

Rosetta Input and Output

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Toward high-resolution prediction and design of transmembrane helical protein structures

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```
../../../../bin/AbinitioRelax.linuxgccrelease -database
../../../../rosetta_database -in:file:fasta ./input_files/1elwA.fasta
-in:file:native ./input_files/1elw.pdb -in:file:frag3
./input_files/aa1elwA03_05.200_v1_3 -in:file:frag9
./input_files/aa1elwA09_05.200_v1_3 -abinitio:relax -relax:fast
-abinitio::increase_cycles 10 -abinitio::rg_reweight 0.5
-abinitio::rsd_wt_helix 0.5 -abinitio::rsd_wt_loop 0.5 -use_filters
true -psipred_ss2 ./input_files/1elwA.psipred_ss2 -kill_hairpins
./input_files/1elwA.psipred_ss2 -out:file:silent 1elwA_silent.out
-nstruct 10
```

How do we get Rosetta?

- <https://www.rosettacommons.org/software/license-and-download>
- Weekly Releases: (e.g. “2016.37”)
 - Latest version of the code, released roughly every week
 - Every revision passes scientific performance tests
- Numbered Releases (e.g. “3.7”)
 - A weekly release that’s relabeled, released roughly every 6 months
- All tutorials use version 2017.36.59679 (December 2017)
- Documentation & Demos:
 - <https://www.rosettacommons.org/docs/latest/Home>
 - <https://www.rosettacommons.org/demos/latest/Home>

The Rosetta Suite

Applications:

- rosetta_scripts
- score_jd2
- relax
- loop_model

Scripts:

- clean_pdb.py
- pdb_renumber.py
- molfile_to_params.py
- make_symmdef_file.pl

What goes in, what comes out

```
../../../../bin/AbinitioRelax.linuxgccrelease -database  
../../../../rosetta_database -in:file:fasta ./input_files/1elwA.fasta  
-in:file:native ./input_files/1elw.pdb -in:file:frag3  
./input_files/aa1elwA03_05.200_v1_3 -in:file:frag9  
./input_files/aa1elwA09_05.200_v1_3 -abinitio:relax -relax:fast  
-abinitio::increase_cycles 10 -abinitio::rg_reweight 0.5  
-abinitio::rsd_wt_helix 0.5 -abinitio::rsd_wt_loop 0.5 -use_filters  
true -psipred_ss2 ./input_files/1elwA.psipred_ss2 -kill_hairpins  
./input_files/1elwA.psipred_ss2 -out:file:silent 1elwA_silent.out  
-nstruct 10
```

Applications

Options



Types of Options

<https://www.rosettacommons.org/docs/latest/full-options-list>

- Types of options:
 - Input files and directories (e.g. “-in:file:fasta”, “-in:file:s”)
 - Output files and directories (e.g. “-out:path:pdb”, “-out:nstruct”)
 - Application specific options (e.g. “-relax:range:angle_max 0.2”)
- How to enter options:

- Command line:

```
score_jd2.default.linuxgccrelease -in:file:s  
test.pdb
```

- Options file (either tab- or space-delimited):

```
score_jd2.default.linuxgccrelease @options.txt
```

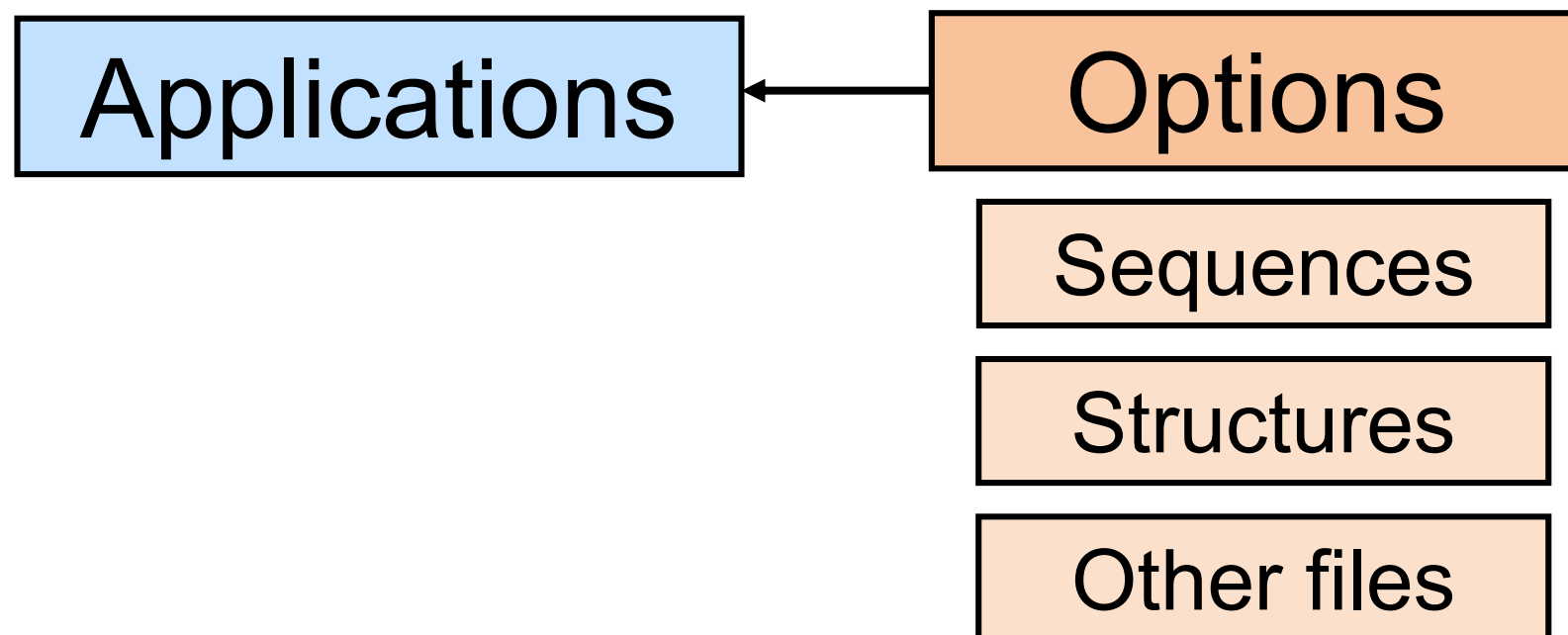
What goes in, what comes out

```
../../bin/AbinitioRelax.linuxgccrelease @options.txt
```

options.txt

```
-database ../../rosetta_database
-in
  -file
    -fasta ./input_files/1elwA.fasta
    -native ./input_files/1elw.pdb
    -frag3 ./input_files/aa1elwA03_05.200_v1_3
    -frag9 ./input_files/aa1elwA09_05.200_v1_3
-abinitio
  -relax
  -increase_cycles 10
  -rg_reweight 0.5
  -rsd_wt_helix 0.5
  -rsd_wt_loop 0.5
-relax:fast
-use_filters true
-psipred_ss2 ./input_files/1elwA.psipred_ss2
-kill_hairpins
-out
  -nstruct 10
  -file
    -silent 1elwA_silent.out
```

What goes in, what goes out



Protein Structure Data

PDB files

- International standard
- Readable by PyMol, MOE, Chimera, etc
- One line per atom
- Useful for small number of structures
- Full info:
www.wwpdb.org/documentation/file-format
- **Must be processed with `clean_pdb.py` prior to use in Rosetta**

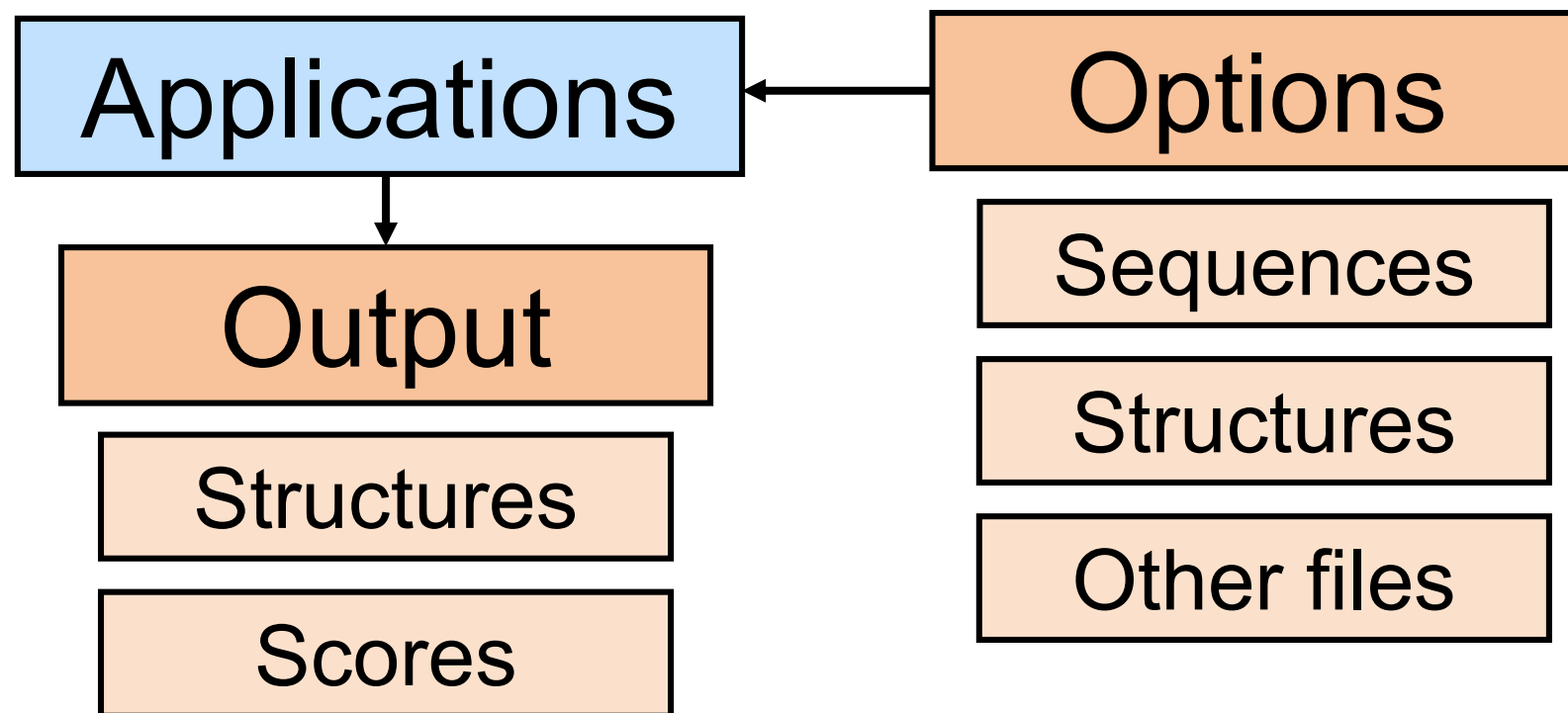
Silent files

- Specific to Rosetta
- Compact
- One line per residue
- Useful for archiving many structures
- Binary silent files: more compact, but not human-readable
- Full info:
https://www.rosettacommons.org/docs/latest/rosetta_basics/file_types/silent-file

Other files: application-specific

- Span File: Defines which residues are in the membrane
- Loops File: Identifies the loop residues for loop closure
- Params File: Custom parameters for small molecules or non-canonical amino acids
- Constraint File: Experimentally derived restraints
- Fragment File: Short protein segments used for comparative modeling and de novo folding
- Res Files: Indicates which residue positions should be designed

What goes in, what goes out



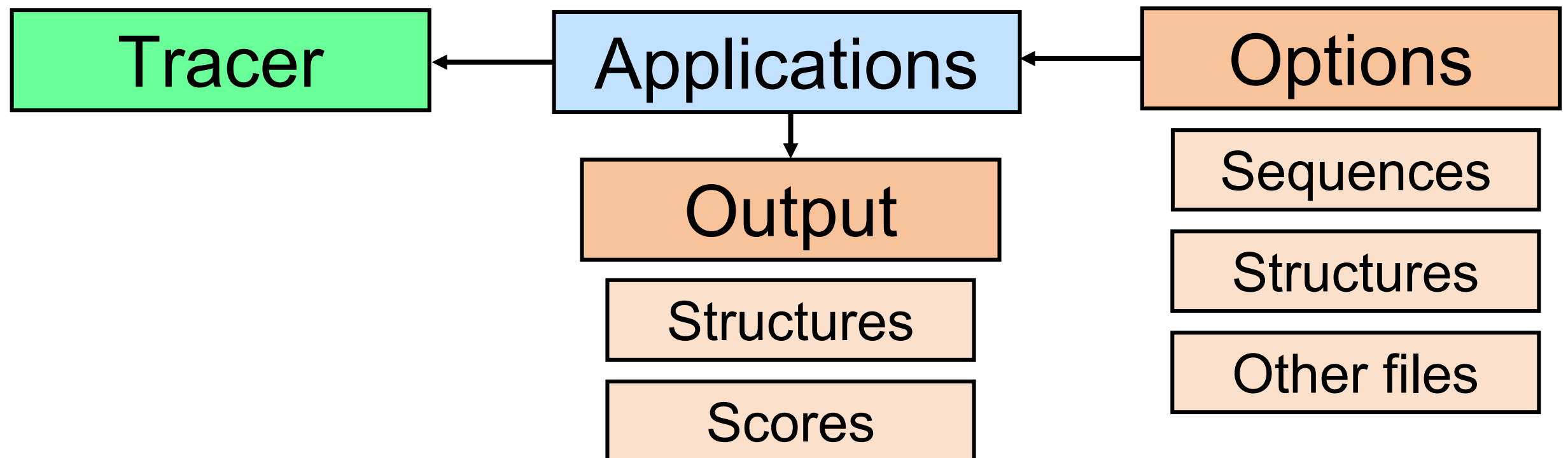
Score tables in output score files

```
SEQUENCE:|
SCORE:  score      fa_atr      fa_rep      fa_sol      fa_intra_rep  fa_elec      ...      omega      fa_dun      p_aa_pp      ref      description
SCORE: -1217.209 -2778.696  266.309  1545.149      5.900  -301.320  ...      63.032  684.989  -109.110  -32.534  3gbm_HA_3gbn_Ab_full_0011
SCORE: -1217.028 -2792.422  263.906  1549.738      5.867  -295.799  ...      66.036  682.694  -108.402  -32.534  3gbm_HA_3gbn_Ab_full_0012
SCORE: -1204.280 -2760.354  259.175  1534.072      5.913  -293.050  ...      65.391  674.840  -108.393  -32.534  3gbm_HA_3gbn_Ab_full_0013
SCORE: -1207.127 -2768.191  260.443  1541.857      5.881  -301.847  ...      67.951  686.381  -110.919  -32.534  3gbm_HA_3gbn_Ab_full_0014
SCORE: -1208.390 -2769.872  262.398  1539.668      5.879  -297.571  ...      64.073  681.731  -109.633  -32.534  3gbm_HA_3gbn_Ab_full_0015
SCORE: -1214.352 -2763.475  252.977  1531.781      5.920  -295.620  ...      65.883  676.240  -109.111  -32.534  3gbm_HA_3gbn_Ab_full_0016
SCORE: -1219.655 -2789.629  264.179  1549.529      5.885  -298.401  ...      63.134  682.856  -108.031  -32.534  3gbm_HA_3gbn_Ab_full_0017
SCORE: -1186.718 -2801.397  279.206  1561.481      5.934  -295.056  ...      67.359  681.528  -105.381  -32.534  3gbm_HA_3gbn_Ab_full_0018
SCORE: -1215.503 -2758.727  255.909  1532.410      5.903  -299.673  ...      66.402  678.984  -111.856  -32.534  3gbm_HA_3gbn_Ab_full_0019
SCORE: -1217.883 -2782.742  259.590  1550.245      5.889  -299.331  ...      63.274  680.028  -108.206  -32.534  3gbm_HA_3gbn_Ab_full_0020
SCORE: -1198.782 -2777.296  263.448  1541.979      5.968  -297.280  ...      68.332  687.685  -109.097  -32.534  3gbm_HA_3gbn_Ab_full_0021
SCORE: -1209.557 -2779.964  261.169  1556.555      5.846  -302.588  ...      63.881  681.855  -109.275  -32.534  3gbm_HA_3gbn_Ab_full_0023
SCORE: -1224.909 -2776.609  259.690  1543.340      5.874  -298.333  ...      63.170  675.545  -110.378  -32.534  3gbm_HA_3gbn_Ab_full_0024
SCORE: -1202.468 -2771.633  263.260  1547.001      5.909  -298.973  ...      65.652  683.601  -109.045  -32.534  3gbm_HA_3gbn_Ab_full_0026
SCORE: -1216.261 -2775.841  257.923  1542.257      5.900  -299.608  ...      66.459  682.661  -109.199  -32.534  3gbm_HA_3gbn_Ab_full_0027
SCORE: -1209.306 -2779.799  262.576  1547.355      5.901  -297.681  ...      65.276  682.562  -109.749  -32.534  3gbm_HA_3gbn_Ab_full_0028
SCORE: -1221.261 -2783.969  262.440  1549.503      5.855  -302.005  ...      64.895  684.862  -108.807  -32.534  3gbm_HA_3gbn_Ab_full_0029
SCORE: -1202.380 -2774.027  259.636  1537.434      5.915  -292.278  ...      66.615  682.911  -108.091  -32.534  3gbm_HA_3gbn_Ab_full_0030
SCORE: -1201.713 -2771.522  259.725  1540.804      5.904  -295.524  ...      67.195  681.868  -108.624  -32.534  3gbm_HA_3gbn_Ab_full_0031
SCORE: -1195.317 -2786.103  273.621  1547.012      5.911  -292.683  ...      68.143  680.827  -107.152  -32.534  3gbm_HA_3gbn_Ab_full_0032
SCORE: -1209.027 -2766.003  256.911  1536.377      5.926  -298.778  ...      64.564  685.533  -109.246  -32.534  3gbm_HA_3gbn_Ab_full_0033
SCORE: -1206.444 -2780.299  265.236  1543.936      5.886  -297.829  ...      64.436  682.950  -107.925  -32.534  3gbm_HA_3gbn_Ab_full_0035
SCORE: -1209.361 -2774.235  259.464  1541.286      5.888  -296.928  ...      67.864  679.797  -109.848  -32.534  3gbm_HA_3gbn_Ab_full_0036
SCORE: -1209.428 -2774.683  264.095  1545.204      5.899  -301.183  ...      65.623  683.858  -107.948  -32.534  3gbm_HA_3gbn_Ab_full_0037
SCORE: -1209.120 -2784.944  266.037  1543.980      5.879  -295.598  ...      65.160  685.062  -109.819  -32.534  3gbm_HA_3gbn_Ab_full_0038
SCORE: -1204.681 -2773.288  264.079  1538.727      5.878  -297.499  ...      65.903  683.761  -108.878  -32.534  3gbm_HA_3gbn_Ab_full_0039
SCORE: -1210.196 -2771.337  263.743  1538.364      5.901  -299.579  ...      65.708  683.140  -109.715  -32.534  3gbm_HA_3gbn_Ab_full_0041
SCORE: -1211.073 -2776.715  259.882  1547.542      5.863  -303.553  ...      67.405  685.284  -108.160  -32.534  3gbm_HA_3gbn_Ab_full_0042
SCORE: -1214.648 -2780.396  261.300  1544.135      5.889  -300.337  ...      66.263  685.718  -109.501  -32.534  3gbm_HA_3gbn_Ab_full_0043
SCORE: -1216.096 -2779.447  260.645  1545.806      5.872  -299.687  ...      66.893  679.556  -108.300  -32.534  3gbm_HA_3gbn_Ab_full_0044
SCORE: -1227.359 -2790.062  261.244  1549.745      5.894  -299.397  ...      63.919  682.009  -109.613  -32.534  3gbm_HA_3gbn_Ab_full_0045
SCORE: -1224.560 -2787.163  263.018  1541.368      5.879  -297.468  ...      65.586  683.252  -109.746  -32.534  3gbm_HA_3gbn_Ab_full_0046
SCORE: -1207.967 -2773.475  261.557  1546.365      5.920  -301.947  ...      66.652  682.649  -109.787  -32.534  3gbm_HA_3gbn_Ab_full_0047
SCORE: -1210.521 -2773.902  257.256  1543.895      5.887  -296.454  ...      66.742  675.904  -107.866  -32.534  3gbm_HA_3gbn_Ab_full_0048
SCORE: -1203.967 -2767.613  263.371  1541.055      5.876  -297.629  ...      64.674  681.230  -110.923  -32.534  3gbm_HA_3gbn_Ab_full_0049
SCORE: -1206.728 -2759.167  259.854  1529.948      5.906  -297.720  ...      65.498  683.356  -110.453  -32.534  3gbm_HA_3gbn_Ab_full_0050
```

Score tables in output PDB files

```
ATOM 3378 HB THR L 227 -36.166 22.580 28.848 1.00 0.00 H
ATOM 3379 HG1 THR L 227 -34.994 19.987 29.136 1.00 0.00 H
ATOM 3380 1HG2 THR L 227 -34.138 22.579 30.246 1.00 0.00 H
ATOM 3381 2HG2 THR L 227 -35.593 22.831 31.238 1.00 0.00 H
ATOM 3382 3HG2 THR L 227 -34.799 21.240 31.213 1.00 0.00 H
TER
# All scores below are weighted scores, not raw scores.
#BEGIN_POSE_ENERGIES_TABLE 3gbn_Ab_0005.pdb
label fa_atr fa_rep fa_sol fa_intra_rep fa_elec pro_close hbond_sr_bb hbond_lr_bb hbond_bb_sc hbond_sc dslf_fa13 rama omega fa_dun p_aa_pp yhh_planarity ref total
weights 1 0.55 0.9375 0.005 0.875 1.25 1.17 1.17 1.17 1.1 1.25 0.25 0.625 0.7 0.4 0.625 1 NA
pose -994.338 137.719 561.027 2.15688 -112.612 19.7634 -12.2069 -79.5391 -24.1449 -23.4441 -1.15166 -7.47192 71.8572 276.633 -29.8673 0.09431 13.9828 -201.541
GLU:NtermProteinFull_1 -1.58225 0.53996 1.45283 0.00353 0.06909 0 0 0 0 0 0 0 0.01109 6.53174 0 0 -1.96094 5.06505
VAL_2 -3.34255 0.45648 1.46378 0.01322 -0.08167 0 0 0 0 0 0 -0.16095 0.87346 0.30715 0.39992 0 0.97964 0.90848
GLN_3 -2.79445 0.10936 1.74929 0.00451 -0.52743 0 0 0 -0.35772 0 0 -0.09682 0.35321 2.59775 0.02034 0 -1.51717 -0.45911
LEU_4 -5.13483 0.73792 1.6574 0.00685 -0.16379 0 0 0 0 0 0 0.06265 0.2281 2.29891 -0.1217 0 0.76113 0.33264
VAL_5 -2.72905 0.12167 1.72074 0.00789 -0.45069 0 0 0 0 0 0 -0.27382 0.01969 0.02557 -0.49649 0 0.97964 -1.07485
...
TYR_205 -9.68927 0.6599 4.04398 0.02918 -1.11866 0 0 0 -0.69927 -0.4197 0 -0.03371 0.01485 1.86931 -0.07409 0.02555 0.1625 -5.22942
TYR_206 -8.27907 0.53027 3.95082 0.03533 -0.75969 0 0 0 0 0 0 -0.10219 0.77773 2.1235 -0.06518 0.00994 0.1625 -1.61604
CYS:disulfide_207 -4.8779 0.37363 2.6835 0.00127 -0.70663 0 0 0 -0.56501 0 -0.29622 -0.22449 0.0286 1.4135 -0.08388 0 0.44379 -1.80984
ALA_208 -4.48831 0.2957 1.92707 0.00107 -0.48653 0 0 0 0 0 0 0.05006 0.28785 0 -0.24738 0 0.77374 -1.88673
THR_209 -5.73046 0.81574 3.59921 0.00829 -1.2848 0 0 0 -0.46497 0 0 0.23162 0.01866 0.16545 -0.28654 0 0.20134 -2.72646
...
THR_224 -6.10085 0.26779 3.79175 0.00865 -0.91162 0 0 0 -0.45219 -0.61107 0 0.02255 0.07826 0.06259 -0.14086 0 0.20134 -3.78367
LYS_225 -3.90687 0.70976 2.6297 0.00615 -0.81559 0 0 0 0 0 0 -0.04424 0.00136 0.98794 0.09041 0 -0.35857 -0.69994
LEU_226 -5.97934 0.46605 2.34857 0.02903 -0.32933 0 0 0 0 0 0 -0.08426 0.1675 2.62906 -0.15244 0 0.76113 -0.14405
THR:CtermProteinFull_227 -3.2336 0.44967 3.66532 0.00842 -0.88667 0 0 0 -0.13737 0 0 0 0.062 0 0 0.20134 0.1291
#END_POSE_ENERGIES_TABLE 3gbn_Ab_0005.pdb
bref_irms 0.0777809
cen_irms 0.0777809
final_chainbreak 0.143091
final_looprelax_score -201.541
irms 0.0630764
```

What goes in, what goes out



Tracer Output

```
core.init: Rosetta version exported from http://www.rosettacommons.org
core.init: command: /dors/meilerlab/apps/rosetta/rosetta_2016.08.58479/main/source/bin/rosetta_scripts.default.linuxgccrelease @docking.options -parser:protocol docking
core.init: 'RNG device' seed mode, using '/dev/urandom', seed=1059677151 seed_offset=0 real_seed=1059677151
core.init.random: RandomGenerator:init: Normal mode, seed=1059677151 RG_type=mt19937
core.init: Resolved executable path: /dors/meilerlab/apps/rosetta/rosetta_2016.08.58479/main/source/build/src/release/linux/2.6/64/x86/gcc/5.2/default/rosetta_scripts.d
core.init: Looking for database based on location of executable: /dors/meilerlab/apps/rosetta/rosetta_2016.08.58479/main/database/
protocols.jd2.PDBJobInputter: Instantiate PDBJobInputter
protocols.jd2.PDBJobInputter: PDBJobInputter::fill_jobs
protocols.jd2.PDBJobInputter: pushed 3gbm_HA_3gbn_Ab.pdb nstruct indices 1 - 50
protocols.evaluation.ChiWellRmsdEvaluatorCreator: Evaluation Creator active ...
protocols.jd2.JobDistributor: Parser is present. Input mover will be overwritten with whatever the parser creates.
protocols.jd2.PDBJobInputter: PDBJobInputter::pose_from_job
protocols.jd2.PDBJobInputter: filling pose from PDB 3gbm_HA_3gbn_Ab.pdb
core.chemical.ResidueTypeSet: Finished initializing fa_standard residue type set. Created 384 residue types
core.chemical.ResidueTypeSet: Total time to initialize 0.43 seconds.
core.conformation.Conformation: Found disulfide between residues 7 461
...
protocols.rosetta_scripts.ParsedProtocol.REPORT: =====End report for =====
protocols.rosetta_scripts.ParsedProtocol.REPORT: =====Begin report for =====
protocols.rosetta_scripts.ParsedProtocol.REPORT: =====End report for =====
protocols.jd2.JobDistributor: 3gbm_HA_3gbn_Ab_full_0050 reported success in 381 seconds
protocols.jd2.JobDistributor: no more batches to process...
protocols.jd2.JobDistributor: 50 jobs considered, 50 jobs attempted in 16297 seconds
~
~
```

Options to control tracer output:

- Silence certain tracers:
 - mute core.chemical.ResidueTypeSet
- Change verbosity level (Error/Warning/Info/Debug/Trace)
 - out:levels all:Warning core.init:Info

Any Questions?