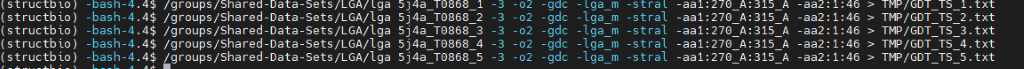
3, 4, 6 en 7 uitschrijven

I created the 5j4a\_T0868\_1 … \_5   files in the MOL2 folder… and used this command line for 1 till 5:



|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Model | Range solution | Range model | DOPE | GDT\_TS |
| 1 | 315\_A:270\_A | 01:46 | -332,95 | 73,37 |
| 2 | 315\_A:270\_A | 01:46 | -340,90 | 72,28 |
| 3 | 315\_A:270\_A | 01:46 | -333,18 | 74,46 |
| 4 | 315\_A:270\_A | 01:46 | -345,55 | 76,63 |
| 5 | 315\_A:270\_A | 01:46 | -335,34 | 74,46 |

The greener, the more the model structure looked like the solution according to the measure. So the DOPE score seems to predict the best model pretty good. For the rest of the models, the DOPE score is not very predictive for the GDT\_TS score.

Pairwise sequence alignment - Lianne

1. I used the LOCAL (I think local is needed because the alignment from the slide looks also local, and there is probably not a large set of the protein that is a match, so it's better to look for smaller ranges that match, to at least get some matches) Water EMBOSS pairwise sequence alignment (random choice) to generate the alignment: https://www.ebi.ac.uk/Tools/psa/emboss\_water/ . Input files were seq\_3zih and seq\_T0868. I choose the pearson/fasta output..
2. I pasted the result in the alignment.ali file.. this needs to be converted to pir format and altered to match the PDB file
3. First the pir file looked like this:

**>P1;T0868**

**sequence:T0868: . : . : . :.: : : :**

**LGGTLQRAPQGSSVDFVFSSGPNNGKTVDFMLTPDTVAQAAKINQFFDKN\***

**>P1;3zih**

**structure:3zih.pdb:114:A:139:A: : : :**

**IGGDIQRI--GSDI---------------FLCTPDNVDVSGTISELISED\***

4) After alterations the pir file looked like this:

**>P1;T0868**

**sequence:T0868: . : . : . :.: : : :**

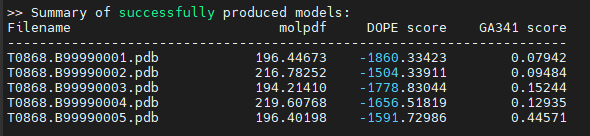
**LGGTLQRAPQGSSVDFVFSSGPNNGKTVDFMLTPDTVAQAAKI\***

**>P1;3zih**

**structure:3zih.pdb:114:A:139:A: : : :**

**IGGDIQRI--GSDI---------------FLCTPDNVDVSGTI\***

The dope scores in the results look like this:



Model 1 has lowest DOPE score.. So model 1 will be compared with the solution (5j4a.pdb).. This generated the following GDT\_TS score:

Used the following commandline to get the GDT\_TS score: 33.721

Quesiont 8, local want het zegt niks anders..