|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Sample | MuPyV |   |   | MuPyV-Fab |   |   |
| Map composition | capsid | capsomer (pentavalent) | capsomer (hexavalent) | capsid | capsomer (pentavalent) | capsomer (hexavalent) |
| Particle number | 15,499 | 185,988 | 929,940 | 9,146 | 109,752 | 548,769 |
| Symmetry imposed | I1 | C5 | C1 | I1 | C5 | C1 |
| Map resolution (Å) | 3.9Å | 2.9 | 2.9 | 4.2Å | 3.2 | 3.3 |
| Local resolution (Å) |   | 2.7 – 3.1 | 2.7 – 3.1 |   | 2.9 – 3.8 | 3.0 – 3.8 |
| Model composition |   | VP1  | VP1  |   | VP1, 8A7H5 Fab | VP1, 8A7H5 Fab |
|   |   |   |   |   |   |   |
| VP1 |   | chain F (x5) | chain A-E |   | chain F (x5) | chain A-E |
| Protein residues |   | 1660 | 1687 |   | 1660 | 1687 |
| RMS bonds (Å) |   | 0.0044 | 0.0043 |   | 0.0073 | 0.0078 |
| RMS angles (°) |   | 0.76 | 0.72 |   | 0.82 | 0.84 |
| Validation |   |   |   |   |   |   |
| Molprobity Score |   | 2.97 | 2.67 |   | 2.86 | 2.82 |
| Clashscore |   | 11.99 | 9.16 |   | 11.59 | 9.98 |
| Rotamer outliers (%) |   | 11.60 | 8.09 |   | 9.29 | 9.10 |
| Ramachandran plot |   |   |   |   |   |   |
| Favored (%) |   | 89.43 | 91.91 |   | 90.06 | 89.33 |
| Outliers (%) |   | 0.29 | 0.39 |   | 0.29 | 0.34 |
|   |   |   |   |   |   |   |
| Fab |   |   |   |   | 1x | 5x |
| Protein residues |   |   |   |   | 215 | 1070 |
| RMS bonds (Å) |   |   |   |   | 0.0043 | 0.0048 |
| RMS angles (°) |   |   |   |   | 0.74 | 0.85 |
| Validation |   |   |   |   |   |   |
| Molprobity Score |   |   |   |   | 2.95 | 3.35 |
| Clashscore |   |   |   |   | 18.74 | 16.71 |
| Rotamer outliers (%) |   |   |   |   | 8.33 | 19.27 |
| Ramachandran plot |   |   |   |   |   |   |
| Favored (%) |   |   |   |   | 92.31 | 85.78 |
| Outliers (%) |   |   |   |   | 0.00 | 0.46 |