



Central European Institute of Technology  
BRNO | CZECH REPUBLIC

# Validation - trends

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EUROPEAN UNION  
EUROPEAN REGIONAL DEVELOPMENT FUND  
INVESTING IN YOUR FUTURE

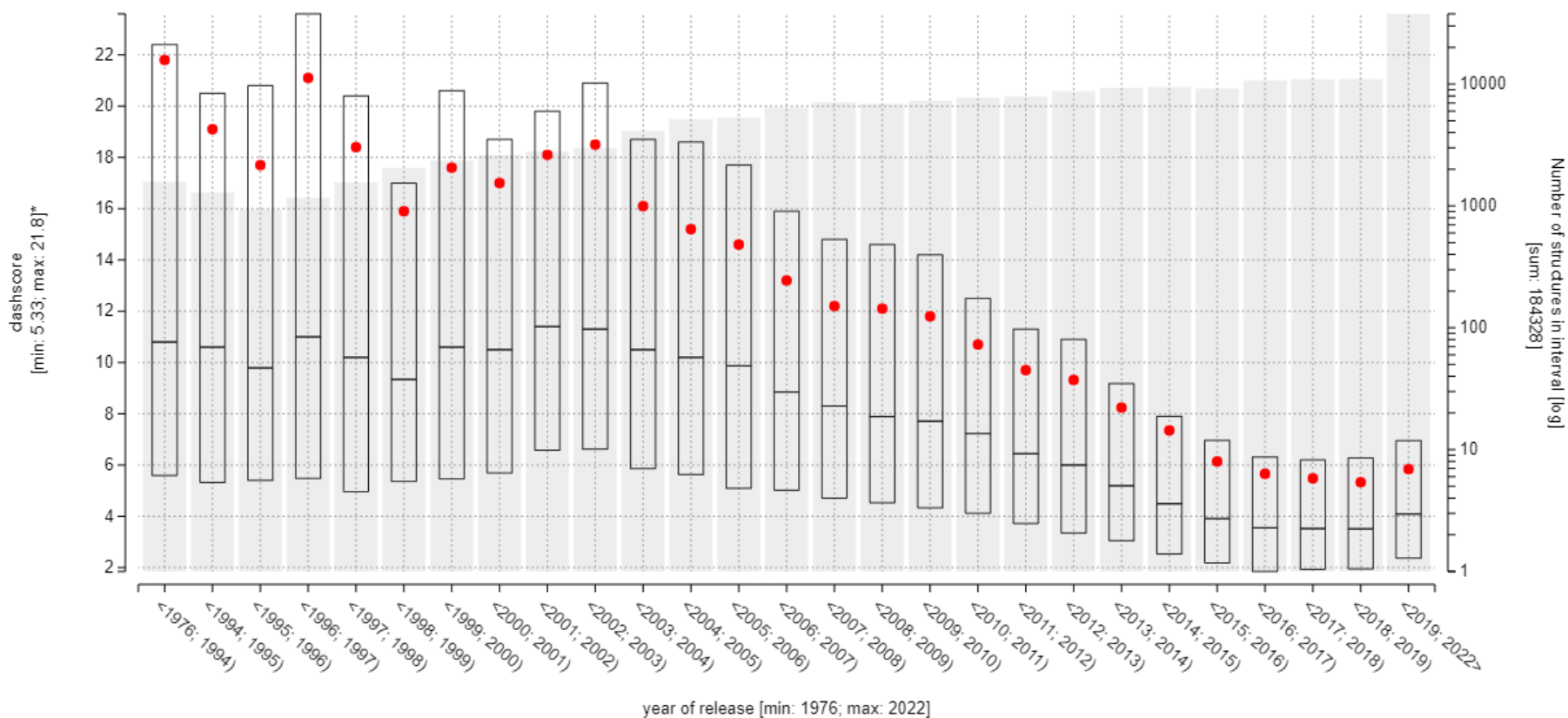


**OP Research and  
Development for Innovation**



# ValTrendsDB

- Database of biomacromolecular structure validation trends
- Based on structures from Protein Data Bank, automatic update
- <http://ncbr.muni.cz/ValTrendsDB>



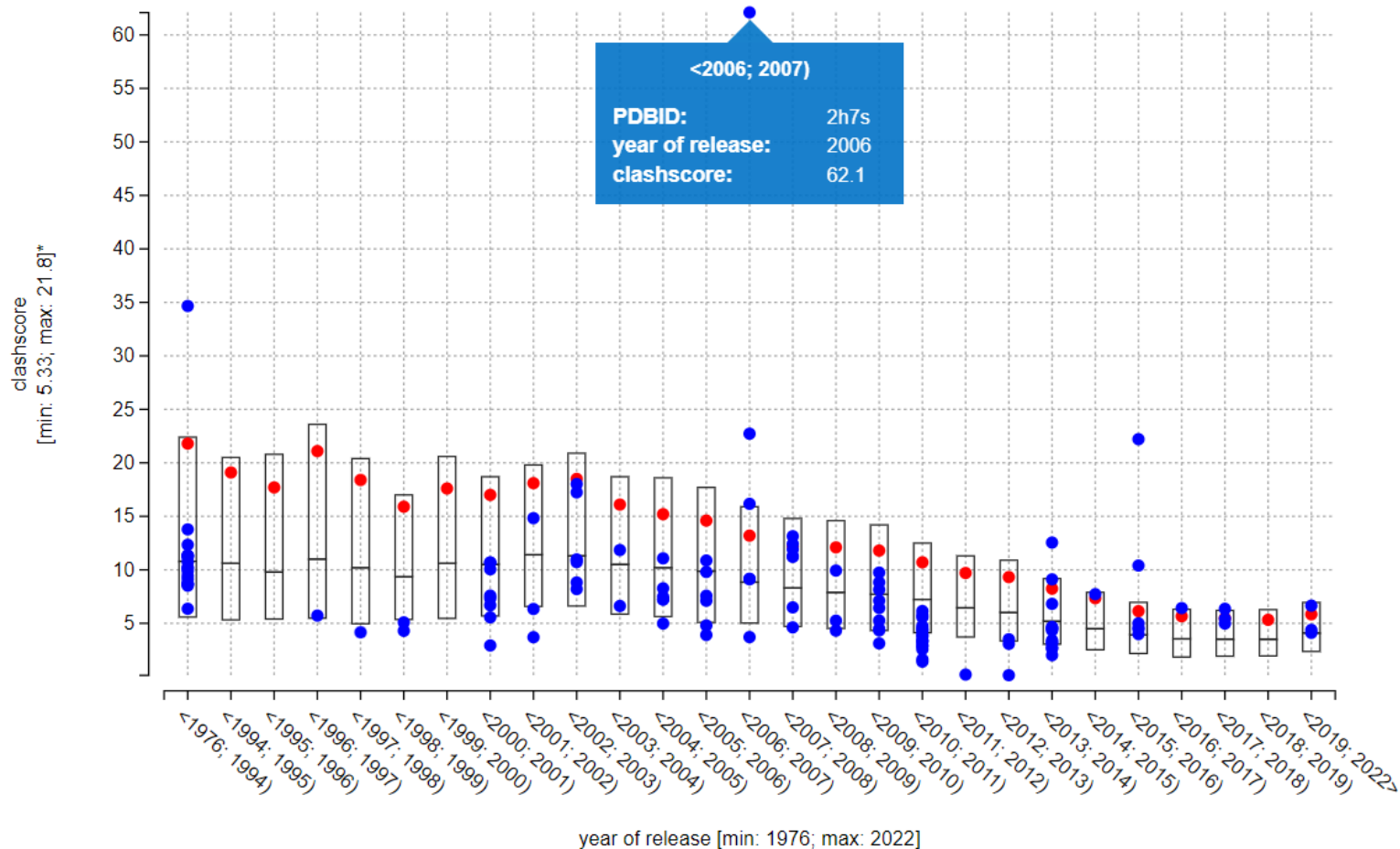
\*clashscore structure quality factor

current 2022-01-20

Horský V., Bendová V., Toušek D., Koča J. Svobodová R., 2019. ValTrendsDB: bringing Protein Data Bank validation information closer to the user. *Bioinformatics*, 35(24), 5389-5390. 

# ValTrendsDB

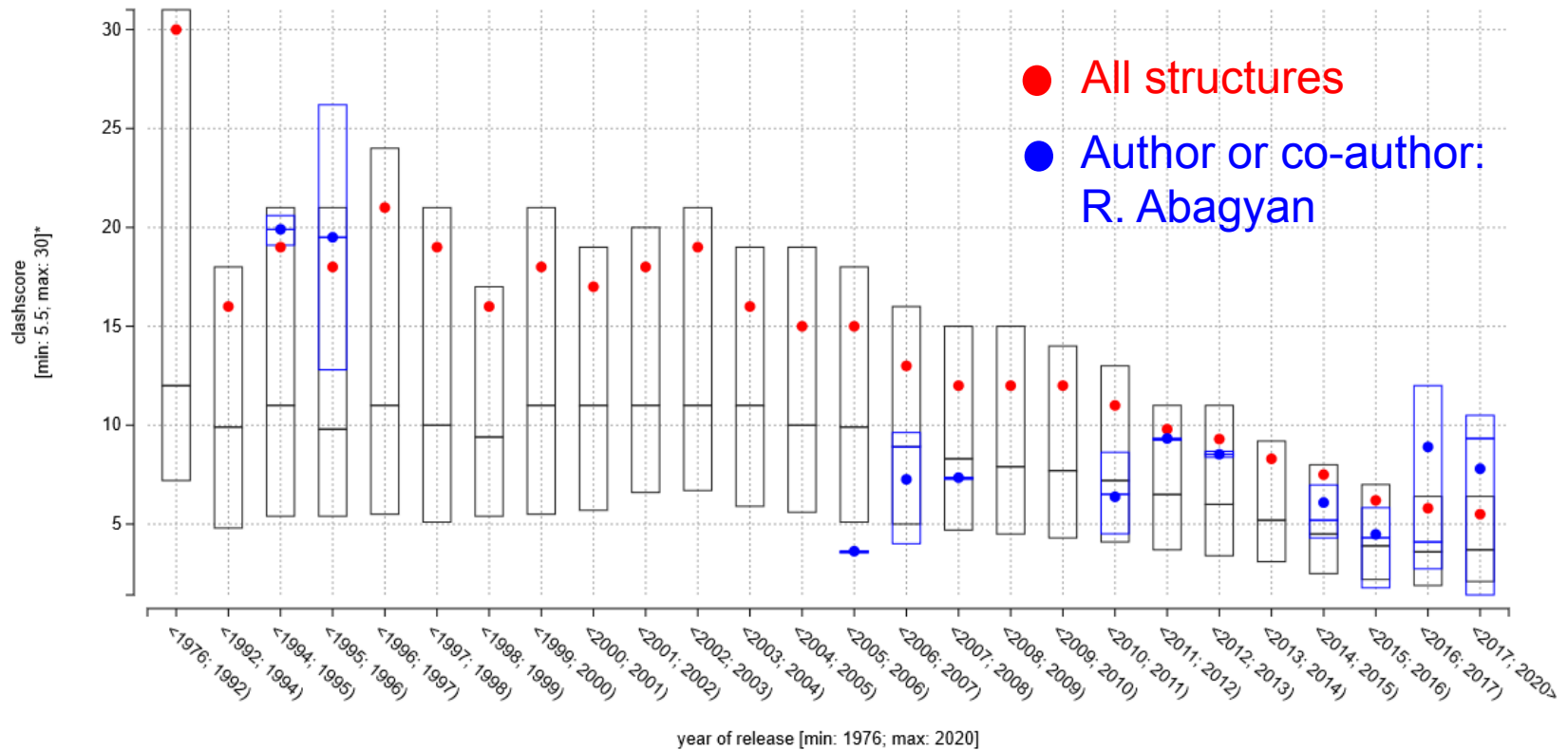
- Validation of cytochromes P450 – overview of the whole family



Blue points are structures of cytochromes P450-cam  
Red points show a common trend

# Other projects: ValTrendsDB

- Database of biomacromolecular structure validation trends
- Based on structures from Protein Data Bank, automatic update
- <http://ncbr.muni.cz/ValTrendsDB>



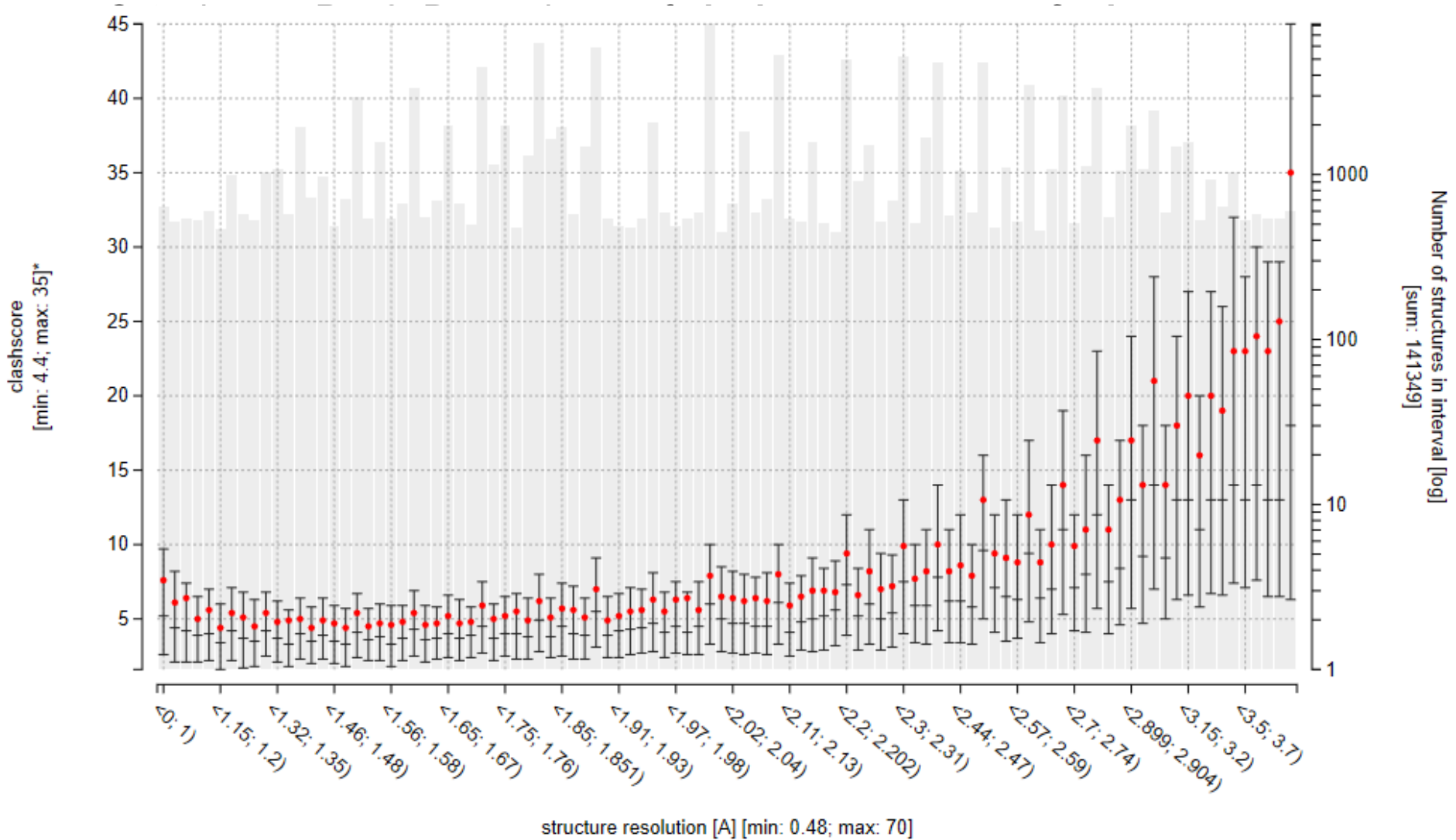
\*clashscore structure quality factor

current 2020-01-02

Horský V., Bendová V., Toušek D., Koča J. Svobodová R., 2019. ValTrendsDB: bringing Protein Data Bank validation information closer to the user. *Bioinformatics*, 35(24), 5389-5390. 

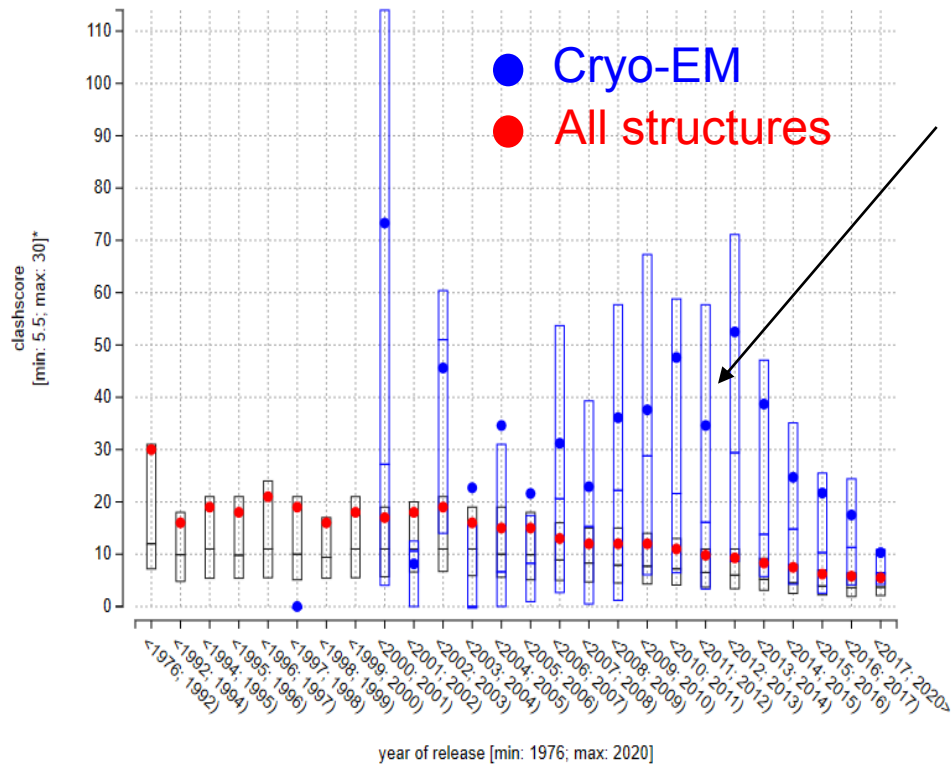
# ValTrendsDB

## Protein quality and resolution :-)



# ValTrendsDB

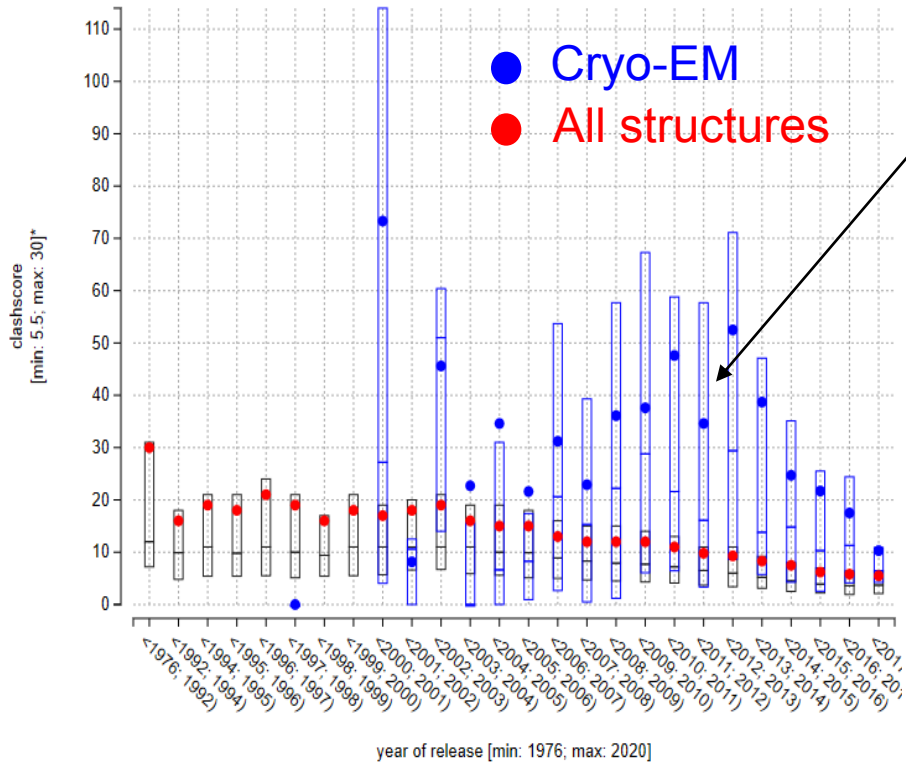
## Example of analysis



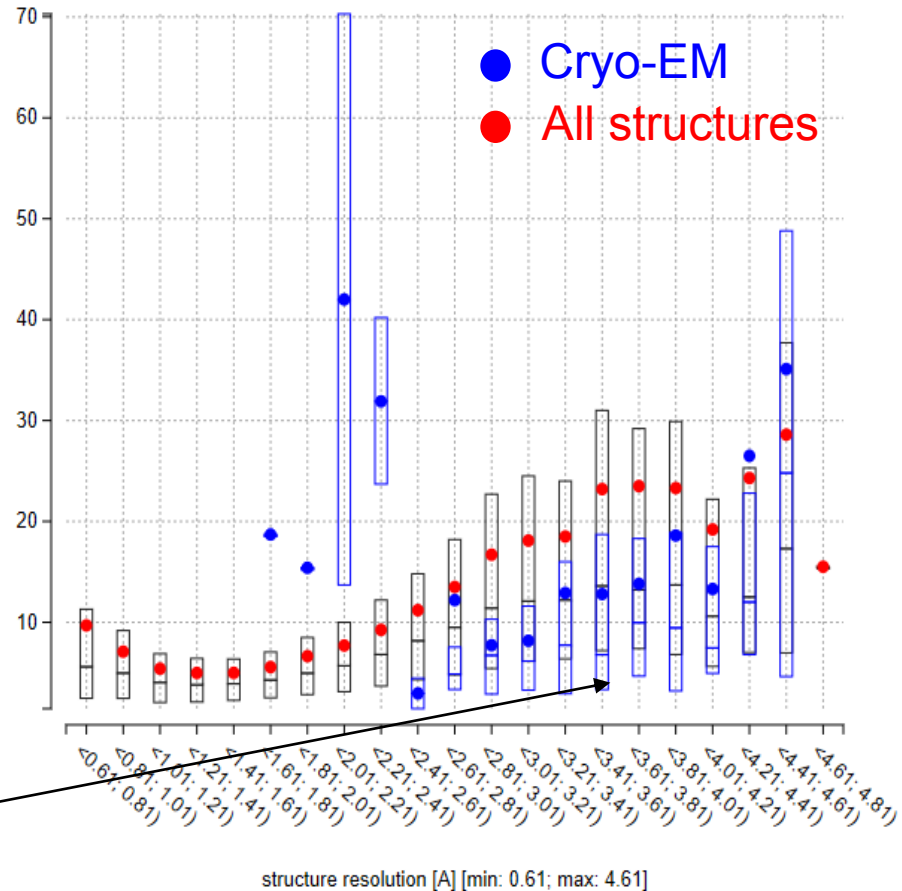
It looks, Cryo-EM structures have much lower quality than common structures

# ValTrendsDB

## Example of analysis



It looks, Cryo-EM structures have much lower quality than common structures



But when we take into account a resolution, Cryo-EM structures have (for resolution > 2.4 Å) higher quality