Supplementary Table S1: List of the structures of non-nucleoside inhibitor complexes of the RNA dependent RNA polymerase of Hepatitis C Virus.

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| Binding Sites | PDB IDs | Formula | Inhibitor name |
| Palm Site (55 Complexes) | 3CDE | C21 H23 N5 O6 S3 | N-{3-[5-hydroxy-2-(3-methylbutyl)-3-oxo-6-thiophen-2-yl-2,3-dihydropyridazin-4-yl]-1,1-dioxido-2H-1,2,4-benzothiadiazin-7-yl}methanesulfonamide |
| 3CWJ | C22 H24 N4 O6 S3 | N-{3-[5-hydroxy-2-(3-methylbutyl)-3-oxo-6- thiophen-2-yl-2,3-dihydropyridazin-4-yl]- 1,1-dioxido-2H-1,4-benzothiazin-7-yl}methanesulfonamide |
| 2YOJ | C25 H14 F2 N4 O5 | 4-fluoranyl-6-[(7-fluoranyl-4-oxidanylidene-3H-quinazolin-6-yl)methyl]-8-(2-oxidanylidene-1H-pyridin-3-yl)furo[2,3-e]indole-7-carboxylic acid |
| 3BR9 | C23 H25 N5 O6 S2 | (2R)-2-({3-[5-hydroxy-2-(3-methylbutyl)-3-oxo-6-thiophen-2-yl-2,3-dihydropyridazin-4-yl]-1,1-dioxido-2H-1,2,4-benzothiadiazin-7-yl}oxy)propanamide |
| 3BSA | C21 H22 N6 O6 S2 | 2-({3-[5-hydroxy-2-(3-methylbutyl)-3-oxo-6-(1,3-thiazol-5-yl)-2,3-dihydropyridazin-4-yl]-1,1-dioxido-2H-1,2,4-benzothiadiazin-7-yl}oxy)acetamide |
| 3CO9 | C20 H23 N5 O6 S2 | N-{3-[4-hydroxy-1-(3-methylbutyl)-2-oxo-1,2-dihydropyrrolo[1,2-b]pyridazin-3-yl]-1,1-dioxido-2H-1,2,4-benzothiadiazin-7-yl}methanesulfonamide |
| 3CVK | C21 H29 N5 O6 S2 | N-{3-[1-(3,3-Dimethyl-butyl)-4-hydroxy-2-oxo-1,2,4a,5,6,7-hexahydro-pyrrolo[1,2-b]pyridazin-3-yl]-1,1-dioxo-1,2-dihydro-1lambda6-benzo[1,2,4]thiadiazin-7-yl}-methanesulfonamide |
| 3D28 | C21 H20 N2 O4 S | (5S)-1-benzyl-3-(1,1-dioxido-1,2-benzisothiazol-3-yl)-4-hydroxy-5-(1-methylethyl)-1,5-dihydro-2H-pyrrol-2-one |
| 3D5M | C24 H25 Cl F N3 O6 S2 | N-({3-[(5S)-5-tert-butyl-1-(3-chloro-4-fluorobenzyl)-4-hydroxy-2-oxo-2,5-dihydro-1H-pyrrol-3-yl]-1,1-dioxido-1,2-benzisothiazol-7-yl}methyl)methanesulfonamide |
| 3E51 | C21 H28 N6 O6 S2 | N-{3-[5-hydroxy-2-(3-methylbutyl)-3-oxo-6-pyrrolidin-1-yl-2,3-dihydropyridazin-4-yl]-1,1-dioxido-2H-1,2,4-benzothiadiazin-7-yl}methanesulfonamide |
| 3G86 | C25 H19 F2 N3 O6 S2 | N-{3-[6-fluoro-1-(4-fluorobenzyl)-4-hydroxy-2-oxo-1,2-dihydroquinolin-3-yl]-1,1-dioxido-4H-1,4-benzothiazin-7-yl}methanesulfonamide |
| 3GYN | C24 H34 N4 O6 S2 | N-{3-[(5R)-1-cyclopentyl-4-hydroxy-5-methyl-5-(3-methylbutyl)-2-oxo-1,2,5,6-tetrahydropyridin-3-yl]-1,1-dioxido-4H-1,2,4-benzothiadiazin-7-yl}methanesulfonamide |
| 3H2L | C23 H23 F N4 O6 S2 | N-{3-[(4ar,7as)-1-(4-fluorobenzyl)-4-hydroxy-2-oxo-2,4a,5,6,7,7a-hexahydro-1H-cyclopenta[b]pyridin-3-yl]-1,1-dioxido-2H-1,2,4-benzothiadiazin-7-yl}methanesulfonamide |
| 3H59 | C26 H30 F N3 O6 S2 | N-{3-[(5S)-5-(1,1-dimethylpropyl)-1-(4-fluoro-3-methylbenzyl)-4-hydroxy-2-oxo-2,5-dihydro-1H-pyrrol-3-yl]-1,1-dioxido-4H-1,4-benzothiazin-7-yl}methanesulfonamide |
| 3H5S | C27 H30 F N3 O6 S2 | (5S)-5-tert-butyl-1-(4-fluoro-3-methylbenzyl)-4-hydroxy-3-[8-(methylsulfonyl)-1,1-dioxido-6,7,8,9-tetrahydroisothiazolo[4,5-h]isoquinolin-3-yl]-1,5-dihydro-2H-pyrrol-2-one |
| 3H5U | C24 H26 F N3 O6 S2 | N-({3-[(5S)-5-tert-butyl-1-(4-fluorobenzyl)-4-hydroxy-2-oxo-2,5-dihydro-1H-pyrrol-3-yl]-1,1-dioxido-1,2-benzisothiazol-7-yl}methyl)methanesulfonamide |
| 3H98 | C19 H22 N6 O6 S2 | N-{3-[5-hydroxy-8-(3-methylbutyl)-7-oxo-7,8-dihydroimidazo[1,2-a]pyrimidin-6-yl]-1,1-dioxido-4H-1,2,4-benzothiadiazin-7-yl}methanesulfonamide |
| 3HKW | C30 H32 F N3 O6 S | (11S)-10-[(2,5-dimethyl-1,3-oxazol-4-yl)carbonyl]-11-{2-fluoro-4-[(2-methylprop-2-en-1-yl)oxy]phenyl}-3,3-dimethyl-2,3,4,5,10,11-hexahydrothiopyrano[3,2-b][1,5]benzodiazepin-6-ol 1,1-dioxide |
| 3HKY | C30 H32 F N3 O6 S | (11S)-10-[(2,5-dimethyl-1,3-oxazol-4-yl)carbonyl]-11-{2-fluoro-4-[(2-methylprop-2-en-1-yl)oxy]phenyl}-3,3-dimethyl-2,3,4,5,10,11-hexahydrothiopyrano[3,2-b][1,5]benzodiazepin-6-ol 1,1-dioxide |
| 3LKH | C23 H29 F N2 O4 | 2-(2-{[(1S)-1-benzyl-2-hydroxyethyl]amino}-2-oxoethoxy)-N-butyl-6-fluoro-N-methylbenzamide |
| 3SKA | C21 H15 F3 N4 O3 | 1-[(2-aminopyridin-4-yl)methyl]-3-(2-oxo-1,2-dihydropyridin-3-yl)-5-(trifluoromethyl)-1H-indole-2-carboxylic acid |
| 3SKE | C22 H14 F3 N5 O4 S | 1-[(2-aminopyridin-4-yl)methyl]-3-(2,4-dioxo-1,2-dihydrothieno[3,4-d]pyrimidin-3(4H)-yl)-5-(trifluoromethyl)-1H-indole-2-carboxylic acid |
| 3SKH | C22 H15 Cl F N O2 | 1-benzyl-5-chloro-3-(2-fluorophenyl)-1H-indole-2-carboxylic acid |
| 3TYQ | C23 H18 F N3 O5 | 5-ethyl-1-(2-fluoro-5-nitrobenzyl)-3-(2-oxo-1,2-dihydropyridin-3-yl)-1H-indole-2-carboxylic acid |
| 3TYV | C25 H20 F3 N3 O4 S | N-(cyclopropylsulfonyl)-1-(2,5-difluorobenzyl)-6-fluoro-5-methyl-3-(2-oxo-1,2-dihydropyridin-3-yl)-1H-indole-2-carboxamide |
| 3U4O | C20 H15 Cl N4 O3 | 1-[(2-aminopyridin-4-yl)methyl]-5-chloro-3-(2-oxo-1,2-dihydropyridin-3-yl)-1H-indole-2-carboxylic acid |
| 3U4R | C27 H23 Cl N6 O6 S2 | 1-[(2-aminopyridin-4-yl)methyl]-5-chloro-N-({3-[(methylsulfonyl)amino]phenyl}sulfonyl)-3-(2-oxo-1,2-dihydropyridin-3-yl)-1H-indole-2-carboxamide |
| 3UPH | C24 H19 F2 N3 O5 S | 6-(2,5-difluorobenzyl)-N-(methylsulfonyl)-8-(2-oxo-1,2-dihydropyridin-3-yl)-3,6-dihydro-2H-furo[2,3-e]indole-7-carboxamide |
| 3UPI | C25 H21 F2 N3 O5 S | (3S)-6-(2,5-difluorobenzyl)-3-methyl-N-(methylsulfonyl)-8-(2-oxo-1,2-dihydropyridin-3-yl)-3,6-dihydro-2H-furo[2,3-e]indole-7-carboxamide |
| 4EAW | C24 H37 N4 O6 P S | N-{(1S)-3-[(5S)-5-tert-butyl-1-(3,3-dimethylbutyl)-4-hydroxy-2-oxo-2,5-dihydro-1H-pyrrol-3-yl]-1-ethoxy-1-oxido-1,4-dihydro-2,4,1-benzodiazaphosphinin-7-yl}methanesulfonamide |
| 4IH5 | C11 H10 N6 | 4-(2-phenylhydrazinyl)-1H-pyrazolo[3,4-d]pyrimidine |
| 4IH6 | C17 H24 N2 O2 | (5S)-3-(4-tert-butylbenzyl)-5-(propan-2-yl)imidazolidine-2,4-dione |
| 4IH7 | C15 H17 N O | 3-(3-tert-butylphenyl)pyridin-2(1H)-one |
| 4KAI | C27 H25 B F2 N2 O6 S | [4-({[5-cyclopropyl-2-(4-fluorophenyl)-3-(methylcarbamoyl)-1-benzofuran-6-yl](methylsulfonyl)amino}methyl)-2-fluorophenyl]boronic acid |
| 4KB7 | C29 H28 B F N2 O6 S | 5-cyclopropyl-2-(4-fluorophenyl)-6-[{2-[(3R)-1-hydroxy-1,3-dihydro-2,1-benzoxaborol-3-yl]ethyl}(methylsulfonyl)amino]-N-methyl-1-benzofuran-3-carboxamide |
| 4KBI | C28 H25 B F2 N2 O6 S | 5-cyclopropyl-6-{[(7-fluoro-1-hydroxy-1,3-dihydro-2,1-benzoxaborol-5-yl)methyl](methylsulfonyl)amino}-2-(4-fluorophenyl)-N-methyl-1-benzofuran-3-carboxamide |
| 4KE5 | C27 H25 B F2 N2 O6 S | [4-({[5-cyclopropyl-2-(4-fluorophenyl)-3-(methylcarbamoyl)-1-benzofuran-6-yl](methylsulfonyl)amino}methyl)-2-fluorophenyl]boronic acid |
| 4KHM | C27 H25 B F2 N2 O6 S | [4-({[5-cyclopropyl-2-(4-fluorophenyl)-3-(methylcarbamoyl)-1-benzofuran-6-yl](methylsulfonyl)amino}methyl)-2-fluorophenyl]boronic acid |
| 4KHR | C27 H25 B F2 N2 O6 S | [4-({[5-cyclopropyl-2-(4-fluorophenyl)-3-(methylcarbamoyl)-1-benzofuran-6-yl](methylsulfonyl)amino}methyl)-2-fluorophenyl]boronic acid |
| 4MIB | C25 H32 N4 O4 S | N-({(3S)-1-[6-tert-butyl-5-methoxy-8-(2-oxo-1,2-dihydropyridin-3-yl)quinolin-3-yl]pyrrolidin-3-yl}methyl)methanesulfonamide |
| 4MK8 | C25 H30 N2 O4 S | N-(4-{2-[3-tert-butyl-2-methoxy-5-(2-oxo-1,2-dihydropyridin-3-yl)phenyl]ethyl}phenyl)methanesulfonamide |
| 4MK9 | C24 H25 N3 O5 S | N-{2-[3-tert-butyl-2-methoxy-5-(2-oxo-1,2-dihydropyridin-3-yl)phenyl]-1,3-benzoxazol-5-yl}methanesulfonamide |
| 4MKA | C26 H26 N2 O6 S | N-{3-[3-tert-butyl-2-methoxy-5-(2-oxo-1,2-dihydropyridin-3-yl)phenyl]-1-oxo-1H-isochromen-7-yl}methanesulfonamide |
| 4MKB | C24 H27 N3 O4 S | N-(4-{(E)-2-[3-tert-butyl-2-methoxy-5-(3-oxo-2,3-dihydropyridazin-4-yl)phenyl]ethenyl}phenyl)methanesulfonamide |
| 4MZ4 | C25 H17 Cl F N3 O3 | 1-[(2-chloroquinolin-3-yl)methyl]-6-fluoro-5-methyl-3-(2-oxo-1,2-dihydropyridin-3-yl)-1H-indole-2-carboxylic acid |
| 5PZK | C38 H38 N4 O5 | (2E)-3-(4-{[(1-{[(13-cyclohexyl-6-oxo-6,7-dihydro-5H-indolo[1,2-d][1,4]benzodiazepin-10-yl)carbonyl]amino}cyclopentyl)carbonyl]amino}phenyl)prop-2-enoic acid |
| 5PZL | C23 H21 F N4 O6 S | 2-({3-[1-(2-cyclopropylethyl)-6-fluoro-4-hydroxy-2-oxo-1,2-dihydroquinolin-3-yl]-1,1-dioxo-1,4-dihydro-1lambda~6~,2,4-benzothiadiazin-7-yl}oxy)acetamide |
| C23 H21 F N4 O6 S | 2-({3-[1-(2-cyclopropylethyl)-6-fluoro-4-hydroxy-2-oxo-1,2-dihydroquinolin-3-yl]-1,1-dioxo-1,4-dihydro-1lambda~6~,2,4-benzothiadiazin-7-yl}oxy)acetamide |
| 5PZN | C27 H25 F N2 O3 | 5-[3-(tert-butylcarbamoyl)phenyl]-2-(4-fluorophenyl)-N-methyl-1-benzofuran-3-carboxamide |
| 5PZN | C38 H38 N4 O5 | (2E)-3-(4-{[(1-{[(13-cyclohexyl-6-oxo-6,7-dihydro-5H-indolo[1,2-d][1,4]benzodiazepin-10-yl)carbonyl]amino}cyclopentyl)carbonyl]amino}phenyl)prop-2-enoic acid |
| 3FQK | C22 H23 F N2 O5 S | 5-cyclopropyl-2-(4-fluorophenyl)-6-[(2-hydroxyethyl)(methylsulfonyl)amino]-N-methyl-1-benzofuran-3-carboxamide |
| 3FQL | C22 H23 F N2 O5 S | 5-cyclopropyl-2-(4-fluorophenyl)-6-[(2-hydroxyethyl)(methylsulfonyl)amino]-N-methyl-1-benzofuran-3-carboxamide |
| 4JY0 | C27 H32 N4 O3 S | (4S,5R)-1-(4-tert-butylbenzoyl)-2-(2-methylpropyl)-4-pyrazin-2-yl-5-(1,3-thiazol-2-yl)-L-proline |
| 2GIQ | C21 H18 F N3 O4 S | 1-(2-cyclopropylethyl)-3-(1,1-dioxido-2h-1,2,4-benzothiadiazin-3-yl)-6-fluoro-4-hydroxyquinolin-2(1h)-one |
| 2AWZ | C16 H13 Br N2 O3 S3 | 5r-(4-bromophenylmethyl)-3-(benzenesulfonylamino)-4-oxo-2-thionothiazolidine |
| 2AX0 | C19 H18 N2 O3 S3 | 5r-(2e-methyl-3-phenyl-allyl)-3-(benzenesulfonylamino)-4-oxo-2-thionothiazolidine |
| 2AX1 | C14 H10 Cl2 N2 O3 S4 | 5r-(3,4-dichlorophenylmethyl)-3-(2-thiophenesulfonylamino)-4-oxo-2-thionothiazolidine |
| Thumb Site  (44 Complexes) | 2D3U | C19 H14 N2 O4 S2 | 5-(4-cyanophenyl)-3-{[(2-methylphenyl)sulfonyl]amino}thiophene-2-carboxylic acid |
| 2D3Z | C18 H14 F N O4 S2 | 5-(4-fluorophenyl)-3-{[(4-methylphenyl)sulfonyl]amino}thiophene-2-carboxylic acid |
| 2D41 | C19 H17 N O5 S3 | 5'-acetyl-4-{[(2,4-dimethylphenyl)sulfonyl]amino}-2,2'-bithiophene-5-carboxylic acid |
| 2HWH | C16 H14 N2 O4 S2 | 4-methyl-n-{(5e)-5-[(5-methyl-2-furyl)methylene]-4-oxo-4,5-dihydro-1,3-thiazol-2-yl}benzenesulfonamide |
| 2HWI | C18 H15 F N2 O4 S | (2s)-({(5z)-5-[(5-ethyl-2-furyl)methylene]-4-oxo-4,5-dihydro-1,3-thiazol-2-yl}amino)(4-fluorophenyl)acetic acid |
| 1NHU | C24 H18 Cl2 F3 N O3 | (2s)-2-[(2,4-dichloro-benzoyl)-(3-trifluoromethyl-benzyl)-amino]-3-phenyl-propionic acid |
| 2DXS | C27 H30 N2 O4 | N-[(13-cyclohexyl-6,7-dihydroindolo[1,2-d][1,4]benzoxazepin-10-yl)carbonyl]-2-methyl-l-alanine |
| 2O5D | C24 H19 F N4 O7 S2 | (2s)-2-({(5z)-5-[(5-ethyl-2-furyl)methylene]-4-oxo-4,5-dihydro-1,3-thiazol-2-yl}amino)-2-(4-fluorophenyl)-n-[(4-nitrophenyl)sulfonyl]acetamide |
| 2WHO | C20 H15 BR N2 O3 | 2-(3-bromophenyl)-6-[(2-hydroxyethyl)amino]-1h-benzo[de]isoquinoline-1,3(2h)-dione |
| 3CIZ | C7 H6 Br N O2 | 2-amino-5-bromobenzoic acid |
| 3CJ0 | C9 H9 Br N2 O3 | 4-[(5-bromopyridin-2-yl)amino]-4-oxobutanoic acid |
| 3CJ2 | C14 H19 Br N2 O | 4-bromo-2-{[(3R,5S)-3,5-dimethylpiperidin-1-yl]carbonyl}aniline |
| 3CJ3 | C18 H18 Br Cl N2 O | 4-bromo-2-{[(2R)-2-(2-chlorobenzyl)pyrrolidin-1-yl]carbonyl}aniline |
| 3CJ4 | C18 H23 Br N2 O4 | 4-[(4-bromo-2-{[(3R,5S)-3,5-dimethylpiperidin-1-yl]carbonyl}phenyl)amino]-4-oxobutanoic acid |
| 3CJ5 | C22 H30 Br N3 O4 | N-(4-bromo-2-{[(3R,5S)-3,5-dimethylpiperidin-1-yl]carbonyl}phenyl)-4-morpholin-4-yl-4-oxobutanamide |
| 3FRZ | C29 H37 N5 O3 | (6R)-6-cyclopentyl-6-[2-(2,6-diethylpyridin-4-yl)ethyl]-3-[(5,7-dimethyl[1,2,4]triazolo[1,5-a]pyrimidin-2-yl)methyl]-4-hydroxy-5,6-dihydro-2H-pyran-2-one |
| 3FRZ | C35 H39 N3 O7 | N-[(benzyloxy)carbonyl]-L-alpha-glutamyl-N-[(1S)-4-oxo-4-phenyl-1-propylbut-2-en-1-yl]-L-phenylalaninamide |
| 3MF5 | C24 H24 O2 S | 3-[2-(trans-4-methylcyclohexyl)phenyl]-5-phenylthiophene-2-carboxylic acid |
| 3Q0Z | C38 H38 N4 O5 | (2E)-3-(4-{[(1-{[(13-cyclohexyl-6-oxo-6,7-dihydro-5H-indolo[1,2-d][1,4]benzodiazepin-10-yl)carbonyl]amino}cyclopentyl)carbonyl]amino}phenyl)prop-2-enoic acid |
| 4DRU | C32 H38 N4 O5 S | 13-cyclohexyl-3-methoxy-17,22-dimethyl-7H-10,6-(methanoiminothioiminobutanoiminomethano)indolo[2,1-a][2]benzazepine-14,23-dione 16,16-dioxide |
| 4EO6 | C22 H31 N O3 S | 5-(3,3-dimethylbut-1-yn-1-yl)-3-{[(trans-4-methylcyclohexyl)carbonyl](propan-2-yl)amino}thiophene-2-carboxylic acid |
| 4EO8 | C21 H30 N2 O3 S | 5-(3,3-dimethylbut-1-yn-1-yl)-3-{2,2-dimethyl-1-[(trans-4-methylcyclohexyl)carbonyl]hydrazinyl}thiophene-2-carboxylic acid |
| 4IZ0 | C10 H7 Cl3 N2 O3 S | 2,4,5-trichloro-N-(5-methyl-1,2-oxazol-3-yl)benzenesulfonamide |
| 4J02 | C16 H17 Cl2 N O3 | [(1R)-5,8-dichloro-1-propyl-1,3,4,9-tetrahydropyrano[3,4-b]indol-1-yl]acetic acid |
| 4J04 | C13 H7 Cl4 N O4 S | 4-chloro-2-{[(2,4,5-trichlorophenyl)sulfonyl]amino}benzoic acid |
| 4J06 | C11 H7 Br Cl N O4 S2 | 2-{[(5-bromothiophen-2-yl)sulfonyl]amino}-4-chlorobenzoic acid |
| 4J08 | C20 H17 N O5 S | 2-{[(4-methylphenyl)sulfonyl]amino}-5-phenoxybenzoic acid |
| 4J0A | C20 H17 N O5 S | 2-{[(4-methylphenyl)sulfonyl]amino}-4-phenoxybenzoic acid |
| 4JJS | C25 H28 F3 N O4 | 2-{[(trans-4-methylcyclohexyl)carbonyl](propan-2-yl)amino}-5-[2-(trifluoromethyl)phenoxy]benzoic acid |
| 4JJU | C21 H12 F5 N3 O2 | 1-(2,4-difluorobenzyl)-6-{[3-(trifluoromethyl)pyridin-2-yl]oxy}quinazolin-4(1H)-one |
| 4JU3 | C21 H17 N O7 S | 5-(4-carboxyphenoxy)-2-{[(4-methylphenyl)sulfonyl]amino}benzoic acid |
| 4JU4 | C19 H13 Br F N O5 S | 2-{[(4-bromo-2-fluorophenyl)sulfonyl]amino}-5-phenoxybenzoic acid |
| 4JU6 | C24 H29 N O4 | 2-{[(trans-4-methylcyclohexyl)carbonyl](propan-2-yl)amino}-5-phenoxybenzoic acid |
| 4JU7 | C24 H29 N O4 | 2-{[(trans-4-methylcyclohexyl)carbonyl](propan-2-yl)amino}-5-phenoxybenzoic acid |
| 4JVQ | C32 H36 N2 O6 | 5-{4-[(4-methoxybenzoyl)amino]phenoxy}-2-{[(trans-4-methylcyclohexyl)carbonyl](propan-2-yl)amino}benzoic acid |
| 4OBC | C6 H13 N O4 S | 2-(n-morpholino)-ethanesulfonic acid |
| C12 H26 O6 | 1-(2-methoxy-ethoxy)-2-{2-[2-(2-methoxy-ethoxy]-ethoxy}-ethane |
| 4TLR | C24 H33 N O5 S | 3-{(2R,5R)-5-cyclohexyl-2-[(2R)-2-hydroxypropyl]-3-oxomorpholin-4-yl}-5-(3,3-dimethylbut-1-yn-1-yl)thiophene-2-carboxylic acid |
| C22 H23 F N2 O5 S | 5-cyclopropyl-2-(4-fluorophenyl)-6-[(2-hydroxyethyl)(methylsulfonyl)amino]-N-methyl-1-benzofuran-3-carboxamide |
| 2BRK | C27 H30 N2 O4 | 3-cyclohexyl-1-(2-morpholin-4-yl-2-oxoethyl)-2-phenyl-1h-indole-6-carboxylic acid |
| 2BRL | C31 H39 N3 O3 | 3-cyclohexyl-1-(2-{methyl[(1-methylpiperidin-3-yl)methyl]amino}-2-oxoethyl)-2-phenyl-1h-indole-6-carboxylic acid |
| 2HAI | C5 H11 N O3 S2 | S,s-(2-hydroxyethyl)thiocysteine |
| C3 H7 N O4 S | 3-sulfinoalanine |
| C21 H27 F O4 | (6s)-6-cyclopentyl-6-[2-(3-fluoro-4-isopropoxyphenyl)ethyl]-4-hydroxy-5,6-dihydro-2h-pyran-2-one |
| 2I1R | C18 H15 F N6 O2 S | (5z)-5-[(5-ethyl-2-furyl)methylene]-2-{[(s)-(4-fluorophenyl)(1h-tetrazol-5-yl)methyl]amino}-1,3-thiazol-4(5h)-one |
| 2WRM | C18 H18 N2 O4 | (3r)-3-(4-methyl-1,3-dioxo-1,3-dihydro-2h-pyrrolo[3,4-c]quinolin-2-yl)hexanoic acid |
| 3HVO | C20 H15 BR N2 O3 | 2-(3-bromophenyl)-6-[(2-hydroxyethyl)amino]-1h-benzo[de]isoquinoline-1,3(2h)-dione |
| 2WCX | C20 H21 N O2 S | 6-cyclohexyl-4-methyl-5-phenyl-4h-thieno[3,2-b]pyrrole-2-carboxylic acid |
| 2GIR | C22 H27 N O3 S | 3-{isopropyl[(trans-4-methylcyclohexyl)carbonyl]amino}-5-phenylthiophene-2-carboxylic acid |
| Primer Grip (3 Complexes) | 2IJN | C12 H9 F6 N3 O S | (2r,3r)-3-{[3,5-bis(trifluoromethyl)phenyl]amino}-2-cyano-3-thioxopropanamide |
| 5TWM | C28 H29 F N4 O3 | 5-[3-(tert-butylcarbamoyl)phenyl]-6-(ethylamino)-2-(4-fluorophenyl)-N-methylfuro[2,3-b]pyridine-3-carboxamide |
| 1YVF | C22 H16 Br N O4 | (2z)-2-(benzoylamino)-3-[4-(2-bromophenoxy)phenyl]-2-propenoic acid |
| Subdomains interfaces  (7 Complexes) | 2GC8 | C12 H15 Cl N2 O4 S | 1-[(2-amino-4-chloro-5-methylphenyl)sulfonyl]-l-proline |
| 3GNW | C34 H32 F N3 O5 S | (11S)-11-[4-(benzyloxy)-2-fluorophenyl]-3,3-dimethyl-10-[(6-methylpyridin-2-yl)carbonyl]-2,3,4,5,10,11-hexahydrothiopyrano[3,2-b][1,5]benzodiazepin-6-ol 1,1-dioxide |
| 3QGF | C38 H38 N4 O5 | (2E)-3-(4-{[(1-{[(13-cyclohexyl-6-oxo-6,7-dihydro-5H-indolo[1,2-d][1,4]benzodiazepin-10-yl)carbonyl]amino}cyclopentyl)carbonyl]amino}phenyl)prop-2-enoic acid |
| C24 H23 Cl F3 N5 O5 S | (2R)-4-(6-chloropyridazin-3-yl)-N-(4-methoxybenzyl)-1-{[4-(trifluoromethoxy)phenyl]sulfonyl}piperazine-2-carboxamide |
| 3QGH | C28 H26 F6 N6 O6 S | N-cyclopropyl-6-[(3R)-3-{[4-(trifluoromethoxy)benzyl]carbamoyl}-4-{[4-(trifluoromethoxy)phenyl]sulfonyl}piperazin-1-yl]pyridazine-3-carboxamide |
| 3QGI | C29 H30 F6 N6 O6 S | N-[(2S)-butan-2-yl]-6-[(3R)-3-{[4-(trifluoromethoxy)benzyl]carbamoyl}-4-{[4-(trifluoromethoxy)phenyl]sulfonyl}piperazin-1-yl]pyridazine-3-carboxamide |
| 5TRI | C22 H16 Cl N O4 | 3-[(4-chlorophenyl)methoxy]-2-(1-oxo-1,3-dihydro-2H-isoindol-2-yl)benzoic acid |
| C38 H38 N4 O5 | (2E)-3-(4-{[(1-{[(13-cyclohexyl-6-oxo-6,7-dihydro-5H-indolo[1,2-d][1,4]benzodiazepin-10-yl)carbonyl]amino}cyclopentyl)carbonyl]amino}phenyl)prop-2-enoic acid |
| 5TRK | C23 H19 Cl N2 O5 | N-{3-[(benzenecarbonyl)amino]-4-[(4-chlorophenyl)methoxy]benzene-1-carbonyl}glycine |
| C38 H38 N4 O5 | (2E)-3-(4-{[(1-{[(13-cyclohexyl-6-oxo-6,7-dihydro-5H-indolo[1,2-d][1,4]benzodiazepin-10-yl)carbonyl]amino}cyclopentyl)carbonyl]amino}phenyl)prop-2-enoic acid |