Links for Refl1D:

https://github.com/reflectometry/refl1d

https://github.com/bumps/bumps

https://refl1d.readthedocs.io/en/latest/

https://pages.nist.gov/reflectometry-calculators/reflectivity-calculator.html

Here is the model file:

```python
from refl1d.names import *
from refl1d.probe import make_probe
from numpy import *
# LOAD DATA AND CREATE A PROBE

probe = load4('ORSO_example_quick.ort',L=10.0,dL=0.1,FWHM=True)

#Polymer
polymer_rho = 2.7
polymer_t = 259
polymer_sig = 5

# SiO2
SiO_t= 30
SiO_sig= 5
SiO_rho = 3.545

# Si
Si_sig = 5.0 #Interfacial roughness
Si_rho = 2.069

# D2O
D2O_rho = 6.4024

polymer = SLD(name="polymerO",rho=polymer_rho)
SiO = SLD(name="SiO",rho=SiO_rho)
Si = SLD(name="Si",rho=Si_rho)
D2O = SLD(name="D2O", rho=D2O_rho)

sample=(D2O(100,3)
|polymer(polymer_t,polymer_sig)
|SiO(SiO_t,SiO_sig)
|Si)
# CONSTRAINTS
# probe.theta_offset.value = th
probe.intensity.value = 1
```

```python
probe.background.value = 1e-8
# probe.theta_offset = probe.pp.theta_offset


# FIT PARAMETERS
# offsets
probe.intensity.range(0.5,5)
probe.background.range(1e-11,1e-6)
#probe.theta_offset.range(-0.2,0.2)
# probe.sample_broadening.range(0,0.1)

polymer.rho.pmp(5)
polymer.irho.range(0,2)
sample[polymer].interface.pmp(5)
sample[polymer].thickness.pmp(5)

sample[SiO].interface.range(1,50)
sample[SiO].thickness.range(1,100)

# EQUALITY CONSTRAINTS:
#sample[Si].interface = sample[SiO].interface

# EXPRESSION CONSTRAINTS
#sample[Si].interface = sample[SiO].interface + 2.0

#GGG
sample[Si].interface.range(1,50)
# sample[GGG].rho.pmp(4)
# sample[GGG].magnetism.rhoM.range(0,4)



# PROBLEM DEFINITION
zed = 2 # microslabbing bin size, in A
alpha = 0.0 # integration factor - leave this at zero
step = False
M = Experiment(sample=sample, probe=probe, dz=zed,dA=alpha,step_interfaces=step)


problem = FitProblem(M)
problem.name = "OopsieItUpsideDown"
```
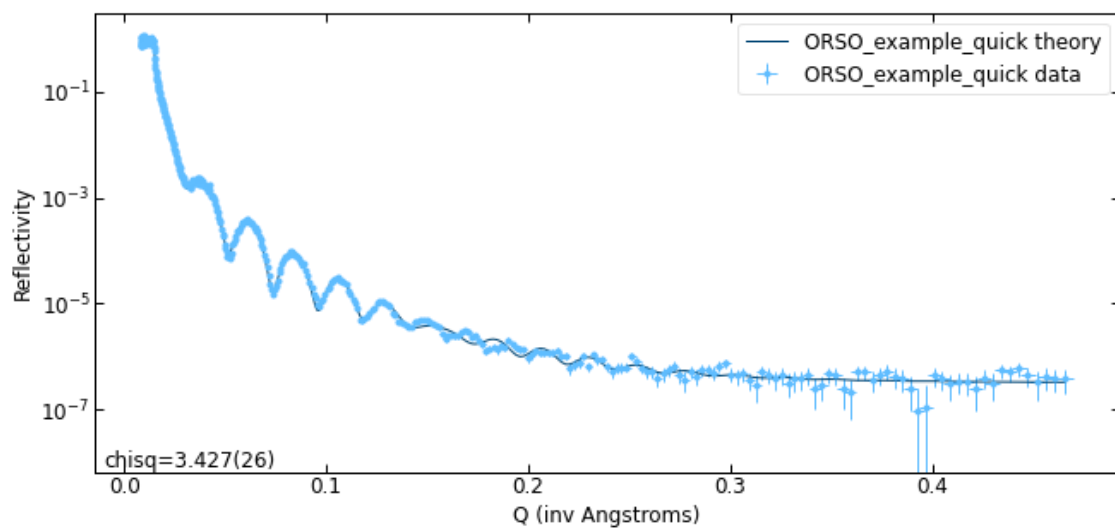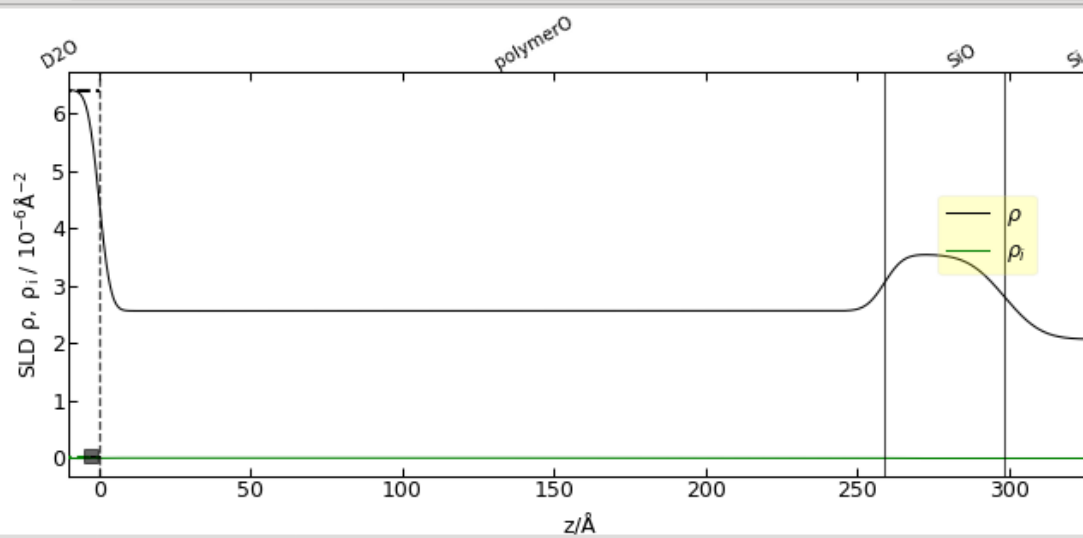
And here are the results:

File  Help  Fitting  Reflectivity

**Reflectivity** ⊠

chisq=3.427(26)

ORSO_example_quick theory
ORSO_example_quick data

Reflectivity

Q (inv Angstroms)

x=0.4496 y=0.000120516

◄ Profile ⊠ | Parameters | Summary | Log | Convergence | Uncertainty | Correlations | Parameter Trace ►

D2O          polymerO                    SiO      Si

SLD ρ, ρᵢ / 10⁻⁶Å⁻²

ρ
ρᵢ

z/Å

x:116  y:6.00

Fit status: Co...

| Fit Parameter | Value | Minimum | Maximum |
|---|---|---|---|
| background | | 3.24600000000001e-11 | |
| intensity | | 0.8857 | 0.5 |
| polymerO interface | | 4.833 | 4.75 |
| polymerO irho | | 0.00613799999990 | |
| polymerO rho | | 2.561 | 2.56 |
| polymerO thickness | | 259.0 | 246 |
| SiO interface | | 9.57200000000001 | |
| SiO thickness | | 39.56 | 1 |
| Si interface | | 13.5400000000001 | |

**Parameters** | **Summary** | **Log** | **Convergence** | **Uncertainty** | **Correlations** | **Parameter Trace** ⊠ | **Model** ▶

x=109.47 y=6.63e−07



**Log** | **Convergence** | **Uncertainty** | **Correlations** | **Parameter Trace** | **Model Uncertainty** ⊠
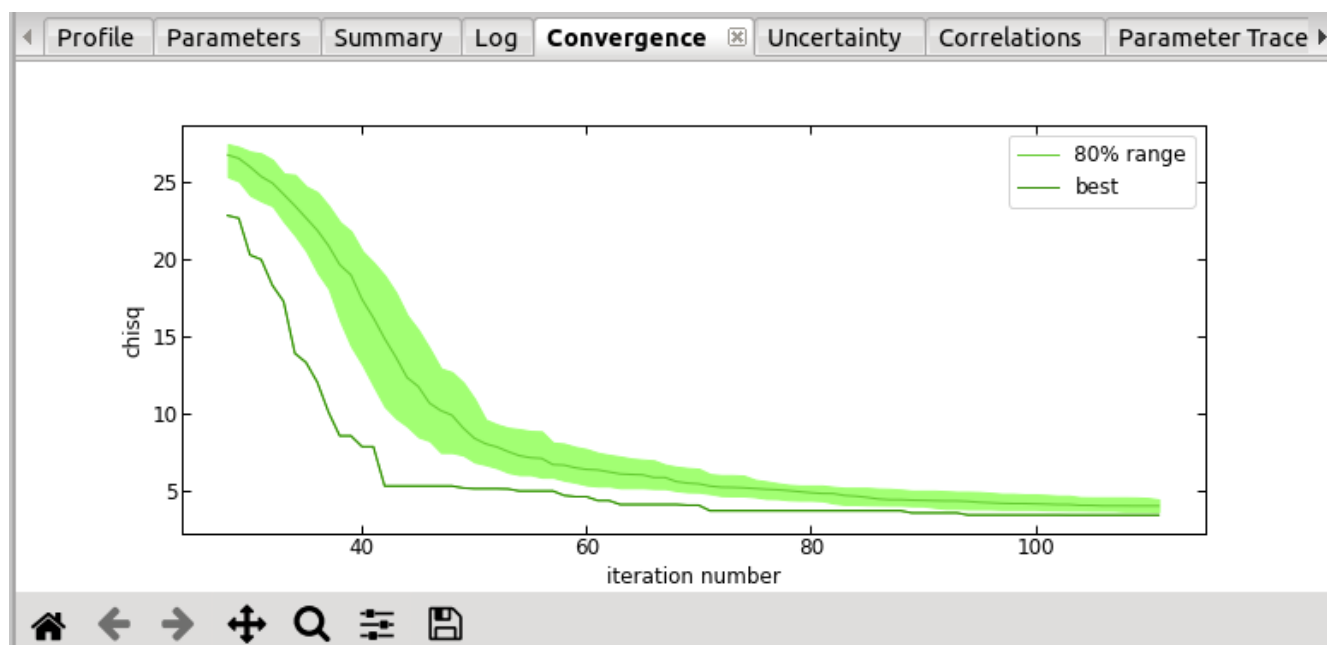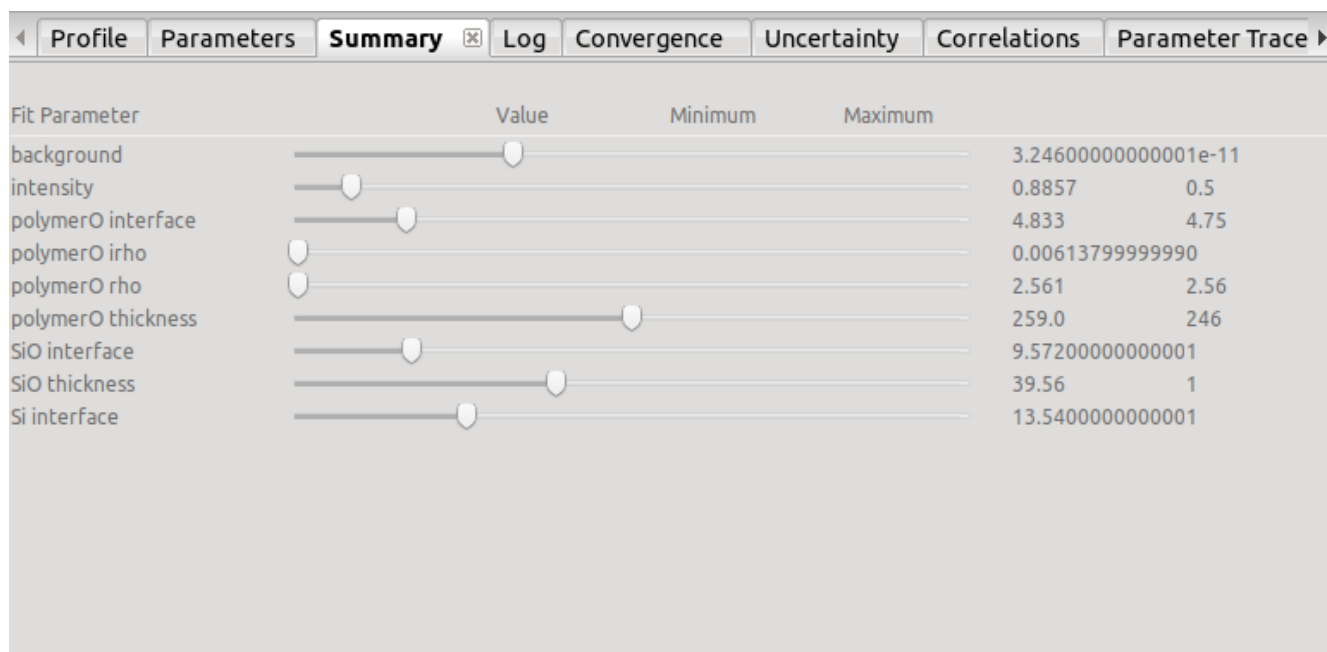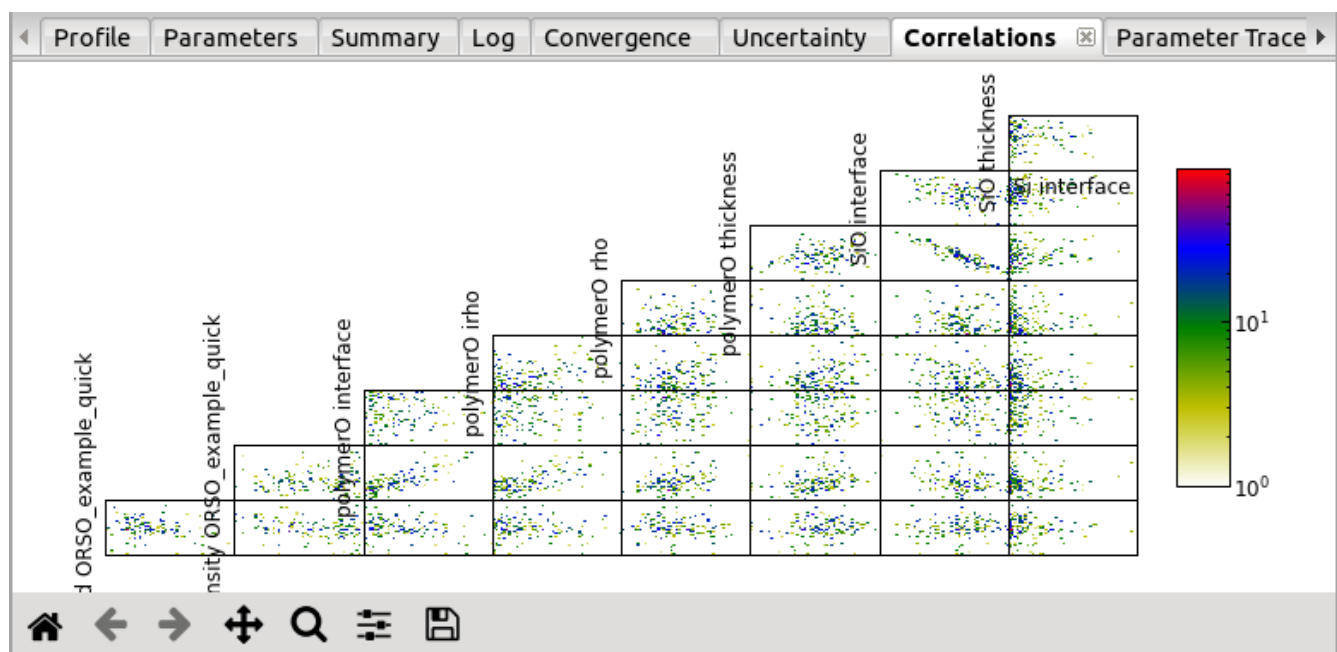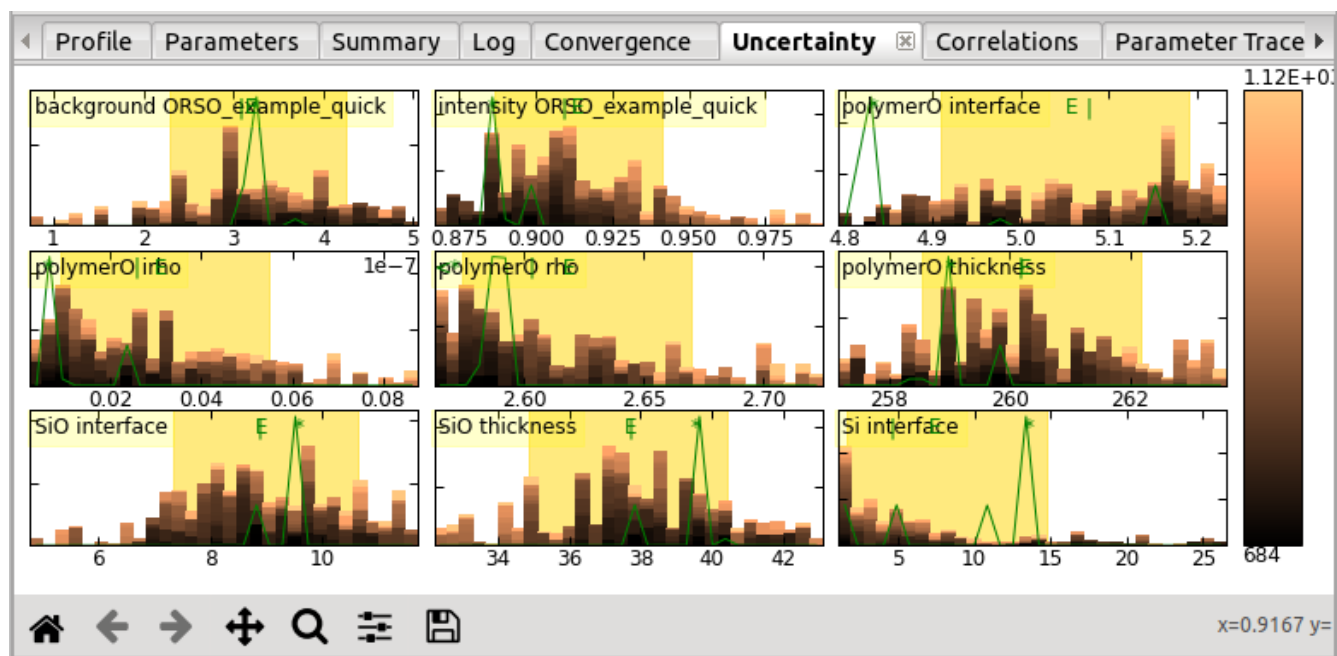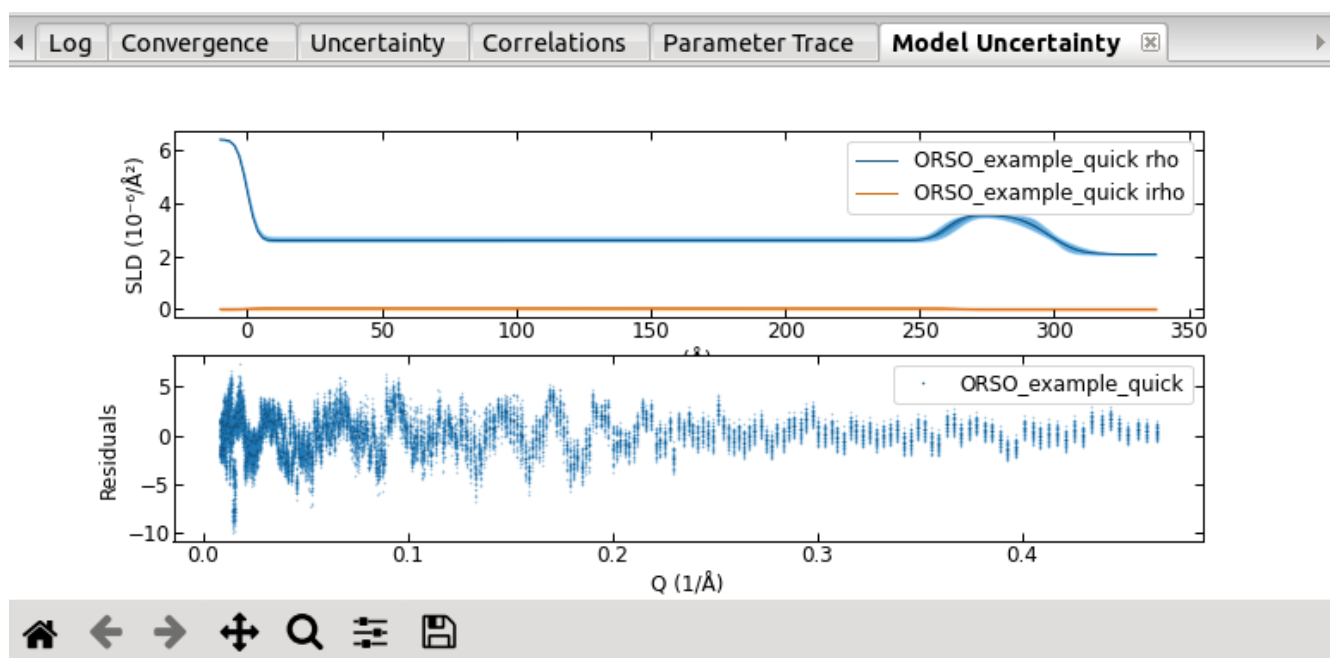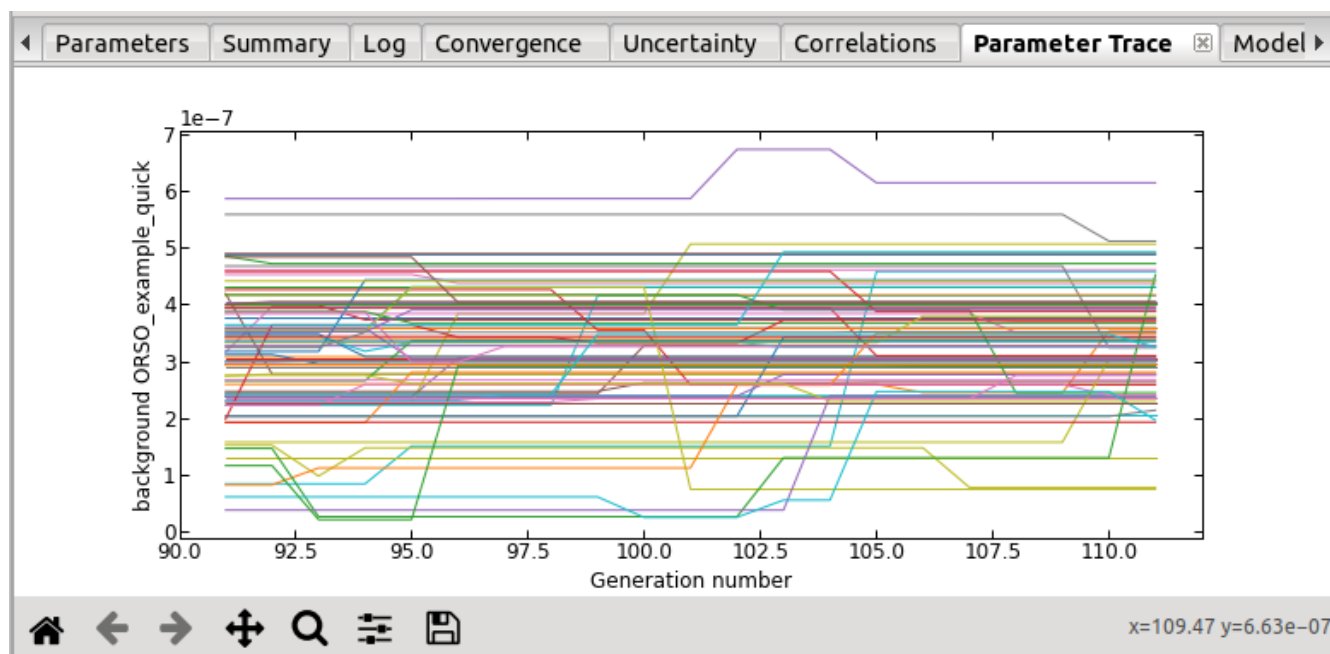
← → C 🔒 pages.nist.gov/reflectometry-calculators/reflectivity-calculator.html ☆ 🗀 ⚙ 👤 ⋮

Load (*.refl) datafile: [Choose Files] ORSO_example_quick.ort [generate Refl1D script] refl1d_script.py [help] [undo]

⦿ reflectivity ○ phase

qmin `0.008060` qmax `0.465555` nPts `251` bkg `3e-7`

○ y-scale: linear ⦿ log

| thickness (Å) | roughness (above, Å) | SLDn (Å⁻²) x10⁻⁶ | iSLDn (Å⁻²) x10⁻⁶ | |
|---|---|---|---|---|
| 0.0000 | 10.000 | 6.3600 | 0.0000 | +after x |
| 279.86 | 12.563 | 2.4447 | 0.0000 | +after x |
| 11.309 | 0.0000 | 5.2945 | 0.0000 | +after x |
| 0.0000 | 0.0000 | 2.0700 | 0.0000 | +after x |

[export table] [import table]

[start fit] log:

```
thickness_3 =    11.3091 +/- 1.66378
thickness_2 =   279.859 +/- 2.02607
roughness_3 =    0.00000 +/- 1.01975e+6
roughness_2 =   12.5633 +/- 1.44124
sld_3 = 5.29455 +/- 0.323862
sld_2 = 2.44465 +/- 0.0350960

reduced chi-squared =   3.50662
iterations =    161
```

R (I/I₀) — Q (Å⁻¹)

theory
data

0.49034, 0.19238

[export calc] [export svg]

SLD (10⁻⁶ A⁻²), θ (π rad) — z (Ångström, from substrate)

[export profile] [export svg]

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⊘ This type of file can harm your computer. Do you want to keep refl1d_script (....py anyway? [Keep] [Discard]

[Show all] ✕