ORSO example fit

We use the anaklasis package to fit the ORSO example data (data file *ORSO_example.ort*) that contains 4-column data (*Q,R,dR,dQ*). The data come from a Neutron Reflectivity measurement of a Si/SiO2/Polymer/D2O system.

we first import *anaklasis.ref*

In [1]:
```
from anaklasis import ref
```

we then name the project, import input data, set *Q* units in Angstrom (as they are in the input file) and also set pointwise resolution since our file contains *dQ* data.

In [2]:
```
project='ORSO_example'
in_file=['ORSO_example.ort']
units=['A'] # Angstrom units
resolution=[-1] # poitwise resolution
```

we then create our model where we assume that the polymer layer has no solvent penetration.

In [3]:
```
model=[
        # Re_sld Im_sld  thk  rough solv description
        [  2.07e-6, 0.0,  0,    'p0', 0.0, 'Si'],
        [  3.47e-6, 0.0, 'p1', 'p2', 0.0, 'SiO2'],
        [   'p3',   0.0, 'p4', 'p5', 0.0, 'Polymer'],
        [  6.35e-6, 0.0,  0,     0,   1.0, 'D2O'],
        ]
```

We have a single model in the system covering uniformly the whole substrate (single patch), so

In [4]:
```
system=[model]
patches=[1.0]
```

we have entered 6 parameters in total in the model. Let's define their bounds together with their descriptions. Note that we consider that all parameters have a uniform probability to assume a value between the declared bounds.

In [5]:
```
global_param = [
    # param  min  max  description    type
        ['p0', 0, 5, 'Si_SiO2_roughness','uniform'],
        ['p1', 0, 100, 'SiO2_thickness','uniform'],
        ['p2', 0, 50, 'SiO2_Polymer_roughness','uniform'],
        ['p3', -0.5e-6, 3.0e-6, 'Polymer_sld','uniform'],
        ['p4', 0, 700, 'Polymer_thickness','uniform'],
        ['p5', 0, 80, 'Polymer_D2O_roughness','uniform'],
        ]
```

although not necesary, we may require that the thickness of the SiO2 and polymer layers stays always larger than their roughness. We can do that using two inequality constraints

In [6]:
```
constraints = ['p1>p2','p4>p5']
```

We have no multi-parameters to declare (they are usually used for multiple contrast refinements), so

In [7]:
```
multi_param = [] # no multi-parameters
```

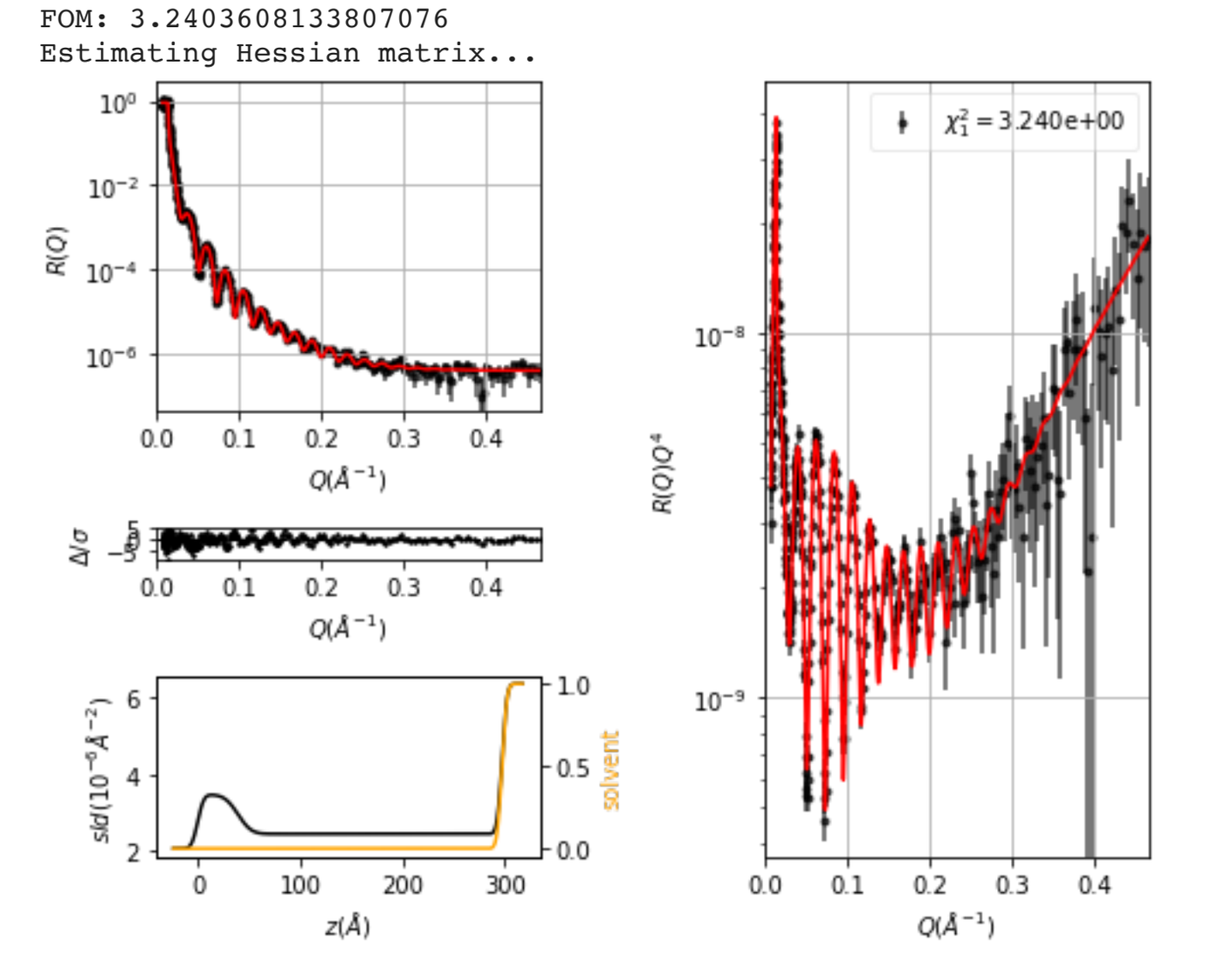
We then leave the scale and the background a bit free to vary during the refinemenet

In [8]:
```
background = [[0.0,1.0e-6,'uniform']]
scale = [[0.9,1.1,'uniform']]
```

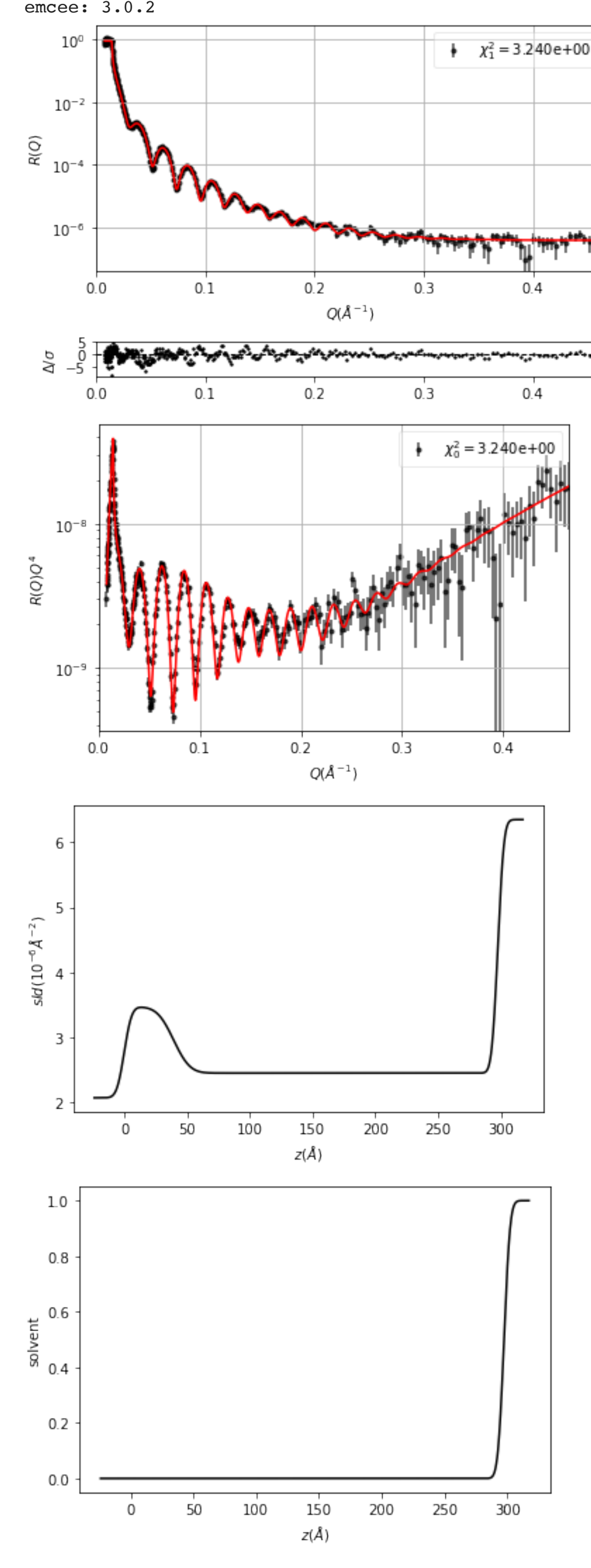
Then we set the fit details and call the *ref.fit* function to perform the data refinement

In [9]:
```
fit_mode=0 # using FOM1
fit_weight=[1]
method = 'simple' # Uncertainty estimated through Hessian matrix

res = ref.fit(project, in_file, units, fit_mode,
fit_weight,method,resolution,patches, system,
global_param,multi_param, constraints,
background,scale,experror=True)
```

```
--------------------------------------------------------------------
Program ANAKLASIS - Fit Module for X-ray/Neutron reflection datasets
version 1.4, June 2021
developed by Dr. Alexandros Koutsioumpas. JCNS @ MLZ
for bugs and requests contact: a.koutsioumpas[at]fz-juelich.de
--------------------------------------------------------------------
Project name: ORSO_example
Using chi squared with errors figure of merit (FOM)
Fast fit mode. Using small differential evolution population size
Parameter uncertainity calculation by Hessian matrix estimation
A plot summarizing results will pop-up after the end of the calculation


Directory already exists.. overwriting data..
file#0 experimental points: 408
Q units in inverse A
dQ/Q pointwise
fit weight:  1
free parameters =  8


list of free parameters: p0 (Si_SiO2_roughness),p1 (SiO2_thickness),p2 (SiO2_Polymer_roughness),p3 (Polymer_sld),p4 (Polymer_thickness),p5 (Polymer_D
2O_roughness),bkg curve#0,scale curve#0,

Running differential evolution minimization...
/n
Success: True
Number of evaluation: 5799
Number of iterations: 50
FOM: 3.2403608133807076
Estimating Hessian matrix...
```



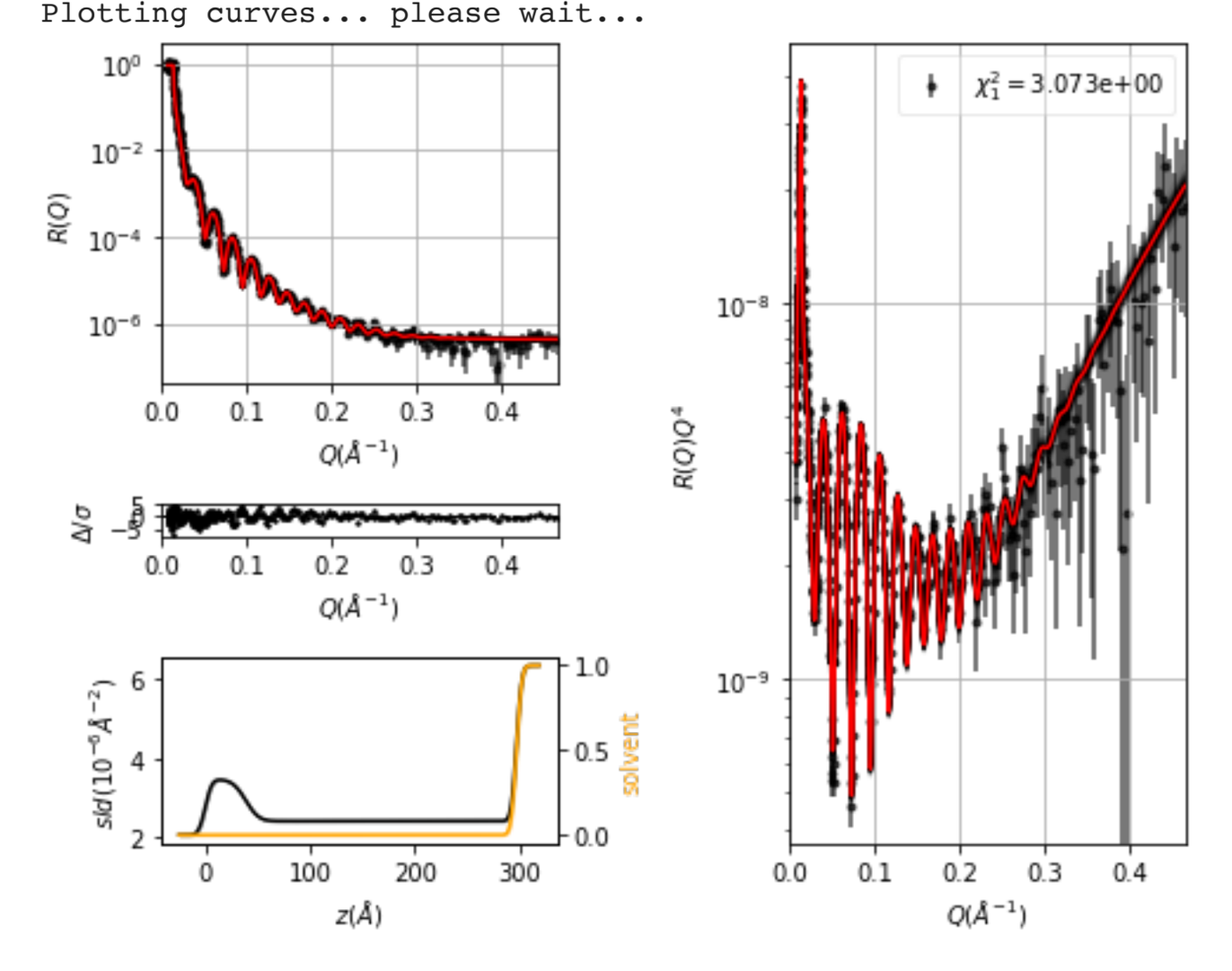

```
--------------------------------------------------------------------
Final model parameters
--------------------------------------------------------------------


Curve #0


Instrumental Resolution, dQ/Q: pointwise
fit weigth: 1
--------------------------------------------------------------------
Si real sld (10^-6 A^-2)      = 2.07 (fixed)
Si imaginary sld (10^-6 A^-2) = 0.00 (fixed)
Si thickness (A)              = 0.00 (fixed)
Si/SiO2 roughness (A) = 4.69 (parametric), -> p0
Si solvent volume fraction    = 0.00 (fixed)
--------------------------------------------------------------------
SiO2 real sld (10^-6 A^-2)      = 3.47 (fixed)
SiO2 imaginary sld (10^-6 A^-2) = 0.00 (fixed)
SiO2 thickness (A)              = 39.30 (parametric), -> p1
SiO2/Polymer roughness (A) = 10.21 (parametric), -> p2
SiO2 solvent volume fraction    = 0.00 (fixed)
--------------------------------------------------------------------
Polymer real sld (10^-6 A^-2)      = 2.45 (parametric), -> p3
Polymer imaginary sld (10^-6 A^-2) = 0.00 (fixed)
Polymer thickness (A)              = 258.18 (parametric), -> p4
Polymer/D2O roughness (A) = 3.79 (parametric), -> p5
Polymer solvent volume fraction    = 0.00 (fixed)
--------------------------------------------------------------------
D2O real sld (10^-6 A^-2)      = 6.35 (fixed)
D2O imaginary sld (10^-6 A^-2) = 0.00 (fixed)
D2O solvent volume fraction    = 1.00 (fixed)
--------------------------------------------------------------------


Background:  = 3.87e-07 ± 3.05e-07, bounds: 0.0 -> 1e-06 (uniform)
Scale:  = 9.04e-01 ± 4.03e-02, bounds: 0.9 -> 1.1 (uniform)


Parameters:

Si_SiO2_roughness: p0 = 4.69e+00 ± 5.65e+00, bounds: 0.0 -> 5.0 (uniform)
SiO2_thickness: p1 = 3.93e+01 ± 2.47e+00, bounds: 0.0 -> 100.0 (uniform)
SiO2_Polymer_roughness: p2 = 1.02e+01 ± 5.36e+00, bounds: 0.0 -> 50.0 (uniform)
Polymer_sld: p3 = 2.45e-06 ± 7.14e-07, bounds: -5e-07 -> 3e-06 (uniform)
Polymer_thickness: p4 = 2.58e+02 ± 1.83e+00, bounds: 0.0 -> 700.0 (uniform)
Polymer_D2O_roughness: p5 = 3.79e+00 ± 1.28e+00, bounds: 0.0 -> 80.0 (uniform)


curve#0 chi^2 = 3.24e+00



Note: reported chi^2 is given by 1/N x sum[((R-R_exp)/sigma_exp)^2]
      where: N is the number of experimental points, sigma_exp the experimental uncertainty
      R and R_exp the theoretical and experimental reflectivity respectively.


Total calculation time (sec):  13

Library versions used for the calculations:
numpy: 1.20.1
scipy: 1.6.0
numdifftools: 0.9.39
sympy: 1.7.1
emcee: 3.0.2
```



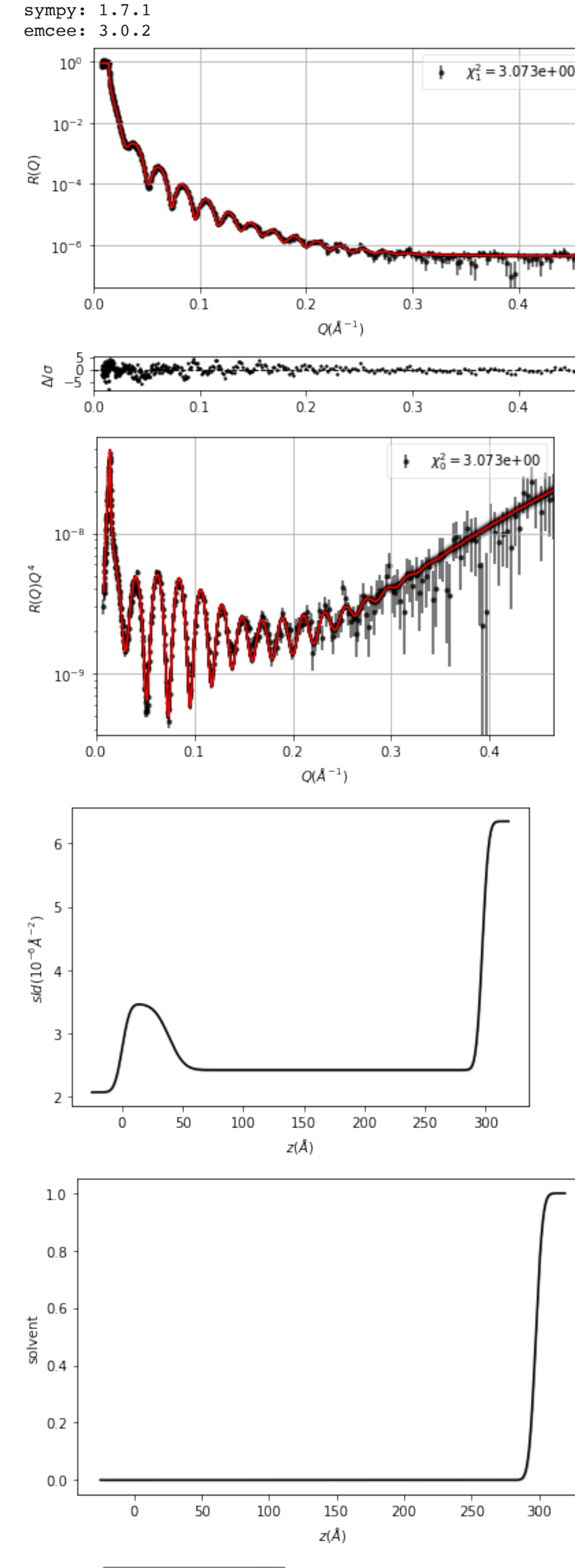
We get a relatively good fit of the data using the declared model. We can go futher and run an MCMC sampling of the system in order to get an even better estimation of parameter correlation and uncertainity comparing to our previous estimation of uncertainity using a Hessian matrix evaluation.

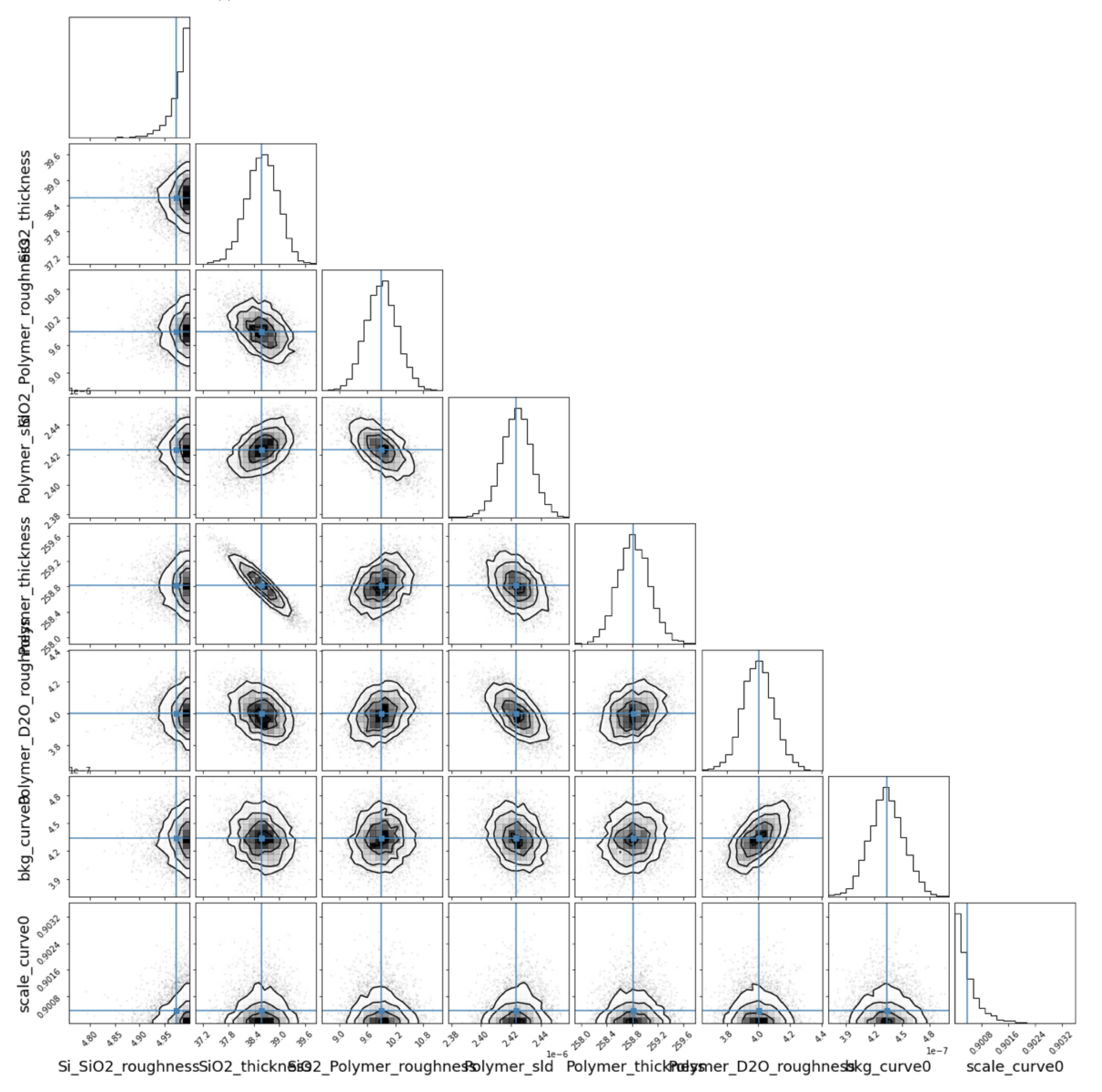
In [10]:
```
fit_mode=0 # using FOM1
fit_weight=[1]
method = 'mcmc' # Markov chain Monte Carlo sampling

res = ref.fit(project, in_file, units, fit_mode,
fit_weight,method,resolution,patches, system,
global_param,multi_param, constraints,
background,scale,experror=True)
```

```
--------------------------------------------------------------------
Program ANAKLASIS - Fit Module for X-ray/Neutron reflection datasets
version 1.4, June 2021
developed by Dr. Alexandros Koutsioumpas. JCNS @ MLZ
for bugs and requests contact: a.koutsioumpas[at]fz-juelich.de
--------------------------------------------------------------------
Project name: ORSO_example
Using chi squared with errors figure of merit (FOM)
Fast fit mode. Using small differential evolution population size
Parameter uncertainity calculation using Markov Chain Monte Carlo
A plot summarizing results will pop-up after the end of the calculation


Directory already exists.. overwriting data..
file#0 experimental points: 408
Q units in inverse A
dQ/Q pointwise
fit weight:  1
free parameters =  8


list of free parameters: p0 (Si_SiO2_roughness),p1 (SiO2_thickness),p2 (SiO2_Polymer_roughness),p3 (Polymer_sld),p4 (Polymer_thickness),p5 (Polymer_D
2O_roughness),bkg curve#0,scale curve#0,

Running differential evolution minimization...
/n
Success: True
Number of evaluation: 7367
Number of iterations: 64
FOM: 3.305833342758203
Running Markov Chain Monte Carlo sampling...
Initializing MCMC walkers..
MCMC test run..
100%|██████████| 500/500 [00:21<00:00, 23.06it/s]
WARNING:root:The chain is shorter than 50 times the integrated autocorrelation time for 8 parameter(s). Use this estimate with caution and run a long
er chain!
N/50 = 10;
tau: [51.139 34.231 64.271 64.022 32.202 65.341 68.163 55.276]
  0%|          | 3/4080 [00:00<03:11, 21.25it/s]
MCMC production run..
100%|██████████| 4080/4080 [02:49<00:00, 24.03it/s]
Calculating mean curves...
  0%|          | 0/139 [00:00<?, ?it/s]

100%|██████████| 139/139 [00:21<00:00,  6.53it/s]
Plotting curves... please wait...
```




```
--------------------------------------------------------------------
Final model parameters
--------------------------------------------------------------------


Curve #0


Instrumental Resolution, dQ/Q: pointwise
fit weigth: 1
--------------------------------------------------------------------
Si real sld (10^-6 A^-2)      = 2.07 (fixed)
Si imaginary sld (10^-6 A^-2) = 0.00 (fixed)
Si thickness (A)              = 0.00 (fixed)
Si/SiO2 roughness (A) = 5.00 (parametric), -> p0
Si solvent volume fraction    = 0.00 (fixed)
--------------------------------------------------------------------
SiO2 real sld (10^-6 A^-2)      = 3.47 (fixed)
SiO2 imaginary sld (10^-6 A^-2) = 0.00 (fixed)
SiO2 thickness (A)              = 38.12 (parametric), -> p1
SiO2/Polymer roughness (A) = 8.41 (parametric), -> p2
SiO2 solvent volume fraction    = 0.00 (fixed)
--------------------------------------------------------------------
Polymer real sld (10^-6 A^-2)      = 2.47 (parametric), -> p3
Polymer imaginary sld (10^-6 A^-2) = 0.00 (fixed)
Polymer thickness (A)              = 259.67 (parametric), -> p4
Polymer/D2O roughness (A) = 3.39 (parametric), -> p5
Polymer solvent volume fraction    = 0.00 (fixed)
--------------------------------------------------------------------
D2O real sld (10^-6 A^-2)      = 6.35 (fixed)
D2O imaginary sld (10^-6 A^-2) = 0.00 (fixed)
D2O solvent volume fraction    = 1.00 (fixed)
--------------------------------------------------------------------


Background:  = 4.33e-07 ± 1.95e-08, bounds: 0.0 -> 1e-06 (uniform)
Scale:  = 9.00e-01 ± 3.70e-04, bounds: 0.9 -> 1.1 (uniform)


Parameters:

Si_SiO2_roughness: p0 = 5.00e+00 ± 2.56e-02, bounds: 0.0 -> 5.0 (uniform)
SiO2_thickness: p1 = 3.81e+01 ± 3.62e-01, bounds: 0.0 -> 100.0 (uniform)
SiO2_Polymer_roughness: p2 = 8.41e+00 ± 3.41e-01, bounds: 0.0 -> 50.0 (uniform)
Polymer_sld: p3 = 2.47e-06 ± 9.54e-09, bounds: -5e-07 -> 3e-06 (uniform)
Polymer_thickness: p4 = 2.60e+02 ± 2.47e-01, bounds: 0.0 -> 700.0 (uniform)
Polymer_D2O_roughness: p5 = 3.39e+00 ± 9.31e-02, bounds: 0.0 -> 80.0 (uniform)


curve#0 chi^2 = 3.07e+00



Note: reported chi^2 is given by 1/N x sum[((R-R_exp)/sigma_exp)^2]
      where: N is the number of experimental points, sigma_exp the experimental uncertainty
      R and R_exp the theoretical and experimental reflectivity respectively.


Total calculation time (sec):  227

Library versions used for the calculations:
numpy: 1.20.1
scipy: 1.6.0
numdifftools: 0.9.39
sympy: 1.7.1
emcee: 3.0.2
```





As you may see almost all parameters of the model are not correlated, with the small exception of the SiO2 thickness and Polymer thickness where a moderate covariance is observed.