GAG-POL POLYPROTEIN	1.36 A	4	B 123 LEU - A 87 LEU B 132 VAL - A 121 VAL B 182 VAL - A 98 VAL B 184 ILE - A 100 ILE	L
	HIV-1 PROTEASE	0.85 A	3	B 49 GLY - A 184 GLY B 50 ILE - A 231 ILE B 81 PRO - A 237 PRO	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.76 A	3	B 147 ILE - A 19 ILE B 149 GLY - A 55 GLY B 150 ILE - A 58 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.97 A	3	A 49 GLY - A 230 GLY A 50 ILE - A 231 ILE A 81 PRO - A 301 PRO	L
	FIV PROTEASE;FIV PROTEASE	0.93 A	3	B 33 ALA - A 281 ALA B 35 ILE - A 285 ILE B 37 VAL - A 208 VAL	R
Ritonavir	PROTEASE;PROTEASE	0.84 A	3	B 47 ILE – A 19 ILE B 49 GLY – A 55 GLY B 50 ILE – A 58 ILE	R
	GAG-POL POLYPROTEIN;GAG-POL POLYPROTEIN	0.81 A	3	A 47 ILE – A 228 ILE A 49 GLY – A 230 GLY A 50 ILE – B 5 ILE	R
	POL POLYPROTEIN;POL POLYPROTEIN	0.69 A	3	A 47 ILE - A 182 ILE A 49 GLY - A 184 GLY A 50 ILE - A 231 ILE	L
	PROTEASE;PROTEASE	0.93 A	3	B 47 ILE - A 228 ILE B 49 GLY - A 275 GLY B 50 ILE - A 300 ILE	R
Saquinavir	PROTEASE;PROTEASE	0.81 A	3	B 32 VAL - A 121 VAL B 81 PRO - A 103 PRO B 82 THR - A 124 THR	L

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	PROTEASE;PROTEASE	0.76 A	3	B 147 ILE - A 19 ILE B 149 GLY - A 55 GLY B 150 ILE - A 58 ILE	R
	PROTEASE E35D-SQV;PROTEASE E35D-SQV	0.84 A	3	B 47 ILE - A 182 ILE B 49 GLY - A 184 GLY B 50 ILE - A 231 ILE	L
	PROTEASE;PROTEASE	0.91 A	3	B 147 ILE - A 228 ILE B 149 GLY - A 275 GLY B 150 ILE - A 300 ILE	R
Amprenavir	PROTEASE;PROTEASE	0.87 A	3	A 47 ILE - A 19 ILE A 49 GLY - A 55 GLY A 50 ILE - A 58 ILE	R
	PROTEASE	0.93 A	3	B 23 LEU - A 87 LEU B 32 VAL - A 121 VAL B 84 ILE - A 100 ILE	R
	PROTEASE;PROTEASE	1.29 A	4	A 23 LEU - A 87 LEU A 32 VAL - A 121 VAL A 82 VAL - A 98 VAL A 84 ILE - A 100 ILE	L
	PROTEASE;PROTEASE	0.97 A	3	A 47 ILE - A 182 ILE A 49 GLY - A 184 GLY A 50 VAL - A 185 VAL	L
Lopinavir	PROTEASE;PROTEASE	0.96 A	3	B 47 ILE - A 19 ILE B 49 GLY - A 55 GLY B 50 ILE - A 58 ILE	L
	HIV-1 PROTEASE	0.85 A	3	A 48 GLY - B 4 GLY A 49 GLY - A 230 GLY A 50 ILE - A 231 ILE	L
	PROTEASE	0.78 A	3	B 47 ILE - A 182 ILE B 49 GLY - A 184 GLY B 50 ILE - A 231 ILE	L
	HIV-1 PROTEASE	0.97 A	3	A 48 GLY - A 188 GLY A 49 GLY - A 186 GLY A 50 ILE - A 231 ILE	L
	HIV-1 PROTEASE	0.90 A	3	A 48 GLY - B 2 GLY A 49 GLY - B 4 GLY A 50 ILE - B 5 ILE	R
Tipranavir	PROTEASE	0.94 A	3	A 47 ILE - A 182 ILE A 49 GLY - A 184 GLY A 50 VAL - A 185 VAL	L
	HIV-1 PROTEASE	0.72 A	3	A 47 ILE - A 182 ILE A 49 GLY - A 184 GLY A 50 ILE - A 231 ILE	R
	HIV-1 PROTEASE	0.95 A	3	A 47 ILE - A 228 ILE A 49 GLY - A 230 GLY A 50 ILE - B 5 ILE	L
	HIV-1 PROTEASE	0.90 A	3	A 47 ILE - A 19 ILE A 49 GLY - A 55 GLY A 50 ILE - A 58 ILE	R
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.85 A	3	A 47 ILE - A 182 ILE A 49 GLY - A 184 GLY A 50 ILE - A 231 ILE	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.93 A	3	A 47 ILE - A 19 ILE A 49 GLY - A 55 GLY A 50 ILE - A 58 ILE	L
	PROTEASE RETROPEPSIN	0.67 A	3	B 8 ARG - A 306 ARG B 23 LEU - A 113 LEU B 82 VAL - A 85 VAL	R

Supplementary Tables

Supplementary Table 16. Possible binding sites of 4MX2 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Darunavir	HIV-1 PROTEASE	0.65 A	3	B 49 GLY - C 414 GLY B 50 ILE - C 467 ILE B 81 PRO - C 202 PRO	R
Ritonavir	CYTOCHROME P450 3A4	0.67 A	3	A 108 PHE - C 145 PHE A 215 PHE - C 232 PHE A 481 GLY - C 234 GLY	R

Supplementary Tables

Supplementary Table 17. Possible binding sites of 4O2Z against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.86 A	3	A 47 ILE - A 60 ILE A 48 GLY - A 59 GLY A 49 GLY - A 56 GLY	L
	POL POLYPROTEIN;POL POLYPROTEIN	0.68 A	3	A 47 ILE - A 267 ILE A 48 GLY - A 268 GLY A 49 GLY - A 290 GLY	R
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.21 A	3	A 81 PRO - A 44 PRO A 82 VAL - A 43 VAL A 84 ILE - A 75 ILE	R
Atazanavir	PROTEASE;PROTEASE	1.10 A	3	B 81 PRO - A 44 PRO B 82 VAL - A 43 VAL B 84 ILE - A 75 ILE	R
Saquinavir	HIV-1 PROTEASE	0.72 A	3	A 32 VAL - A 211 VAL A 81 PRO - A 252 PRO A 84 ILE - A 212 ILE	R
	PROTEASE;PROTEASE	1.15 A	3	B 129 ASP - A 233 ASP B 148 GLY - A 162 GLY B 180 THR - A 345 THR	R
	HIV-1 PROTEASE	1.37 A	4	A 23 LEU - A 311 LEU A 81 PRO - A 299 PRO A 82 VAL - A 298 VAL A 84 ILE - A 294 ILE	L
	PROTEASE E35D-SQV;PROTEASE E35D-SQV	1.15 A	3	B 32 VAL - A 275 VAL B 81 PRO - A 270 PRO B 84 ILE - A 274 ILE	R
	PROTEASE;PROTEASE	0.64 A	3	B 32 VAL - A 275 VAL B 81 PRO - A 219 PRO B 84 ILE - A 274 ILE	L
Lopinavir	HIV-1 PROTEASE	1.11 A	3	A 48 GLY - A 290 GLY A 49 GLY - A 268 GLY A 50 ILE - A 263 ILE	R
	HIV-1 PROTEASE	1.00 A	3	A 48 GLY - A 290 GLY A 49 GLY - A 268 GLY A 50 ILE - A 267 ILE	R
	PROTEASE;PROTEASE	1.24 A	3	A 32 VAL - A 182 VAL A 81 PRO - A 131 PRO A 84 ILE - A 192 ILE	L
	PROTEASE;PROTEASE	0.96 A	3	A 32 VAL - A 275 VAL A 81 PRO - A 219 PRO A 84 ILE - A 274 ILE	L
	PROTEASE	1.15 A	3	A 47 ILE - A 234 ILE A 49 GLY - A 238 GLY A 50 ILE - A 240 ILE	L
Ritonavir	PROTEASE	1.23 A	3	A 8 ARG - A 174 ARG A 81 PRO - A 218 PRO A 82 VAL - A 232 VAL	R
Darunavir	PROTEASE	0.98 A	3	B 123 LEU - A 92 LEU B 125 ASP - A 96 ASP B 184 ILE - A 95 ILE	L
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.92 A	3	B 29 ASP - A 96 ASP B 80 THR - A 130 THR B 81 PRO - A 131 PRO	R
	PROTEASE RETROPEPSIN	1.17 A	3	B 29 ASP - A 371 ASP B 80 THR - A 130 THR B 81 PRO - A 131 PRO	R
Amprenavir	PROTEASE	1.06 A	3	B 23 LEU - A 163 LEU B 32 VAL - A 156 VAL B 84 ILE - A 159 ILE	L
	PROTEASE	1.07 A	3	B 23 LEU - A 292 LEU B 32 VAL - A 298 VAL B 84 ILE - A 294 ILE	L

Supplementary Tables

Supplementary Table 18. Possible binding sites of 4S1E against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	1.10 A	3	A 29 ASP - A 159 ASP A 81 PRO - A 81 PRO A 82 VAL - A 79 VAL	R
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.05 A	3	A 81 PRO - A 81 PRO A 82 VAL - A 79 VAL A 84 ILE - A 85 ILE	R
Darunavir	GAG-POL POLYPROTEIN	1.30 A	4	B 123 LEU - A 47 LEU B 132 VAL - A 154 VAL B 182 VAL - A 29 VAL B 184 ILE - A 45 ILE	L
	HIV-1 PROTEASE	1.00 A	3	B 128 ALA - A 52 ALA B 130 ASP - A 51 ASP B 132 VAL - A 113 VAL	R
Ribavirin	RNA POLYMERASE	1.00 A	3	A 308 THR - A 56 THR A 309 THR - A 55 THR A 312 ASN - A 58 ASN	L
Saquinavir	PROTEASE;PROTEASE	0.67 A	3	A 8 ARG - A 78 ARG A 32 VAL - A 161 VAL A 80 THR - A 138 THR	L
Atazanzvir	PROTEASE;PROTEASE	0.90 A	3	B 81 PRO - A 81 PRO B 82 VAL - A 79 VAL B 84 ILE - A 85 ILE	R
Amprenavir	PROTEASE	0.83 A	3	B 23 LEU - B 47 LEU B 32 VAL - B 154 VAL B 84 ILE - B 45 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.23 A	4	A 23 LEU - A 47 LEU A 32 VAL - A 154 VAL A 82 VAL - A 29 VAL A 84 ILE - A 45 ILE	L

Supplementary Tables

Supplementary Table 19. Possible binding sites of 4S1J against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	1.09 A	3	A 29 ASP - B 159 ASP A 81 PRO - B 81 PRO A 82 VAL - B 79 VAL	R
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.04 A	3	A 81 PRO - B 81 PRO A 82 VAL - B 79 VAL A 84 ILE - B 85 ILE	R
Darunavir	FIV PROTEASE;FIV PROTEASE	1.04 A	3	B 33 ALA - A 33 ALA B 35 ILE - A 164 ILE B 37 VAL - A 160 VAL	R
	GAG-POL POLYPROTEIN	1.34 A	4	B 123 LEU - A 47 LEU B 132 VAL - A 154 VAL B 182 VAL - A 29 VAL B 184 ILE - A 45 ILE	L
	HIV-1 PROTEASE	1.00 A	3	B 128 ALA - B 52 ALA B 130 ASP - B 51 ASP B 132 VAL - B 113 VAL	R
	FIV PROTEASE;FIV PROTEASE	0.90 A	3	B 33 ALA - B 33 ALA B 35 ILE - B 43 ILE B 37 VAL - B 160 VAL	R
	FIV PROTEASE;FIV PROTEASE	1.11 A	3	B 33 ALA - B 33 ALA B 35 ILE - B 35 ILE B 37 VAL - B 179 VAL	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.01 A	3	A 23 LEU - B 120 LEU A 32 VAL - B 117 VAL A 82 VAL - B 154 VAL	L
Ribavirin	RNA POLYMERASE	1.00 A	3	A 308 THR - B 56 THR A 309 THR - B 55 THR A 312 ASN - B 58 ASN	L
Saquinavir	PROTEASE	0.67 A	3	A 8 ARG - B 78 ARG A 32 VAL - B 161 VAL A 80 THR - B 138 THR	L
Atazanavir	PROTEASE;PROTEASE	0.87 A	3	B 81 PRO - B 81 PRO B 82 VAL - B 79 VAL B 84 ILE - B 85 ILE	R
Amprenavir	PROTEASE	0.84 A	3	B 23 LEU - B 47 LEU B 32 VAL - B 154 VAL B 84 ILE - B 45 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.27 A	4	A 23 LEU - A 47 LEU A 32 VAL - A 154 VAL A 82 VAL - A 29 VAL A 84 ILE - A 45 ILE	L
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.89 A	3	C1041 GLN - A 133 GLN C1058 GLY - A 97 GLY C1137 GLY - A 131 GLY	R

Supplementary Tables

Supplementary Table 20. Possible binding sites of 5C4Q against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.83 A	3	C1057 HIS - B 12 HIS C1078 VAL - B 72 VAL C1081 ASP - B 69 ASP	L
Amprenavir	HIV-1 PROTEASE	1.14 A	3	B 129 ASP - B 27 ASP B 176 LEU - B 80 LEU B 182 VAL - B 72 VAL	L
	HIV-1 PROTEASE	1.19 A	3	B 129 ASP - B 75 ASP B 176 LEU - B 54 LEU B 182 VAL - B 36 VAL	L
	HIV-1 PROTEASE	1.03 A	3	B 129 ASP - A 27 ASP B 176 LEU - A 107 LEU B 182 VAL - A 72 VAL	L
	HIV-1 PROTEASE	1.36 A	3	B 129 ASP - B 53 ASP B 176 LEU - B 78 LEU B 182 VAL - B 47 VAL	R

Supplementary Tables

Supplementary Table 21. Possible binding sites of 5CFK against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Darunavir	HIV-1 PROTEASE	0.68 A	3	B 49 GLY - F 127 GLY B 50 ILE - F 128 ILE B 81 PRO - F 234 PRO	L
	PROTEASE;PROTEASE	0.77 A	3	B 47 VAL - F 225 VAL B 49 GLY - F 240 GLY B 50 ILE - F 241 ILE	L
	WILD-TYPE HIV-1 PROTEASE DIMER	0.77 A	3	B 23 LEU - E 75 LEU B 32 VAL - E 23 VAL B 82 VAL - E 16 VAL	L
Amprenavir	PROTEASE;PROTEASE	1.30 A	4	A 23 LEU - E 22 LEU A 32 VAL - E 16 VAL A 82 VAL - E 23 VAL A 84 ILE - E 19 ILE	L
	PROTEASE	0.82 A	3	B 149 GLY - F 127 GLY B 150 ILE - F 128 ILE B 181 PRO - F 234 PRO	R
	PROTEASE	0.82 A	3	B 23 LEU - A 247 LEU B 32 VAL - A 244 VAL B 84 ILE - A 241 ILE	R
	PROTEASE	0.71 A	3	B 147 VAL - F 225 VAL B 149 GLY - F 240 GLY B 150 ILE - F 241 ILE	L

Supplementary Tables

Supplementary Table 22. Possible binding sites of 5CX2 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Darunavir	PROTEASE	0.61 A	3	B 123 LEU - B 472 LEU B 132 ILE - C 510 ILE B 182 ILE - C 507 ILE	L
Amprenavir	PROTEASE;PROTEASE	1.32 A	3	A 23 LEU - C 475 LEU A 32 VAL - A 479 VAL A 84 ILE - D 507 ILE	R
	PROTEASE	1.46 A	3	B 23 LEU - B 472 LEU B 32 VAL - A 503 VAL B 84 ILE - A 507 ILE	R

Supplementary Tables

Supplementary Table 23. Possible binding sites of 5FEA against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	**Known similar target**	**RMSD**	**No. of binding residues**	**3D-interface residues**	**Superposition type**
Saquinavir	PROTEASE	1.17 A	3	A 8 ARG - B 37 ARG A 32 VAL - B 46 VAL A 80 THR - B 42 THR	L
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.17 A	3	B 29 ASP - A 95 ASP B 30 ASN - A 96 ASN B 80 THR - B 42 THR	L
Amprenavir	PROTEASE;PROTEASE	1.46 A	3	A 23 LEU - B 94 LEU A 32 VAL - A 46 VAL A 84 ILE - B 97 ILE	R
	HIV-1 PROTEASE	1.16 A	3	B 129 ASP - B 112 ASP B 176 LEU - B 90 LEU B 182 VAL - A 70 VAL	L

Supplementary Tables

Supplementary Table 24. Possible binding sites of 5OSG against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	1.05 A	3	A 29 ASP - h 106 ASP A 81 PRO - h 122 PRO A 82 VAL - h 121 VAL	R
Saquinavir	PROTEASE;PROTEASE	0.86 A	3	B 129 ASP - h 69 ASP B 148 GLY - h 65 GLY B 180 THR - h 117 THR	L
Darunavir	ASPARTYL PROTEASE	1.29 A	3	B 23 LEU - h 107 LEU B 32 VAL - h 121 VAL B 82 VAL - h 59 VAL	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.10 A	3	A 23 LEU - h 200 LEU A 32 VAL - h 187 VAL A 82 VAL - h 202 VAL	L
	ASPARTYL PROTEASE	1.32 A	3	B 23 LEU - h 119 LEU B 32 VAL - h 57 VAL B 82 VAL - h 121 VAL	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.23 A	3	A 23 LEU - h 156 LEU A 32 VAL - h 160 VAL A 82 VAL - h 153 VAL	R
	WILD-TYPE HIV-1 PROTEASE DIMER	0.99 A	3	B 23 LEU - h 107 LEU B 32 VAL - h 121 VAL B 82 VAL - h 118 VAL	L
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	1.16 A	3	A1123 ARG - P 224 ARG A1157 ALA - P 222 ALA A1159 SER - P 218 SER	R

Supplementary Tables

Supplementary Table 25. Possible binding sites of 5TCK against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Nevirapine	HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT	1.20 A	3	A 179 VAL - A 230 VAL A 181 TYR - A 223 TYR A 188 TYR - A 222 TYR	L
Rilpivirine	REVERSE TRANSCRIPTASE/RIBONU CLEAS E H	1.24 A	3	A 179 VAL - A 230 VAL A 181 TYR - A 223 TYR A 188 TYR - A 222 TYR	L
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	1.24 A	3	A 8 ARG - A 290 ARG A 23 LEU - A 283 LEU A 25 ASP - A 280 ASP	L
Darunavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.67 A	3	B 125 ASP - B 279 ASP B 127 GLY - B 295 GLY B 128 ALA - B 296 ALA	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.15 A	3	A 23 LEU - B 283 LEU A 32 VAL - B 278 VAL A 82 VAL - B 235 VAL	R
Saquinavir	PROTEASE	1.18 A	3	A 8 ARG - B 241 ARG A 32 VAL - B 171 VAL A 80 THR - B 167 THR	R
	PROTEASE;PROTEASE	1.26 A	3	B 8 ARG - B 290 ARG B 23 LEU - B 283 LEU B 25 ASP - B 280 ASP	L
	PROTEASE;PROTEASE	0.64 A	3	B 25 ASP - B 279 ASP B 27 GLY - B 295 GLY B 28 ALA - B 296 ALA	R
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.65 A	3	B 25 ASP - B 279 ASP B 27 GLY - B 295 GLY B 28 ALA - B 296 ALA	R
Tipranavir	HIV-1 PROTEASE	0.63 A	3	B 25 ASP - B 279 ASP B 27 GLY - B 295 GLY B 28 ALA - B 296 ALA	R
Amprenavir	PROTEASE;PROTEASE	0.69 A	3	A 25 ASP - B 279 ASP A 27 GLY - B 295 GLY A 28 ALA - B 296 ALA	R
	HIV-1 PROTEASE	1.04 A	3	B 129 ASP - B 245 ASP B 176 LEU - B 177 LEU B 182 VAL - B 188 VAL	L
	HIV-1 PROTEASE	1.04 A	3	B 129 ASP - A 245 ASP B 176 LEU - A 211 LEU B 182 VAL - A 190 VAL	L
	HIV-1 PROTEASE	1.06 A	3	B 129 ASP - B 182 ASP B 176 LEU - B 211 LEU B 182 VAL - B 190 VAL	L
	HIV-1 PROTEASE	1.48 A	3	B 129 ASP - A 233 ASP B 176 LEU - A 289 LEU B 182 VAL - A 278 VAL	L

Supplementary Tables

Supplementary Table 26. Possible binding sites of 5TCM against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Ritonavir	POL POLYPROTEIN;POL POLYPROTEIN	0.97 A	3	A 25 ASP - A 18 ASP A 28 ALA - A 27 ALA A 29 ASP - A 50 ASP	R
Lopinavir	PROTEASE	1.07 A	3	A 25 ASP - C 18 ASP A 28 ALA - C 27 ALA A 29 ASP - C 50 ASP	R
Saquinavir	PROTEASE;PROTEASE	1.09 A	3	B 8 ARG - B 47 ARG B 23 LEU - B 78 LEU B 25 ASP - B 75 ASP	R
Atazanavir	PROTEASE	1.11 A	3	A 25 ASP - A 18 ASP A 28 ALA - A 27 ALA A 29 ASP - A 50 ASP	R
Amprenavir	HIV-1 PROTEASE	1.07 A	3	B 129 ASP - A 22 ASP B 176 LEU - A 51 LEU B 182 VAL - A 30 VAL	L
	HIV-1 PROTEASE	1.24 A	3	B 129 ASP - A 75 ASP B 176 LEU - A 51 LEU B 182 VAL - A 30 VAL	L

Supplementary Tables

Supplementary Table 27. Possible binding sites of 5USF against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.76 A	3	A 47 ILE - B 499 ILE A 48 GLY - B 496 GLY A 49 GLY - B 134 GLY	L
	POL POLYPROTEIN;POL POLYPROTEIN	0.68 A	3	A 29 ASP - B 236 ASP A 81 PRO - B 274 PRO A 82 VAL - B 275 VAL	L
	PROTEIN (PROTEASE);PROTEIN (PROTEASE)	0.77 A	3	A 47 ILE - A 89 ILE A 49 GLY - A 93 GLY A 50 ILE - A 97 ILE	L
	PROTEASE	0.73 A	3	A 39 VAL - A 68 VAL A 91 LEU - A 111 LEU A 98 TRP - A 70 TRP	R
Ritonavir	POL POLYPROTEIN	0.61 A	3	B 47 ILE - B 89 ILE B 49 GLY - B 93 GLY B 50 ILE - B 97 ILE	L
Darunavir	HIV-1 PROTEASE	0.63 A	3	A 47 ILE - B 89 ILE A 49 GLY - B 93 GLY A 50 ILE - B 97 ILE	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.67 A	3	B 125 ASP - A 263 ASP B 127 GLY - A 264 GLY B 128 ALA - A 265 ALA	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.47 A	3	A 49 GLY - B 474 GLY A 50 ILE - B 475 ILE A 81 PRO - B 368 PRO	R
	PROTEASE	0.75 A	3	B 123 LEU - A 86 LEU B 132 ILE - A 91 ILE B 182 ILE - A 89 ILE	L
Saquinavir	PROTEASE;PROTEASE	0.69 A	3	B 25 ASP - A 263 ASP B 27 GLY - A 264 GLY B 28 ALA - A 265 ALA	L
	PROTEASE;PROTEASE	0.63 A	3	B 147 ILE - B 89 ILE B 149 GLY - B 93 GLY B 150 ILE - B 97 ILE	R
	HIV-1 PROTEASE	1.43 A	4	A 23 LEU - A 208 LEU A 81 PRO - A 205 PRO A 82 VAL - A 206 VAL A 84 ILE - A 178 ILE	L
	HIV-1 PROTEASE	1.43 A	4	A 23 LEU - A 322 LEU A 81 PRO - A 274 PRO A 82 VAL - A 275 VAL A 84 ILE - A 245 ILE	R
	PROTEASE;PROTEASE	1.00 A	4	B 28 ALA - B 72 ALA B 47 ILE - B 89 ILE B 49 GLY - B 93 GLY B 50 ILE - B 97 ILE	R
Nelfinavir	ASPARTYLPROTEASE;ASPARTYL PROTEASE	1.46 A	4	B 23 LEU - B 86 LEU B 25 ASP - B 73 ASP B 32 VAL - B 92 VAL B 84 ILE - B 89 ILE	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.69 A	3	B 25 ASP - A 263 ASP B 27 GLY - A 264 GLY B 28 ALA - A 265 ALA	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.67 A	3	A 47 ILE - B 89 ILE A 49 GLY - B 93 GLY A 50 ILE - B 97 ILE	L
Atazanavir	PROTEASE;PROTEASE	0.70 A	3	B 47 ILE - A 89 ILE B 49 GLY - A 93 GLY B 50 ILE - A 97 ILE	L

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Lopinavir	PROTEASE;PROTEASE	0.63 A	3	B 47 ILE - A 89 ILE B 49 GLY - A 93 GLY B 50 ILE - A 97 ILE	L
	HIV-1 PROTEASE	0.52 A	3	A 48 GLY - A 496 GLY A 49 GLY - A 134 GLY A 50 ILE - A 133 ILE	L
Amprenavir	PROTEASE;PROTEASE	0.67 A	3	A 25 ASP - A 263 ASP A 27 GLY - A 264 GLY A 28 ALA - A 265 ALA	L
	PROTEASE	0.47 A	3	B 149 GLY - B 474 GLY B 150 ILE - B 475 ILE B 181 PRO - B 368 PRO	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.71 A	3	A 47 ILE - B 89 ILE A 49 GLY - B 93 GLY A 50 ILE - B 97 ILE	L
Tipranavir	HIV-1 PROTEASE	0.61 A	3	B 47 ILE - A 89 ILE B 49 GLY - A 93 GLY B 50 ILE - A 97 ILE	L

Supplementary Tables

Supplementary Table 28. Possible binding sites of 5ZWY against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Darunavir	POL POLYPROTEIN	1.01 A	3	B 147 ILE - A 122 ILE B 149 GLY - B 39 GLY B 150 VAL - B 38 VAL	R
	HIV-1 PROTEASE	1.02 A	3	B 49 GLY - B 22 GLY B 50 ILE - B 161 ILE B 81 PRO - B 186 PRO	R
Saquinavir	PROTEASE;PROTEASE	0.78 A	3	B 129 ASP - B 241 ASP B 148 GLY - B 238 GLY B 180 THR - B 217 THR	R
	HIV-1 PROTEASE	0.98 A	3	A 47 ILE - A 122 ILE A 49 GLY - B 39 GLY A 50 VAL - B 38 VAL	R
	PROTEASE	0.77 A	3	A 80 THR - B 165 THR A 81 PRO - B 134 PRO A 82 THR - B 133 THR	R
Tipranavir	PROTEASE	0.87 A	3	A 47 ILE - B 122 ILE A 49 GLY - A 39 GLY A 50 VAL - A 38 VAL	R
Lopinavir	HIV-1 PROTEASE	1.04 A	3	A 48 GLY - B 79 GLY A 49 GLY - B 81 GLY A 50 ILE - B 85 ILE	R
Amprenavir	PROTEASE;PROTEASE	0.90 A	3	A 47 ILE - A 122 ILE A 49 GLY - B 39 GLY A 50 VAL - B 38 VAL	R
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.98 A	3	C1041 GLN - A 158 GLN C1058 GLY - A 55 GLY C1137 GLY - A 282 GLY	R
	NS3 PROTEASE, NS4A PROTEIN	0.75 A	3	C1041 GLN - B 315 GLN C1058 GLY - B 52 GLY C1137 GLY - B 275 GLY	L
	NS3 PROTEASE, NS4A PROTEIN	0.74 A	3	C1041 GLN - B 315 GLN C1058 GLY - B 52 GLY C1137 GLY - B 313 GLY	R
	NS3 PROTEASE, NS4A PROTEIN	0.93 A	3	C1041 GLN - B 58 GLN C1058 GLY - B 282 GLY C1137 GLY - B 275 GLY	R
	NS3 PROTEASE, NS4A PROTEIN	0.76 A	3	C1041 GLN - A 158 GLN C1058 GLY - A 22 GLY C1137 GLY - A 53 GLY	R

Supplementary Tables

Supplementary Table 29. Possible binding sites of 6ADO against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	**Known similar target**	**RMSD**	**No. of binding residues**	**3D-interface residues**	**Superposition type**
Darunavir	PROTEASE	0.95 A	3	B 123 LEU - A 472 LEU B 132 ILE - A 465 ILE B 182 ILE - B 510 ILE	R
Saquinavir	PROTEASE;PROTEASE	1.42 A	3	B 8 ARG - B 471 ARG B 23 LEU - B 475 LEU B 25 ASP - A 506 ASP	R
Amprenavir	PROTEASE	1.22 A	3	B 23 LEU - C 472 LEU B 32 VAL - B 503 VAL B 84 ILE - B 507 ILE	L

Supplementary Tables

Supplementary Table 30. Possible binding sites of 6ADZ against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Nelfinavir	PROTEASE RETROPEPSIN	0.92 A	3	B 8 ARG - C 471 ARG B 23 LEU - C 475 LEU B 82 VAL - D 503 VAL	R

Supplementary Tables

Supplementary Table 31. Possible binding sites of 6AH6 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Amprenavir	PROTEASE;PROTEASE	1.33 A	3	A 23 LEU - C 475 LEU A 32 VAL - A 479 VAL A 84 ILE - D 507 ILE	L
	PROTEASE	1.31 A	3	B 23 LEU - B 472 LEU B 32 VAL - A 503 VAL B 84 ILE - A 507 ILE	R

Supplementary Tables

Supplementary Table 32. Possible binding sites of 6AZ1 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Saquinavir	HIV-1 PROTEASE	0.57 A	3	A 32 VAL - H 164 VAL A 81 PRO - H 94 PRO A 84 ILE - H 163 ILE	L
	PROTEASE	0.95 A	4	A 23 LEU - E 232 LEU A 81 PRO - E 237 PRO A 82 VAL - E 236 VAL A 84 VAL - E 234 VAL	R
	PROTEASE;PROTEASE	1.05 A	4	B 28 ALA - L 57 ALA B 47 ILE - L 71 ILE B 49 GLY - L 94 GLY B 50 ILE - L 96 ILE	L
	PROTEASE;PROTEASE	0.68 A	3	B 25 ASP - G 38 ASP B 27 GLY - G 39 GLY B 28 ALA - G 40 ALA	R
	PROTEASE;PROTEASE	0.54 A	3	B 25 ASP - E 85 ASP B 27 GLY - E 82 GLY B 28 ALA - E 81 ALA	L
Lopinavir	PROTEASE	0.59 A	3	B 47 ILE - g 283 ILE B 49 GLY - g 297 GLY B 50 ILE - g 303 ILE	R
	PROTEASE	0.61 A	3	A 47 ILE - E 192 ILE A 49 GLY - E 190 GLY A 50 ILE - E 189 ILE	R
	HIV-1 PROTEASE	0.71 A	3	A 48 GLY - g 213 GLY A 49 GLY - g 212 GLY A 50 ILE - g 241 ILE	L
Darunavir	GAG-POL POLYPROTEIN	1.30 A	4	B 123 LEU - P 91 LEU B 132 VAL - P 125 VAL B 182 VAL - P 85 VAL B 184 ILE - P 94 ILE	L
	GAG-POL POLYPROTEIN	0.93 A	4	B 123 LEU - P 130 LEU B 132 VAL - P 102 VAL B 182 VAL - P 125 VAL B 184 ILE - P 122 ILE	R
	GAG-POL POLYPROTEIN	1.37 A	4	B 123 LEU - T 88 LEU B 132 VAL - T 118 VAL B 182 VAL - T 92 VAL B 184 ILE - T 122 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.52 A	3	B 125 ASP - E 85 ASP B 127 GLY - E 82 GLY B 128 ALA - E 81 ALA	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.69 A	3	B 125 ASP - G 38 ASP B 127 GLY - G 39 GLY B 128 ALA - G 40 ALA	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.66 A	3	B 147 ILE - L 71 ILE B 149 GLY - L 94 GLY B 150 ILE - L 96 ILE	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.69 A	3	B 147 ILE - g 283 ILE B 149 GLY - g 297 GLY B 150 ILE - g 303 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.68 A	3	B 147 ILE - E 192 ILE B 149 GLY - E 190 GLY B 150 ILE - E 189 ILE	R
	PROTEASE (RETROPEPSIN);PROTEASE (RETROPEPSIN)	0.53 A	3	A 25 ASN - g 135 ASN A 27 GLY - g 138 GLY A 28 ALA - g 137 ALA	L
	HIV-1 PROTEASE	0.68 A	3	B 128 ALA - H 186 ALA B 130 ASP - H 110 ASP	L

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				B 132 VAL - H 125 VAL	
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.21 A	4	B 8 ARG - J 78 ARG B 23 LEU - J 126 LEU B 82 VAL - J 33 VAL B 84 ILE - J 110 ILE	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.55 A	3	B 25 ASP - E 85 ASP B 27 GLY - E 82 GLY B 28 ALA - E 81 ALA	L
Amprenavir	PROTEASE;PROTEASE	0.53 A	3	A 25 ASP - E 85 ASP A 27 GLY - E 82 GLY A 28 ALA - E 81 ALA	L
	PROTEASE;PROTEASE	0.68 A	3	A 25 ASP - G 38 ASP A 27 GLY - G 39 GLY A 28 ALA - G 40 ALA	R
	PROTEASE;PROTEASE	1.09 A	4	A 23 LEU - U 122 LEU A 32 VAL - U 90 VAL A 82 VAL - U 124 VAL A 84 ILE - U 101 ILE	L
	PROTEASE;PROTEASE	0.71 A	3	A 47 ILE - F 142 ILE A 49 GLY - F 126 GLY A 50 ILE - F 125 ILE	L
	PROTEASE;PROTEASE	0.72 A	4	B 123 LEU - K 78 LEU B 132 VAL - K 184 VAL B 182 VAL - K 102 VAL B 184 VAL - K 104 VAL	R
	PROTEASE	0.72 A	3	B 23 LEU - U 122 LEU B 32 VAL - U 90 VAL B 84 ILE - U 101 ILE	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.87 A	4	A 23 LEU - P 130 LEU A 32 VAL - P 102 VAL A 82 VAL - P 125 VAL A 84 ILE - P 122 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.37 A	4	A 23 LEU - T 88 LEU A 32 VAL - T 118 VAL A 82 VAL - T 92 VAL A 84 ILE - T 122 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.33 A	4	A 23 LEU - P 91 LEU A 32 VAL - P 125 VAL A 82 VAL - P 85 VAL A 84 ILE - P 94 ILE	L
Tipranavir	HIV-1 PROTEASE	0.69 A	3	A 47 ILE - g 283 ILE A 49 GLY - g 297 GLY A 50 ILE - g 303 ILE	L
	HIV-1 PROTEASE	0.48 A	3	B 25 ASP - E 85 ASP B 27 GLY - E 82 GLY B 28 ALA - E 81 ALA	L
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.57 A	3	A1123 ARG - C 172 ARG A1157 ALA - C 99 ALA A1159 SER - C 34 SER	L
	NS3 PROTEASE, NS4A PROTEIN	0.71 A	3	C1041 GLN - J 98 GLN C1058 GLY - F 157 GLY C1137 GLY - F 154 GLY	L
Indinavir	POL POLYPROTEIN	0.56 A	3	B 47 ILE - g 283 ILE B 49 GLY - g 297 GLY B 50 ILE - g 303 ILE	R
Ritonavir	POL POLYPROTEIN;POL POLYPROTEIN	0.62 A	3	A 47 ILE - g 283 ILE A 49 GLY - g 297 GLY A 50 ILE - g 303 ILE	R
Simeprevir	GENOME POLYPROTEIN	0.58 A	3	A 57 HIS - g 64 HIS A 58 GLY - g 63 GLY A 81 ASP - g 86 ASP	R
	GENOME POLYPROTEIN	0.56 A	3	A 57 HIS - g 149 HIS A 58 GLY - g 148 GLY A 81 ASP - g 173 ASP	R

Supplementary Tables

Supplementary Table 33. Possible binding sites of 6BYA against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Ritonavir	POL POLYPROTEIN;POL POLYPROTEIN	1.00 A	3	A 25 ASP - D 21 ASP A 28 ALA - D 30 ALA A 29 ASP - D 53 ASP	R
Lopinavir	PROTEASE	1.09 A	3	A 25 ASP - D 21 ASP A 28 ALA - D 30 ALA A 29 ASP - D 53 ASP	R
Saquinavir	PROTEASE;PROTEASE	1.11 A	3	B 8 ARG - C 50 ARG B 23 LEU - C 81 LEU B 25 ASP - C 78 ASP	R
Atazanavir	PROTEASE	1.13 A	3	A 25 ASP - D 21 ASP A 28 ALA - D 30 ALA A 29 ASP - D 53 ASP	R

Supplementary Tables

Supplementary Table 34. Possible binding sites of 6ICR against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD-Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Amprenavir	PROTEASE	1.39 A	3	B 23 LEU - C 472 LEU B 32 VAL - A 503 VAL B 84 ILE - A 507 ILE	R
	PROTEASE;PROTEASE	1.37 A	3	A 23 LEU - C 475 LEU A 32 VAL - B 479 VAL A 84 ILE - A 507 ILE	R

Supplementary Tables

Supplementary Table 35. Possible binding sites of 6K90 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Saquinavir	PROTEASE;PROTEASE	0.93 A	3	B 129 ASP - B 77 ASP B 148 GLY - A 17 GLY B 180 THR - A 283 THR	L
	ENDOTHIAPEPSIN	0.82 A	3	A 35 ASP - A 231 ASP A 80 GLY - A 17 GLY A 222 THR - A 227 THR	R
Darunavir	PROTEASE (RETROPEPSIN);PROTEASE (RETROPEPSIN)	0.95 A	3	A 25 ASN - B 72 ASN A 27 GLY - B 68 GLY A 28 ALA - B 71 ALA	R
	PROTEASE	0.93 A	3	B 123 LEU - B 69 LEU B 132 ILE - A 52 ILE B 182 ILE - B 65 ILE	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.98 A	3	A 23 LEU - B 82 LEU A 32 VAL - B 115 VAL A 82 VAL - B 7 VAL	L
	ASPARTYL PROTEASE	0.89 A	3	B 23 LEU - B 257 LEU B 32 VAL - B 295 VAL B 82 VAL - B 256 VAL	R
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	1.25 A	4	A1057 HIS - B 16 HIS A1058 GLY - B 17 GLY A1078 VAL - A 35 VAL A1081 ASP - A 36 ASP	R
Tipranavir	HIV-1 PROTEASE	0.83 A	3	B 25 ASP - B 231 ASP B 27 GLY - B 20 GLY B 28 ALA - B 23 ALA	R
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.71 A	3	A 47 ILE - A 265 ILE A 48 GLY - A 269 GLY A 49 GLY - A 268 GLY	R
	POL POLYPROTEIN;POL POLYPROTEIN	0.95 A	3	A 29 ASP - B 36 ASP A 81 PRO - A 50 PRO A 82 VAL - A 51 VAL	R
Simeprevir	GENOME POLYPROTEIN	0.67 A	3	A 57 HIS - B 16 HIS A 58 GLY - B 17 GLY A 81 ASP - A 36 ASP	L
Dolutegravir	PFV INTEGRASE	0.85 A	3	A 128 ASP - B 119 ASP A 185 ASP - B 231 ASP A 187 GLY - B 20 GLY	L

Supplementary Tables

Supplementary Table 36. Possible binding sites of 6L2B against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Darunavir	GAG-POL POLYPROTEIN	1.43 A	4	B 123 LEU - A 47 LEU B 132 VAL - A 154 VAL B 182 VAL - A 29 VAL B 184 ILE - A 45 ILE	L
	HIV-1 PROTEASE	0.97 A	3	B 128 ALA - A 52 ALA B 130 ASP - A 51 ASP B 132 VAL - A 113 VAL	R
Ribavirin	RNA POLYMERASE	1.00 A	3	A 308 THR - A 56 THR A 309 THR - A 55 THR A 312 ASN - A 58 ASN	L
Saquinavir	PROTEASE	0.71 A	3	A 8 ARG - A 78 ARG A 32 VAL - A 161 VAL A 80 THR - A 138 THR	L
	PROTEASE	1.18 A	3	A 8 ARG - A 42 ARG A 23 LEU - A 187 LEU A 80 THR - A 64 THR	L
Amprenavir	PROTEASE	0.89 A	3	B 23 LEU - A 47 LEU B 32 VAL - A 154 VAL B 84 ILE - A 45 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.36 A	4	A 23 LEU - A 47 LEU A 32 VAL - A 154 VAL A 82 VAL - A 29 VAL A 84 ILE - A 45 ILE	L

Supplementary Tables

Supplementary Table 37. Possible binding sites of 6L6O against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Ritonavir	GAG-POL POLYPROTEIN;GAG-POL POLYPROTEIN	0.96 A	3	A 47 ILE - A 121 ILE A 49 GLY - A 88 GLY A 50 ILE - A 16 ILE	R
Indinavir	HIV-II PROTEASE	0.78 A	3	A 47 VAL - A 17 VAL A 49 GLY - A 88 GLY A 50 ILE - A 120 ILE	L
Darunavir	PROTEASE	0.96 A	3	B 147 VAL - A 17 VAL B 149 GLY - A 88 GLY B 150 ILE - A 120 ILE	L
	FIV PROTEASE;FIV PROTEASE	1.20 A	3	B 33 ALA - A 156 ALA B 35 ILE - A 29 ILE B 37 VAL - A 124 VAL	R
Amprenavir	PROTEASE;PROTEASE	1.16 A	3	A 47 ILE - A 29 ILE A 49 GLY - A 125 GLY A 50 ILE - A 95 ILE	L
	PROTEASE	0.95 A	3	B 147 VAL - A 17 VAL B 149 GLY - A 88 GLY B 150 ILE - A 120 ILE	L
Tipranavir	HIV-1 PROTEASE;HIV-1 PROTEASE	1.09 A	3	B 8 ARG - A 60 ARG B 23 LEU - A 62 LEU B 82 THR - A 12 THR	L
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.84 A	3	A1123 ARG - A 60 ARG A1157 ALA - A 11 ALA A1159 SER - A 13 SER	R

Supplementary Tables

Supplementary Table 38. Possible binding sites of 6TCZ against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.29 A	3	A 47 ILE - d 133 ILE A 48 GLY - d 134 GLY A 49 GLY - d 135 GLY	R
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.36 A	4	A 47 ILE - h 187 ILE A 48 GLY - h 185 GLY A 49 GLY - h 183 GLY A 50 ILE - h 57 ILE	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.47 A	4	A 47 ILE - i 161 ILE A 48 GLY - i 159 GLY A 49 GLY - i 157 GLY A 50 ILE - i 32 ILE	L
	POL POLYPROTEIN	1.33 A	4	B 47 ILE - c 170 ILE B 49 GLY - c 84 GLY B 50 VAL - c 85 VAL B 81 PRO - c 158 PRO	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.93 A	4	A 25 ASP - D 165 ASP A 28 ALA - D 160 ALA A 81 PRO - E 155 PRO A 84 ILE - D 169 ILE	R
Darunavir	POL POLYPROTEIN;POL POLYPROTEIN	1.42 A	4	A 8 ARG - D 233 ARG A 23 LEU - D 194 LEU A 82 VAL - D 229 VAL A 84 ILE - D 190 ILE	L
	GAG-POL POLYPROTEIN	1.31 A	4	B 123 LEU - G 165 LEU B 132 VAL - G 48 VAL B 182 VAL - G 163 VAL B 184 ILE - G 137 ILE	R
	HIV-1 PROTEASE	0.50 A	3	B 49 GLY - c 79 GLY B 50 ILE - c 78 ILE B 81 PRO - c 244 PRO	L
Saquinavir	PROTEASE;PROTEASE	1.30 A	4	B 28 ALA - j 15 ALA B 47 ILE - j 112 ILE B 49 GLY - j 110 GLY B 50 ILE - j 109 ILE	R
	HIV-1 PROTEASE	1.43 A	4	A 47 ILE - H 187 ILE A 48 GLY - H 185 GLY A 49 GLY - H 183 GLY A 50 ILE - H 57 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	1.49 A	4	B 27 GLY - F 241 GLY B 29 ASP - F 245 ASP B 48 GLY - E 260 GLY B 80 THR - E 263 THR	L
	PROTEASE;PROTEASE	1.19 A	4	B 28 ALA - H 217 ALA B 47 ILE - H 187 ILE B 49 GLY - H 183 GLY B 50 ILE - H 57 ILE	L
	PROTEASE	1.38 A	4	A 47 ILE - H 57 ILE A 48 THR - H 56 THR A 49 GLY - H 185 GLY A 50 ILE - H 187 ILE	L
Amprenavir	HIV-1 PROTEASE;HIV-1 PROTEASE	1.30 A	4	A 23 LEU - g 165 LEU A 32 VAL - g 48 VAL A 82 VAL - g 163 VAL A 84 ILE - g 137 ILE	R
Lopinavir	HIV-1 PROTEASE	0.45 A	3	A 48 GLY - e 272 GLY A 49 GLY - e 271 GLY A 50 ILE - e 270 ILE	L
	HIV-1 PROTEASE	0.48 A	3	A 48 GLY - L 109 GLY A 49 GLY - L 110 GLY A 50 ILE - L 111 ILE	L

Supplementary Tables

Supplementary Table 39. Possible binding sites of 7CMJ against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.82 A	3	A 47 ILE - A 70 ILE A 48 GLY - A 183 GLY A 49 GLY - A 181 GLY	L
	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	1.00 A	4	A 47 ILE - A 70 ILE A 48 GLY - A 183 GLY A 49 GLY - A 181 GLY A 50 ILE - A 180 ILE	L
	PROTEASE RETROPEPSIN	0.73 A	3	B 147 ILE - A 70 ILE B 149 GLY - A 181 GLY B 150 ILE - A 180 ILE	R
	PROTEASE RETROPEPSIN	0.85 A	3	B 147 ILE - B 180 ILE B 149 GLY - B 183 GLY B 150 ILE - B 70 ILE	R
Ritonavir	PROTEASE;PROTEASE	0.67 A	3	B 47 ILE - A 70 ILE B 49 GLY - A 181 GLY B 50 ILE - A 180 ILE	R
	POL POLYPROTEIN;POL POLYPROTEIN	0.84 A	3	A 47 ILE - B 180 ILE A 49 GLY - B 183 GLY A 50 ILE - B 70 ILE	R
Darunavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.92 A	3	A 23 LEU - A 122 LEU A 32 VAL - A 88 VAL A 82 VAL - A 124 VAL	L
	FIV PROTEASE;FIV PROTEASE	0.91 A	3	B 33 ALA - A 93 ALA B 35 ILE - A 91 ILE B 37 VAL - A 64 VAL	L
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.64 A	3	B 147 ILE - A 70 ILE B 149 GLY - A 181 GLY B 150 ILE - A 180 ILE	R
	PROTEASE	0.96 A	3	B 123 LEU - A 27 LEU B 132 ILE - A 180 ILE B 182 ILE - A 196 ILE	L
Saquinavir	PROTEASE;PROTEASE	0.86 A	3	A 47 ILE - B 180 ILE A 49 GLY - B 183 GLY A 50 ILE - B 70 ILE	R
	PROTEASE;PROTEASE	0.54 A	3	B 147 ILE - A 70 ILE B 149 GLY - A 181 GLY B 150 ILE - A 180 ILE	R
	HIV-1 PROTEASE	0.97 A	4	A 47 ILE - A 70 ILE A 48 GLY - A 183 GLY A 49 GLY - A 181 GLY A 50 ILE - A 180 ILE	R
Amprenavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.66 A	3	A 47 ILE - A 70 ILE A 49 GLY - A 181 GLY A 50 ILE - A 180 ILE	R
Lopinavir	PROTEASE;PROTEASE	0.73 A	3	B 47 ILE - A 70 ILE B 49 GLY - A 181 GLY B 50 ILE - A 180 ILE	L
	HIV-1 PROTEASE	0.89 A	3	A 48 GLY - A 183 GLY A 49 GLY - A 181 GLY A 50 ILE - A 180 ILE	R
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.72 A	3	A 47 ILE - B 70 ILE A 49 GLY - B 181 GLY A 50 ILE - B 180 ILE	L
Atazanavir	PROTEASE;PROTEASE	0.73 A	3	B 47 ILE - A 70 ILE B 49 GLY - A 181 GLY B 50 ILE - A 180 ILE	R
Tipranavir	HIV-1 PROTEASE	0.73 A	3	A 47 ILE - A 70 ILE A 49 GLY - A 181 GLY A 50 ILE - A 180 ILE	R

Supplementary Tables

Supplementary Table 40. Possible binding sites of 7WHR against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Ritonavir	GAG-POL POLYPROTEIN;GAG-POL POLYPROTEIN	0.64 A	3	A 47 ILE - A 305 ILE A 49 GLY - A 288 GLY A 50 ILE - A 270 ILE	L
Amprenavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.67 A	3	A 47 ILE - A 305 ILE A 49 GLY - A 288 GLY A 50 ILE - A 270 ILE	L
	PROTEASE;PROTEASE	0.59 A	3	A 23 LEU - F 357 LEU A 32 VAL - F 322 VAL A 84 ILE - F 339 ILE	L
Lopinavir	PROTEASE	0.64 A	3	B 47 ILE - E 305 ILE B 49 GLY - E 288 GLY B 50 ILE - E 270 ILE	L
Nelfinavir	PROTEASE RETROPEPSIN	0.74 A	3	B 8 ARG - B 173 ARG B 23 LEU - B 175 LEU B 82 VAL - B 168 VAL	R
Darunavir	PROTEASE	0.74 A	3	B 123 LEU - D 357 LEU B 132 ILE - D 342 ILE B 182 ILE - D 339 ILE	R
Tipranavir	HIV-1 PROTEASE	0.65 A	3	A 47 ILE - A 305 ILE A 49 GLY - A 288 GLY A 50 ILE - A 270 ILE	R
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.72 A	3	A1132 ILE - D 46 ILE A1136 LYS - D 50 LYS A1137 GLY - D 53 GLY	R
Saquinavir	PROTEASE E35D-SQV;PROTEASE E35D-SQV	0.70 A	3	B 47 ILE - A 305 ILE B 49 GLY - A 288 GLY B 50 ILE - A 270 ILE	R

Supplementary Tables

Supplementary Table 41. Possible binding sites of 7ZHV against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Ritonavir	PROTEASE	0.58 A	3	A 47 ILE - A 304 ILE A 49 GLY - A 355 GLY A 50 ILE - A 527 ILE	L
Darunavir	HIV-1 PROTEASE	0.59 A	3	A 47 ILE - A 304 ILE A 49 GLY - A 355 GLY A 50 ILE - A 527 ILE	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.78 A	3	B 125 ASP - A 159 ASP B 127 GLY - A 152 GLY B 128 ALA - A 153 ALA	R
	FIV PROTEASE	1.01 A	4	A 32 GLY - A 204 GLY A 33 ALA - A 205 ALA A 34 ASP - A 164 ASP A 35 ILE - A 167 ILE	L
Indinavir	PROTEIN (PROTEASE);PROTEIN (PROTEASE)	0.77 A	3	A 47 ILE - A 304 ILE A 49 GLY - A 355 GLY A 50 ILE - A 527 ILE	R
	HIV-II PROTEASE;HIV-II PROTEASE	1.14 A	4	B 25 ASP - B 540 ASP B 28 ALA - B 539 ALA B 32 ILE - B 401 ILE B 84 ILE - B 543 ILE	R
Saquinavir	PROTEASE	0.49 A	3	A 48 ILE - A 304 ILE A 50 GLY - A 355 GLY A 51 ILE - A 527 ILE	L
	PROTEASE	0.92 A	4	B 125 ASP - A 159 ASP B 127 GLY - A 152 GLY B 128 ALA - A 153 ALA B 130 ASP - A 155 ASP	R
	PROTEASE;PROTEASE	0.77 A	3	B 25 ASP - A 159 ASP B 27 GLY - A 152 GLY B 28 ALA - A 153 ALA	R
Amprenavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.74 A	3	A 47 ILE - A 304 ILE A 49 GLY - A 355 GLY A 50 ILE - A 527 ILE	R
	PROTEASE;PROTEASE	0.76 A	3	A 25 ASP - A 159 ASP A 27 GLY - A 152 GLY A 28 ALA - A 153 ALA	R
	PROTEASE;PROTEASE	0.78 A	3	A 23 LEU - A 435 LEU A 32 VAL - A 282 VAL A 84 ILE - A 417 ILE	L
	PROTEASE	0.70 A	3	B 149 GLY - A 303 GLY B 150 ILE - A 304 ILE B 181 PRO - A 526 PRO	R
	PROTEASE	1.01 A	4	B 25 ASP - A 159 ASP B 27 GLY - A 152 GLY B 28 ALA - A 153 ALA B 30 ASP - A 155 ASP	R
	PROTEASE	1.32 A	4	B 23 LEU - A 516 LEU B 32 ILE - A 304 ILE B 82 ILE - A 519 ILE B 84 ILE - A 305 ILE	L
Nelfinavir	PROTEASE RETROPEPSIN;PROTEASE RETROPEPSIN	0.78 A	3	B 25 ASP - A 159 ASP B 27 GLY - A 152 GLY B 28 ALA - A 153 ALA	R
	PROTEASE RETROPEPSIN	0.60 A	3	B 47 ILE - A 304 ILE B 49 GLY - A 355 GLY B 50 ILE - A 527 ILE	L
Atazanavir	PROTEASE;PROTEASE	0.60 A	3	B 47 ILE - A 304 ILE B 49 GLY - A 355 GLY	L

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				B 50 ILE - A 527 ILE	
Lopinavir	PROTEASE;PROTEAS E	0.59 A	3	B 47 ILE - A 304 ILE B 49 GLY - A 355 GLY B 50 ILE - A 527 ILE	R
Tipranavir	HIV-1 PROTEASE	0.74 A	3	B 25 ASP - A 159 ASP B 27 GLY - A 152 GLY B 28 ALA - A 153 ALA	R
	HIV-1 PROTEASE	0.64 A	3	B 47 ILE - A 304 ILE B 49 GLY - A 355 GLY B 50 ILE - A 527 ILE	R
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.58 A	3	A1132 ILE - B 290 ILE A1136 LYS - B 406 LYS A1137 GLY - B 405 GLY	L

Supplementary Tables

Supplementary Table 42. Possible binding sites of 8B5U against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.78 A	3	A 47 ILE - A 136 ILE A 48 GLY - A 81 GLY A 49 GLY - A 80 GLY	R
	POL POLYPROTEIN;POL POLYPROTEIN	0.84 A	3	A 47 ILE - A 136 ILE A 48 GLY - A 137 GLY A 49 GLY - A 139 GLY	R
	POL POLYPROTEIN	1.10 A	3	B 8 ARG - A 209 ARG B 81 PRO - A 160 PRO B 82 ALA - A 163 ALA	R
Lopinavir	HIV-1 PROTEASE	0.98 A	3	A 48 GLY - A 80 GLY A 49 GLY - A 81 GLY A 50 ILE - A 136 ILE	R
Saquinavir	PROTEASE;PROTEASE	0.75 A	3	B 129 ASP - A 85 ASP B 148 GLY - A 80 GLY B 180 THR - A 140 THR	L
	PROTEASE;PROTEASE	0.91 A	3	A 8 ARG - A 226 ARG A 32 VAL - A 196 VAL A 80 THR - A 191 THR	R
Tipranavir	PROTEASE	0.99 A	3	A 28 ALA - A 163 ALA A 29 ASP - A 162 ASP A 30 ASP - A 117 ASP	L
Amprenavir	PROTEASE;PROTEASE	0.89 A	3	A 23 LEU - A 121 LEU A 32 VAL - A 4 VAL A 84 ILE - A 72 ILE	R
Darunavir	FIV PROTEASE;FIV PROTEASE	1.07 A	3	B 33 ALA - A 126 ALA B 35 ILE - A 218 ILE B 37 VAL - A 219 VAL	L
	FIV PROTEASE;FIV PROTEASE	1.11 A	3	B 33 ALA - A 9 ALA B 35 ILE - A 7 ILE B 37 VAL - A 74 VAL	R
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.77 A	3	C1041 GLN - A 98 GLN C1058 GLY - A 77 GLY C1137 GLY - A 8 GLY	R

Supplementary Tables

Supplementary Table 43. Possible binding sites of 8C79 against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.51 A	3	A 47 ILE - B 373 ILE A 48 GLY - B 131 GLY A 49 GLY - B 132 GLY	R
Saquinavir	HIV-1 PROTEASE	0.72 A	3	A 8 ARG - B 155 ARG A 80 THR - B 367 THR A 82 VAL - B 172 VAL	R
	PROTEASE;PROTEASE	0.71 A	3	A 8 ARG - A 32 ARG A 32 VAL - A 29 VAL A 80 THR - A 37 THR	L
	HIV-1 PROTEASE	0.85 A	3	A 47 ILE - B 287 ILE A 49 GLY - A 276 GLY A 50 VAL - A 275 VAL	L
Ritonavir	PROTEASE RETROPEPSIN	0.70 A	3	A 8 ARG - A 169 ARG A 81 PRO - A 362 PRO A 82 ALA - A 363 ALA	R
Tipranavir	PROTEASE	0.78 A	3	A 47 ILE - B 287 ILE A 49 GLY - A 276 GLY A 50 VAL - A 275 VAL	L
Darunavir	PROTEASE (RETROPEPSIN);PROTEASE (RETROPEPSIN)	0.80 A	3	A 25 ASN - B 249 ASN A 27 GLY - B 248 GLY A 28 ALA - B 247 ALA	R
	HIV-1 PROTEASE;HIV-1 PROTEASE	0.83 A	3	A 49 GLY - A 446 GLY A 50 ILE - B 259 ILE A 81 PRO - B 426 PRO	L
Atazanavir	PROTEASE;PROTEASE	0.61 A	3	A 8 ARG - A 169 ARG A 81 PRO - A 362 PRO A 82 ALA - A 363 ALA	R
Amprenavir	PROTEASE;PROTEASE	0.75 A	3	A 47 ILE - B 287 ILE A 49 GLY - A 276 GLY A 50 VAL - A 275 VAL	L
	PROTEASE	0.80 A	3	B 23 LEU - B 75 LEU B 32 VAL - B 29 VAL B 84 ILE - B 6 ILE	L
	PROTEASE	1.35 A	4	B 23 LEU - B 117 LEU B 32 ILE - B 100 ILE B 82 ILE - B 86 ILE B 84 ILE - B 99 ILE	R
	PROTEASE	0.85 A	3	B 147 VAL - A 184 VAL B 149 GLY - A 128 GLY B 150 ILE - A 129 ILE	L
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.69 A	3	C1041 GLN - B 110 GLN C1058 GLY - B 126 GLY C1137 GLY - B 103 GLY	L
	NS3 PROTEASE, NS4A PROTEIN	0.84 A	3	C1041 GLN - B 110 GLN C1058 GLY - B 179 GLY C1137 GLY - B 128 GLY	L

Supplementary Tables

Supplementary Table 44. Possible binding sites of 8CTM against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.76 A	3	A 29 ASP - A 15 ASP A 81 PRO - A 62 PRO A 82 VAL - A 61 VAL	L
	HIV-II PROTEASE	0.71 A	3	A 47 VAL - B 45 VAL A 49 GLY - B 12 GLY A 50 ILE - B 13 ILE	L
Darunavir	PROTEASE (RETROPEPSIN);PROTEASE (RETROPEPSIN)	0.77 A	3	A 25 ASN - C 266 ASN A 27 GLY - B 267 GLY A 28 ALA - B 268 ALA	R
	HIV-1 PROTEASE	0.55 A	3	B 49 GLY - D 12 GLY B 50 ILE - D 13 ILE B 81 PRO - D 242 PRO	R
	FIV PROTEASE	1.01 A	4	A 32 GLY - C 24 GLY A 33 ALA - C 306 ALA A 34 ASP - C 305 ASP A 35 ILE - C 304 ILE	R
Amprenavir	PROTEASE	0.46 A	3	B 23 LEU - B 7 LEU B 32 VAL - B 63 VAL B 84 ILE - B 33 ILE	L
Saquinavir	PROTEASE;PROTEASE	0.74 A	3	B 32 VAL - C 207 VAL B 81 PRO - C 214 PRO B 82 THR - C 212 THR	L
Grazoprevir	NS3 PROTEASE, NS4A PROTEIN	0.69 A	3	C1057 HIS - D 177 HIS C1078 VAL - D 261 VAL C1081 ASP - D 262 ASP	L

Supplementary Tables

Supplementary Table 45. Possible binding sites of 8J6E against known anti-viral drugs. Features of different drug binding motifs. HIV-1-Human Immunodeficiency virus 1, RMSD- Root Mean Square Deviation, Å-angstrom, Amino acids are represented by standard three letter code.

Drugs	Known similar target	RMSD	No. of binding residues	3D-interface residues	Superposition type
Indinavir	POL POLYPROTEIN;POL POLYPROTEIN	0.74 A	3	A 47 ILE - A 301 ILE A 48 GLY - A 302 GLY A 49 GLY - A 324 GLY	R
	HIV-II PROTEASE;HIV-II PROTEASE	1.08 A	3	B 47 VAL - A 172 VAL B 49 GLY - A 174 GLY B 50 ILE - A 175 ILE	R
Saquinavir	PROTEASE;PROTEASE	1.07 A	3	B 129 ASP - A 192 ASP B 148 GLY - A 189 GLY B 180 THR - A 183 THR	R
	HIV-1 PROTEASE	0.98 A	3	A 47 ILE - A 241 ILE A 49 GLY - A 221 GLY A 50 VAL - A 222 VAL	R
Tipranavir	PROTEASE	0.97 A	3	A 47 ILE - A 241 ILE A 49 GLY - A 221 GLY A 50 VAL - A 222 VAL	R
	PROTEASE	1.07 A	3	A 47 ILE - A 195 ILE A 49 GLY - A 174 GLY A 50 VAL - A 150 VAL	L
	HIV-1 PROTEASE	0.85 A	3	B 25 ASP - A 119 ASP B 27 GLY - A 69 GLY B 28 ALA - A 68 ALA	L
Darunavir	HIV-1 PROTEASE;HIV-1 PROTEASE	0.95 A	3	A 23 LEU - A 50 LEU A 32 VAL - A 42 VAL A 82 VAL - A 63 VAL	R
	PROTEASE	1.10 A	3	B 147 VAL - A 172 VAL B 149 GLY - A 174 GLY B 150 ILE - A 175 ILE	L
	FIV PROTEASE;FIV PROTEASE	0.95 A	3	B 33 ALA - A 207 ALA B 35 ILE - A 175 ILE B 37 VAL - A 149 VAL	R
	FIV PROTEASE;FIV PROTEASE	0.78 A	3	B 33 ALA - A 153 ALA B 35 ILE - A 175 ILE B 37 VAL - A 194 VAL	R
Amprenavir	PROTEASE;PROTEASE	0.92 A	3	A 47 ILE - A 241 ILE A 49 GLY - A 221 GLY A 50 VAL - A 222 VAL	R
	PROTEASE;PROTEASE	1.32 A	4	B 123 LEU - A 83 LEU B 132 VAL - A 35 VAL B 182 VAL - A 74 VAL B 184 VAL - A 71 VAL	R