



JOURNAL OF  
APPLIED  
CRYSTALLOGRAPHY

**Volume 54 (2021)**

**Supporting information for article:**

***SHELIXIR*: automation of experimental phasing procedures using  
*SHELX C/D/E***

**Petr Kolenko, Jan Stránský, Tomáš Koval', Martin Malý and Jan Dohnálek**

## S1. List of command-line arguments

### S1.1. SAD - Heme PAS sensor domain of Ec DOS

```
shelixir -prefix 137 -sad 137.HKL -sfac Fe -ntry 10000 -find 20  
-Epar "-h -a10 -m10 -e -q -z" -bravais oP -solv 30 70 5 -nproc 11
```

### S1.2. MAD - Fragment of the plakin domain of plectin (Cys->Ala mutant)

```
shelixir -prefix 2odv -peak 2ODV_SeMet_peak_235A.ahkl -ntry 1000  
-hrem 2ODV_SeMet_remote_230A.ahkl -sfac Se -find 20 -bravais oP  
-Epar "-h -a5 -m5 -e -s0.5 -z"
```

### S1.3. MAD - Structure genomics project

```
shelixir -prefix 4jgl -peak 4jgl-peak.HKL -infl 4jgl-infl.HKL  
-hrem 4jgl-hrem.HKL -sfac Se -ntry 1000 -find 20 -Epar "-h -a5 -m20  
-e -z" -bravais hP -solv 30 70 5 -nproc 11
```

```
shelixir -prefix 4nzk -peak 4nzk-peak.HKL -infl 4nzk-infl.HKL -hrem  
4nzk-hrem.HKL -sfac Se -ntry 1000 -find 20 -Epar "-h -a5 -m20  
-z" -bravais hP -solv 30 70 5 -nproc 11
```

### S1.4. MAD – Thaumatin

```
shelixir -prefix bessy-tutorial -peak bessy-tutorial-peak.HKL -infl  
bessy-tutorial-infl.HKL -hrem bessy-tutorial-hrem.HKL -lrem bessy-  
tutorial-lrem.HKL -find 20 -sfac Br -ntry 1000 -bravais tP -Epar "-h  
-a5 -m5 -z" -solv 30 70 5 -nproc 11
```

### S1.5. MAD - Regulatory protein GerE from *Bacillus subtilis*

```
shelixir -prefix gere-short -peak gere_peak.sca -infl gere_infl.sca  
-hrem gere_hrem.sca -lrem gere_lrem.sca -nat gere_nat.sca -find 15 -  
ntry 100 -bravais mC -Epar "-m10 -a1 -h -z"  
-solv 30 70 5 -wavelength 0.98 -nproc 12
```

### S1.6. SIRAS - N-terminal domain of UL21

```
shelixir -prefix 140_xds_3 -nat 140-xds.HKL -sira 141-xds.HKL  
-sfac Hg -find 10 -ntry 10000 -Epar "-h -a5 -m10 -z" -bravais hP  
-solv 30 70 5 -nproc 11 -res 999 3
```

**S1.7. SIRAS - Helicase-like transcription factor**

```
shelixir -prefix 4s0n-s -nat 4s0n-nat.HKL -sira 4s0n-sira.HKL
-sfac Se -find 10 -ntry 1000 -Epar "-h -a3 -m5 -z" -list P21 -solv
30 70 5 -nproc 11 -fix_low 999 -screen_high "2.0 2.2 2.4 2.6 2.8
3.0"
```

**S1.8. UV-RIP – Thaumatin**

```
shelixir -prefix thau-rip -before thau-before.HKL -after
thau-after.HKL -ntry 1000 -bravais tP -sfac S -find 20 -Epar "-h -a5
-m5 -q -z" -solv 30 70 5 -nproc 11
```

**S2. SIRAS - Helicase-like transcription factor**

Optimal search at various high-resolution limits was run with command:

```
shelixir -prefix 4s0n-s -nat 4s0n-nat.HKL -sira 4s0n-sira.HKL
-sfac Se -find 20 -ntry 1000 -Epar "-h -a3 -m5 -z" -list P21 -solv
30 70 5 -nproc 11 -fix_low 999 -screen_high "2.0 2.2 2.4 2.6 2.8
3.0"
```

**Table S1** List of optimal SC values for various high-resolution limits for the data from the HIRAN domain of the helicase-like transcription factor.

High-resolution limit [ $\text{\AA}$ ]	2.0	2.2	2.4	2.6	2.8	3.0
Optimal SC value [%]	40	40	50	35	45	50
Atoms built	2101	2051	1991	2046	2046	1622