



# Structural Biology

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Uniquely positioned to drive Integrated  
Drug Discovery (IDD) program for small and large molecules

Gene to Structural Programs | Complex Targets |  
Design to Enhance Crystallizability



## Gene to co-crystal structure service

- Screen in high throughput fashion for co-crystals
  - Micro and macro seeding for co-crystals
  - Soaking with small molecules
- Synchrotron data collection for high resolution information
- Molecular replacement structure determination

## Gene to novel structure service

- Crystallize novel targets, domain antibody-antigen complexes and protein-protein complexes
- 10,000 unique conditions to screen for initial hits and high throughput optimization
- Molecular replacement or experimental phasing and structure determination from data collected at a synchrotron

## Quality attributes to be targeted

- 2.6 Å or better resolution
- >85% completeness
- $I/\text{Sig } I > 1.5$  (in highest resolution bin)
- 20 or better  $R_{\text{work}}$
- 25 or better and  $R_{\text{free}}$
- Bond angle RMSD 0.02
- Bond length RMSD 1.5
- >80% Average correlation co-efficient
- Discernable electron density of ligand (if present)

