



STRUCTURAL
BIOLOGY

Volume 76 (2020)

Supporting information for article:

A practical overview of molecular replacement: *Clostridioides difficile* PilA1, a difficult case study

Adam D. Crawshaw, Arnaud Baslé and Paula S. Salgado

Table S1 PISA server interfaces

N#	Structure 1				Structure 2				Interface area Å ²	CSS	
	Range	N _{at}	N _{res}	Surface Å ²	Range	Symmetry op.	N _{at}	N _{res}			Surface Å
1	B	61	20	7240	A	-y+2, x+2, -z+1/2	61	17	7118	588.3	0
2	A	61	22	7118	B	-y+3/2, x-1/2, z+1/4	61	18	7240	515.8	0
3	C	59	15	7101	C	-y+3/2, x-1/2, z+1/4	57	22	7101	496.2	0
4	A	48	17	7118	A	-y+2, x+2, -z+1/2	49	17	7118	459.8	0
5	C	37	14	7101	B	x, y, z	40	14	7240	371.4	0
6	B	28	11	7240	A	x, y, z	33	11	7118	274.3	0
7	C	37	13	7101	B	-y+3/2, x-1/2, z+1/4	22	9	7240	227.6	0
8	C	11	5	7101	A	x, y, z	8	4	7118	78.0	0

Job 3: Basic Molecular Replacement - PHASER The job is Pending

Input Results Comments

Input data Simple options Extra steps Keywords

Job title: Basic MR - PHASER

Use data from job [] as input below..

Reflections

Reflections: 1 /p1a/4 [] [] []

Use Intensity (I) or amplitude (F) ML target: I []

Composition

Composition of asymmetric unit: Provided as full specification by sequence []

Crystal contents: 4 Asu content file from Define crystal contents [] [] []

Specify crystal contents []

Select one or more sequences ☒

Search model

Search: 2 Edited search model [] [] [] Copies: 3 []

Similarity of ensemble to target: read from header of PDB []

Already placed coordinates ☐

Annotations:

- Output from Aimless (points to Reflections field)
- Input sequence using FASTA (points to Specify crystal contents button)
- Search model PDB (points to Search field)
- Number of copies in ASU (points to Copies field)

Figure S1 PHASER input form in the CCP4i2 suite. Basic molecular replacement requires scaled reflections, here selected from the AIMLESS task output, the crystal contents to be defined by input of a FASTA sequence of the target and a search model which has been selected from the output from SCULPTOR. Alignment information was included in the header of the output from SCULPTOR but can also be defined as sequence identity (0.1-0.9) or RMS value. Information must also be given regarding the expected number of molecules in the asymmetric unit.

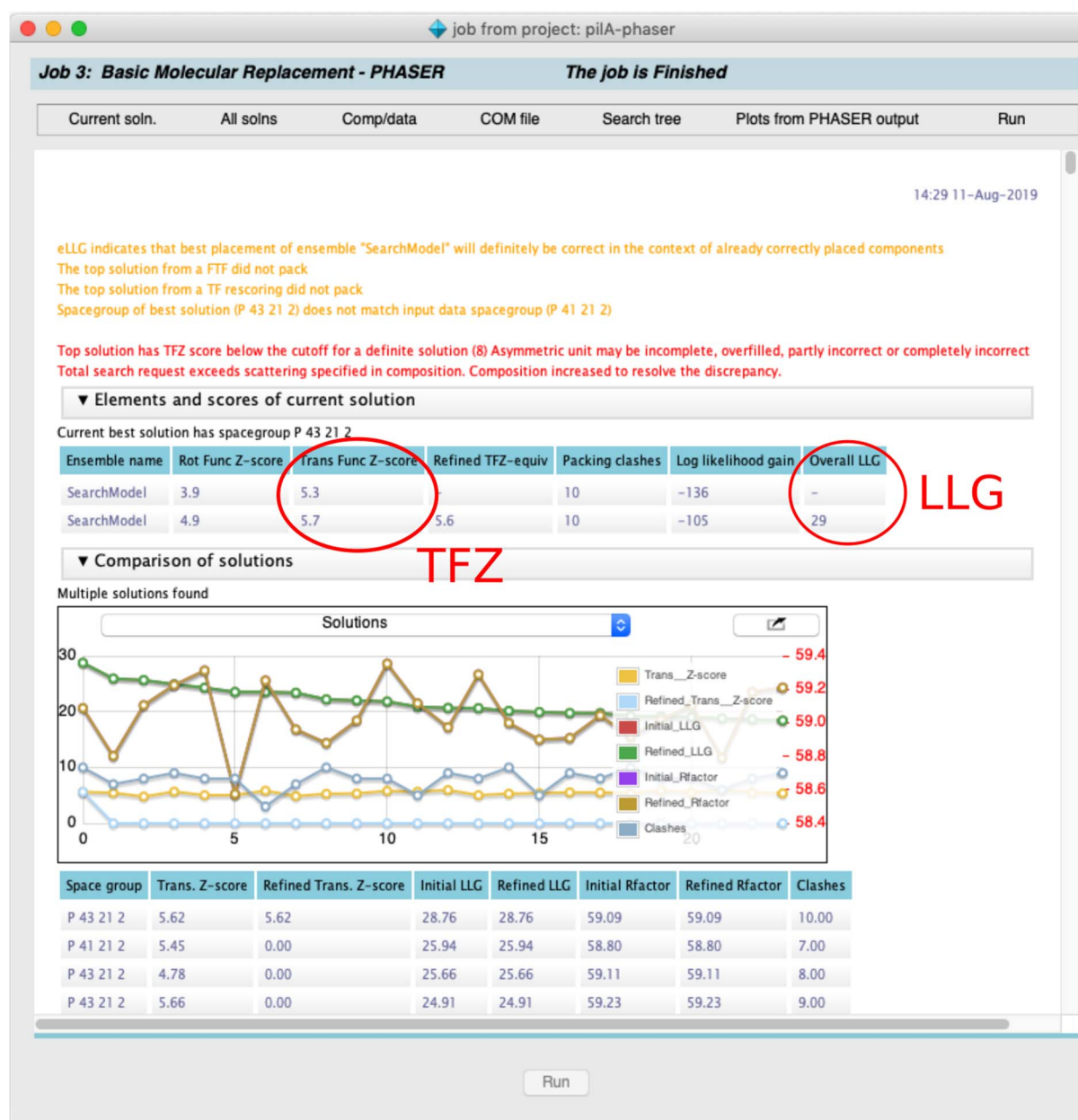


Figure S2 The output from PHASER viewed in CCP4i2 showing the statistics for the best result. The most important of these, the TFZ and LLG are circled in red. In the case of this process, the TFZ was 5.7 and LLG 29, indicating that a correct solution had not been found, as highlighted in the program output comments.