Hydrogen Bond Occupancy

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| Quercetin |  |  |
| Donor | Acceptor | Occupancy |
| QUE275-Side | VAL95-Main | 9.20% |
| QUE275-Side | LYS41-Side | 5.96% |
| QUE275-Side | ILE76-Side | 3.80% |
| QUE275-Side | GLU63-Side | 0.00% |
| LYS41-Side | QUE275-Side | 2.28% |
| VAL95-Main | QUE275-Side | 2.01% |
| ASP158-Main | QUE275-Side | 0.26% |
| PHE159-Main | QUE275-Side | 0.00% |
| QUE275-Side | VAL26-Side | 3.40% |
| GLU99-Main | QUE275-Side | 10.40% |
| QUE275-Side | ALA39-Side | 7.75% |
| QUE275-Side | GLY19-Main | 6.15% |
| QUE275-Side | ALA96-Main | 1.91% |
| QUE275-Side | ILE157-Side | 6.35% |
| QUE275-Side | MET143-Side | 1.85% |
| QUE275-Side | LEU92-Side | 15.47% |
| GLY98-Main | QUE275-Side | 5.30% |
| QUE275-Side | GLY98-Main | 26.60% |
| QUE275-Side | GLU99-Side | 9.70% |
| QUE275-Side | GLY97-Main | 11.87% |
| QUE275-Side | LEU18-Main | 5.97% |
| QUE275-Side | ASP158-Main | 0.03% |
| QUE275-Side | LEU18-Side | 4.38% |
| QUE275-Side | VAL95-Side | 2.19% |
| QUE275-Side | SER20-Main | 2.22% |
| SER20-Main | QUE275-Side | 1.60% |
| QUE275-Side | GLY21-Main | 0.41% |
| QUE275-Side | ALA96-Side | 0.13% |
| QUE275-Side | LEU94-Side | 0.16% |
| QUE275-Side | ASP158-Side | 0.42% |
| QUE275-Side | GLU93-Main | 8.58% |
| QUE275-Side | GLU99-Main | 0.18% |
| GLY97-Main | QUE275-Side | 3.23% |
| QUE275-Side | LEU144-Main | 14.62% |
| LEU144-Main | QUE275-Side | 0.57% |
| GLY19-Main | QUE275-Side | 0.35% |
| QUE275-Side | ALA39-Main | 1.02% |
| QUE275-Side | MET143-Main | 0.24% |
| QUE275-Side | LEU145-Main | 0.80% |
| QUE275-Side | LYS155-Side | 6.06% |
| QUE275-Side | LEU145-Side | 0.94% |
| QUE275-Side | ALA40-Main | 0.03% |
| QUE275-Side | LYS41-Main | 0.00% |
| QUE275-Side | LYS27-Main | 0.01% |
| ARG147-Side | QUE275-Side | 1.02% |
| QUE275-Side | LEU92-Main | 0.00% |
| LYS41-Main | QUE275-Side | 0.00% |
| QUE275-Side | LYS155-Main | 0.00% |
| QUE275-Side | LEU94-Main | 0.03% |
| QUE275-Side | ARG147-Side | 0.11% |
| QUE275-Side | ALA24-Side | 2.47% |
| QUE275-Side | ALA24-Main | 2.84% |
| GLY21-Main | QUE275-Side | 0.01% |
| QUE275-Side | ASP102-Side | 0.23% |
| QUE275-Side | GLU140-Main | 0.04% |
| QUE275-Side | GLU140-Side | 0.00% |
| QUE275-Side | VAL25-Main | 0.06% |

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| Kaemferol |  |  |
| Donor | Acceptor | Occupancy |
| DRG275-Side | LYS41-Side | 0.02% |
| DRG275-Side | ILE157-Side | 4.80% |
| DRG275-Side | GLU63-Side | 0.00% |
| DRG275-Side | ILE76-Side | 15.49% |
| VAL95-Main | DRG275-Side | 6.90% |
| ASP158-Main | DRG275-Side | 0.01% |
| PHE159-Main | DRG275-Side | 0.00% |
| DRG275-Side | GLU99-Side | 19.15% |
| DRG275-Side | GLU93-Main | 8.44% |
| DRG275-Side | VAL95-Main | 1.98% |
| DRG275-Side | ALA39-Side | 4.31% |
| DRG275-Side | ALA96-Main | 3.25% |
| DRG275-Side | LEU18-Main | 2.68% |
| DRG275-Side | LEU18-Side | 1.08% |
| DRG275-Side | ALA96-Side | 0.10% |
| DRG275-Side | LEU92-Side | 6.12% |
| DRG275-Side | VAL26-Side | 2.86% |
| GLY97-Main | DRG275-Side | 29.91% |
| DRG275-Side | MET143-Side | 2.62% |
| DRG275-Side | GLY19-Main | 3.94% |
| DRG275-Side | GLY97-Main | 12.15% |
| DRG275-Side | GLY98-Main | 1.95% |
| ARG147-Side | DRG275-Side | 5.56% |
| DRG275-Side | VAL95-Side | 0.55% |
| DRG275-Side | GLU99-Main | 0.07% |
| GLY19-Main | DRG275-Side | 0.19% |
| DRG275-Side | ARG147-Side | 3.99% |
| GLY98-Main | DRG275-Side | 0.01% |
| DRG275-Side | ASP102-Side | 0.13% |
| GLU99-Main | DRG275-Side | 0.17% |
| DRG275-Side | LEU94-Main | 0.02% |
| DRG275-Side | LEU94-Side | 0.01% |
| GLU93-Main | DRG275-Side | 0.01% |
| LYS41-Side | DRG275-Side | 0.05% |
| SER20-Main | DRG275-Side | 0.77% |
| DRG275-Side | SER20-Main | 0.16% |
| DRG275-Side | GLY21-Main | 0.03% |
| GLY21-Main | DRG275-Side | 0.01% |
| DRG275-Side | LYS28-Side | 0.00% |

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| Fisetin |  |  |
| Donor | Acceptor | Occupancy |
| DRG275-Side | LYS41-Side | 0.11% |
| DRG275-Side | ILE157-Side | 0.93% |
| DRG275-Side | GLU63-Side | 0.01% |
| LYS41-Side | DRG275-Side | 0.04% |
| VAL95-Main | DRG275-Side | 18.77% |
| ASP158-Main | DRG275-Side | 0.06% |
| PHE159-Main | DRG275-Side | 0.01% |
| DRG275-Side | ASN141-Side | 7.84% |
| DRG275-Side | GLU140-Side | 20.90% |
| DRG275-Side | LEU92-Side | 12.28% |
| DRG275-Side | ILE76-Side | 6.23% |
| DRG275-Side | GLU140-Main | 5.69% |
| DRG275-Side | ALA24-Side | 0.08% |
| DRG275-Side | ASP158-Side | 21.07% |
| DRG275-Side | ALA24-Main | 0.19% |
| DRG275-Side | ASN141-Main | 4.79% |
| DRG275-Side | ALA39-Side | 7.69% |
| DRG275-Side | LYS138-Side | 0.35% |
| DRG275-Side | ASP158-Main | 0.00% |
| DRG275-Side | GLY21-Main | 0.08% |
| DRG275-Side | LEU18-Main | 8.37% |
| DRG275-Side | VAL26-Side | 6.71% |
| DRG275-Side | GLY19-Main | 24.61% |
| DRG275-Side | SER20-Main | 4.61% |
| DRG275-Side | VAL95-Side | 0.46% |
| DRG275-Side | VAL95-Main | 12.29% |
| GLY21-Main | DRG275-Side | 0.19% |
| DRG275-Side | LEU18-Side | 3.72% |
| LYS138-Side | DRG275-Side | 0.19% |
| DRG275-Side | ILE157-Main | 1.38% |
| DRG275-Side | GLU93-Main | 15.47% |
| DRG275-Side | MET143-Side | 1.25% |
| SER20-Main | DRG275-Side | 4.80% |
| ASN141-Side | DRG275-Side | 2.03% |
| GLY19-Main | DRG275-Side | 1.05% |
| DRG275-Side | SER20-Side | 0.03% |
| SER20-Side | DRG275-Side | 0.01% |
| DRG275-Side | LEU94-Main | 0.32% |
| DRG275-Side | GLU99-Side | 0.49% |
| DRG275-Side | ALA96-Side | 1.86% |
| DRG275-Side | ALA96-Main | 17.81% |
| DRG275-Side | LEU94-Side | 2.02% |
| ALA96-Main | DRG275-Side | 3.95% |
| DRG275-Side | GLY97-Main | 0.43% |
| DRG275-Side | ALA39-Main | 0.02% |
| DRG275-Side | LEU92-Main | 0.02% |
| GLY98-Main | DRG275-Side | 0.84% |
| DRG275-Side | GLY98-Main | 0.02% |

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| Compound A |  |  |
| Donor | Acceptor | Occupancy |
| UNK275-Side | LYS41-Side | 1.16% |
| UNK275-Side | GLU63-Side | 1.04% |
| UNK275-Side | MET143-Side | 29.71% |
| ASP158-Main | UNK275-Side | 26.87% |
| LYS41-Side | UNK275-Side | 1.16% |
| UNK275-Side | LEU18-Side | 1.13% |
| UNK275-Side | VAL95-Main | 16.17% |
| UNK275-Side | ILE76-Side | 1.55% |
| UNK275-Side | LEU90-Side | 0.05% |
| UNK275-Side | ASP158-Main | 0.26% |
| UNK275-Side | LEU67-Side | 0.70% |
| VAL95-Main | UNK275-Side | 1.05% |
| GLY97-Main | UNK275-Side | 20.92% |
| UNK275-Side | PHE159-Side | 0.02% |
| PHE159-Side | UNK275-Side | 0.01% |
| UNK275-Side | ILE157-Side | 0.73% |
| UNK275-Side | ALA96-Side | 0.02% |
| UNK275-Side | LEU92-Side | 0.71% |
| UNK275-Side | LEU18-Main | 0.16% |
| UNK275-Side | GLY19-Main | 0.08% |
| UNK275-Side | ALA39-Side | 1.58% |
| UNK275-Side | ASP158-Side | 13.72% |
| GLY19-Main | UNK275-Side | 0.05% |
| UNK275-Side | VAL95-Side | 0.07% |
| UNK275-Side | LEU78-Side | 0.06% |
| UNK275-Side | GLY97-Main | 20.67% |
| UNK275-Side | ALA96-Main | 0.04% |
| UNK275-Side | VAL26-Side | 0.11% |
| UNK275-Side | GLU93-Main | 13.67% |
| GLY98-Main | UNK275-Side | 0.00% |
| PHE103-Side | UNK275-Side | 2.26% |
| UNK275-Side | GLY98-Main | 0.58% |
| UNK275-Side | ILE157-Main | 0.00% |
| UNK275-Side | PHE103-Side | 0.01% |
| ARG147-Side | UNK275-Side | 0.82% |
| GLU99-Main | UNK275-Side | 0.23% |
| UNK275-Side | GLU99-Side | 49.69% |
| ARG53-Side | UNK275-Side | 5.97% |
| SER20-Main | UNK275-Side | 0.02% |

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| Compound B |  |  |
| Donor | Acceptor | Occupancy |
| UNK275-Side | VAL95-Main | 0.96% |
| UNK275-Side | GLU93-Main | 132.71% |
| UNK275-Side | ILE157-Side | 0.21% |
| UNK275-Side | LEU94-Main | 0.01% |
| UNK275-Side | GLU63-Side | 212.74% |
| VAL95-Main | UNK275-Side | 0.62% |
| LEU94-Main | UNK275-Side | 0.00% |
| GLU93-Main | UNK275-Side | 22.66% |
| ASP158-Main | UNK275-Side | 54.66% |
| PHE159-Main | UNK275-Side | 59.66% |
| UNK275-Side | LYS41-Side | 4.01% |
| PHE159-Side | UNK275-Side | 16.04% |
| UNK275-Side | LEU18-Main | 0.58% |
| LYS41-Side | UNK275-Side | 3.12% |
| UNK275-Side | ILE76-Side | 3.80% |
| UNK275-Side | PHE159-Side | 0.08% |
| UNK275-Side | MET143-Side | 6.66% |
| UNK275-Side | LEU92-Side | 0.94% |
| UNK275-Side | ASP158-Main | 3.52% |
| UNK275-Side | ALA39-Side | 0.20% |
| UNK275-Side | LEU90-Side | 0.24% |
| UNK275-Side | LEU67-Side | 0.11% |
| UNK275-Side | PHE159-Main | 0.09% |
| GLY160-Main | UNK275-Side | 0.03% |
| UNK275-Side | ASP158-Side | 0.27% |
| GLY19-Main | UNK275-Side | 0.22% |
| UNK275-Side | LEU18-Side | 0.01% |
| UNK275-Side | VAL26-Side | 0.01% |
| UNK275-Side | ILE156-Main | 0.22% |
| GLY97-Main | UNK275-Side | 0.00% |

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| Compound C |  |  |
| Donor | Acceptor | Occupancy |
| UNK275-Side | GLU99-Side | 135.91% |
| UNK275-Side | LEU18-Main | 3.38% |
| UNK275-Side | ILE157-Side | 0.35% |
| UNK275-Side | LYS41-Side | 1.01% |
| LYS41-Side | UNK275-Side | 12.09% |
| VAL95-Main | UNK275-Side | 2.38% |
| ASP158-Main | UNK275-Side | 33.71% |
| PHE159-Side | UNK275-Side | 0.02% |
| GLY19-Main | UNK275-Side | 0.37% |
| UNK275-Side | GLY19-Main | 0.44% |
| UNK275-Side | GLU140-Main | 0.03% |
| UNK275-Side | ASP158-Side | 6.02% |
| UNK275-Side | VAL26-Side | 0.86% |
| UNK275-Side | ILE76-Side | 0.03% |
| UNK275-Side | GLY97-Main | 1.05% |
| UNK275-Side | LEU92-Side | 0.33% |
| UNK275-Side | ASP158-Main | 1.73% |
| UNK275-Side | VAL95-Main | 0.77% |
| UNK275-Side | MET143-Side | 0.72% |
| UNK275-Side | LEU18-Side | 0.07% |
| PHE159-Main | UNK275-Side | 0.00% |
| UNK275-Side | GLU63-Side | 0.00% |
| VAL26-Main | UNK275-Side | 0.00% |
| GLY21-Main | UNK275-Side | 0.13% |
| UNK275-Side | ALA24-Main | 0.01% |
| UNK275-Side | SER20-Main | 0.12% |
| SER20-Main | UNK275-Side | 0.10% |
| UNK275-Side | ALA24-Side | 0.11% |
| UNK275-Side | GLY21-Main | 0.00% |
| UNK275-Side | VAL95-Side | 0.52% |
| UNK275-Side | ILE157-Main | 0.06% |
| GLY97-Main | UNK275-Side | 8.98% |
| GLU99-Main | UNK275-Side | 19.57% |
| UNK275-Side | GLY98-Main | 0.02% |
| LYS28-Main | UNK275-Side | 0.01% |
| UNK275-Side | GLU99-Main | 0.00% |
| UNK275-Side | ASP102-Side | 0.01% |