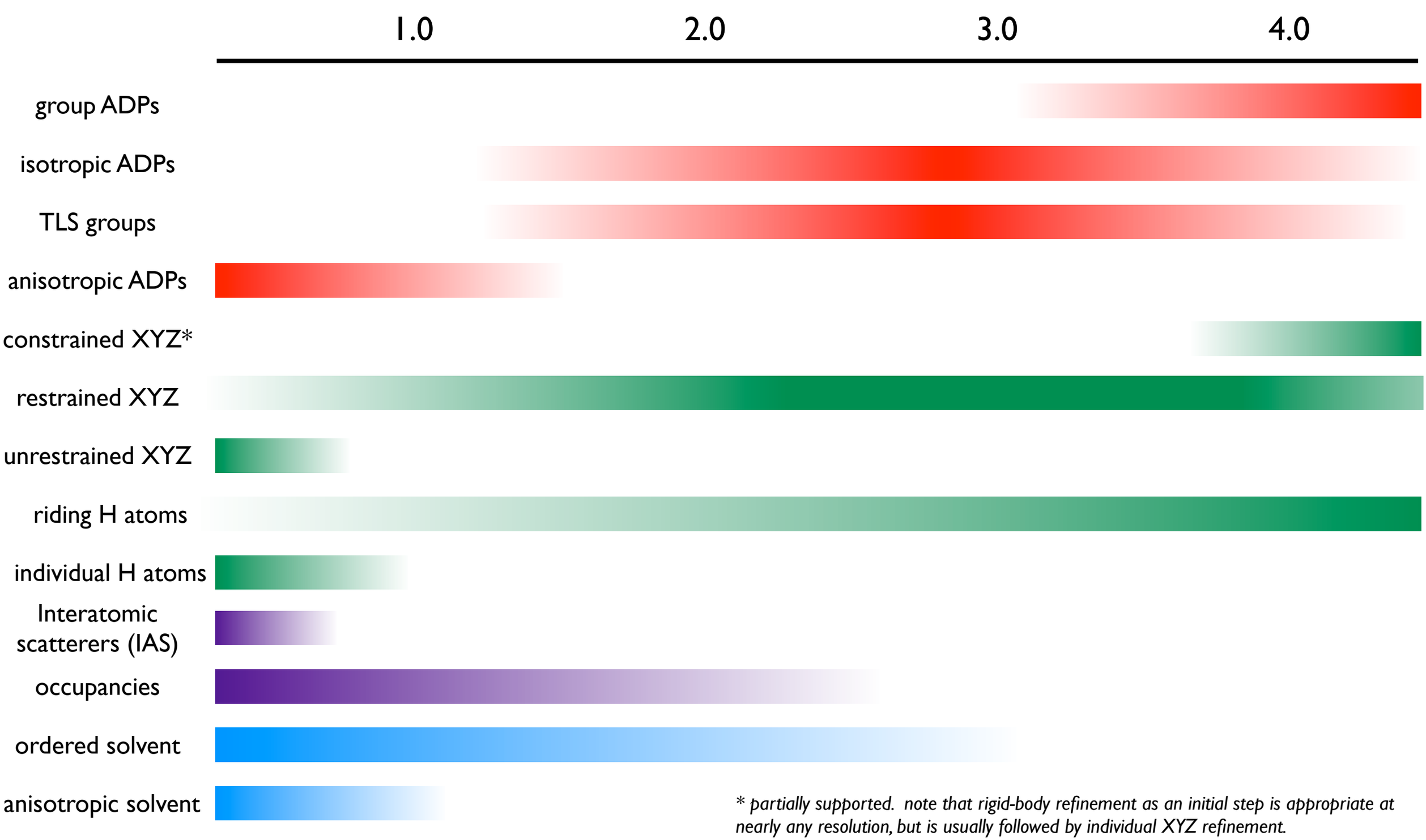
Refinement strategy versus resolution

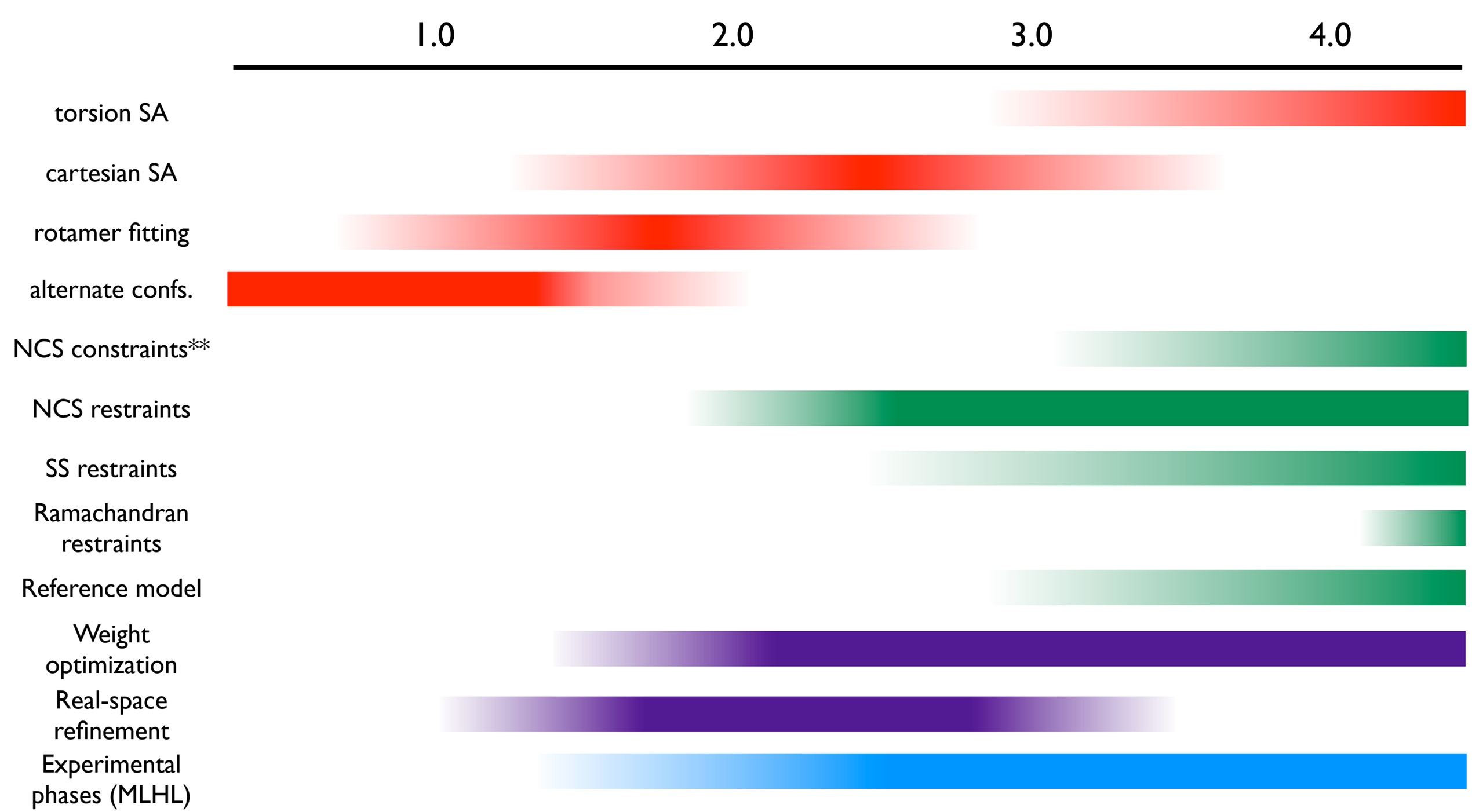


** partially supported. note that rigid-body refinement as an initial step is appropriate at nearly any resolution, but is usually followed by individual XYZ refinement.*

***Very** approximate - more dependent on # of observations than absolute resolution!*

Model quality also needs to be considered

Other options versus resolution



** *not yet available in PHENIX*

Three common scenarios: resolution

- **4.0 Å ("low resolution"):** individual sites, individual or grouped B-factors, TLS, reciprocal-space minimization, very tightly restrained with weight optimization (if applicable: NCS, reference model, secondary structure, experimental phases)
- **2.5Å ("medium resolution"):** individual sites, individual isotropic B-factors, TLS, real-space and reciprocal-space minimization, rotamer fitting, solvent picking, NCS restraints, experimental phases
  - later in refinement: add weight optimization, no real-space
- **1.0Å ("atomic resolution"):** individual sites, anisotropic B-factors, reciprocal-space minimization, explicit hydrogens, occupancies for alternate conformations; loosely restrained

(note: these options are specific to phenix.refine, but many have equivalents in other programs)