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Supporting information for article:

The X-ray crystallography phase problem solved thanks to *AlphaFold* and *RoseTTAFold* models: a case-study report

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Legends to supplementary figures

Figure S1 : Space group assignment.

The contrast values of the molecular replacement solutions obtained in the three space groups from the $P3_121$ Laue group, using the MOLREP program and the truncated AlphaFold model as search model, clearly show the much better contrast values in space group $P3_221$.

Figure S2 : Comparison of the different statistics calculated by MOLREP for the molecular replacement solutions obtained for each search model.

A. Score values of the molecular replacement solutions obtained with MOLREP. Correct solutions are highlighted as dark colors while incorrect solutions are in light colors. The color code is shown above the graph and is also used for the other panels.

B. TF/sigma values of the molecular replacement solutions obtained with MOLREP.

C. LLG values of the molecular replacement solutions obtained with PHASER.

Figure S3 : Comparison of the LLG values calculated by BUSTER during the refinement of the molecular replacement solutions.

A. LLG values calculated by BUSTER after the refinement of the molecular replacement solutions obtained with MOLREP.

B. LLG values calculated by BUSTER after the refinement of the molecular replacement solutions obtained with PHASER.

Figure S4 : Analysis of the crystal content.

2.5 µg of purified *Kl*Nmd4 (lane 1) or six crystals of *Kl*Nmd4 rinsed twice in the crystallization solution and then dissolved in water (lane 2) were loaded on a 12% SDS-PAGE. The gel was stained with Coomassie Blue.

Table S1. Primers and plasmid used for cloning and heterologous expression of *Kl*Nmd4.

Plasmid name	Backbone (Antibiotic resistance)	Primers	Sequence	Restriction site	Protein expressed
pMG897	pET28-His_6-ZZ-3C (Kan^R)	oMG593	CCTGGGATCCATCCTCAATTTCATC ATAGACTCGT	BamHI	His_6-ZZ-3C-*Kl*Nmd4
		oMG594	TATACTCGAGTCAAGATTTATTCTTG GCCGAAGTTG	XhoI	

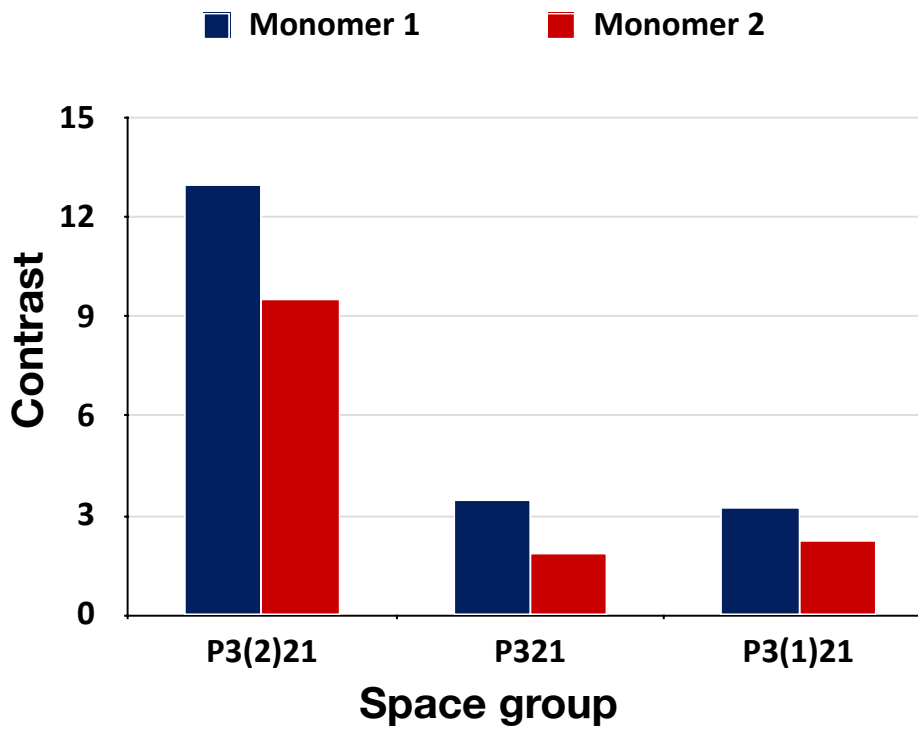
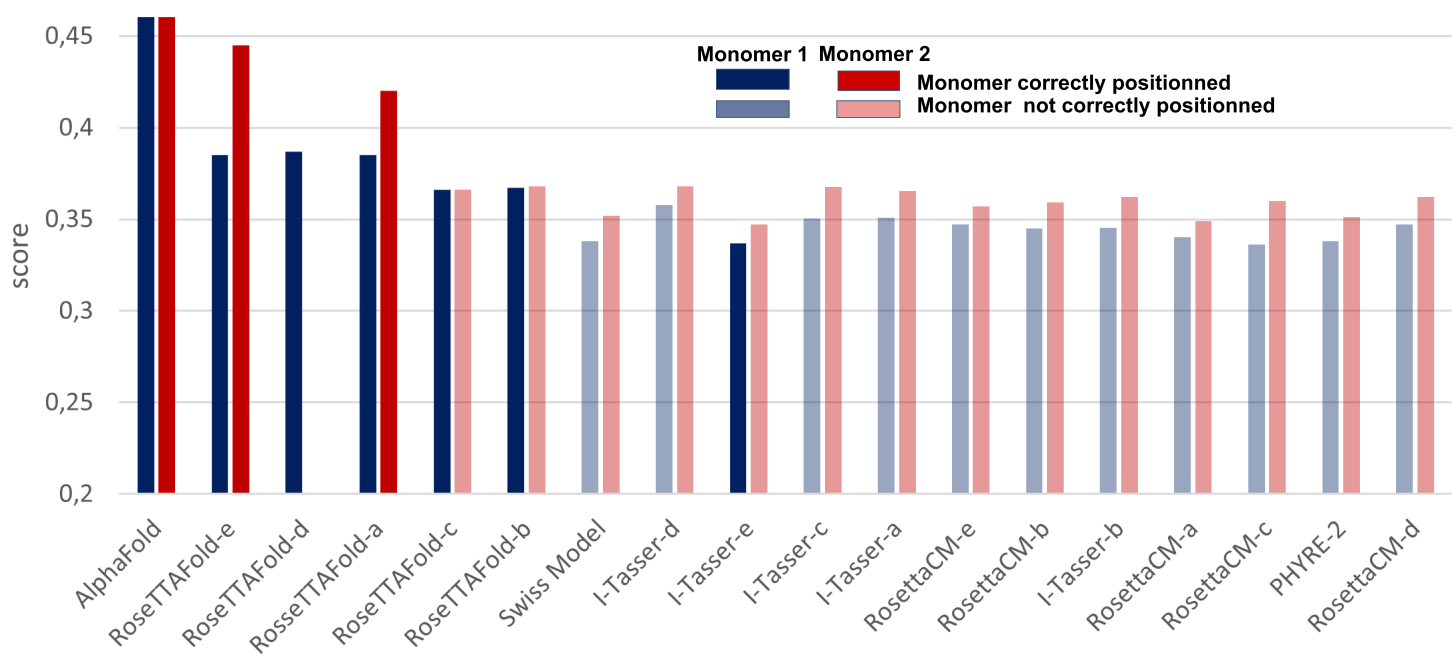
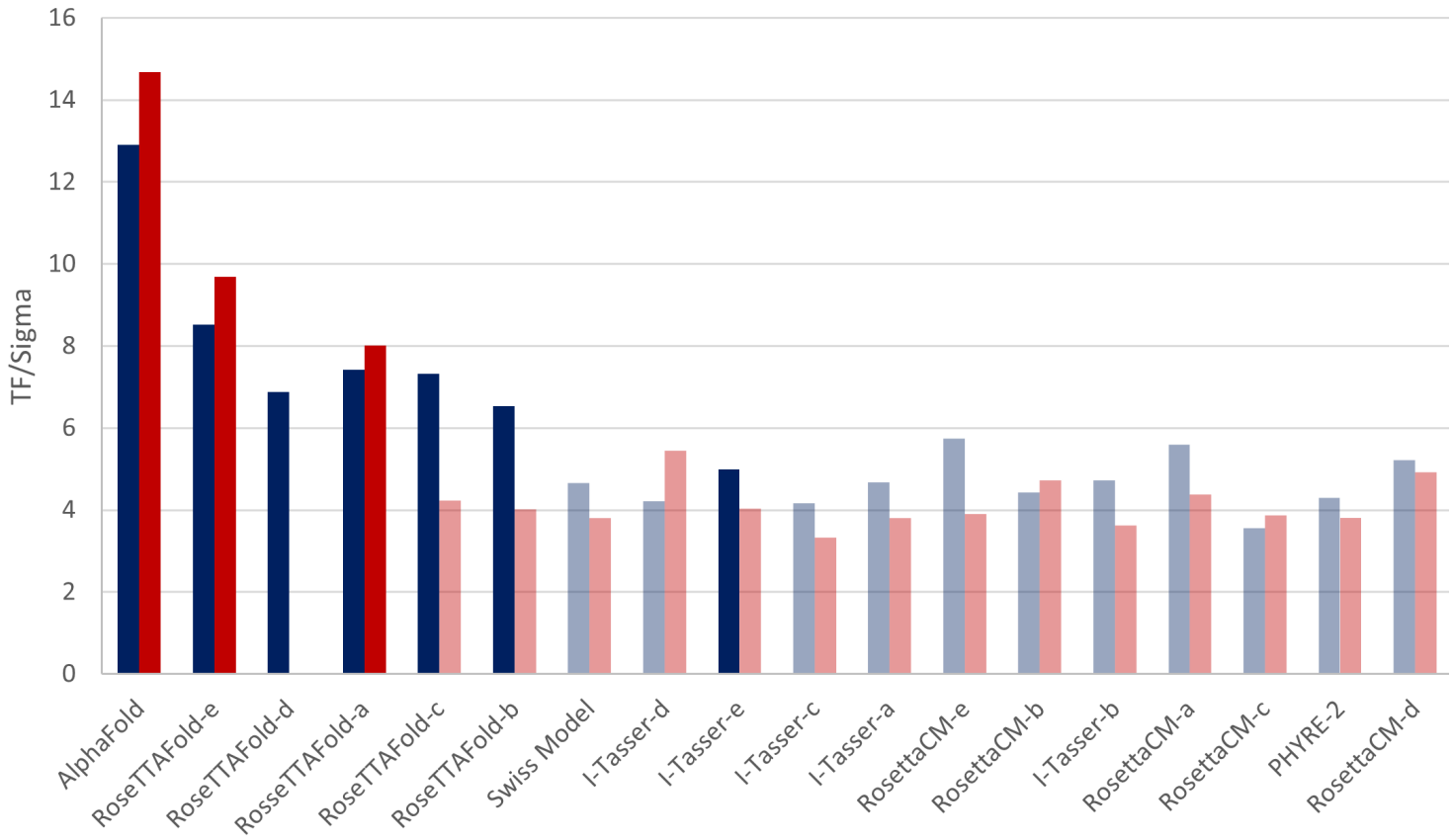

Monomer 1
Monomer 2
15
12
9
6
3
0
Contrast
P3(2)21
P321
P3(1)21
Space group

Figure S1

A.



B.



C.

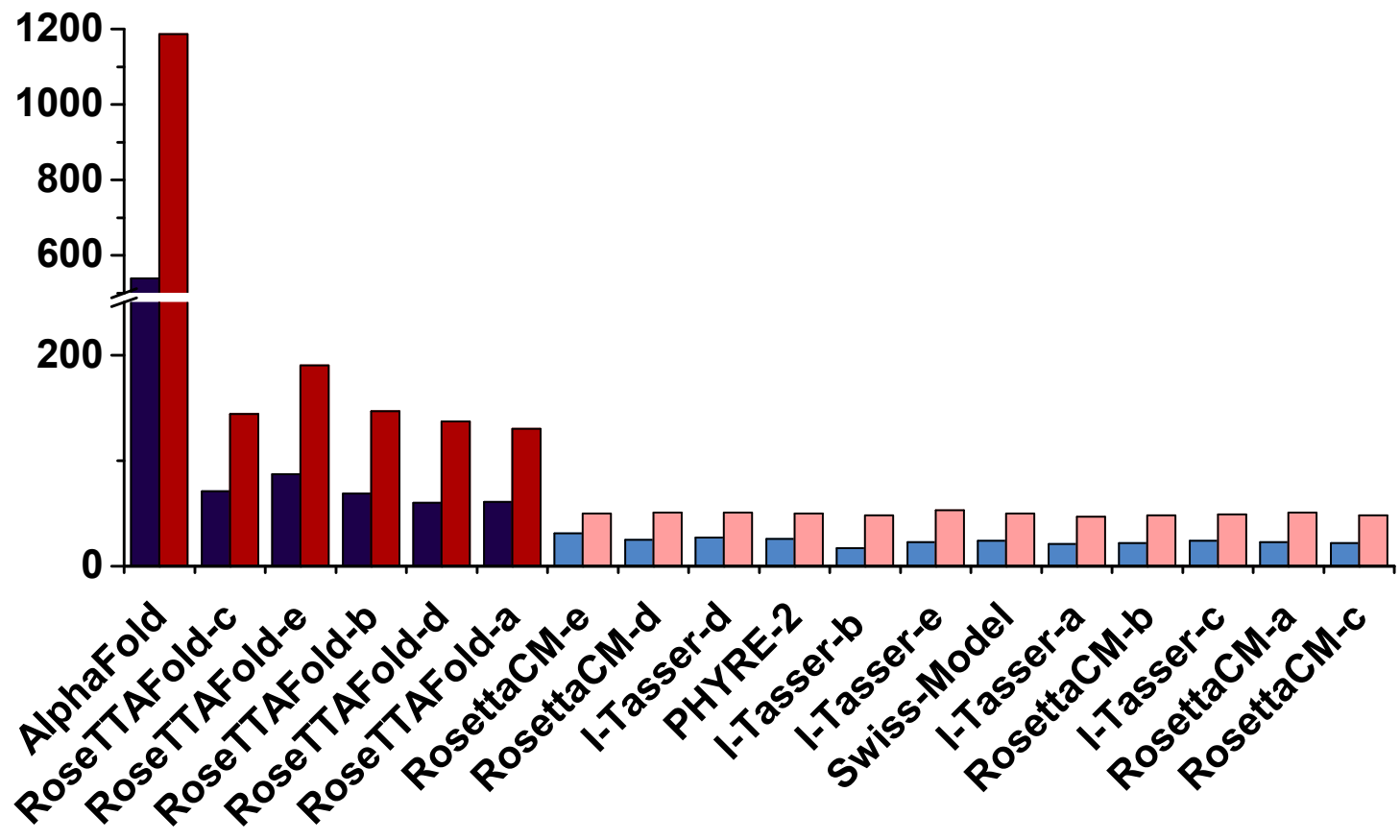
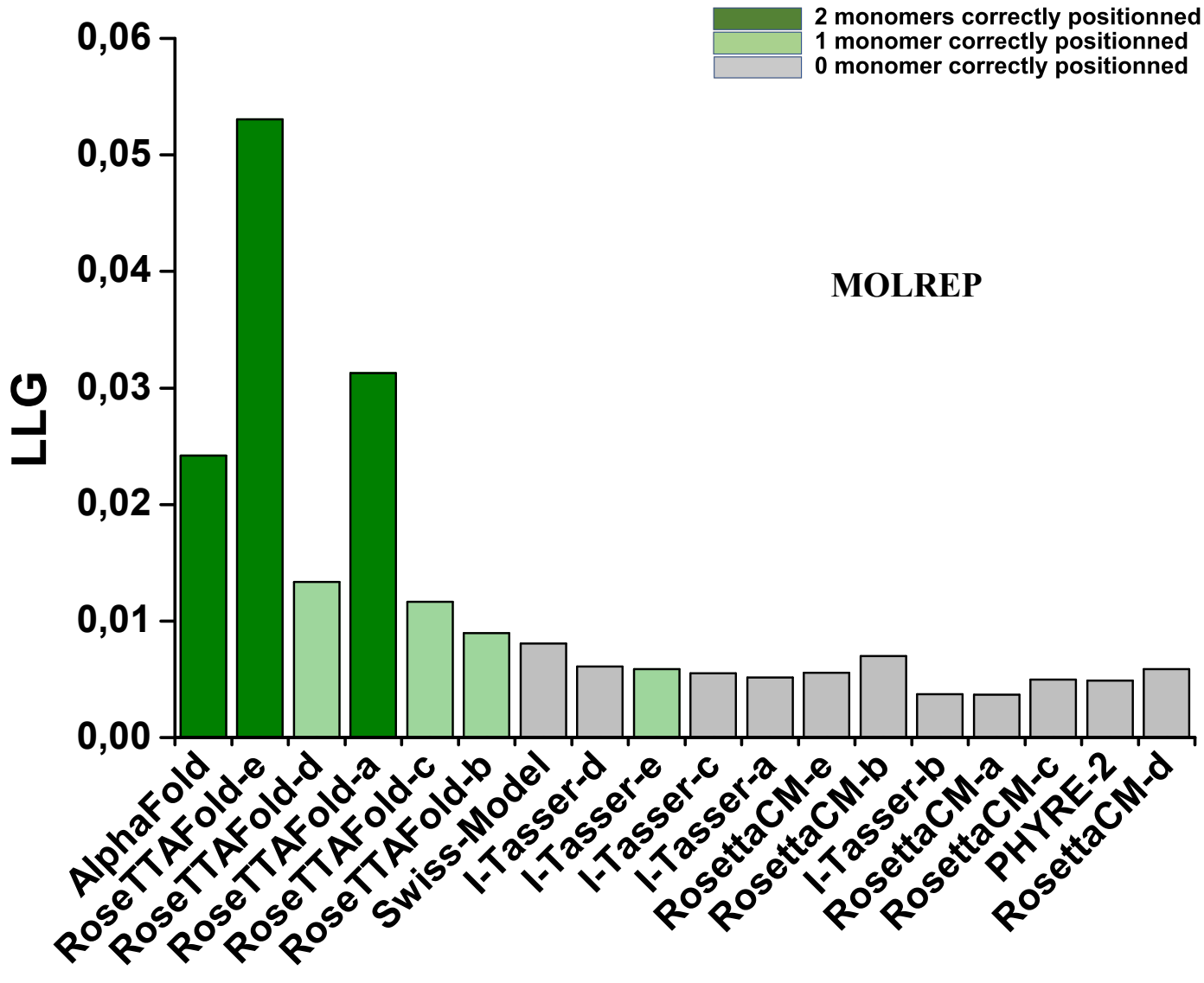


Figure S2

A.


2 monomers correctly positionned
1 monomer correctly positionned
0 monomer correctly positionned
MOLREP
LLG
0,06
0,05
0,04
0,03
0,02
0,01
0,00
AlphaFold
RoseTTAFold-e
RoseTTAFold-d
RoseTTAFold-a
RoseTTAFold-c
RoseTTAFold-b
Swiss-Model
I-Tasser-d
I-Tasser-e
I-Tasser-c
I-Tasser-a
RosettaCM-e
RosettaCM-b
I-Tasser-b
RosettaCM-a
RosettaCM-c
PHYRE-2
RosettaCM-d

B.

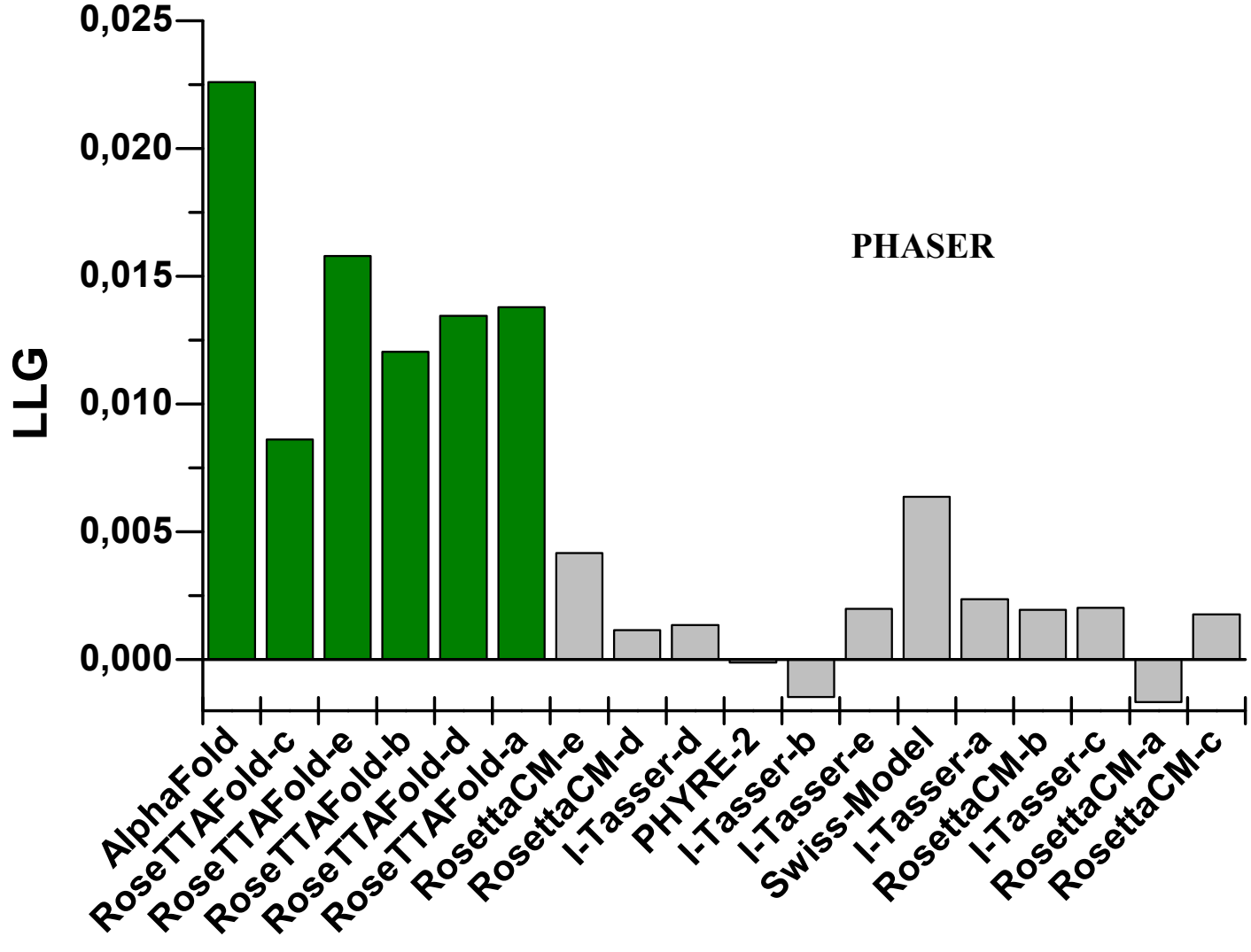

PHASER
LLG
0,025
0,020
0,015
0,010
0,005
0,000
AlphaFold
RoseTTAFold-c
RoseTTAFold-e
RoseTTAFold-b
RoseTTAFold-d
RoseTTAFold-a
RosettaCM-e
RosettaCM-d
I-Tasser-d
PHYRE-2
I-Tasser-b
I-Tasser-e
Swiss-Model
I-Tasser-a
RosettaCM-b
I-Tasser-c
RosettaCM-a
RosettaCM-c

Figure S3

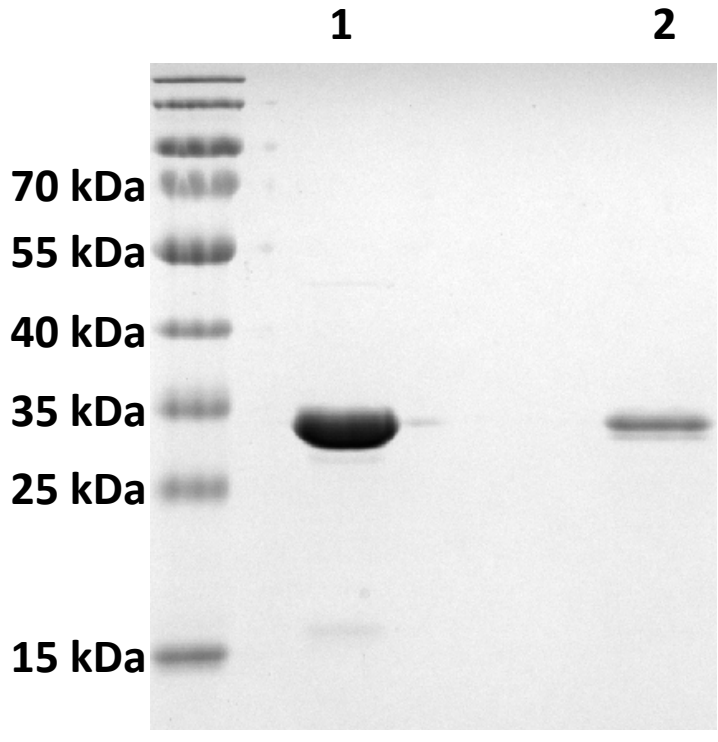


Figure S4