# An overview of the web infrastructure for the 2019 Model Metrics Challenge

[this document is available by clicking on the HELP link in any of the Results pages]

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# General information

### Entry webpage for Results of all cryo-EM model Challenges

Evaluation results for all cryo-EM model challenges are available from the EMDataResource website <u>https://model-compare.emdataresource.org</u>:



Results of the latest challenge are accessible by clicking on the '2019' block of target images.

### Overall scheme of the 2019 Metrics Challenge

The evaluation system for 2019 Model Metrics Challenge is based on the 2016/2017 Model Challenge system (*Kryshtafovych A, Adams PD, Lawson CL, Chiu W. (2018). Evaluation system and web infrastructure for the second cryo-EM model challenge. J Struct Biol. 204, 96-108. doi: 10.1016/j.jsb.2018.07.006. PMID:30017700*). The 2019 system was significantly redesigned with inclusion of new evaluation measures and analysis tools. The overall organization of the redesigned system is described in this Help document.

Submitted models are evaluated in 4 different tracks:

- exclusively from coordinates (stereochemistry and energy-based),
- evaluating model-to-map fit,
- comparing to reference structure(s),
- checking agreement with other submitted models.

Each track uses its own software tools, and evaluation results are grouped accordingly in 4 classes. A general evaluation scheme is presented below:



### List of software tools used in different evaluation tracks

### Exclusively from coordinates

- PHENIX <sup>1</sup> (phenix.model\_statistics),
- Molprobity<sup>2</sup> (phenix.molprobity, phenix.cbetadev),
- CaBLAM<sup>3</sup> (phenix.cablam),
- ProQ3 <sup>4</sup> (machine learning energy and geometry-based single-model accuracy assessment method).

### Model-to-map fit

- PHENIX <sup>1</sup> (phenix.map\_model\_cc),
- TEMPy <sup>5-8</sup> (global and local model-map fit),
- EMRinger <sup>9</sup> (global and local model-map fit based on side-chain fit),
- Q-score<sup>10</sup>,
- Atom Inclusion score (reimplemented from EMDB Visual Analysis pages<sup>11</sup>, e.g., <u>https://www.ebi.ac.uk/pdbe/entry/emdb/EMD-10101/analysis</u> – thanks to Zhe Wang and Ardan Patwardhan from EBI).

### Comparing to reference structure(s)

- QS-score <sup>12</sup> (multimers),
- LGA <sup>13</sup> (used for generating GDT-family based scores),
- LDDT <sup>14</sup> (superposition-free measure; compares difference in distance patterns),
- CAD score <sup>15</sup> (superposition-free measure; compares difference in contact areas),
- Hydrogen-bond score (hydrogen bonds identified with HBPLUS<sup>16</sup>).

### Agreement between the models

• Davis QAconsensus <sup>17</sup>.

### Targets /reference structures / EM maps

Results for each target can be visited by clicking on the target pictograph /name

Targets in the 2019 edition of the challenge are numbered consecutively, from T0101 to T0104 (targets in the previous challenge started from T00. .). In the results tables, biological target name is provided together with the target ID.

The extended target ID includes PDB ID of the reference structure and the name of the representative chain used in the evaluations. Several reference structures can be used for the same target. Results for the reference structures are highlighted in grey in all results tables.

Map EMDB ID is shown in a separate column of the target-specific evaluation results. Unlike the previous challenge, results for different maps of the same protein are organized as different targets, e.g. Apoferritin comprises three targets (T0101-T0103) corresponding to maps at different resolution.



### Models

All models in the 2019 Challenge were submitted through the Challenges EMDataResource gateway at Rutgers. Information on the submissions with full metadata is available from:

https://challenges.emdataresource.org/sites/default/files/model\_metrics\_challenge\_metadata.xlsx

Model summary statistics can be found here:

https://challenges.emdataresource.org/sites/default/files/Submissions-Analysis.html

Files used in the evaluation (models, targets, maps) and results (plain text files as generated by evaluation programs) are available by following the 'data repositorium' link

https://model-compare.emdataresource.org/data/2019)



The Model ids used in the Results tables (e.g. T0104EM010\_1) are formed according to the following scheme:

- T0104 [target name]
- EM [electron microscopy]
- 010 [predictor group number (see below)]
- \_1 [model number 1 from this predictor for this target]

### Predictors

Each group participating in the EM Model Challenge is assigned a unique number. Predictor IDs corresponding to each model are encoded in the model name (see above). Before the June 2019 Face-to-Face Model Metrics Workshop, the group\_ID – group\_name correspondence was concealed from everyone but the organizers. The group names were revealed at the meeting and are now shown in the Group Name column on all Results pages.

### Hierarchical organization of the results

As described above, models are evaluated in 4 different tracks: exclusively from coordinates, model-to-map fit, versus reference structure(s), and agreement between models. Evaluation results in each of the tracks are reported separately under four different tabs provided at the highest level of the Results page hierarchy:

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  | Resol.<br>Orig.<br>Model<br>1.980  | (FSC=0.5)  | EMRinger     score     8.299   | Q-1<br>♦ Orig.<br>Model<br>0.830   | score  | Ator<br>Orig.<br>Mode<br>0.802  
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  | Resol.           ♦ Orig.           Model           1.980           1.984           2.000           1.988           1.996           2.012   | (FSC=0.5)  | €EMRinger<br>score<br>8.299<br>7.690<br>7.149<br>6.603<br>6.737<br>7.594   | <ul> <li>Q-s</li> <li>♦ Orig.<br/>Model</li> <li>0.830</li> <li>0.841</li> <li>0.835</li> <li>0.827</li> <li>0.819</li> <li>0.629</li> </ul>   | score<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.824  | Ator<br>Orig.<br>Mode<br>0.802<br>0.805<br>0.784<br>0.784<br>0.411  
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  | ¢LAP<br>0.393<br>0.399<br>0.395<br>0.386<br>0.386<br>0.384<br>0.393<br>0.383  | Crig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.092<br>0.092<br>0.997  
  | TemPy<br>ENV<br>1 ◆ noH<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997  | ¢111<br>0.012<br>0.010<br>0.011<br>0.011<br>0.011<br>0.012<br>0.012  | ♦ MI<br>(ov) 0.067 0.067 0.068 0.061 0.065 0.065 0.067  | SI<br>◆ Orig.<br>Model<br>0.624<br>0.625<br>0.618<br>0.616<br>0.588<br>0.612   
                         | MOC<br>0.624<br>0.626<br>0.625<br>0.618<br>0.612  | ▶ Orig.<br>Mode<br>0.717<br>0.727<br>0.732<br>0.676<br>0.684<br>0.708<br>0.708  | ox CC<br>0.725<br>0.725<br>0.732<br>0.719<br>0.716<br>0.708<br>0.706   | CCC<br>◆ Orig.<br>Model<br>0.873<br>0.836<br>0.811<br>0.837<br>0.845<br>0.794<br>0.789   | C(mask)<br>BF=0<br>0.810<br>0.809<br>0.802<br>0.799<br>0.794<br>0.786  | Ph<br>Cr<br>Model<br>0.847<br>0.818<br>0.810<br>0.818<br>0.818<br>0.824<br>0.790<br>0.786   | C(vol)   | CC(<br>♦ Orig.<br>Model<br>0.757<br>0.775<br>0.768<br>0.705<br>0.715<br>0.740<br>0.741  |   
  | Resol.   | (FSC=0.5)  | €EMRinger<br>score<br>8.299<br>7.690<br>7.149<br>6.603<br>6.737<br>7.584<br>8.299  | Q-1  | 0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.824<br>0.806  | Ator<br>Orig.<br>Mode<br>0.802<br>0.806<br>0.805<br>0.784<br>0.784<br>0.411<br>0.785  
  | downloa<br>All   | ad cs<br>on<br>• BE<br>0.94!<br>0.95:<br>0.94!<br>0.93:<br>0.93!<br>0.93!<br>0.94!<br>0.94!  |
| * • Model<br>T0101EM028_<br>T0101EM010_<br>T0101EM041_<br>T0101EM041_<br>T0101EM042_<br>T0101EM082_<br>T0101EM082_  |  | Metho<br>ab-initio/<br>optimized<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio   | d<br>◆ auto/<br>man.<br>man.<br>man.<br>auto<br>auto<br>auto<br>auto   | EM Ma  | ♦ Res<br>ol. <ol> <li>1.8</li> </ol>   
   | ♦ CCC<br>0.579<br>0.579<br>0.577<br>0.577<br>0.575<br>0.572<br>0.569<br>0.569  | ♦ CCC<br>(ov) 0.264 0.263 0.263 0.260 0.265 0.258 0.264  
   
   | ◆ LAP<br>0.393<br>0.399<br>0.395<br>0.386<br>0.384<br>0.383<br>0.383<br>0.386   | ♦ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.092<br>0.002  
   | TemPy<br>ENV<br>€NV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997  | ◆1/11<br>0.012<br>0.010<br>0.011<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012  | ♦ MI<br>(ov) 0.067 0.067 0.068 0.061 0.065 0.065 0.067 0.067 0.064  | SI           ♦ Orig.           Model           0.624           0.625           0.618           0.588           0.612           0.583   | MOC<br>0.624<br>0.626<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.612<br>0.617     
  |   | 0.725<br>0.725<br>0.725<br>0.732<br>0.719<br>0.716<br>0.708<br>0.706<br>0.693  | CC   | C(mask)<br>↓ ◆ BF=0<br>0.810<br>0.809<br>0.802<br>0.794<br>0.786<br>0.775  | Ph<br>Crig.<br>Model<br>0.847<br>0.818<br>0.810<br>0.818<br>0.818<br>0.824<br>0.790<br>0.786<br>0.797   | enix<br>C(vol)<br>• 8F=0<br>0.808<br>0.809<br>0.809<br>0.800<br>0.797<br>0.795<br>0.772  | CC(<br>Orig.<br>Model<br>0.757<br>0.768<br>0.705<br>0.768<br>0.705<br>0.715<br>0.740<br>0.741<br>0.735  | peaks)   
   | Resol.           ♦ Orig.           Model           1.984           2.000           1.988           1.996           2.012           2.020           2.004   | (FSC=0.5)<br>♦ BF=0<br>2.016<br>1.996<br>2.000<br>2.016<br>2.020<br>2.012<br>2.020<br>2.020  | ◆ EMRinger<br>score<br>8.299<br>7.590<br>7.149<br>6.603<br>6.737<br>7.584<br>8.299<br>7.486  | <ul> <li>Q-1</li> <li>♦ Orig.<br/>Model</li> <li>0.830</li> <li>0.841</li> <li>0.835</li> <li>0.827</li> <li>0.819</li> <li>0.689</li> <li>0.806</li> <li>0.667</li> </ul>   | score<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.824<br>0.806<br>0.801  | Ator<br>Mode<br>0.802<br>0.806<br>0.805<br>0.784<br>0.784<br>0.784<br>0.785<br>0.406   
   | downloa<br>All<br>0.802<br>0.806<br>0.805<br>0.784<br>0.784<br>0.785<br>0.783  | ad cs<br>Dn<br>0.94!<br>0.95:<br>0.94!<br>0.93:<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.94!   |
| Model     T0101EM028     T0101EM010     T0101EM091     T0101EM091     T0101EM041     T0101EM082     T010EM082   |  | Metho<br>+ ab-initio/<br>optimized<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio  | d  | EM Ma  |  
  | ♦ CCC<br>0.579<br>0.577<br>0.577<br>0.577<br>0.575<br>0.572<br>0.569<br>0.569<br>0.569   | ♦ CCCC<br>(ov) 0.264 0.263 0.263 0.265 0.265 0.258 0.264 0.270  
   
  | ♦ LAP 0.393 0.395 0.386 0.386 0.383 0.386 0.386 0.386 0.386 0.386 0.372   | ♦ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002  
  | TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997   | ¢111<br>0.012<br>0.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012<br>0.012   | ♦ MI<br>(ov) 0.067 0.067 0.068 0.061 0.065 0.067 0.067 0.067 0.064 0.074  | Si<br>Orig.<br>Model<br>0.626<br>0.625<br>0.618<br>0.616<br>0.588<br>0.612<br>0.583<br>0.607<br>0.525     0.612     0.625     0.612     0.625     0.625     0.612     0.625     0.612     0.612     0.583     0.607     0.583     0.607     0.57   | MOC<br>0.624<br>0.626<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.617<br>0.607<br>0.607   
   | b<br>♦ Orig.<br>Mode<br>0.717<br>0.722<br>0.732<br>0.676<br>0.684<br>0.708<br>0.708<br>0.696<br>0.542<br>0.722  | ox CC<br>0.725<br>0.725<br>0.732<br>0.719<br>0.716<br>0.706<br>0.706<br>0.693<br>0.694   | CC   | C(mask)  | Ph<br>Crig.<br>Model<br>0.817<br>0.818<br>0.810<br>0.818<br>0.810<br>0.818<br>0.810<br>0.818<br>0.824<br>0.790<br>0.786<br>0.797<br>0.786   | enix<br>C(vol)<br>• 8F=0<br>0.808<br>0.809<br>0.809<br>0.800<br>0.797<br>0.796<br>0.785<br>0.772<br>0.769<br>0.769   | CC(   | ▶ eaks) ♦ BF=0 0.759 0.760 0.766 0.763 0.740 0.740 0.740 0.738 0.722 0.721   | Resol.   | (FSC=0.5)<br>¢
BF=0<br>2.016<br>2.020<br>2.012<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.00 | ◆ EMRinger<br>score 8.299 7.690 7.149 6.603 6.737 7.584 8.299 7.486 7.415 7.475  | Q-1<br>♦ Orig.<br>Model<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.689<br>0.866<br>0.866<br>0.866<br>0.866<br>0.867<br>0.731  | score<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.824<br>0.806<br>0.801<br>0.705   | Ator  
  | downloa<br>m Inclusic<br>All<br>0.802<br>0.805<br>0.784<br>0.784<br>0.785<br>0.783<br>0.779<br>0.779   | ad cs  |
| Model     T0101EM028_1     T0101EM010_     T0101EM041_     T0101EM041_     T0101EM042_2     T0101EM042_2     T0101EM043     T0101EM035     T010EM035     T010EM035     T010EM035     T010EM035     T010EM035      T010EM035  | Group<br>Name<br>ccpem<br>yu<br>chiu<br>arpwarp<br>rosetta<br>singharcy<br>rosetta<br>phenix<br>fzjuelich<br>cdm/  | Metho<br>to ab-initio/<br>optimized<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio  | d  | EM Ma  | ♦ Res ol. 1.8   
   | ♦ CCC 0.579 0.577 0.577 0.575 0.572 0.569 0.569 0.567 0.567 0.567 0.567 0.567  | ♦ CCCC<br>(ov) 0.264 0.263 0.263 0.265 0.265 0.258 0.264 0.279 0.249 0.279 0.249 0.255   
   
   | ◆ LAP<br>0.393<br>0.399<br>0.395<br>0.384<br>0.393<br>0.383<br>0.386<br>0.373<br>0.386<br>0.373<br>0.345  | ♦ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002  
   | TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997  | ◆1/11<br>0/012<br>0.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012<br>0.012<br>0.011   | ♦ MI<br>(ov) 0.067 0.068 0.061 0.065 0.067 0.064 0.067 0.064 0.063 0.061 0.065 0.064 0.065 0.065 0.065  | Si<br>Orig.<br>Model<br>0.624<br>0.625<br>0.618<br>0.616<br>0.616<br>0.612<br>0.612<br>0.623<br>0.612<br>0.625<br>0.612<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.626<br>0.612<br>0.583<br>0.607<br>0.589      0. | MOC<br>0.624<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.617<br>0.607<br>0.607<br>0.607  
  | b   | ox CC<br>0.725<br>0.725<br>0.732<br>0.719<br>0.716<br>0.706<br>0.693<br>0.691<br>0.689   | CC   | C(mask)  | Ph<br>Crig.<br>Model<br>0.847<br>0.818<br>0.810<br>0.818<br>0.824<br>0.790<br>0.786<br>0.797<br>0.716<br>0.797<br>0.716   | enix<br>C(vol)<br>♦ BF=0<br>0.808<br>0.807<br>0.809<br>0.790<br>0.790<br>0.772<br>0.772<br>0.769<br>0.772  | CC(<br>♦ Orig.<br>Model<br>0.757<br>0.775<br>0.768<br>0.705<br>0.745<br>0.741<br>0.735<br>0.555<br>0.765<br>0.765   | peaks)   | Resol.           ♦ Orig.           Model           1.980           1.984           2.001           2.012           2.004           2.045           1.988   | (FSC=0.5)<br>♦ BF=0<br>2.016<br>1.996<br>2.016<br>2.020<br>2.012<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.025   
   | ◆ EMRinger<br>score 8.299 7.499 6.603 6.737 7.584 8.299 7.486 7.415 7.707 7.733  | Q-1<br>♦ Orig.<br>Model<br>0.830<br>0.841<br>0.827<br>0.819<br>0.827<br>0.819<br>0.806<br>0.667<br>0.791<br>0.6791<br>0.759  | score<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.824<br>0.806<br>0.801<br>0.791<br>0.759  | Ator<br>Mode<br>0.802<br>0.806<br>0.805<br>0.806<br>0.805<br>0.784<br>0.784<br>0.411<br>0.784<br>0.406<br>0.406<br>0.406<br>0.479<br>0.405   
   | downloa<br>m Inclusic<br>All<br>1.1 ♦ noH<br>0.802<br>0.805<br>0.784<br>0.784<br>0.785<br>0.783<br>0.779<br>0.778<br>0.779<br>0.773  | ad cs<br>on<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.94!<br>0.93:<br>0.94!<br>0.94!<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.94!<br>0.95:<br>0.94!<br>0.94!<br>0.95:<br>0.94!<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.94!<br>0.95:<br>0.94!<br>0.94!<br>0.95:<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95! |
|   |  | Metho<br>to ab-initio/<br>optimized<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio   | d  | EM Ma  | ■P<br>■ Res<br>ol.      1.8  
  1.8     1.8 <td>♦ CCCC<br/>0.579<br/>0.577<br/>0.577<br/>0.577<br/>0.575<br/>0.569<br/>0.569<br/>0.569<br/>0.569<br/>0.562<br/>0.557<br/>0.556</td> <td>♦ CCCC<br/>(ov) 0.264 0.263 0.263 0.258 0.264 0.279 0.249 0.249 0.255 0.255 0.252</td> <td>◆ LAP 0.393 0.399 0.395 0.386 0.386 0.386 0.373 0.385 0.345 0.365</td> <td>♦ Orig.<br/>Mode<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.002<br/>0.997<br/>0.002<br/>0.997</td> <td>TemPy<br/>ENV<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997</td> <td>◆ 111<br/>0.012<br/>0.010<br/>0.011<br/>0.011<br/>0.012<br/>0.012<br/>0.012<br/>0.012<br/>0.011<br/>0.011</td> <td>♦ MI<br/>(ov) 0.067 0.067 0.068 0.061 0.067 0.067 0.064 0.073 0.061 0.055 0.061</td> <td></td> <td>MOC<br/>0.624<br/>0.625<br/>0.618<br/>0.616<br/>0.623<br/>0.612<br/>0.617<br/>0.607<br/>0.607<br/>0.589<br/>0.595</td> <td></td> <td>ox CC<br/>↓ ◆ BF=0<br/>0.725<br/>0.725<br/>0.725<br/>0.719<br/>0.716<br/>0.708<br/>0.708<br/>0.693<br/>0.691<br/>0.694<br/>0.685</td> <td>CC<br/>♦ Orig.<br/>Model<br/>0.873<br/>0.836<br/>0.837<br/>0.845<br/>0.794<br/>0.784<br/>0.818<br/>0.818<br/>0.818<br/>0.818<br/>0.818<br/>0.818<br/>0.839<br/>0.740<br/>0.839<br/>0.740<br/>0.807</td> <td>C(mask)<br/>♦ BF=0<br/>0.810<br/>0.809<br/>0.809<br/>0.799<br/>0.794<br/>0.775<br/>0.769<br/>0.775<br/>0.769<br/>0.775<br/>0.769<br/>0.775</td> <td>Ph<br/>Crig.<br/>Model<br/>0.847<br/>0.818<br/>0.810<br/>0.818<br/>0.818<br/>0.824<br/>0.790<br/>0.786<br/>0.797<br/>0.716<br/>0.819<br/>0.746</td> <td>enix<br/>C(vol)<br/>♦ BF=0<br/>0.808<br/>0.807<br/>0.808<br/>0.800<br/>0.797<br/>0.790<br/>0.772<br/>0.772<br/>0.776<br/>0.777<br/>0.769<br/>0.777<br/>0.761</td> <td>CC(<br/>♦ Orig.<br/>Model<br/>0.757<br/>0.765<br/>0.705<br/>0.740<br/>0.740<br/>0.735<br/>0.735<br/>0.735<br/>0.735<br/>0.765<br/>0.761<br/>0.695<br/>0.744</td> <td><b>peaks)</b> ♦ BF=0 0.759 0.760 0.766 0.753 0.749 0.738 0.722 0.721 0.723 0.695 0.713</td> <td>Resol.           ● Orig.           Model           1.980           1.984           2.001           2.012           2.004           2.045           1.988           2.076</td> <td>(FSC=0.5)<br/>♦ BF=0<br/>2.016<br/>1.996<br/>2.016<br/>2.020<br/>2.016<br/>2.020<br/>2.020<br/>2.020<br/>2.020<br/>2.020<br/>2.0245<br/>2.024<br/>2.025<br/>2.037</td> <td></td> <td>Q-3     ΦOrig.     Model     0.830     0.841     0.827     0.819     0.869     0.866     0.667     0.791     0.671     0.759     0.774</td> <td>score<br/>0.830<br/>0.841<br/>0.825<br/>0.825<br/>0.829<br/>0.824<br/>0.806<br/>0.801<br/>0.791<br/>0.799<br/>0.774</td> <td>Ator<br/>Mode<br/>0.802<br/>0.806<br/>0.805<br/>0.784<br/>0.784<br/>0.411<br/>0.784<br/>0.406<br/>0.406<br/>0.779<br/>0.405<br/>0.744</td> <td>downloa<br/>m Inclusic<br/>All<br/>● noH<br/>0.802<br/>0.806<br/>0.805<br/>0.784<br/>0.799<br/>0.785<br/>0.783<br/>0.779<br/>0.778<br/>0.778<br/>0.778<br/>0.778<br/>0.778</td> <td>ad cs<br/>on<br/>0.94!<br/>0.95:<br/>0.94!<br/>0.93!<br/>0.93!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.94!<br/>0.93!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!<br/>0.94!</td> | ♦ CCCC<br>0.579<br>0.577<br>0.577<br>0.577<br>0.575<br>0.569<br>0.569<br>0.569<br>0.569<br>0.562<br>0.557<br>0.556   | ♦ CCCC<br>(ov) 0.264 0.263 0.263 0.258 0.264 0.279 0.249 0.249 0.255 0.255 0.252  
   
  | ◆ LAP 0.393 0.399 0.395 0.386 0.386 0.386 0.373 0.385 0.345 0.365   | ♦ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997                  
  | TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997   | ◆ 111<br>0.012<br>0.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012<br>0.012<br>0.011<br>0.011  | ♦ MI<br>(ov) 0.067 0.067 0.068 0.061 0.067 0.067 0.064 0.073 0.061 0.055 0.061  |  
                         | MOC<br>0.624<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.617<br>0.607<br>0.607<br>0.589<br>0.595  |   | ox CC<br>↓ ◆ BF=0<br>0.725<br>0.725<br>0.725<br>0.719<br>0.716<br>0.708<br>0.708<br>0.693<br>0.691<br>0.694<br>0.685   | CC<br>♦ Orig.<br>Model<br>0.873<br>0.836<br>0.837<br>0.845<br>0.794<br>0.784<br>0.818<br>0.818<br>0.818<br>0.818<br>0.818<br>0.818<br>0.839<br>0.740<br>0.839<br>0.740<br>0.807                    | C(mask)<br>♦ BF=0<br>0.810<br>0.809<br>0.809<br>0.799<br>0.794<br>0.775<br>0.769<br>0.775<br>0.769<br>0.775<br>0.769<br>0.775  | Ph<br>Crig.<br>Model<br>0.847<br>0.818<br>0.810<br>0.818<br>0.818<br>0.824<br>0.790<br>0.786<br>0.797<br>0.716<br>0.819<br>0.746  | enix<br>C(vol)<br>♦ BF=0<br>0.808<br>0.807<br>0.808<br>0.800<br>0.797<br>0.790<br>0.772<br>0.772<br>0.776<br>0.777<br>0.769<br>0.777<br>0.761  | CC(<br>♦ Orig.<br>Model<br>0.757<br>0.765<br>0.705<br>0.740<br>0.740<br>0.735<br>0.735<br>0.735<br>0.735<br>0.765<br>0.761<br>0.695<br>0.744  | <b>peaks)</b> ♦ BF=0 0.759 0.760 0.766 0.753 0.749 0.738 0.722 0.721 0.723 0.695 0.713  
  | Resol.           ● Orig.           Model           1.980           1.984           2.001           2.012           2.004           2.045           1.988           2.076   | (FSC=0.5)<br>♦ BF=0<br>2.016<br>1.996<br>2.016<br>2.020<br>2.016<br>2.020<br>2.020<br>2.020<br>2.020<br>2.020<br>2.0245<br>2.024<br>2.025<br>2.037   |  | Q-3     ΦOrig.     Model     0.830     0.841     0.827     0.819     0.869     0.866     0.667     0.791     0.671     0.759     0.774   | score<br>0.830<br>0.841<br>0.825<br>0.825<br>0.829<br>0.824<br>0.806<br>0.801<br>0.791<br>0.799<br>0.774   | Ator<br>Mode<br>0.802<br>0.806<br>0.805<br>0.784<br>0.784<br>0.411<br>0.784<br>0.406<br>0.406<br>0.779<br>0.405<br>0.744  
  | downloa<br>m Inclusic<br>All<br>● noH<br>0.802<br>0.806<br>0.805<br>0.784<br>0.799<br>0.785<br>0.783<br>0.779<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778   | ad cs<br>on<br>0.94!<br>0.95:<br>0.94!<br>0.93!<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.94!<br>0.93!<br>0.94!<br>0.93!<br>0.94!<br>0.94!<br>0.93!<br>0.94!<br>0.94!<br>0.93!<br>0.94!<br>0.94!<br>0.93!<br>0.94!<br>0.94!<br>0.94!<br>0.93!<br>0.94!<br>0.94!<br>0.93!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94! |
| Model     T0101EM028_     T0101EM010_     T0101EM010_     T0101EM041_     T0101EM041_     T0101EM042_     T0101EM082_     T0101EM082_     T0101EM082_     T0101EM082_     T0101EM084_      T0101EM084_     T010EM084_     T010EM084_     T010EM084_     T010EM084_     T0 | Group<br>Name<br>yu<br>chiu<br>arpwarp<br>rosetta<br>phenix<br>fzjuelich<br>cdmd<br>-  | Methi  | d  | EM Ma  | ■ P PRes ol. 1.8   
  | ♦ CCC<br>0.579<br>0.577<br>0.577<br>0.575<br>0.575<br>0.569<br>0.569<br>0.569<br>0.567<br>0.567<br>0.557<br>0.555<br>0.557   | ♦ CCC<br>(ov) 0.264 0.263 0.263 0.268 0.268 0.264 0.279 0.249 0.249 0.249 0.255 0.255 0.252 0.258   
   
  | ◆ LAP 0.393 0.399 0.395 0.386 0.386 0.386 0.383 0.386 0.382 0.345 0.365 0.373   | ♦ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.997<br>0.997   
  | TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997   | ◆ 111<br>0.012<br>0.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012<br>0.012<br>0.011<br>0.011<br>0.011<br>0.010  | ★ MII<br>(ov) 0.067 0.067 0.068 0.065 0.065 0.064 0.067 0.064 0.073 0.061 0.055 0.061 0.065   | SI           Model           0.624           0.625           0.616           0.588           0.616           0.583           0.607           0.573           0.595           0.560   | MOC<br>0.624<br>0.626<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.617<br>0.607<br>0.606<br>0.589<br>0.595<br>0.594  
   |   | ox CC<br>0.725<br>0.725<br>0.732<br>0.716<br>0.708<br>0.708<br>0.708<br>0.693<br>0.691<br>0.694<br>0.685<br>0.670  | CC<br>♦ Orig.<br>Model<br>0.873<br>0.836<br>0.813<br>0.845<br>0.794<br>0.794<br>0.845<br>0.818<br>0.818<br>0.818<br>0.818<br>0.839<br>0.718<br>0.839<br>0.777                                      | C(mask)<br>♦ BF=0<br>0.810<br>0.809<br>0.809<br>0.799<br>0.799<br>0.794<br>0.775<br>0.769<br>0.775<br>0.769<br>0.775<br>0.769<br>0.775<br>0.769<br>0.775                           | Ph<br>Cr<br>4<br>0.817<br>0.818<br>0.818<br>0.818<br>0.818<br>0.790<br>0.786<br>0.790<br>0.716<br>0.819<br>0.716<br>0.819<br>0.726<br>0.759   | enix<br>C(vol)<br>• BF=0<br>0.808<br>0.809<br>0.809<br>0.809<br>0.790<br>0.790<br>0.790<br>0.795<br>0.770<br>0.769<br>0.770<br>0.761<br>0.748  | CC(<br>♦ Orig.<br>Model<br>0.757<br>0.765<br>0.705<br>0.740<br>0.740<br>0.735<br>0.735<br>0.761<br>0.695<br>0.761<br>0.679  | ▶ eaks)  | Resol.           ♦ Orig.           Model           1.980           1.982           2.000           2.001           2.012           2.012           2.020           2.045           1.988           2.076           2.028   | (FSC=0.5)<br>♦ BF=0<br>2.016<br>1.996<br>2.000<br>2.016<br>2.000<br>2.012<br>2.020<br>2.020<br>2.022<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.033   
  | ◆ EMRinger<br>score 8.299 7.690 7.690 6.603 6.737 7.584 8.299 7.486 8.299 7.486 7.415 7.707 7.743 7.943  | Q-3<br>♦ Orig.<br>Model<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.689<br>0.669<br>0.669<br>0.669<br>0.669<br>0.791<br>0.671<br>0.774<br>0.639  | ◆ not     0.830     0.841     0.835     0.827     0.819     0.806     0.801     0.791     0.795     0.774     0.775  | Ator  
  | downloa<br>m Inclusic<br>All<br>◆ noH<br>0.802<br>0.806<br>0.805<br>0.784<br>0.799<br>0.783<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.764<br>0.753   | ad cs<br>Dn<br>• BE<br>0.94!<br>0.95:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.94!<br>0.95:<br>0.95!<br>0.94!<br>0.95:<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!<br>0.95!  |
| Model     T0101EM028     T0101EM010     T0101EM010     T0101EM041     T0101EM041     T0101EM042     T0101EM032     T0101EM032     T0101EM032     T0101EM034     T0101EM034     T0101EM034     T0101EM034  |  | Metha<br>ab-initio<br>optimized<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>optimized<br>ab-initio<br>optimized<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio  | d  | EM Ma<br>+ MapID<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>em | ◆Resol. <ol> <li>1.8</li> </ol>  
   | ♦ CCC 0.579 0.577 0.577 0.575 0.569 0.569 0.569 0.567 0.562 0.556 0.5547 0.4777 0.4777   | ♦ CCCC<br>(ov) 0.264 0.263 0.260 0.265 0.264 0.265 0.264 0.279 0.249 0.249 0.255 0.252 0.253 0.214   
   
   | ♦ LAP <ul> <li>0.393</li> <li>0.395</li> <li>0.386</li> <li>0.383</li> <li>0.383</li> <li>0.386</li> <li>0.373</li> <li>0.382</li> <li>0.345</li> <li>0.373</li> <li>0.289</li> </ul>   | ♦ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.092<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002   
   | TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.97 | ◆ 111         0012         0012         0.011         0.011         0.012         0.012         0.012         0.012         0.011         0.010         0.011         0.010         0.011         0.010         0.011         0.012         0.012         0.011         0.012         0.012         0.012         0.011         0.012         0.01         0.012         0.01         0.01         0.01         0.01         0.01         0.01         0.01         0.01         0.01         0.01         0.01         0.01         0.01         0.01         0.01         0.01 | ★ MII<br>(ov) 0.067 0.067 0.068 0.065 0.065 0.064 0.067 0.064 0.073 0.061 0.055 0.061 0.065 0.061 0.065 0.061 0.065 0.064 0.065 0.061 0.065 0.064 0.065 0.061 0.065 0.064 0.065 0.061 0.065 0.064 0.065 0.061 0.065 0.064 0.065 0.061 0.065 0.064 0.065 0.061 0.065 0.064 0.065 0.061 0.065 0.064 0.065 0.064 0.065 0.061 0.065 0.064   | SI           ♦ Orig.           Model           0.624           0.625           0.618           0.612           0.588           0.612           0.573           0.595           0.596           0.596           0.596           0.596           0.596   | MOC<br>0.624<br>0.626<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.617<br>0.607<br>0.606<br>0.595<br>0.594<br>0.506   
  | b<br>♦ Orig.<br>Mode<br>0.717<br>0.727<br>0.676<br>0.684<br>0.708<br>0.708<br>0.542<br>0.542<br>0.699<br>0.723<br>0.699<br>0.723<br>0.699<br>0.701<br>0.548<br>0.559  | ox CC  | € Orig.<br>Model<br>0.873<br>0.836<br>0.811<br>0.837<br>0.845<br>0.789<br>0.789<br>0.789<br>0.789<br>0.789<br>0.789<br>0.789<br>0.777<br>0.845<br>0.777<br>0.645                                   | 2(mask)  | Ph<br>CC<br>Model<br>0.847<br>0.818<br>0.818<br>0.818<br>0.824<br>0.790<br>0.786<br>0.797<br>0.716<br>0.747<br>0.759<br>0.634<br>   | enix<br>C(vol)<br>• BF=0<br>0.808<br>0.807<br>0.808<br>0.809<br>0.800<br>0.790<br>0.790<br>0.790<br>0.790<br>0.770<br>0.770<br>0.747<br>0.748<br>0.633<br>0.748  | CC(<br>♦ Orig.<br>Model<br>0.757<br>0.775<br>0.765<br>0.705<br>0.741<br>0.735<br>0.555<br>0.761<br>0.995<br>0.741<br>0.655<br>0.761<br>0.995<br>0.764<br>0.679<br>0.584   | ▶ BF=0 0.759 0.760 0.766 0.749 0.740 0.721 0.722 0.721 0.723 0.695 0.713 0.697 0.577   
   | Resol.           ♦ Orig.           Model           1.980           1.984           2.000           2.012           2.020           2.045           1.988           2.075           2.016           2.028           2.028           2.028   | (FSC-0.5)<br>♦ BF=0<br>2.016<br>1.996<br>2.000<br>2.012<br>2.020<br>2.022<br>2.022<br>2.022<br>2.024<br>2.075<br>2.033<br>2.193<br>2.033   | € EMRinger<br>score<br>8.299<br>7.690<br>6.737<br>7.584<br>8.299<br>7.496<br>7.415<br>7.743<br>7.743<br>7.237<br>7.943<br>6.447<br>7.943   | Q-3<br>♦ Orig.<br>Model<br>0.830<br>0.845<br>0.827<br>0.839<br>0.689<br>0.689<br>0.689<br>0.689<br>0.689<br>0.689<br>0.689<br>0.671<br>0.791<br>0.671<br>0.759<br>0.779<br>0.639<br>0.639<br>0.639<br>0.639  | ◆ not<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.826<br>0.806<br>0.801<br>0.791<br>0.775<br>0.759<br>0.774  | Ator   
   | downloa<br>m Inclusic<br>All   | ad cs<br>Dn<br>• BE<br>0.94!<br>0.95:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.93:<br>0.94!<br>0.94!<br>0.93:<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!<br>0.94!  |
| Model     T0101EM028     T0101EM010     T0101EM041     T0101EM041     T0101EM041     T0101EM032     T0101EM032     T0101EM038     T0101EM038     T0101EM038     T0101EM038     T0101EM038     T0101EM054     S T0101EM054     S T0101EM054     S T0101EM054   |  | Methn<br>ab-inlio/<br>optimized<br>ab-inlio<br>ab-inlio<br>ab-inlio<br>ab-inlio<br>ab-inlio<br>ab-inlio<br>optimized<br>ab-inlio<br>optimized<br>optimized<br>ab-inlio<br>ab-inlio<br>ab-inlio<br>ab-inlio<br>ab-inlio<br>ab-inlio<br>ab-inlio<br>ab-inlio   | d  | EM Ma<br>MapID     emd_20026_1     emd_2002  | ♦ Res<br>ol. <ol> <li>1.8</li> </ol>   
   | ♦ CCCC 0.579 0.577 0.577 0.575 0.575 0.572 0.569 0.569 0.567 0.562 0.556 0.547 0.547 0.4477 0.4477 0.4460 0.394  | ♦ CCCC<br>(ov) 0.264 0.263 0.260 0.265 0.258 0.249 0.255 0.252 0.252 0.258 0.214 0.254 0.214 0.214 0.249 0.255 0.258 0.214 0.249 0.255 0.258 0.214 0.249 0.255 0.258 0.214 0.249 0.255 0.258 0.214 0.249 0.255 0.258 0.214 0.249 0.255 0.258 0.214 0.249 0.255 0.258 0.214 0.249 0.255 0.258 0.214 0.249 0.255 0.258 0.214 0.249 0.255 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.214 0.249 0.258 0.258 0.214 0.249 0.258 0.214 0.258 0.258 0.258 0.258 0.258 0.258 0.258 <td>♦ LAP <ul> <li>0.393</li> <li>0.395</li> <li>0.386</li> <li>0.383</li> <li>0.383</li> <li>0.386</li> <li>0.373</li> <li>0.382</li> <li>0.345</li> <li>0.373</li> <li>0.289</li> <li>0.289</li> <li>0.190</li> </ul></td> <td><ul> <li>♦ Orig.<br/>Mode</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.002</li> <li>0.997</li> <li>0.997</li></ul></td>
<td>TemPy<br/>ENV<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.997<br/>0.97</td> <td>¢111<br/>0.012<br/>1.010<br/>0.011<br/>0.011<br/>0.012<br/>0.012<br/>0.012<br/>0.012<br/>0.011<br/>0.011<br/>0.011<br/>0.011<br/>0.010</td> <td>♦ MI<br/>(ov) 0.067 0.067 0.068 0.061 0.065 0.064 0.067 0.064 0.061 0.065 0.065 0.061 0.065 0.0661 0.065 0.066 0.065 0.066 0.035</td> <td>SI           ↓ Orig.           Model           0.626           0.625           0.616           0.866           0.616           0.583           0.617           0.573           0.589           0.589           0.589           0.590           0.595           0.475           0.479           0.304</td> <td>MOC</td> <td>b<br/>♦ Orig.<br/>Mode<br/>0.717<br/>0.722<br/>0.676<br/>0.684<br/>0.708<br/>0.708<br/>0.708<br/>0.708<br/>0.708<br/>0.708<br/>0.708<br/>0.723<br/>0.699<br/>0.723<br/>0.699<br/>0.741<br/>0.644<br/>0.559<br/>0.559<br/>0.524<br/>0.427<br/>0.427<br/>0.645<br/>0.645<br/>0.645<br/>0.645<br/>0.645<br/>0.765<br/>0.645<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.755<br/>0.75</td> <td>ox CC           0.725           0.725           0.732           0.716           0.708           0.708           0.708           0.693           0.691           0.663           0.669           0.670           0.564           0.524</td> <td>€ Crig.<br/>Model<br/>0.873<br/>0.836<br/>0.811<br/>0.837<br/>0.845<br/>0.789<br/>0.818<br/>0.779<br/>0.818<br/>0.779<br/>0.818<br/>0.839<br/>0.740<br/>0.839<br/>0.777<br/>0.646<br/>0.574</td> <td>C(mask)<br/>0.810<br/>0.810<br/>0.809<br/>0.799<br/>0.794<br/>0.769<br/>0.775<br/>0.769<br/>0.775<br/>0.769<br/>0.776<br/>0.762<br/>0.740<br/>0.620<br/>0.574<br/>0.454</td> <td>Ph<br/>CC<br/>0.847<br/>0.848<br/>0.818<br/>0.818<br/>0.824<br/>0.790<br/>0.776<br/>0.797<br/>0.746<br/>0.797<br/>0.747<br/>0.747<br/>0.747<br/>0.759<br/>0.634<br/>0.634</td> <td>enix<br/>C(vol)<br/>♦ BF=0<br/>0.808<br/>0.807<br/>0.809<br/>0.809<br/>0.790<br/>0.790<br/>0.772<br/>0.769<br/>0.772<br/>0.761<br/>0.747<br/>0.633<br/>0.633<br/>0.633<br/>0.593<br/>0.489</td> <td>CC(</td> <td>peaks)</td> <td>Resol.           ♦ Orig.           Model           1.980           1.984           2.000           2.012           2.020           2.044           2.075           2.016           2.028           2.193           2.243</td> <td>(FSC-0.5)</td> <td>€ EMRinger<br/>score<br/>8.299<br/>7.480<br/>6.603<br/>6.603<br/>6.603<br/>6.737<br/>7.584<br/>8.299<br/>7.485<br/>7.707<br/>7.745<br/>7.745<br/>7.237<br/>7.943<br/>7.237<br/>7.943<br/>7.237<br/>7.943<br/>7.237</td> <td>Q-3     Q-3     Q-3</td> <td>score 0.830 0.841 0.835 0.824 0.824 0.824 0.806 0.801 0.791 0.795 0.774 0.775 0.643 0.673 0.463</td>
<td>Ator<br/>Mode<br/>0.802<br/>0.806<br/>0.805<br/>0.784<br/>0.406<br/>0.779<br/>0.406<br/>0.779<br/>0.406<br/>0.779<br/>0.406<br/>0.779<br/>0.406<br/>0.779<br/>0.406<br/>0.779<br/>0.406<br/>0.784<br/>0.339<br/>0.515<br/>0.391<br/>0.319<br/>0.515<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.315<br/>0.31</td> <td>downloa<br/>m Inclusic<br/>All</td> <td>ad cs<br/>on<br/>0.941<br/>0.955<br/>0.944<br/>0.935<br/>0.934<br/>0.935<br/>0.934<br/>0.935<br/>0.934<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.945<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.935<br/>0.944<br/>0.945<br/>0.945<br/>0.944<br/>0.935<br/>0.946<br/>0.945<br/>0.946<br/>0.945<br/>0.946<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947<br/>0.947</td> | ♦ LAP <ul> <li>0.393</li> <li>0.395</li> <li>0.386</li> <li>0.383</li> <li>0.383</li> <li>0.386</li> <li>0.373</li> <li>0.382</li> <li>0.345</li> <li>0.373</li> <li>0.289</li> <li>0.289</li> <li>0.190</li> </ul>   | <ul> <li>♦ Orig.<br/>Mode</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.002</li> <li>0.997</li> <li>0.997</li></ul>   |
TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.97 | ¢111<br>0.012<br>1.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012<br>0.012<br>0.011<br>0.011<br>0.011<br>0.011<br>0.010  | ♦ MI<br>(ov) 0.067 0.067 0.068 0.061 0.065 0.064 0.067 0.064 0.061 0.065 0.065 0.061 0.065 0.0661 0.065 0.066 0.065 0.066 0.035   | SI           ↓ Orig.           Model           0.626           0.625           0.616           0.866           0.616           0.583           0.617           0.573           0.589           0.589           0.589           0.590           0.595           0.475           0.479           0.304   | MOC   
   | b<br>♦ Orig.<br>Mode<br>0.717<br>0.722<br>0.676<br>0.684<br>0.708<br>0.708<br>0.708<br>0.708<br>0.708<br>0.708<br>0.708<br>0.723<br>0.699<br>0.723<br>0.699<br>0.741<br>0.644<br>0.559<br>0.559<br>0.524<br>0.427<br>0.427<br>0.645<br>0.645<br>0.645<br>0.645<br>0.645<br>0.765<br>0.645<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.755<br>0.75 | ox CC           0.725           0.725           0.732           0.716           0.708           0.708           0.708           0.693           0.691           0.663           0.669           0.670           0.564           0.524                  | € Crig.<br>Model<br>0.873<br>0.836<br>0.811<br>0.837<br>0.845<br>0.789<br>0.818<br>0.779<br>0.818<br>0.779<br>0.818<br>0.839<br>0.740<br>0.839<br>0.777<br>0.646<br>0.574                          | C(mask)<br>0.810<br>0.810<br>0.809<br>0.799<br>0.794<br>0.769<br>0.775<br>0.769<br>0.775<br>0.769<br>0.776<br>0.762<br>0.740<br>0.620<br>0.574<br>0.454                            | Ph<br>CC<br>0.847<br>0.848<br>0.818<br>0.818<br>0.824<br>0.790<br>0.776<br>0.797<br>0.746<br>0.797<br>0.747<br>0.747<br>0.747<br>0.759<br>0.634<br>0.634  | enix<br>C(vol)<br>♦ BF=0<br>0.808<br>0.807<br>0.809<br>0.809<br>0.790<br>0.790<br>0.772<br>0.769<br>0.772<br>0.761<br>0.747<br>0.633<br>0.633<br>0.633<br>0.593<br>0.489                                     | CC(   | peaks)   | Resol.           ♦ Orig.           Model           1.980           1.984           2.000           2.012           2.020           2.044           2.075           2.016           2.028           2.193           2.243   | (FSC-0.5)   
  | € EMRinger<br>score<br>8.299<br>7.480<br>6.603<br>6.603<br>6.603<br>6.737<br>7.584<br>8.299<br>7.485<br>7.707<br>7.745<br>7.745<br>7.237<br>7.943<br>7.237<br>7.943<br>7.237<br>7.943<br>7.237   | Q-3  | score 0.830 0.841 0.835 0.824 0.824 0.824 0.806 0.801 0.791 0.795 0.774 0.775 0.643 0.673 0.463  | Ator<br>Mode<br>0.802<br>0.806<br>0.805<br>0.784<br>0.406<br>0.779<br>0.406<br>0.779<br>0.406<br>0.779<br>0.406<br>0.779<br>0.406<br>0.779<br>0.406<br>0.779<br>0.406<br>0.784<br>0.339<br>0.515<br>0.391<br>0.319<br>0.515<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.315<br>0.31 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|
| Model     T0101EM028     T0101EM020     T0101EM010     T0101EM091     T0101EM091     T0101EM091     T0101EM092     T0101EM035     T0101EM035     T0101EM035     T0101EM054     T0101EM054     T0101EM054     T0101EM054     T0101EM060     T0101EM060   |  | Methre<br>ab-initio/<br>optimized<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio  | d  | EM Ma<br>+ MapiD<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>em | P<br>★Res<br>ol.<br>1.8<br>1.8<br>1.8<br>1.8<br>1.8<br>1.8<br>1.8<br>1.  
  | ♦ CCC 0.579 0.577 0.577 0.575 0.569 0.569 0.569 0.562 0.556 0.556 0.477 0.450 0.372  | ♦ CCCC<br>(ov) 0.264 0.263 0.268 0.268 0.268 0.258 0.258 0.258 0.249 0.249 0.249 0.249 0.249 0.242 0.255 0.252 0.254 0.244 0.240 0.214 0.240 0.1144   
   
  | ◆ LAP 0.393 0.399 0.395 0.384 0.383 0.383 0.382 0.345 0.345 0.365 0.373 0.289 0.269 0.170   | <ul> <li>♦ Orig.</li> <li>Mode</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.997</li> <li>0.002</li>
<li>0.997</li> <li>0.002</li> <li>0.997</li> <li>0.002</li> <li>0.997</li> <li>0.002</li> <li>0.997</li> </ul>  | TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997  | ♦ 111<br>0.012<br>0.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.011<br>0.011<br>0.011<br>0.010<br>0.011<br>0.010  | ♦ MII<br>(ov) 0.067 0.068 0.061 0.065 0.067 0.064 0.067 0.064 0.065 0.065 0.065 0.066 0.065 0.066 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.065 0.064 0.065 0.065 0.065 0.065 0.064 0.065 0.064 0.065 0.064 0.065 0.065 0.065 0.064 0.065 0.065 0.064 0.065 0.064 0.065 0.065 0.064 0.065 |  |
MOC<br>0.624<br>0.626<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.617<br>0.606<br>0.589<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.595<br>0.5 |   | ox CC           0.725           0.725           0.732           0.719           0.708           0.708           0.693           0.691           0.669           0.665           0.564           0.524           0.404                                  | CC<br>♦ Orig.<br>Model<br>0.873<br>0.836<br>0.845<br>0.794<br>0.794<br>0.845<br>0.794<br>0.818<br>0.718<br>0.718<br>0.740<br>0.646<br>0.574<br>0.646<br>0.574<br>0.428                             | 2(mask)<br>→ BF=0<br>0.810<br>0.809<br>0.802<br>0.794<br>0.786<br>0.775<br>0.769<br>0.775<br>0.769<br>0.775<br>0.769<br>0.775<br>0.762<br>0.753<br>0.620<br>0.574<br>0.424         | Ph<br>Crig.<br>Model<br>0.847<br>0.818<br>0.818<br>0.818<br>0.818<br>0.818<br>0.790<br>0.786<br>0.796<br>0.716<br>0.716<br>0.716<br>0.716<br>0.746<br>0.759<br>0.765<br>0.593<br>0.463  | enix<br>C(vol)<br>♦ BF=0<br>0.808<br>0.809<br>0.809<br>0.809<br>0.790<br>0.790<br>0.797<br>0.790<br>0.772<br>0.769<br>0.772<br>0.769<br>0.774<br>0.747<br>0.747<br>0.747<br>0.633<br>0.633<br>0.693<br>0.463 | CC(   | peaks)           ◆ BF=0           0.759           0.760           0.763           0.749           0.740           0.722           0.723           0.695           0.713           0.695           0.577           0.531           0.398  
   | Resol.   | (FSC=0.5)  | € EMRinger<br>score<br>8.299<br>7.149<br>6.603<br>7.149<br>6.603<br>7.418<br>7.415<br>7.415<br>7.415<br>7.415<br>7.415<br>7.415<br>7.415<br>7.445<br>4.447<br>3.447<br>1.599   | Q-3<br>♦ Orig.<br>Model<br>0.830<br>0.841<br>0.835<br>0.825<br>0.819<br>0.667<br>0.791<br>0.671<br>0.671<br>0.791<br>0.759<br>0.774<br>0.503<br>0.553<br>0.416<br>0.553<br>0.44  | score<br>0.830<br>0.841<br>0.835<br>0.827<br>0.827<br>0.829<br>0.824<br>0.806<br>0.801<br>0.791<br>0.795<br>0.759<br>0.775<br>0.643<br>0.573<br>0.428                    | Ator<br>Mode<br>0.802<br>0.806<br>0.805<br>0.784<br>0.406<br>0.779<br>0.406<br>0.779<br>0.406<br>0.779<br>0.406<br>0.743<br>0.743<br>0.743<br>0.764<br>0.339<br>0.515<br>0.331   
   | downlos<br>m Inclusic<br>All<br>◆ noH<br>0.802<br>0.806<br>0.805<br>0.784<br>0.799<br>0.783<br>0.779<br>0.778<br>0.778<br>0.773<br>0.774<br>0.753<br>0.628<br>0.586<br>0.462<br>0.462  | ad cs<br>0.944<br>0.955<br>0.954<br>0.933<br>0.944<br>0.933<br>0.944<br>0.934<br>0.944<br>0.934<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.944<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.946<br>0.9466<br>0.9466<br>0.9466<br>0.9466<br>0.9466<br>0.9466<br>0.9466<br>0.94666       |
| Model     ToiotEuko2,     ToiotEuko2,     ToiotEuko1,     ToiotEuko1,     ToiotEuko1,     ToiotEuko1,     ToiotEuko1,     ToiotEuko1,     ToiotEuko2,     | Group<br>Name<br>ccpem<br>yu<br>chiu<br>arpwarp<br>arosetta<br>singharoy<br>rosetta<br>singharoy<br>rosetta<br>kihara<br>kihara<br>deeptracer<br>deeptracer  | Methn<br>db-intio/<br>optimized<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio<br>ab-intio  |  | EM Ma<br># MapiD<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1<br>emd_20026_1  | ↓ Res<br>ol. 1.8   
  | ♦ CCC 0.579 0.577 0.577 0.575 0.569 0.569 0.569 0.562 0.557 0.556 0.5477 0.4470 0.4450 0.394 0.372   | ♦ CCCC<br>(ov) 0.264 0.263 0.268 0.268 0.268 0.264 0.274 0.249 0.249 0.255 0.252 0.252 0.252 0.254 0.214 0.240 0.172 0.144  
   
  | ♦ LAP <ul> <li>0.393</li> <li>0.395</li> <li>0.386</li> <li>0.383</li> <li>0.383</li> <li>0.382</li> <li>0.345</li> <li>0.365</li> <li>0.365</li> <li>0.365</li> <li>0.269</li> <li>0.190</li> <li>0.172</li> </ul>   | ◆
Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.997<br>0.002<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002 | TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997   | ¢111<br>0.012<br>0.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.011<br>0.011<br>0.011<br>0.011<br>0.010<br>0.010   | ♦ MII<br>(ov) 0.067 0.068 0.065 0.065 0.067 0.066 0.067 0.067 0.067 0.061 0.065 0.065 0.065 0.065 0.065 0.046 0.055 0.046 0.059 0.035 0.025   | SI   
   | MOC<br>0.624<br>0.626<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.617<br>0.607<br>0.607<br>0.607<br>0.595<br>0.594<br>0.594<br>0.594<br>0.594<br>0.483<br>0.400<br>0.377  | b<br>♦ Orig.<br>10.727<br>0.732<br>0.676<br>0.708<br>0.708<br>0.686<br>0.542<br>0.701<br>0.648<br>0.689<br>0.701<br>0.648<br>0.559<br>0.5524<br>0.427<br>0.404  | ox CC<br>↓ ◆ BF=0<br>0.725<br>0.725<br>0.732<br>0.716<br>0.706<br>0.706<br>0.693<br>0.694<br>0.694<br>0.685<br>0.670<br>0.564<br>0.524<br>0.524<br>0.427<br>0.404  | CC<br>♦ Orig.<br>Model<br>0.873<br>0.835<br>0.845<br>0.794<br>0.794<br>0.845<br>0.794<br>0.818<br>0.718<br>0.818<br>0.718<br>0.740<br>0.646<br>0.574<br>0.454<br>0.428                             | C(mask)<br>■ ♥BF=0<br>0.810<br>0.809<br>0.799<br>0.799<br>0.796<br>0.775<br>0.766<br>0.775<br>0.760<br>0.775<br>0.762<br>0.753<br>0.620<br>0.574<br>0.454<br>0.428                 | Ph<br>Crig.<br>0.847<br>0.818<br>0.818<br>0.818<br>0.818<br>0.818<br>0.790<br>0.786<br>0.796<br>0.716<br>0.716<br>0.716<br>0.759<br>0.634<br>0.593<br>0.489<br>0.463  | C(vol)   | CCC(<br>♦ Orig.<br>Model<br>0.757<br>0.775<br>0.768<br>0.741<br>0.741<br>0.355<br>0.761<br>0.555<br>0.761<br>0.555<br>0.764<br>0.679<br>0.531<br>0.424<br>0.398   | ▶         ▶         BF=0           0.759         0.760         0.766           0.749         0.749         0.749           0.721         0.721         0.723           0.695         0.713         0.695           0.577         0.531         0.424           0.398         0.895         0.721  
  | Resol.           ♦ Orig.           Model           1.980           1.984           2.000           2.012           2.020           2.020           2.045           2.045           2.046           2.076           2.028           2.193           2.242           3.413           3.597                 | (FSC-0.5)  | € EMRinger<br>score<br>8.299<br>7.690<br>7.149<br>8.299<br>7.415<br>7.584<br>8.299<br>7.415<br>7.743<br>7.237<br>7.743<br>7.237<br>7.245<br>7.743<br>6.447<br>1.599<br>1.481   | Q-3           ♦ Orig.<br>Model           0.830           0.841           0.837           0.819           0.806           0.667           0.774           0.639           0.553           0.416           0.384   | ★ not<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.826<br>0.806<br>0.801<br>0.795<br>0.759<br>0.759<br>0.774<br>0.775<br>0.643<br>0.573<br>0.6573<br>0.461<br>0.428 | Ator  
  | downlos<br>All<br>0.802<br>0.806<br>0.805<br>0.784<br>0.784<br>0.785<br>0.783<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.778<br>0.768<br>0.628<br>0.462<br>0.446 | ad cs<br>on<br>0.944<br>0.955<br>0.944<br>0.955<br>0.944<br>0.933<br>0.943<br>0.933<br>0.944<br>0.933<br>0.944<br>0.933<br>0.944<br>0.935<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.934<br>0.935<br>0.934<br>0.934<br>0.934<br>0.935<br>0.934<br>0.934<br>0.935<br>0.934<br>0.934<br>0.935<br>0.934<br>0.935<br>0.934<br>0.935<br>0.934<br>0.935<br>0.934<br>0.935<br>0.934<br>0.935<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.936<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.956<br>0.9566<br>0.9566<br>0.956<br>0.9566<br>0.9566<br>0.9566<br>0.9566<br>0.9566   |
| Model     T010EW028     T010EW010     T010EW01     T010EW01     T010EW01     T010EW01     T010EW01     T010EW02     T | Group<br>Name<br>copen<br>yu<br>chlu<br>arpwarp<br>cosetta<br>singharoy<br>rosetta<br>singharoy<br>rosetta<br>tiphenix<br>tiphenix<br>tiphenix<br>tiphenix<br>tiphenix<br>tiphenix<br>tiphenix<br>tiphenix<br>deptracer<br>deeptracer  | Metho<br>optimized<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio   | d  | EM Ma<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1   | ◆ Res<br>ol. <ol> <li>1.8</li> </ol>   
   | ♦ CCCC 0.579 0.577 0.577 0.577 0.572 0.569 0.567 0.566 0.557 0.556 0.547 0.450 0.450 0.394 0.372   | ♦ CCCC<br>(ov) 0.264 0.263 0.263 0.265 0.258 0.264 0.279 0.249 0.255 0.252 0.258 0.252 0.258 0.252 0.258 0.2144 0.240 0.172 0.144  
   
   | ◆ LAP 0.393 0.395 0.386 0.383 0.386 0.382 0.382 0.382 0.385 0.385 0.289 0.190 0.172   | ♦ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.002<br>0.002<br>0.002<br>0.997<br>0.002<br>0.002  
   | TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997  | ¢11<br>0.012<br>0.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012<br>0.012<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011   | ♦ MI<br>(ov) 0.067 0.068 0.065 0.065 0.067 0.064 0.073 0.061 0.065 0.065 0.065 0.066 0.065 0.065 0.046 0.059 0.035 0.029  | SI   | MOC<br>0.624<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.617<br>0.607<br>0.606<br>0.599<br>0.595<br>0.594<br>0.506<br>0.483<br>0.400<br>0.377  
  | b   | x CC<br>0.725<br>0.725<br>0.732<br>0.716<br>0.708<br>0.708<br>0.708<br>0.693<br>0.694<br>0.669<br>0.669<br>0.669<br>0.670<br>0.524<br>0.524<br>0.524<br>0.427<br>0.404   | CCC<br>♦ Orig.<br>Miodel<br>0.833<br>0.836<br>0.837<br>0.845<br>0.799<br>0.848<br>0.740<br>0.839<br>0.740<br>0.839<br>0.740<br>0.839<br>0.740<br>0.807<br>0.574<br>0.454<br>0.428                  | C(mask)<br>0.810<br>0.810<br>0.809<br>0.799<br>0.799<br>0.798<br>0.775<br>0.760<br>0.775<br>0.775<br>0.775<br>0.762<br>0.753<br>0.620<br>0.574<br>0.454<br>0.428                   | Ph<br>C<br>C<br>0.847<br>0.818<br>0.824<br>0.790<br>0.795<br>0.776<br>0.776<br>0.747<br>0.747<br>0.747<br>0.747<br>0.747<br>0.747<br>0.747<br>0.749<br>0.634<br>0.489<br>0.483  | enix<br>C(vol)<br>♦ BF=0<br>0.808<br>0.807<br>0.809<br>0.800<br>0.790<br>0.790<br>0.790<br>0.770<br>0.769<br>0.772<br>0.769<br>0.777<br>0.761<br>0.747<br>0.747<br>0.761<br>0.633<br>0.489<br>0.483          | CCC(  | ◆ BF=0<br>0.759<br>0.760<br>0.766<br>0.763<br>0.749<br>0.749<br>0.749<br>0.738<br>0.722<br>0.721<br>0.723<br>0.695<br>0.713<br>0.697<br>0.577<br>0.577<br>0.531<br>0.531   | Resol.           ♦ Orig.           filodel           1.980           1.984           2.002           2.012           2.020           2.042           2.045           1.988           2.075           2.016           2.028           2.193           2.193           3.413           3.597               | (FSC-0.5)<br>♦
BF=0<br>2.016<br>1.996<br>2.000<br>2.016<br>2.020<br>2.012<br>2.020<br>2.045<br>2.027<br>2.027<br>2.045<br>2.027<br>2.033<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.293<br>2.193<br>2.294<br>2.193<br>2.193<br>2.295<br>2.033<br>2.193<br>2.295<br>2.193<br>2.295<br>2.193<br>2.295<br>2.193<br>2.295<br>2.193<br>2.295<br>2.193<br>2.295<br>2.193<br>2.295<br>2.193<br>2.295<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.193<br>2.1  | € EMRinger<br>score<br>8 299<br>7 690<br>6 683<br>6 6737<br>7 584<br>8 299<br>7 690<br>7 584<br>8 299<br>7 7584<br>8 299<br>7 7584<br>8 299<br>7 7584<br>8 299<br>7 485<br>7 485 | Q-1<br>◆ Orig.<br>Model<br>0.830<br>0.841<br>0.835<br>0.827<br>0.89<br>0.866<br>0.667<br>0.791<br>0.667<br>0.791<br>0.667<br>0.791<br>0.653<br>0.633<br>0.653<br>0.653<br>0.633<br>0.653<br>0.634<br>0.634   | € not<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.806<br>0.801<br>0.795<br>0.775<br>0.775<br>0.775<br>0.775<br>0.775<br>0.775<br>0.643<br>0.643<br>0.643<br>0.643  | Ator<br>Mode<br>0.802<br>0.806<br>0.805<br>0.784<br>0.411<br>0.785<br>0.406<br>0.779<br>0.405<br>0.743<br>0.764<br>0.391<br>0.391<br>0.373   | downlos<br>m Inclusic<br>All<br>0.802<br>0.806<br>0.805<br>0.784<br>0.784<br>0.784<br>0.783<br>0.778<br>0.778<br>0.778<br>0.773<br>0.773<br>0.773<br>0.628<br>0.586<br>0.462<br>0.446  | ad cs   
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| Model     ToioteWol2,     | Group<br>Name<br>ccpem<br>yu<br>chiu<br>arpwarp<br>z arpwarp<br>z kara<br>khara<br>khara<br>d deptracer<br>d deptracer | Metha  | d  | EM Ma<br>+ MapID<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>em | ◆ Res<br>ol. 1.8 1   
  | ¢ CCCC<br>0.579<br>0.577<br>0.577<br>0.577<br>0.572<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.567<br>0.562<br>0.567<br>0.562<br>0.567<br>0.564<br>0.557<br>0.574<br>0.574<br>0.579<br>0.579<br>0.579<br>0.579<br>0.579<br>0.577<br>0.577<br>0.577<br>0.577<br>0.572<br>0.572<br>0.579<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.572<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.569<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.559<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.559<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359<br>0.359 | ♦ CCC<br>(ov) 0.264 0.280 0.280 0.280 0.285 0.284 0.279 0.249 0.255 0.258 0.258 0.258 0.258 0.258 0.258 0.258 0.258 0.258 0.258 0.258 0.258 0.258 0.258 0.251 0.252 0.258 0.252 0.258 0.240 0.172 0.144   
   
  | ♦ LAP 0.393 0.395 0.386 0.384 0.383 0.383 0.384 0.383 0.384 0.385 0.373 0.385 0.373 0.289 0.190 0.172   | ◆ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.092<br>0.002<br>0.002<br>0.002  |
TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.97 | ♥ 11<br>0.012<br>0.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012<br>0.012<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011   | ♦ MI<br>(ov) 0.067 0.067 0.068 0.068 0.069 0.067 0.064 0.067 0.064 0.061 0.065 0.061 0.065 0.061 0.046 0.059 0.029  | SI<br>♦ Orig.<br>Model<br>0.624<br>0.625<br>0.618<br>0.618<br>0.618<br>0.612<br>0.588<br>0.612<br>0.583<br>0.607<br>0.589<br>0.585<br>0.589<br>0.595<br>0.595<br>0.595<br>0.475<br>0.479<br>0.394<br>0.371   | MOC<br>0.624<br>0.626<br>0.625<br>0.616<br>0.623<br>0.617<br>0.607<br>0.607<br>0.606<br>0.599<br>0.594<br>0.594<br>0.594<br>0.594<br>0.594<br>0.594<br>0.483<br>0.400<br>0.377  
   | b<br>♦ Orig.<br>Mode<br>0.717<br>0.727<br>0.732<br>0.676<br>0.684<br>0.708<br>0.686<br>0.542<br>0.701<br>0.689<br>0.701<br>0.689<br>0.559<br>0.524<br>0.424<br>0.404  | ox CC  | CC<br>♦ Orig.<br>Model<br>0.873<br>0.836<br>0.811<br>0.837<br>0.845<br>0.748<br>0.748<br>0.748<br>0.740<br>0.777<br>0.777<br>0.646<br>0.574<br>0.454<br>0.454<br>0.458                             | (mask)<br>● BF=0<br>0.810<br>0.802<br>0.799<br>0.775<br>0.769<br>0.775<br>0.769<br>0.775<br>0.769<br>0.775<br>0.762<br>0.520<br>0.574<br>0.428                                     | Ph<br>Crig.<br>Model<br>0.847<br>0.818<br>0.810<br>0.818<br>0.824<br>0.796<br>0.776<br>0.716<br>0.776<br>0.716<br>0.789<br>0.779<br>0.716<br>0.769<br>0.759<br>0.634<br>0.593<br>0.483  | enix<br>C(vol)<br>• BF=0<br>0.808<br>0.807<br>0.809<br>0.790<br>0.790<br>0.772<br>0.769<br>0.7747<br>0.761<br>0.747<br>0.633<br>0.633<br>0.593<br>0.489<br>0.463   | CC(<br>♦ Orig.<br>0.757<br>0.775<br>0.775<br>0.775<br>0.741<br>0.741<br>0.741<br>0.745<br>0.755<br>0.744<br>0.745<br>0.755<br>0.744<br>0.695<br>0.744<br>0.695<br>0.744<br>0.555<br>0.764<br>0.555<br>0.764<br>0.424<br>0.398 | ▶ caks)  | Resol.           ♦ Orig.           1.980           1.984           2.000           2.012           2.020           2.020           2.042           2.045           1.986           2.075           2.016           2.0208           2.193           2.243           3.413           3.597                | (FSC-0.5)<br>♦ BF=0<br>2.016<br>1.996<br>2.000<br>2.012<br>2.020<br>2.022<br>2.022<br>2.025<br>2.037<br>2.037<br>2.033<br>2.193<br>2.243<br>3.597   
  | € EMRinger<br>score<br>7.680<br>7.149<br>6.603<br>6.737<br>7.584<br>8.299<br>7.416<br>8.299<br>7.418<br>8.299<br>7.418<br>7.418<br>7.418<br>7.418<br>7.418<br>6.447<br>7.237<br>7.943<br>6.447<br>1.599<br>1.481   | Q-1<br>• Orig.<br>Model<br>0.830<br>0.841<br>0.835<br>0.827<br>0.819<br>0.689<br>0.866<br>0.667<br>0.791<br>0.679<br>0.774<br>0.639<br>0.759<br>0.774<br>0.633<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.504<br>0.503<br>0.503<br>0.504<br>0.503<br>0.504<br>0.503<br>0.504<br>0.503<br>0.504<br>0.503<br>0.503<br>0.503<br>0.504<br>0.504<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0.503<br>0. | € ore  | Ator<br>• Orig.<br>• Mode<br>0.802<br>0.806<br>0.784<br>0.784<br>0.784<br>0.411<br>0.785<br>0.406<br>0.779<br>0.405<br>0.743<br>0.743<br>0.764<br>0.339<br>0.515<br>0.339<br>0.373   | downlos<br>m Inclusic<br>All<br>● noH<br>0.802<br>0.806<br>0.805<br>0.784<br>0.799<br>0.785<br>0.785<br>0.783<br>0.779<br>0.778<br>0.773<br>0.764<br>0.562<br>0.628<br>0.622<br>0.446  | ad cs   
  |
| Model     T0101EW028     T0101EW029     T0101EW04      T0101EW04      T0101EW04     T0101EW04   | Group<br>Name<br>copen<br>yu<br>chu<br>arpwarp<br>arpwarp<br>arpwarp<br>trosetta<br>phenix<br>rosetta<br>phenix<br>tzjuelich<br>codmd<br>kihara<br>deeptracer<br>deeptracer  | Metho<br>* ab-initio/<br>optimized<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>ab-initio<br>a                                     | d  | EM Ma<br>+ MapIO<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_20028_1<br>emd_2008_1<br>emd_2008_1<br>emd_2008_1<br>emd_2008_1<br>emd_2008_1<br>emd_200 | P<br>◆Res<br>ol.<br>1.8<br>1.8<br>1.8<br>1.8<br>1.8<br>1.8<br>1.8<br>1.  
  | ◆ CCCC     0.579     0.579     0.579     0.577     0.575     0.575     0.562     0.569     0.567     0.567     0.567     0.556     0.547     0.477     0.450     0.372     stitute   |   
   
  | ♦ LAP 0.393 0.395 0.386 0.384 0.383 0.383 0.384 0.385 0.373 0.385 0.373 0.289 0.190 0.172 eral Me   | ♦ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002   
  | TemPy<br>ENV<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997  | ◆ 011<br>0.012<br>0.011<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012<br>0.012<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011<br>0.011  | ♦ MII<br>(ov) 0.067 0.067 0.068 0.068 0.068 0.069 0.064 0.061 0.061 0.061 0.065 0.061 0.062 0.062 0.064 0.065 0.061 0.065 0.061 0.065 0.029 GMS)  | SI           ● Orig.           Model           0.626           0.625           0.618           0.626           0.612           0.633           0.607           0.573           0.599           0.560           0.479           0.394           0.371   | ▲ noH           0.624           0.626           0.625           0.618           0.612           0.617           0.617           0.606           0.595           0.594           0.506           0.483           0.400   
   | b           ♦ Orig.<br>Mode           0.717           0.727           0.732           0.676           0.684           0.708           0.696           0.542           0.723           0.686           0.559           0.524           0.404   | ox CC           ◆ BF=0           0.725           0.732           0.719           0.716           0.708           0.708           0.693           0.694           0.689           0.684           0.524           0.524           0.427           0.404 | CC<br>♦ Orig.<br>Model<br>0.873<br>0.836<br>0.837<br>0.845<br>0.718<br>0.818<br>0.819<br>0.718<br>0.879<br>0.748<br>0.574<br>0.646<br>0.574<br>0.428   | 2(mask)  | Ph<br>C<br>C<br>Model<br>0.847<br>0.818<br>0.810<br>0.818<br>0.824<br>0.790<br>0.797<br>0.716<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.799<br>0.796<br>0.799<br>0.799<br>0.799<br>0.799<br>0.796<br>0.799<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.799<br>0.796<br>0.593<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.499<br>0.4990<br>0.4990000000000 | enix<br>C(vol)<br>♦ BF=0<br>0.809<br>0.809<br>0.809<br>0.809<br>0.809<br>0.790<br>0.790<br>0.790<br>0.772<br>0.765<br>0.772<br>0.776<br>0.777<br>0.770<br>0.747<br>0.763<br>0.633<br>0.489<br>0.463          | CC(   | ▶         ▶         ▶         ▶         ₽         BF=0         0.759         0.760         0.760         0.763         0.749         0.721         0.722         0.721         0.722         0.721         0.723         0.6897         0.531         0.4531         0.4531         0.4531         0.4531         0.4388         0.3388         < | Resol.           ♥ Orig.           Model           1.964           2.000           2.000           2.000           2.001           2.002           2.004           2.076           2.028           2.193           2.242           3.413           3.597   | (FSC-0.5)<br>♦ BF=0<br>2016<br>1.996<br>2.000<br>2.010<br>2.020<br>2.020<br>2.022<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.024<br>2.025<br>2.024<br>2.025<br>2.024<br>2.025<br>2.024<br>2.025<br>2.024<br>2.025<br>2.024<br>2.025<br>2.024<br>2.027<br>2.025<br>2.024<br>2.027<br>2.025<br>2.024<br>2.027<br>2.025<br>2.024<br>2.027<br>2.025<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>2.027<br>3.413<br>3.597  
  | <b>EMRinger</b><br>8.299<br>7.690<br>6.737<br>7.584<br>8.299<br>7.485<br>8.299<br>7.485<br>7.745<br>7.745<br>7.743<br>7.237<br>7.543<br>7.237<br>7.543<br>7.237<br>1.459<br>1.459<br>1.459<br>1.459  | Q-3     Q-3     Q-1     Q-3     Q-1     Q-1     Q-1     Q-2  | €COFE  | Ator   | downlos<br>m Inclusic<br>All<br>● noH<br>0.802<br>0.806<br>0.805<br>0.784<br>0.784<br>0.785<br>0.785<br>0.783<br>0.779<br>0.778<br>0.773<br>0.778<br>0.773<br>0.764<br>0.586<br>0.462<br>0.446   | ad cs<br>0<br>0<br>0<br>0<br>0<br>0<br>0<br>0<br>0<br>0<br>0<br>0<br>0  
  |
| • Model           ToinEW029           ToinEW010           ToinEW011           ToinEW012           ToinEW012           ToinEW012           ToinEW012           ToinEW012           ToinEW012           ToinEW012           ToinEW012           ToinEW023           ToinEW024           ToinEW025           ToinEW025           ToinEW025           ToinEW025           ToinEW025           ToinEW025           ToinEW025           ToinEW025           ToinEW025   |  | Methr<br>* ab-initio/<br>optimized<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-inito<br>ab-i 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| € Res of the second se   
   | ◆ CCCC     0.579     0.577     0.577     0.577     0.577     0.575     0.569     0.569     0.562     0.557     0.547     0.477     0.450     0.372     stitute     querie  | ← CCC<br>(ov)<br>0.284<br>0.280<br>0.283<br>0.285<br>0.285<br>0.285<br>0.285<br>0.285<br>0.285<br>0.284<br>0.240<br>0.279<br>0.242<br>0.252<br>0.252<br>0.252<br>0.252<br>0.254<br>0.240<br>0.252<br>0.254<br>0.254<br>0.263<br>0.265<br>0.264<br>0.279<br>0.245<br>0.254<br>0.256<br>0.258<br>0.264<br>0.259<br>0.259<br>0.259<br>0.259<br>0.259<br>0.259<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.265<br>0.258<br>0.265<br>0.258<br>0.265<br>0.258<br>0.265<br>0.258<br>0.265<br>0.258<br>0.265<br>0.258<br>0.265<br>0.258<br>0.265<br>0.258<br>0.265<br>0.258<br>0.265<br>0.258<br>0.265<br>0.258<br>0.258<br>0.265<br>0.258<br>0.258<br>0.258<br>0.258<br>0.258<br>0.258<br>0.255<br>0.258<br>0.255<br>0.258<br>0.255<br>0.258<br>0.254<br>0.279<br>0.240<br>0.279<br>0.240<br>0.172<br>0.144<br>0.172<br>0.144 0.172 0.144 0.172 0.144 0.172 0.144 0.155 0.156 0.1   
   
   | <ul> <li>◆LAP</li> <li>0.393</li> <li>0.395</li> <li>0.386</li> <li>0.383</li> <li>0.386</li> <li>0.373</li> <li>0.385</li> <li></li></ul> | ◆ Orig.<br>Mode<br>0.997<br>0.997<br>0.997<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.997<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002<br>0.002 | TemPy<br>ENV<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997<br>0.997   
   | ◆ 1/1<br>0.012<br>1.010<br>0.011<br>0.011<br>0.012<br>0.012<br>0.012<br>0.011<br>0.011<br>0.011<br>0.011<br>0.010<br>0.011<br>0.010<br>0.010   |   | Si           ● Orig.           Model           0.624           0.625           0.618           0.616           0.583           0.617           0.583           0.503           0.599           0.580           0.590           0.591           0.592           0.593           0.594           0.394           0.371   | MOC<br>• noH<br>0.624<br>0.626<br>0.625<br>0.618<br>0.616<br>0.623<br>0.612<br>0.617<br>0.606<br>0.595<br>0.595<br>0.596<br>0.483<br>0.400<br>0.377   | ●         Orig.           Model         0.717           0.727         0.676           0.684         0.708           0.708         0.708           0.708         0.723           0.696         0.524           0.559         0.524           0.427         0.404   
   | ox CC           0.725           0.725           0.725           0.732           0.719           0.708           0.708           0.693           0.694           0.669           0.670           0.524           0.427           0.404                  | CC<br>● Orig.<br>Mlodel<br>0.873<br>0.836<br>0.811<br>0.845<br>0.794<br>0.784<br>0.718<br>0.718<br>0.718<br>0.719<br>0.818<br>0.714<br>0.839<br>0.777<br>0.846<br>0.777<br>0.574<br>0.454<br>0.428 | (mask)<br>♦ BF=0<br>0.810<br>0.802<br>0.794<br>0.786<br>0.775<br>0.775<br>0.775<br>0.775<br>0.775<br>0.775<br>0.775<br>0.775<br>0.775<br>0.753<br>0.620<br>0.574<br>0.454<br>0.428 | Ph<br>Crig.<br>Model<br>0.847<br>0.818<br>0.818<br>0.824<br>0.796<br>0.776<br>0.716<br>0.716<br>0.716<br>0.716<br>0.776<br>0.776<br>0.776<br>0.776<br>0.776<br>0.778<br>0.634<br>0.633<br>0.463   | enix<br>C(vol)<br>♦ BF=0<br>0.808<br>0.807<br>0.790<br>0.790<br>0.790<br>0.772<br>0.7769<br>0.777<br>0.7769<br>0.774<br>0.747<br>0.748<br>0.633<br>0.489<br>0.463  | CC(   | ♥ BF=0<br>7.759<br>0.760<br>0.766<br>0.776<br>0.770<br>0.721<br>0.722<br>0.721<br>0.723<br>0.695<br>0.577<br>0.531<br>0.424<br>0.398   | Resol.           ♦ Orig.           Model           1.984           2.000           1.986           2.012           2.020           2.045           2.052           2.045           2.075           2.076           2.078           2.078           2.078           2.078           3.413           3.597 | (FSC=0.5)  | ♦ EMRinger<br>score 8.299 7.690 6.603 7.405 6.737 7.455 7.475 7.743 7.743 7.2415 7.743 7.475 7.743 7.475 7.475 7.475 7.475 7.475 7.475
7.475 7.  | <ul> <li>Q-1</li> <li>♦ Orig.<br/>Model</li> <li>0.841</li> <li>0.835</li> <li>0.847</li> <li>0.819</li> <li>0.806</li> <li>0.667</li> <li>0.774</li> <li>0.759</li> <li>0.774</li> <li>0.639</li> <li>0.553</li> <li>0.416</li> <li>0.384</li> </ul>  | Core   | Ator<br>Mode<br>0.802<br>0.806<br>0.805<br>0.778<br>0.784<br>0.778<br>0.779<br>0.405<br>0.779<br>0.405<br>0.779<br>0.405<br>0.779<br>0.405<br>0.779<br>0.405<br>0.339<br>0.515<br>0.339  | downlos<br>m Inclusic<br>All<br>◆ noH<br>0.802<br>0.806<br>0.805<br>0.784<br>0.799<br>0.783<br>0.779<br>0.778<br>0.773<br>0.773<br>0.773<br>0.773<br>0.628<br>0.462<br>0.446   | ad cs  
   |

Evaluation data are available as sortable score tables or interactive (clickable) graphs.

Additionally, a *Comparative Analyses* Tab is available to the right of the four main tabs. Under this tab, a user can view summaries of relative accuracies of models, compare scores of models in different evaluation tracks or check correlations between pairs of scores.

### Switching between targets

Switching to results for a different target can be done by returning to the main Challenge page and clicking on the desired target pictograph (see the *Models* section above) or by accessing the "Target" drop-down menu on any of the target-specific results pages.

	EM Model Challenge - 2019																														
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	A 11-1-1	Group	Metho		CM M	ap				E	NV			SM	IOC	bo	x CC	CC(	mask)	C	C(vol)	CC(	eaks)	Resol	(FSC=0.5)	EMRinger	Q-s	core	1	All	
	◆ MOUEI	Name	♦ ab-initio/ optimized	¢ man.	MapID	¢ol.	¢CCC	¢(ov)	\$LAP	¢Orig. Model	¢ noH	¢MI	\$(ov)	¢Orig. Model	¢ noH	♦ Orig.	\$ BF=0	¢Orig.	\$ BF=0	¢Orig. Model	♣ BF=0	♦ <sup>Orig.</sup>	\$ BF=0	¢Orig. Model	<b>♦</b> BF=0	score	♦ <sup>Orig.</sup>	¢ noH	¢Orig. Model	\$ noH	¢BB
1	T0104EM035_1	phenix	ab-initio	man.	emd_0406	2.9	0.321	0.491	0.197	0.985	0.985	0.038	0.240	0.741	0.741	0.640	0.778	0.847	0.848	0.846	0.840	0.558	0.763	2.985	3.012	5.151	0.652	0.652	0.650	0.650	0.765
2	T0104EM027_1	kumar	ab-initio	man.	emd_0406	2.9	0.321	0.489	0.196	0.985	0.985	0.038	0.241	0.739	0.739	0.651	0.777	0.853	0.844	0.851	0.837	0.574	0.760	3.003	3.040	4.780	0.648	0.648	0.644	0.644	0.758
4	T0104EM010_1	chiu	ap-meo optimized	man. man.	emd_0406	2.9	0.319	0.484	0.196	0.985	0.985	0.036	0.230	0.734	0.734	0.736	0.766	0.892	0.831	0.880	0.825	0.703	0.746	2.950	2.967	4.000	0.653	0.653	0.639	0.639	0.746
5	T0104EM041_1	arpwarp	ab-initio	man.	emd_0406	2.9	0.318	0.477	0.194	0.985	0.985	0.038	0.227	0.731	0.731	0.775	0.765	0.905	0.832	0.883	0.823	0.757	0.744	2.967	3.012	3.033	0.642	0.642	0.630	0.630	0.743
6	T0104EM073_1 T0104EM041_2	singharoy	optimized ab initio	auto	emd_0406	2.9	0.316	0.482	0.193	0.985	0.985	0.037	0.229	0.723	0.723	0.760	0.759	0.822	0.820	0.816	0.815	0.735	0.734	3.012	3.012	5.581	0.635	0.635	0.626	0.626	0.760
8	T0104EM090_1	mbaker	ab-initio	man.	emd_0406	2.9	0.314	0.465	0.181	0.985	0.985	0.036	0.208	0.709	0.709	0.608	0.734	0.797	0.800	0.797	0.793	0.507	0.701	3.077	3.106	2.621	0.607	0.607	0.608	0.608	0.748
9	T0104EM028_1	ccpem	ab-initio	man.	emd_0406	2.9	0.313	0.483	0.191	0.985	0.985	0.038	0.231	0.715	0.715	0.730	0.754	0.904	0.816	0.891	0.811	0.695	0.728	2.950	3.030	4.838	0.632	0.632	0.618	0.618	0.742
11	T0104EM025_1	rosetta	ab-initio	auto man.	emd_0406 emd_0406	2.9	0.313	0.488	0.180	0.965	0.985	0.037	0.244	0.663	0.707	0.735	0.748	0.879	0.821	0.864	0.810	0.699	0.720	2.985	3.040	9.202	0.498	0.634	0.327	0.644	0.754
	TOTOTOTOTO	rosetta	ab-initio	man	emd 0406	2.9	0.312	0.486	0 193	0.983	0.985	0.039	0.239	0.662	0 729	0.757	0 749	0.878	0.825	0.856	0.813	0 734	0.723	2 967	3 030	5.048	0.505	0.643	0.325	0.641	0.748

### Sorting tables

Results tables can be sorted on any column by clicking on the column name (the column header will be highlighted). A repeat click will reorder the data in the reverse order.

0.594 0.456 0.405 0.448 0.347

0.594 0.600 0.502 0.454 0.533 0.303 0.489 0.454 0.470 0.289

3.125 3.751 3.425 2.179 3.333 3.386 3.425 2.779 3.571 1.610

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		model coordinates only     fit to EM map     vs reference structure     vs other models     Comparative Analyses       Geometry Scores     ADPs Histogram     Accuracy Estimate																								
1	arget: Hum	Geometry Scores       ADPs Histogram       Accuracy Estimate         Human Apofemtin: T0101 (emd 20026 1)       Image: Comparison of the state																								
•	ilter by meth	od: ⊻ ab-	-initio ⊠ oj	otimized	CryoEM	model	⊠fi	ully autor	nated	⊠partia	lly auto	mated,	with son	ne manu	ual step	is fi	ter								dow	nload csv
ŀ	ilter by meth	iod: ⊠ ab-	Mett	nod	CryoEM	model	⊻fi	ully autor	nated	⊠ partia	Ily auto	mated,	with son	ie manu	ual step	is fi	ter	Pite de la			м	lolprobity			<b>dow</b> Cablam	nload csv
ł	Amodel	¢Gr.Name	Mett ¢ab-initio/ optimized	nod auto/ man.	¢rmsd	Bonds	⊵ fi	ully autor	Angles \$max	de partia	Deviation	mated, n from id Chirality	eal model	¢rmsd	Jal step Planarit ♦ max	y ¢count	¢rmsd	Dihedral	¢ count	▲Clash	M ¢Rot-ou	lolprobity t ∳Rama-out	◆Rama-fv	¢Conf-out	dow Cablam ♦Conf-disfy	nload csv ♦Ca-out
# 1	Model     T0101EM054_2	¢Gr.Name 2 kihara	Mett ab-initio/ ab-initio/ ab-initio	aod ¢auto/ man. man.	¢rmsd 0.020	Bonds	✓ fr	ully autor ¢rmsd 1.509	Angles Angles max 15.032	d partia ¢count 1943	Deviation	n from id Chirality 0.318	eal model ( \$count 204	¢rmsd 0.008	Planarit Planarit Planarit 0.027	y 257 fil y ¢count 257	¢rmsd 9.347	Dihedral ¢max 77.749	¢count 871	▲Clash 0.000	M \$Rot-out 0.000	lolprobity t   \$Rama-out 0.590	◆Rama-fv 96.470	¢Conf-out 1.20	dow Cablam ♦Conf-disfv 4.80	nload csv ¢Cα-out 0.00
# 1 2		¢ Gr.Name 2 kihara 1 singharoy	Mett ab-initio/ optimized	nod auto/ man. auto	¢rmsd 0.020 0.022	Bonds I ♦max 0.142 0.071	✓ fr	ully autor	Angles ¢max 15.032 9.235	✓ partia ♦ count 1943 1945	Deviation Trmsd 0.096 0.138	n from id Chirality I 🗣 max 0.318 0.476	eal model ( \$count 204 204	♦ rmsd 0.008 0.018	Planarit Planarit O.027 0.128	y ∳ count 257 258	♦rmsd 9.347 22.110	Dihedral ♦ max 77.749 178.516	¢count 871 872	Clash 0.000 0.000	M \$Rot-out 0.000 1.310	lolprobity t ≑Rama-out 0.590 0.000	♦ Rama-fv 96.470 99.410	♦Conf-out 1.20 1.20	dow Cablam ♦ Conf-disfy 4.80 2.40	nload csv ¢Cα-out 0.00 0.00
# 1 2 3	Model     T0101EM054_3     T0101EM073_     T0101EM073_	¢Gr.Name 2 kihara 1 singharoy 1 chiu	Mett ab-initio/ optimized optimized	nod auto/ man. auto man.	cryoEM ♦ rmsd 0.020 0.022 0.005	Bonds I €max 0.142 0.071 0.028	€ count 1442 1443 1513	↓ + + + + + + + + + + + + + + + + + + +	Angles ¢max 15.032 9.235 8.655	¢count 1943 1945 2051	Deviation	mated, n from id Chirality I ♦ max 0.318 0.476 0.139	eal model count 204 204 215	♦ rmsd 0.008 0.018 0.005	Planarit	y ∳ count 257 258 272	♦rmsd 9.347 22.110 18.238	Dihedral ♦ max 77.749 178.516 177.040	¢count 871 872 940	Clash 0.000 0.340	M \$Rot-our 0.000 1.310 0.000	lolprobity t	♦ Rama-fv 96.470 99.410 98.240	♦ Conf-out 1.20 1.20 0.60	dow Cablam Cablam Conf-disfy 4.80 2.40 1.80	■ Ca-out 0.00 0.00 0.00
# 1 2 3 4	Model     T0101EM054_1     T0101EM054_2     T0101EM054_2     T0101EM025_     T0101EM025_	<ul> <li>♦ Gr.Name</li> <li>2 kihara</li> <li>1 singharoy</li> <li>1 chiu</li> <li>1 chiu</li> <li>1 chiu</li> </ul>	Mett ab-initio/ optimized optimized optimized	nod ∳auto/ man. auto man. auto	¢rmsd 0.020 0.022 0.016 0.020	Bonds ■	€ count 1442 1443 1513 1442		Angles ¢ max 15.032 9.235 8.655 10.746 10.656	¢count 1943 1945 2051 1942	Deviation	mated, n from id Chirality 0.318 0.476 0.139 0.502	eal model	rmsd 0.008 0.018 0.012 0.020	Planarit	y ◆ count 257 258 272 258 272 258 272 258	♦ rmsd 9.347 22.110 18.238 17.637 20.545	Dihedral \$max 77.749 178.516 177.040 177.003 177.003	¢count 871 872 940 872	▲Clash 0.000 0.340 0.360 0.360	M \$Rot-our 0.000 1.310 0.000 1.960 1.210	lolprobity t = Rama-out 0.590 0.000 0.000 0.000 0.000	♦ Rama-fv 96.470 99.410 98.240 97.060 09.200	♦ Conf-out 1.20 1.20 0.60 1.20	Cablam           ♦ Conf-disfy           4.80           2.40           1.80           2.40	Ca-out     0.00
# 123456	Model     T0101EM054_2     T0101EM054_3     T0101EM051_     T0101EM03_     T0101EM035_     T0101EM035_     T0101EM035_	ood: ⊠ ab- od: ⊠ ab- chiana	Mett ab-initio optimized optimized optimized optimized optimized	timized → auto/ man. auto man. auto auto auto		Bonds Bonds I ♦max 0.142 0.071 0.028 0.075 0.165 0.219	€ count 1442 1443 1513 1442 1443	<ul> <li>\$rmsd</li> <li>1.509</li> <li>2.310</li> <li>0.817</li> <li>2.165</li> <li>1.979</li> <li>1.989</li> </ul>	Angles ¢ max 15.032 9.235 8.655 10.746 18.628 53.8627	¢count 1943 1945 2051 1942 1945 1945	Peviation	mated, n from id Chirality 0.318 0.476 0.139 0.502 0.362 0.391	eal model	rmsd 0.008 0.018 0.005 0.012 0.020	Planarit Planarit Planarit	y ∳ count 257 258 272 258 272 256 258 272 256 258	◆rmsd 9.347 22.110 18.238 17.637 20.545 10.725	Dihedral	¢count 871 872 940 872 872 868	▲Clash 0.000 0.340 0.360 0.360	M \$Rot-out 0.000 1.310 0.000 1.960 1.310 0.000	lolprobity t	◆Rama-fv 96.470 99.410 98.240 97.060 98.820 98.820 98.820	♦ Conf-out 1.20 1.20 0.60 1.20 1.20 1.20	dow <u>Cablam</u> ♦ Conf-disfy 4.80 2.40 2.40 2.40 2.40 3.60	
# 1 2 3 4 5 6 7	Model     T0101EM054_2     T0101EM073_     T0101EM073_     T0101EM023_     T010EM03_     T010EM		Mett ab-initio optimized optimized optimized optimized ab-initio ab-initio	nod auto/ man. auto auto auto auto auto auto		Bonds ■ 0.142 0.071 0.028 0.075 0.165 0.219 0.219			Angles	¢count 1943 1945 2051 1942 1945 1945 1942 1945 1932	Peviation	mated, n from id Chirality 0.318 0.476 0.139 0.502 0.363 0.291 0.305	eal model	rmsd 0.008 0.018 0.012 0.020 0.012 0.020 0.009	Planarit	y ¢ count 257 258 272 258 258 255 255 255 255	¢rmsd 9.347 22.110 18.238 17.637 20.545 10.727 11.041	Dihedral \$\Phi max 77.749 178.516 177.040 177.03 174.284 137.135 137.410	¢count 871 872 940 872 872 868 868	▲Clash 0.000 0.000 0.340 0.360 0.360 0.360 0.360	M Rot-ou: 0.000 1.310 0.000 1.310 0.000 1.310 0.000 0.000	lolprobity t   ◆Rama-out 0.590 0.000 0.000 0.590 0.590 0.590 0.590 0.590	◆ Rama-fv 99.410 98.240 97.060 98.820 98.820 98.820 98.820 98.820	♦ Conf-out 1.20 1.20 0.80 1.20 1.20 1.20 1.20	Cablam Cablam Conf-disfy 4.80 2.40 2.40 2.40 3.60 3.60	nload csv ♦ Cα-out 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
# 1 2 3 4 5 6 7 8	Model     T0101EM054     T0101EM073     T0101EM073     T0101EM075     T0101EM082     T0101EM08     T010EM08     T0EM08     T0EM08     T0EM08     T0EM08     T0EM08     T0EM	odd: M ab- ♦ Gr.Name 2 kihara 1 singharoy 1 chiu 1 cdmd 1 fzjuelich 2 rosetta 1 rosetta 1 vu	Mett ab-initio/ optimized optimized optimized optimized optimized optimized ab-initio ab-initio	auto man. auto auto auto auto auto auto auto auto	¢rmsd 0.020 0.022 0.005 0.016 0.032 0.017 0.032 0.017 0.022 0.004	Bonds 0.142 0.071 0.028 0.075 0.165 0.219 0.219 0.033	✓ fr ♦ count 1442 1443 1513 1442 1443 1435 1435	¢rmsd 1.509 2.310 2.165 1.979 1.989 1.989 1.985	Angles		Deviation	mated, n from id Chiralify 0.476 0.139 0.502 0.363 0.291 0.305 0.156	eal model ¢ count 204 204 204 204 204 204 204 202 202	rmsd 0.008 0.012 0.020 0.009 0.009 0.009 0.009	Planarit	y ∳ count 257 258 275 256 256 255 255 255	¢rmsd 9.347 22.110 18.238 17.637 20.545 10.727 11.041 13.527	Dihedral ¢max 77.749 178.516 177.040 177.003 174.284 137.410 140.426	♦ count 871 872 940 872 872 868 868 868	▲Clash 0.000 0.340 0.360 0.360 0.360 0.730 1.090	M \$ Rot-out 0.000 1.310 0.000 1.310 0.000 0.000 0.000	lolprobity t \$Rama-out 0.590 0.000 0.000 0.590 0.590 0.590 0.590 0.000	◆ Rama-fv 96.470 99.410 98.240 97.060 98.820 98.820 98.820 98.820 98.820	♦ Conf-out 1.20 1.20 1.20 1.20 1.20 1.20 1.20 1.20	Cablam           ♦ Conf-disfy           4.80           2.40           2.40           3.60           3.60           2.40	PCα-out     0.00     0.
# 1 2 3 4 5 6 6 7 8 9	Model     T0101EM054		Metti	nod auto/ man. auto auto auto auto auto auto auto auto	◆rmsd 0.020 0.022 0.005 0.016 0.032 0.017 0.022 0.004	Bonds 0.142 0.071 0.028 0.075 0.219 0.219 0.033	✓ fr	↓ autor ↓ ↓ 1.509 2.310 0.817 2.165 1.979 1.989 1.994 0.665 0.937	Angles ¢ max 15.032 9.235 10.746 18.628 53.667 53.105 7.188 6.602	¢count 1943 1945 2051 1942 1945 1932 1932 1932 2051	Deviation	mated, n from id Chirality (	eal model ¢ count 204 204 204 204 204 204 204 204	rmsd 0.008 0.018 0.0012 0.020 0.012 0.020 0.009 0.009 0.009	Planarit	y ∳ count 257 258 272 256 255 255 255 255 272	♦ rmsd 9.347 22.110 18.238 17.637 20.545 10.727 11.041 13.527 20.746	Dihedral ¢max 77.749 178.516 177.040 177.003 174.284 137.135 137.410 140.426 179.679	♦ count 871 872 940 872 868 868 868 868 868 940	▲Clash 0.000 0.340 0.360 0.360 0.360 0.360 0.360 0.730 1.090	M	lolprobity ↓ ◆Rama-out 0.590 0.000 0.000 0.590 0.590 0.590 0.590 0.000 0.000	◆ Rama-fv 96.470 99.410 98.240 97.060 98.820 98.820 98.820 98.820 98.220 98.240	♦ Conf-out 1.20 1.20 0.60 1.20 1.20 1.20 1.20 1.80 0.60	Cablam           ♦ Conf-disfy           4.80           2.40           1.80           2.40           3.60           3.60           2.40           1.80	Provide the second se
# 1 2 3 4 5 6 7 8 9 1	Model     T0101EM054_2     T0101EM054_2     T0101EM051_     T0101EM052_     T0101EM082_     T010EM082_     T0101EM082_     T0101EM082_     T0101EM082_		Mett ab-initio optimized ab-initio optimized optimized optimized ab-initio ab-initio ab-initio	nod auto/ man. auto man. auto auto auto auto auto auto man. - man.	◆rmsd 0.020 0.022 0.005 0.016 0.032 0.017 0.022 0.004 0.002	Bonds 0.142 0.071 0.028 0.075 0.165 0.219 0.219 0.033 0.033 0.091	✓ fri 1442 1443 1513 1442 1435 1435 1435 1435 1513 1513	♦ rmsd 1.509 2.310 0.817 2.165 1.979 1.989 1.994 0.665 0.937	Angles	¢count 1943 1945 2051 1942 1945 1942 1932 1932 1932 2051 1942	Deviation	mated, n from id Chirality ● max 0.318 0.476 0.139 0.502 0.363 0.291 0.305 0.365 0.316 0.315 0.316	eal model ( \$ count 204 204 204 204 204 204 204 202 202 202	rmsd 0.008 0.018 0.005 0.012 0.020 0.009 0.009 0.009 0.009 0.009	Planarit	y ◆count 257 258 255 255 255 255 255 255 255	♦ rmsd 9.347 22.110 18.238 17.637 20.545 10.727 11.041 13.527 20.746 13.780	Dihedral \$ max 77.749 178.516 177.040 177.003 174.284 137.135 137.410 140.426 179.679 158.268	♦ count 871 872 940 872 872 868 868 868 868 868 868 940 872	▲Clash 0.000 0.340 0.360 0.360 0.360 0.360 0.360 1.370 1.370	M \$ Rot-out 0.000 1.310 0.000 1.310 0.000 0.000 0.000 0.610 0.000	lolprobity 1 \$ Rama-out 0.590 0.000 0.000 0.590 0.590 0.590 0.590 0.000 0.000 0.000 0.000	◆Rama-fv 96.470 99.410 98.240 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820	◆Conf-out 1.20 1.20 1.20 1.20 1.20 1.20 1.20 1.20	dow € Cablam € Conf-disfv 4.80 2.40 2.40 3.60 3.60 2.40 1.80 3.60 3.60 3.60 3.60 3.60 3.60 3.60 3.60	nload csv ♦ Cα-out 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
# 1 2 3 4 5 6 7 8 9 1 1	Model     T0101EM054	od: Mathematical ab- Gr.Name 2 kihara 1 singharoy 1 cdmd 1 cdmd 1 rosetta 1 yu - 2 arpwarp	Mett     Ab-initio/     optimized     optimized     optimized     optimized     ab-initio     ab-initio     ab-initio     -     ab-initio     -	nod	¢rmsd 0.020 0.022 0.005 0.016 0.032 0.0017 0.022 0.004 0.006 0.020 0.012	Bonds ■ model ■ max 0.142 0.071 0.028 0.075 0.165 0.219 0.033 0.038 0.091 0.050	✓ fr ♦ count 1442 1443 1443 1443 1435 1435 1435 1435 1513 1542 1442 1445	¢rmsd 1.509 2.310 0.817 1.979 1.984 0.665 0.937 1.984 0.842	Angles	¢count 1943 1945 2051 1942 1945 1932 1932 2051 1932 2051 1932 1932 2051 1945	Deviation	mated, n from id Chirality (	eal model	♦ rmsd 0.008 0.018 0.005 0.012 0.009 0.009 0.009 0.009 0.009 0.003 0.004 0.011	Planarit		¢rmsd 9.347 22.110 18.238 17.637 20.545 10.727 11.041 13.527 20.746 13.760	Dihedral ¢max 77.749 178.516 177.040 177.003 174.284 137.410 140.426 179.679 158.268 84.049		▲Clash 0.000 0.000 0.340 0.360 0.360 0.360 0.360 1.090 1.370 1.490 3.240	Mi	lolprobity t	◆ Rama-fv 96.470 99.410 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820	♦ Conf-out 1.20 0.60 1.20 1.20 1.20 1.20 1.80 0.60 0.60 0.60 1.20	Cablam Cablam Conf-disfv 4.80 2.40 2.40 3.60 3.60 3.60 3.60 3.60 3.60 3.60 3.60 3.60 3.60	■ nload csv ♦ Cα-out 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00
# 1 2 3 4 5 6 6 7 8 9 1 1 1	Model     T0101EM054     T0101EM073     T0101EM073     T0101EM073     T0101EM023     T0101EM082     T0101EM082     T0101EM083     T0101EM043     T0101EM041     T0101EM041     T0101EM041     T0101EM041     T0101EM041     T0101EM043     T0101EM045      T0101EM045      T0101EM045      T0101EM045      T0101EM045      T0101EM045      T0101EM045      T0101EM045      T0101EM045      T0101EM045      T0101EM045      T010EM045      T010EM045      T010EM045      T010EM045      T010EM045      T010EM045      T010EM045       T010EM045       T010EM045       T010EM045       T010EM045       T010EM045	ood: ⊠ ab- od: ⊠ ab- conservations of the servation of	Metti	and auto/ man. auto auto auto auto auto auto auto auto auto auto auto auto auto auto/ man. auto/ man. auto/ man. auto/ man. auto auto/ man. auto	¢rmsd 0.020 0.022 0.005 0.016 0.022 0.005 0.012 0.022 0.004 0.022 0.004 0.020 0.012 0.012 0.005	Bonds ■ model ■ model 0.142 0.075 0.165 0.219 0.033 0.038 0.091 0.050 0.033		Illy autor \$\phi\$ rmsd 1.509 2.310 0.815 1.989 1.989 1.989 1.989 1.989 1.989 1.984 1.842 0.542	Angles		Deviation           ◆rmsd           0.096           0.138           0.044           0.144           0.093           0.079           0.039           0.072           0.089           0.038	mated, n from id Chirality ● max 0.318 0.476 0.139 0.502 0.305 0.305 0.305 0.312 0.399 0.395 0.312 0.399 0.329 0.329 0.329 0.329 0.329 0.329 0.329 0.325 0.329 0.325 0.355	eal model	♦ rmsd 0.008 0.018 0.005 0.012 0.020 0.009 0.003 0.004 0.011 0.011 0.011	Planarit ◆max 0.027 0.128 0.027 0.058 0.188 0.120 0.016 0.020 0.056 0.101 0.020	y ∳ count 257 258 252 258 255 255 255 272 256 255 255 255 255 255 255 25	¢rmsd 9.347 22.110 18.238 17.637 10.727 11.041 13.527 20.746 13.780 13.068 13.019	Dihedral \$\Phi max\$ 77.749 178.516 177.040 177.040 177.003 174.284 137.410 140.426 179.679 158.268 84.049 179.820	<ul> <li>         ♦ count     </li> <li>871</li> <li>872</li> <li>940</li> <li>872</li> <li>868</li> <li>868</li> <li>940</li> <li>872</li> <li>877</li> <li>877</li> <li>872</li> </ul>	▲ Clash 0.000 0.360 0.360 0.360 0.360 0.360 0.360 0.360 0.360 1.090 1.370 1.440 3.240 4.330	M	t         *Rama-out           0.590         0.000           0.000         0.000           0.590         0.590           0.590         0.590           0.590         0.590           0.590         0.000           0.000         0.000           0.000         0.000           0.000         0.000           0.000         0.000	◆ Rama-fv 96.470 99.410 98.240 98.820 98.820 98.820 98.820 98.220 98.220 98.220 98.240 99.2410 97.080 98.820	◆Conf-out 1.20 1.20 1.20 1.20 1.20 1.20 1.20 1.20	Cablam           € Cont-disty           4.80           2.40           2.40           2.40           3.60           2.40           3.60           3.60           3.60           3.60           3.60           3.60           1.20	♦ Cα-out           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00           0.00
# 1 2 3 4 5 6 6 7 8 9 9 1 1 1 1	Model     T0101EM054_2     T0101EM073_1     T0101EM073_1     T0101EM073_1     T0101EM073_1     T0101EM073_1     T0101EM073_1     T0101EM073_1     T0101EM073_1     T0101EM073_1     T0101EM074_1      T0101EM074_1      T0101EM074_1      T0101	Gr.Name     Gr.Name     Gr.Name     Skhara     Isingharay     Ichiu	Mett ab-initio/ optimized optimized optimized optimized ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio	aod auto/ man. auto auto auto auto auto auto auto man. auto auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto man. auto	¢rmsd 0.020 0.022 0.005 0.016 0.032 0.017 0.022 0.004 0.004 0.004 0.004 0.006 0.020 0.015 0.005 0.027	Bonds I ◆max 0.142 0.071 0.028 0.075 0.219 0.219 0.033 0.038 0.091 0.033 0.038 0.091 0.033 0.135		IIIy autor ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	Angles		Deviation	mated, chiralit, max 0.318 0.476 0.139 0.502 0.363 0.291 0.305 0.156 0.312 0.299 0.395 0.126 0.129	eal model ( \$count 204 204 204 204 204 202 202 202	♦ rmsd 0.008 0.018 0.012 0.020 0.020 0.009 0.009 0.009 0.009 0.003 0.004 0.015 0.015 0.013 0.003 0.010	Planarit ◆ max 0.027 0.128 0.027 0.058 0.121 0.120 0.016 0.020 0.056 0.101 0.019 0.035	y	♦ rmsd 9.347 9.2110 18.238 17.637 20.545 10.727 11.041 13.527 20.746 13.780 13.068 13.019 9.886	Dihedral	<ul> <li>         ♦ count     </li> <li>871</li> <li>872</li> <li>940</li> <li>872</li> <li>868</li> <li>872</li> <li>871</li> </ul>	▲ Clash 0.000 0.340 0.360 0.360 0.360 0.360 1.370 1.440 3.240 3.240 4.330	M \$ Rot-out 0.000 1.310 0.000 1.960 1.310 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000 0.000	Iolprobity ↓	◆Rama-fy 96.470 99.410 98.240 98.820 88.80 88.	€Conf-out 1.20 1.20 1.20 1.20 1.20 1.20 1.20 1.20 0.60 0.60 0.60 0.60 1.250	Cablam ♦ Conf-disfv 4.80 2.40 2.40 3.60 3.60 3.60 3.60 1.80 3.00 3.60 1.20 2.260	
1 1 2 3 4 4 5 6 6 7 8 9 1 1 1 1 1 1 1	Model     TototeMost,	Gr.Name     Gr.Name     Skhara     khara     khara     khara     kinara     tokur     rosetta     rosetta     rosetta     rosetta     rosetta     tokura     khara     appvarp     denxix	Initio Metti dab-initio optimized optimized optimized optimized optimized ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio	nod auto/ man. auto auto auto auto auto man. man.	¢rmsd 0.020 0.022 0.005 0.016 0.032 0.017 0.022 0.006 0.006 0.006 0.006 0.020 0.015 0.007 0.012	Bonds 0.142 0.071 0.229 0.033 0.038 0.091 0.050 0.033 0.033 0.033 0.044 0.044		IIIy autor ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	Angles		Deviation	mated, Chirality € max 0.318 0.476 0.502 0.305 0.156 0.305 0.305 0.305 0.312 0.305 0.395 0.126 0.529 0.324	with son	♦ rmsd 0.008 0.018 0.005 0.012 0.020 0.009 0.009 0.003 0.004 0.0015 0.011 0.001 0.010 0.001 0.010	Planarit ◆ max 0.027 0.028 0.128 0.128 0.121 0.120 0.016 0.020 0.056 0.101 0.020 0.035 0.020		♦ rmsd 9.347 22.110 18.238 18.238 17.637 20.545 10.727 20.746 13.057 13.068 13.019 9.886 13.978 13.019	Dihedral ¢ max 77.749 178.516 177.040 177.040 174.284 137.135 137.410 140.426 179.679 158.268 84.049 179.823 149.523 149.523	♦ count 871 872 940 872 872 868 868 868 868 940 877 877 877 871 877 871 877	▲Clash 0.000 0.340 0.360 0.360 0.360 0.360 0.360 1.990 1.370 1.370 1.370 1.370 4.330 4.340 4.570	M	Iolprobity ↓ € Rama-out 0.590 0.000 0.590 0.590 0.590 0.590 0.000 0.590 0.000 0.000 0.000 0.000 0.000 0.4120 0.000 4.120 0.000 0.000 0.000 0.000 0.000 0.000 0.590 0.000 0.590 0.000 0.590 0.000 0.590 0.000 0.590 0.000 0.000 0.590 0.0000 0.00000 0.0000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000000	♦ Rama-fv 99,410 99,410 98,240 97,080 98,820 99,410 99,410 99,410 98,820 98,820 99,410 99,410 98,820 98,820 98,820 99,410 99,410 98,820 98,820 98,820 98,820 99,410 98,820 98,820 99,820 98,820 99,820 98,820 99,820 99,820 98,820 99,820 98,820 99,820 98,800 98,800 98,800 98,800 98,800 98,800 98,800 98,800 98,800 98,800 98	♦ Conf-out 1.20 1.20 1.20 1.20 1.20 1.20 0.60 0.60 0.60 0.60 0.60 0.60 0.60 0	Cablam                € Cont-disty                 4.80                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                 2.40                    2.40                2.40                 2.40                 2.40                 2.260                 3.60	
1 1 2 3 4 4 5 6 6 7 8 9 1 1 1 1 1 1 1 1	Model     TototEN054     TototEN054     TototEN054     TototEN055     TototEN055     TototEN055     TototEN055     TototEN055     TototEN05     TototEN05     TototEN05     TototEN05     TototEN05     TototEN05     TototEN05	ood: ⊠ ab- od: ⊠ ab- od: ≤ Gr.Name 2 khara 1 singharoy 1 chiu 1 comd 1 r2yaelic 1 rosetta 1 ampwarp 2 depetracer 2 depetracer	Metti d-initio/ d-initio/ d-initio/ d-initio optimized ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio ab-initio	timized ti		Bonds 0.142 0.071 0.028 0.075 0.165 0.219 0.033 0.038 0.091 0.050 0.033 0.035 0.044 0.103 0.044		¢rmsd 1.509 2.310 0.817 2.165 0.937 1.979 1.989 1.999 1.994 0.685 0.937 1.942 0.542 2.468 2.398 2.398	Angles		Deviation + rmsd 0.096 0.138 0.044 0.093 0.079 0.039 0.079 0.039 0.072 0.039 0.028 0.142 0.084 0.08	mated, n from id Chirality (	eal model	rmsd 0.008 0.018 0.002 0.020 0.009 0.003 0.004 0.011 0.011 0.003 0.011 0.007 0.003	Planarit	y ∳ count 257 258 255 255 255 255 255 255 255	♦ rmsd 9.347 22.110 18.238 17.637 20.545 10.727 11.041 13.527 20.746 13.780 13.068 13.019 9.886 13.978 13.978 18.480	Dihedral	<ul> <li>              € count             871          </li> <li>             940         </li> <li>             872         </li> <li>             868         </li> <li>             940         </li> <li>             872         </li> <li>             868         </li> <li>             940         </li> <li>             872         </li> <li>             874         </li> <li>             868         </li> <li>             940         </li> <li>             877         </li> <li>             940         </li> <li>             877         </li> <li>             872         </li> </ul>	▲ Clash 0.000 0.340 0.360 0.360 0.360 0.360 1.370 1.440 3.240 4.330 4.340 4.340 4.340 4.670 36.100	M ◆Rot-out 0.000 1.960 1.960 0.000 0.610 0.000 0.610 0.0000 0.0000000 0.00000 0.00000000	Instantian State	◆ Rama-fy 96.470 99.410 98.240 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 98.820 88.820 98.820 88.820 98.820 98.820 98.820 98.820 98.820	◆Conf-out 1.20 1.20 1.20 1.20 1.20 1.20 0.60 0.60 0.60 0.60 0.60 1.20 0.60 0.60 1.20 0.60	Cablam           ◆ Conf-disfv           ↓ 60           ↓ 240           1.80           2.40           1.80           3.60           3.60           3.60           3.60           3.60           3.60           3.60           3.60           3.60           3.60           2.40           1.20           22.60           0.00	

### Filtering models

Results for all models, or only the models built using specific modeling techniques

ab initio / optimization

or

automatic / manual

can be displayed by marking the appropriate checkboxes and clicking on the 'filter' button.



			opunized	indir.		01.		(01)		Model	V HOI		(01)	Model	<b>•</b> 11011	Mode	al 🕶 Di -C	Mode	el 🗸 Di -0	Mod	CChurk						_		1	al Thom	1
1	T0104EM035_1	phenix	ab-initio	man.	emd_04	06 2.9	0.32	0.49	0.20	0.98	0.98	0.04	0.24	0.74	0.74	0.64	0.78	0.85	0.85	0.85	CC(VOID	ime):	<i>m</i> ·	(0.1).						0.65	0.77
2	T0104EM027_1	kumar	ab-initio	man.	emd_04	06 2.9	0.32	0.49	0.20	0.98	0.98	0.04	0.24	0.74	0.74	0.65	0.78	0.85	0.84	0.85	Cross C	orrelation	coefficient	(U-1) Detv	een a moo	iei and targe	t density ma	p regions	with	0.64	0.76
3	T0104EM010_1	yu	ab-initio	man.	emd_04	06 2.9	0.32	0.48	0.20	0.98	0.98	0.04	0.24	0.74	0.74	0.74	0.77	0.89	0.83	0.87	the high	iest densit	y values. I	he region i	s defined b	ly the N high	iest value po	ints in th	e/	0.64	0.75
4	T0104EM091_1	chiu	optimized	man.	emd 04	06 2.9	0.32	0.48	0.20	0.98	0.98	0.04	0.23	0.73	0.73	0.74	0.77	0.89	0.83	0.88	model-	calculated	map, with	N being th	ne number	of grid poin	ts inside the	molecula	/	0.64	0.76
5	T0104EM041_1	arpwarp	ab-initio	man.	emd_04	06 2.9	0.32	0.48	0.19	0.98	0.98	0.04	0.23	0.73	0.73	0.78	0.77	0.91	0.83	0.88	mask. [l	PMID:3019	8894]							0.63	0.74
6	T0104EM073_1	singharoy	optimized	auto	emd_04	06 2.9	0.32	0.48	0.19	0.98	0.98	0.04	0.23	0.72	0.72	0.76	0.76	0,82	0.82	0.82	[larger i	s better]	<b>— —</b>							0.63	0.76
7	T0104EM041_2	arpwarp	ab-initio	auto	emd_04	06 2.9	0.32	0.47	0.19	0.99	0.99	0.04	0.22	0.73	0.73	0.74	0.75	0.89	0.82	0.86	0.80	0.70	0.71	2.99	3.05	3.96	0.63	63	0.62	0.62	0.74
8	T0104EM090_1	mbaker	ab-initio	man.	emd_04	06 2.9	0.31	0.46	0.18	0.98	0.98	0.04	0.21	0.71	0.71	0.61	0.73	0.80	0.80	0.80	0.79	0.51	0.70	3.08	3.11	2.62	0.61	0.61	0.61	0.61	0.75
9	T0104EM028_1	ccpem	ab-initio	man.	emd_04	06 2.9	0.31	0.48	0.19	0.98	0.98	0.04	0.23	0.71	0.71	0.73	0.76	0.90	0.82	0.89	0.81	0.69	0.73	2.95	3.03	4.84	0.63	0.63	0.62	0.62	0.74
1	0 T0104EM025_1	cdmd	optimized	auto	emd_04	06 2.9	0.31	0.46	0.18	0.98	0.98	0.04	0.21	0.71	0.71	0.73	0.73	0.79	0.79	0.79	0.79	0.70	0.70	3.12	3.12	4.25	0.60	0.60	0.61	0.61	0.75
1	1 T0104EM082 1	rosetta	ab-initio	man.	emd 04	06 2.9	0.31	0.49	0.19	0.98	0.98	0.04	0.24	0.66	0.73	0.73	0.75	0.88	0.82	0.86	0.81	8.70	0.72	2.98	3.04	5.11	0.50	0.63	0.33	0.64	0.75
1	2 T0104EM082_2	rosetta	ab-initio	man.	emd_04	06 2.9	0.31	0.49	0.19	0.98	0.98	0.04	0.24	0.66	0.73	0.76	0.75	0.88	0.82	0.86	0.81	0.73	0.72	2.97	3.03	5.05	0.51	0.64	0.32	0.64	0.75
1	3 T0104EM073_2	singharoy	optimized	auto	emd_04	06 2.9	0.31	0.45	0.18	0.98	0.98	0.04	0.19	0.69	0.69	9.73	0.73	0.78	0.78	0.78	0.78	0.69	0.69	3.11	3.11	3.92	0.60	0.60	0.61	0.60	0.75
1	4 T0104EM6nbb	-	-	-	emd_04	06 2.9	0.31	0.45	0.18	0.98	0.98	0.04	0.20	0.70	0.70	0.69	0.73	0.84	0.78	0.83	0.78	0.63	0.69	3.09	3.12	3.75	0.59	0.59	0.60	0.60	0.75
1	5 T0104EM060 1	deeptracer	ab-initio	man.	emd 04	06 2.9	0.29	0.41	0.15	0.98	0.98	0.03	0.15	0.62	0.68	0.64	0.64	0.67	0.67	0.68	0.68	0.56	0.56	3.42	3.42	2.18	0.46	0.50	0.45	0.54	0.71
1	6 T0104EM054 2	kihara	ab-initio	man.	emd 04	06 2.9	0.29	0.44	0.16	0.98	0.98	0.04	0.18	0.59	0.65	0.65	0.66	0.75	0.70	0.73	0.70	0.58	0.59	3.31	3.33	3.39	0.41	0.53	0.30	0.56	0.69
1	7 T0104EM060_2	deeptracer	ab-initio	man.	emd_04	06 2.9	0.28	0.40	0.14	0.98	0.98	0.03	0.15	0.61 /	0.62	0.62	0.62	0.66	0.66	0.66	0.66	0.55	0.55	3.42	3.42	2.79	0.45	0.49	0.45	0.54	0.70
1	8 T0104EM054_1	kihara	ab-initio	man.	emd_04	06 2.9	0.27	0.41	0.14	0.98	0.98	0.03	0.15	0.56	0.61	0.61	0.61	0.67	0.63	0.6	0.64	0.53	0.52	3.57	3.57	1 61	0.35	0.47	0.29	0.51	0.65
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### Brief descriptions of scores

Hovering mouse over the column name pops up a window with a brief description of the selected measure. A more detailed description can be found by consulting this document or original papers. PMIDs are provided in the pop-up window.

### Downloading results as text files

Results presented in the interactive tables can be downloaded as text files in comma separated format by clicking on the 'download csv' link above the scores table.

### Local accuracy plot: zoom in to region of interest

Per-residue scatter plots can be explored in more detail by narrowing the view to a region of interest.

In the lower (line-only) graph, place the cursor over the plot area (marker should turn into cross) and then click above the first residue of the desired interval, then drag cursor to the end residue (the area of interest will be highlighted grey) and release it – the top plot will change accordingly. The width of the selected window can be increased /decreased by placing the cursor at the edge of the grey box (marker will become a two-sided arrow) and then clicking and dragging the edge. Once the width of the grey window is selected (40 residues as shown), you can move this window along the whole graph by clicking on the main (upper) plot and moving the cursor to the left and right. Scrolling while the cursor is in the upper plot expands /narrows the selected window of residues.



## Evaluation based on model coordinates only

#### **Overview**

This group evaluates models based exclusively on their atomic coordinates. Phenix and MolProbity report agreement of stereo-chemical features of the models with those of high-resolution experimental structures, while ProQ3 estimates global and local accuracy of the models based on knowledge-based potentials and features derived from the models and predicted from target's sequence.

#### Measures

#### PHENIX (phenix.model\_statistics)<sup>1</sup>

PHENIX model\_statistics quantifies deviations of *bond distances, angles, chirality, planarity* and *dihedral angles* from ideal values <sup>18</sup>. For each parameter, three values are provided: RMSD, maximum deviation (in Ångstroms for distances or degrees for angles), and number of measured bonds, angles, etc.

#### Molprobity scores <sup>2</sup>

MolProbity validates agreement of model geometric parameters with high-resolution experimental structures (2 Å or better). Four Molprobity scores are reported:

*Clash score* reports the number of serious steric clashes per 1000 atoms. A clash is considered "serious" if steric overlap between any two atoms is > 0.4 Å. A good quality structure typically has clash-score < 20.

*Rot-out* reports the percentage of sidechains classified as poor rotamers, from those sidechains that can be evaluated. A sidechain conformation is poor if its set of torsion angles falls outside the bounds of the rotamer definition.

**Ram-out** quantifies the percentage of residues with backbone conformations classified as outliers (i.e., those for which the combination of  $\varphi$  and  $\psi$  torsion angles is unusual), while

*Ram-fav* quantifies percentage of residues with conformations in favored Ramachandran plot regions, from those residues that can be evaluated.

#### CaBLAM scores<sup>3</sup>

*CaBLAM* (or Cα Based Low-resolution Annotation Method) is a tool for validating lowresolution structures. In the 2.5–4.0Å resolution range, CaBLAM can be more robust in validating protein backbone than the Ramachandran analysis; for high-quality models, it typically provides little information beyond the Ramachandran validation.

*Ca-out* reports the percentage of Ca geometry outliers.

*Conf-out* quantifies the percentage of backbone conformations classified as outliers.

*Conf-disfav* quantifies percentage of disfavored conformations (including outliers), from those residues that can be evaluated.

#### ProQ3 (a-priori model accuracy assessment)

**ProQ3**<sup>19</sup> is based on a machine learning algorithm that combines knowledge-based Rosetta energy terms <sup>20</sup> with comparison of predicted and observed structural features, including contacts between different atom types, secondary structure and surface accessibility, and features predicted from sequence profiles. Local, per-residue accuracy is described in terms of S-score (0-1) <sup>21</sup>, and global accuracy is a normalized sum of the local values (in 0-1 range). Higher values correspond to more reliable estimates.

#### Model coordinates only web infrastructure

The *model coordinates only* tab of the website provides results in three subsections: Geometry Scores, ADP Histogram and Accuracy Estimate.

### model coordinates only $\rightarrow$ Geometry Scores

The *Geometry Scores* tab reports scores calculated using the measures discussed in this section.

		EM Model Challenge - 2019	
Results			
model coord	inates only	/ fit to EM map vs reference structure vs other models Comparative Analyses	nelp
Geome	etry Scores	s ADPs Histogram Accuracy Estimate	
Target: Human Apof	erritin: T0101	1 (emd 20026 1)	

Filter by method: 🗹 ab-initio 🗹 optimized cryoEM model 🛛 fully automated 🖓 partially automated, with some manual steps 🛛 filter

			Meth	od							Deviation	from id	eal mode								Me	Incohitu			Cablam	
#	Model	<b>≑</b> Gr.Name	ab-initio/	auto/		Bonds			Angles			Chirality	1		Planarity	/		Dihedral			MC	aprobity			Cabiam	
			optimized	▼man.	<b>¢</b> rmsd	¢max	<b>≑</b> count	<b>≑</b> rmsd	♦ max	<b>≑</b> count	<b>≑</b> rmsd	max	¢count	<b>¢</b> rmsd	max	<b>≑</b> count	<b>¢</b> rmsd	¢max	♦ count	▲Clash	<b>♦</b> Rot-out		Rama-fv	Conf-out	Conf-disfv	¢Cα-out
1	T0101EM054_2	kihara	ab-initio	man.	0.020	0.142	1442	1.509	15.032	1943	0.096	0.318	204	0.008	0.027	257	9.347	77.749	871	0.000	0.000	0.590	96.470	1.20	4.80	0.00
2	T0101EM073_1	singharoy	optimized	auto	0.022	0.071	1443	2.310	9.235	1945	0.138	0.476	204	0.018	0.128	258	22.110	178.516	872	0.000	1.310	0.000	99.410	1.20	2.40	0.00
3	T0101EM091_1	chiu	optimized	man.	0.005	0.028	1513	0.817	8.655	2051	0.044	0.139	215	0.005	0.027	272	18.238	177.040	940	0.340	0.000	0.000	98.240	0.60	1.80	0.00
4	T0101EM025_1	cdmd	optimized	auto	0.016	0.075	1442	2.165	10.746	1942	0.144	0.502	204	0.012	0.058	256	17.637	177.003	872	0.360	1.960	0.000	97.060	1.20	2.40	0.00
5	T0101EM038_1	fzjuelich	optimized	auto	0.032	0.165	1443	1.979	18.628	1945	0.093	0.363	204	0.020	0.188	258	20.545	174.284	872	0.360	1.310	0.590	98.820	1.20	2.40	0.00
6	T0101EM082_2	rosetta	ab-initio	auto	0.017	0.219	1435	1.989	53.667	1932	0.069	0.291	202	0.009	0.121	255	10.727	137.135	868	0.360	0.000	0.590	98.820	1.20	3.60	0.00
7	T0101EM082_1	rosetta	ab-initio	auto	0.022	0.219	1435	1.994	53.105	1932	0.079	0.305	202	0.009	0.120	255	11.041	137.410	868	0.730	0.000	0.590	98.820	1.80	3.60	0.00
8	T0101EM010_1	yu	ab-initio	man.	0.004	0.033	1435	0.665	7.188	1932	0.039	0.156	202	0.003	0.016	255	13.527	140.426	868	1.090	0.000	0.000	98.220	0.60	2.40	0.00
9	T0101EM3ajo	-	-	-	0.006	0.038	1513	0.937	6.602	2051	0.072	0.312	215	0.004	0.020	272	20.746	179.679	940	1.370	0.610	0.000	98.240	0.60	1.80	0.00
10	T0101EM028_1	ccpem	ab-initio	man.	0.020	0.091	1442	1.984	8.885	1942	0.105	0.299	204	0.015	0.056	256	13.780	158.268	872	1.440	0.000	0.000	99.410	0.60	3.00	0.00
11	T0101EM041_2	arpwarp	ab-initio	auto	0.012	0.050	1450	1.842	9.831	1953	0.089	0.395	205	0.011	0.101	258	13.068	84.049	877	3.240	3.250	1.170	97.080	1.20	3.60	0.00
12	T0101EM035_1	phenix	ab-initio	man.	0.005	0.033	1442	0.542	4.975	1942	0.038	0.126	204	0.003	0.019	256	13.019	179.820	872	4.330	0.000	0.000	98.820	0.60	1.20	0.00
13	T0101EM054_1	kihara	ab-initio	man.	0.027	0.135	1442	2.468	22.996	1943	0.142	0.529	204	0.010	0.035	257	9.886	65.923	871	4.340	0.000	4.120	86.470	12.50	22.60	2.38
14	T0101EM041_1	arpwarp	ab-initio	man.	0.012	0.044	1450	1.800	11.573	1953	0.084	0.324	205	0.007	0.020	258	13.978	149.523	877	4.670	2.600	0.580	96.490	2.40	3.60	0.00
15	T0101EM060_2	deeptracer	ab-initio	man.	0.031	0.103	1442	2.398	11.128	1942	0.135	0.461	204	0.003	0.039	256	18.480	179.994	872	36.100	0.000	0.000	94.710	5.40	10.10	1.79
16	T0101EM060_3	deeptracer	ab-initio	man.	0.031	0.103	1442	2.430	11.790	1942	0.115	0.348	204	0.002	0.017	256	18.410	179.991	872	41.160	0.000	0.000	95.290	6.00	8.90	2.38
17	T0101EM060_1	deentracer	ab-initio	auto	0.047	0.400	1443	2 572	58 192	1944	0.246	1 574	204	0.019	0.092	257	9 760	59 867	873	42 280	0.650	2 940	92 940	7 10	10 70	0.60

download csv

### model coordinates only $\rightarrow$ Atomic displacement parameters (ADP)

The *ADP Histogram* tab presents a histogram of ADPs (B-factors) for the model selected in the 'Model' dropdown menu.



#### model coordinates only $\rightarrow$ Accuracy Estimate

The *Accuracy Estimate* tab shows color-coded barplots of the predicted local accuracy of each residue in the model in terms of the ProQ3 error S-function (see above). Residue numbers are provided in the header section of the plot. The cumulative accuracy estimate for the model *(ProQ score)* is provided to the left of the barplot.



# Evaluation versus EM maps

### Overview

Evaluation of each model's fit to its cryo-EM density map includes calculation of global and perresidue goodness-of-fit scores generated with PHENIX  $^1$ , TEMPy  $^{5-8}$ , EMRinger<sup>9</sup>, Q-score<sup>10</sup> and Atom Inclusion  $^{11}$ .

Some scores are highly sensitive to the presence/absence of hydrogen atoms in the model. For such measures, scores are calculated both for models including all atoms (*Orig.Model*) and for models stripped of their hydrogen atoms (*noH*).

The calculation of cross-correlation scores implicitly takes into account ADP/B-factors as well as x,y,z coordinates. Since some models were submitted with unreasonable (or missing) ADP/B-factors, we calculated the cross-correlations with the B-factors as submitted by modelers (*Orig.Model*) and without them (BF=0).

### Measures

### PHENIX suite of scores for analysis of cryo-EM atomic models <sup>22</sup>

*Box CC*: real space cross-correlation coefficient (0-1) between a model and entire target density map. Higher values usually signify a better fit to map. Low values do not necessarily mean that the model does not fit the map well, but may instead indicate that there are uninterpreted map regions or poorly connected densities.

*CC(mask)*: cross-correlation coefficient (0-1) between a model and target density map values inside a mask calculated around the macromolecule.

*CC(vol)*: cross-correlation coefficient (0-1) between a model and target density map regions with the highest density values. The regions are defined by the N highest value points in the model-calculated map, with N being the number of grid points inside the molecular mask.

*CC(peaks)*: cross-correlation coefficient (0-1) between a model and target density map regions with the highest density values. The regions are defined by the N highest value points in the model-calculated map and the N highest value points in the experimental map.

*Resol. (FSC=0.5):* model-map Fourier Shell Correlation resolution at FSC = 0.5.

The cross-correlation scores are calculated with originally submitted B-factors and with B-factors set to 0.

#### TEMPy scores 5-8

*CCC (cross-correlation coefficient)* scores goodness of fit between the original map and the map calculated from the model coordinates at the author-specified resolution of the

experimental map (or an updated user-provided map). *CCC* is calculated by the array multiplication of density values at the same points in the model and target maps.

*LAP* (*Laplacian-filtered CCC*) is computed similarly to CCC, using density maps preprocessed with a Laplacian filter.

*ENV* (*Envelope*) estimates how much of the density map is filled with atoms, and penalizes protrusions from the map envelope. Larger *ENV* values denote better fits.

*MI*: *(Mutual Information)* is a statistical measure that quantifies the extent of register between two binned densities relative to their background distributions.

**SMOC** (Segment Mander's Overlap Coefficient) is a per-residue model-to-map fit measure, which calculates the Mander's overlap coefficient for overlapping residue fragments and assigns the score to the central residue in the fragment. The score is in [0-1] range with higher values indicating a better fit (*Note: The score can also take negative values when the density values in one of the maps are negative*). The SMOC score is also calculated for the whole structure by averaging the per-residue scores.

The *ENV* and *SMOC* scores are calculated for all atoms and non-hydrogen atoms. The other TEMPy scores are insensitive to the presence of hydrogen atoms in models.

#### EMRinger score 9

*EMringer* evaluates accuracy of side-chain placement within map density. There is a strong (negative) correlation between resolution and the overall EMRinger score. Side chain density is generally only resolvable for resolutions better than 4.5 Å. In general, for maps better than 3.5 Å resolution, the minimum expected score is 1. Most structures which have been carefully refined score above 1.5, with some getting scores above 3.

#### Q- score 10

*Q-score* measures the resolvability of atomic-model features in a density map at each model atom position (non-hydrogen atoms only). Per-residue *Q-scores* are generalized into the global *Q-score* for the whole model. The global *Q-score* generally correlates well with the estimated resolution of a density map.

#### Atom Inclusion scores 11

*Atom Inclusion* reports the fraction of atoms within the target map contour. An atom is within the contour if its position in the map has a density value above the current threshold. Several variants of the score are calculated: *All:Orig.Model* is calculated on all atoms present in the submitted model; *All:noH* is calculated on all non-hydrogen atoms; *BB* is calculated on backbone atoms only.

### Fit to EM map web infrastructure

The *fit to EM map* tab provides evaluation results for overall model-to-map fit (under *Global Accuracy* tab) and fit on a per-residue basis (*Local Accuracy* tab).

The *Global Accuracy* results calculated with the measures discussed above are presented under the *Scores* and *Plots* tabs.

# fit to EM map $\rightarrow$ Global Accuracy $\rightarrow$ Scores

The *Scores* table provide all scores calculated in the 'fit to EM map' evaluation track. Values in five columns of the *Scores* table (Resol. (2), EMRinger and Atom Inclusion (2)) are clickable.



Clicking on the scores in one of the five clickable columns brings up associated plots for these models, e.g. for T0104EM041\_2 (highlighted in yellow):



The *Fit to EM map: Global Accuracy: Plots* tab includes results of the *FSC versus Resolution* calculations and *Atom Inclusion* plots.

### fit to EM map $\rightarrow$ Global Accuracy $\rightarrow$ Plots $\rightarrow$ FSC versus Resolution

In the *FSC versus Resolution* plots, the lines for all submitted models are shown by default with model legends provided beneath the graph Lines for post-processed models with B-factors set to 0 (bf0) are not shown but listed in light grey beneath the original models. The visibility of a line in the graph can be changed by clicking on the model name in the model list. The table to the right of the graph shows resolution values corresponding to FSC=0.5. Moving the mouse along the selected curve shows corresponding coordinates for this model



### fit to EM map $\rightarrow$ Global Accuracy $\rightarrow$ Plots $\rightarrow$ Atom Inclusion

In the *Atom Inclusion* plots, the lines for all submitted models are shown by default with model legends provided beneath the graph. Model names and atom inclusion ratios for different contour levels are shown with hovering mouse over the curve(s). For each model, two curves can be shown: one considering all atoms in the model (all) and the other backbone atoms only (bb). Status of a line in the graph (visible /invisible) can be changed by clicking on the model name in the model list (model names in black /grey correspond to visible /invisible lines, correspondingly).

Results			
model coordinates only fit to EM map vs ref	erence structure	vs other models	Comparative Analyses
Giobal Accuracy Local Accuracy			<u>}</u>
Scores Plots			
FSC vs Resolution Atom Inclus	ion		
Target: Horse Liver Alcohol Dehydrogenase: T0104 (emd 0406) 💌			filmer
Trace by meanor, is accurate in optimized dryoed mode	1 0.9 0.8 0.7 0.8 0.7 0.8 0.7 0.8 0.5 0.4 0.3 0.2 0.1 0 0 0.03 0.2 0.1 0 0 0.03 0.02 0.1 0 0 0.03 0.02 0.1 0 0 0.03 0.02 0.1 0 0 0.03 0.02 0.1 0 0 0.03 0.02 0.1 0 0 0.03 0.03 0.02 0.1 0 0 0.03 0.02 0.1 0 0 0.03 0.02 0.03 0.02 0.03 0.02 0.03 0.02 0.03 0.02 0.03 0.02 0.03 0.02 0.03 0.02 0.03 0.02 0.1 0 0.04 0.03 0.02 0.1 0 0.04 0.03 0.02 0.1 0 0.04 0.03 0.02 0.1 0 0.04 0.03 0.02 0.1 0 0.04 0.03 0.02 0.1 0 0.1 0 0 0.03 0.02 0.1 0 0 0.03 0.02 0 0 0 0 0 0 0 0 0 0 0 0 0	-0.01 0 T0104EM041_2(bb) T0104EM041_2(bb) T0104EM073_1(bb) T0104EM027_1(bb) T0104EM027_1(bb) T0104EM027_1(bb) T0104EM025_1(bb) T0104EM025_1(bb) T0104EM025_2(bb) T0104EM022_2(bb)	O.O2         O.O2           0.01         0.02           0.02         T0104EM082_1(bb)           0.01         0.02           0.01         0.02           0.01         T0104EM060_1(bb)           0.02         T0104EM060_1(bb)           0.01         0.02           0.01         T0104EM060_1(bb)           0.01         0.02           0.0104EM073_2(all)         T0104EM060_1(all)           0.01         0.02           0.0104EM073_2(all)         T0104EM073_2(bb)           0.01         T0104EM082_1(all)           0.01         0.02           0.01         0.02           0.01         0.02           0.01         0.02           0.01         0.02           0.01         0.02           0.01         0.02           0.0104EM073_2(all)         T0104EM073_2(bb)           0.0104EM025         T0104EM082_1(all)           0.0104EM025_2(all)         T0104EM028_1(bb)           0.0104EM024_2(all)         T0104EM024_2(bb)           0.0104EM025_2(all)         T0104EM024_2(bb)           0.0104EM025_1(all)         T0104EM025_2(bb)           0.0104EM029_1(all)         T0104EM029_1(bb)

The *Fit to EM map: Local Accuracy* results are presented through seven tabs: *Per-chain Summary, TemPy, Phenix, EMRinger, Q-score, Atom Inclusion* and *All scores.* 

### fit to EM map $\rightarrow$ Local Accuracy $\rightarrow$ Per-chain Summary

While the *Global Accuracy*  $\rightarrow$  *Scores* tab shows scores for the whole multimeric model, the *Local Accuracy*  $\rightarrow$  *Per-chain Summary* tab provides model-to-map fit scores for separate chains. Scores in TemPy (SMOC) and PHENIX (box CC) columns are clickable. The links take users to score-specific pages for the selected model (see below).

Results	
model coordinates only fit to EM map vs reference structu	re vs other models Comparative Analyses help
Global Accuracy Local Accuracy	
Per-chain Summary TemPy Phenix EMRinger	Q-score Atom Inclusion All scores
Target: Horse Liver Alcohol Dehydrogenase: T0104 (emd 0406) 🖂	

Filter by method: 🗹 ab-initio 🗹 optimized cryoEM model 🛛 fully automated 🖓 partially automated, with some manual steps

#### os filter download csv

			Meth	od		EM Map	TemPy	Phenix
#	Model	Gr.Name	<ul> <li>ab-initio/ optimized</li> </ul>	¢ auto/ man.	♥ Chain	MapID	♦ SMOC	box CC
1	T0104EM041_2	arpwarp	ab-initio	auto	A	emd_0406	0.73	0.84
2	T0104EM041_2	arpwarp	ab-initio	auto	в	emd_0406	0.73	0.85
3	T0104EM025_1	cdmd	optimized	auto	A	emd_0406	0.71	0.79
4	T0104EM025_1	cdmd	optimized	auto	в	emd_0406	0.70	0.78
5	T0104EM073_1	singharoy	optimized	auto	A	emd_0406	0.72	0.81
6	T0104EM073_1	singharoy	optimized	auto	в	emd_0406	0.72	0.81
7	T0104EM073_2	singharoy	optimized	auto	A	emd_0406	0.69	0.78
8	T0104EM073_2	singharoy	optimized	auto	в	emd_0406	0.70	0.78
9	T0104EM060_1	deeptracer	ab-initio	man.	A	emd_0406	0.62	0.67
10	T0104EM060_1	deeptracer	ab-initio	man.	в	emd_0406	0.62	0.67
11	T0104EM010_1	yu	ab-initio	man.	A	emd_0406	0.74	0.84
12	T0104EM010_1	yu	ab-initio	man.	в	emd_0406	0.74	0.84
13	T0104EM027_1	kumar	ab-initio	man.	A	emd_0406	0.74	0.78
14	T0104EM027_1	kumar	ab-initio	man.	в	emd_0406	0.74	0.78
15	T0104EM028_1	copem	ab-initio	man.	A	emd_0406	0.71	0.86
16	T0104EM028_1	copem	ab-initio	man.	в	emd_0406	0.72	0.86
17	T0104EM035_1	phenix	ab-initio	man.	A	emd_0406	0.74	0.77
18	T0104EM035_1	phenix	ab-initio	man.	в	emd_0406	0.74	0.77
19	T0104EM041_1	arpwarp	ab-initio	man.	A	emd_0406	0.73	0.87
20	T0104EM041_1	arpwarp	ab-initio	man.	в	emd_0406	0.73	0.88
21	T0104EM054_1	kihara	ab-initio	man.	A	emd_0406	0.55	0.63
22	T0104EM054_1	kihara	ab-initio	man.	в	emd_0406	0.56	0.65
23	T0104EM054 2	kihara	ab-initio	man.	A	emd 0406	0.60	0.71
24	T0104EM054 2	kihara	ab-initio	man.	в	emd 0406	0.59	0.70
25	T0104EM060 2	deeptracer	ab-initio	man.	A	emd 0406	0.60	0.65
26	T0104EM060 2	deeptracer	ab-initio	man.	в	emd 0406	0.61	0.65
27	T0104EM082 1	rosetta	ab-initio	man.	A	emd 0406	0.66	0.83
28	T0104EM082 1	rosetta	ab-initio	man.	в	emd 0406	0.66	0.83
29	T0104EM082 2	rosetta	ab-initio	man.	A	emd 0406	0.66	0.84
30	T0104EM082 2	rosetta	ab-initio	man.	в	emd 0406	0.66	0.84
31	T0104EM090 1	mbaker	ab-initio	man.	A	emd 0406	0.71	0.73
32	T0104EM090_1	mbaker	ab-initio	man	в	emd 0406	0.71	0.73
33	T0104EM091_1	chiu	ontimized	man	A	emd 0406	0.73	0.85
34	T0104EM091 1	chiu	ontimized	man	B	emd_0408	0.73	0.85
35	T0104EM8pbb	-			Δ	emd_0408	0.69	0.79
36	T0104EM6nbb	-	-	-	в	emd 0406	0.70	0.79

### fit to EM map $\rightarrow$ Local Accuracy $\rightarrow$ TemPy /Phenix /EMRinger /Q-score /Atom Inclusion

The five score-specific tabs show different local (per-residue) scores for models.

If a specific model is selected in the dropdown menu then the plot shows data for one chain of this model by default. Clicking on the chain name in the chain list beneath the plot hides /unhides lines for other chains. The cumulative per-chain scores are shown to the right of the plot.



If all models are selected, the plot shows evaluation data for one chain in each of the models (the representative chain name is listed after the model name in parenthesis). Lines for models can be hidden unhidden by clicking on the model name in the model list.



All graphs are shown as scatter plots by default. The view can be switched to colored bars by clicking on the '*colored bars*' radio button (see Q-score and Atom Inclusion pages as examples below). Hovering over a bar shows value of the score for the selected residue.



### fit to EM map $\rightarrow$ Local Accuracy $\rightarrow$ All Scores

This tab shows all five local scores (see above) for a selected model in one web page.

Results							
model coordinates only fit to EM map vs reference structure vs other models <i>Comparative Analyses</i>							
Global Accuracy Local Accuracy							
Per-chain Summary TemPy Phenix EMRinger Q-score Atom Inclusion All scores							
Target: Horse Liver Alcohol Dehvdrogenase: T0104 (emd 0406) 🗸							
Filter by method: 🗹 ab-initio 🗌 optimized cryoEM model 🛛 fully automated 🗹 partially automated, with some manual steps 🛛 filter							
Model: T0104EM010 1 V Chart type: O scatter   Colored bars							
Chain: A 🛩							
(0.8; 1.0) (0.6; 0.8) (0.4; 0.6) (0.2; 0.4) (0.0; 0.2) N/A							
#         Score           • Name         • Value           1. SMOC         0.74           2. box, CC         0.84           3. ENRinger         4.9           4.9							

Assessment of models versus reference structure(s) is carried out at two levels:

- Monomeric: accuracy of separate subunits (protein chains) are evaluated;
- Multimeric: model-reference agreement is evaluated for the whole multimeric structure.

### Evaluation versus reference structure (monomeric mode)

### Overview

Submitted multimeric models are first split into chains. The separate chains are checked for similarity to each other, and all differing chain-based models are evaluated separately.

Comparisons to reference structures are made using rigid-body superposition-based measures (RMSD, GDT\_TS, GDT\_HA and GDC-SC), and local-based superposition-free measures (LDDT and CAD).

#### Measures

### Superposition-based LGA family of scores (GDT\_TS <sup>13,23</sup>, GDT\_HA, GDC\_SC <sup>24</sup>)

GDT\_TS, GDT\_HA and GDC\_SC scores are all calculated with the LGA package.

 $GDT_TS$  (Global Distance Test – Total Score) reports the average percentage of model C $\alpha$  atoms that can be superimposed with the reference structure under 1, 2, 4, and 8 Å distance cutoffs. Only well-modeled regions contribute to the GDT\_TS score, in contrast to RMSD, where all residues contribute, including superposition outliers. The GDT\_TS score is in the range [0-100] with higher scores corresponding to better fit. GDT\_TS scores over 50 indicate structures with significant similarity, while scores below 25 indicate unrelated structures.

*GDT\_HA* (*Global Distance Test – High Accuracy*) is a modification of the GDT\_TS score that uses tighter distance cut-offs (0.5, 1, 2 and 4 Å) and thus is better suited for the evaluation of high accuracy models. GDT\_HA scores are in the range 0-100; they are highly correlated with GDT\_TS scores, usually 10-20 points lower for the same models.

 $GDC\_SC$  (Global Distance Calculation for Side Chains) measure is calculated similarly to GDT\_TS but using a characteristic atom near the end of each side chain as a residue representative (instead of C $\alpha$ ). This measure implicitly brings the accuracy of side chain modeling into the scoring formula. GDC\_SC is scaled in the range 0-100.

#### Superposition-independent structure-based family of scores (LDDT, CADaa)

LDDT and CAD scores are superposition-free measures of local structure; they are more effective in assessing quality of multi-domain models. While rigid body superposition-based scores (e.g., GDT\_TS) are very sensitive to relative domain orientation (as superposition of two multi-domain structures is usually dominated by one of the domains), these local measures are

practically insensitive to spatial inter-domain arrangements and therefore are well suited for evaluation of model quality in such cases.

*LDDT*<sup>14</sup> is based on comparison of all-atom distance maps between model and target structures. The algorithm determines the percentage of preserved distances between all pairs of atoms in the target structure that are closer in space than a predefined cutoff. The final score is the average of the percentages of the preserved distances under four distance tolerance cutoffs (0.5, 1, 2 and 4 Å). The LDDT score range is [0-1].

*CAD-score*<sup>15</sup> estimates similarity of two structures based on differences in inter-residueresidue contact areas. The inter-residue contact areas can be defined for any subset of atoms in a residue (e.g., backbone or side-chain-only). In our system we report a variant of the CAD-score that is based on comparison of contact areas for all atoms in a residue (*CADaa*). The contact areas are calculated using the Voronyi tessellation approach in the target and the model separately, and then per-residue differences are summed and normalized to the [0-1] interval. Based on CASP evaluation data, the CAD-score has a bell-shaped distribution with around 90% of scores falling in the range [0.3; 0.7]. CAD score has a desired feature of favoring models with better stereo-chemical arrangements<sup>25</sup>.

#### Guide to web infrastructure

The vs reference structure  $\rightarrow$  Monomers tab provides evaluation results for overall similarity of the monomeric subunits of the model to the reference structures (under *Global Accuracy* tab) and their similarity on a per-residue basis (*Local Accuracy* tab).

#### vs reference structure $\rightarrow$ Monomers $\rightarrow$ Global Accuracy $\rightarrow$ Scores

The *Scores* tab reports all scores calculated in the 'vs reference structure  $\rightarrow$  Monomers' evaluation track. Values in the GDT\_TS column are clickable. Clicking on a GDT\_TS value for the selected model brings up a GDT plot showing the percentage of fit residues for distance cutoffs from 0 to 10 Å (see comments in the *Monomers*  $\rightarrow$  *Global Accuracy*  $\rightarrow$  *Plots* tab below).

Results	
model coordinates only fit to EM map vs reference	e structure vs other models Comparative Analyses
Multimer Monomers	
Global Accuracy Local Accuracy	
Scores Plots	
Target: Horse Liver Alcohol Dehydrogenase: T0104 6nbb A 💟	

Filter by method: 🗹 ab-initio 🗹 optimized cryoEM model

I fully automated partially automated, with some manual steps filter

								\			
#	\$ Model	<b>≑</b> Gr.Name	Method		Superposition-free measures (similarity of local geometric features)		Superposition-based measures (rigid body similarity)				
			ab-initio/ optimized	auto/ man.	<b>≑</b> LDDT	<b>≑CAD</b>	<b>♦</b> RMSD	<b>♦</b> GDT_TS	<b>♦</b> GDT_HA	<b>♦</b> GDC_ALL	<b>♦</b> GDC_SC
1	T0104EM041_2_A	arpwarp	ab-initio	auto	0.80	0.79	0.45	98.40	93.25	86.49	71.49
2	T0104EM025_1_A	cdmd	optimized	auto	0.91	0.83	0.45	99.67	94.92	89.09	72.90
3	T0104EM073_1_A	singharoy	optimized	auto	0.93	0.85	0.42	99.53	96.12	91.70	77.94
4	T0104EM073_2_A	singharoy	optimized	auto	0.95	0.89	0.37	99.60	97.59	94.12	84.81
5	T0104EM060_1_A	deeptracer	ab-initio	man.	0.83	0.75	0.66	98.40	85.16	79.00	58.96
6	T0104EM010_1_A	yu	ab-initio	man.	0.92	0.83	0.42	99.53	95.86	90.13	75.76
7	T0104EM027_1_A	kumar	ab-initio	man.	0.93	0.84	0.42	99.60	96.06	91.12	76.85
8	T0104EM028_1_A	ccpem	ab-initio	man.	0.90	0.81	0.48	99.33	94.78	87.85	69.11
9	T0104EM035_1_A	phenix	ab-initio	man.	0.92	0.84	0.38	99.00	95.59	89.99	74.83
10	T0104EM041_1_A	arpwarp	ab-initio	man.	0.90	0.82	0.46	99.60	95.32	88.22	70.56
11	T0104EM054_1_A	kihara	ab-initio	man.	0.54	0.53	3.34	69.65	51.74	45.22	33.11
12	T0104EM054_2_A	kihara	ab-initio	man.	0.63	0.61	2.93	78.61	66.38	59.85	46.84
13	T0104EM060_2_A	deeptracer	ab-initio	man.	0.83	0.75	0.74	97.53	84.16	78.13	58.24
14	T0104EM082_1_A	rosetta	ab-initio	man.	0.92	0.83	0.44	99.60	95.12	90.17	75.69
15	T0104EM082_2_A	rosetta	ab-initio	man.	0.92	0.83	0.43	99.53	95.45	90.01	74.22
16	T0104EM090_1_A	mbaker	ab-initio	man.	0.86	0.78	0.57	99.27	89.77	84.29	68.06
17	T0104EM091_1_A	chiu	optimized	man.	0.94	0.86	0.42	99.40	96.93	92.41	80.45

#### vs reference structure $\rightarrow$ Monomers $\rightarrow$ Global Accuracy $\rightarrow$ Plots

Accuracy of the model versus the reference structure is visually summarized by GDT plots showing percentage of residues in the model that can be superimposed into the target under the specified residue-residue distance cutoff. A larger area under the curve indicates a more accurate model. An ideal model would be represented by a line going straight up and then staying horizontally across the whole range of distance cutoffs. Graphs are interactive: lines can be switched on and off and the underlying scores can be shown using the techniques described in the General Information section.



### vs reference structure $\rightarrow$ Monomers $\rightarrow$ Local Accuracy $\rightarrow$ LGA /LDDT

There are two tabs under the Local Accuracy– LGA and LDDT. Clicking on either tab shows per-residue accuracy of models as color-coded bars. The LGA tab displays  $C\alpha$ - $C\alpha$  distances between corresponding residues in model and target after their optimal LGA superposition, while the LDDT tab shows per-residue LDDT score. Clicking on a data bar shows structural superposition of the model and the target colored the same way as the underlying bar.

Desite	
Results	
model coordinates only fit to EM map vs reference structure vs other models Comparative Analyses	help
Multimer	
Global Accuracy	
LGA LDDT	
Target: Horse Liver Alcohol Dehydrogenase: T0104 6nbb A 🖂	
Filter by method: 🗹 ab-initio 🗹 optimized cryot Model 🛛 fully automated 🖄 partially automated, with some manual steps 🔰 filter	
Model-Target CA-CA distances	
(0; 1) (1; 2) (2; 4) (4; 8) >8 N/A	
Method	
# \$Model \$\phi_0 = 0 = 0 = 0 = 0 = 0 = 0 = 0 = 0 = 0 =	270 . 300 330 360 .
1. T0104EM041_2_A ab-initio auto 98.40 93.25 0.45 2. T0104EM025_1_A optimized auto 99.67 94.92 45	
3. T0104EM073_1_A optimized auto 99.53 96.12 0 2 4 4. T0104EM073_2_A optimized auto 99.60 97.59 0.37	
5. T0104EM060_1_A ab-initio man. 98.40 85.16 0.68 6. T0104EM010_1_A ab-initio man. 99.53 95.86 0.42	
7. T0104EM027_1_A ab-initio man. 99.60 96.06 0.42 8. T0104EM028_1_A ab-initio man. 99.33 94.78 0.48	
9. T0104Ell035_1_A ab-initio man. 99.00 95.59 0.38 10. T0104Ell041_1_A ab-initio man. 99.60 95.32 0.46	
11. 10104EN054_2_A ab-initio man. 68.65 51.74 3.34 12. T0104EN054_2_A ab-initio man. 78.61 66.38 2.93	
13. 10104EM000_2_A ab-initio man. 97:55 64:16 07:4 14. T0104EM082_1_A ab-initio man. 99:55	
16. T014EM092A ab-initio man. 99.27 17. T014EM091 A ab-initio man. 99.40 17. T014EM091 A optimized man. 99.40 for model T0104EM054 2 A (thin line)	
structurally aligned to target T0104_6nbb_A (thick line)	
The regions of the target and the model are colored according to the following color map:	
(0; 1) (1; 2) (2; 4) (4; 8) >8 N/A	

# Evaluation versus reference structure (multimeric mode)

### **Overview**

Submitted multimeric models are evaluated as single units.

Comparison to the reference structures is made with rigid-body superposition-based measures (GDT\_TS, GDT\_HA, GDC\_ALL and GDC\_SC, RMSD), local-based superposition-free measures (QS-best, QS-global, LDDTo and LDDTw), descriptive statistical measures (N\_close, N\_far, CA\_score and Seq.match) and hydrogen bonding similarity measures (precision and Jaccard\_coefficient).

### Measures

### QS scores

Evaluation of multimers vs the reference structure is carried out using the QS<sup>12</sup> suite of measures (QS stands for Quaternary Structure). The score quantifies the similarity between quaternary structures in terms of shared interfacial contacts of their subunits. The package first finds the best mapping between the target and model chains using the structure symmetry, and then reports five scores:

**QS\_best:** fraction of interchain contacts (C $\beta$ -C $\beta$ <12A) shared between two structures for best fitting interface;

**QS\_global:** fraction of interchain contacts shared between two structures for all interfaces;

*RMSD* calculated on the whole aligned structure (Ca's of all common chains);

**LDDTo** (Local Distance Difference Test, oligomeric): the LDDT score (see monomeric section) calculated on whole oligomeric structure;

*LDDTw* (*Local Distance Difference Test, weighted*): the LDDT score calculated first on each chain separately and then length-weighted for the whole multimeric structure.

The LDDT scores described above were adapted for multimeric structures in a way that does not penalize for over-prediction, e.g. a tetrameric model (containing a perfect dimeric model) vs the dimeric target is giving a perfect score. QS-scores are ranked in [0-1] interval. Scores above 0.7 indicate highly similar quaternary structures, while scores below 0.3 indicate low assembly similarity.

### Superposition-based LGA family of scores (GDT\_TS<sup>13,23</sup>, GDT\_HA, GDC\_SC<sup>24</sup>, GDC\_ALL)

LGA scores for multimeric structures are calculated similarly to monomeric ones (see monomeric section), using the chain correspondence established with the QS-tool (above).

#### phenix.chain\_comparison module

PHENIX's chain\_comparison module calculates the proximity of model and target structures, once coordinates of both are optimally fit to the density. This is important when analyzing *ab initio* models, which may be incomplete, have sequence errors, or have regions of unassigned sequence. The method reports

N(close) –number of Ca atoms within 3Å of corresponding atoms in the target;

N(far) – number of Cas further than 3Å;

*CA\_score* – number of Cas within 3Å of the target divided by the rmsd;

*Seq.match* % - percentage of Ca atoms with correct residue name.

#### Hydrogen bonds scores

Hydrogen bond scores report accuracy of reproducing the target's hydrogen bonds. Hydrogen bonds are first identified with HBPLUS <sup>16</sup> and then compared with precision and Jaccard coefficient statistics.

**Precision** (>0) = TP/(TP+FP) is the fraction of correctly reproduced hydrogen bonds in a model. TP is the number of correctly reproduced hydrogen bonds in the model; FP is the number of hydrogen bonds in the model that are absent in the target;

*Precision (>6):* the precision measure (above) calculated on a subset of non-local hydrogen bonds (minimal sequence separation of six residues);

*Jaccard coefficient (>0)* = TP/(TP+FP+FN) is a statistical measure of similarity of hydrogen bonds in a model and the target. The measure is stricter than the precision as it additionally penalizes models for not reproducing hydrogen bonds present in the target (FN is the number of hydrogen bonds in the target that were not reproduced in the model).

*Jaccard coefficient (>6):* the Jaccard coefficient measure (above) calculated on a subset of non-local hydrogen bonds (minimal sequence separation of six residues).

### Guide to web infrastructure

The vs reference structure  $\rightarrow$  Multimers tab provides evaluation results on similarity of whole submitted models to reference structures.

Please note that the term 'multimers' is used here in a wider sense meaning whole models and whole targets. If a target is monomeric and the evaluation results make sense for both multimeric and monomeric structures, then results would appear under the *Multimers* tab. This pertains to the *phenix.chain\_comparison* and *hydrogen bonds* calculations. The 'Target' dropdown menu for these two analyses allows switching between all targets including multimers and monomers. However, if the results of multimeric calculations do not make sense in the monomeric context (e.g. QS score) or the results of multimeric calculations are the same as monomeric (LGA scores for monomers) then these results are not shown under the *Multimers* tab and the 'Target' dropdown menu contains only the list of multimeric targets.

### vs reference structure $\rightarrow$ Multimers $\rightarrow$ QS score /LGA /chain\_comparison /Hbonds



# Comparison versus other models

### **Overview**

If several models are submitted on the same target, higher level of model conservancy (global and local) can be an indicator of higher model reliability (overall or per-residue). Evaluation in this regime includes calculation of pairwise GDT\_TS scores (all-against-all models) and inter-residue distances (as reported in the LGA's optimal superposition).

#### Measures

**Davis\_QA** score <sup>17</sup> estimates accuracy of a model based on its similarity to other models submitted on the target. The method superimposes all models pairwise by running LGA in the sequence dependent mode. For each model, the quality score is calculated by averaging the GDT\_TS scores from all pairwise comparisons. In the local mode, per-residue scores are obtained by averaging the S-function-transformed distances <sup>21</sup> between the corresponding residues in pairwise LGA superpositions of the selected model with the other models submitted on the target.

### Guide to web infrastructure

The vs other models tab provides global DAVIS QA score and per-residue similarity scores in the form of color-coded bars. Clicking on a data bar shows structural superposition of the model and the target colored according to the underlying bar.



# Comparative analyses

### Overview

This tab provides a web resource for comparing methods, models and scores from different evaluation tracks.

### Guide to web infrastructure

### Comparative analyses → Models Pair-wise Comparison

Visual comparison of a models' accuracy according to different evaluation scores can be performed using the slider tool. The sliders enable visualization of all major scores for all models submitted to a single target in one page. The default view has 'all' models selected in the 'Model' dropdown menu. Scores are shown as semi-transparent grey diamonds. Overlapping diamonds make grey color more intense. Hovering over a diamond identifies model(s) and shows the score value (if scores are identical, all models are listed). Scores in different evaluation tracks are grouped together (e.g., 'Reference-free scores' or 'vs EM Map Scores').



Selecting a model from the *Model* dropdown menu marks scores for the model with red triangles in the lower halves of all slider bars. At the same time, a second *Model* menu appears allowing selection of a different model and comparison of the two sets of scores. Scores for the second model are marked in the upper halves of the slider bars by blue triangles.



#### Comparative analyses $\rightarrow$ Scores Pair-wise Comparison $\rightarrow$ Scatter Plots

This page allows pairwise comparisons of different per-target scores, so that one can evaluate correlation (or lack thereof) for any pair of scores. Six panels are shown. By default, these panels show relation between six different scores (y axis) and the PHENIX's Box\_CC score (x-axis). Scatter plot for the desired pair of scores can be drawn by selecting the scores from the dropdown menu beneath each panel and clicking on the 'Redraw all plots with updated XY' button. Each point in the plot represents a model. Model scores and names can be identified by hovering the mouse over the point of interest. Each graph has a separate menu that appears after placing the mouse in the plot area. Meaning of symbols in the menu are explained with the hovering mouse. Graphs also can be zoomed in and out by selecting a rectangular area in the plot (click on the desired corner of the area and drag the mouse to the opposite corner).



#### Comparative analyses $\rightarrow$ Scores Pair-wise Comparison $\rightarrow$ Correlation Summary

The *Correlation Summary* page shows Pearson's correlation coefficients between different evaluation scores calculated on all submitted models for all targets.

The Comparative analyses  $\rightarrow$  Scores Pair-wise Comparison  $\rightarrow$  Correlation Summary  $\rightarrow$ Selected scores tab shows correlation coefficients between preselected scores in four different evaluation tracks. Scores within each evaluation track are marked with the black squares. The DAVIS QA score (a vs other models score) is placed in the 'vs reference structure – Monomers' block.



Four evaluation-track specific subtables of the Comparative analyses  $\rightarrow$  Scores Pair-wise Comparison  $\rightarrow$  Correlation Summary page (i.e., Geometry Scores, fit to EM map, vs reference structure (multi), and vs reference structure (mono)) show correlation coefficients for all evaluation scores within the selected evaluation track. The correlation table for the 'fit to EM map' track is shown as an example below.



#### *Comparative analyses* $\rightarrow$ *Model ranks (per target)*

#### Page under development.

This page enables ranking of models on each target according to the user-selected combination of measures.

For each target, the original (raw) scores are transferred into the distribution-normalized z-scores (standard scores). Values of the z-scores depend on the raw score and the mean and standard deviation of the target's score population:

$$z\_score(model) = \frac{raw\_score(model) - Mean}{StandardDeviation.}$$

A z-score shows relative accuracy of a model with respect to other models submitted on the target. Z-scores can take any values and are dimensionless so that they can be combined with desired weights. This way each model can be assigned a cumulative ranking score in separate assessment tracks (e.g. for model-to-map fit) or for a combination of the assessment tracks.

### *Comparative analyses* $\rightarrow$ *Group ranks (across targets)*

Page under development.

This page enables ranking of prediction methods on all attempted targets according to the userselected combination of measures. Per-target z-scores (see above) from a group (modeling method) are summed or averaged and ranked accordingly.

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