

Supplemental Table 3: Data collection and refinement statistics for N-terminus of R2-mutant PRV pUL37

PRV UL37N-R2	
Data collection^a	
Space group	P2221
Cell dimensions	
a, b, c (Å)	51.28, 68.70, 156.23
α, β, γ (°)	90, 90, 90
Resolution (Å)	48.72-2.48 (2.54-2.48)
R _{sym} or R _{merge}	0.126 (0.262)
I/σI	14.8 (3.5)
Completeness (%)	96.5 (67.4)
Redundancy	5.6 (2.2)
Refinement	
Resolution (Å)	48.72-2.50
No. reflections (free)	19218 (1719)
R _{work} / R _{free^b}	0.1781/0.2366
No. atoms	3742
Protein	3610
Solvent	132
B-factors	45.81
Protein	45.94
Solvent	42.25
RMS ^c deviations	
Bond lengths (Å)	0.007
Bond angles (°)	0.779
Ramachandran plot	
Favored (%)	97.69
Allowed (%)	2.31
Outliers (%)	0.0

^aValues in parentheses are for highest-resolution shell.

^bR_{work} and R_{free} are defined as $\Sigma |F_{obs}| - |F_{calc}| / \Sigma |F_{obs}|$ for the reflections in the working or the test set, respectively.

^cRMS, root mean square.

^dAs determined using Molprobity (molprobity.biochem.duke.edu) [Davis IW, Leaver-Fay A, Chen VB, Block JN, Kapral GJ, Wang X, et al. MolProbity: all-atom contacts and structure validation for proteins and nucleic acids. Nucleic Acids Res 2007 Jul;35(Web Server issue):W375-83. PMID: 17452350]