mini/bin/holes.linuxgccrelease

```
RosettaHoles:      tag    holes   resl    decoy     rmsd    score
RosettaHoles: 1a19_0001 2.14604 1.8894 0.473602 0.645096 -147.615
```

Option Name	Details
-holes:dalphaball	location of DAlphaBall program (/work/sheffler/bin/DAlphaBall.icc on digs)
-holes:make_pdb	make a pdb with the per-atom scores in the temperature column
-holes:make_voids	put explicit rep. of cavities into PDB (slow)
-packstat:cavity_burial_probe_radius	Radius to define cavity burial -- exposed cavities are pruned away (default 1.6Å)
-packstat:include_water	Don't throw away waters before doing void calculation
-packstat:surface_accessibility	Compute surface accessibility of cavities (SLOW)

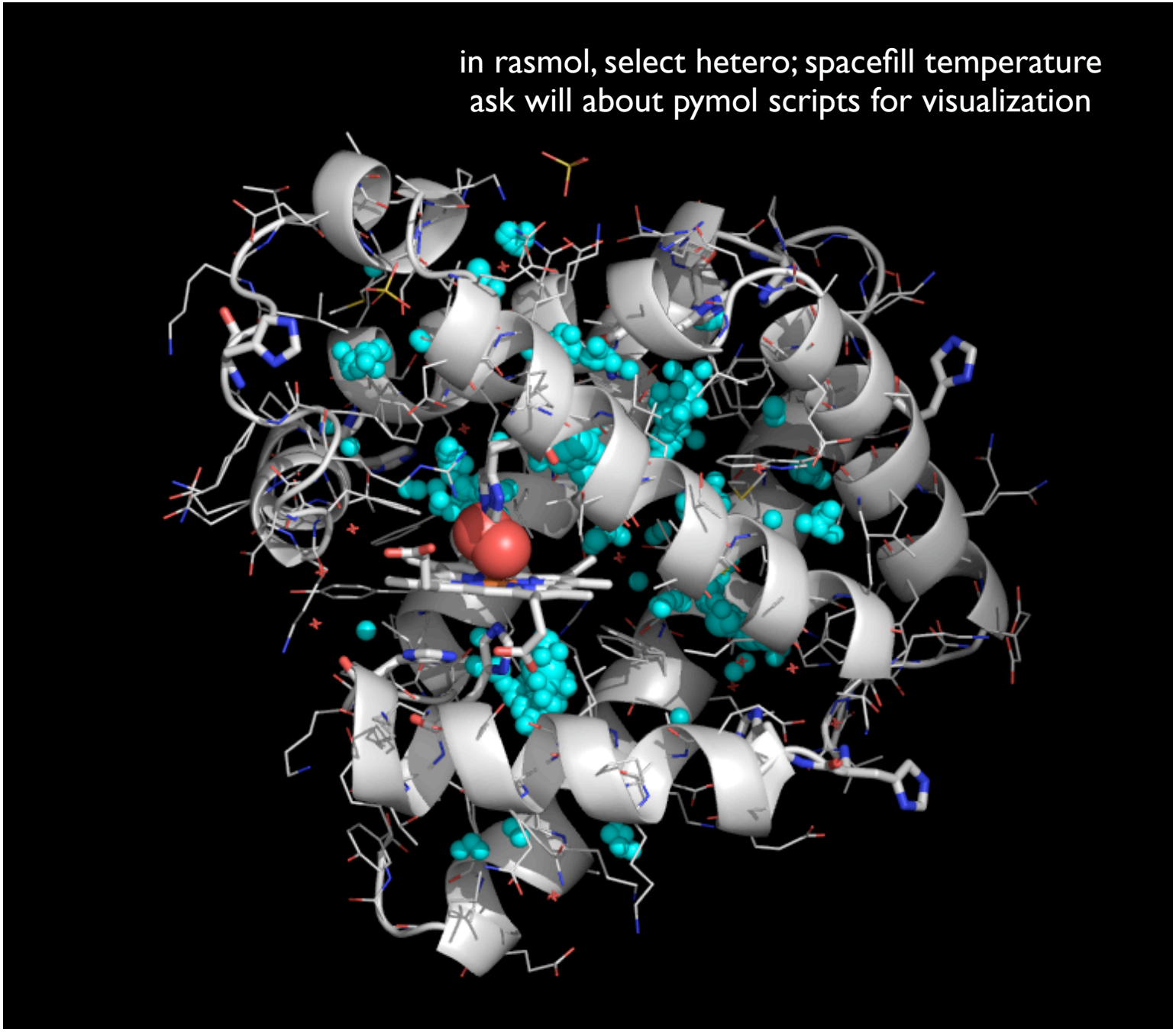
Also available as **holes**, **holes_resl**, and **holes_decoy** ScoreTypes*

*if your decoy isn't relaxed after 4 hours, consult a physician

The packing scores

score	range	interpretation
decoy	-5 to 5	discriminatory, low if native-like
Pdecoy	0 to 1	sigmoid(decoy score)
resl	0 to 4	correlates w/ X-ray Resolution
holes	0 to 7	resl. score + 3 * Pdecoy

output from -hoes:make_voids



core/scoring/packing/compute_holes_score.hh

```
/// the result class holding the three scores and the per-atom scores
class HolesResult : public utility::pointer::ReferenceCount {
public:
   HolesResult() : score(0.0),decoy_score(0.0),resl_score(0.0) {}
   core::Real score, decoy_score, resl_score;
   core::id::AtomID_Map< core::Real > atom_scores;
};

/// for the standard scores
HolesResult
compute_rosettaholes_score(
   pose::Pose const & pose
);

/// if you have custom parameters, or want per-atom scores for a specific score
/// result goes into the "score" field
HolesResult
compute_holes_score(
   pose::Pose  const & pose,
   HolesParams const & params
);

/// computes the cartesian space derivative WRT the given params
HolesResult
compute_holes_deriv(
   pose::Pose  const & pose,
   HolesParams const & params,
   core::id::AtomID_Map< numeric::xyzVector<core::Real> > & deriv
);
```