**S3 Table.** Data collection and refinement statistics for Fab667-(NPNA)3 and Fab668-Junc crystal structures.

|  |  |  |
| --- | --- | --- |
| Data collection | Fab668-Junc | Fab667-(NPNA)3 |
| Beamline | SSRL12-2 | SSRL12-2 |
| Wavelength (Å) | 0.97946 | 0.97946 |
| Space group | P1 | P3221 |
| Unit cell parameters (Å, °) | a=58.07, b=60.13, c=76.34 | a=b=70.40, c=186.49 |
|  | α=72.43, β=68.07, γ=83.58 |  |
| Resolution (Å) | 50.00-1.57 (1.60-1.57)a | 50.00-2.05 (2.09-2.05)a |
| Unique Reflections | 111,126 (5,151)a | 32,790 (1,304)a |
| Multiplicity | 7.0 (4.6)a | 9.8 (3.2)a |
| Completeness (%) | 86.8 (80.7)a | 97.7 (78.8)a |
| <I/σI> | 23.3 (2.2)a | 12.0 (1.1)a |
| Rsymb (%) | 18.1 (77.3)a | 17.1 (75.9)a |
| Rpimb (%) | 7.2 (38.9)a | 5.4 (43.2)a |
| CC1/2c (%) | 90.7 (70.3)a | 90.7 (70.6)a |
| Refinement statistics |  |  |
| Resolution (Å) | 35.05-1.57 | 43.53-2.06 |
| Reflections (work) | 105,599 | 31,104 |
| Reflections (test) | 5483 | 1605 |
| Rcrystd / Rfreee (%) | 17.7/21.2 | 20.2/25.8 |
| No. of atoms |  |  |
| Protein | 6741 | 3320 |
| Water | 778 | 166 |
| Buffer | 8 | 16 |
| Average B-value (Å2) |  |  |
| Fab | 25 ± 9 | 53 ± 12 |
| Peptide | 27 ± 9 | 55 ± 9 |
| Water | 34 ± 9 | 55 ± 12 |
| Buffer | 43 ± 4 | 82 ± 12 |
| Wilson B-value (Å2) | 18 | 42 |
| RMSD from ideal geometry |  |  |
| Bond length (Å) | 0.014 | 0.002 |
| Bond angle (°) | 1.40 | 0.53 |
| Ramachandran statisticsf |  |  |
| Favored (%) | 97.92 | 98.14 |
| Outliers (%) | 0.00 | 0.23 |
| Clashscore | 3.75 | 1.83 |

a Numbers in parentheses refer to the highest resolution shell.

b *R*sym = Σ*hkl* Σ*i* | I*hkl,i* - <I*hkl*> | / Σ*hkl* Σ*i* I*hkl,i* and R*pim* = Σ*hkl* (1/(n-1))1/2 Σ*i* | I*hkl,i* - <I*hkl*> | / Σ*hkl* Σ*i* I*hkl,i*, where I*hkl,i* is the scaled intensity of the ith measurement of reflection h, k, l, <I*hkl*> is the average intensity for that reflection, and *n* is the redundancy.

c CC1/2 = Pearson correlation coefficient between two random half datasets.

*d R*cryst = Σ*hkl* | *F*o - *F*c | / Σ*hkl* | *F*o | x 100, where *F*o and *F*c are the observed and calculated structure factors, respectively.

e *R*free calculated as for *R*cryst, but on a test set comprising 5% of the data excluded from refinement.

f From MolProbity (*41*).