**Supplementary file 2 | Bound nucleotide test.**

|  |  |  |  |
| --- | --- | --- | --- |
|  |  | average real space correlation coefficienta |  |
| structure | nominal resolution(Å) | nucleotide (+Mg2+ if modelled) + contact residuesb | (avgoriginal - avgtest)[(avgoriginal+avgtest)/2](%) |
| L2(ADP) | 4.0 | avgoriginal | 0.7140 | -0.13 |
| L2(ATPtest) | avgtest | 0.7231 |
|  |
| C1(ATP) | 3.9 | avgoriginal | 0.8018 | 3.5 |
| C1(ADPtest) | avgtest | 0.7745 |
|  |
| C2(ATP) | 3.5 | avgoriginal | 0.9053 | 2.5 |
| C2(ADPtest) | avgtest | 0.8826 |
|  |
| C3(ADP) | 4.0 | avgoriginal | 0.8558 | -0.023 |
| C3(ATPtest) | avgtest | 0.8560 |
|  |
| C4(ADP) | 3.6 | avgoriginal | 0.8338 | 1.2 |
| C4(ATPtest) | avgtest | 0.8239 |
|  |
| C5(ATP) | 3.4 | avgoriginal | 0.9064 | 2.3 |
| C5(ADPtest) | avgtest | 0.8857 |

aCalculated using validation tools in PHENIX (Adams et al., 2010).

bThe listed correlation coefficient is an average of the value for the nucleotide, the Mg2+-ion (if modelled), and the following Mfd residues that contact the nucleotide in at least one of the structures: F597, F599, E600, T602, Q605, D629, G631, F632, G633, K634, T635, E636, H665, D729, E730, P780, R783, G874, R902, R905.