2OZK reprocessing

**Before reprocessing**

* **Resolution:**2.90 Å
* **R-Value Free:**0.301
* **R-Value Work:**0.243
* **Bonds:** 0.011
* **Angles:** 1.485

Molprobity

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| All-Atom Contacts | Clashscore, all atoms: | 12.16 | | 96th percentile\* (N=97, 2.90Å ± 0.25Å) |
| Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 169 | 16.02% | Goal: <0.3% |
| Favored rotamers | 699 | 66.26% | Goal: >98% |
| Ramachandran outliers | 28 | 2.37% | Goal: <0.05% |
| Ramachandran favored | 1025 | 86.72% | Goal: >98% |
| MolProbity score^ | 3.14 | | 60th percentile\* (N=3760, 2.90Å ± 0.25Å) |
| Cβ deviations >0.25Å | 9 | 0.80% | Goal: 0 |
| Bad bonds: | 0 / 9575 | 0.00% | Goal: 0% |
| Bad angles: | 6 / 12974 | 0.05% | Goal: <0.1% |
| Peptide Omegas | Cis Prolines: | 0 / 44 | 0.00% | Expected: ≤1 per chain, or ≤5% |
| Cis nonProlines: | 7 / 1146 | 0.61% | Goal: <0.05% |
| Twisted Peptides: | 1 / 1190 | 0.08% | Goal: 0 |
| Low-resolution Criteria | CaBLAM outliers | 66 | 5.7% | Goal: <1.0% |
| CA Geometry outliers | 7 | 0.60% | Goal: <0.5% |
| Additional validations | Chiral volume outliers | 0/1516 | |  |
| Waters with clashes | 0/0 | 0.00% | See UnDowser table for details |

**After reprocessing**

* **Resolution:**2.90 A
* **R-Value Free:** 0.211
* **R-Value Work:** 0.256
* **Bonds:** 0.0105
* **Angles:**  1.808

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| All-Atom Contacts | Clashscore, all atoms: | 7.03 | | 98th percentile\* (N=97, 2.90Å ± 0.25Å) |
| Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 30 | 2.79% | Goal: <0.3% |
| Favored rotamers | 891 | 82.88% | Goal: >98% |
| Ramachandran outliers | 14 | 1.17% | Goal: <0.05% |
| Ramachandran favored | 1114 | 92.83% | Goal: >98% |
| MolProbity score^ | 2.19 | | 98th percentile\* (N=3760, 2.90Å ± 0.25Å) |
| Cβ deviations >0.25Å | 15 | 1.31% | Goal: 0 |
| Bad bonds: | 1 / 9737 | 0.01% | Goal: 0% |
| Bad angles: | 67 / 13197 | 0.51% | Goal: <0.1% |
| Peptide Omegas | Cis Prolines: | 0 / 44 | 0.00% | Expected: ≤1 per chain, or ≤5% |
| Twisted Peptides: | 4 / 1211 | 0.33% | Goal: 0 |
| Low-resolution Criteria | CaBLAM outliers | 37 | 3.1% | Goal: <1.0% |
| CA Geometry outliers | 4 | 0.34% | Goal: <0.5% |
| Additional validations | Chiral handedness swaps | 1/1319 | 0.08% | See Chiral volume report for details |
| Waters with clashes | 6/104 | 5.77% | See UnDowser table for details |

Main differences

A picture containing weapon

Description automatically generatedA close up of a necklace

Description automatically generated

Green = reprocessed Blue = original. Properly formed beta sheet on chain C residues 276-294 and rebuilt loop between sheets.

A picture containing table

Description automatically generatedA picture containing table, room, flower

Description automatically generated

Green = reproessed, Blue = original. Loop rebuilding on C 237-247.

The same changes as above were also made on chain D

A picture containing weapon

Description automatically generated