**Table S3: Summary of steriochemical properties of ICP 7035 using PROCHECK**

|  |  |
| --- | --- |
| **Steriochemical properties of ICP 7035** | **Steriochemical properties of ICPL 84023** |
| **Ramachandran plot** | 95.4% core3.9% allow0.0% gener0.7% disall | **Ramachandran plot** | 93.3% core 6.1% allow 0.0% gener 0.6% disall |
| **All Ramachandrans** | 2 labelled Residues | **All Ramachandrans** | 3 labelled Residues |
| **Chi1-chi2 plots** | 0 labelled residues | **Chi1-chi2 plots** | 1 labelled residues |
| **Side-chain parameters** | 5 better0 inside0 worse | **Side-chain parameters** | 5 better 0 inside 0 worse |
| **Residue properties** | Max.deviation: 4.0Bad contacts: 1Bond len/angle: 3.3Morris et al class: 1,1,2 | **Residue properties** | Max.deviation: 17.4Bad contacts: 1Bond len/angle: 3.8Morris et al class: 1,1,2 |
| **G-factors** | Dihedrals: -0.08Covalent: 0.29Overall: 0.08 | **G-factors** | Dihedrals: -0.08Covalent: 0.23Overall: 0.05 |
| **Planar groups** | 77.3% within limits22.7% highlighted3 off graph | **Planar groups** | 76.5% within limits23.5% highlighted2 off graph |