MobyleNet

http://mobylenet.rpbs.univ-paris-diderot.fr

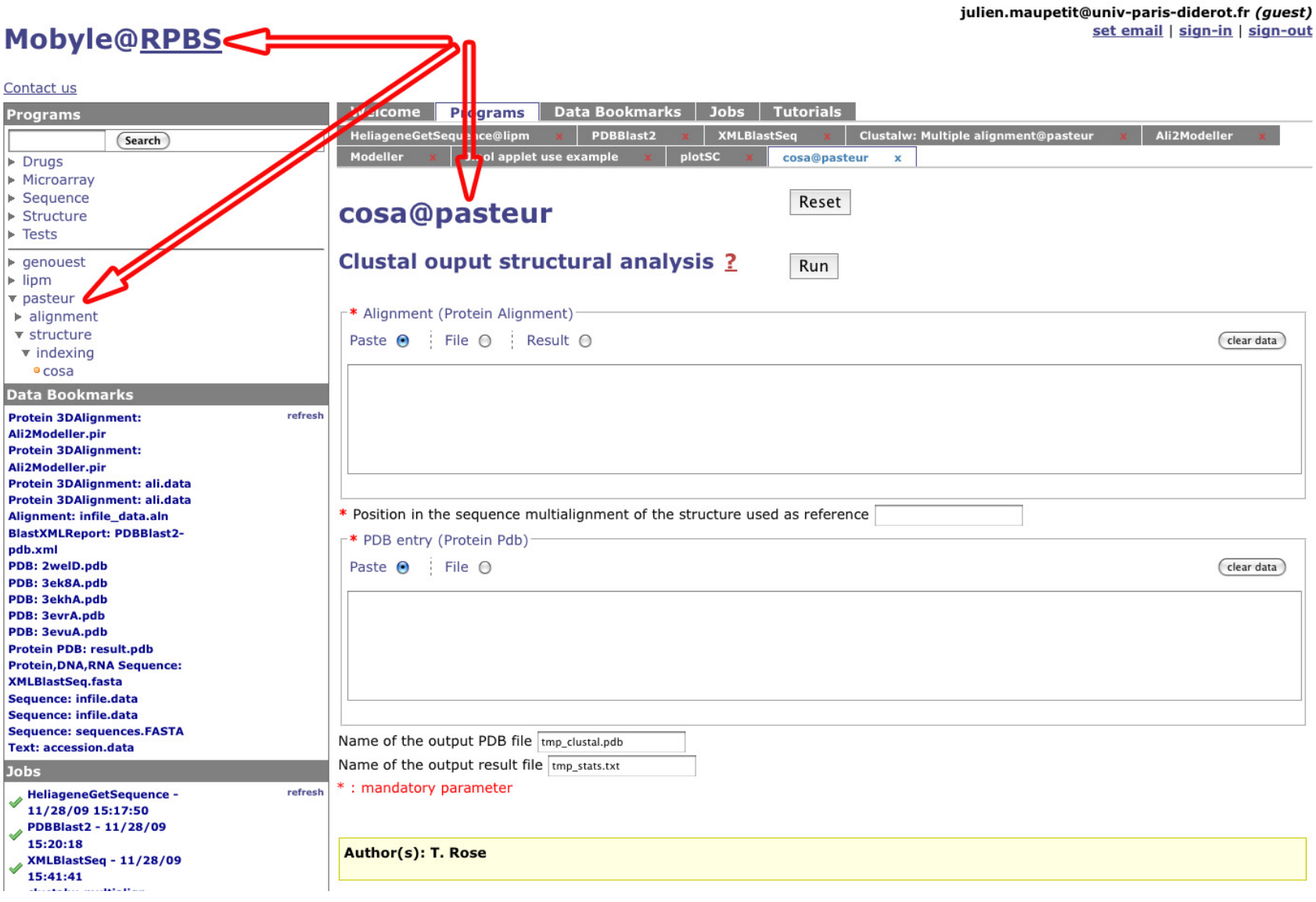
Julien Maupetit, Pierre Tufféry.

-RPBS-

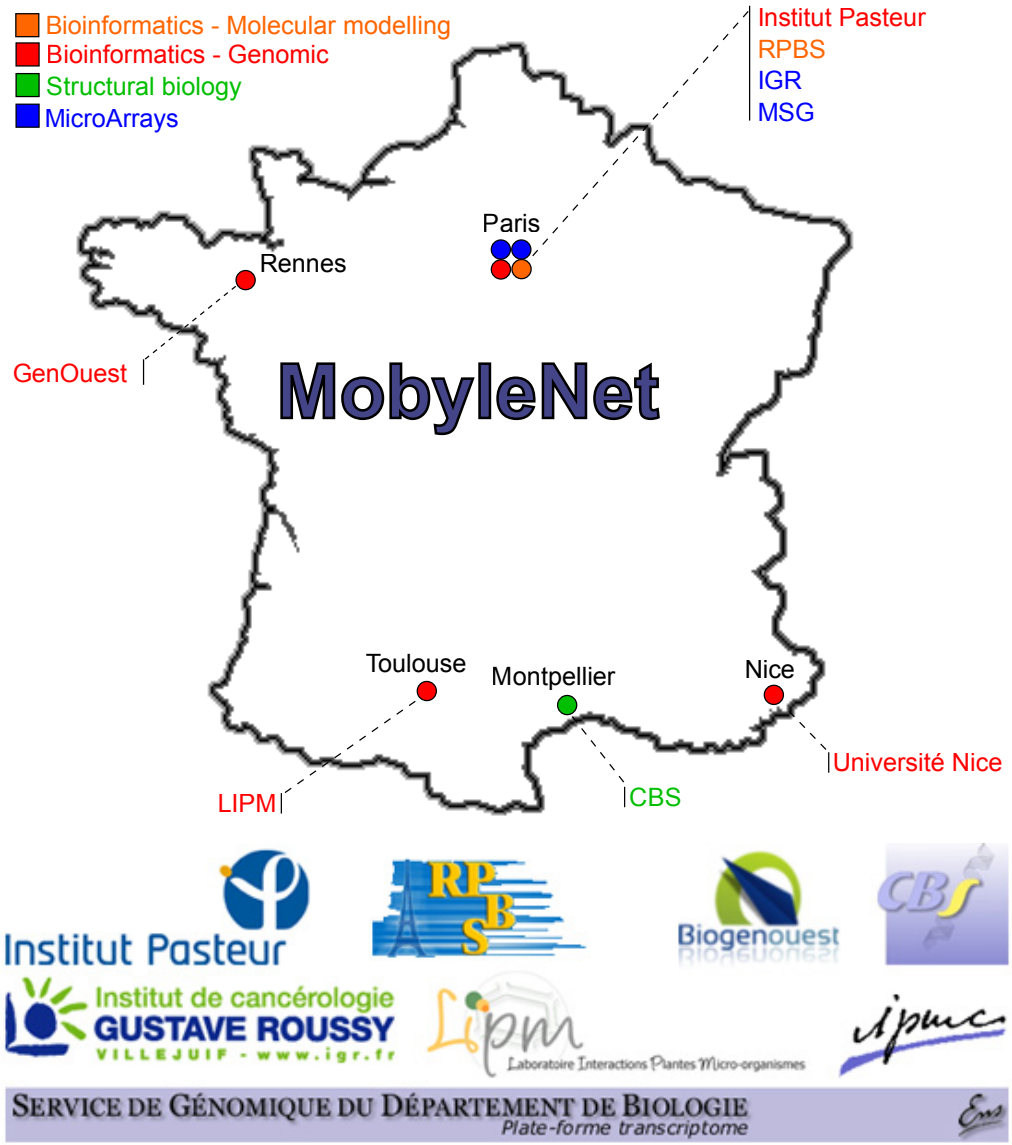
2009/11/13

1 The Mobyle Network

The Mobyle Network



Principles



Distributed mobyle portals

Each portal has its own specificity (banks and programs)

Confidence network

Each portal can import/export a specific service to/from a specific Mobyle portal

User centered

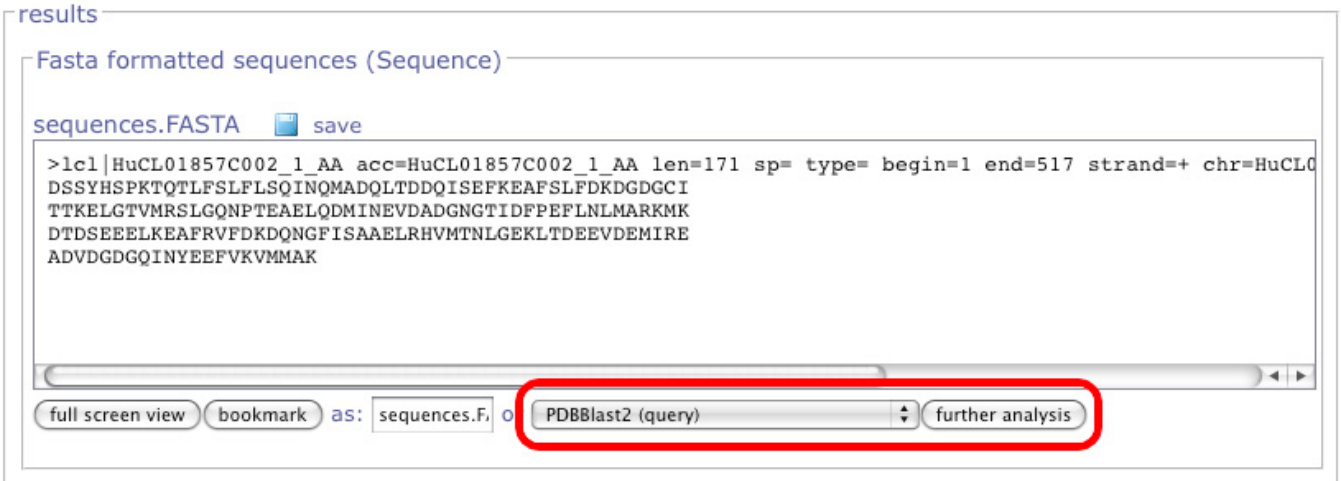
Single interface for multiple portals

→ **Service maintainers are service deployers**

Synopsis

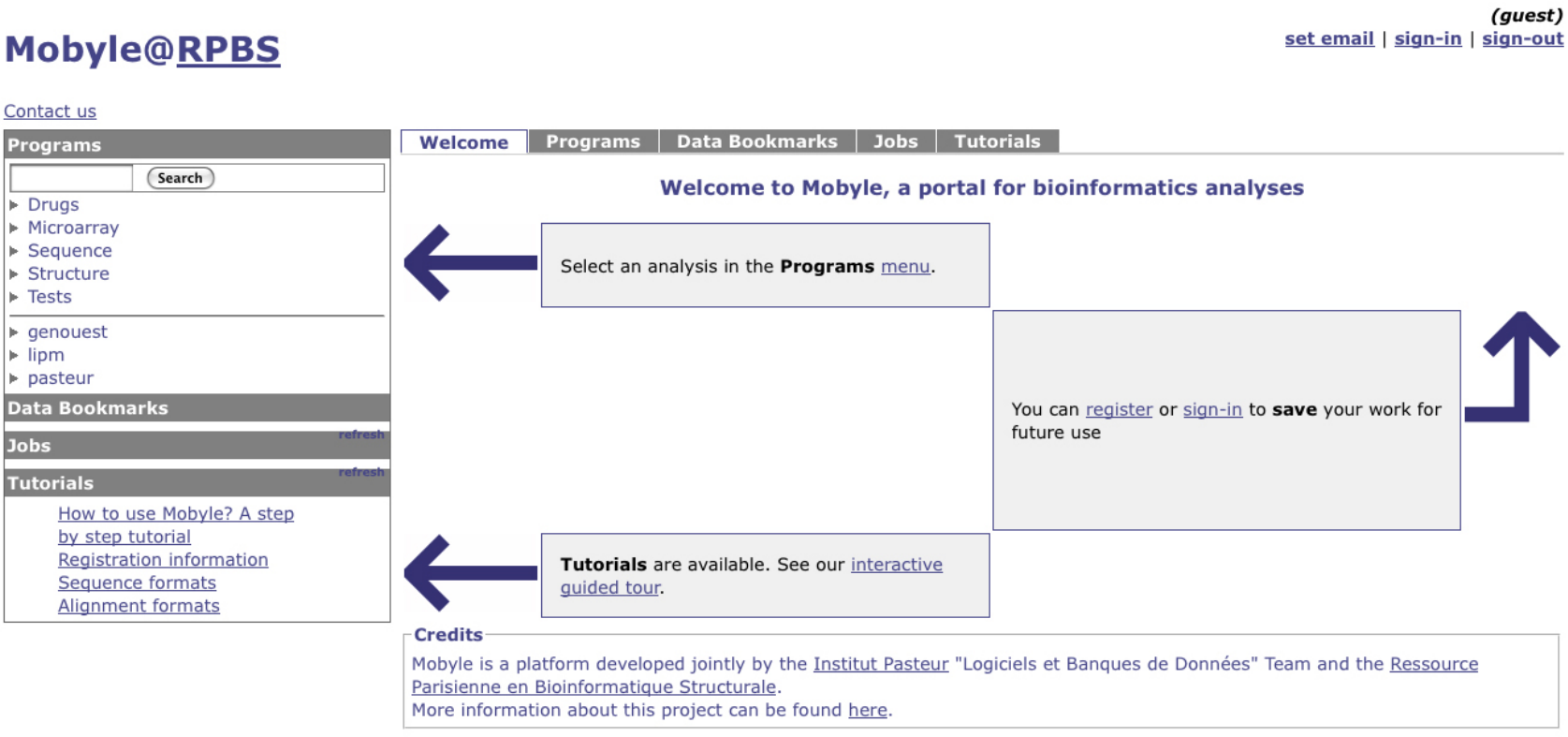
We illustrate here how to take advantage of the MobyleNet to model the 3D structure of the sunflower protein corresponding to the `HuCL01857C002` genomic information.

- tools at the three nodes (LIPM, Pasteur and RPBS) can be chained to complete the modeling
- *nota bene* : all calls are performed within the RPBS (remote imported services) portal

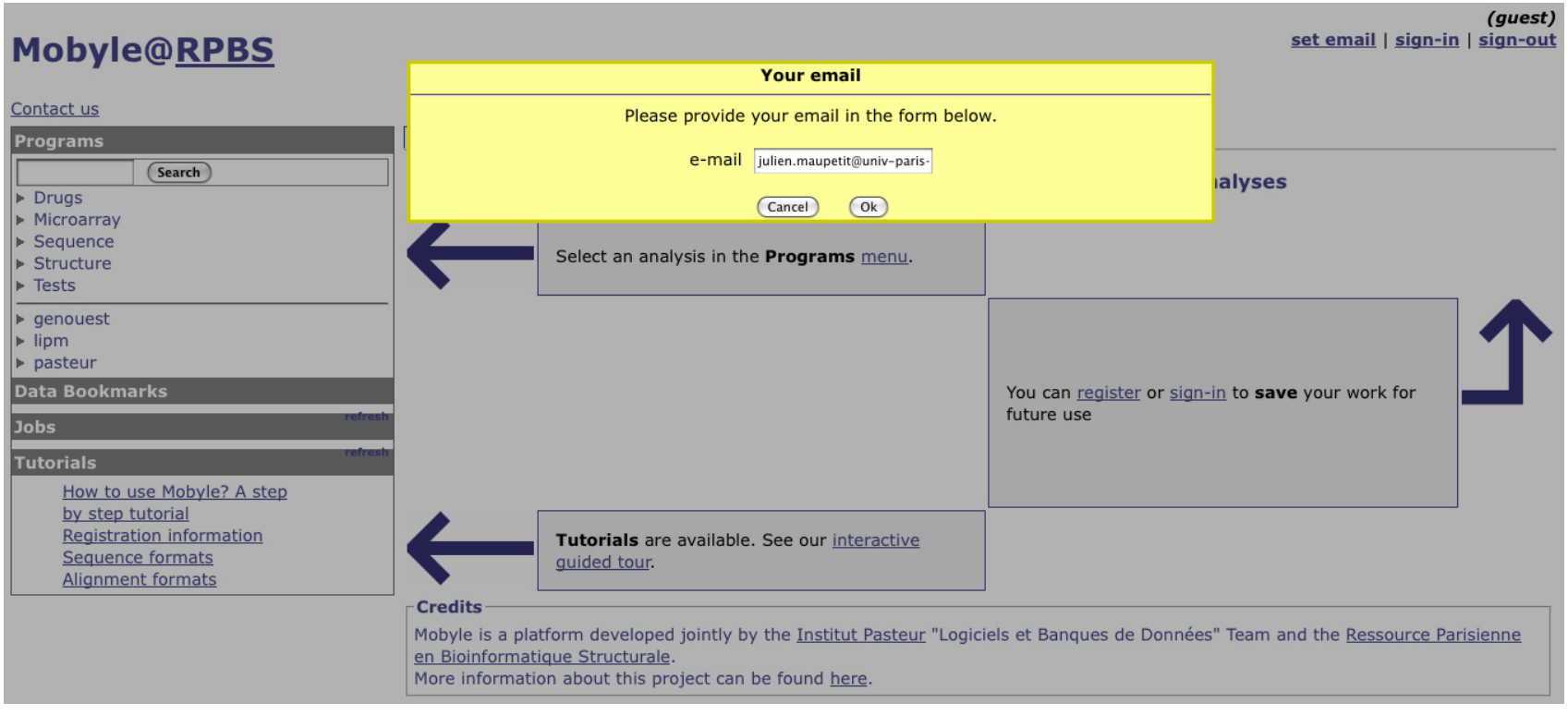


The full tutorial is available at :
`http://mobylenet.rpbs.univ-paris-diderot.fr/doc/tutorials/network.html`

Remote search for sunflower protein sequence



Remote search for sunflower protein sequence



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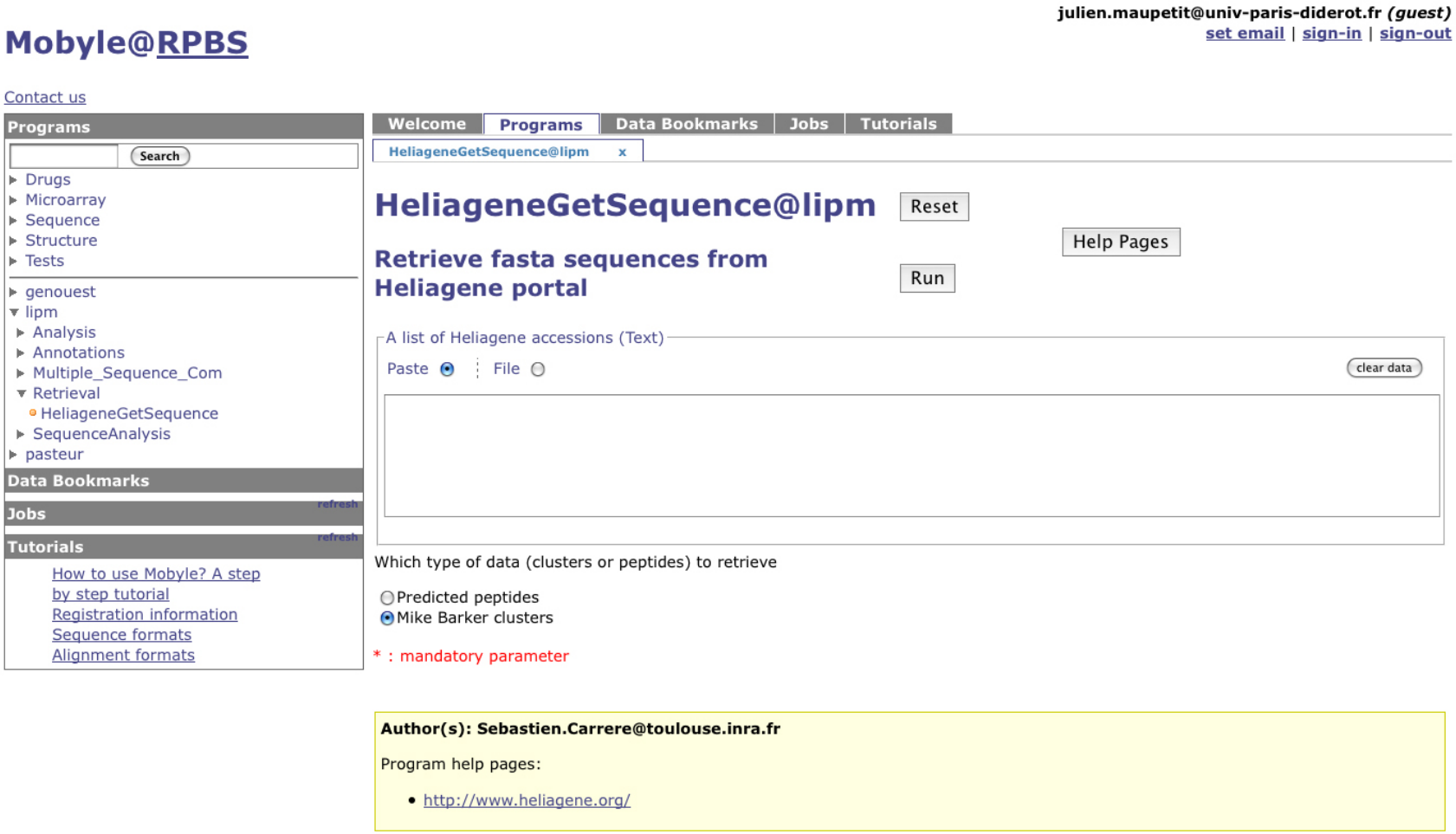

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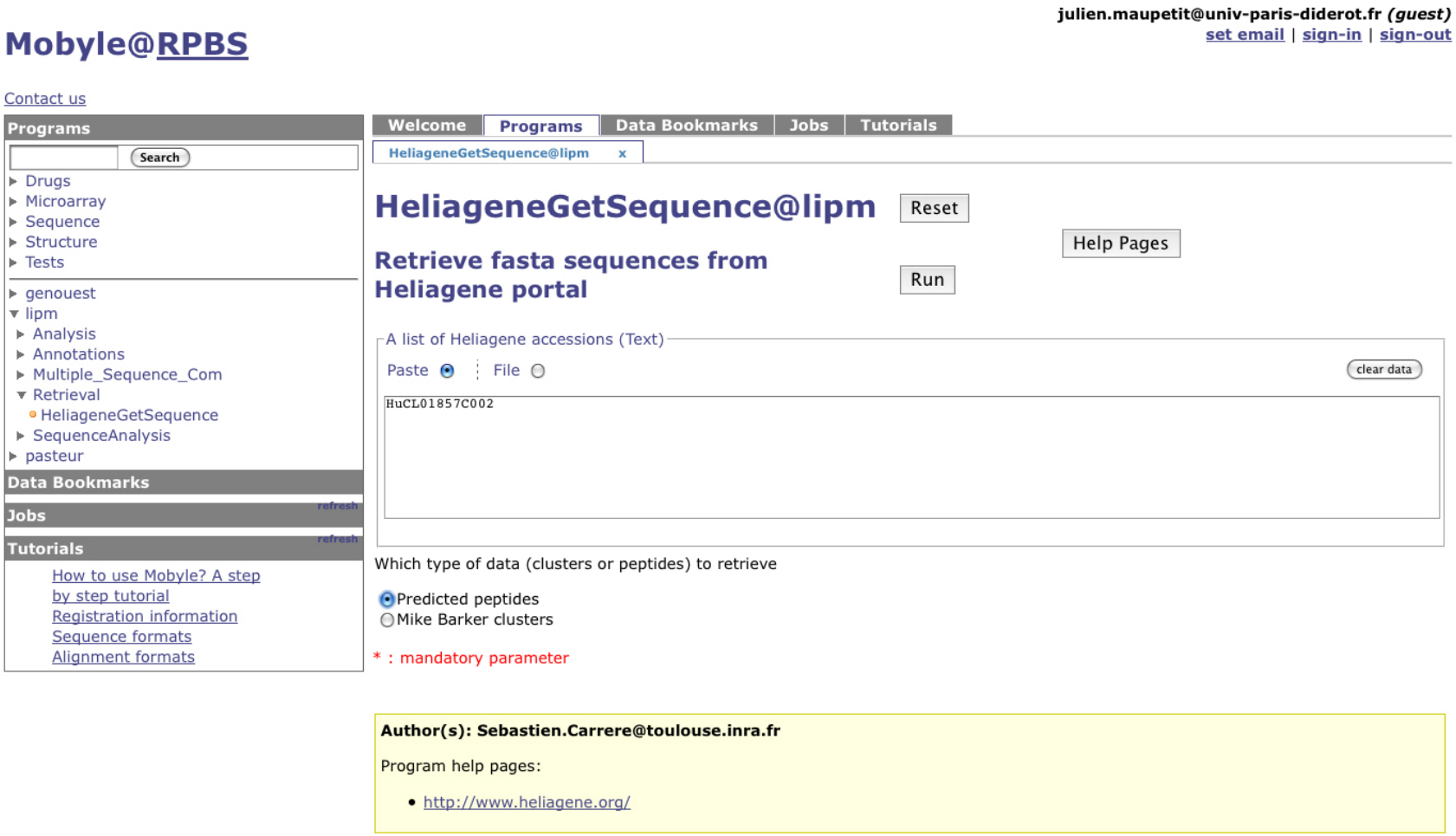

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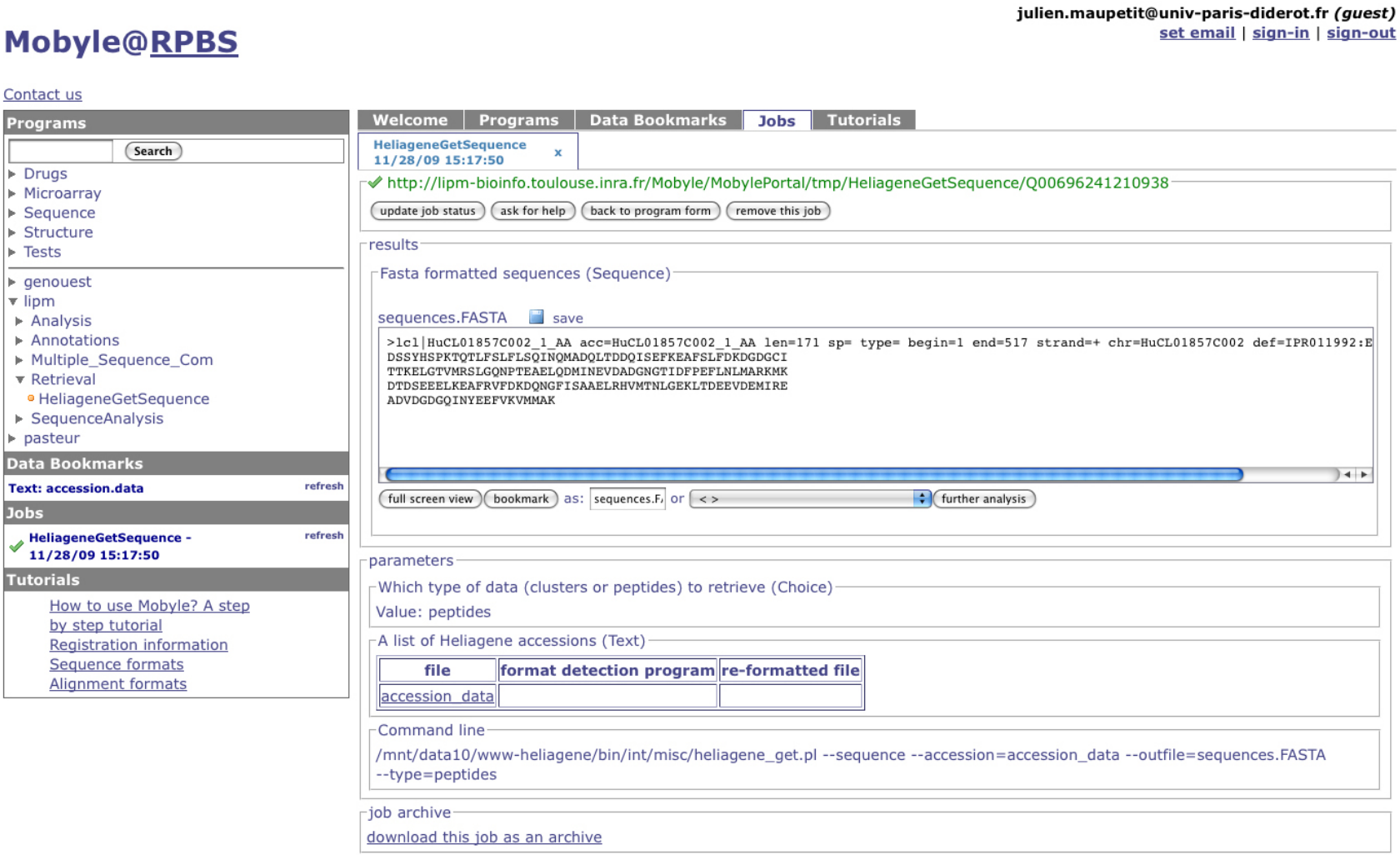

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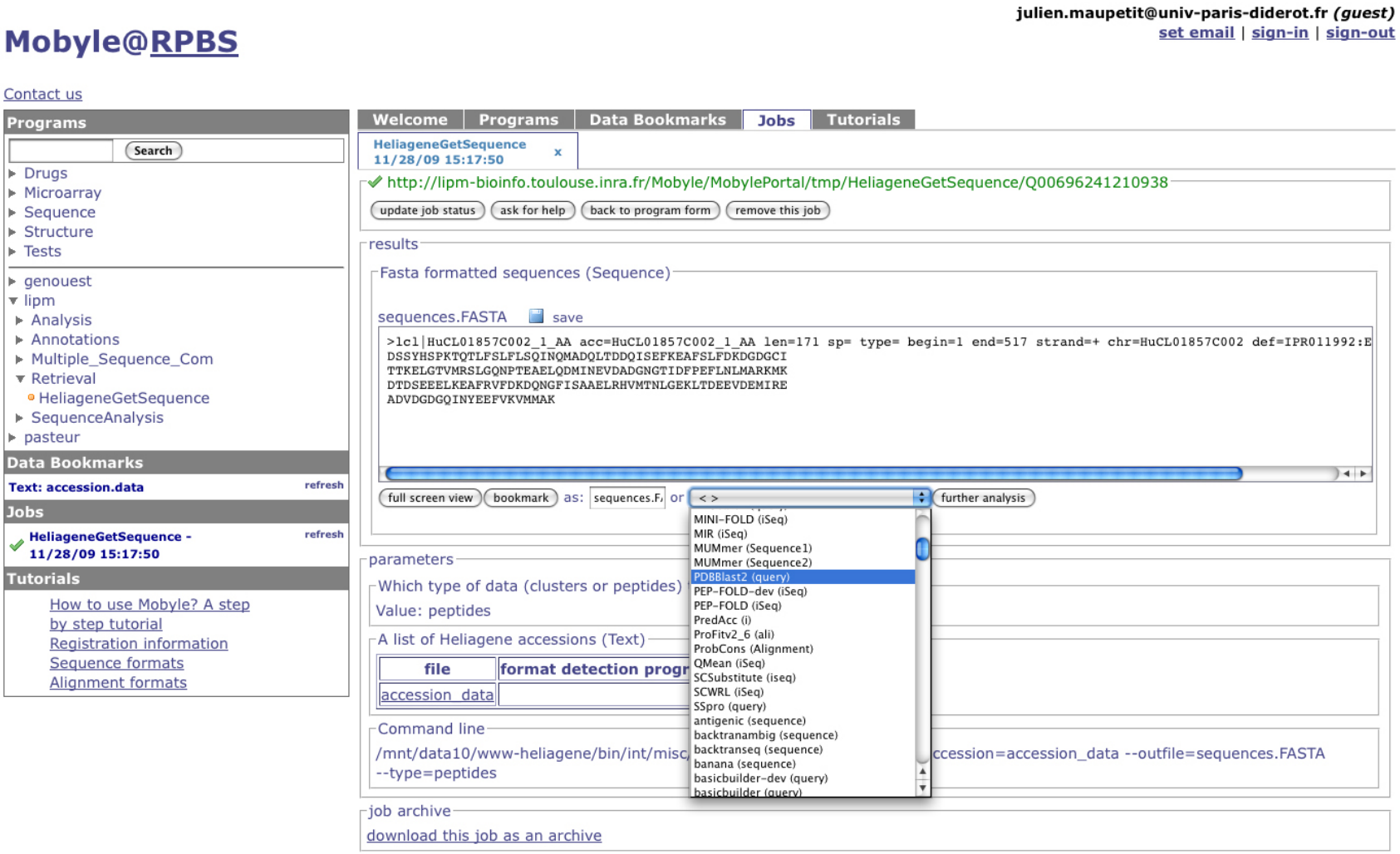

Search for a 3D template

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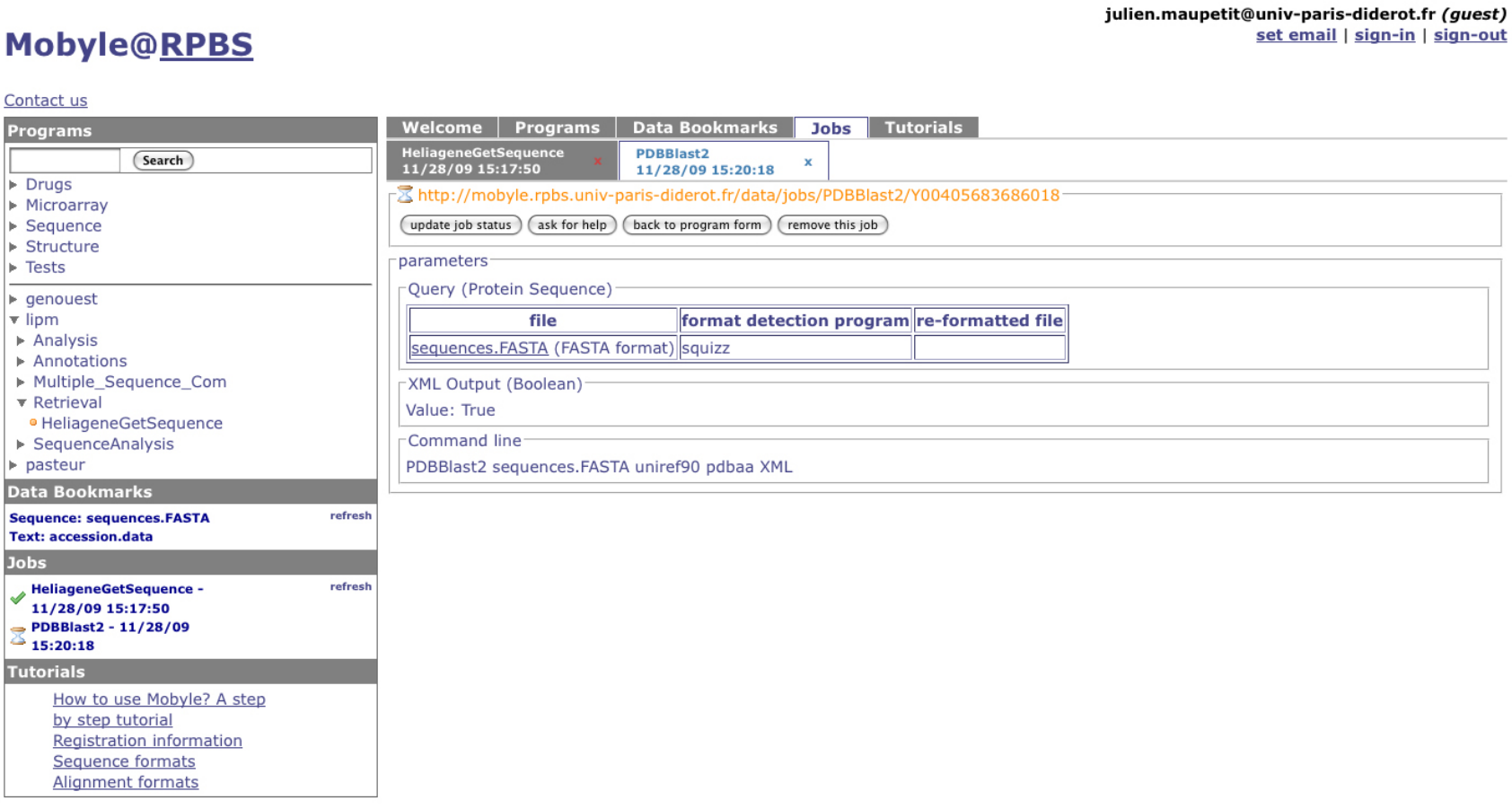

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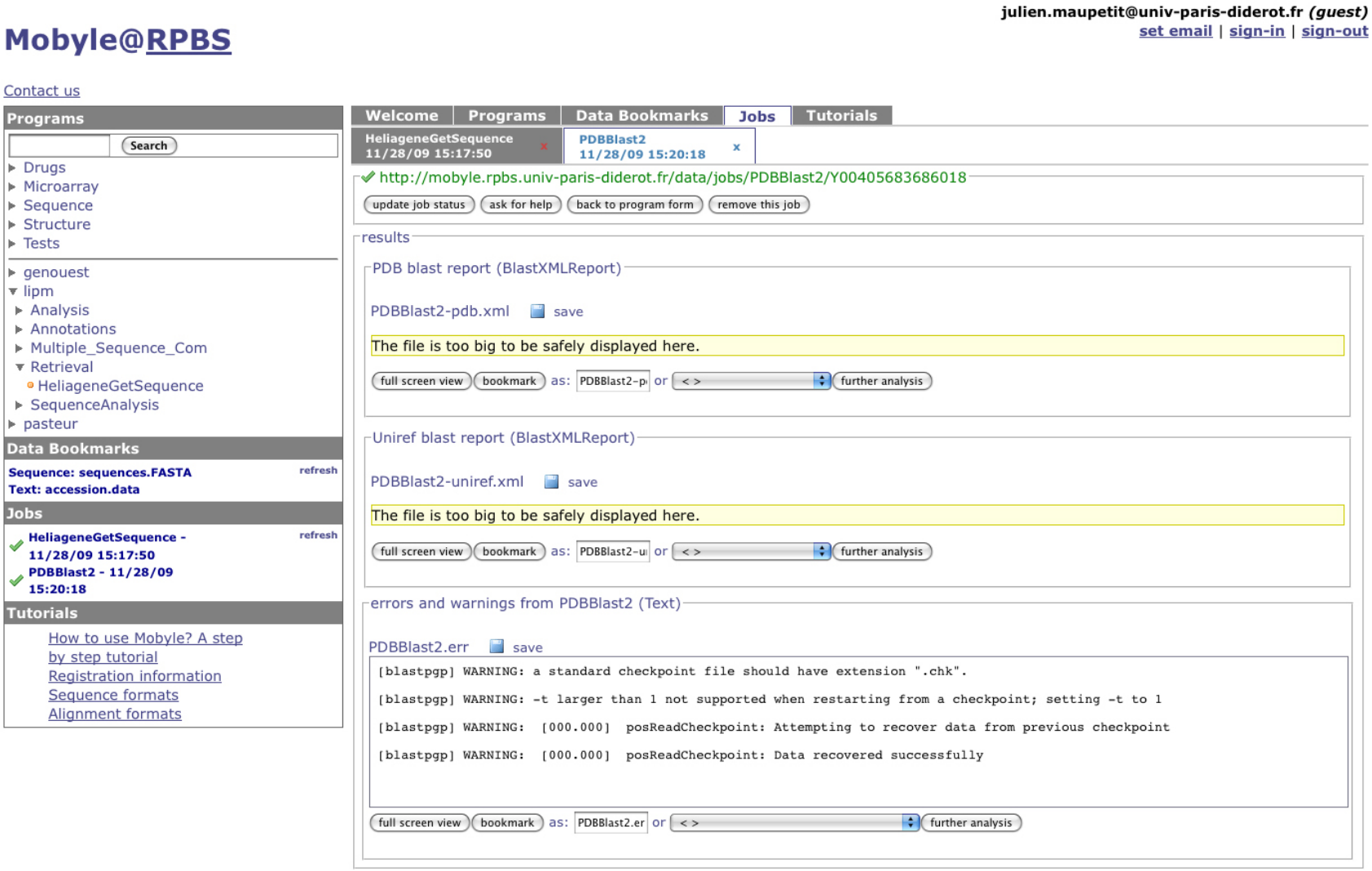

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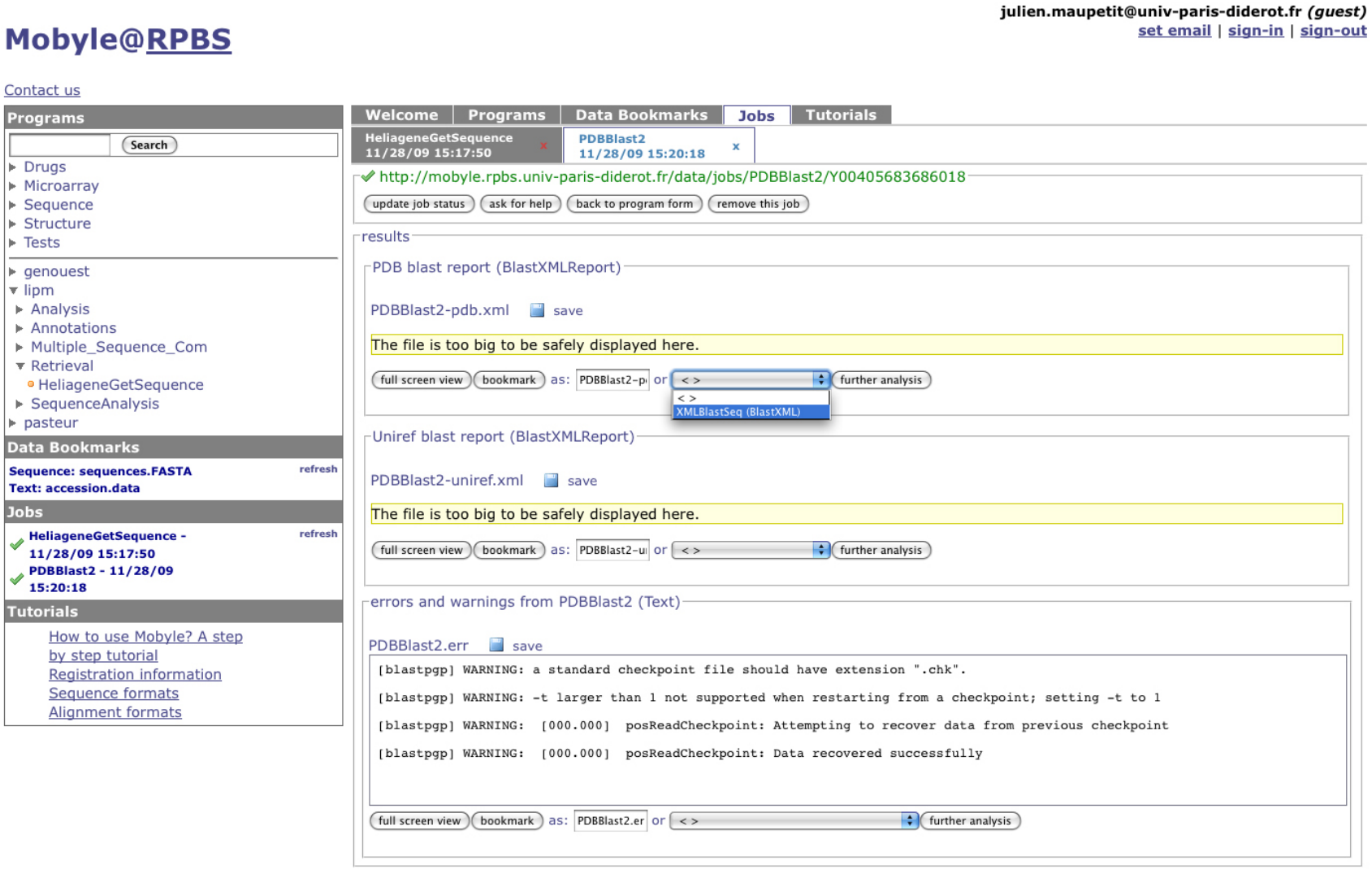
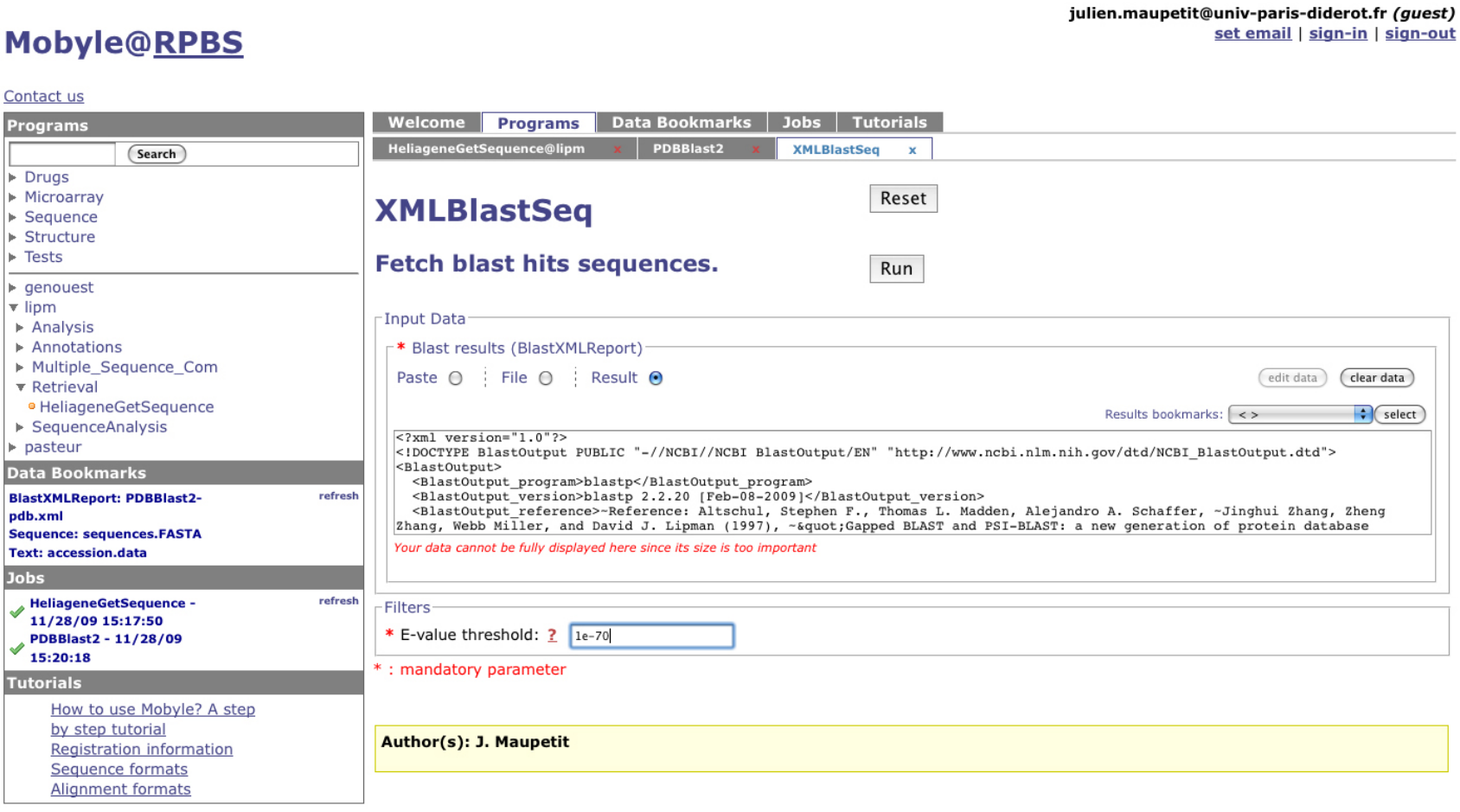


Select templates of interest



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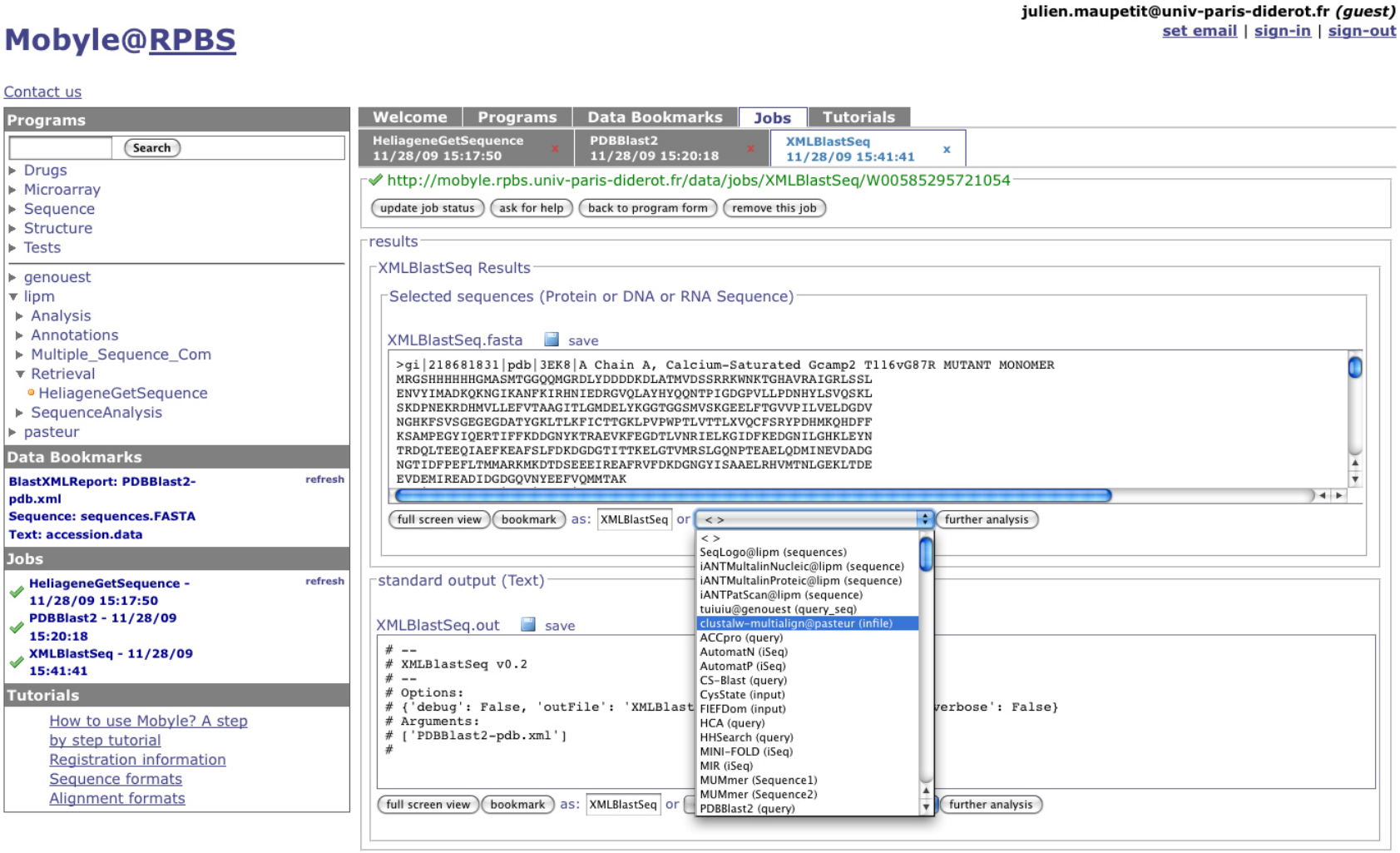
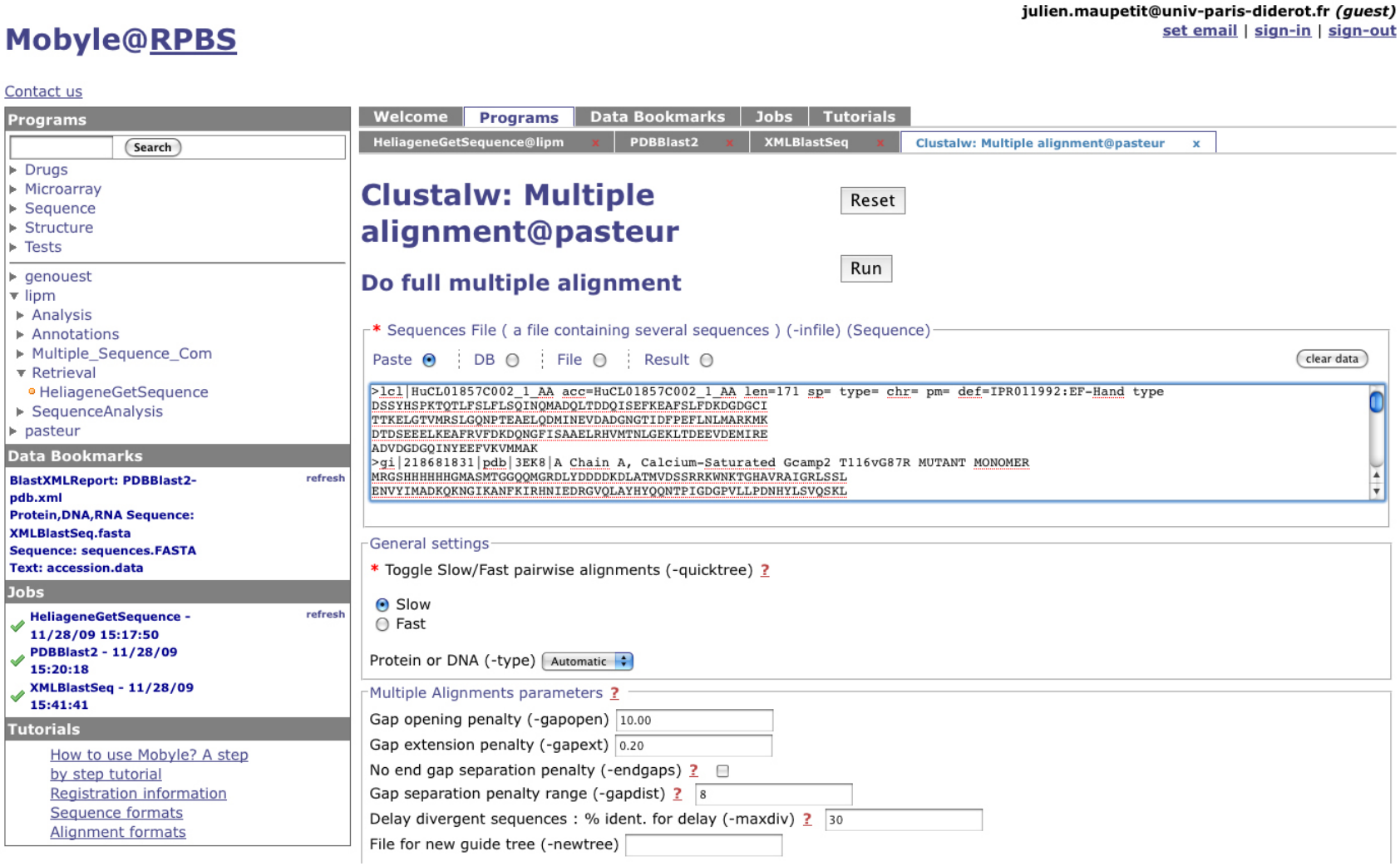
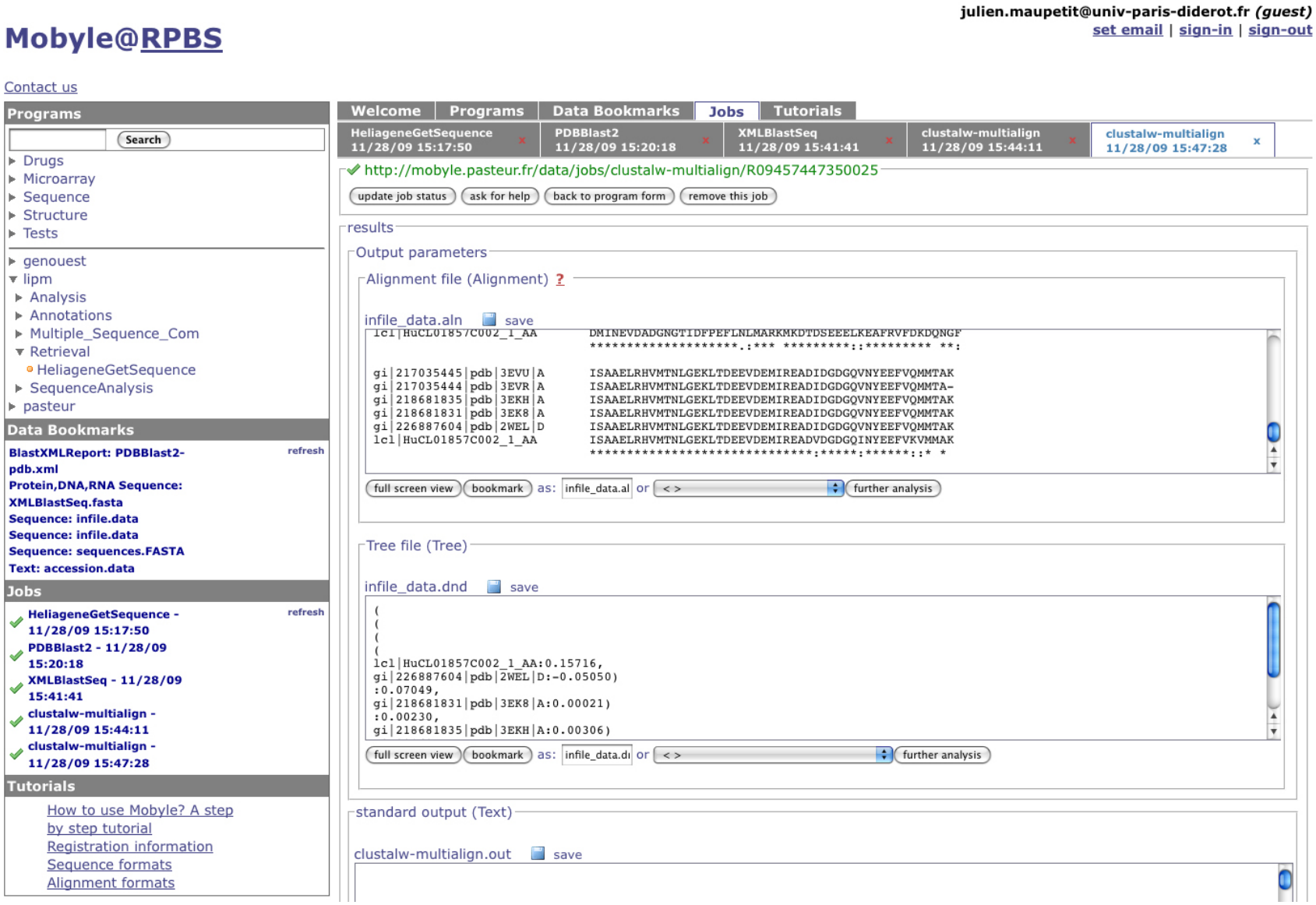


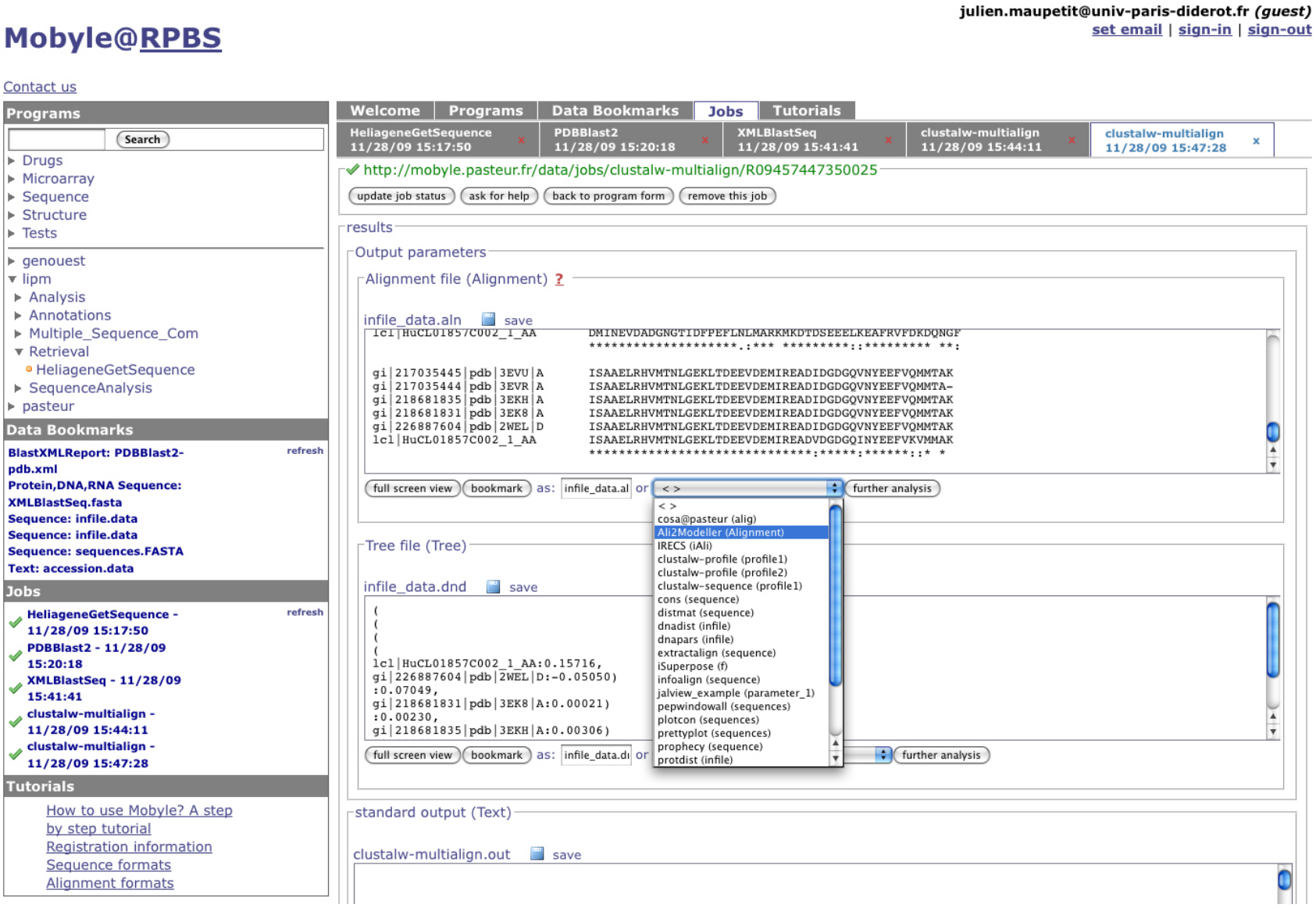
Query/template sequence alignment



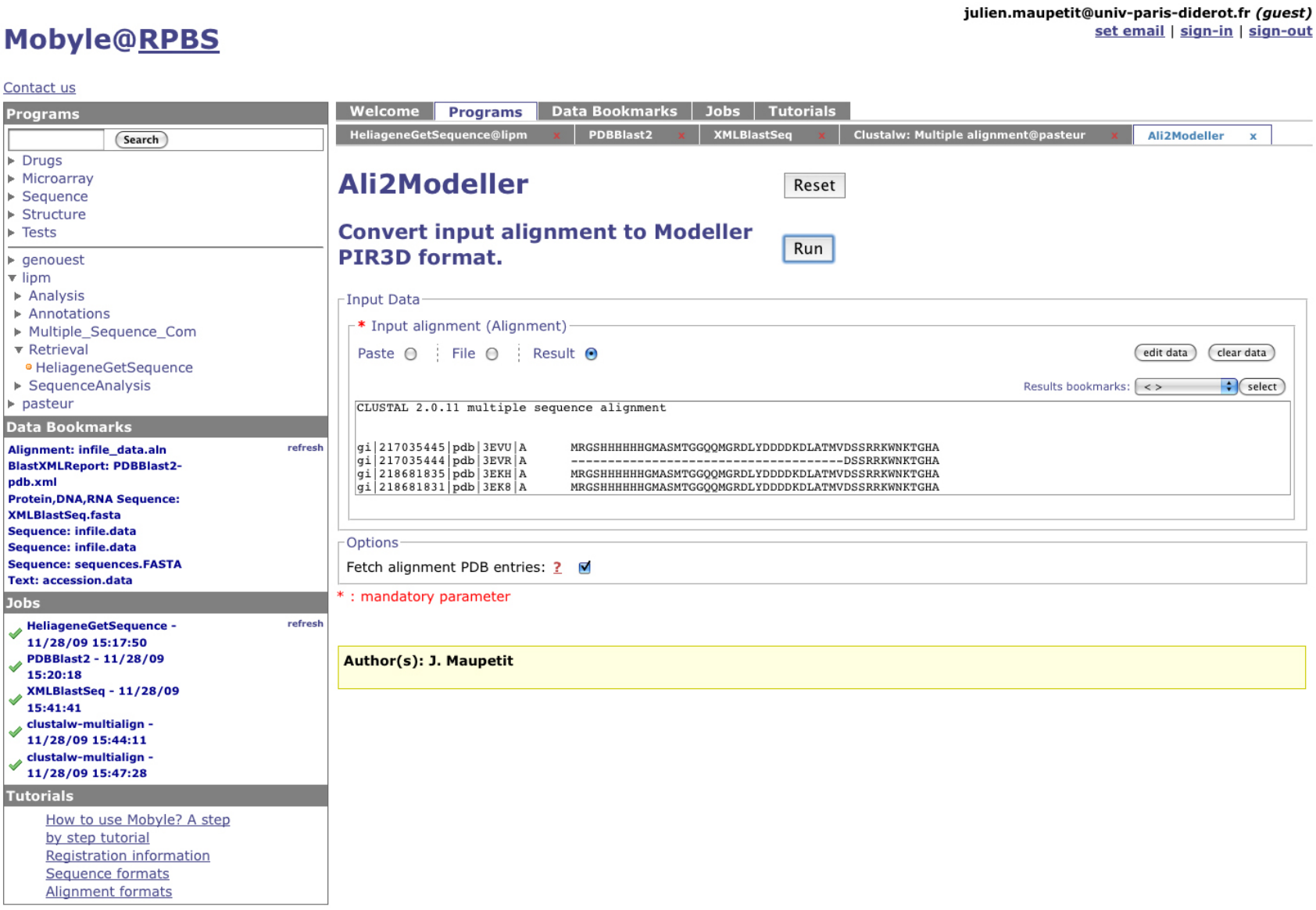
Query/template sequence alignment



Query/template sequence alignment



Preparing modeller input



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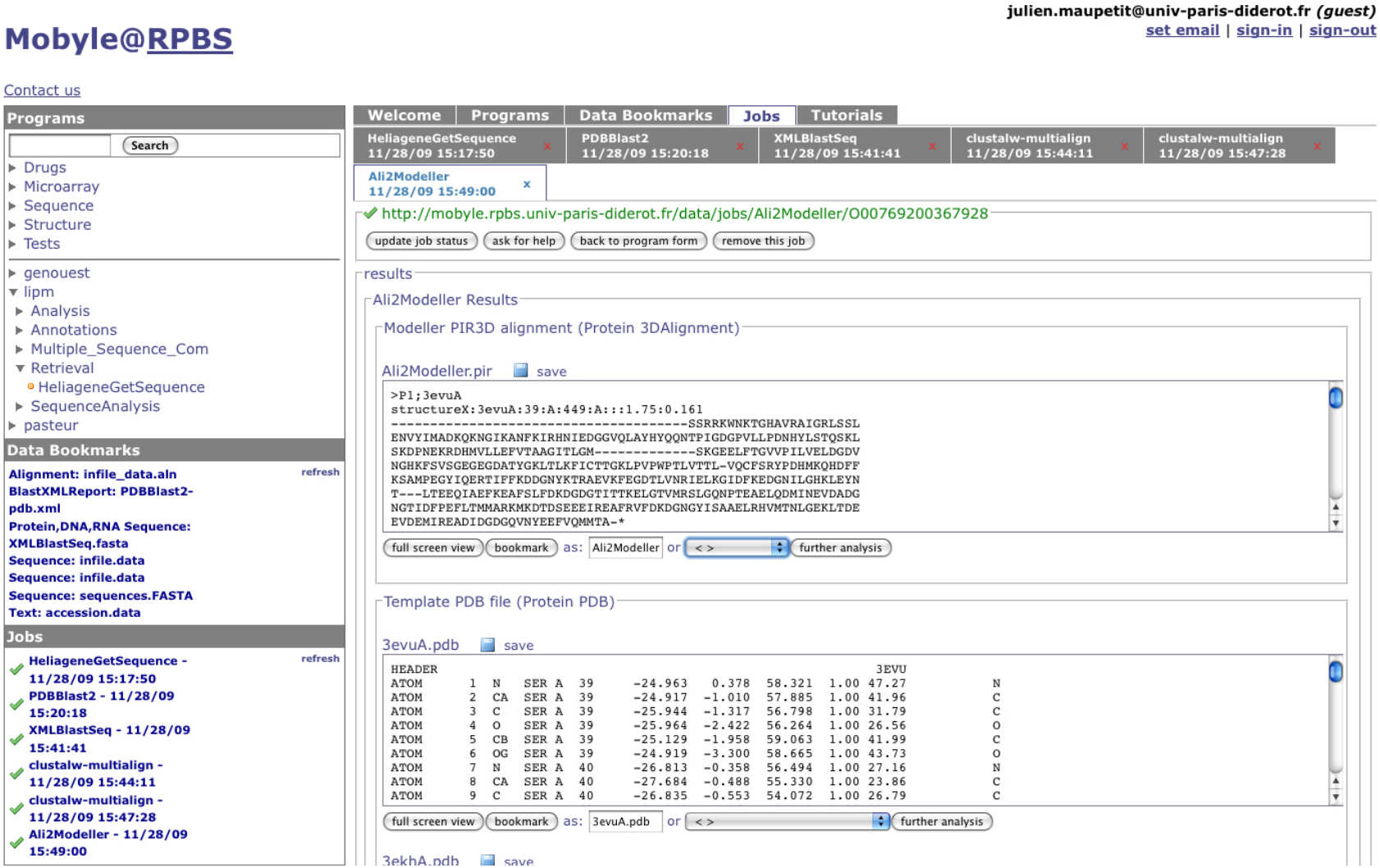

Preparing modeller input

Mobyle@RPBS

julien.maupetit@univ-paris-diderot.fr *(guest)*
set email | sign-in | sign-out

Contact us

Programs

Search

- Drugs
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- genouest
- lipm
  - Analysis
  - Annotations
  - Multiple_Sequence_Com
  - Retrieval
    - HeliageneGetSequence
  - SequenceAnalysis
- pasteur

Data Bookmarks

refresh

Alignment: infile_data.aln
BlastXMLReport: PDBBlast2-pdb.xml
Protein,DNA,RNA Sequence: XMLBlastSeq.fasta
Sequence: infile.data
Sequence: infile.data
Sequence: sequences.FASTA
Text: accession.data

Jobs

refresh

- HeliageneGetSequence - 11/28/09 15:17:50
- PDBBlast2 - 11/28/09 15:20:18
- XMLBlastSeq - 11/28/09 15:41:41
- clustalw-multialign - 11/28/09 15:44:11
- clustalw-multialign - 11/28/09 15:47:28
- Ali2Modeller - 11/28/09 15:49:00

Tutorials

Welcome | Programs | Data Bookmarks | Jobs | Tutorials

HeliageneGetSequence 11/28/09 15:17:50 | PDBBlast2 11/28/09 15:20:18 | XMLBlastSeq 11/28/09 15:41:41 | clustalw-multialign 11/28/09 15:44:11 | clustalw-multialign 11/28/09 15:47:28

Ali2Modeller 11/28/09 15:49:00

http://mobyle.rpbs.univ-paris-diderot.fr/data/jobs/Ali2Modeller/O00769200367928

update job status | ask for help | back to program form | remove this job

results

Ali2Modeller Results

Modeller PIR3D alignment (Protein 3DAlignment)

Ali2Modeller.pir save

```
>P1;3evuA
structureX:3evuA:39:A:449:A:::1.75:0.161
---------------------------------------SSRRKWNKTGHAVRAIGRLSSL
ENVYIMADKQKNGIKANFKIRHNIEDGGVQLAYHYQQNTPIGDGPVLLPDNHYLSTQSKL
SKDPNEKRDHMVLLEFVTAAGITLGM----------SKGEELFTGVVPILVELDGDV
NGHKFSVSGEGEGDATYGKLTLKFICTTGKLPVPWPTLVTTL-VQCFSRYPDHMKQHDFF
KSAMPEGYIQERTIFFKDDGNYKTRAEVKFEGDTLVNRIELKGIDFKEDGNILGHKLEYN
T---LTEEQIAEFKEAFSLFDKDGDGTITTKELGTVMRSLGQNPTEAELQDMINEVDADG
NGTIDFPEFLTMMARKMKDTDSEEEIREAFRVFDKDGNGYISAAELRHVMTNLGEKLTDE
EVDEMIREADIDGDGQVNYEEFVQMMTA-*
```

full screen view | bookmark | as: Ali2Modeller | or < > | further analysis

< >
Modeller (ali)

Template PDB file (Protein PDB)

3evuA.pdb save

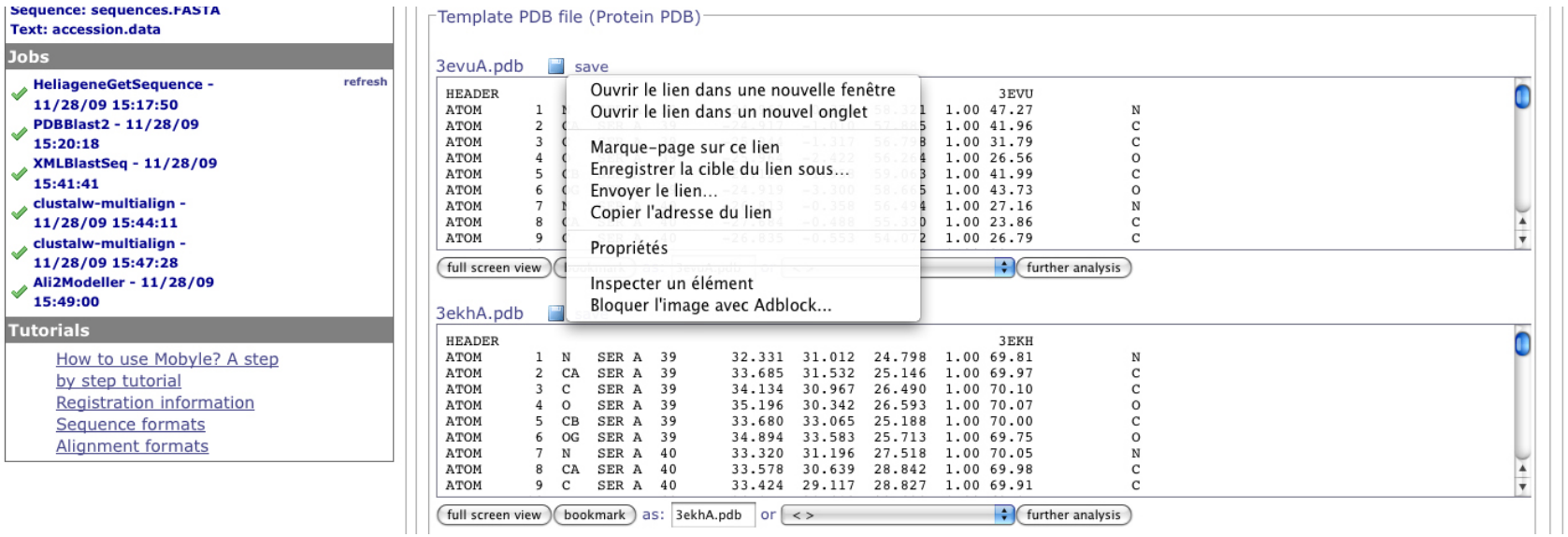
```
HEADER                                                      3EVU
ATOM      1  N   SER A  39     -24.963   0.378  58.321  1.00 47.27           N
ATOM      2  CA  SER A  39     -24.917  -1.010  57.885  1.00 41.96           C
ATOM      3  C   SER A  39     -25.944  -1.317  56.798  1.00 31.79           C
ATOM      4  O   SER A  39     -25.964  -2.422  56.264  1.00 26.56           O
ATOM      5  CB  SER A  39     -25.129  -1.958  59.063  1.00 41.99           C
ATOM      6  OG  SER A  39     -24.919  -3.300  58.665  1.00 43.73           O
ATOM      7  N   SER A  40     -26.813  -0.358  56.494  1.00 27.16           N
ATOM      8  CA  SER A  40     -27.684  -0.488  55.330  1.00 23.86           C
ATOM      9  C   SER A  40     -26.835  -0.553  54.072  1.00 26.79           C
```

full screen view | bookmark | as: 3evuA.pdb | or < > | further analysis

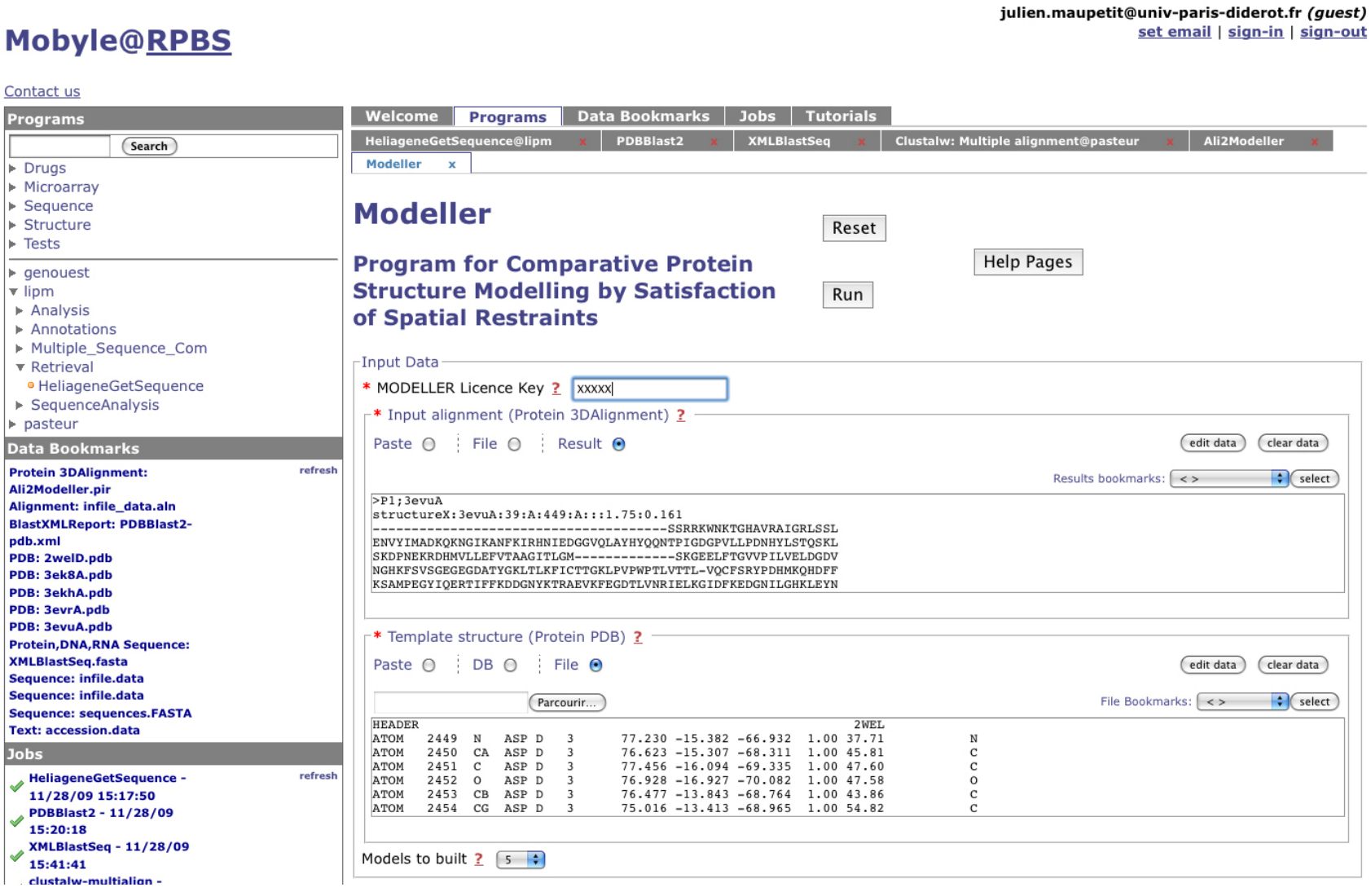
3ekhA.pdb save

```
HEADER                                                      3EKH
```

Preparing modeller input



Perform the 3D modeling



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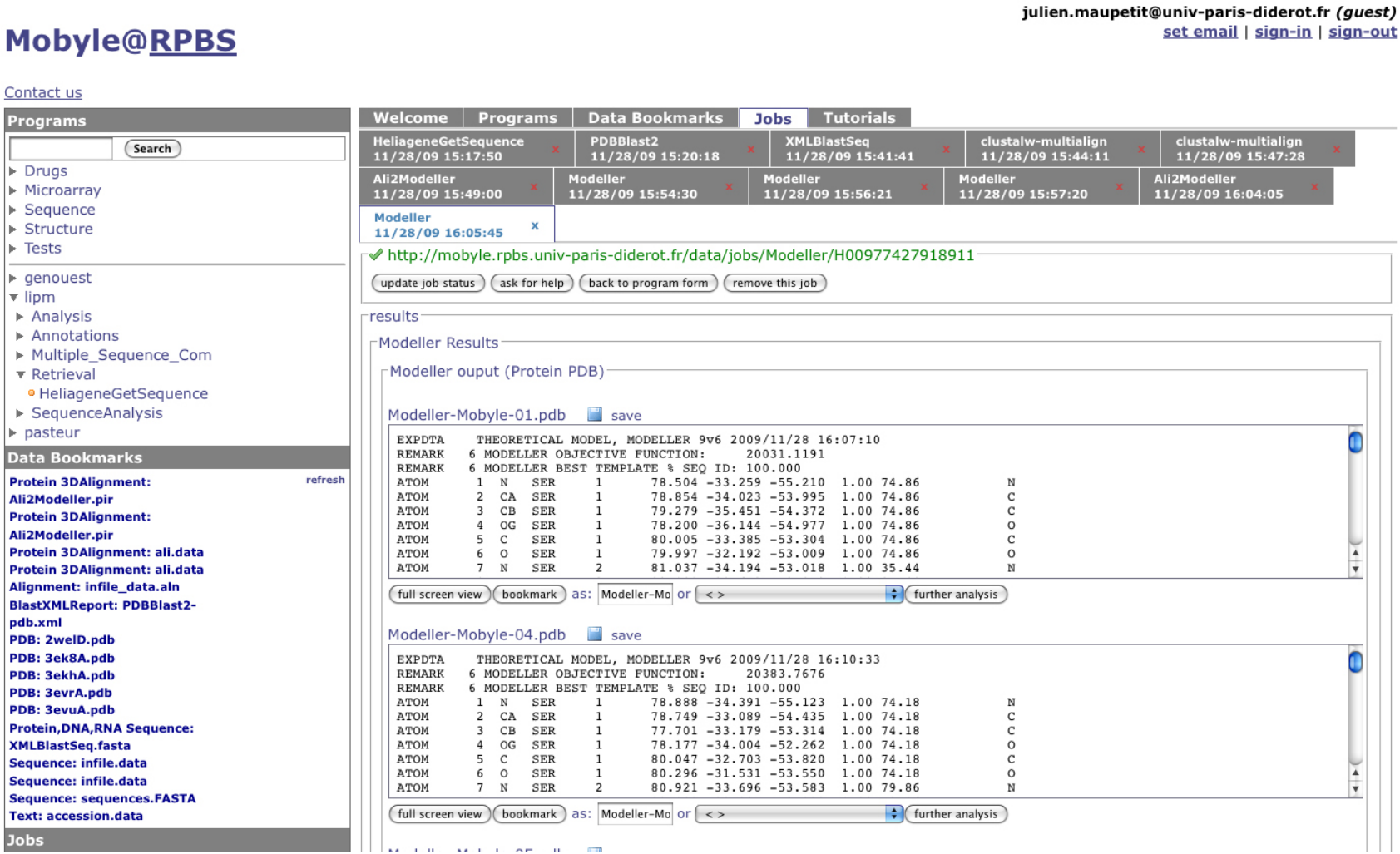

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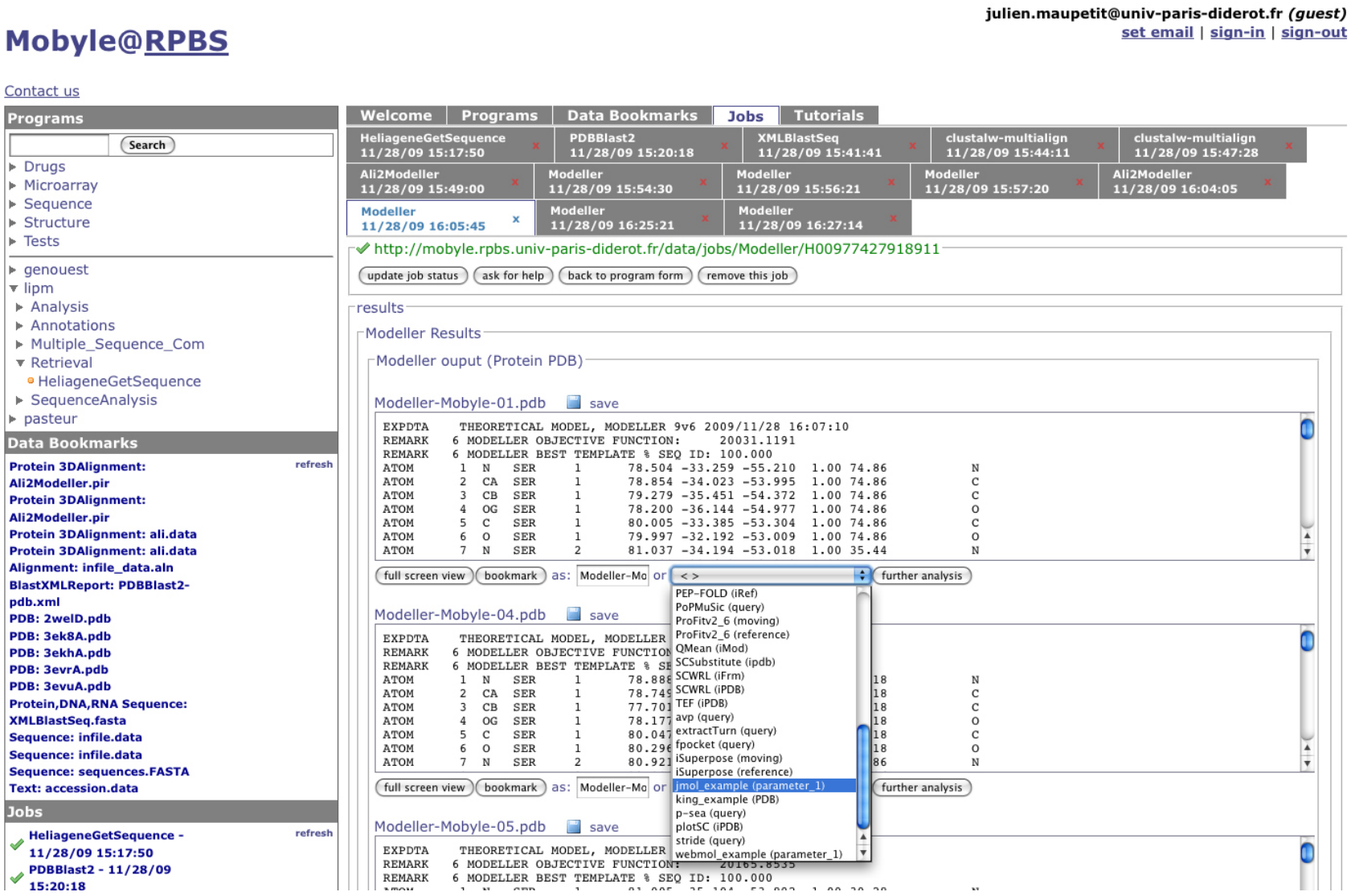
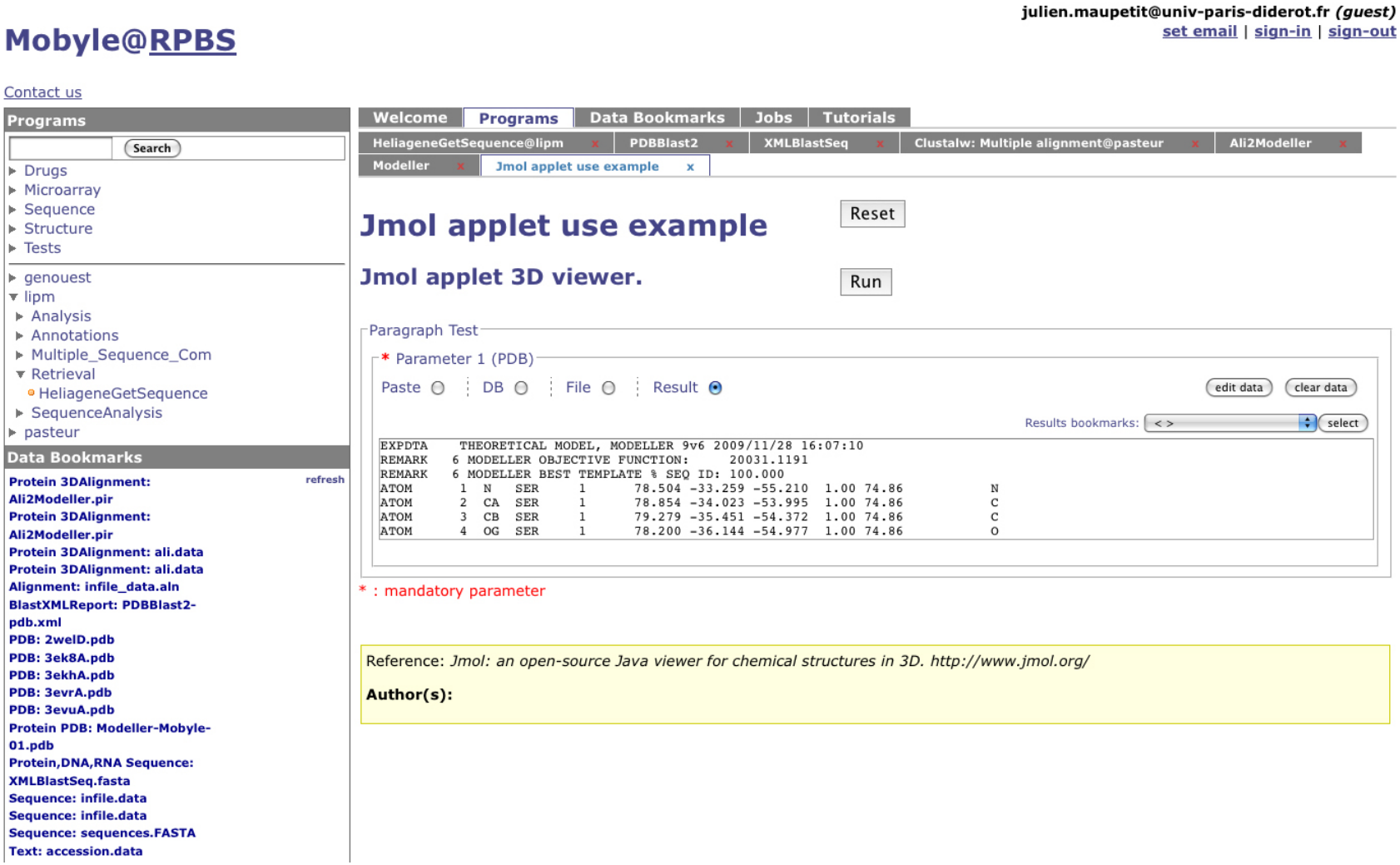
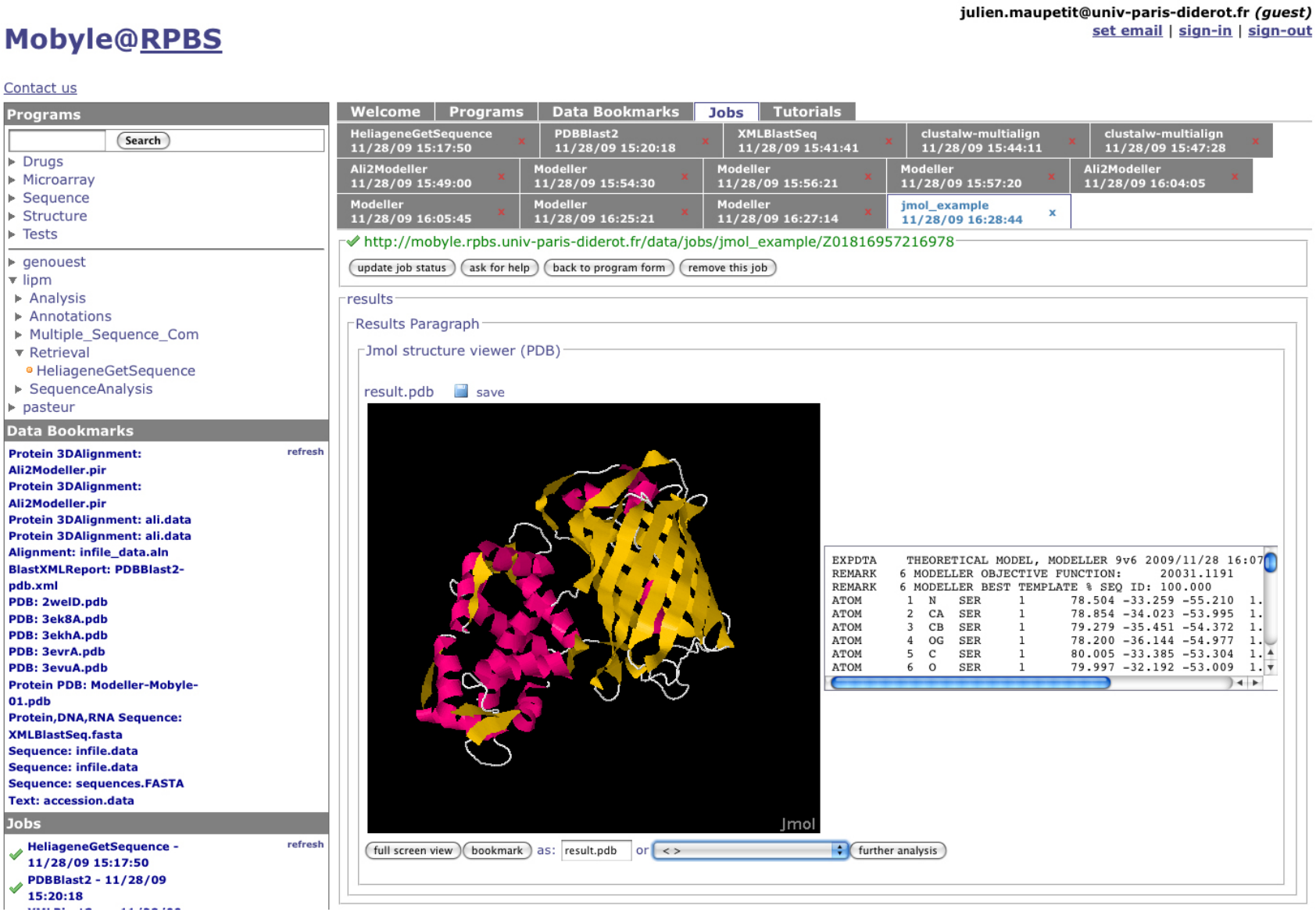


A quick glance at the 3D model



A quick glance at the 3D model



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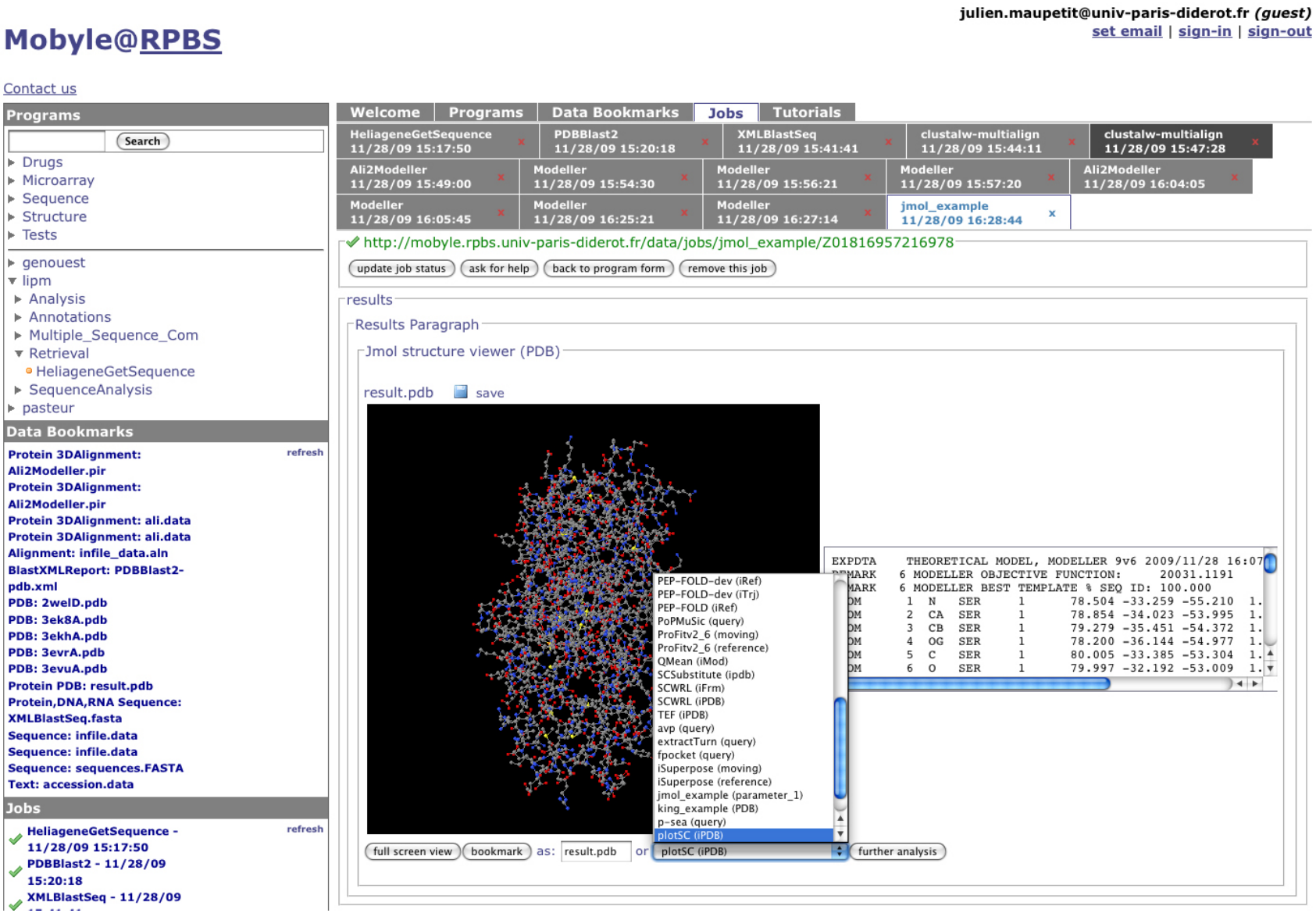
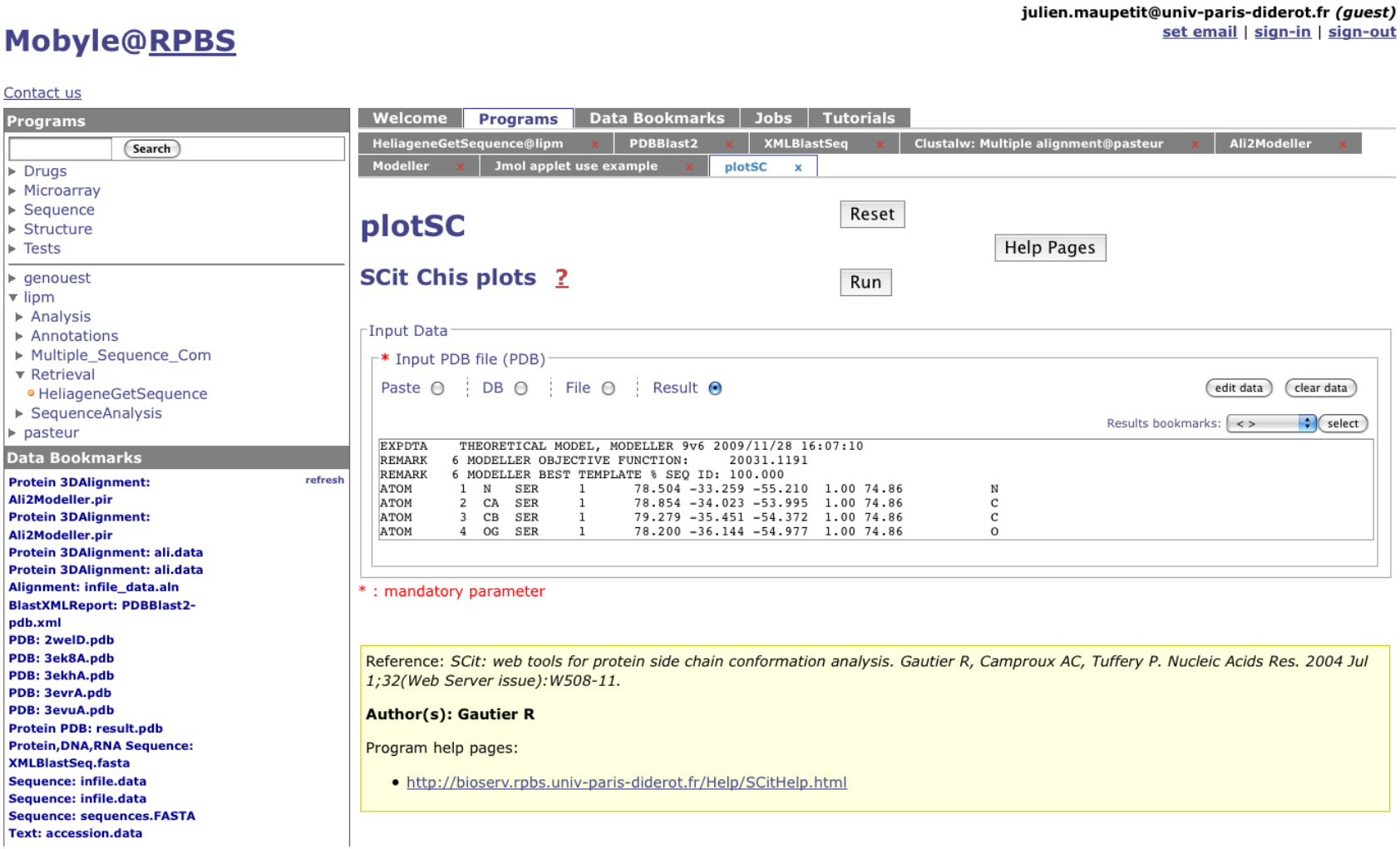


Any further analysis ?



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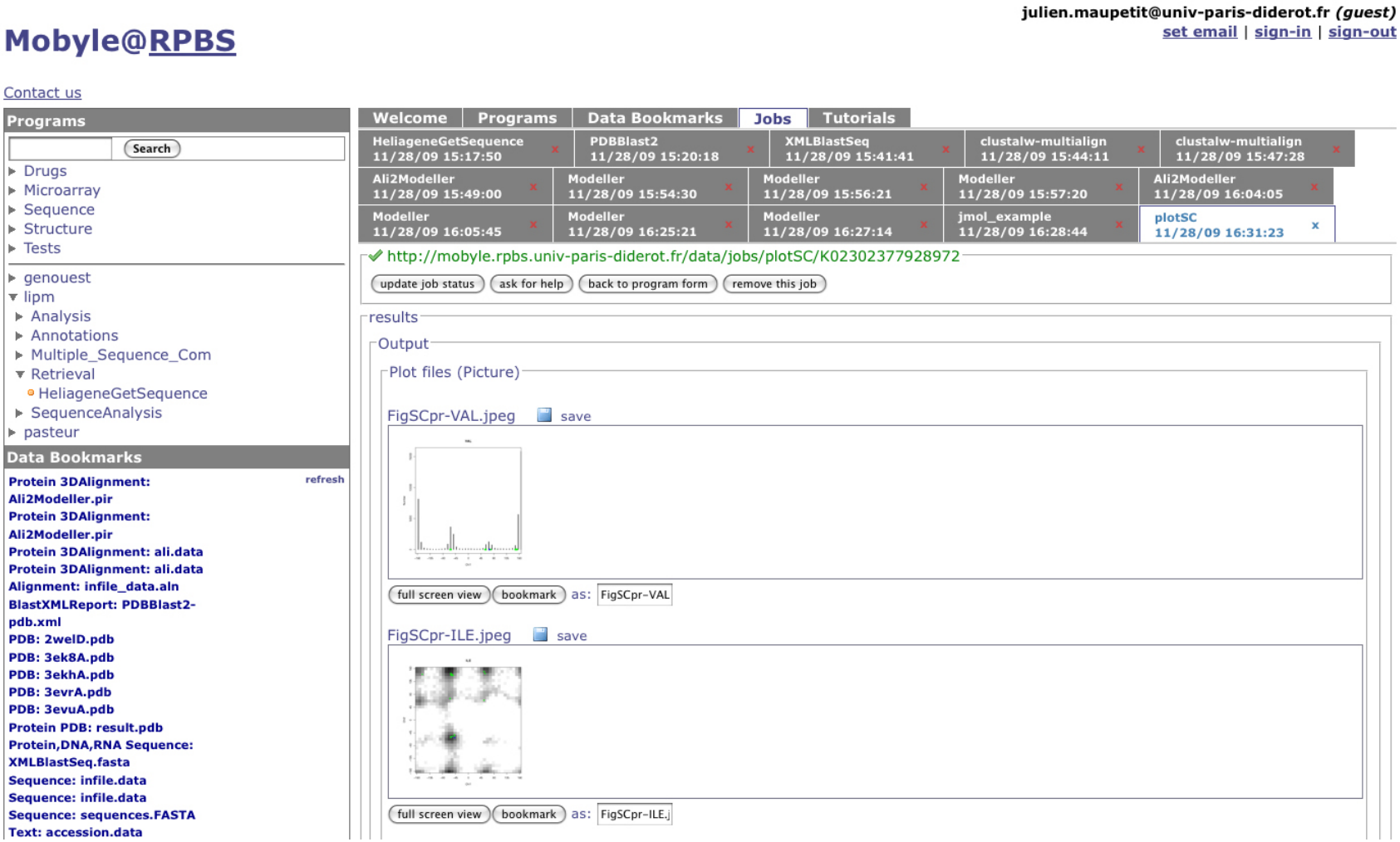
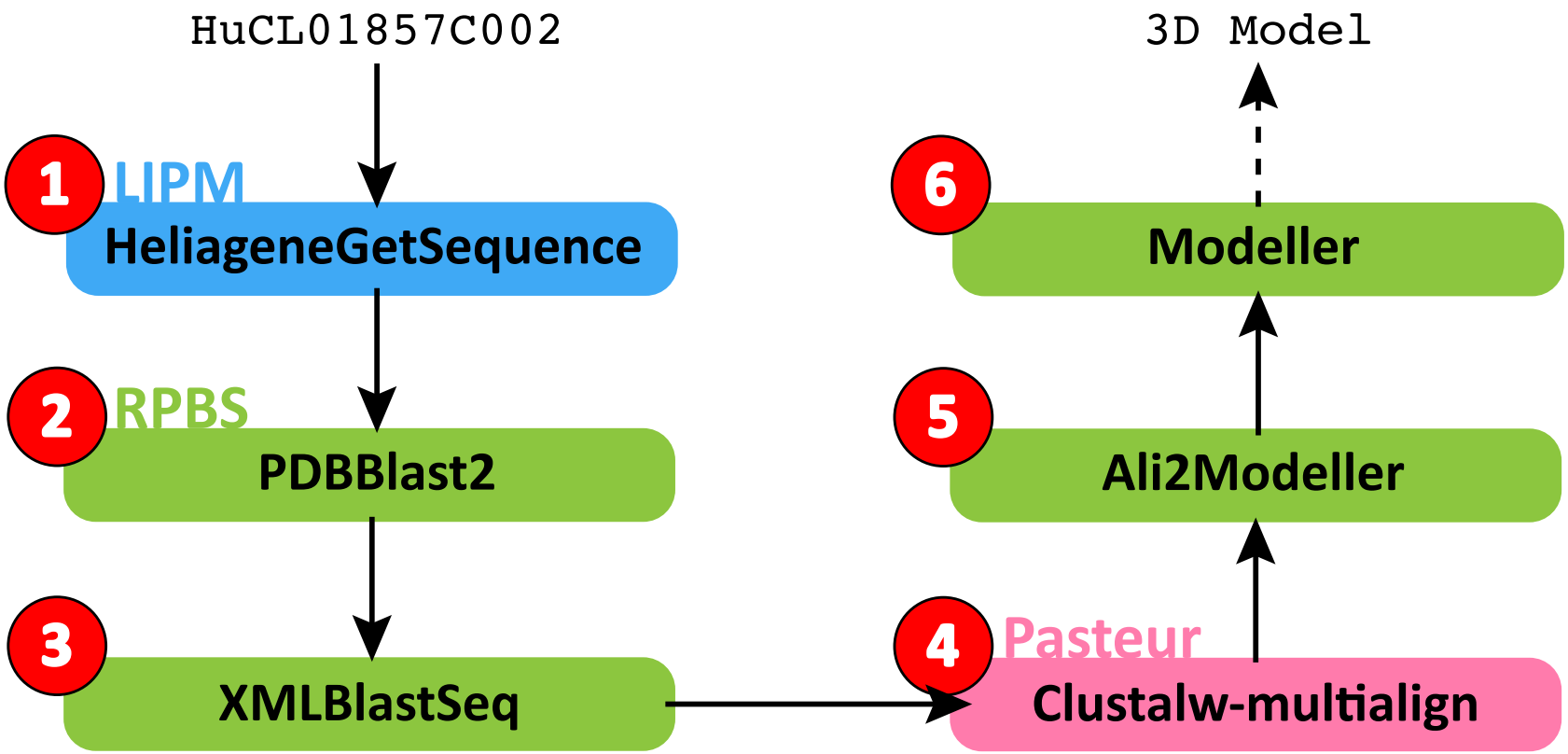


Summary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1 LIPM
HeliageneGetSequence
2 RPBS
PDBBlast2
3
XMLBlastSeq
4 Pasteur
Clustalw-multialign
5
Ali2Modeller
6
Modeller
3D Model