

View Model building

Model building

Imports

- import volumes
- import atomic structure
- import sequence

Preprocess map

- xmipp3 - create 3d mask
- xmipp3 - local MonoRes
- xmipp3 - localdeblur sharpening
- xmipp3 - extract unit cell

Initial model

- chimera - model from template

Rigid fitting

- powerfit_scipion - powerfit
- chimera - chimera rigid fit

Flexible fitting

- phenix - real space refine
- ccp4 - coot refinement
- ccp4 - refmac

Validation

- phenix - emringer
- phenix - molprobity
- phenix - validation_cryoem

Tools-Calculators

- phenix - superpose pdbs
- atomstructutils - operator
- atomstructutils - convert_sym
- chimera - chimera operate
- chimera - chimera restore session
- chimera - contacts

Others

- xmipp3 - 3d bionotes

Exports

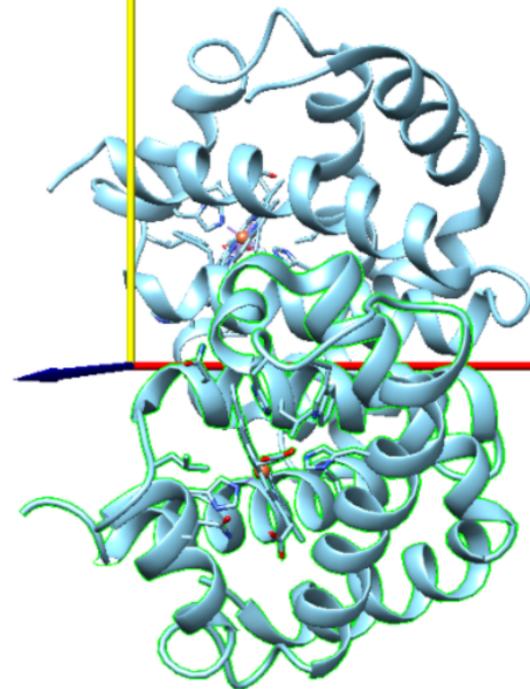
- export to EMDB

Consensus	1	m v L S a a D K t n	11	v k a a W s K i g g	21	H a g e y G A E A L	31	E R M F I g y P T T	41	K T Y F P H F - D I	51
Conservation		- . D K I K A A		V R A W K I G K		A A A G N D A L		S R M V V P Q		K V E R H W P D V	
1pbx_A		M V L S P A D K T N		V K A A W G K V C		A A A G N D A L		S R M V V P Q		K V E R H W P D V	
P69905		- M L T E D D K Q L		I Q H V W E K V L		A A A G N D A L		S R M V V P Q		K V E R H W P D V	
HBA_ALDGI		M V L S A A D K N N		V K G I F T K I A		A A A G N D A L		S R M V V P Q		K V E R H W P D V	
HBA_MELGA		M V L S P A D K T N		I K T A W E K I G		A A A G N D A L		S R M V V P Q		K V E R H W P D V	
HBA_RABIT		M V L S A A D K T N		V K A A W S K V G		A A A G N D A L		S R M V V P Q		K V E R H W P D V	
HBA_HORSE		M V L S A A D K T N									

Consensus	91	h K L R V D P V N F	101	
Conservation		- K L R V D P V N F		
1pbx_A		Y K L R V D P V N F		
P69905		H K L R V D P V N F		
HBA_ALDGI		Y N L R V D P V N F		
HBA_MELGA		H K L R V D P V N F		
HBA_RABIT		H K L R V D P V N F		
HBA_HORSE		H K L R V D P V N F		

UCSF Chimera

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Summary Methods Output Log

Input

inputSequencesToAlign

- 001 (from scipion - import sequence ALDGI -> outputSequence ALDGI)
 - 002 (from scipion - import sequence MELGA -> outputSequence MELGA)
 - 003 (from scipion - import sequence RABIT -> outputSequence RABIT)
 - 004 (from scipion - import sequence HORSE -> outputSequence HORSE)
- pdBfileToBeRefined (from scipion - import atomic structure 1P)

SUMMARY

No output file produced

Command: split #2

Active models: 0 1 2 3 4 5 6 7 8 9 All