# Molecule modeling of EIAV RT based on HIV-1

Group 12

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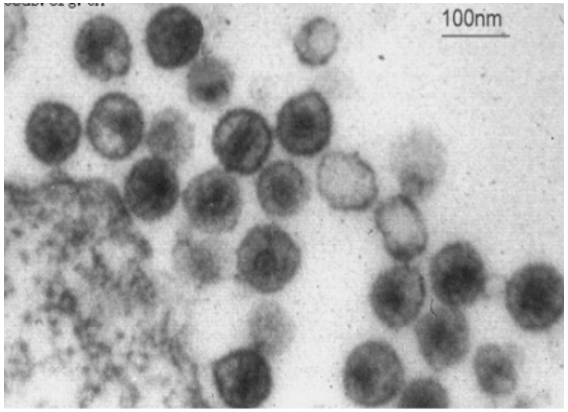
# outlines

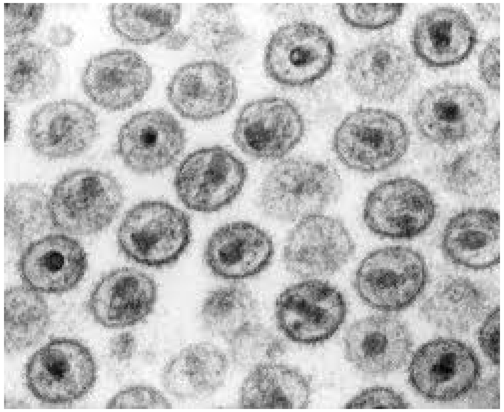
- 1.General information
- 2.charactization of  RT
- 3. preparation for modeling
- 4.molecule modeling
- 5.analysis
- 6.citation

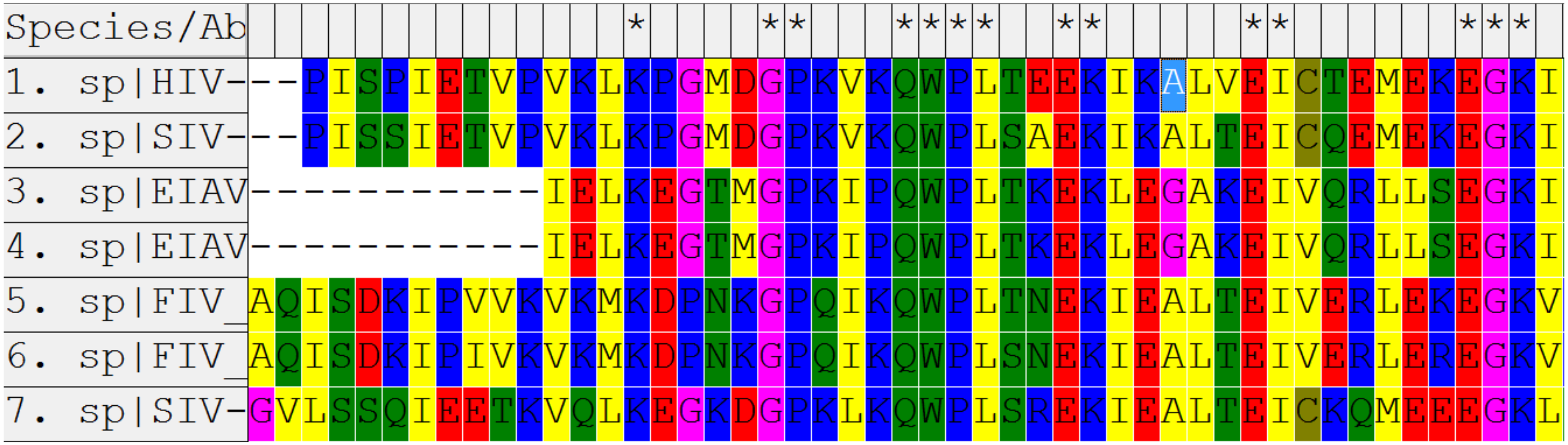
# 1.General information

EIAV :the country cousin of HIV

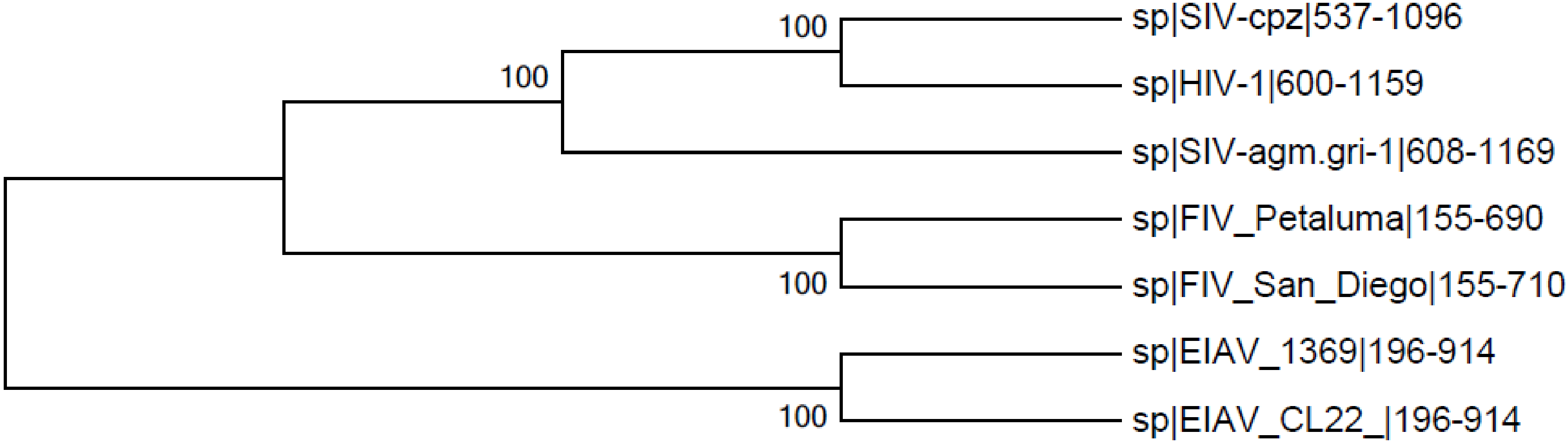
same family ,same genus

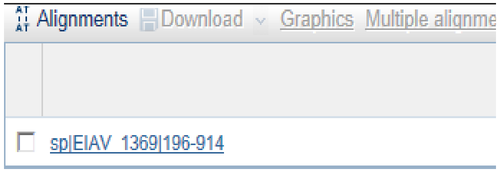




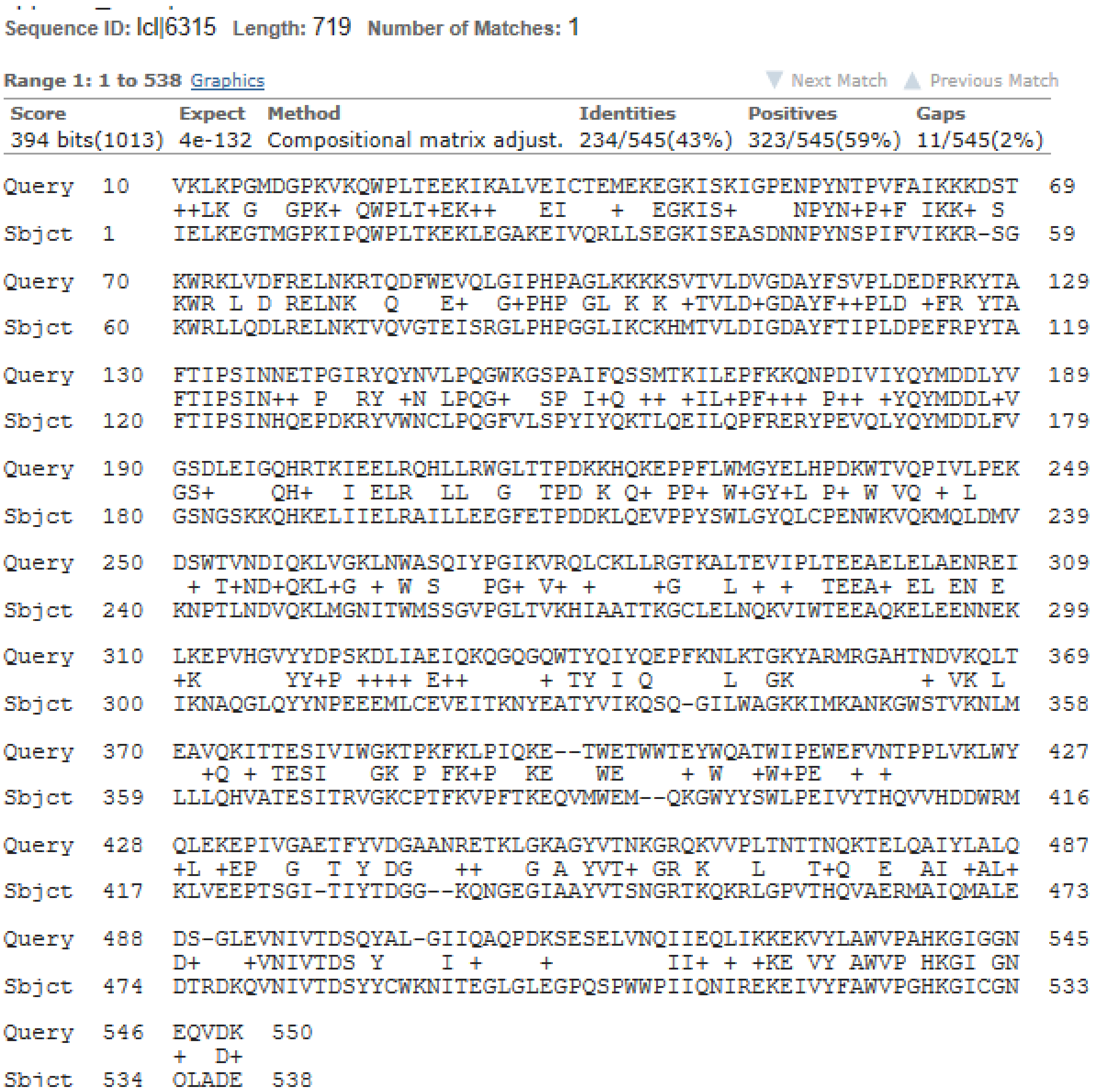


```
Species/Ab              *   **    ****  **     **      ***
1. sp|HIV---PISPIETVPVKLKPGMDGPKVKQWPLTEEKIKALVEICTEMEKEGKI
2. sp|SIV---PISSIETVPVKLKPGMDGPKVKQWPLSAEKIKALTEICQEMEKEGKI
3. sp|EIAV-----------IELKEGTMGPKIPQWPLTKEKLEGAKEIVQRLLSEGKI
4. sp|EIAV-----------IELKEGTMGPKIPQWPLTKEKLEGAKEIVQRLLSEGKI
5. sp|FIV_AQISDKIPVVKVKMKDPNKGPQIKQWPLTNEKIEALTEIVERLEKEGKV
6. sp|FIV_AQISDKIPIVKVKMKDPNKGPQIKQWPLSNEKIEALTEIVERLEREGKV
7. sp|SIV-GVLSSQIEETKVQLKEGKDGPKLKQWPLSREKIEALTEICKQMEEEGKL
```


100
100
100
100
100
sp|SIV-cpz|537-1096
sp|HIV-1|600-1159
sp|SIV-agm.gri-1|608-1169
sp|FIV_Petaluma|155-690
sp|FIV_San_Diego|155-710
sp|EIAV_1369|196-914
sp|EIAV_CL22_|196-914



☐ sp|EIAV_1369|196-914



Sequence ID: lcl|6315 Length: 719 Number of Matches: 1

Range 1: 1 to 538 Graphics

| Score | Expect | Method | Identities | Positives | Gaps |
|---|---|---|---|---|---|
| 394 bits(1013) | 4e-132 | Compositional matrix adjust. | 234/545(43%) | 323/545(59%) | 11/545(2%) |

```
Query  10    VKLKPGMDGPKVKQWPLTEEKIKALVEICTEMEKEGKISKIGPENPYNTPVFAIKKKDST  69
             ++LK G  GPK+ QWPLT+EK++   EI   +  EGKIS+    NPYN+P+F IKK+ S
Sbjct  1     IELKEGTMGPKIPQWPLTKEKLEGAKEIVQRLLSEGKISEASDNNPYNSPIFVIKKR-SG  59

Query  70    KWRKLVDFRELNKRTQDFWEVQLGIPHPAGLKKKKSVTVLDVGDAYFSVPLDEDFRKYTA  129
             KWR L D RELNK  Q   E+  G+PHP GL K K +TVLD+GDAYF++PLD +FR YTA
Sbjct  60    KWRLLQDLRELNKTVQVGTEISRGLPHPGGLIKCKHMTVLDIGDAYFTIPLDPEFRPYTA  119

Query  130   FTIPSINNETPGIRYQYNVLPQGWKGSPAIFQSSMTKILEPFKKQNPDIVIYQYMDDLYV  189
             FTIPSIN++ P  RY +N LPQG+  SP I+Q ++ +IL+PF+++ P++ +YQYMDDL+V
Sbjct  120   FTIPSINHQEPDKRYVWNCLPQGFVLSPYIYQKTLQEILQPFRERYPEVQLYQYMDDLFV  179

Query  190   GSDLEIGQHRTKIEELRQHLLRWGLTTPDKKHQKEPPFLWMGYELHPDKWTVQPIVLPEK  249
             GS+    QH+  I ELR  LL  G  TPD K Q+ PP+ W+GY+L P+ W VQ + L
Sbjct  180   GSNGSKKQHKELIIELRAILLEEGFETPDDKLQEVPPYSWLGYQLCPENWKVQKMQLDMV  239

Query  250   DSWTVNDIQKLVGKLNWASQIYPGIKVRQLCKLLRGTKALTEVIPLTEEAELELAENREI  309
              + T+ND+QKL+G + W S   PG+ V+ +    +G   L + +  TEEA+ EL EN E
Sbjct  240   KNPTLNDVQKLMGNITWMSSGVPGLTVKHIAATTKGCLELNQKVIWTEEAQKELEENNEK  299

Query  310   LKEPVHGVYYDPSKDLIAEIQKQGQGQWTYQIYQEPFKNLKTGKYARMRGAHTNDVKQLT  369
             +K      YY+P ++++ E++     + TY I Q     L  GK         + VK L
Sbjct  300   IKNAQGLQYYNPEEEMLCEVEITKNYEATYVIKQSQ-GILWAGKKIMKANKGWSTVKNLM  358

Query  370   EAVQKITTESIVIWGKTPKFKLPIQKE--TWETWWTEYWQATWIPEWEFVNTPPLVKLWY  427
               +Q + TESI   GK P FK+P  KE   WE    + W  +W+PE  + +
Sbjct  359   LLLQHVATESITRVGKCPTFKVPFTKEQVMWEM--QKGWYYSWLPEIVYTHQVVHDDWRM  416

Query  428   QLEKEPIVGAETFYVDGAANRETKLGKAGYVTNKGRQKVVPLTNTTNQKTELQAIYLALQ  487
             +L +EP  G  T Y DG   ++   G A YVT+ GR K   L   T+Q  E  AI +AL+
Sbjct  417   KLVEEPTSGI-TIYTDGG--KQNGEGIAAYVTSNGRTKQKRLGPVTHQVAERMAIQMALE  473

Query  488   DS-GLEVNIVTDSQYAL-GIIQAQPDKSESELVNQIIEQLIKKEKVYLAWVPAHKGIGGN  545
             D+   +VNIVTDS Y    I +    +        II+ + +KE VY AWVP HKGI GN
Sbjct  474   DTRDKQVNIVTDSYYCWKNITEGLGLEGPQSPWWPIIQNIREKEIVYFAWVPGHKGICGN  533

Query  546   EQVDK  550
             +  D+
Sbjct  534   QLADE  538
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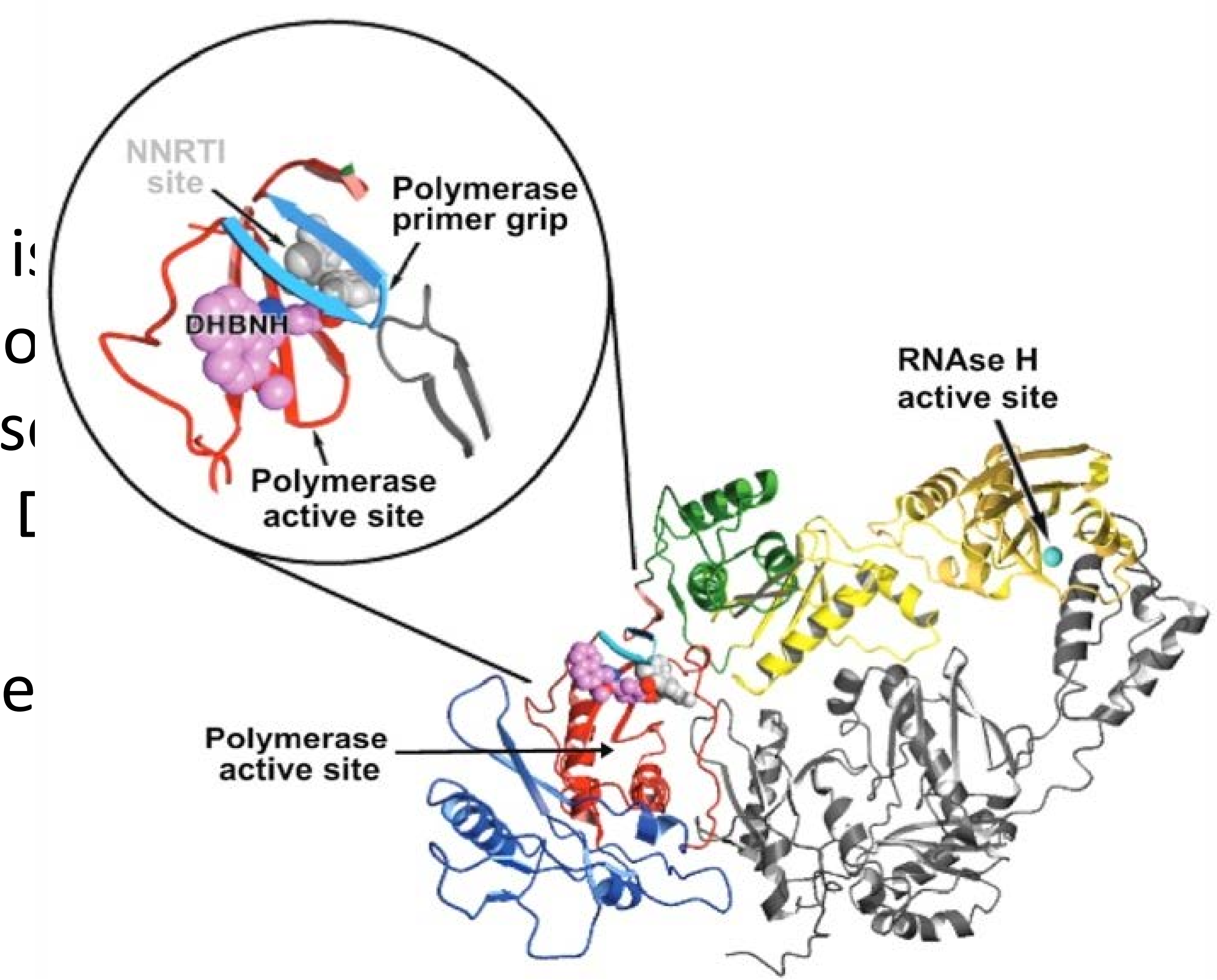

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# 3.preparation for modeling

1.Software

BLAST FASTA

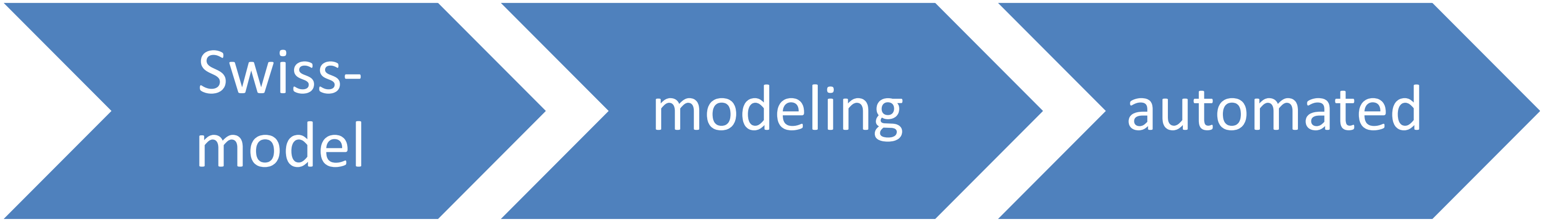
2.Kownledgement of your materials

belongings special quality

shown above

# 4.molecule modeling

1.Tools

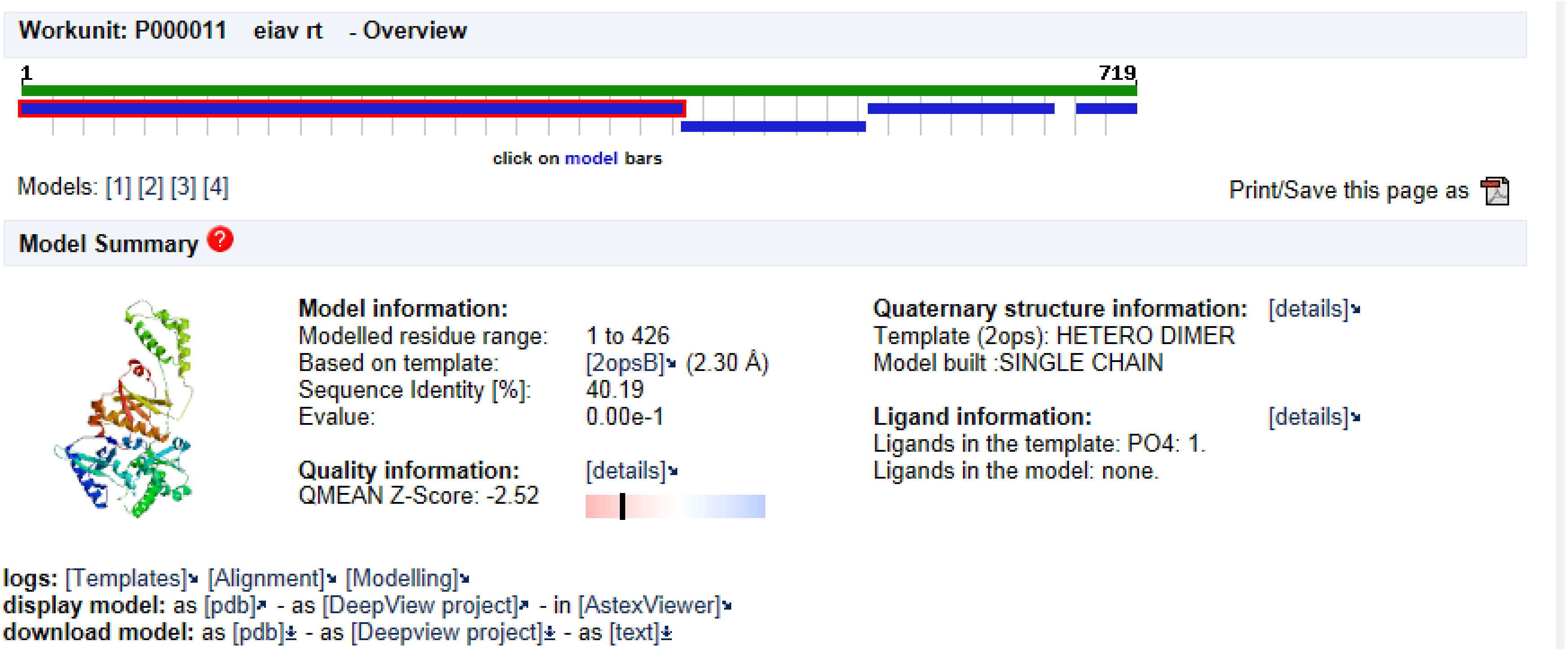


Swiss-model

modeling

automated

# 2.Result (patial)



**Workunit: P000011 eiav rt - Overview**

Models: [1] [2] [3] [4]

Print/Save this page as

**Model Summary**

**Model information:**
Modelled residue range: 1 to 426
Based on template: [2opsB] (2.30 Å)
Sequence Identity [%]: 40.19
Evalue: 0.00e-1

**Quality information:** [details]
QMEAN Z-Score: -2.52

**Quaternary structure information:** [details]
Template (2ops): HETERO DIMER
Model built :SINGLE CHAIN

**Ligand information:** [details]
Ligands in the template: PO4: 1.
Ligands in the model: none.

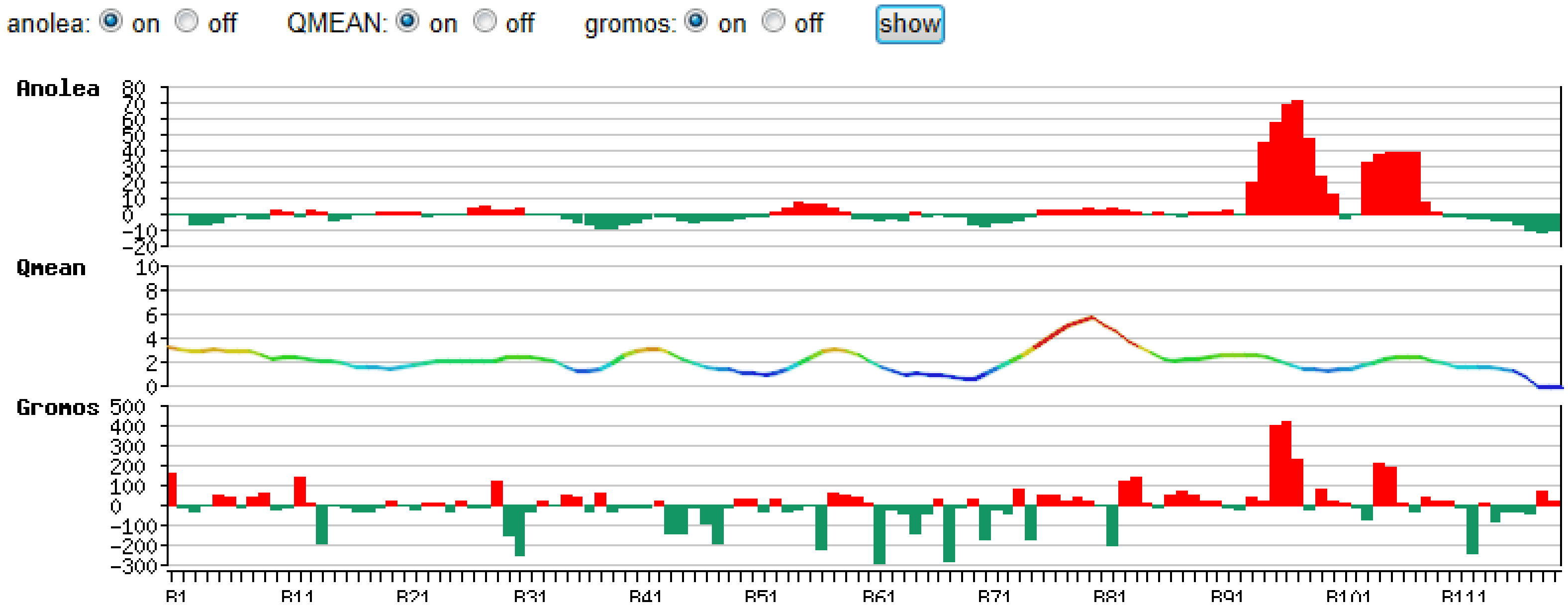
**logs:** [Templates] [Alignment] [Modelling]
**display model:** as [pdb] - as [DeepView project] - in [AstexViewer]
**download model:** as [pdb] - as [Deepview project] - as [text]

# 5.analysis

## 1. QMEAN4 global score(0-1)

| **QMEAN4 global scores:** | | | Local scores | |
|---|---|---|---|---|
| QMEANscore4 | Estimated absolute model quality | Score components | Coloring by residue error | Residue error plot |
| 0.62 | Z-Score: -2.52<br>Plot 1: [save png]<br>Plot 2: [save png] | [save png] | | [save png] |
| | | | Coloring (all chains):<br>[save jpg] [save pdb] | Energy profile:<br>[save raw scores] |

# 2. Local Model Quality Estimation: Anolea / QMEAN / Gromos



anolea: ● on ○ off QMEAN: ● on ○ off gromos: ● on ○ off

（1）.Anolea

assess packing quality of the models.

（2）. QMEAN

a composite scoring function

（3）. Gromos

a general-purpose molecular dynamics computer simulation package

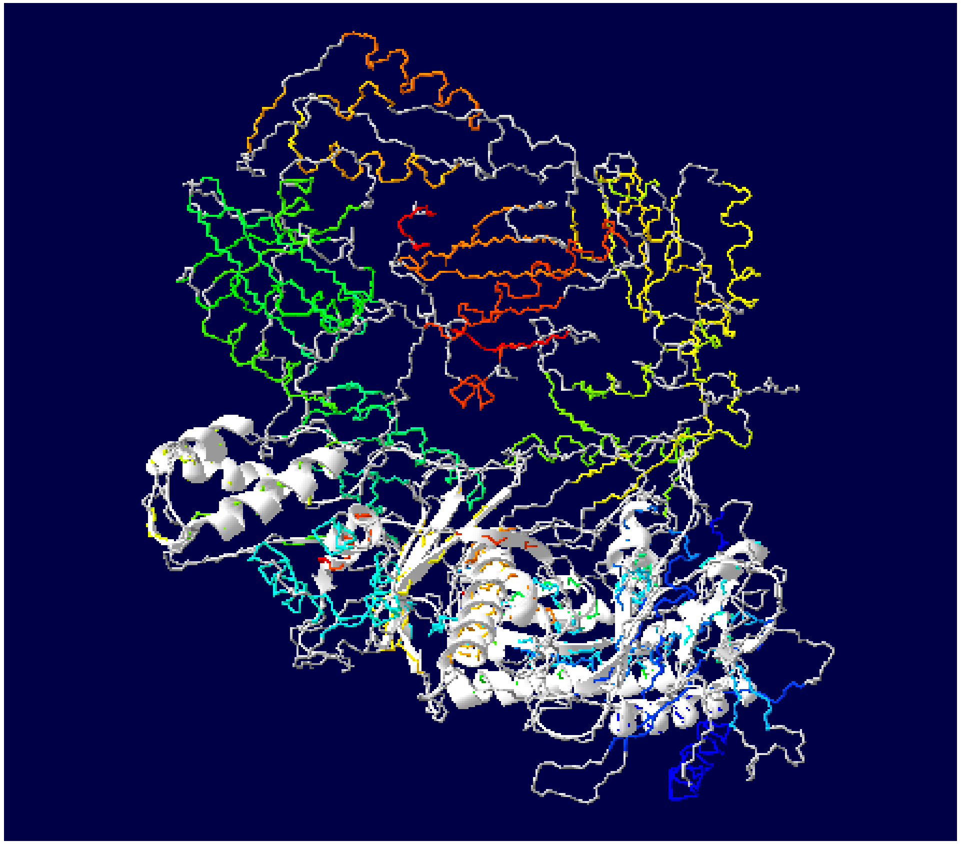
3.Others:

（1）.Alignment Output

（2）.Modeling Log

（3）. Template Selection Log

- Picture conformation



# 6.Citation（略）