Structure Analysis and Deposition Tools in CCP4

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CCP4 is a Structure Solution Suite

- CCP4 contains more than 250 program components
  - ~30% components directly related to structure solution

    MOSFLM, XIA2, DIALS, POINTLESS, AIMLESS, PHASER, MOLREP, AMORE, BEAST, REFMAC, BUCCANEER, PIRATE, DM, PARROT, SOLOMON, MRBUMP, BALBES, CRANK, COOT etc.

  - ~45% components assisting structure solution

    CHAINSAW, HGEN, WATERTIDY, CTRUNCATE, PROFESS, LIBCHECK, SFALL, SKETCHER, JLIGAND, ECALC, RFCORR, DETWIN, SAPI, WATPEAK, SEQWT etc.

  - ~20% related to file transforms and various jiffies

    COORD_FORMAT, PDBSET, PDBCUR, PDB2TO3, COORDCONV, GENSYM, SYMCONV, PHISTATS, STEREO, MTZDUMP, PDB_EXTRACT, F2MTZ, MTZ2CIF, MTZ2VARIOUS, MTZUTILS, SORTMTZ etc.

  - ~5% post-structure solution analysis

    A relatively small subset of the Suite that may be used by structural biologists to aid their research when they have their solved or otherwise obtained structures

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Structure Analysis in CCP4

Coordinate analysis

ACT	*general coordinate analysis: contacts, statistics, selection on B-factors etc*
CONTACT/NCONT	*calculation of various atomic contacts, h-bond candidates etc*
DISTANG	*calculation of interatomic distances and angles*
GEOMCALC	*calculation of various structure features such as planes, deviations from planes, interatomic distances, inter-plane angles, torsions, coordinate transforms and many more*

Domain identification

DYNDOM	*identification of dynamic domains when two protein conformations are available*

Quality checks

PROCHECK	*checks stereochemical quality of protein structures*
ROTAMER	*identification of unusual rotamer configurations*
SFCHECK	*assessment of the agreement between structure and x-ray data*

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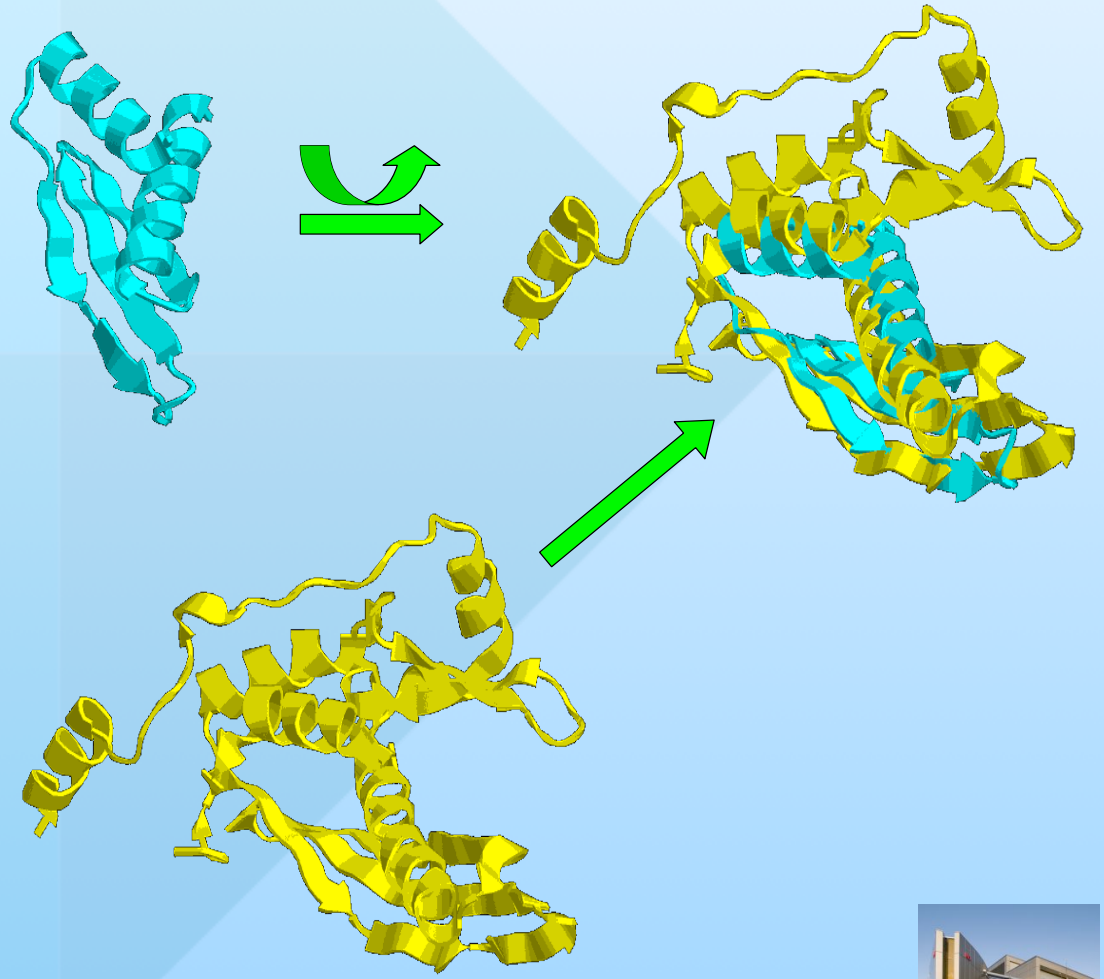
Structure Analysis in CCP4

- Structure alignment, superpositon and comparison

LSQKAB	*superposition of given coordinate subsets*
POLYPOSE	*multiple superposition of same-length structures (conformers)*
TOPP	*topological analysis of protein structures*
SUPERPOSE	*generic structure aligner and superposer, with automatic identification of superposing subsets, based on SSM algorithm*
GESAMT	*generic structure aligner and superposer, with automatic identification of superposing subsets, free from SSM limitations*
PROSMART	*structure aligner and superposer for the calculation of external crystallographic restraints*



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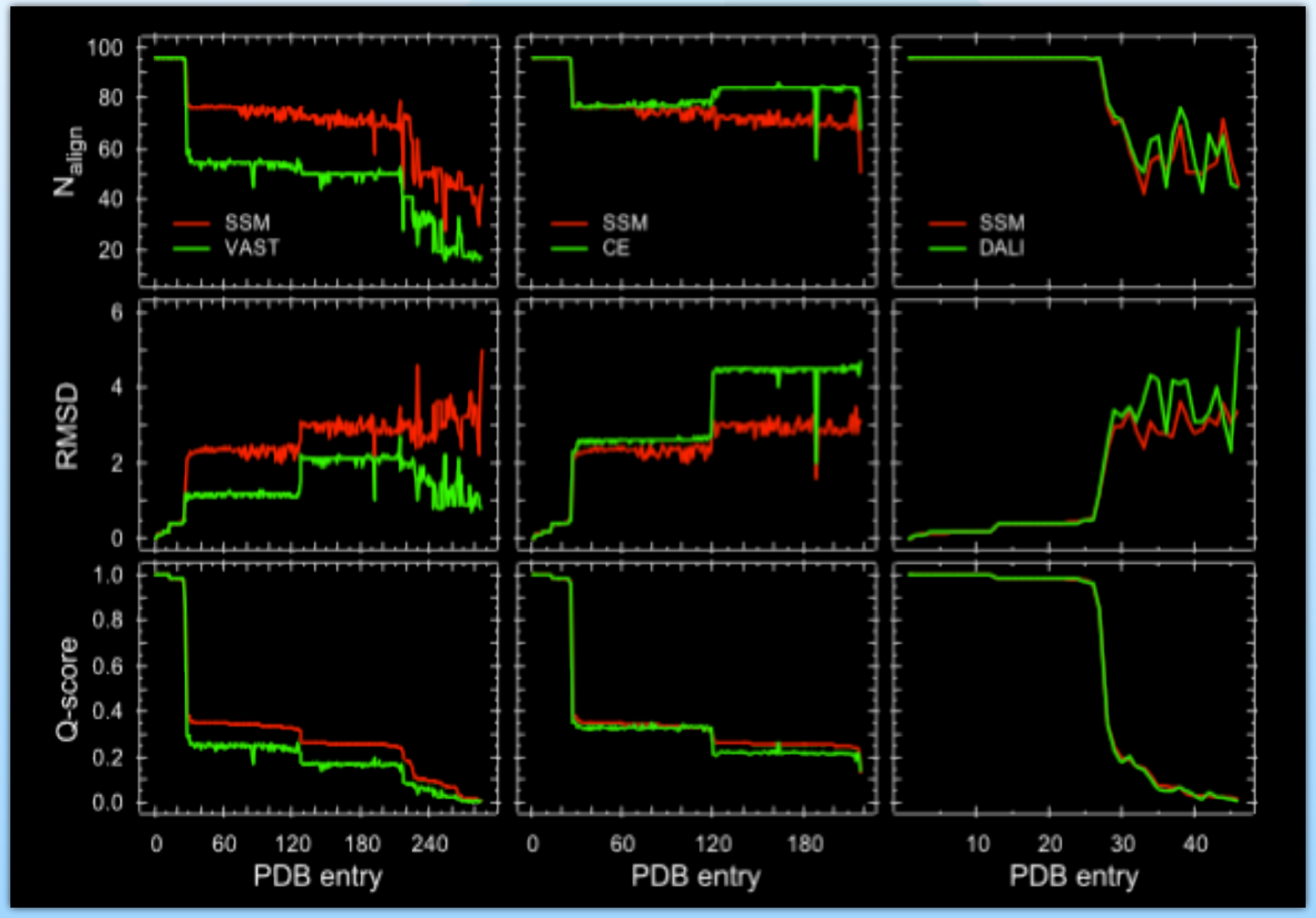
Quality of Structure Alignment

- Often not very well understood
- Depends on measure
- No agreement on the measure

$$Q = \frac{N_{align}^2}{\left(1 + \left(rmsd/R_0\right)^2\right) N_A N_B}$$

Acta Cryst D (2004), **60,** 2256-68



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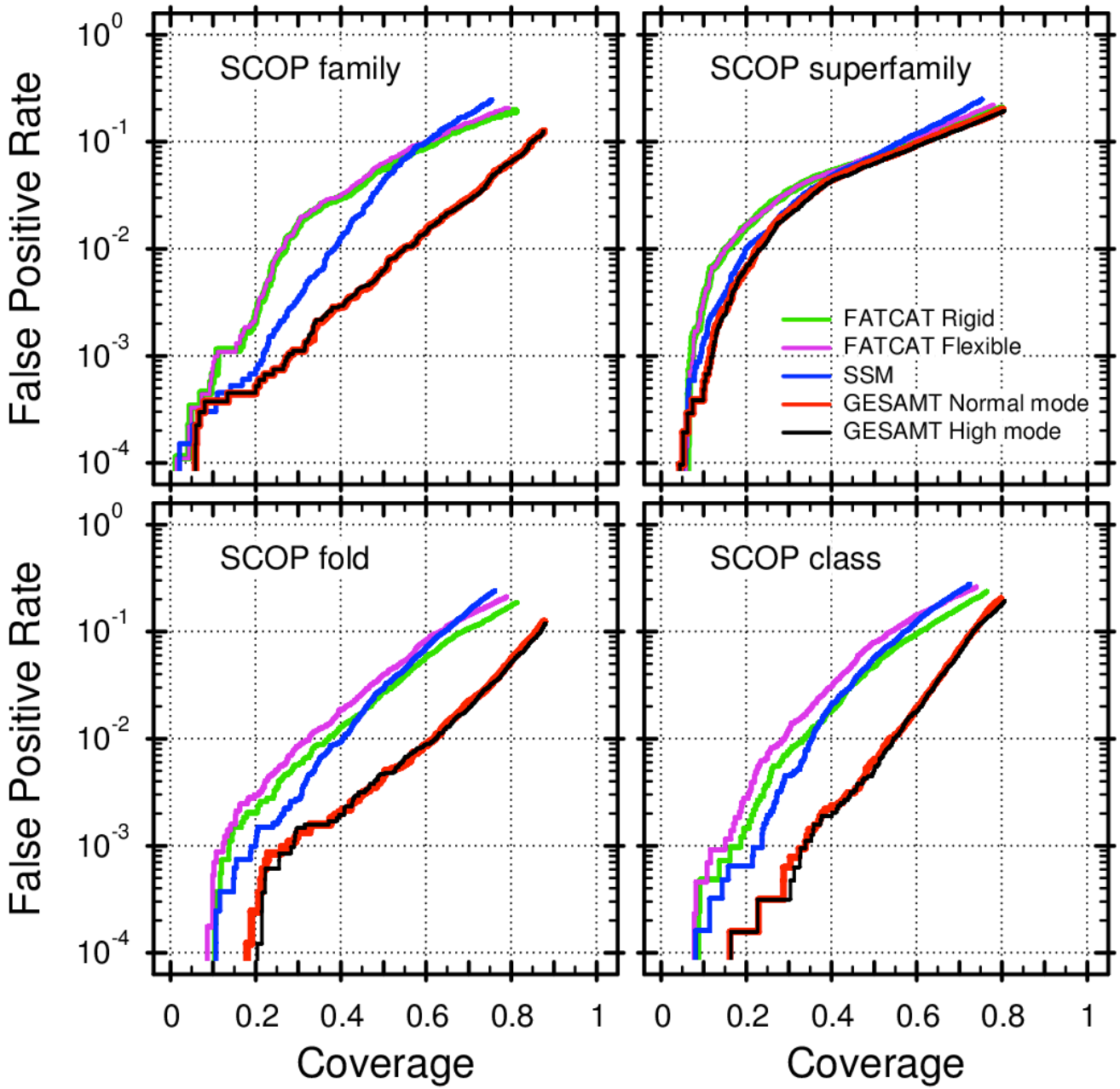
Quality of Structure Alignment



$$FPR = \frac{FP}{TN + FP}$$

$$Coverage = \frac{TP}{TP + FN}$$

TP : True Positives
TN : True Negatives
FP : False Positives
FN : False Negatives

J. Mol. Biochem. (2012), **1,** 76-85

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Structure Analysis in CCP4

Surface analysis

CAVENV	*"visualisation" of cavities (through the generation of a "cavity map")*
SC	*assessment of shape complementarity*
AREAIMOL	*surface and interface area calculations*
SURFACE	*assessment of surface accessibility*
VOLUME	*polyhedral volume of selected part of a protein*

Visualisation

TOPDRAW	*sketchpad for protein topology diagrams (obsoleted)*
CCP4 MG	*advanced Molecular Graphics viewer*

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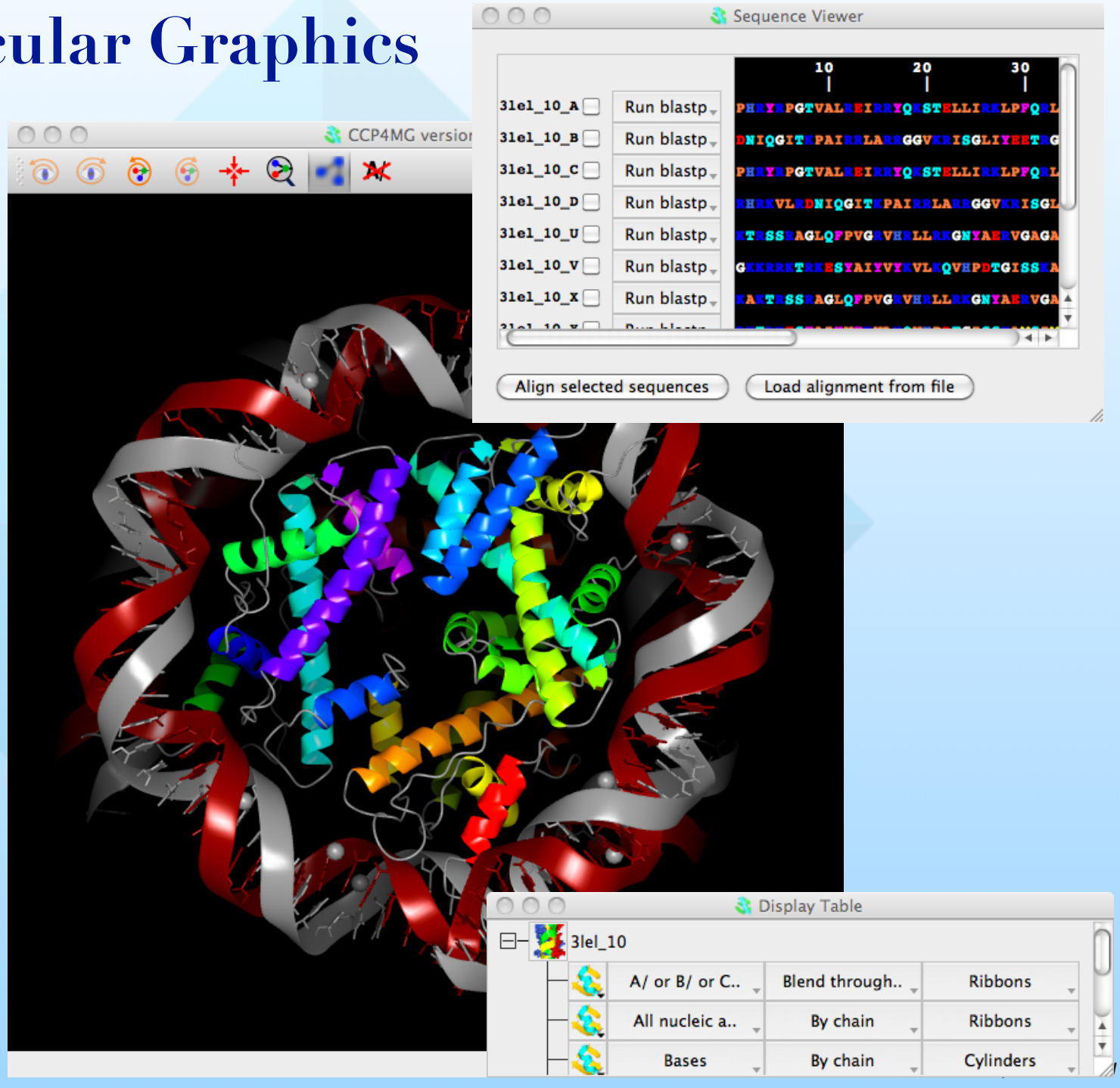
CCP4 Molecular Graphics

Version 2.11.0: Top-Standard Molecular Imaging

- fast and (almost) stable
- highest publication-quality rendering
- flexible image composition
- rich set of tools and options
- developed selection capabilities
- integrated with other CCP4 components, such as SSM and PISA
- connected to external web-services from NIH, PDB, Uppsala and EBI
- stereo capabilities
- integrated structure analysis
- integrated sequence and structure alignment
- normal mode analysis
- movies
- advanced Picture Wizard
- open architecture with PyQt framework



Structure Analysis in CCP4

- Protein interactions and complexes

  PISA *analysis of Protein Interactions, Surfaces and Assemblies*

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