**A Pareto-Optimal Refinement Method for Protein Design Scaffolds**

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**Supporting Information**

**Table S1**

|  |  |  |  |
| --- | --- | --- | --- |
| **Energy term name** | **INPUTS (mean)** | **COORD (mean)** | **Delta** |
| fa\_dun | 404.19 | 245.01 | -159.18 |
| fa\_rep | 207.59 | 117.73 | -89.86 |
| fa\_cust\_pair\_dist | 27.55 | 1.21 | -26.34 |
| omega | 35.57 | 26.20 | -9.37 |
| ch\_bond\_bb\_bb | -19.50 | -27.90 | -8.40 |
| hbond\_bb\_sc | -77.28 | -84.50 | -7.22 |
| hbond\_sc | -25.29 | -31.98 | -6.69 |
| hbond\_lr\_bb | -60.53 | -67.02 | -6.48 |
| fa\_sol | 531.28 | 527.77 | -3.50 |
| rama | 7.05 | 6.02 | -1.04 |
| pro\_close | -14.67 | -15.51 | -0.85 |
| p\_aa\_pp | -17.86 | -18.66 | -0.80 |
| fa\_pair | 0.88 | 0.39 | -0.49 |
| dslf\_ss\_dst | -0.96 | -1.16 | -0.20 |
| hack\_elec | 2.48 | 2.32 | -0.16 |
| dslf\_cs\_ang | 0.18 | 0.05 | -0.13 |
| hbond\_sr\_bb | -21.29 | -21.41 | -0.12 |
| fa\_atr | -1051.68 | -1051.78 | -0.10 |
| dslf\_ss\_dih | 0.13 | 0.08 | -0.06 |
| ref | -19.69 | -19.69 | 0.00 |
| dslf\_ca\_dih | 0.01 | 0.01 | 0.00 |
| coordinate\_constraint | 0.00 | 60.16 | 60.16 |
| total | -91.84 | -352.66 | -260.82 |
| total\_minus\_coord | -91.84 | -412.81 | -320.98 |

**Table S2.**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **label** | **total INPUT** | **total COORD** | **fa\_dun INPUT** | **fa\_dun COORD** | **fa\_rep INPUT** | **fa\_rep COORD** | **Delta Total** | **Delta fa\_dun** | **Delta fa\_rep** |
| V284 | 19.51 | 0.76 | 3.61 | 1.72 | 18.26 | 1.39 | -18.75 | -1.89 | -16.87 |
| Y286 | 17.38 | -0.29 | 1.34 | 1.60 | 19.94 | 2.49 | -17.67 | 0.26 | -17.45 |
| K188 | 13.95 | 0.34 | 15.61 | 1.54 | 0.43 | 0.26 | -13.61 | -14.08 | -0.17 |
| T161 | 12.90 | 0.01 | 5.12 | 0.69 | 9.78 | 0.39 | -12.89 | -4.43 | -9.39 |
| E157 | 7.92 | -1.20 | 1.48 | 1.59 | 10.16 | 0.85 | -9.13 | 0.11 | -9.31 |
| V212 | 6.91 | -1.20 | 1.92 | 0.67 | 7.81 | 0.69 | -8.11 | -1.25 | -7.12 |
| L144 | 4.54 | -2.35 | 0.17 | 0.34 | 7.87 | 0.76 | -6.89 | 0.17 | -7.11 |
| V129 | 6.82 | 1.32 | 6.74 | 1.39 | 1.97 | 1.32 | -5.50 | -5.35 | -0.64 |
| E156 | 5.16 | -0.20 | 8.50 | 2.28 | 0.27 | 0.43 | -5.36 | -6.22 | 0.16 |
| S131 | 4.75 | -0.07 | 4.65 | 0.35 | 2.47 | 0.98 | -4.82 | -4.29 | -1.49 |

**Table S3.**

|  |  |  |
| --- | --- | --- |
| **Protocol** | **fa\_dun** | **Total** |
| No relax (Y) | 3.0 | 0.41 |
| Restrained relax (Y) | 1.34 | -1.17 |
| No relax after enzdes (E) | 1.31 | -1.14 |
| Restrained relax after enzdes (Y) | 0.48 | -1.62 |



**Figure S1.**



**Figure S2.**

**Release info**

Special issue requirements: We have integration test, demo and documentation:

rosetta\_source/doc/apps/public/prepare\_pdb\_for\_rosetta\_with\_relax.dox

rosetta/rosetta\_tests/integration/tests/relax\_w\_allatom\_cst

/work/nivon/rosetta/rosetta\_demos/public/prepare\_pdb\_for\_rosetta\_with\_relax