Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Small Angle X-ray Studies of Short-Range Order in Non-Stoichiometric Pseudoprotic Ionic Liquids: The Influence of Chemical Structure

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## Contents

## S.1: Fitting Procedure for SAXS Data

Here, we report the fitting procedure used to determine peak values presented in the report.

For each dataset, the SAXS signal *S(q)* was fitted to a function consisting of a linear baseline and a sum of five Lorentzian functions:

$$S(q) = a + bq + \sum_{i=1}^{5} \frac{A_i}{(q - q_{0i})^2 + w_i^2} \qquad \text{(S1)}$$

The wavenumber q was expressed in units of $Å^{-1}$. For each dataset, the function was fit using Mathematica 13.0 to implement the above function.

As noted in the text, with few exceptions the local structure peak was well-described either as a single, isolated peak or, where noted, as a pair of peaks consisting of one prominent peak and a low, broad peak at a slightly higher q value. The use of a larger number of Lorentzian functions was driven by the relatively complex structures at high (q>1.0 $Å^{-1}$) wavenumber, and in some cases he presence of a shoulder at low (q<0.2 $Å^{-1}$) q values.

<u>For each mixture, we report:</u>

- A table showing the peak center and width for the local structure
- A complete table of all fitted parameters
- A figure showing the experimental data and fitted function on the same plot (only 1/5$^{th}$ of datapoints are shown)
- A series of plots showing the fitted functions and their residuals

For convenience, we reproduce here Table 1 from the report so that mixtures can be clearly identified.

Table S.1: Notation used in the present study

| **Amines** | | **Acids** | |
|---|---|---|---|
| T2A | Triethylamine | C2A | Acetic acid |
| T6A | Trihexylamine | C6A | Hexanoic acid |
| T8A | Trioctylamine | C8A | Octanoic acid |
| M18A | Octadecylamine | C10A | Decanoic acid |
| D2A | Diethylamine | HBz | Benzoic acid |
| T2OH | Triethanolamine | HSa | Salicylic acid |
| HCyc | Cyclohexanecarboxylic acid | | |
| $\chi$ | Mole fraction of acid in the mixture | | |

## S.2 Fitting Information for Mixtures Presented in Figure 1

**T2A C6A**

### Table S.2: Local Structure Peaks for T2A C6A

| | T2AC6A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | 0 | 0 |
| chi=33 | 0 | 0 |
| chi=50 | 0.348931 | 0.228823 |
| chi=67 | 0.420729 | 0.153419 |
| chi=75 | 0.419965 | 0.128399 |
| chi=83 | 0.418243 | 0.142661 |
| chi=100 | 0.473993 | 0.192415 |

### Table S.3: Fitting Parameters for T2A C6A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.988 | 0.00827 | 0.0573 | 0.366 | 0.0146 | 1.12 | 0.203 | 0.0247 | 1.27 | 0.265 | 0.0153 | 1.62 | 0.398 | 0.0441 | 2.37 | 0.392 | 0.0107 |
| 2.01 | 0.00964 | 0.161 | 0.36 | 0.0322 | 1.12 | 0.139 | 0.00109 | 1.19 | 0.257 | 0.0349 | 1.51 | 0.431 | 0.0735 | 2.48 | 0.499 | 0.0212 |
| 3.05 | -0.00996 | 0.349 | 0.229 | 0.0101 | 1.2 | 0.188 | 0.0082 | 1.4 | 0.5 | 0.116 | 1.44 | 0.379 | 0.0341 | 2.4 | 0.392 | 0.0142 |
| 3.97 | 0.00609 | 0.421 | 0.153 | 0.00673 | 0.703 | 0.173 | 0.00219 | 0.885 | 0.391 | $7.29*10^{-7}$ | 1.41 | 0.403 | 0.143 | 2.35 | 0.5 | 0.0354 |
| 4.98 | 0.01 | 0.42 | 0.128 | 0.00507 | 0.69 | 0.273 | 0.00882 | 1.44 | 0.354 | 0.105 | 1.23 | 0.104 | 0.000326 | 2.31 | 0.5 | 0.0367 |
| 5.97 | -0.00992 | 0.418 | 0.143 | 0.00667 | 1.44 | 0.324 | 0.0919 | 2.45 | 0.452 | 0.0343 | 2 | 0.342 | 0.00756 | 0.693 | 0.253 | 0.00775 |
| 7.01 | -0.0097 | 0.636 | 0.254 | 0.00674 | 1.43 | 0.258 | 0.0544 | 2.42 | 0.499 | 0.0354 | 1.8 | 0.498 | 0.0148 | 0.474 | 0.192 | 0.00688 |

Figure S.1: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T2A C6A

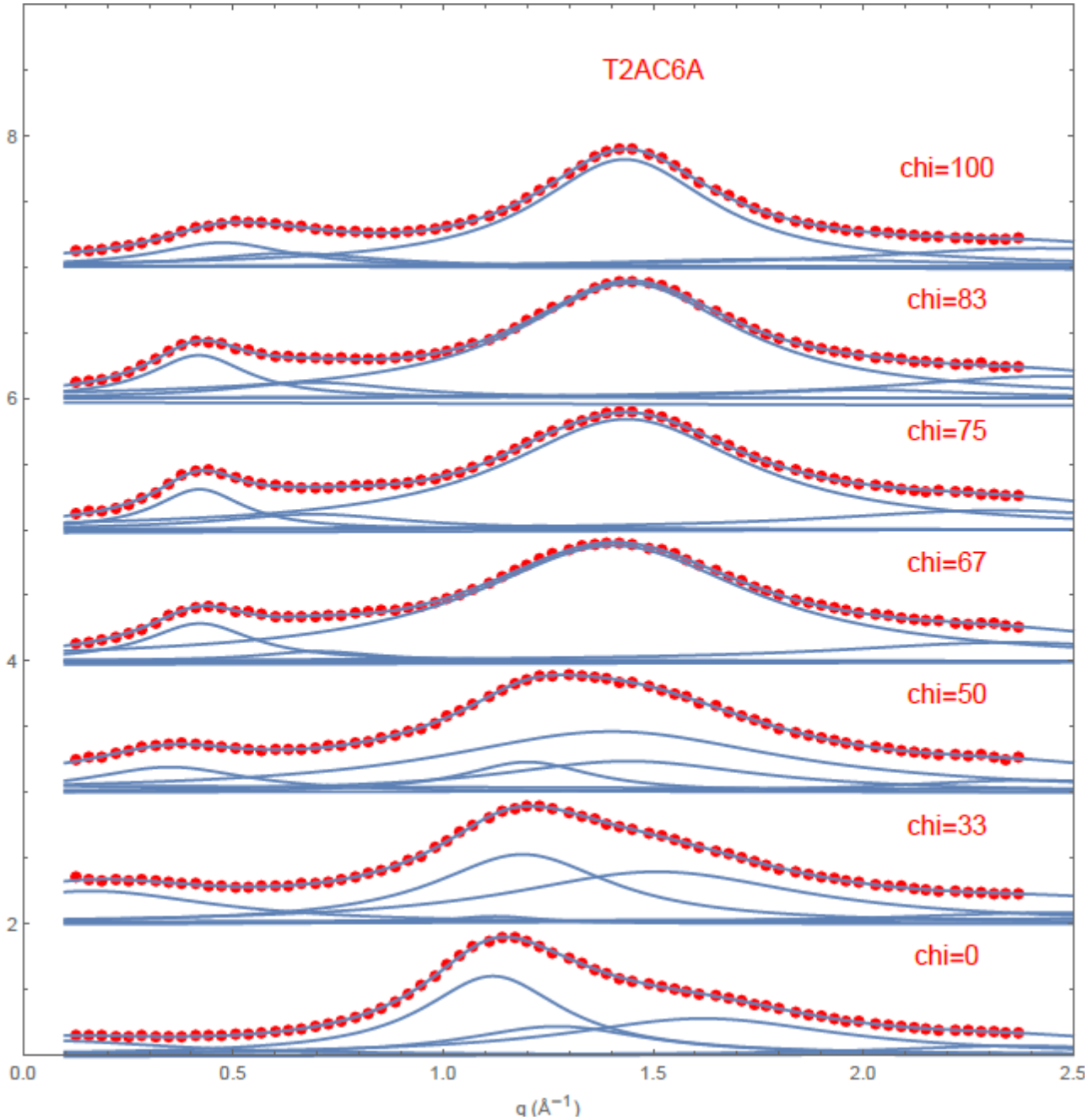
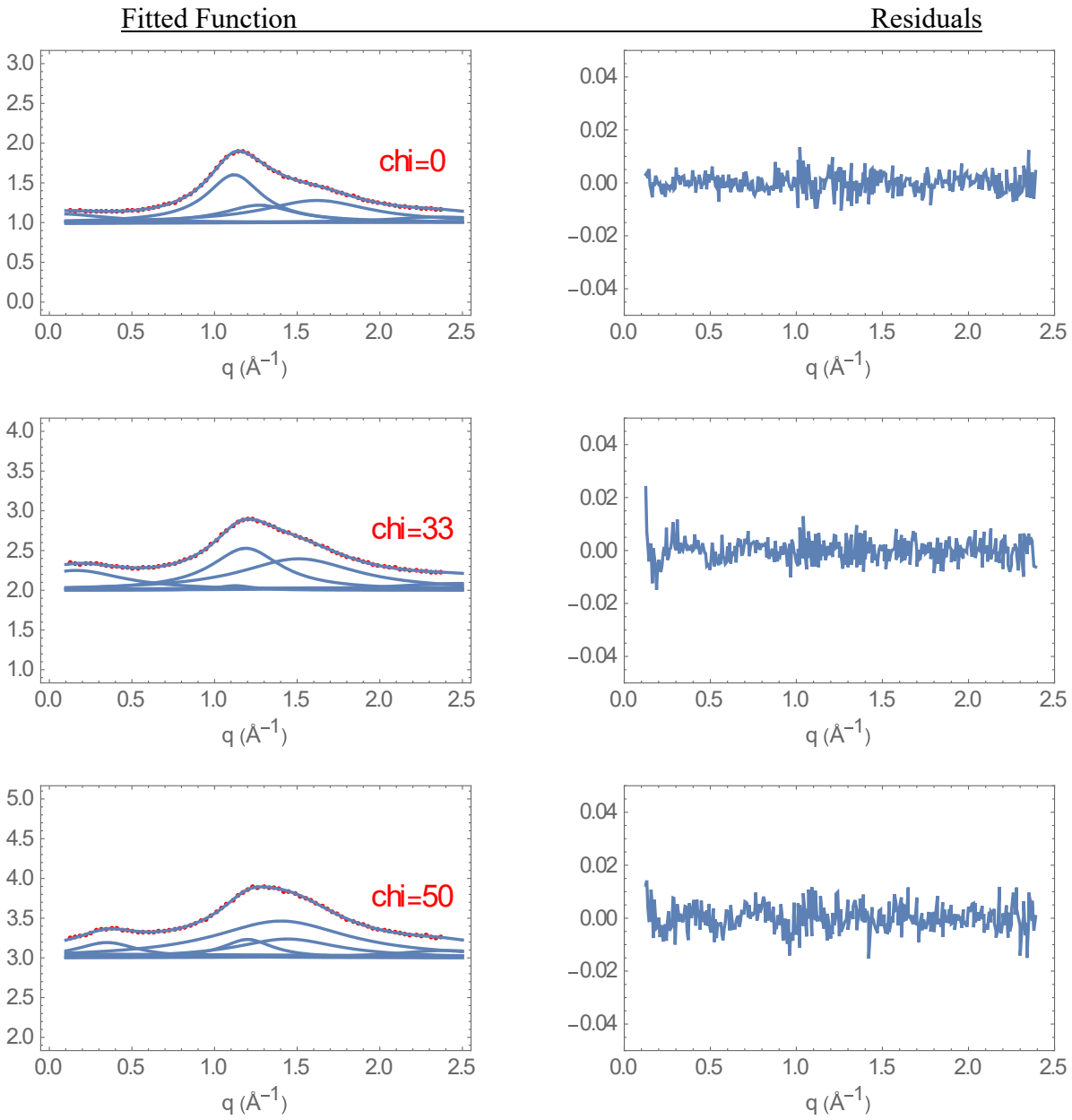
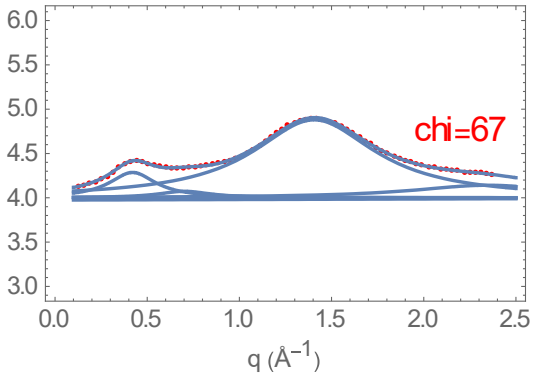
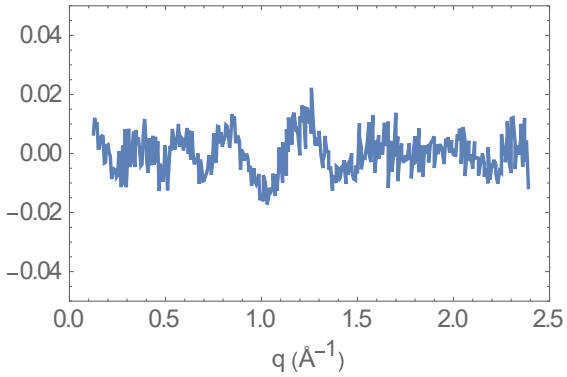
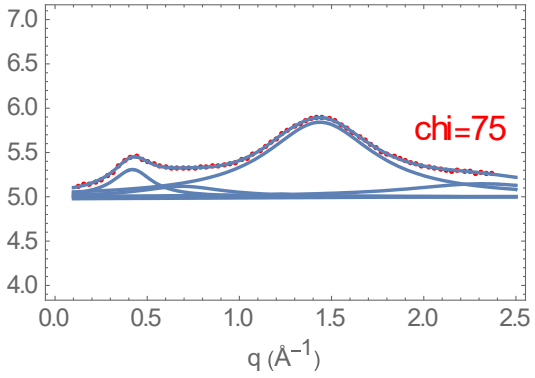


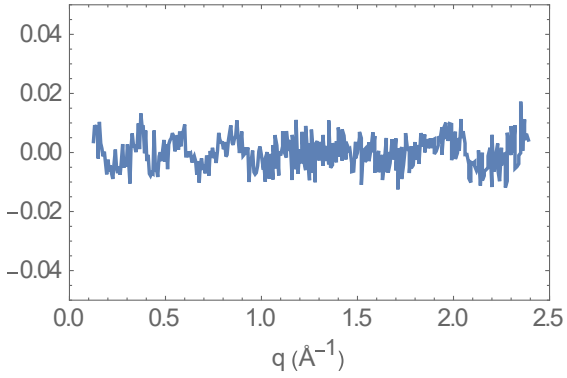
Figure S.2: Fitting functions and residuals for T2A C6A

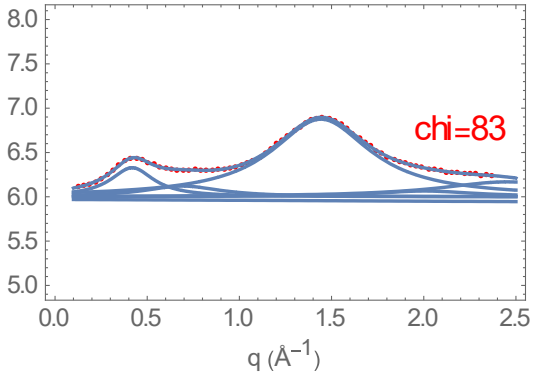


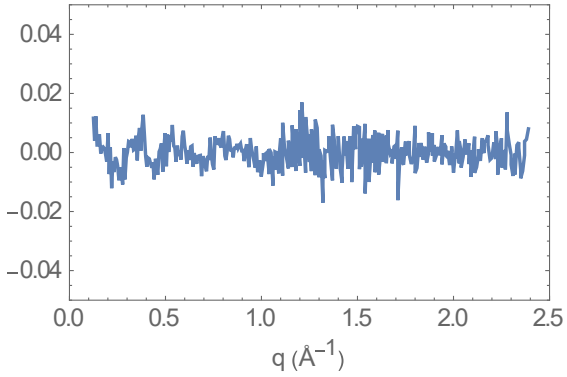

chi=67
q (Å$^{-1}$)

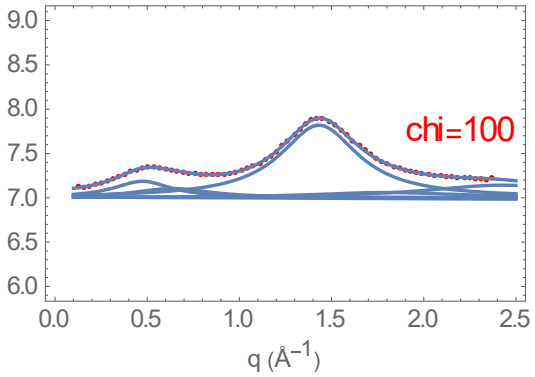

q (Å$^{-1}$)

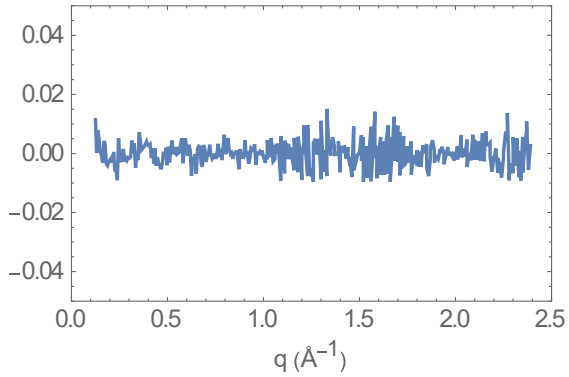

chi=75
q (Å$^{-1}$)


q (Å$^{-1}$)


chi=83
q (Å$^{-1}$)


q (Å$^{-1}$)


chi=100
9.0
8.5
8.0
7.5
7.0
6.5
6.0
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)

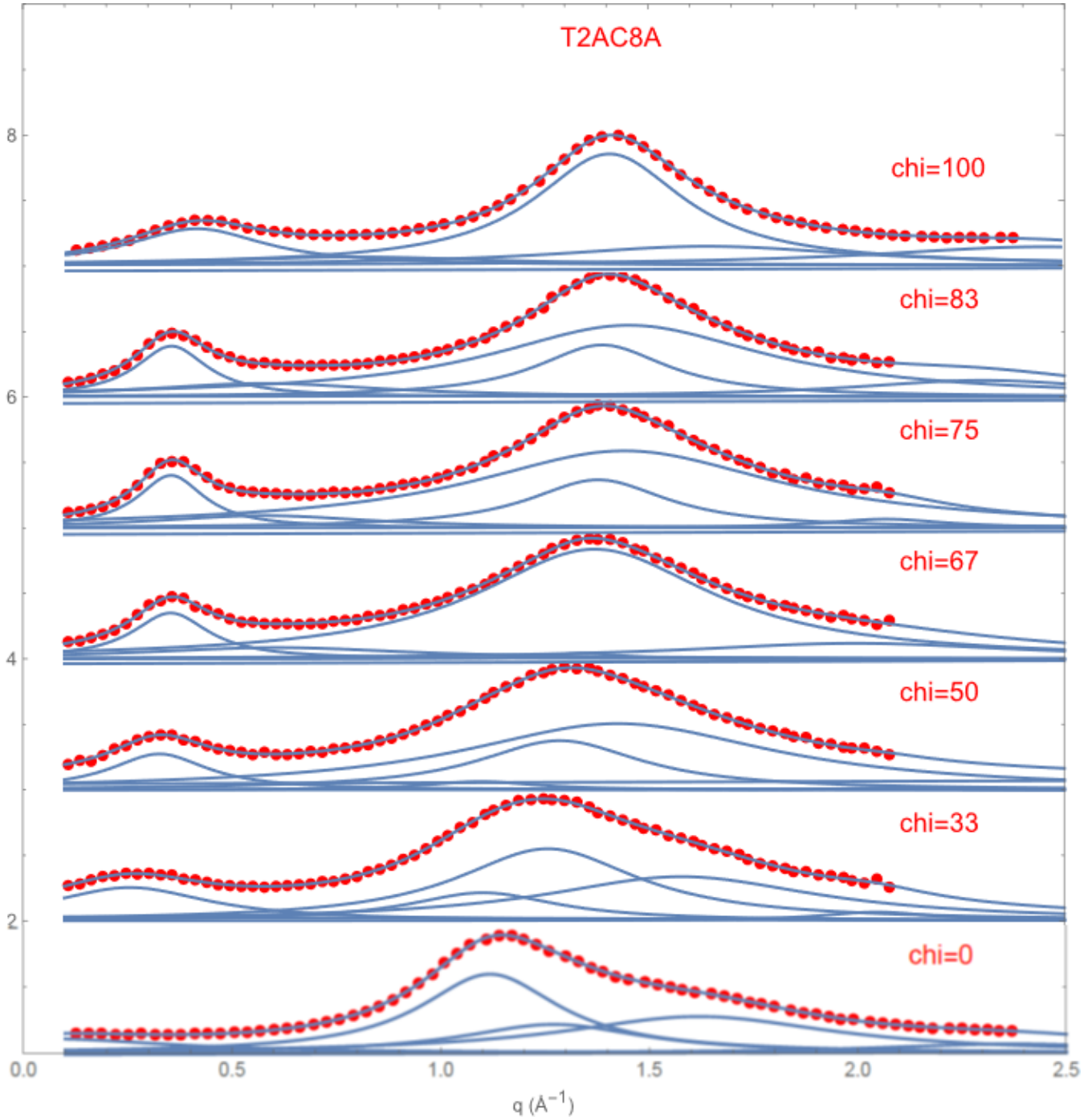
## Table S.4: Local Structure Peaks for T2A C8A

| | T2AC8A | | |
|---|---|---|---|
| | q (Å^-1) | w (Å^-1) | D (A) |
| chi=0 | 0 | 0 | |
| chi=33 | 0.256844 | 0.232381 | 24.46302 |
| chi=50 | 0.327406 | 0.143057 | 19.19079 |
| chi=67 | 0.354867 | 0.111448 | 17.70573 |
| chi=75 | 0.355721 | 0.097582 | 17.66322 |
| chi=83 | 0.356954 | 0.105052 | 17.60221 |
| chi=100 | 0.41763 | 0.185602 | 15.04485 |

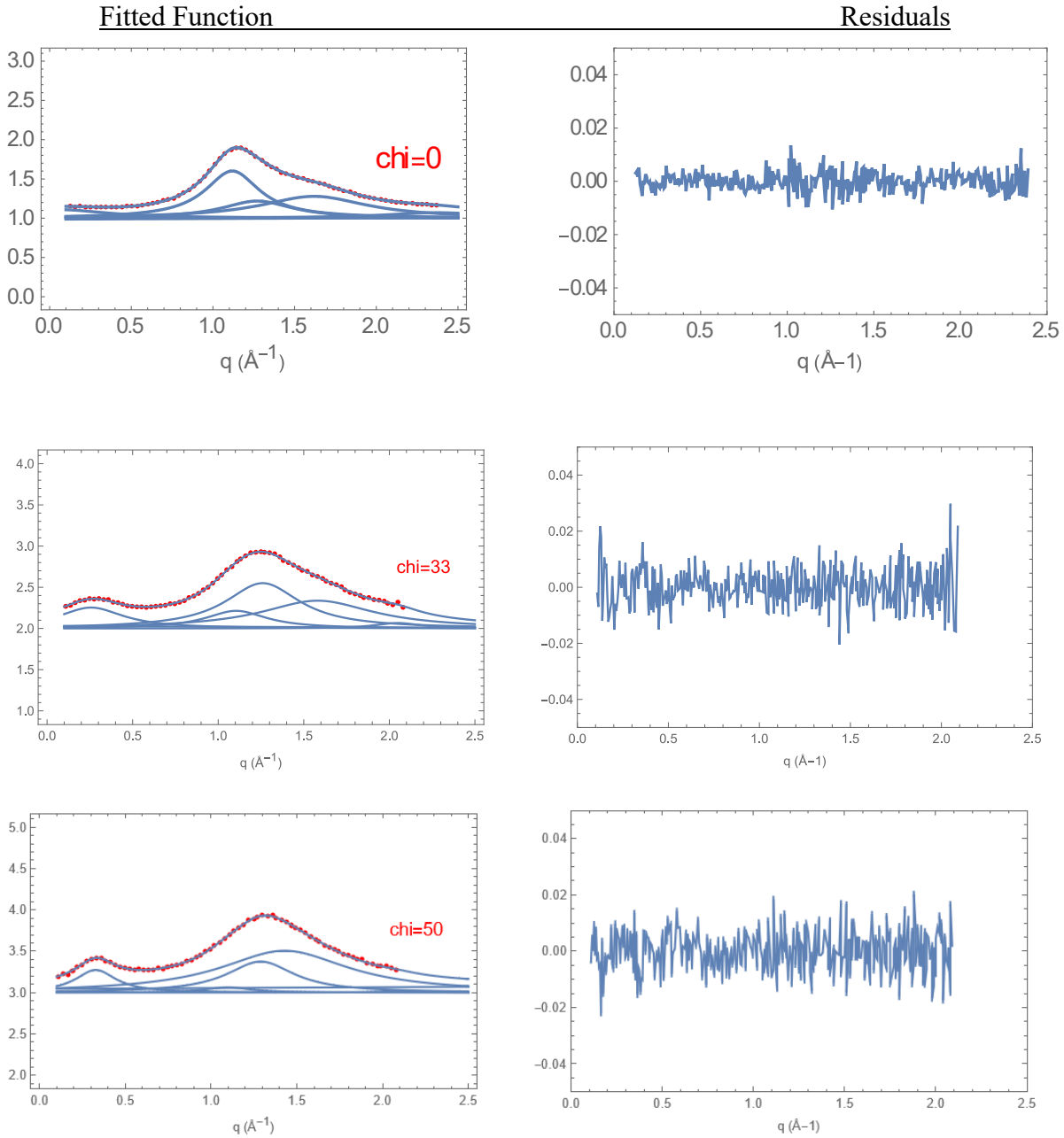
## Table S.5: Fitting Parameters for T2A C8A

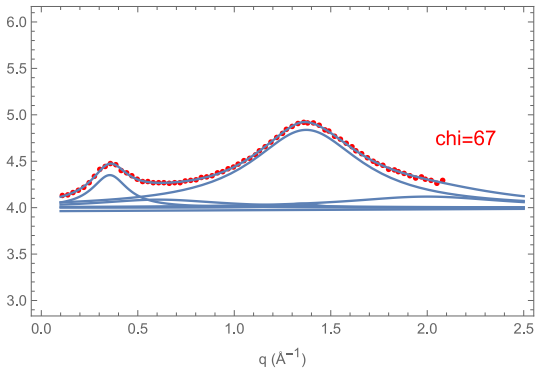
| a | b | q01 | w1 | A1 | q02 | w2 | A2 | q03 | w3 | A3 | q04 | w4 | A4 | q05 | w5 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.988 | 0.00827 | 0.0573 | 0.366 | 0.0146 | 1.12 | 0.203 | 0.0247 | 1.27 | 0.265 | 0.0153 | 1.62 | 0.398 | 0.0441 | 2.37 | 0.3 |
| 2.03 | -0.00957 | 0.257 | 0.232 | 0.0137 | 1.1 | 0.218 | 0.0102 | 1.26 | 0.266 | 0.0388 | 1.58 | 0.399 | 0.0536 | 2.05 | 0.1 |
| 3.04 | 0.00999 | 0.327 | 0.143 | 0.0056 | 1.1 | 0.161 | 0.00163 | 1.43 | 0.454 | 0.104 | 1.29 | 0.239 | 0.0215 | 2.08 | 0. |
| 3.96 | 0.00999 | 0.355 | 0.111 | 0.00435 | 0.61 | 0.396 | 0.0135 | 1.37 | 0.345 | 0.0999 | 1.35 | 0.102 | 0.000446 | 2 | 0 |
| 4.95 | 0.00998 | 0.356 | 0.0976 | 0.00382 | 0.579 | 0.321 | 0.00967 | 1.44 | 0.453 | 0.121 | 1.38 | 0.204 | 0.0153 | 2.07 | 0.1 |
| 5.95 | 0.00998 | 0.357 | 0.105 | 0.00429 | 0.58 | 0.354 | 0.013 | 1.45 | 0.404 | 0.0894 | 1.39 | 0.192 | 0.0147 | 2.31 | 0.3 |
| 6.96 | 0.00948 | 0.418 | 0.186 | 0.0079 | 0.674 | 0.466 | 0.0146 | 2.46 | 0.498 | 0.0303 | 1.41 | 0.218 | 0.0351 | 1.59 | 0.4 |

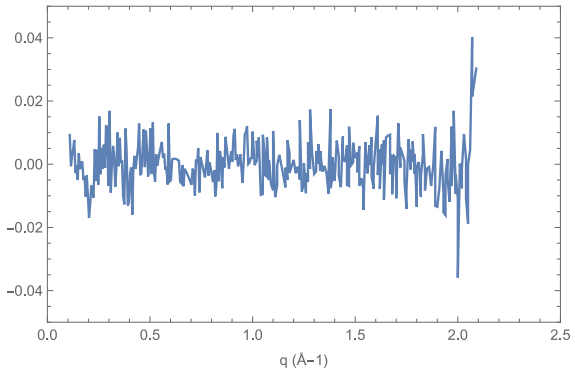
Figure S.3: Fitting functions (blue) and raw data (red, 1/5th of points shown) for T2A C8A

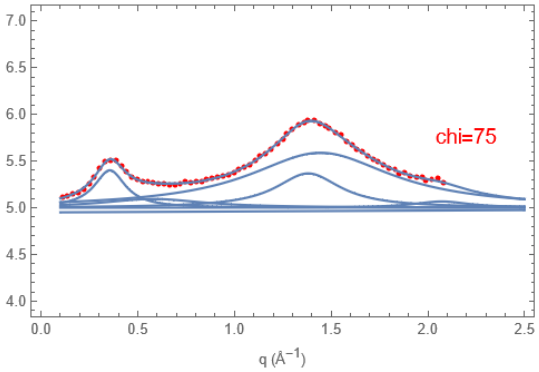


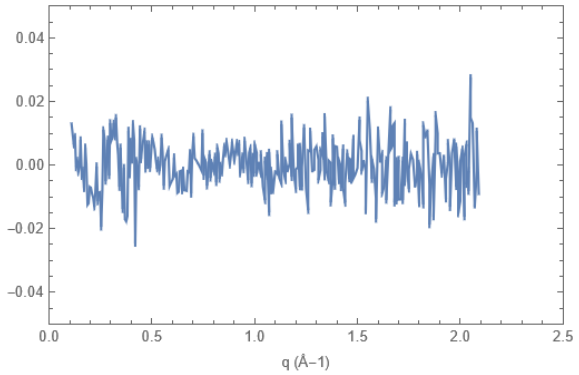
## Figure S.4: Fitting functions and residuals for T2A C8A

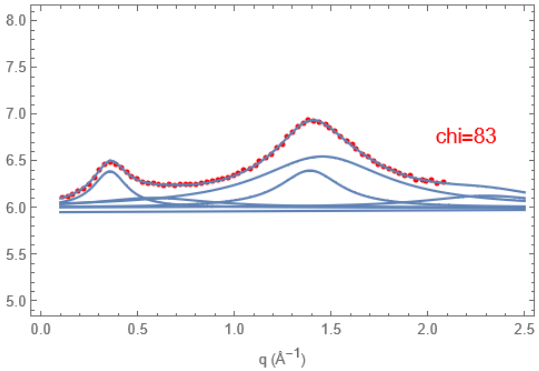


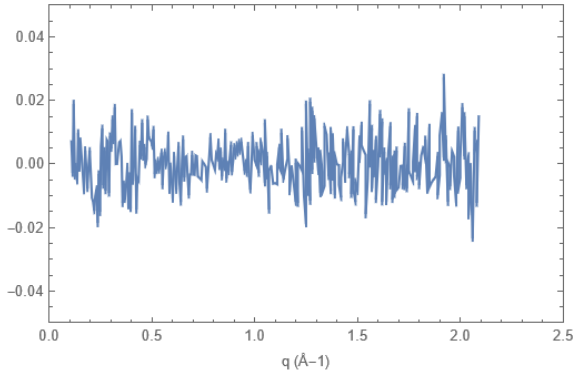

chi=67
q (Å$^{-1}$)


q (Å−1)


chi=75
q (Å$^{-1}$)


q (Å−1)


chi=83
q (Å$^{-1}$)


q (Å−1)

**T2A C10A**

## Table S.6: Local Structure Peaks for T2A C10A

| | T2AC10A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | 0 | 0 |
| chi=33 | 0.263093 | 0.156395 |
| chi=50 | 0.298087 | 0.121944 |
| chi=67 | 0.316413 | 0.100748 |
| chi=75 | 0.319659 | 0.090357 |
| chi=83 | 0.316748 | 0.091768 |

## Table S.7: Fitting Parameters for T2A C10A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.988 | 0.00827 | 0.0573 | 0.366 | 0.0146 | 1.12 | 0.203 | 0.0247 | 1.27 | 0.265 | 0.0153 | 1.62 | 0.398 | 0.0441 | 2.37 | 0.392 | 0.0107 |
| 2.03 | -0.0099 | 0.263 | 0.156 | 0.00671 | 1.25 | 0.299 | 0.0601 | 1.54 | 0.331 | 0.0328 | 1.96 | 0.4 | 0.0119 | 2.4 | 0.3 | 0.0087 |
| 3.05 | 0.01 | 0.298 | 0.122 | 0.00419 | 1.29 | 0.3 | 0.0535 | 1.49 | 0.3 | 0.0258 | 1.8 | 0.3 | 0.00471 | 2.31 | 0.3 | 0.00538 |
| 3.95 | 0.00999 | 0.316 | 0.101 | 0.00398 | 1.38 | 0.281 | 0.0582 | 1.6 | 0.497 | 0.0388 | 0.763 | 0.48 | 0.0226 | 2.4 | 0.5 | 0.0314 |
| 4.95 | 0.00999 | 0.32 | 0.0904 | 0.00365 | 1.4 | 0.272 | 0.0608 | 1.85 | 0.5 | 0.027 | 0.731 | 0.471 | 0.0243 | 2.4 | 0.35 | 0.0128 |
| 5.95 | 0.00998 | 0.317 | 0.0918 | 0.00372 | 1.4 | 0.234 | 0.0391 | 2.36 | 0.5 | 0.0293 | 1.52 | 0.5 | 0.0453 | 0.645 | 0.438 | 0.0181 |

Figure S.5: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T2A C10A

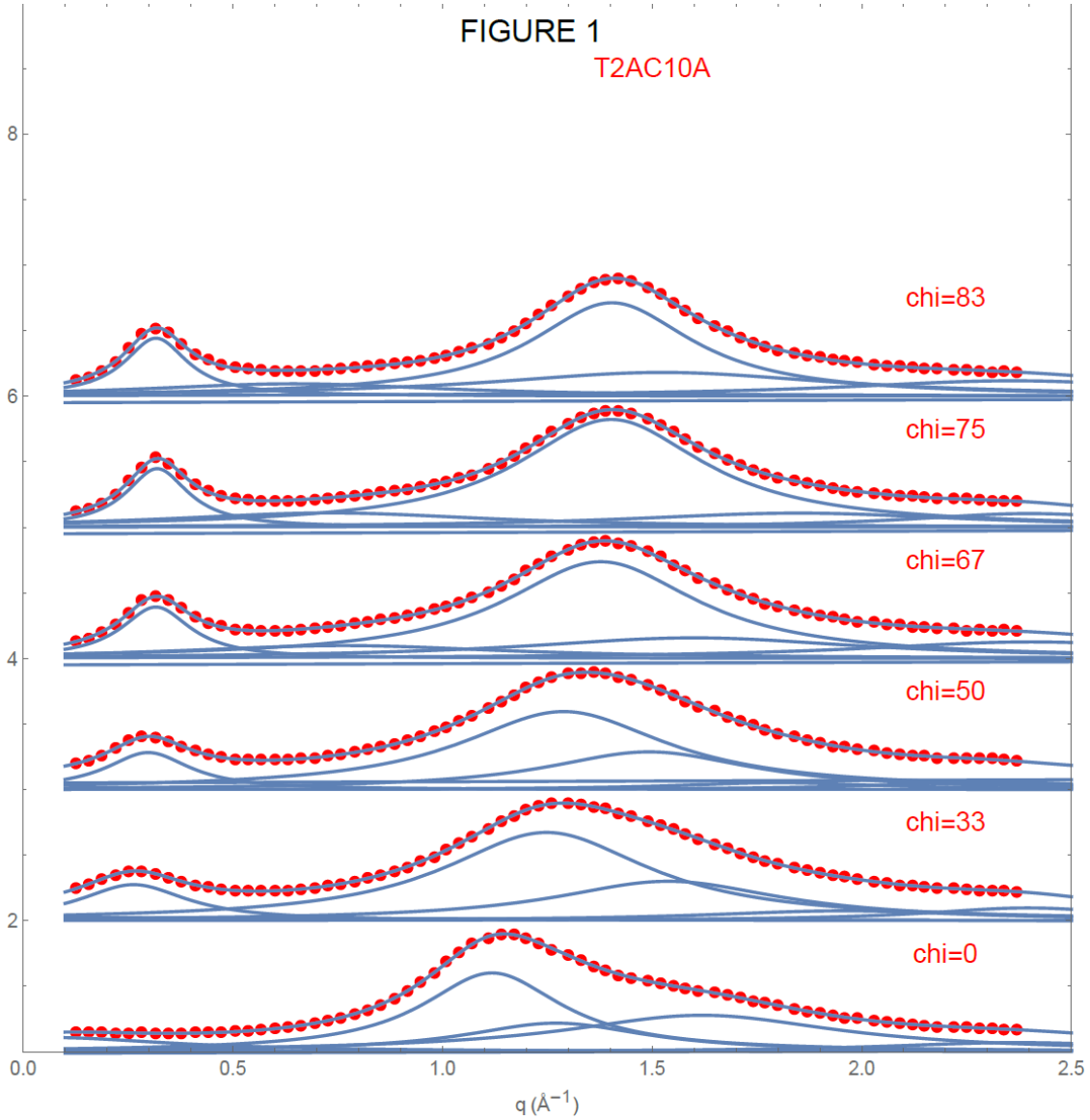
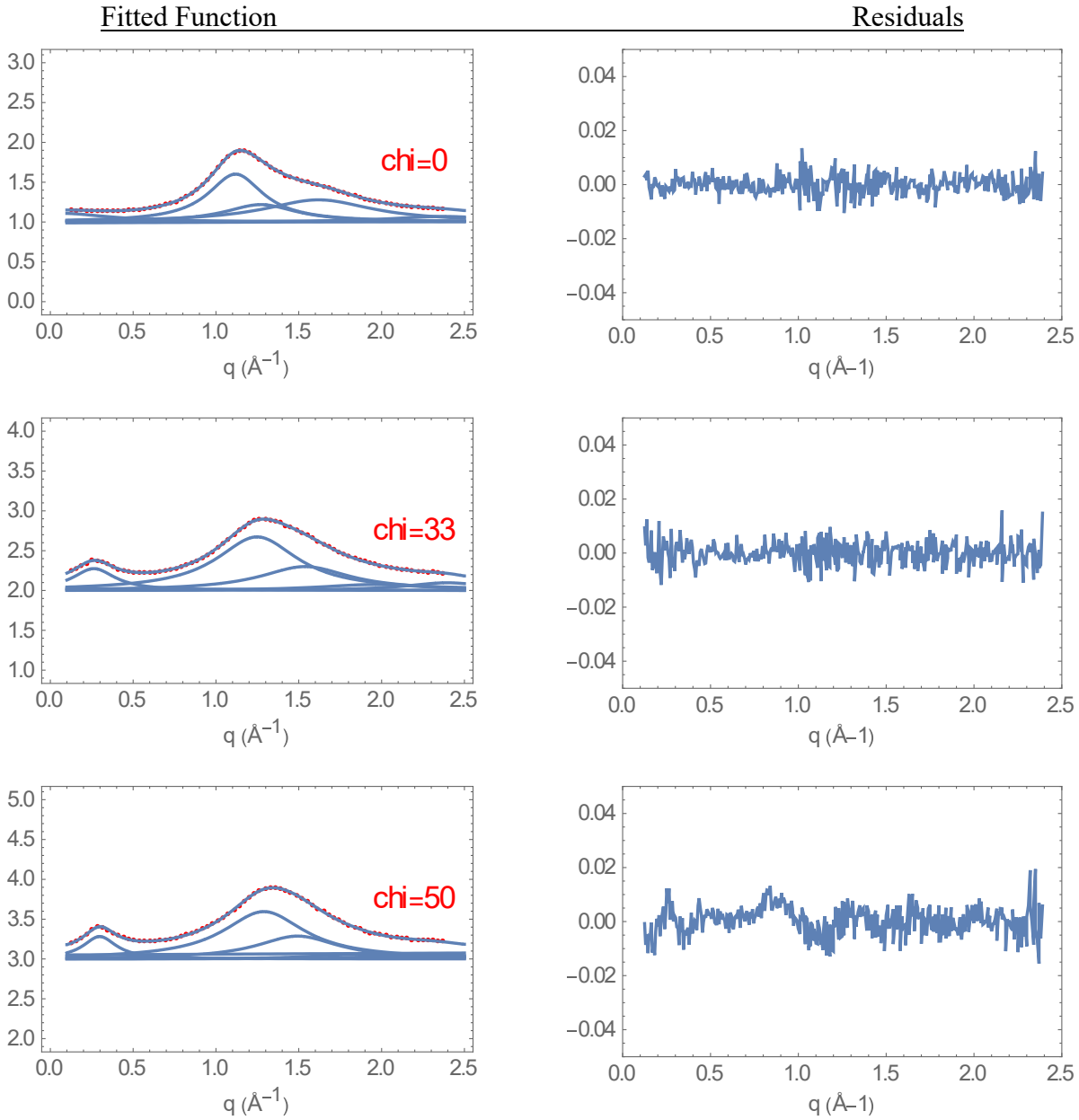
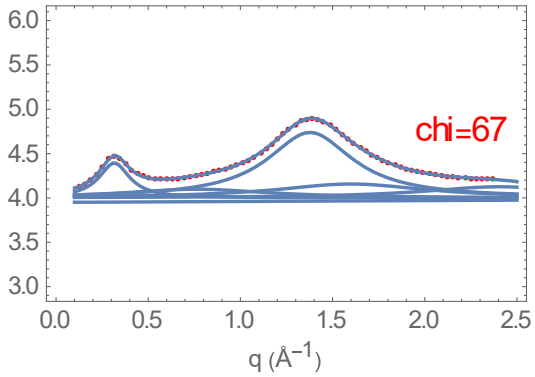
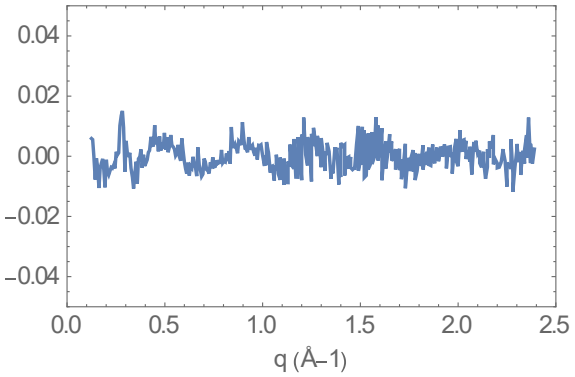
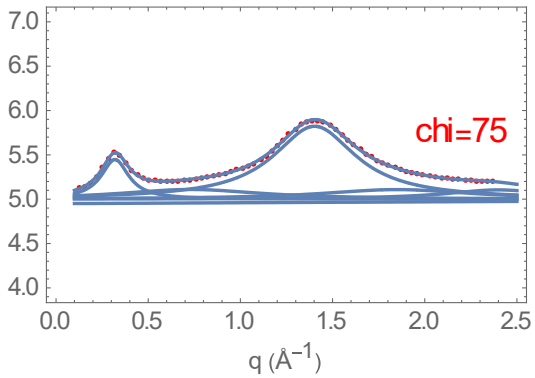


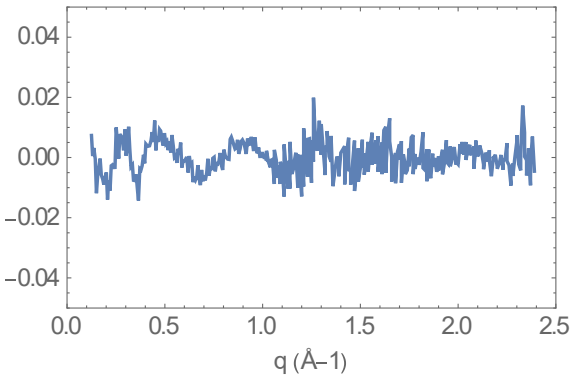
Figure S.6: Fitting functions and residuals for T2A C10A

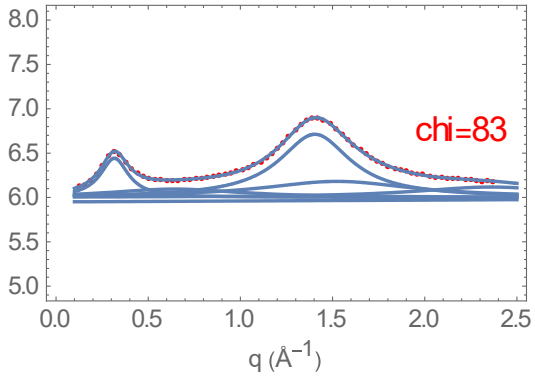


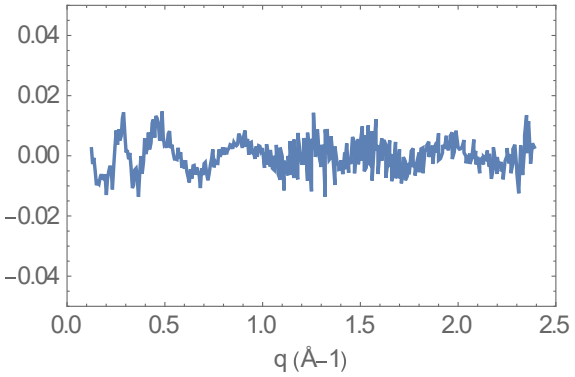

chi=67
q (Å$^{-1}$)


q (Å–1)


chi=75
q (Å$^{-1}$)


q (Å–1)


chi=83
q (Å$^{-1}$)


q (Å–1)

## Table S.8: Local Structure Peaks for T6A C2A

| | T6AC2A | | |
|---|---|---|---|
| | q (Å^-1) | w (Å^-1) | |
| chi=0 | 0.613009 | 0.260993 | |
| chi=33 | 0.573249 | 0.220682 | |
| chi=50 | 0.555645 | 0.200813 | |
| chi=67 | 0.543551 | 0.169751 | 11.5595 |
| chi=75 | 0.523333 | 0.10412 | 12.00608 |
| chi=83 | 0.526188 | 0.108116 | |
| chi=100 | | | |

## Table S.9: Fitting Parameters for T6A C2A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.01 | 0.00886 | 0.142 | 0.0693 | 8.99E-05 | 0.613 | 0.261 | 0.00948 | 1.35 | 0.2 | 0.0187 | 1.42 | 0.312 | 0.0385 | 2.41 | 0.387 | 0.0076 |
| 2.03 | 0.00876 | 0.0679 | 0.088 | 0.00153 | 0.573 | 0.221 | 0.00932 | 1.37 | 0.217 | 0.0234 | 1.47 | 0.293 | 0.0308 | 2.48 | 0.485 | 0.0126 |
| 3.03 | 0.00998 | 0.0788 | 0.0886 | 0.00174 | 0.556 | 0.201 | 0.00985 | 1.38 | 0.22 | 0.0215 | 1.48 | 0.294 | 0.0354 | 2.38 | 0.5 | 0.0141 |
| 4.01 | 0.00987 | 0.544 | 0.17 | 0.0111 | 0.143 | 0.0856 | 0.000399 | 1.45 | 0.262 | 0.0566 | 1.95 | 0.498 | 0.0119 | 2.58 | 0.495 | 0.0185 |
| 5.02 | 0.00998 | 0.523 | 0.104 | 0.00294 | 0.598 | 0.149 | 0.00455 | 1.47 | 0.246 | 0.0455 | 1.6 | 0.5 | 0.022 | 2.39 | 0.5 | 0.0185 |
| 6.03 | 0.0099 | 0.526 | 0.108 | 0.00201 | 0.599 | 0.151 | 0.00505 | 1.49 | 0.234 | 0.0366 | 2.39 | 0.498 | 0.0194 | 1.56 | 0.499 | 0.0416 |
| 7.05 | 0.00975 | 0.00404 | 0.222 | 0.00191 | 0.915 | 0.334 | 0.0246 | 1.65 | 0.347 | 0.0457 | 2.47 | 0.499 | 0.0434 | 1.51 | 0.227 | 0.0214 |

Figure S.7: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T6A C2A

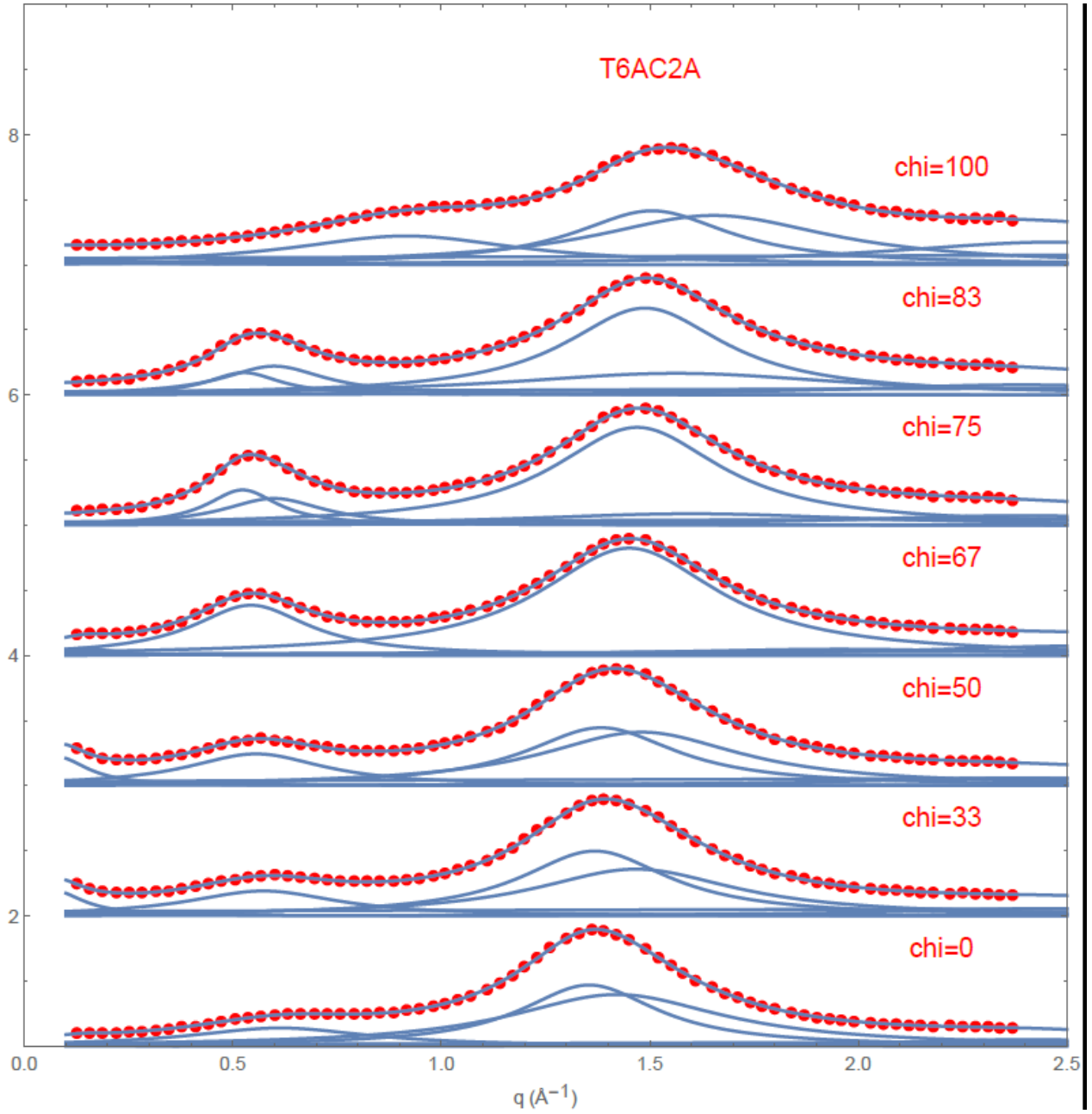
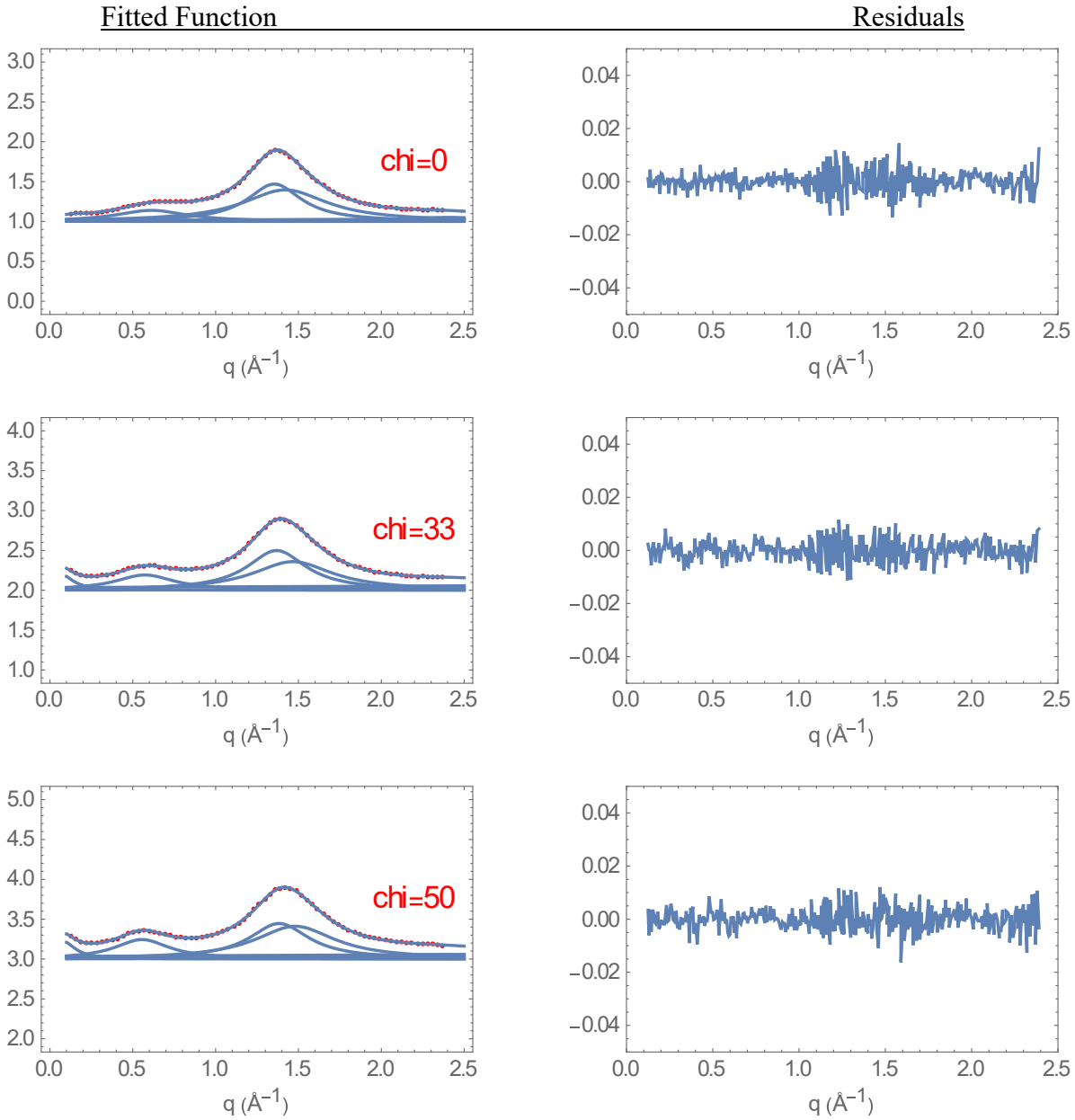
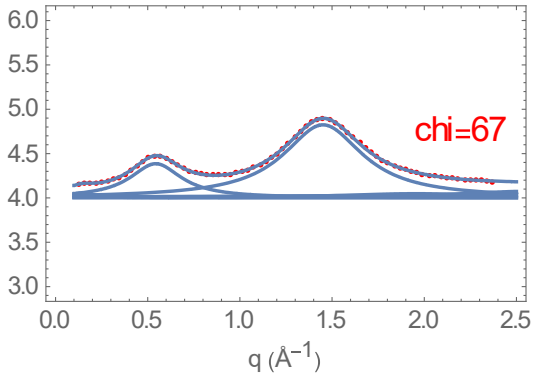
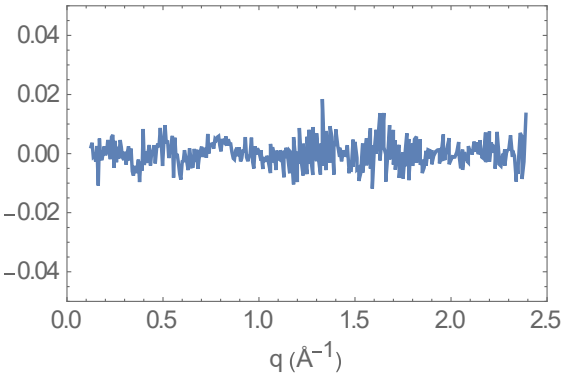
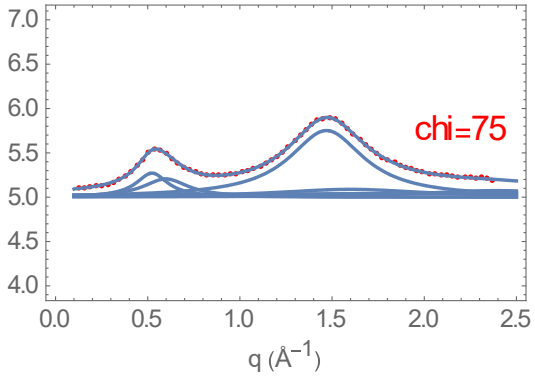


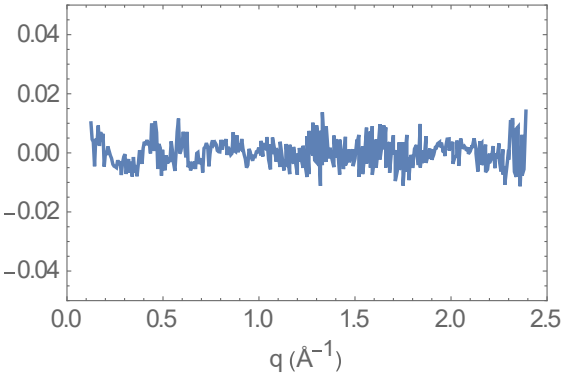
Figure S.8: Fitting functions and residuals for T6A C2A

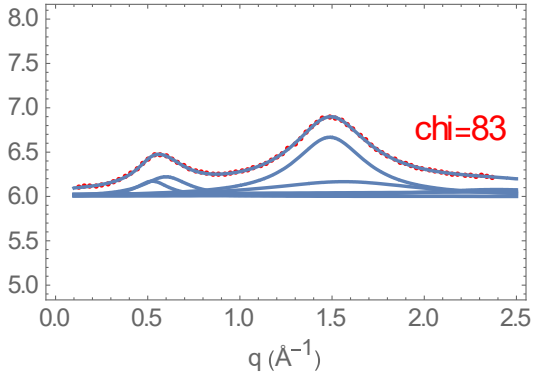


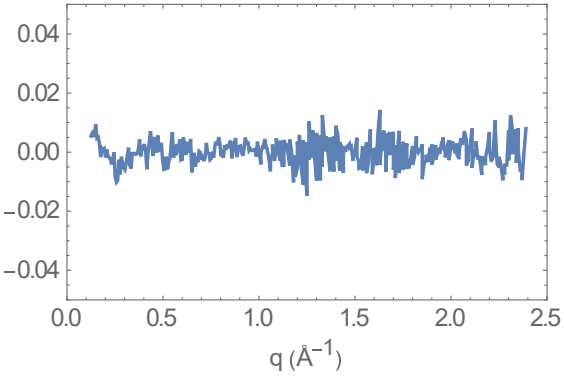

chi=67
q (Å$^{-1}$)

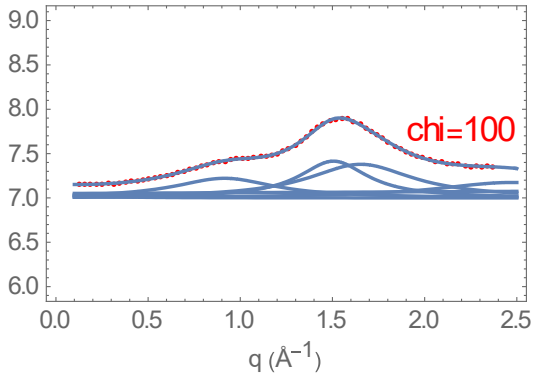

q (Å$^{-1}$)

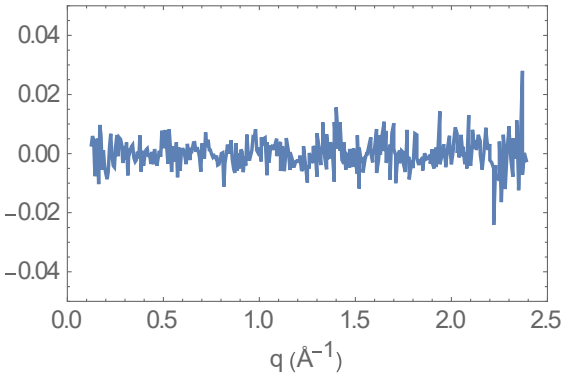

chi=75
q (Å$^{-1}$)


q (Å$^{-1}$)


chi=83
q (Å$^{-1}$)


q (Å$^{-1}$)


chi=100
9.0
8.5
8.0
7.5
7.0
6.5
6.0
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)

## Table S.10: Local Structure Peaks for T6A C6A

| | T6AC6A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | 0.613009 | 0.260993 |
| chi=33 | 0.529271 | 0.244364 |
| chi=50 | 0.529266 | 0.244353 |
| chi=67 | 0.472806 | 0.127198 |
| chi=75 | 0.468122 | 0.106287 |
| chi=83 | 0.458002 | 0.109736 |
| chi=100 | 0.473993 | 0.192415 |

## Table S.11: Fitting Parameters for T6A C6A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.01 | 0.00886 | 0.142 | 0.0693 | 8.99E-05 | 0.613 | 0.261 | 0.00948 | 1.35 | 0.2 | 0.0187 | 1.42 | 0.312 | 0.0385 | 2.41 | 0.387 | 0.0076 |
| 2 | 0.00994 | 0.123 | 0.125 | 0.00112 | 0.529 | 0.244 | 0.0135 | 1.38 | 0.23 | 0.0379 | 1.54 | 0.35 | 0.0198 | 2.43 | 0.5 | 0.0192 |
| 3 | 0.00998 | 0.529 | 0.244 | 0.0135 | 0.123 | 0.125 | 0.00112 | 1.38 | 0.23 | 0.0379 | 1.54 | 0.35 | 0.0198 | 2.43 | 0.5 | 0.0192 |
| 4.03 | -0.00999 | 0.473 | 0.127 | 0.00726 | 0.629 | 0.154 | 0.00114 | 1.41 | 0.231 | 0.0405 | 1.63 | 0.346 | 0.0152 | 2.36 | 0.5 | 0.028 |
| 5.01 | -0.00999 | 0.468 | 0.106 | 0.00523 | 0.577 | 0.188 | 0.00375 | 1.43 | 0.238 | 0.0452 | 1.69 | 0.378 | 0.0157 | 2.36 | 0.5 | 0.0314 |
| 5.99 | -0.00994 | 0.458 | 0.11 | 0.00578 | 0.6 | 0.221 | 0.00483 | 1.44 | 0.246 | 0.0495 | 2.44 | 0.499 | 0.0341 | 1.79 | 0.464 | 0.0198 |
| 7.01 | -0.0097 | 0.636 | 0.254 | 0.00674 | 1.43 | 0.258 | 0.0544 | 2.42 | 0.499 | 0.0354 | 1.8 | 0.498 | 0.0148 | 0.474 | 0.192 | 0.00688 |

Figure S.9: Fitting functions (blue) and raw data (red, 1/5th of points shown) for T6A C6A

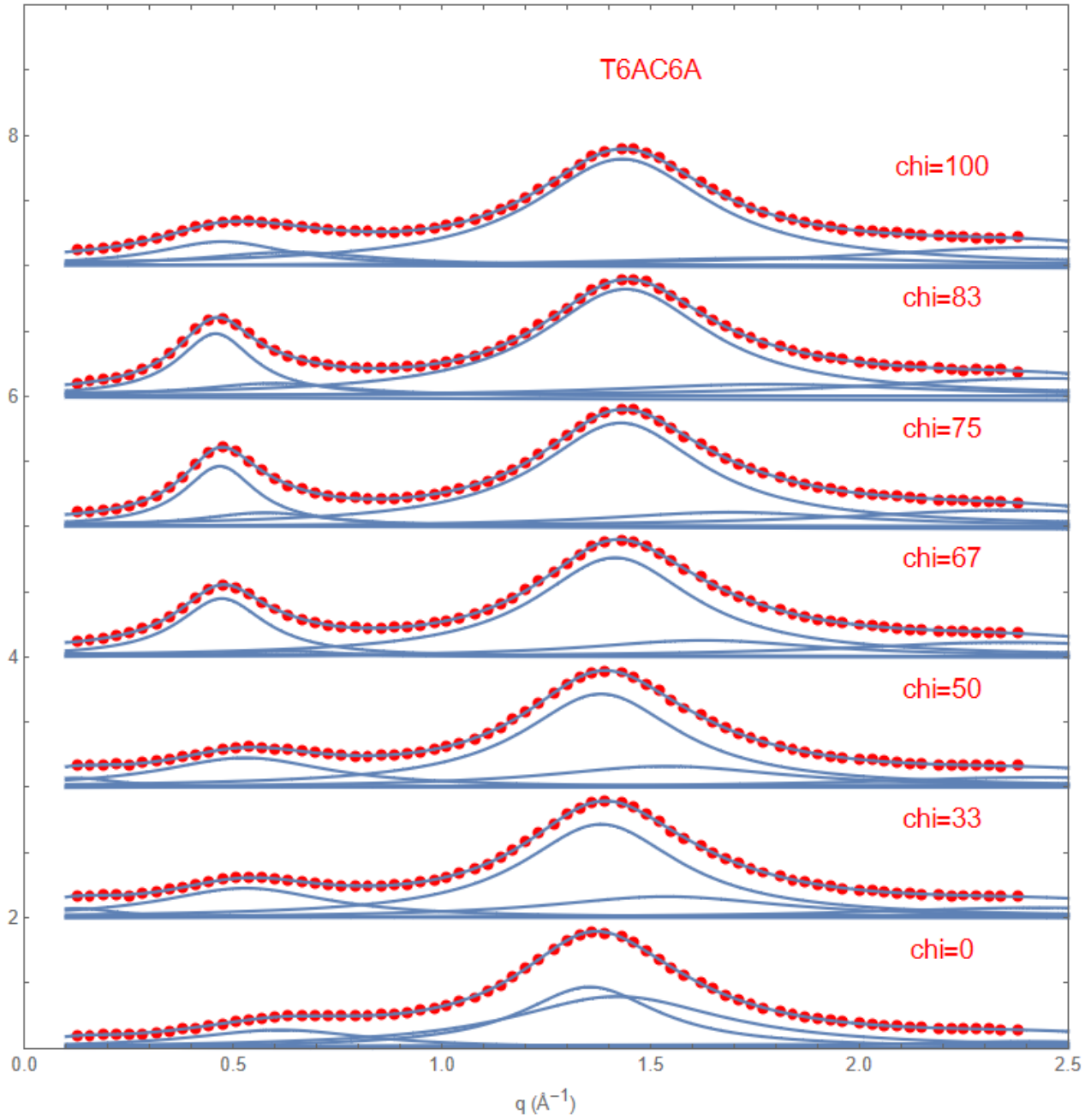
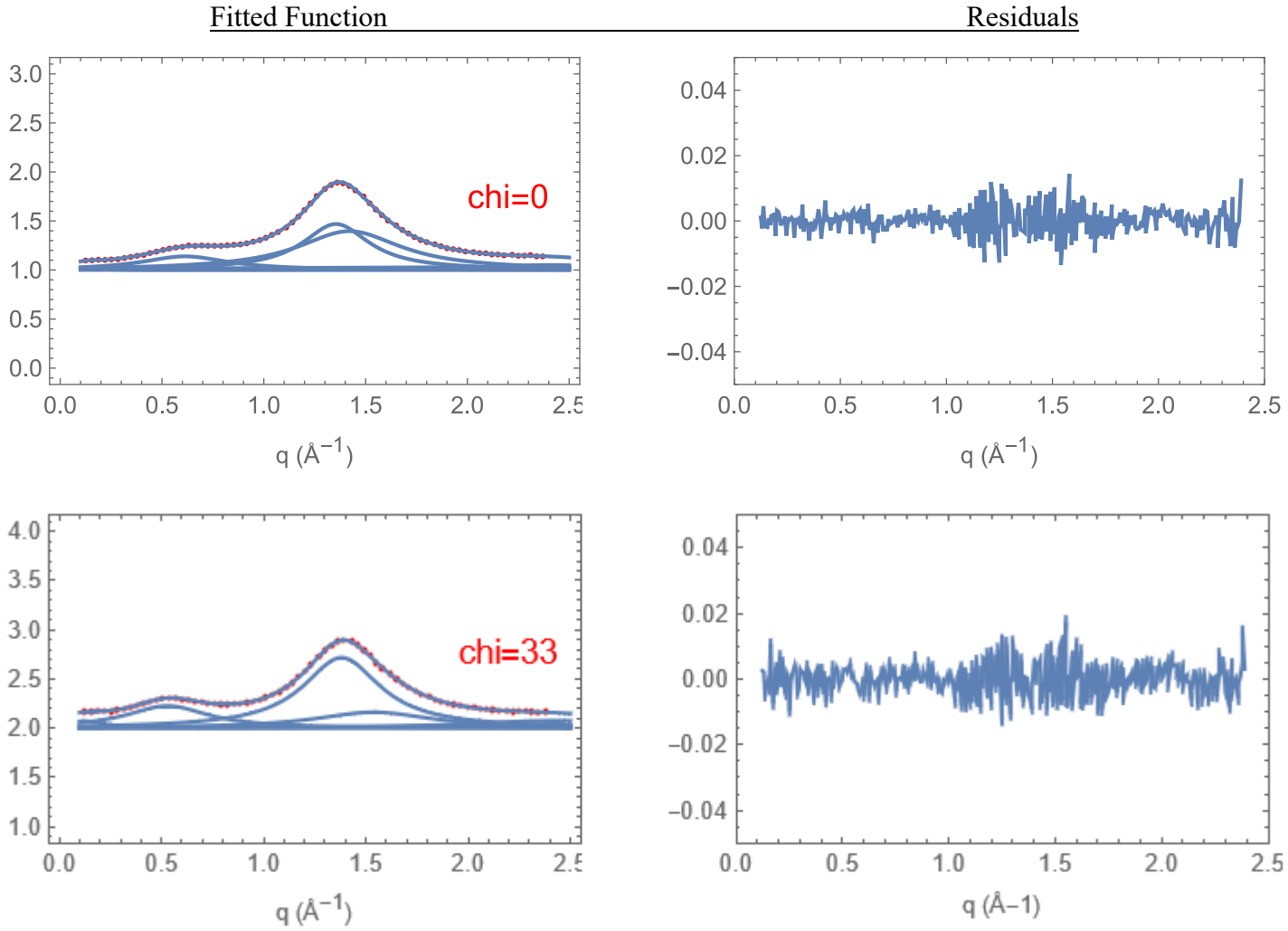
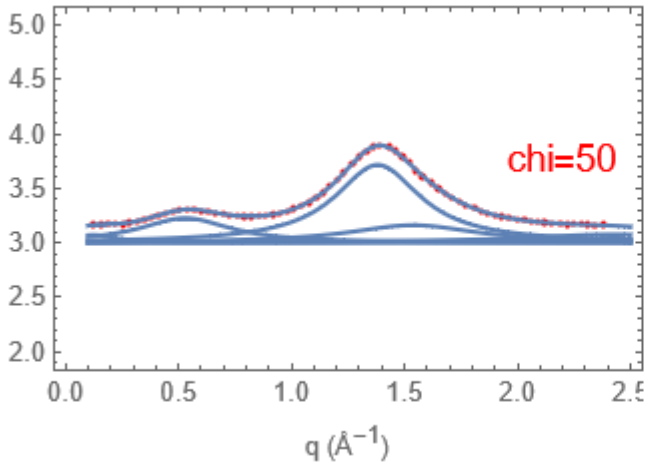
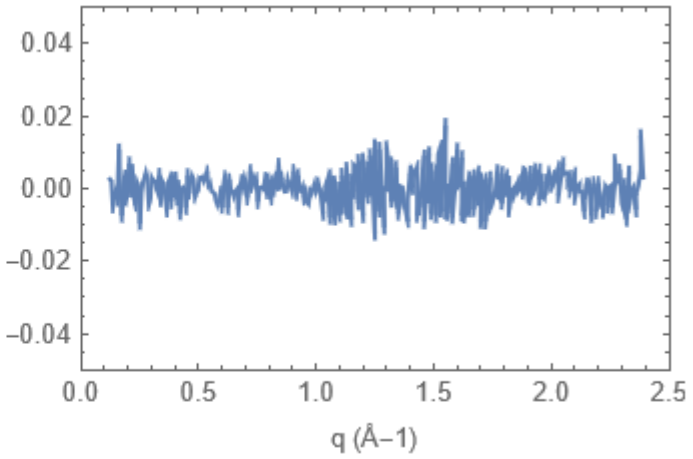
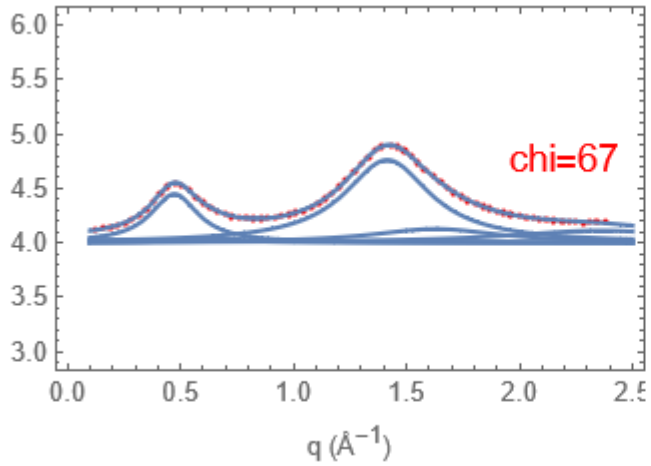


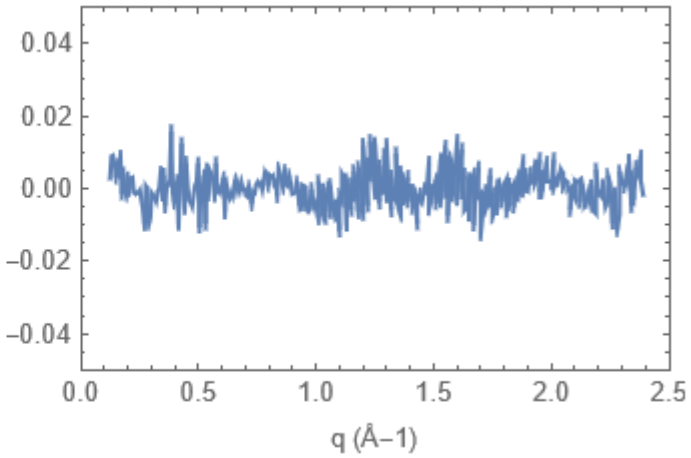
Figure S.10: Fitting functions and residuals for T6A C6A

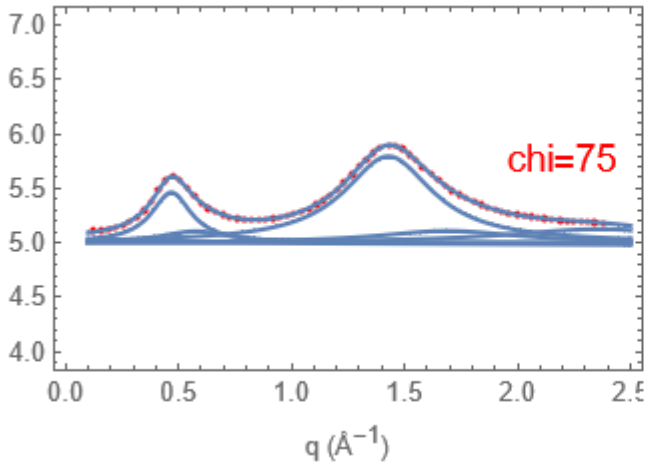


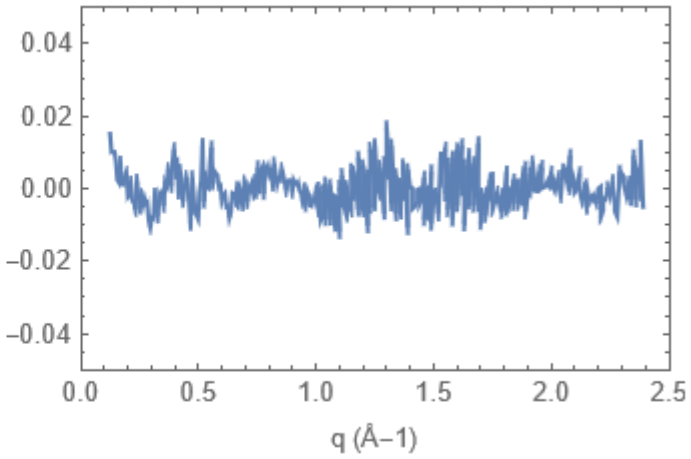

chi=50
q (Å$^{-1}$)

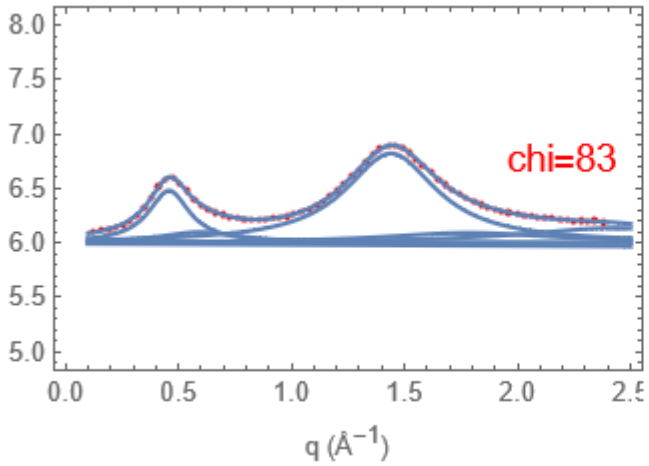

q (Å–1)

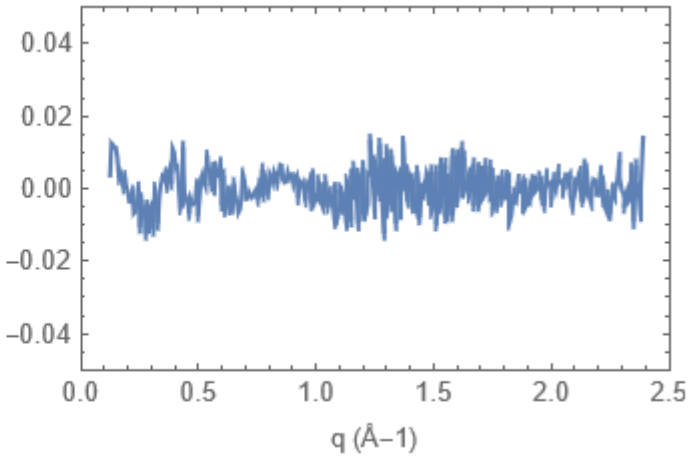

chi=67
q (Å$^{-1}$)

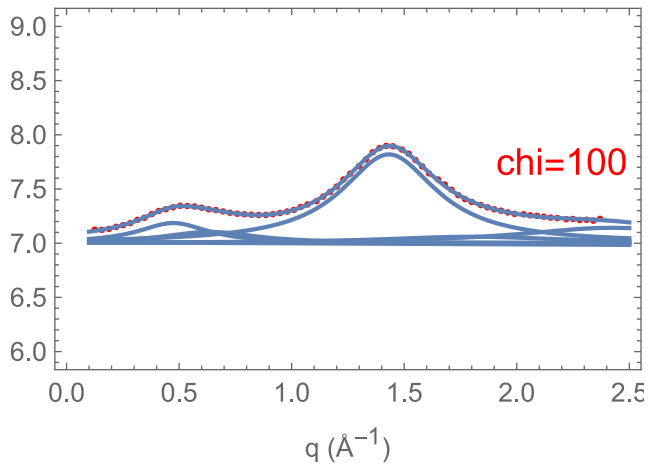

q (Å–1)

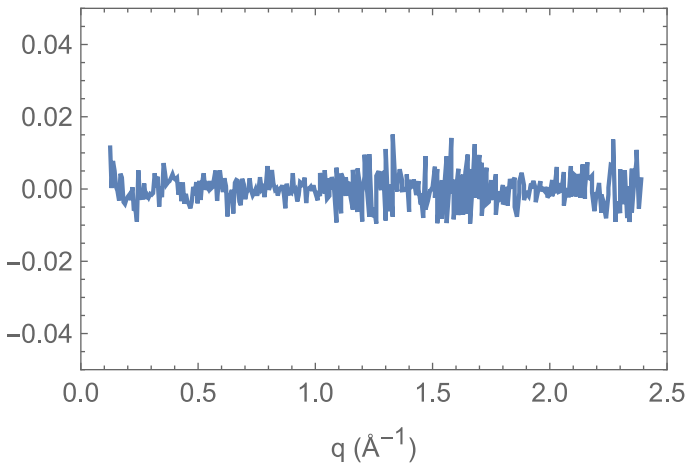

chi=75
q (Å$^{-1}$)


q (Å–1)


chi=83
q (Å$^{-1}$)


q (Å–1)


chi=100
9.0
8.5
8.0
7.5
7.0
6.5
6.0
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)

**T6AC8A**

## Table S.12: Local Structure Peaks for T6A C8A

| | T6AC8A | | |
|---|---|---|---|
| | q (Å^-1) | w (Å^-1) | |
| chi=0 | | | |
| chi=33 | 0.503223 | 0.280679 | |
| chi=50 | 0.458145 | 0.226522 | |
| chi=67 | 0.432352 | 0.131595 | 14.53256 |
| chi=75 | 0.430672 | 0.122167 | 14.58925 |
| chi=83 | 0.418464 | 0.117655 | |
| chi=100 | 0.41763 | 0.185602 | |

## Table S.13: Fitting Parameters for T6A C8A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.01 | 0.00886 | 0.142 | 0.0693 | 8.99E-05 | 0.613 | 0.261 | 0.00948 | 1.35 | 0.2 | 0.0187 | 1.42 | 0.312 | 0.0385 | 2.41 | 0.387 | 0.0076 |
| 2.01 | 0.00994 | 0.0555 | 0.146 | 0.00119 | 0.503 | 0.281 | 0.0159 | 1.38 | 0.215 | 0.032 | 1.53 | 0.329 | 0.0196 | 2.43 | 0.5 | 0.0158 |
| 3.02 | 0.00998 | 0.458 | 0.227 | 0.0136 | 0.0921 | 0.051 | 8.06E-5 | 1.38 | 0.205 | 0.0268 | 1.53 | 0.323 | 0.0246 | 2.42 | 0.5 | 0.0156 |
| 4.01 | 0.01 | 0.432 | 0.132 | 0.00669 | 0.603 | 0.159 | 0.00159 | 0.879 | 0.363 | 4.57e-7 | 1.42 | 0.232 | 0.0444 | 2.09 | 0.5 | 0.021 |
| 5.01 | 0.00998 | 0.431 | 0.122 | 0.00513 | 0.551 | 0.218 | 0.00487 | 1.57 | 0.345 | 0.0232 | 1.41 | 0.209 | 0.0299 | 2.35 | 0.5 | 0.0184 |
| 5.97 | 0.00998 | 0.418 | 0.118 | 0.00564 | 0.582 | 0.27 | 0.00661 | 2.39 | 0.5 | 0.0248 | 1.41 | 0.205 | 0.0286 | 1.56 | 0.41 | 0.0372 |
| 6.96 | 0.00948 | 0.418 | 0.186 | 0.0079 | 0.674 | 0.466 | 0.0146 | 2.46 | 0.498 | 0.0303 | 1.41 | 0.218 | 0.0351 | 1.59 | 0.479 | 0.0353 |

Figure S.11: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T6A C8A

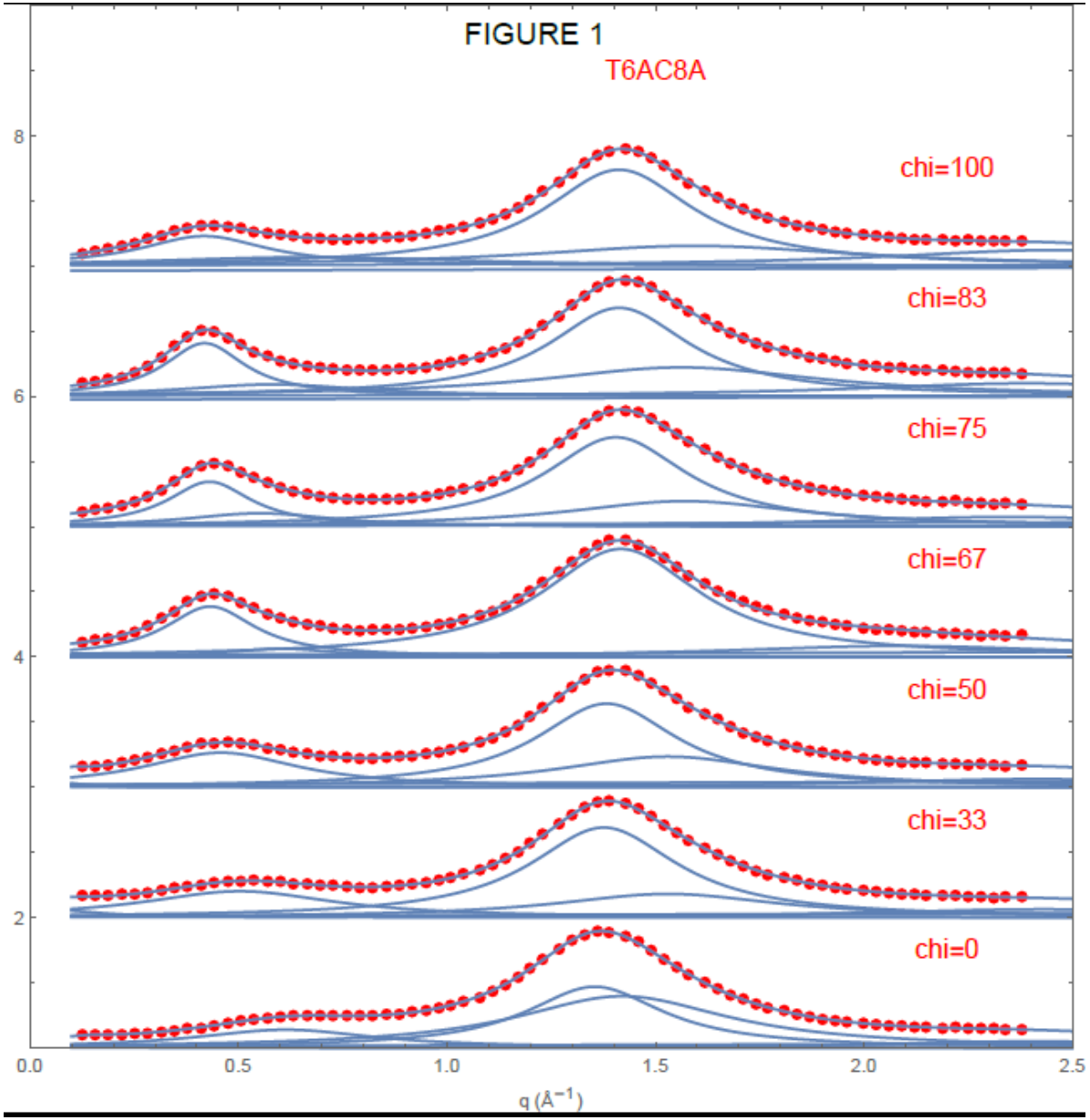
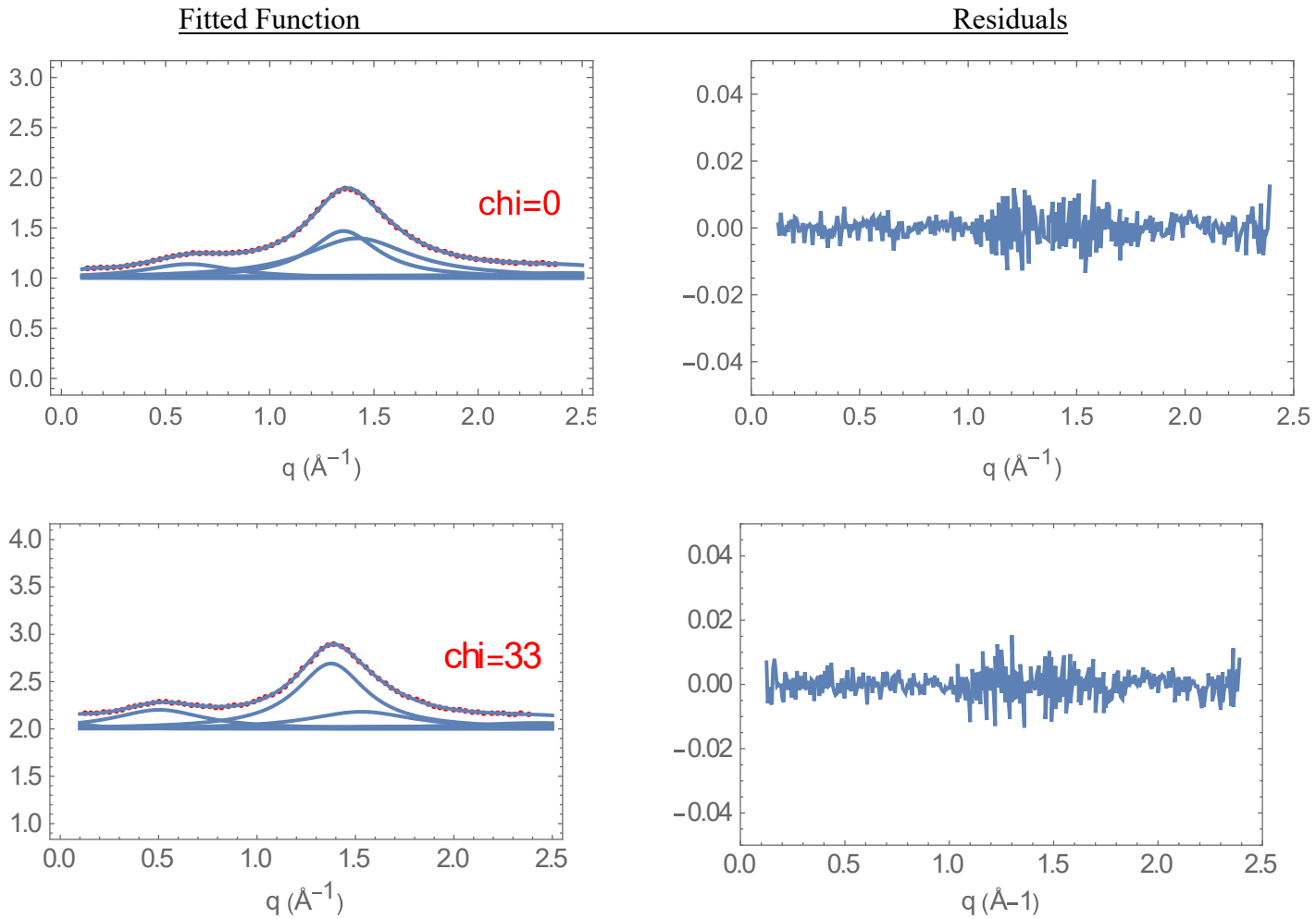
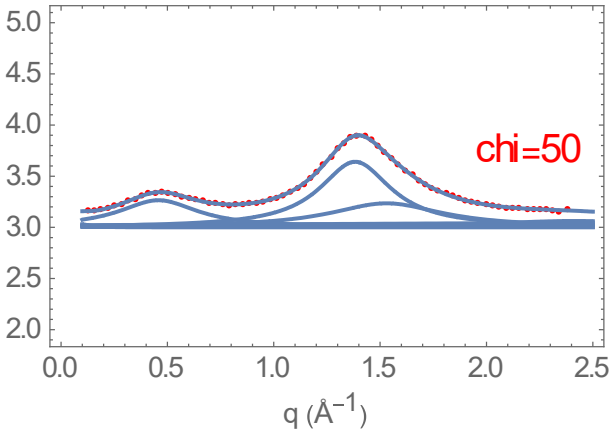
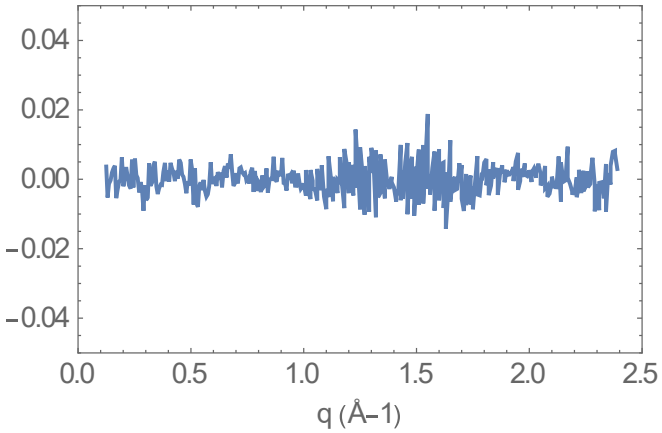
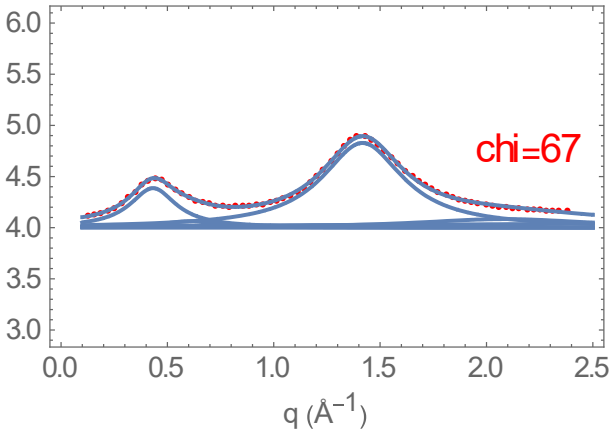


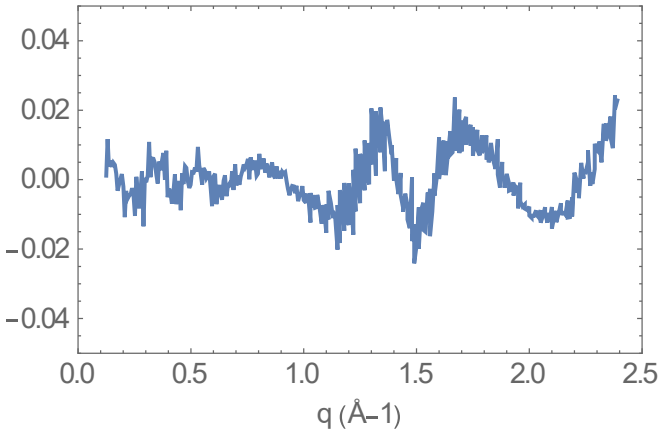
Figure S.12: Fitting functions and residuals for T6A C8A

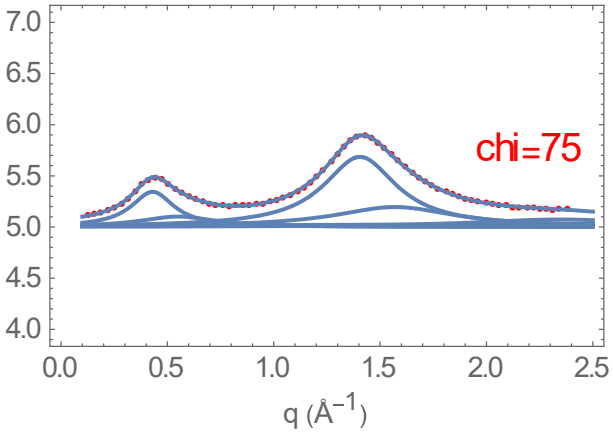


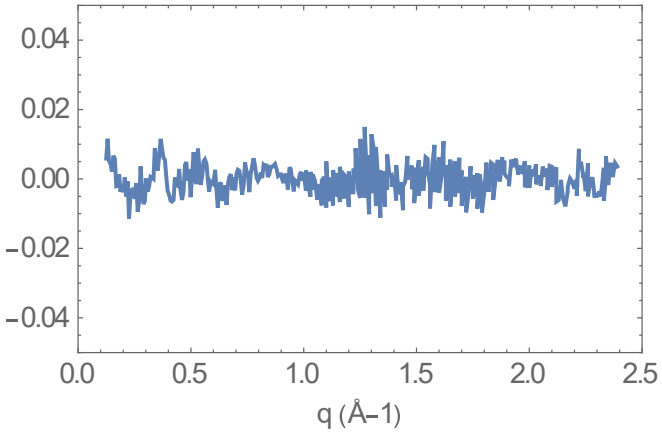

chi=50
q (Å$^{-1}$)

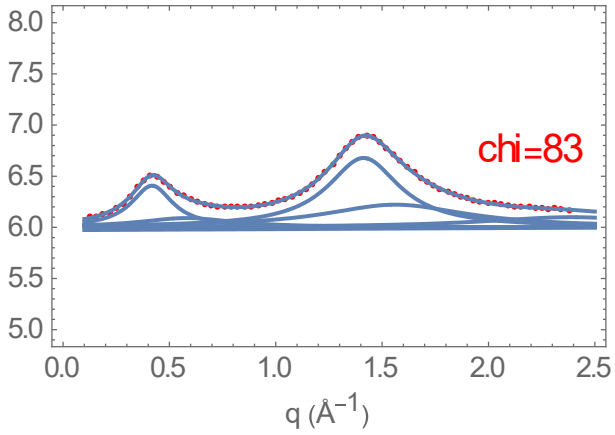

q (Å–1)

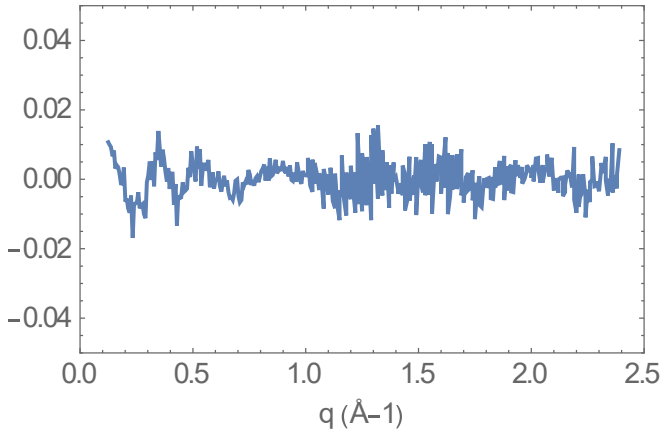

chi=67
q (Å$^{-1}$)

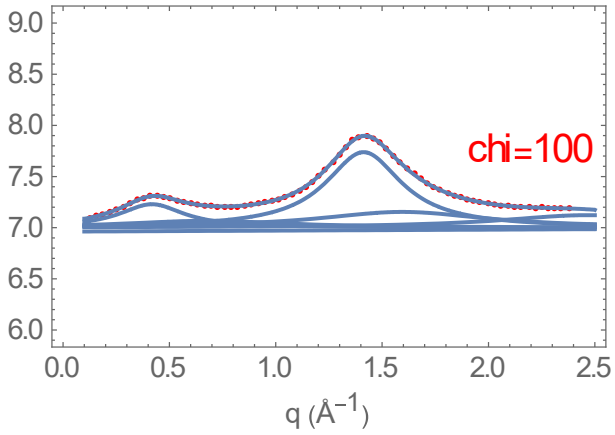

q (Å–1)

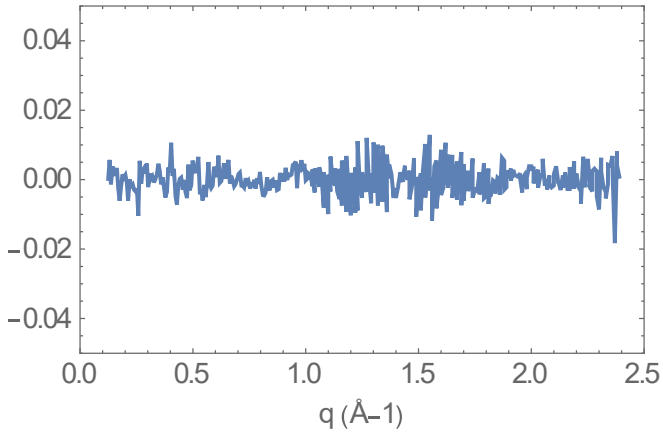

chi=75
q (Å$^{-1}$)


q (Å–1)


chi=83
q (Å$^{-1}$)


q (Å–1)


chi=100
q (Å$^{-1}$)


q (Å–1)

## Table S.14: Local Structure Peaks for T6A C10A

| | T6AC10A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | | |
| chi=33 | 0.486996 | 0.323142 |
| chi=50 | 0.422383 | 0.280071 |
| chi=67 | 0.392374 | 0.142354 |
| chi=75 | 0.395107 | 0.119866 |
| chi=83 | 0.376269 | 0.116727 |

## Table S.15: Fitting Parameters for T6A C10A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.01 | 0.00886 | 0.142 | 0.0693 | 8.99E-05 | 0.613 | 0.261 | 0.00948 | 1.35 | 0.2 | 0.0187 | 1.42 | 0.312 | 0.0385 | 2.41 | 0.387 | 0.0076 |
| 2.05 | -0.00929 | 2.41 | 0.431 | 0.0134 | 1.37 | 0.206 | 0.0238 | 1.48 | 0.228 | 0.0148 | 0.487 | 0.323 | 0.0174 | 1.73 | 0.349 | 0.00785 |
| 2.97 | 0.00999 | 2.48 | 0.499 | 0.0215 | 1.34 | 0.165 | 0.00663 | 1.51 | 0.5 | 0.051 | 0.422 | 0.28 | 0.0212 | 1.44 | 0.21 | 0.021 |
| 3.95 | 0.00708 | 0.586 | 0.343 | 0.0135 | 0.392 | 0.142 | 0.00662 | 2.38 | 0.6 | 0.0433 | 1.62 | 0.379 | 0.019 | 1.41 | 0.223 | 0.0385 |
| 4.95 | 0.00997 | 0.588 | 0.331 | 0.0131 | 0.395 | 0.12 | 0.00536 | 2.36 | 0.5 | 0.0276 | 1.64 | 0.418 | 0.0252 | 1.42 | 0.219 | 0.0374 |
| 5.95 | 0.00999 | 0.604 | 0.335 | 0.012 | 0.376 | 0.117 | 0.00524 | 2.42 | 0.5 | 0.0269 | 1.66 | 0.474 | 0.0309 | 1.43 | 0.22 | 0.038 |

Figure S.13: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T6A C10A

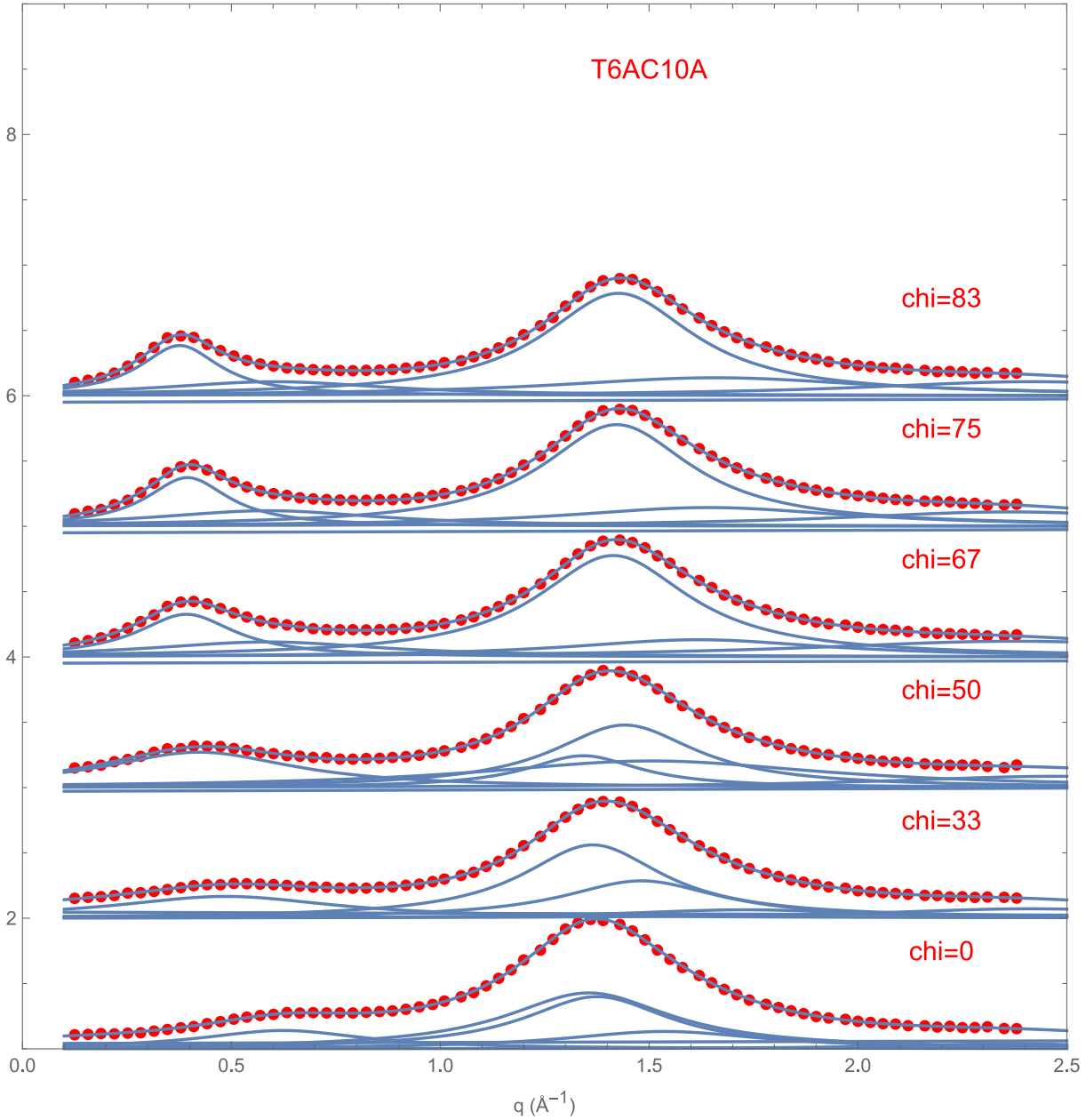
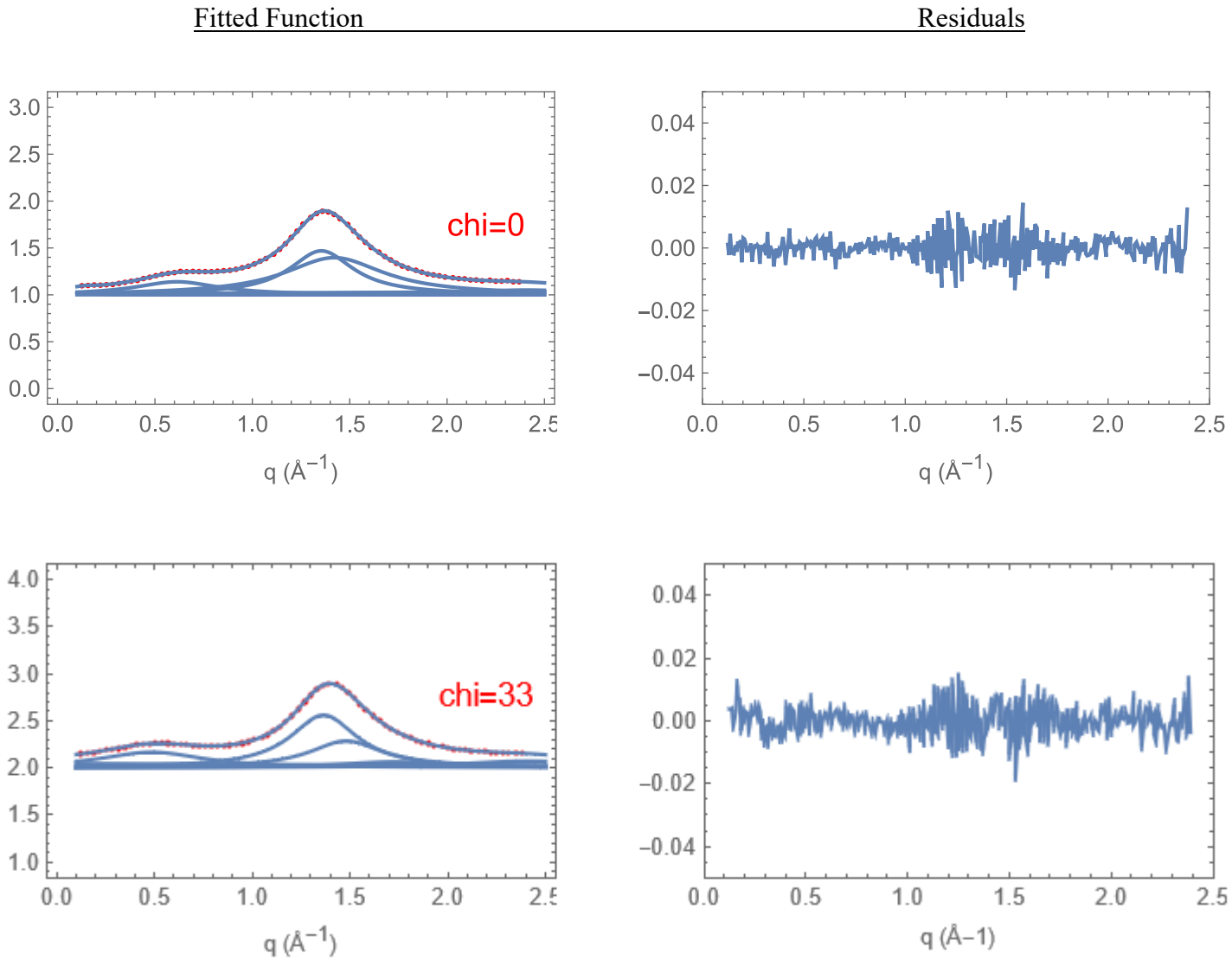
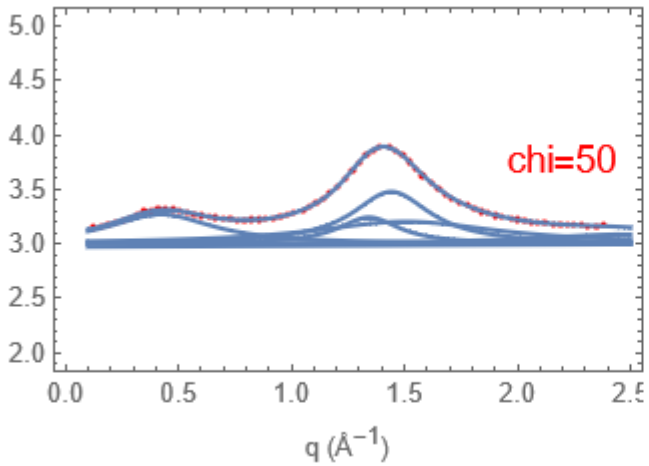
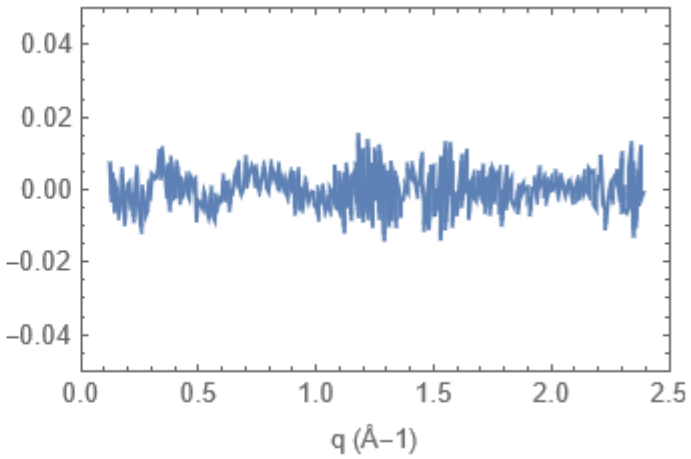
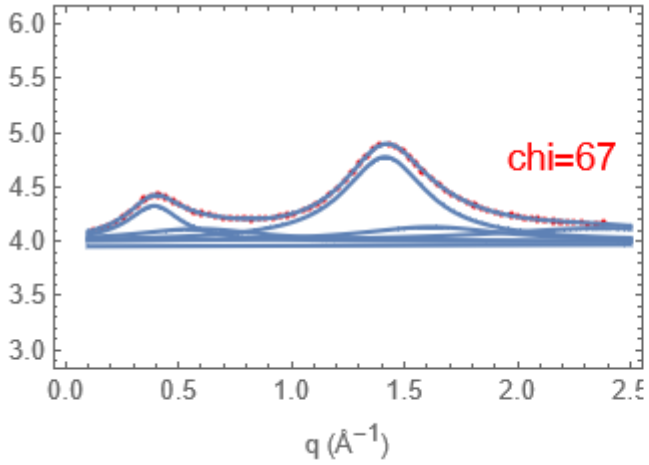


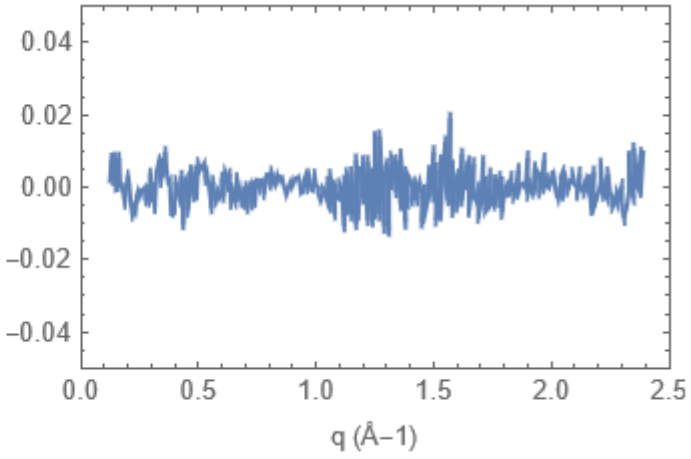
Figure S.14: Fitting functions and residuals for T6A C10A

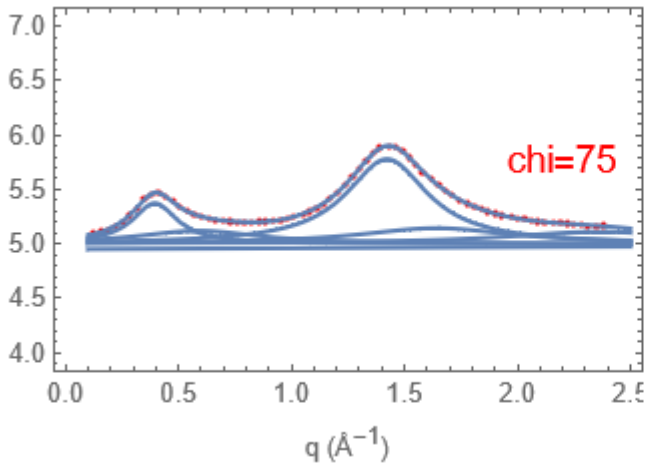


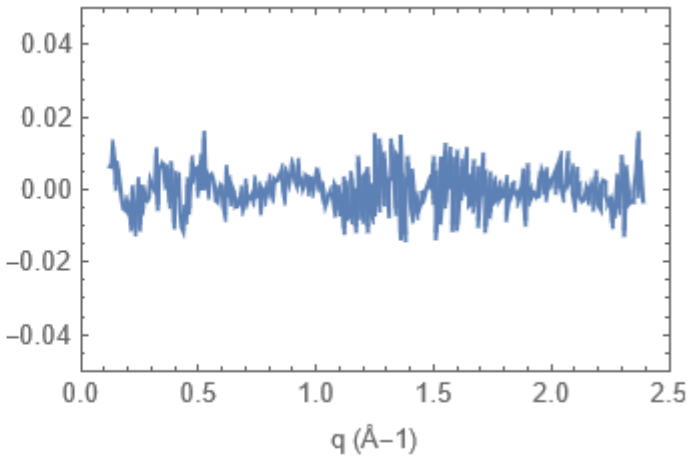

chi=50
q (Å$^{-1}$)

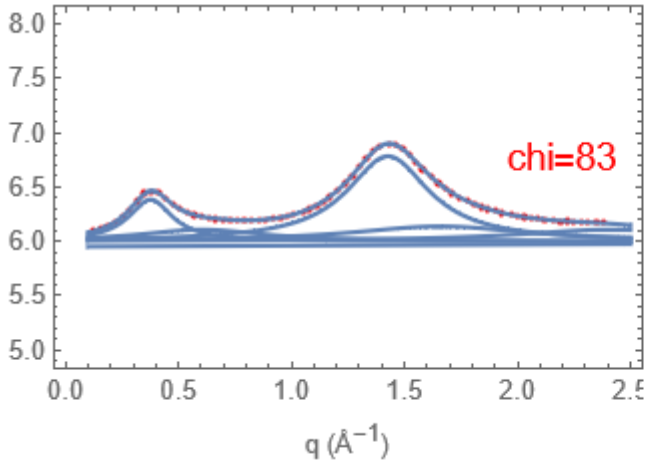

q (Å–1)

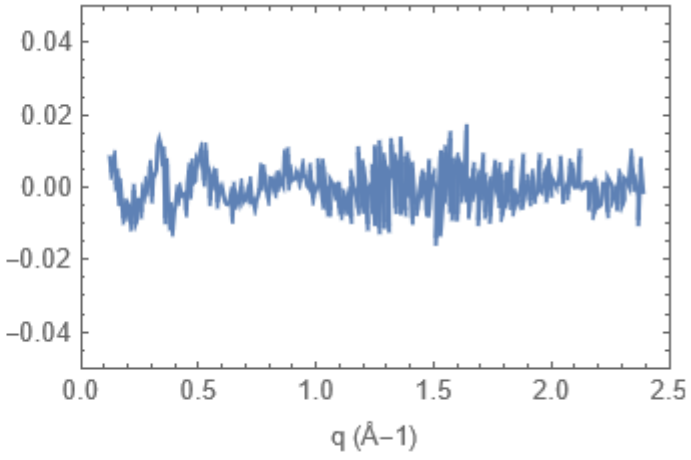

chi=67
q (Å$^{-1}$)


q (Å–1)


chi=75
q (Å$^{-1}$)


q (Å–1)


chi=83
q (Å$^{-1}$)


q (Å–1)

## Table S.16: Local Structure Peaks for T8A C2A

| | T8AC2A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | 0.486889 | 0.197301 |
| chi=33 | 0.449738 | 0.22663 |
| chi=50 | 0.444811 | 0.186806 |
| chi=67 | 0.442315 | 0.135178 |
| chi=75 | 0.454312 | 0.127713 |
| chi=83 | 0.466625 | 0.135289 |
| chi=100 | 0.914855 | 0.333708 |

## Table S.17: Fitting Parameters for T8A C2A

| a | b | q01 | w1 | A1 | q02 | w2 | A2 | q03 | w3 | A3 | q04 | w4 | A4 | q05 | w5 | A5 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.03 | 0.00578 | 0.487 | 0.197 | 0.00348 | 1.3 | 0.283 | 0.0194 | 1.42 | 0.21 | 0.0273 | 1.7 | 0.371 | 0.00438 | 2.4 | 0.373 | 0.00533 |
| 1.97 | 0.00956 | 0.45 | 0.227 | 0.00914 | 0.113 | 0.11 | 0.000961 | 1.37 | 0.39 | 0.0607 | 1.42 | 0.198 | 0.0207 | 2.17 | 0.399 | 0.0104 |
| 2.99 | -0.00839 | 0.445 | 0.187 | 0.00761 | 0.00115 | 0.128 | 0.00339 | 1.36 | 0.426 | 0.0589 | 1.43 | 0.206 | 0.0257 | 2.34 | 0.497 | 0.0301 |
| 4.05 | -0.00996 | 0.442 | 0.135 | 0.00545 | 0.447 | 0.5 | 0.00792 | 1.09 | 0.233 | 0.00338 | 1.45 | 0.232 | 0.0444 | 2.06 | 0.5 | 0.0203 |
| 4.99 | 0.01 | 0.454 | 0.128 | 0.00698 | 1.21 | 0.481 | 0.0421 | 1.45 | 0.191 | 0.0231 | 1.57 | 0.153 | 0.00267 | 1.9 | 0.5 | 0.0292 |
| 6.01 | 0.00951 | 0.467 | 0.135 | 0.00662 | 1.11 | 0.5 | 0.0295 | 1.68 | 0.377 | 0.00867 | 1.48 | 0.219 | 0.0358 | 2.21 | 0.494 | 0.0242 |
| 7.05 | 0.00975 | 0.00404 | 0.222 | 0.00191 | 0.915 | 0.334 | 0.0246 | 1.65 | 0.347 | 0.0457 | 2.47 | 0.499 | 0.0434 | 1.51 | 0.227 | 0.0214 |

Figure S.15: Fitting functions (blue) and raw data (red, 1/5th of points shown) for T8A C2A

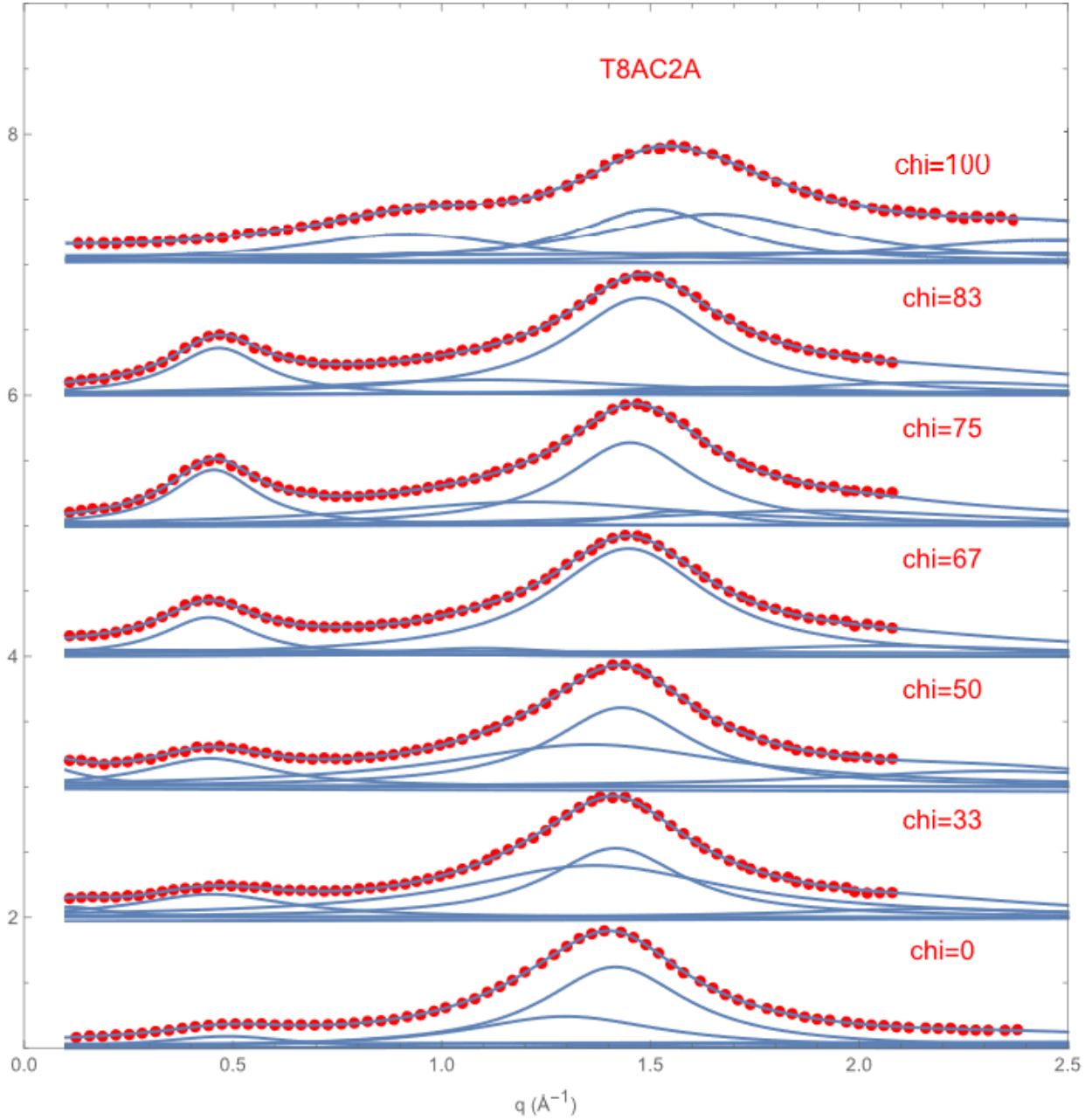
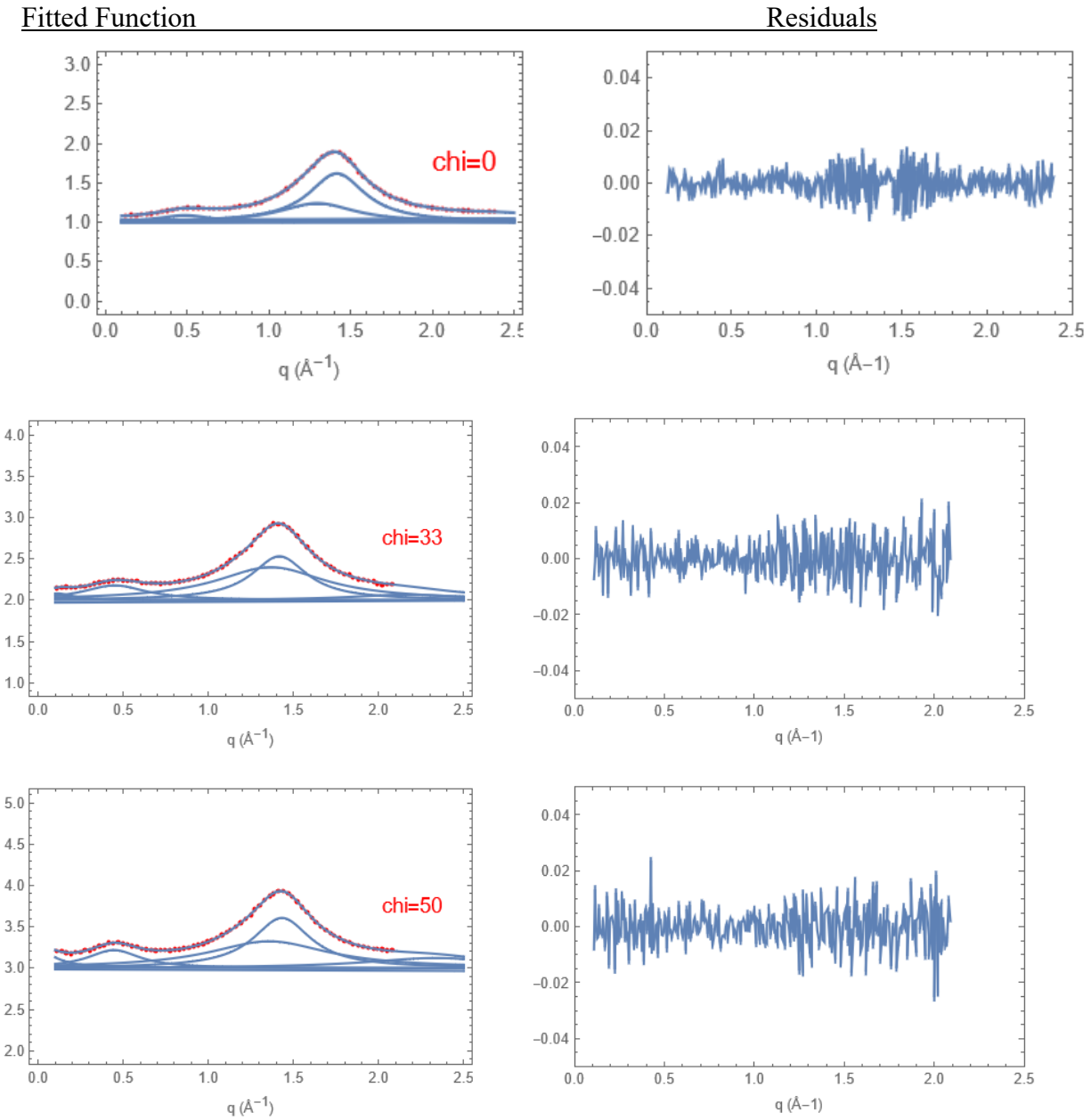
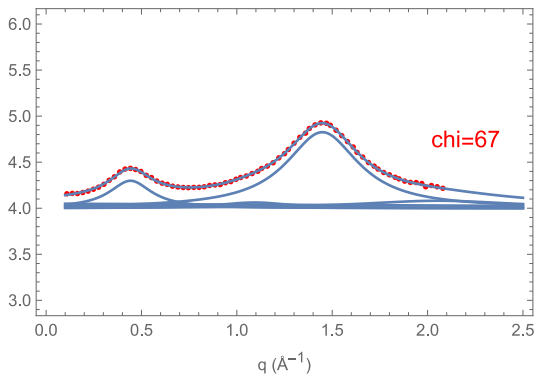
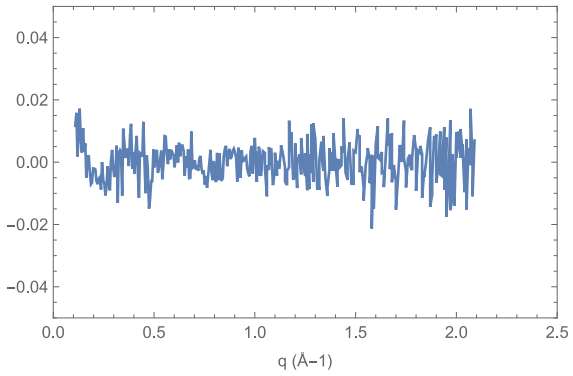
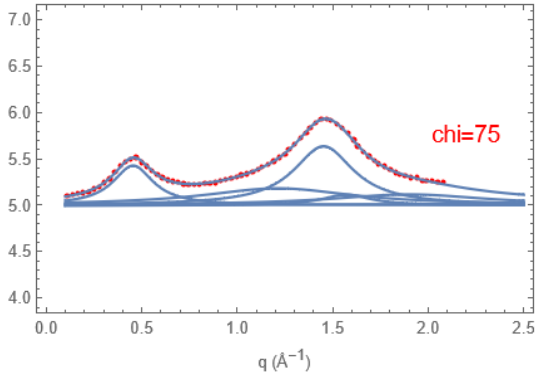


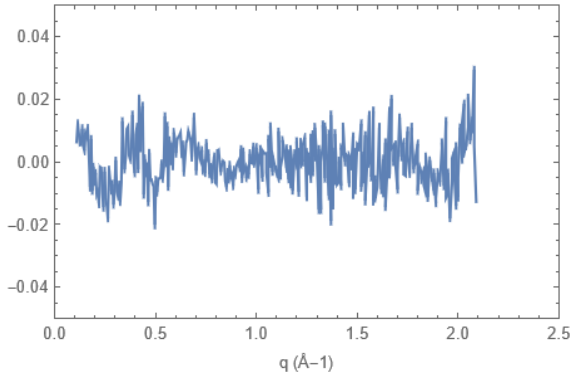
Figure S.16: Fitting functions and residuals for T8A C2A

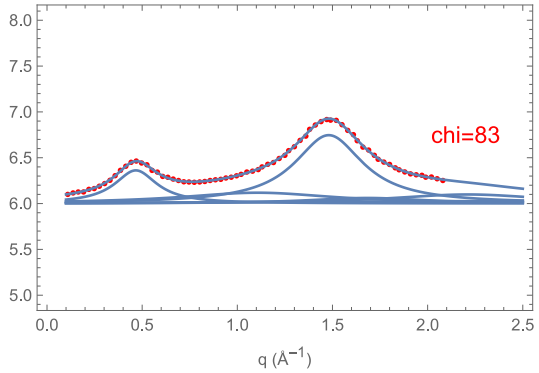


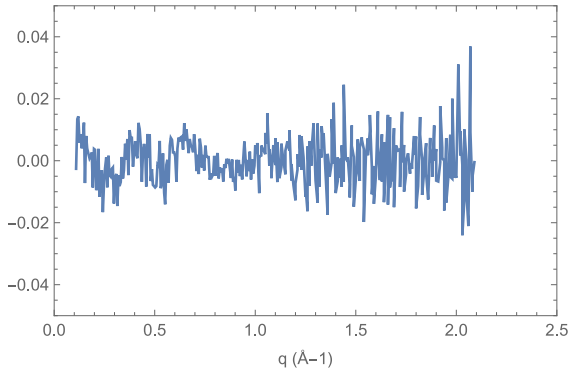

chi=67
q (Å$^{-1}$)

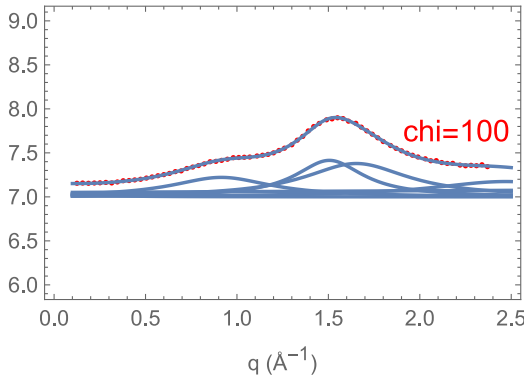

q (Å−1)

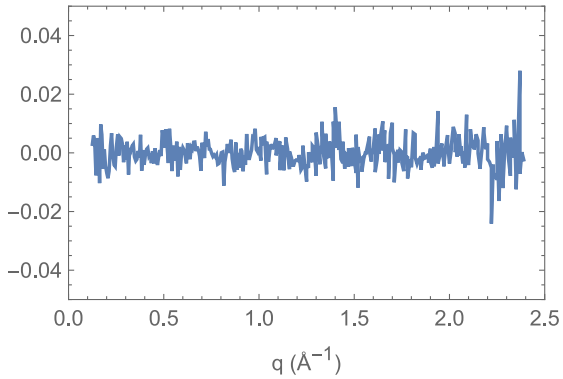

chi=75
q (Å$^{-1}$)


q (Å−1)


chi=83
q (Å$^{-1}$)


q (Å−1)


chi=100
9.0
8.5
8.0
7.5
7.0
6.5
6.0
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)

## Table S.18: Local Structure Peaks for T8A C6A

| | T8AC6A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | | |
| chi=33 | 0.468542 | 0.175375 |
| chi=50 | 0.454399 | 0.194357 |
| chi=67 | 0.431406 | 0.13934 |
| chi=75 | 0.431947 | 0.121119 |
| chi=83 | 0.423076 | 0.082743 |
| chi=100 | 0.476237 | 0.194581 |

## Table S.19: Fitting Parameters for T8A C6A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.03 | 0.00578 | 0.487 | 0.197 | 0.0034 8 | 1.3 | 0.283 | 0.0194 | 1.42 | 0.21 | 0.027 3 | 1.7 | 0.371 | 0.00438 | 2.4 | 0.373 | 0.00533 |
| 2.05 | 0.00773 | 0.469 | 0.175 | 0.0034 3 | 1.23 | 0.228 | 0.0061 1 | 1.42 | 0.21 5 | 0.033 3 | 1.6 | 0.367 | 0.00565 | 2.47 | 0.362 | 0.00349 |
| 3.01 | 0.0083 | 0.454 | 0.194 | 0.0058 4 | 1.43 | 0.158 | 0.0056 1 | 1.39 | 0.28 4 | 0.051 7 | 0.138 | 0.103 | 0.00030 9 | 2.4 | 0.485 | 0.0126 |
| 4.02 | 0.00998 | 0.431 | 0.139 | 0.0065 9 | 1.44 | 0.16 | 0.0053 6 | 1.42 | 0.28 2 | 0.050 9 | 0.11 | 0.088 6 | 0.00023 | 2.34 | 0.5 | 0.0145 |
| 5.04 | 0.00998 | 0.432 | 0.121 | 0.0057 5 | 1.44 | 0.217 | 0.035 | 1.56 | 0.5 | 0.019 1 | 1.2 | 0.185 | 0.00168 | 2.5 | 0.499 | 0.0119 |
| 5.99 | 0.00994 | 0.423 | 0.0827 | 0.0035 | 1.45 | 0.219 | 0.034 | 1.44 | 0.53 | 0.043 2 | 0.49 | 0.137 | 0.00223 | 2.41 | 0.6 | 0.0286 |
| 7.02 | -0.00955 | 0.644 | 0.247 | 0.0098 6 | 1.43 | 0.257 | 0.0891 | 1.76 | 0.49 5 | 0.024 | 0.476 | 0.195 | 0.0121 | 2.41 | 0.499 | 0.0556 |

Figure S.17: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T8A C6A

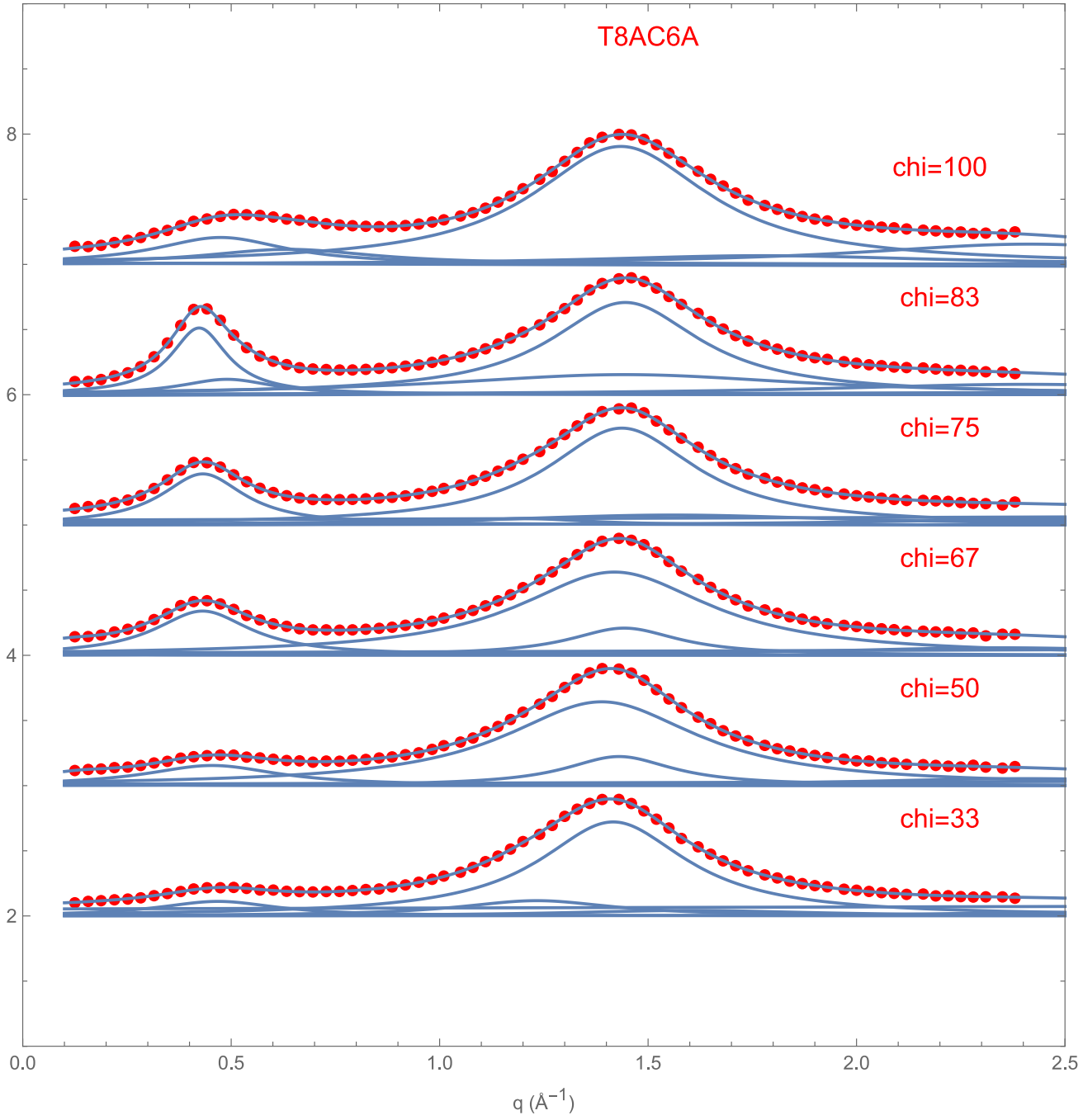
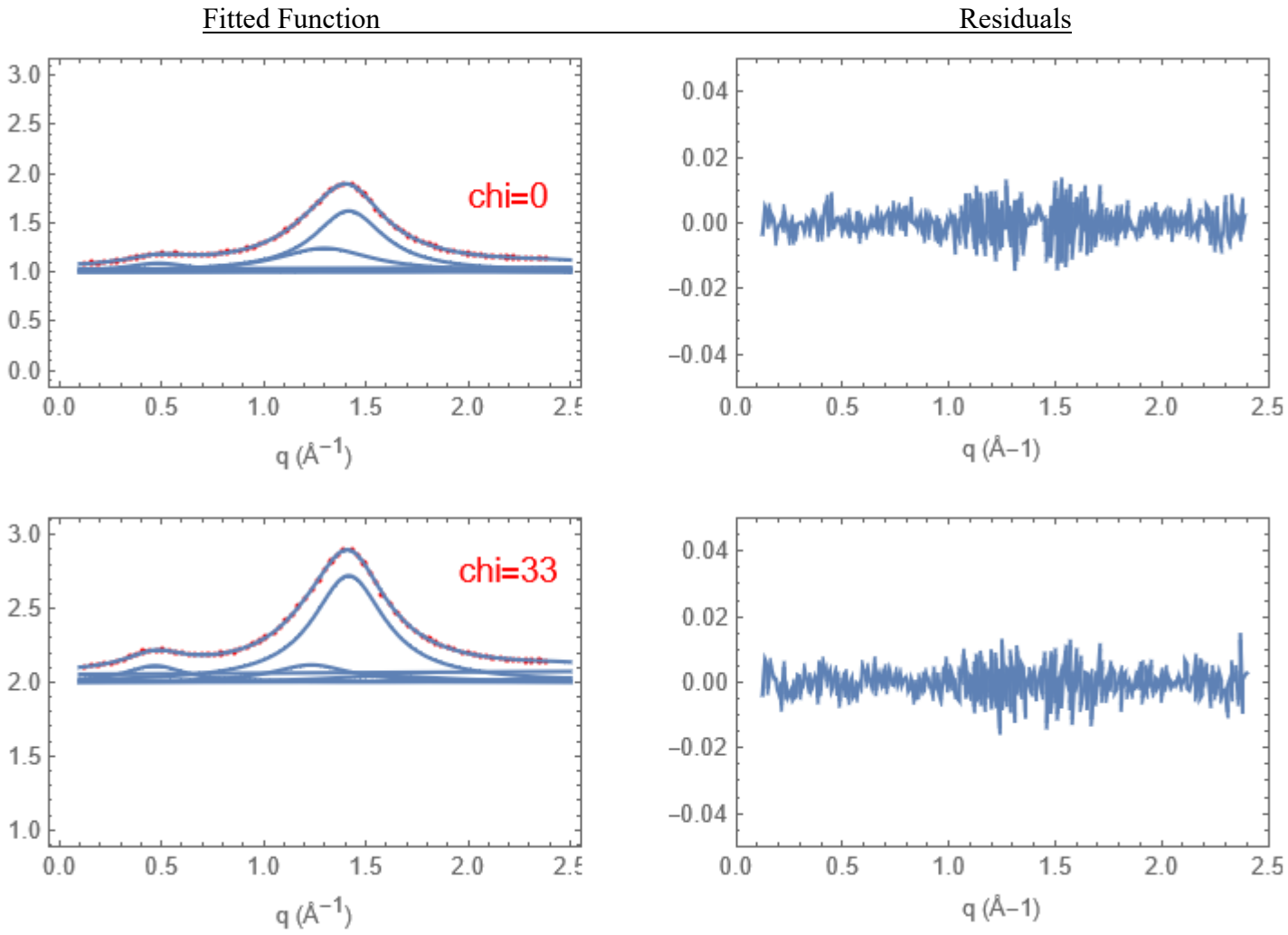
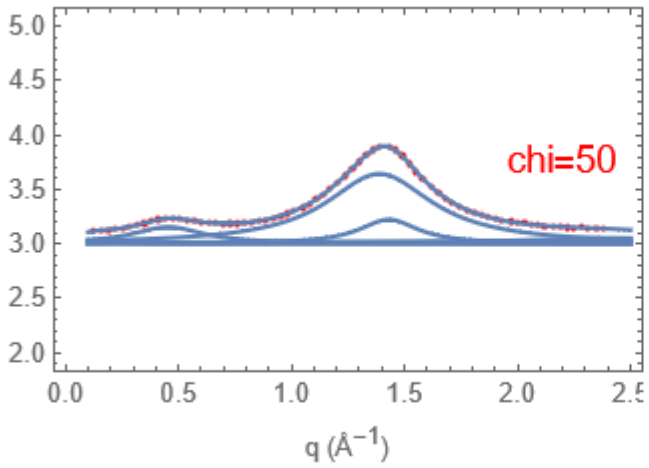
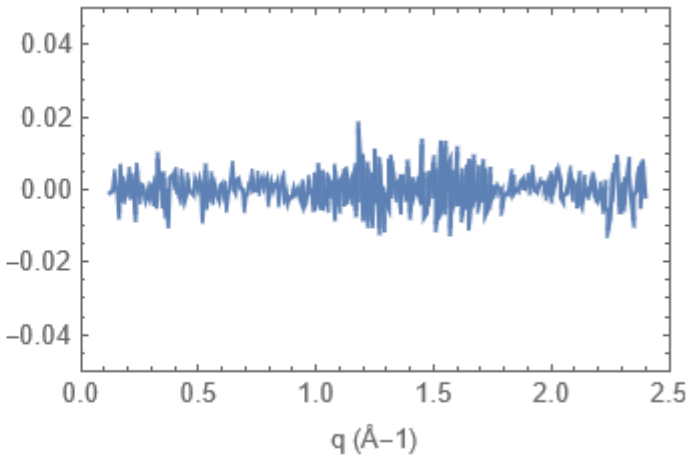
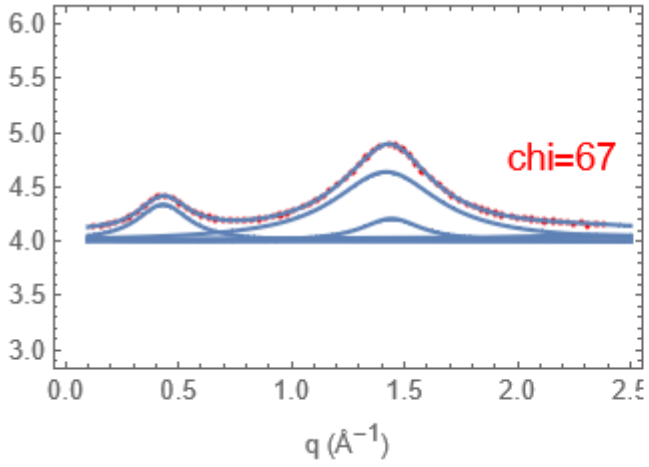


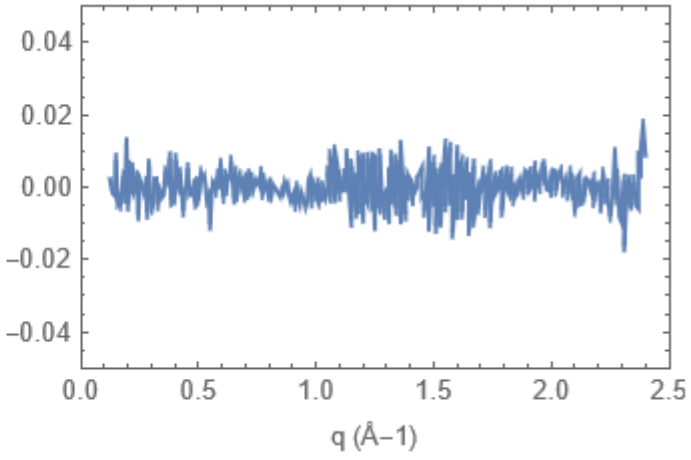
Figure S.18: Fitting functions and residuals for T8A C6A

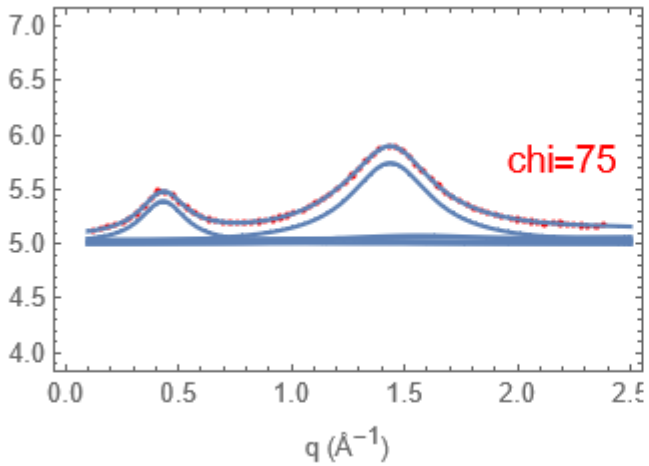


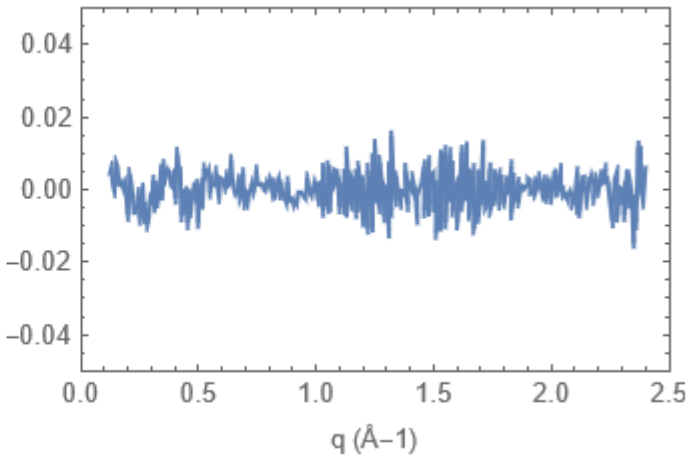

chi=50
q (Å$^{-1}$)

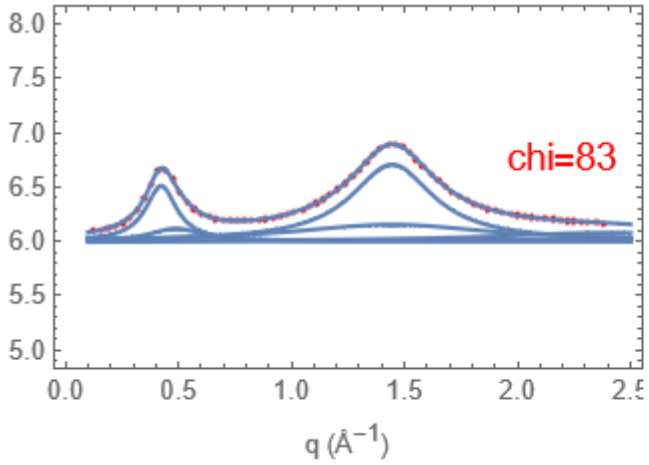

q (Å–1)

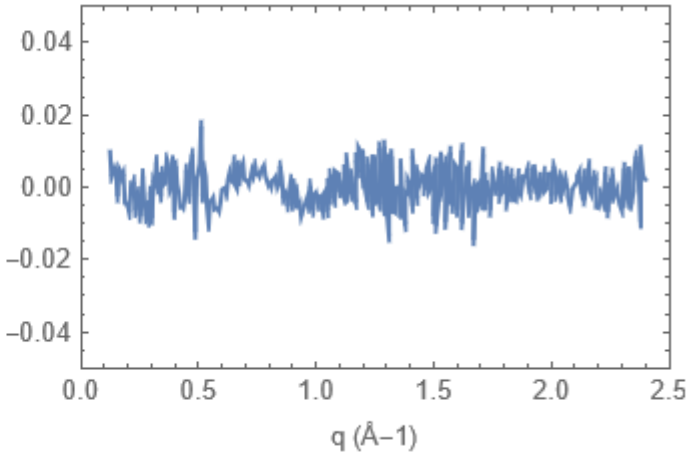

chi=67
q (Å$^{-1}$)

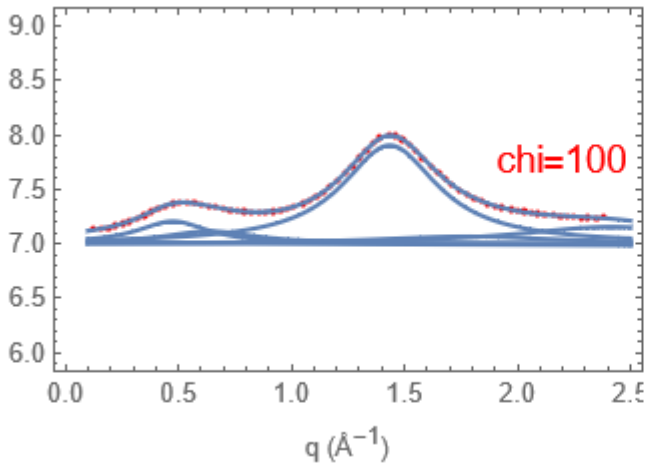

q (Å–1)

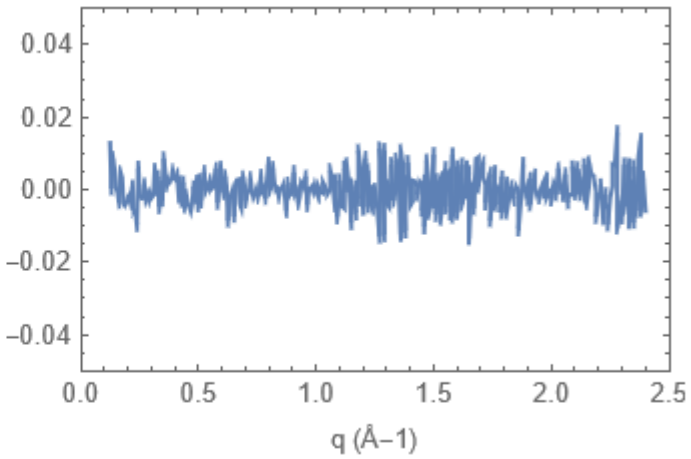

chi=75
q (Å$^{-1}$)


q (Å–1)


chi=83
q (Å$^{-1}$)


q (Å–1)


9.0
8.5
8.0
7.5
7.0
6.5
6.0
0.0
0.5
1.0
1.5
2.0
2.5
chi=100
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
2.5
q (Å−1)

**T8AC8A**

## Table S.20: Local Structure Peaks for T8A C8A

| | T8AC8A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | | |
| chi=33 | 0.44326 | 0.185372 |
| chi=50 | 0.418657 | 0.173421 |
| chi=67 | 0.409713 | 0.155974 |
| chi=75 | 0.408333 | 0.133122 |
| chi=83 | 0.400971 | 0.095243 |
| chi=100 | 0.415004 | 0.201146 |

## Table S.21: Fitting Parameters for T8A C8A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.03 | 0.00578 | 0.487 | 0.197 | 0.00348 | 1.3 | 0.283 | 0.0194 | 1.42 | 0.21 | 0.0273 | 1.7 | 0.371 | 0.00438 | 2.4 | 0.373 | 0.00533 |
| 2.05 | -0.00756 | 0.443 | 0.185 | 0.00428 | 1.21 | 0.228 | 0.00424 | 1.41 | 0.214 | 0.0328 | 1.56 | 0.441 | 0.0183 | 2.42 | 0.459 | 0.0114 |
| 3.05 | -0.00999 | 0.419 | 0.173 | 0.00563 | 1.41 | 0.227 | 0.0413 | 1.72 | 0.392 | 0.0058 | 1.15 | 0.201 | 0.00169 | 2.41 | 0.499 | 0.016 |
| 4.05 | -0.00999 | 0.41 | 0.156 | 0.00592 | 1.41 | 0.222 | 0.0399 | 1.77 | 0.407 | 0.0057 | 1.13 | 0.191 | 0.00148 | 2.46 | 0.495 | 0.0168 |
| 5.03 | -0.00175 | 0.408 | 0.133 | 0.00571 | 1.42 | 0.216 | 0.0356 | 1.63 | 0.497 | 0.0207 | 1.16 | 0.243 | 0.00217 | 2.52 | 0.499 | 0.0168 |
| 5.96 | 0.00998 | 0.401 | 0.0952 | 0.00537 | 1.43 | 0.208 | 0.0313 | 1.53 | 0.5 | 0.0405 | 0.8 | 0.5 | 0.0113 | 2.4 | 0.5 | 0.0225 |
| 6.96 | 0.00943 | 0.415 | 0.201 | 0.0114 | 1.41 | 0.221 | 0.0418 | 1.64 | 0.452 | 0.0299 | 0.8 | 0.42 | 0.0114 | 2.45 | 0.499 | 0.0356 |

Figure S.19: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T8A C8A

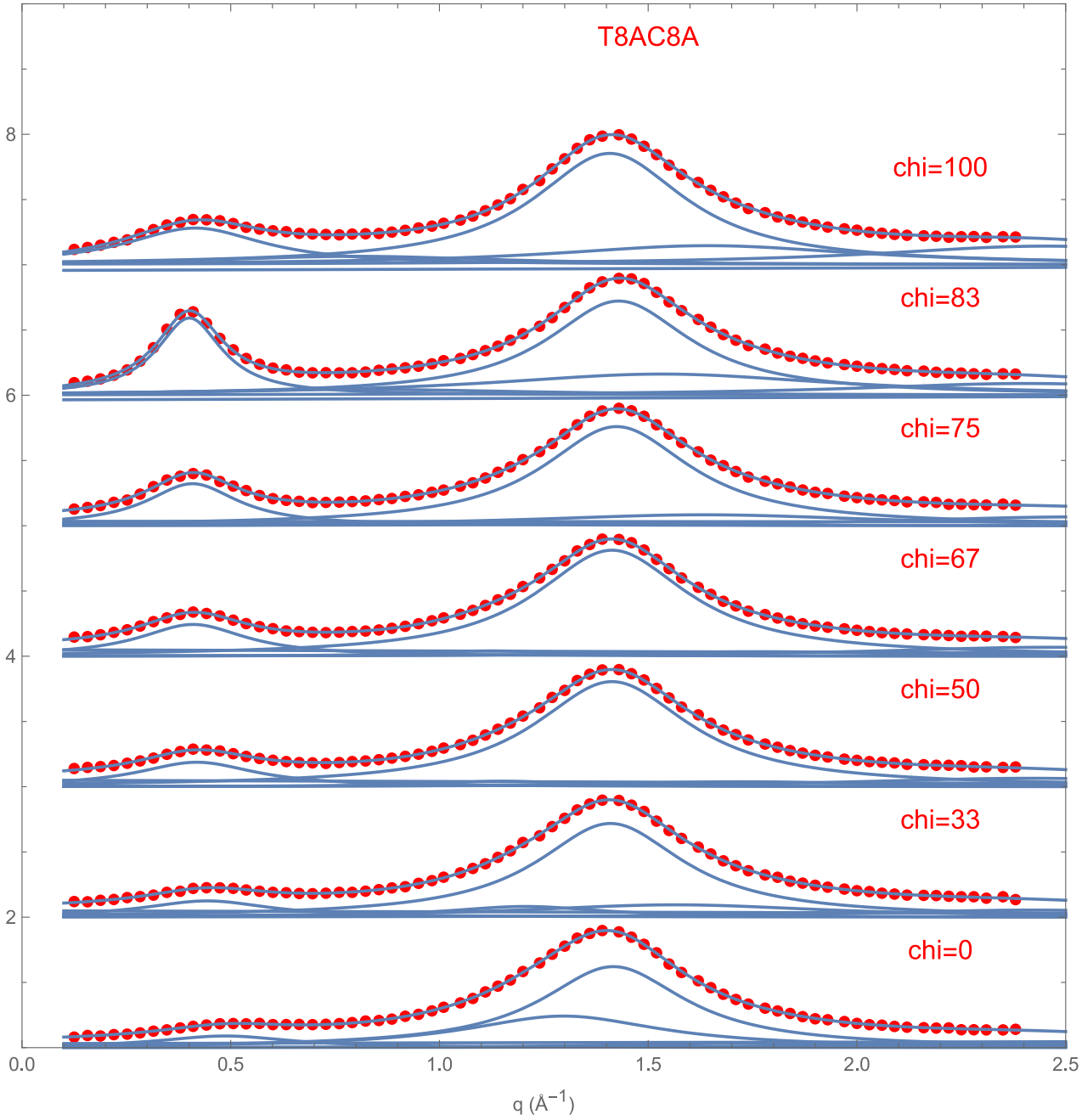
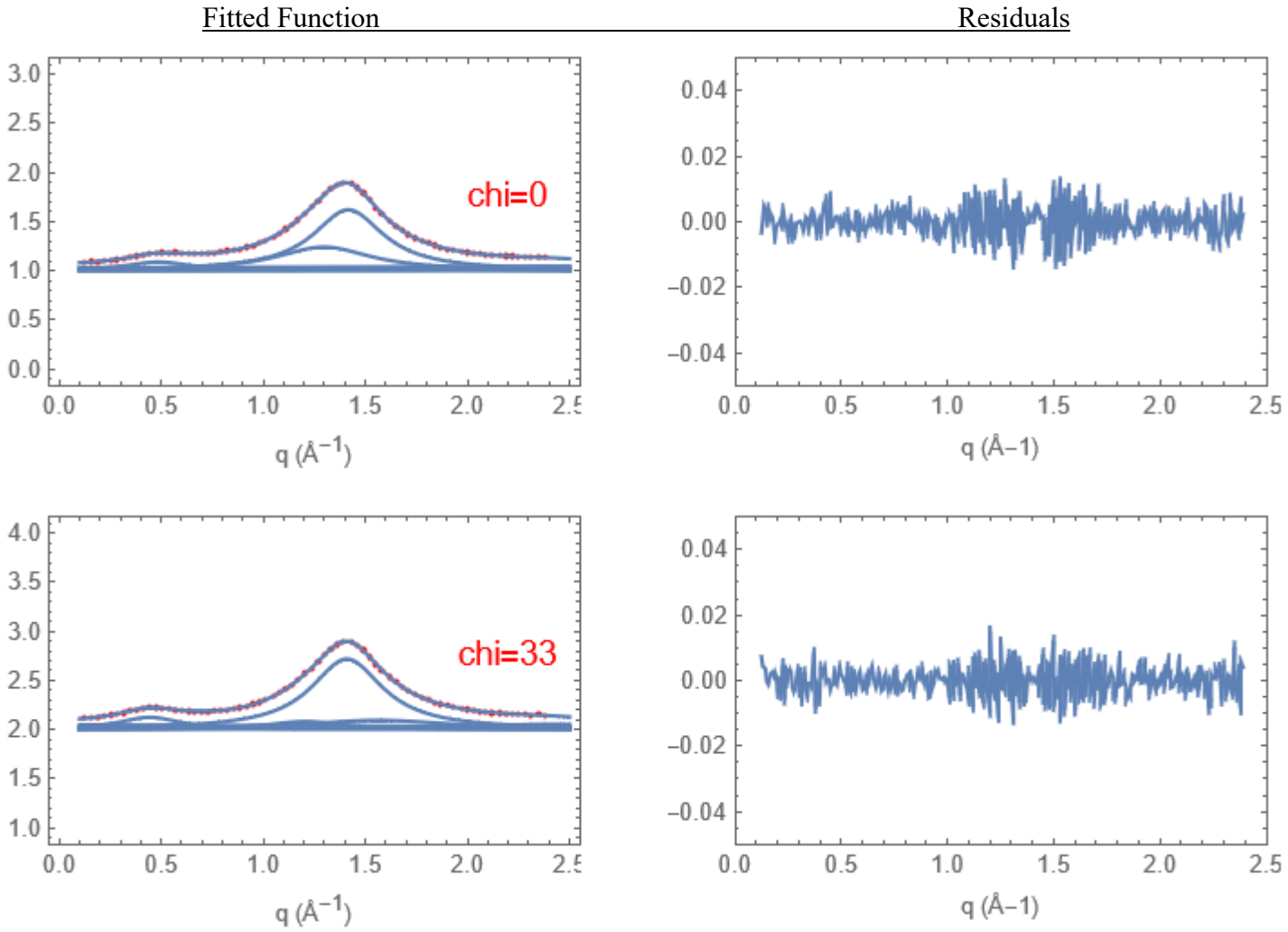
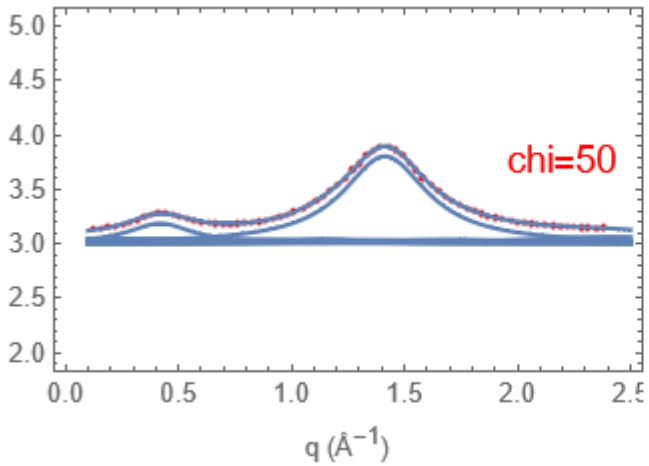
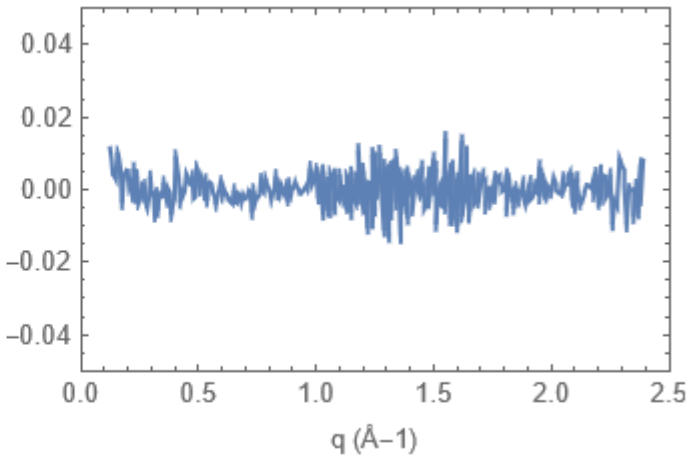
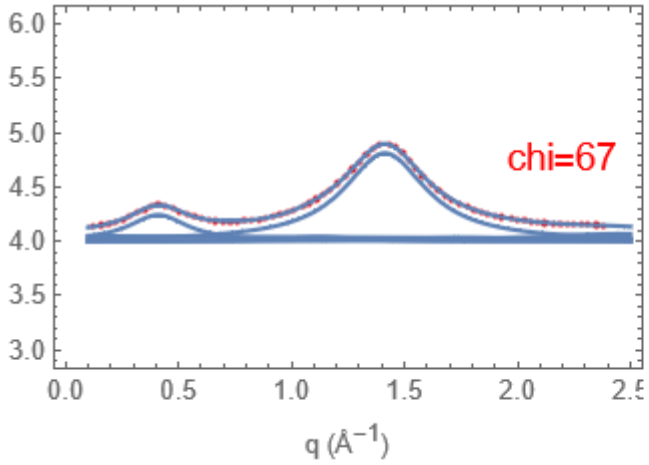


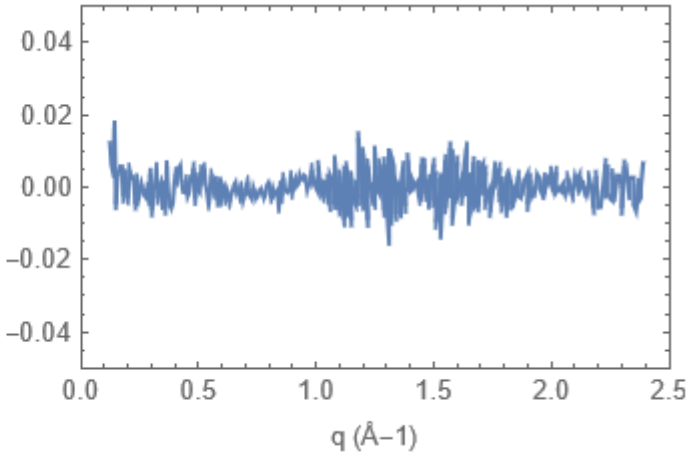
Figure S.20: Fitting functions and residuals for T8A C8A

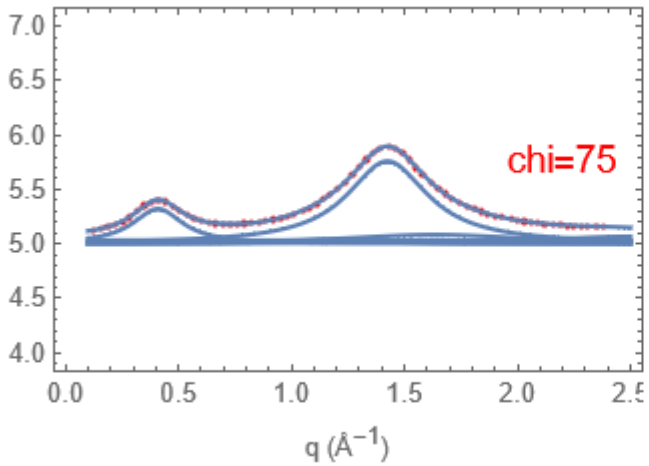


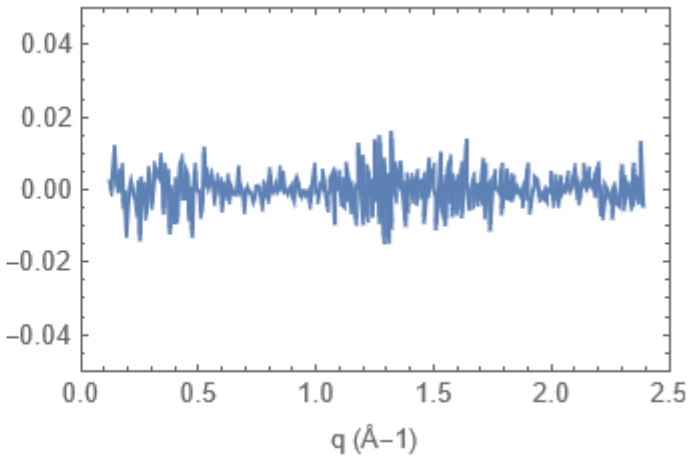

chi=50
q (Å$^{-1}$)

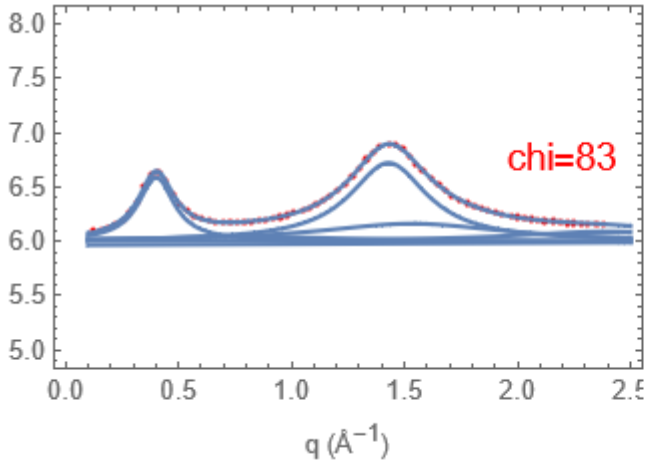

q (Å–1)

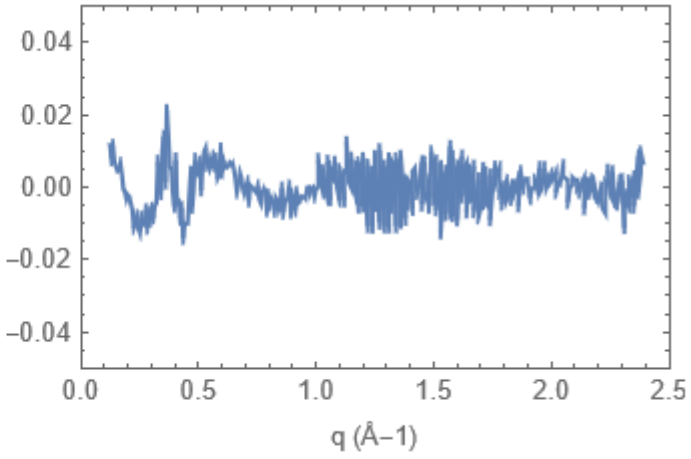

chi=67
q (Å$^{-1}$)

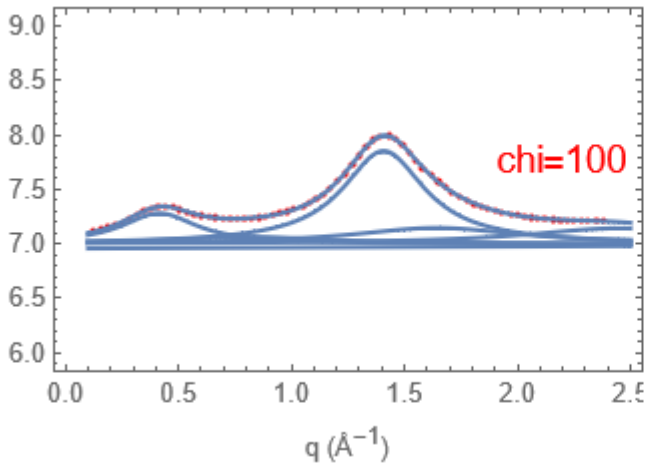

q (Å–1)

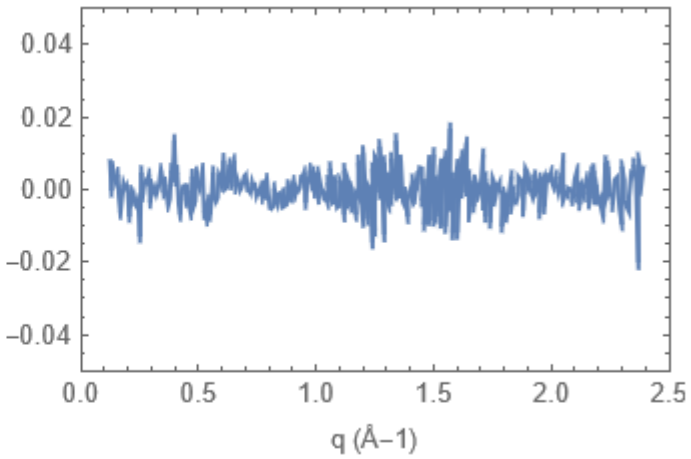

chi=75
q (Å$^{-1}$)


q (Å–1)


chi=83
q (Å$^{-1}$)


q (Å–1)


9.0
8.5
8.0
7.5
7.0
6.5
6.0
chi=100
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
2.5
q (Å−1)

## Table S.22: Local Structure Peaks for T8A C10A

| | T8AC10A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=33 | 0.398975 | 0.0651427 |
| chi=50 | 0.365748 | 0.13925 |
| chi=67 | 0.36291 | 0.0954309 |
| chi=75 | 0.370972 | 0.0910565 |
| chi=83 | 0.365526 | 0.0985632 |

## Table S.23: Fitting Parameters for T8A C10A

| a | b | q01 | w1 | A1 | q02 | w2 | A2 | q03 | w3 | A3 | q04 | w4 | A4 | q05 | w5 | A5 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2.02 | 0.00476 | 0.0623 | 0.0651 | 0.000154 | 0.399 | 0.199 | 0.00691 | 1.35 | 0.286 | 0.0333 | 1.4 | 0.192 | 0.0166 | 2.16 | 0.352 | 0.00466 |
| 3.05 | -0.00944 | 0.366 | 0.139 | 0.00345 | 0.44 | 0.153 | 0.00159 | 1.37 | 0.287 | 0.0263 | 1.4 | 0.197 | 0.0203 | 2.04 | 0.49 | 0.0121 |
| 4. | 0.00935 | 0.363 | 0.0954 | 0.00258 | 0.427 | 0.144 | 0.00275 | 1.45 | 0.695 | 0.0537 | 1.41 | 0.21 | 0.0338 | 2.47 | 0.166 | 0.00625 |
| 4.97 | 0.00922 | 0.371 | 0.0911 | 0.00376 | 0.475 | 0.186 | 0.00227 | 1.44 | 0.697 | 0.0686 | 1.41 | 0.205 | 0.0315 | 2.8 | 0.4 | 0.0366 |
| 5.96 | 0.00877 | 0.366 | 0.0986 | 0.00417 | 1.44 | 0.695 | 0.0628 | 0.5 | 0.245 | 0.00383 | 1.41 | 0.203 | 0.0315 | 2.81 | 0.568 | 0.0565 |
| a | b | q01 | w1 | A1 | q02 | w2 | A2 | q03 | w3 | A3 | q04 | w4 | A4 | q05 | w5 | A5 |
| 2.02 | 0.00476 | 0.0623 | 0.0651 | 0.000154 | 0.399 | 0.199 | 0.00691 | 1.35 | 0.286 | 0.0333 | 1.4 | 0.192 | 0.0166 | 2.16 | 0.352 | 0.00466 |

Figure S.21: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T8A C10A

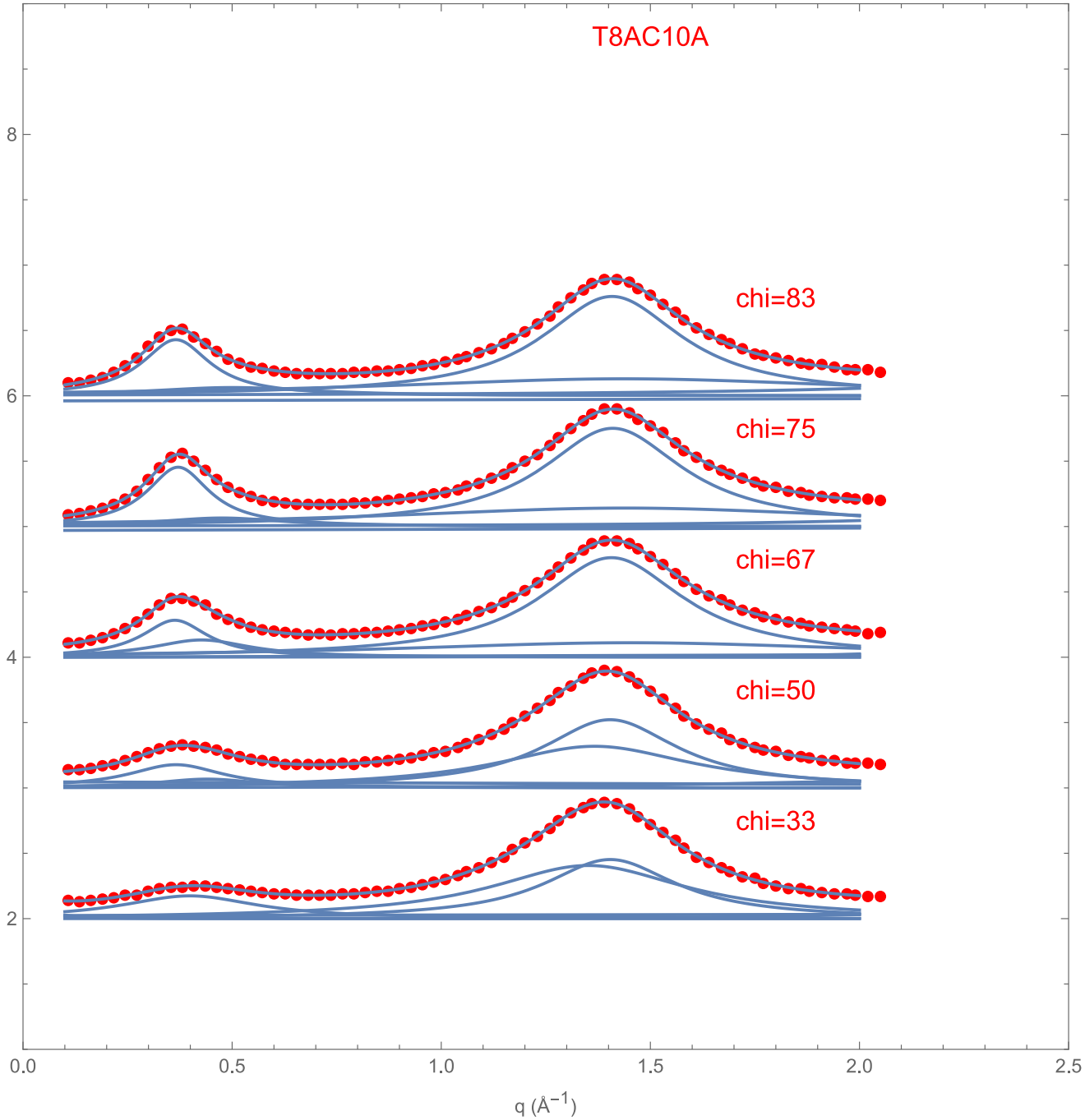
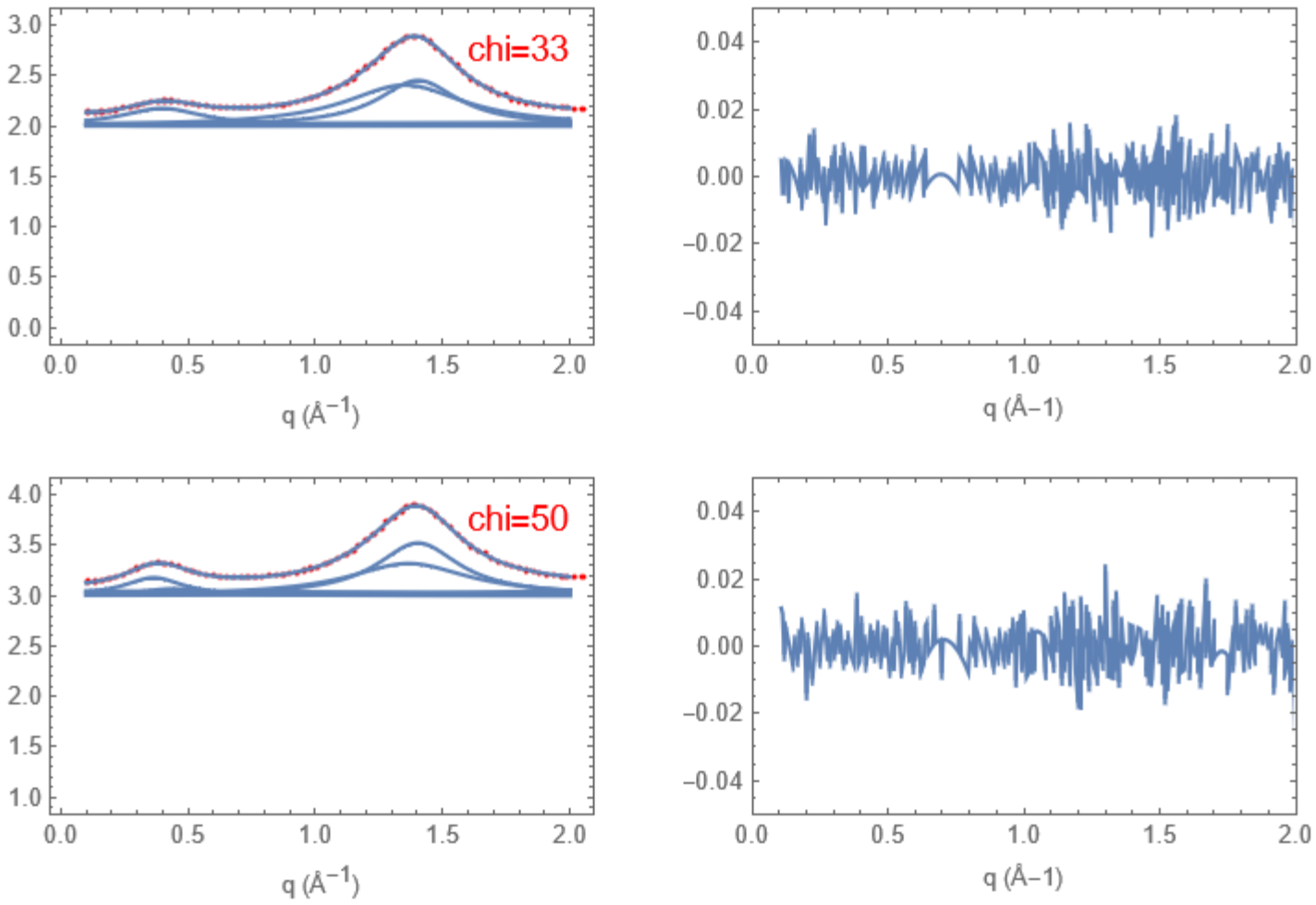
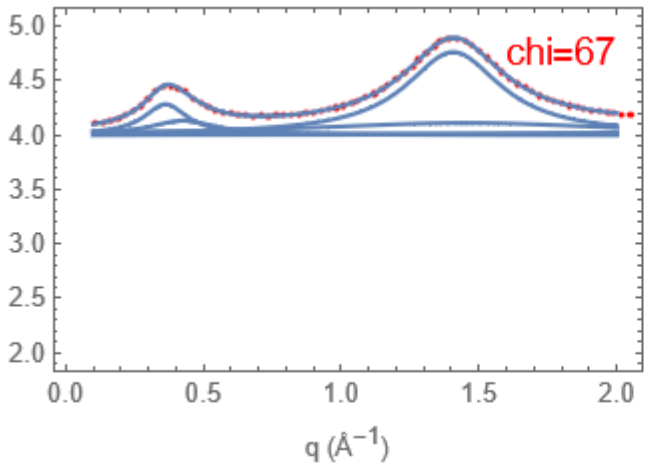
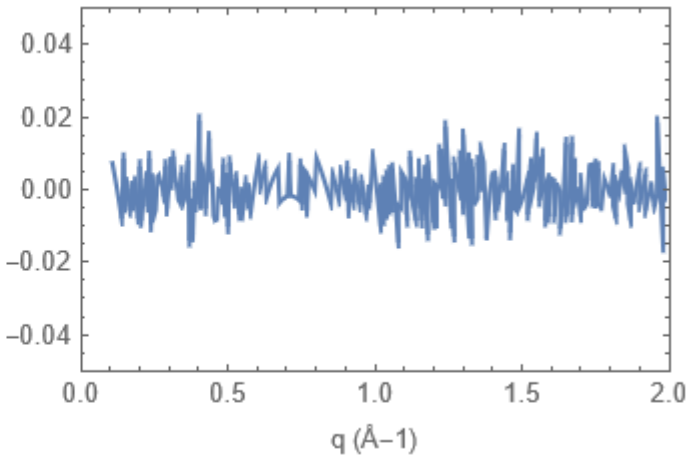
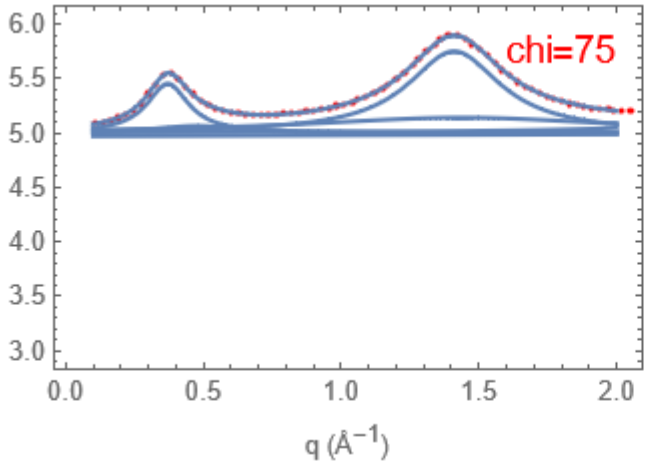


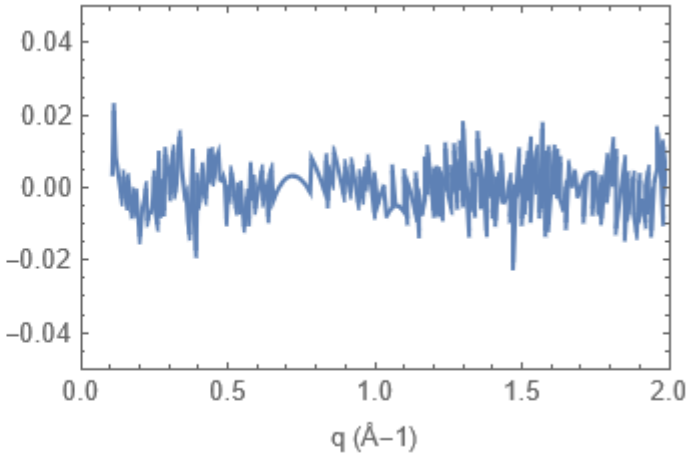
Figure S.22: Fitting functions and residuals for T8A C10A

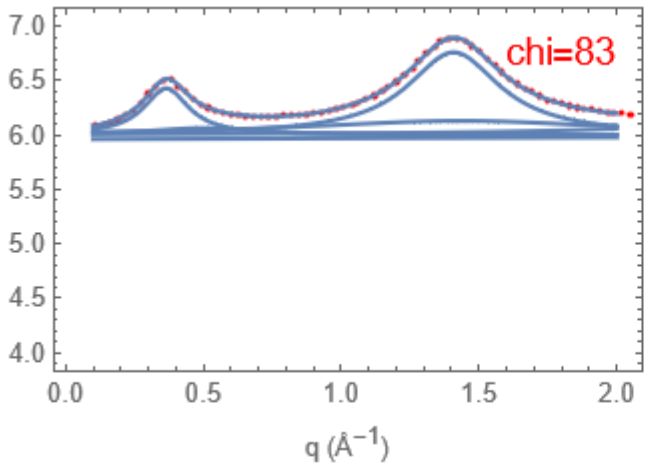


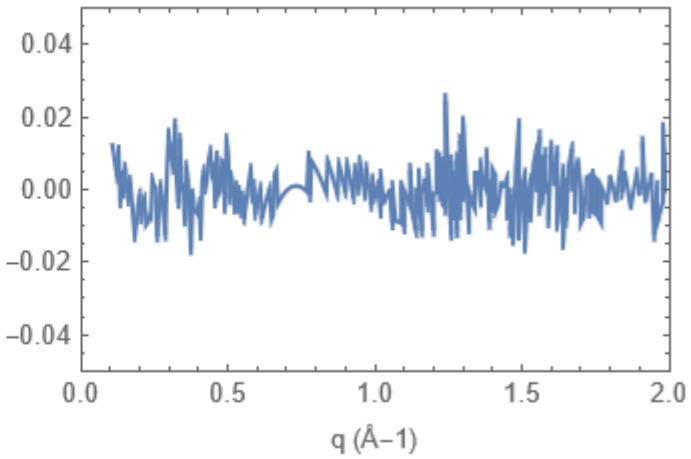

chi=67
5.0
4.5
4.0
3.5
3.0
2.5
2.0
0.0
0.5
1.0
1.5
2.0
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
q (Å−1)


chi=75
6.0
5.5
5.0
4.5
4.0
3.5
3.0
0.0
0.5
1.0
1.5
2.0
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
q (Å−1)


chi=83
7.0
6.5
6.0
5.5
5.0
4.5
4.0
0.0
0.5
1.0
1.5
2.0
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
q (Å−1)

## S.3: Fitting Information for Mixtures Presented in Figure 5

**D2A C6A**

### Table S.24: Local Structure Peaks for D2A C6A

| | D2AC6A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | | |
| chi=33 | 0.435191 | 0.183095 |
| chi=50 | 0.393032 | 0.12822 |
| chi=67 | 0.377885 | 0.122103 |
| chi=75 | 0.417971 | 0.122238 |
| chi=83 | 0.406208 | 0.131294 |
| chi=100 | 0.476237 | 0.194581 |

### Table S.25: Fitting Parameters for D2A C6A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.02 | 0.00603 | 0.12 | 0.253 | 0.00492 | 0.983 | 0.36 | 0.026 | 1.32 | 0.367 | 0.0326 | 1.54 | 0.283 | 0.0568 | 2.38 | 0.384 | 0.0103 |
| 2 | 0.0331 | 0.435 | 0.183 | 0.00866 | 0.822 | 0.343 | 0.0231 | 1.53 | 0.312 | 0.0397 | 1.49 | 0.399 | 0.059 | 2.35 | 0.501 | 0.0189 |
| 2.95 | 0.1 | 0.393 | 0.128 | 0.00569 | 0.745 | 0.357 | 0.0243 | 1.57 | 0.352 | 0.069 | 1.34 | 0.355 | 0.0266 | 1.94 | 0.457 | 0.0157 |
| 3.95 | 0.0999 | 0.378 | 0.122 | 0.00575 | 0.694 | 0.347 | 0.0209 | 1.33 | 0.343 | 0.0205 | 1.51 | 0.318 | 0.0588 | 1.85 | 0.384 | 0.0118 |
| 4.95 | 0.0865 | 0.418 | 0.122 | 0.00529 | 0.669 | 0.377 | 0.0223 | 1.25 | 0.0602 | 3.25E-05 | 1.48 | 0.293 | 0.0666 | 1.97 | 0.353 | 0.00268 |
| 5.95 | 0.0876 | 0.659 | 0.35 | 0.0164 | 1.26 | 0.174 | 0.000819 | 1.48 | 0.283 | 0.0614 | 0.406 | 0.131 | 0.00657 | 1.98 | 0.438 | 0.005 |
| 7.02 | -0.00955 | 0.644 | 0.247 | 0.00986 | 1.43 | 0.257 | 0.0891 | 1.76 | 0.495 | 0.024 | 0.476 | 0.195 | 0.0121 | 2.41 | 0.499 | 0.0556 |

Figure S.23: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for D2A C6A

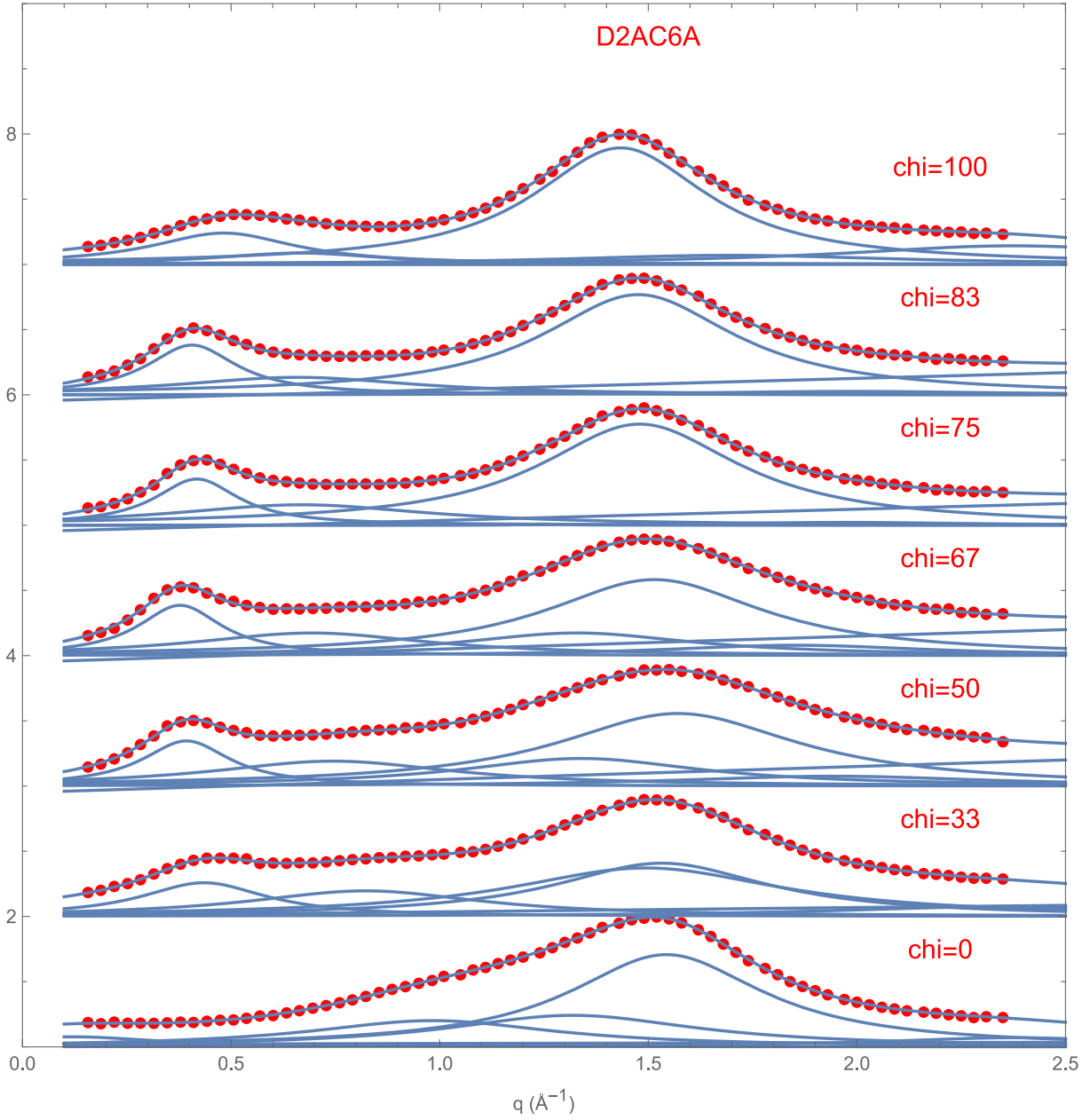
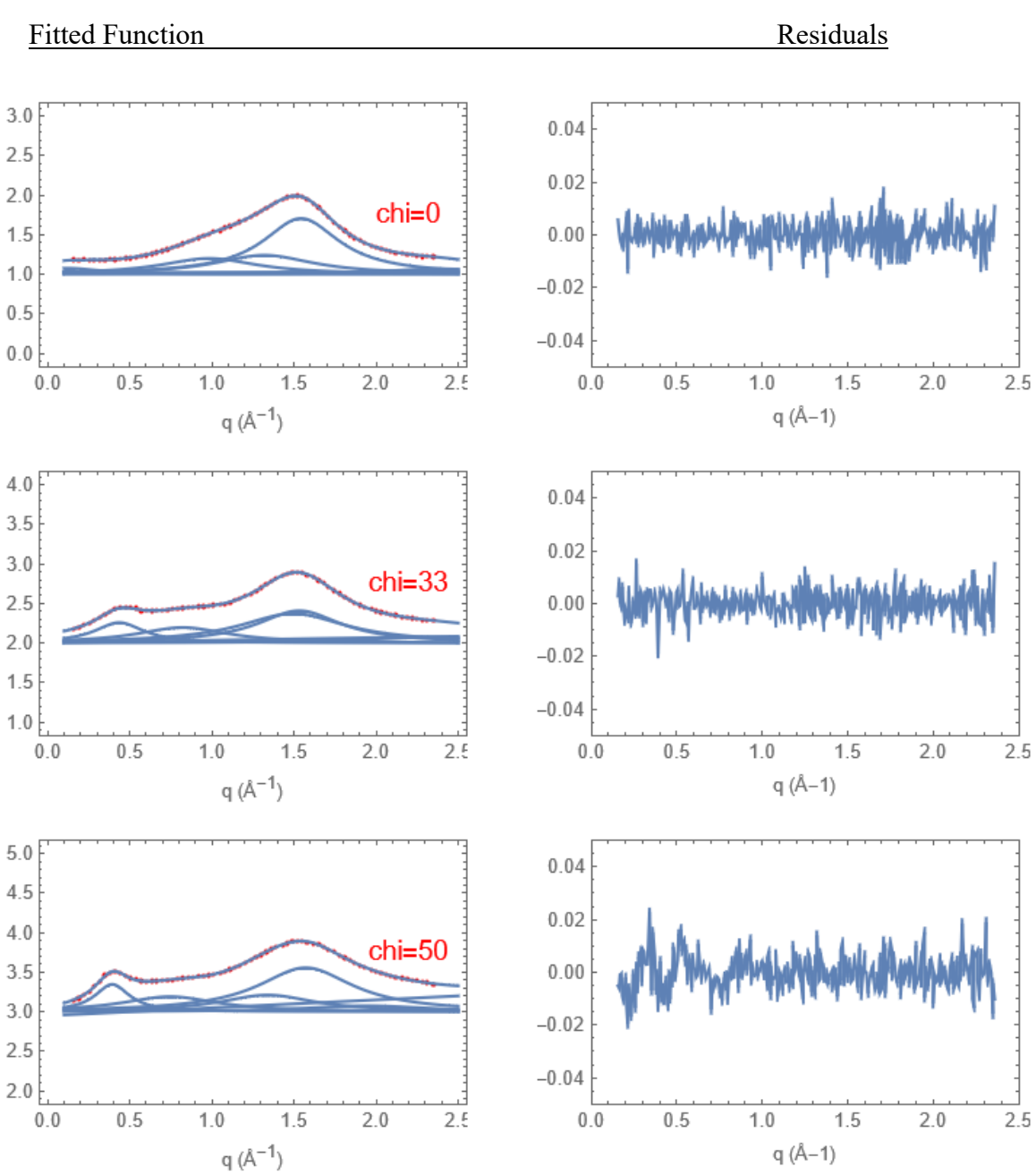
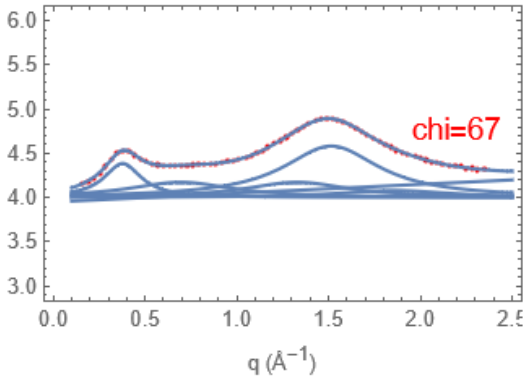
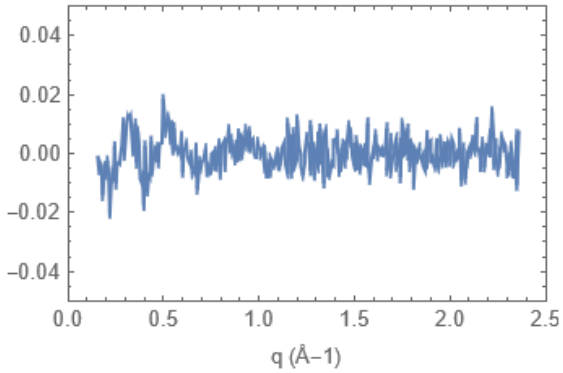
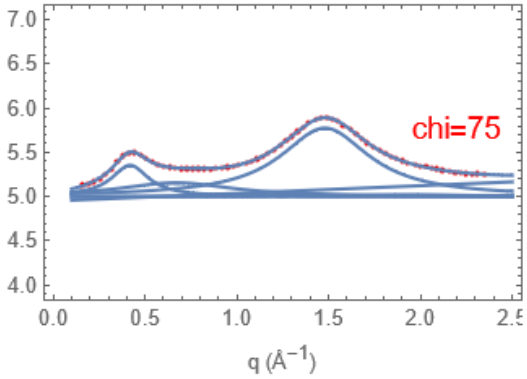


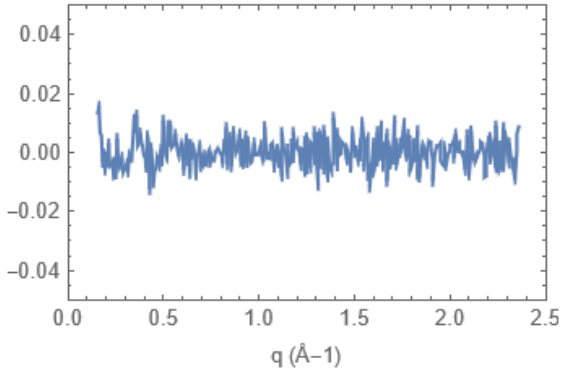
Figure S.24: Fitting functions and residuals for D2A C6A

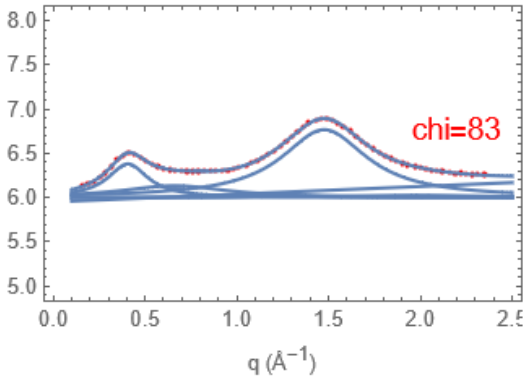


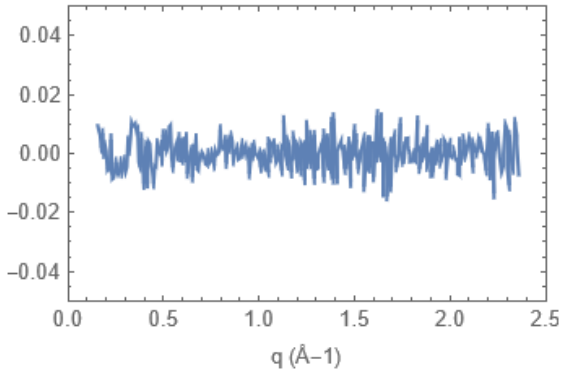

chi=67
q (Å$^{-1}$)

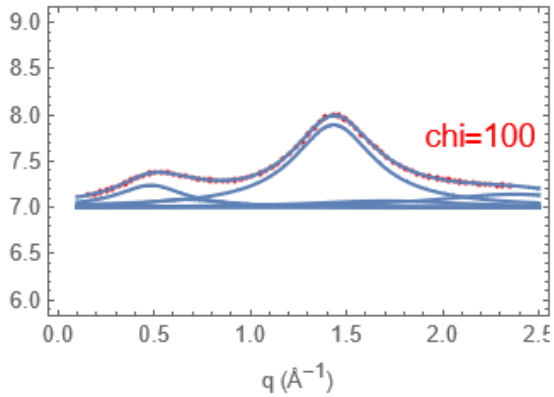

q (Å−1)

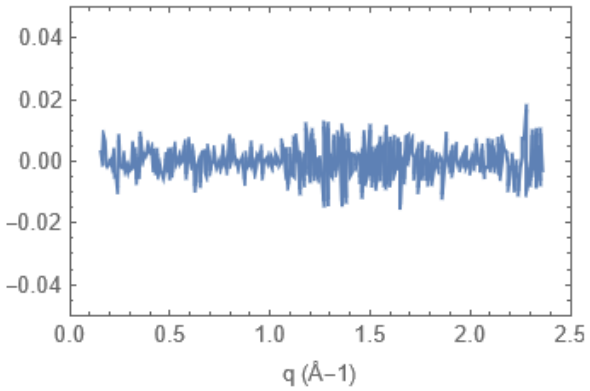

chi=75
q (Å$^{-1}$)


q (Å−1)


chi=83
q (Å$^{-1}$)


q (Å−1)


chi=100
q (Å$^{-1}$)


q (Å–1)

**D2A C8A**

## Table S.26: Local Structure Peaks for D2A C8A

| | D2AC8A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | 0 | 0 |
| chi=33 | 0.37889 | 0.166774 |
| chi=50 | 0.40049 | 0.155585 |
| chi=67 | 0.379101 | 0.119802 |
| chi=75 | 0.374985 | 0.113 |
| chi=83 | 0.377083 | 0.124475 |
| chi=100 | 0.418 | 0.186 |

## Table S.27: Fitting Parameters for D2A C8A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.01 | -0.0088 | 0.0752 | 0.289 | 0.00644 | 2.38 | 0.185 | 0.00273 | 1.05 | 0.399 | 0.0414 | 1.52 | 0.317 | 0.0787 | 2.13 | 0.173 | 0.000949 |
| 1.98 | 0.0359 | 0.379 | 0.167 | 0.00771 | 2.3 | 0.435 | 0.0142 | 0.977 | 0.451 | 0.052 | 1.46 | 0.228 | 0.0253 | 1.6 | 0.325 | 0.0302 |
| 2.95 | 0.0837 | 0.4 | 0.156 | 0.00627 | 1.71 | 0.308 | 0.0105 | 1.03 | 0.479 | 0.0618 | 1.43 | 0.177 | 0.0104 | 1.54 | 0.206 | 0.0136 |
| 3.95 | 0.0761 | 0.379 | 0.12 | 0.00499 | 1.91 | 0.201 | 0.000202 | 0.85 | 0.538 | 0.0415 | 1.43 | 0.158 | 0.00486 | 1.48 | 0.315 | 0.0573 |
| 4.95 | 0.0733 | 0.375 | 0.113 | 0.00512 | 2.39 | 0.0416 | 3.45E-05 | 0.723 | 0.468 | 0.0244 | 1.43 | 0.182 | 0.0107 | 1.47 | 0.345 | 0.0578 |
| 5.95 | 0.0737 | 0.66 | 0.427 | 0.0176 | 2.32 | 0.00363 | 1.99*10^(-7) | 1.42 | 0.177 | 0.01 | 0.377 | 0.124 | 0.00583 | 1.45 | 0.321 | 0.0514 |
| 6.96 | 0.00948 | 0.418 | 0.186 | 0.0079 | 0.674 | 0.466 | 0.0146 | 2.46 | 0.498 | 0.0303 | 1.41 | 0.218 | 0.0351 | 1.59 | 0.479 | 0.0353 |

Figure S.25: Fitting functions (blue) and raw data (red, 1/5th of points shown) for D2A C8A

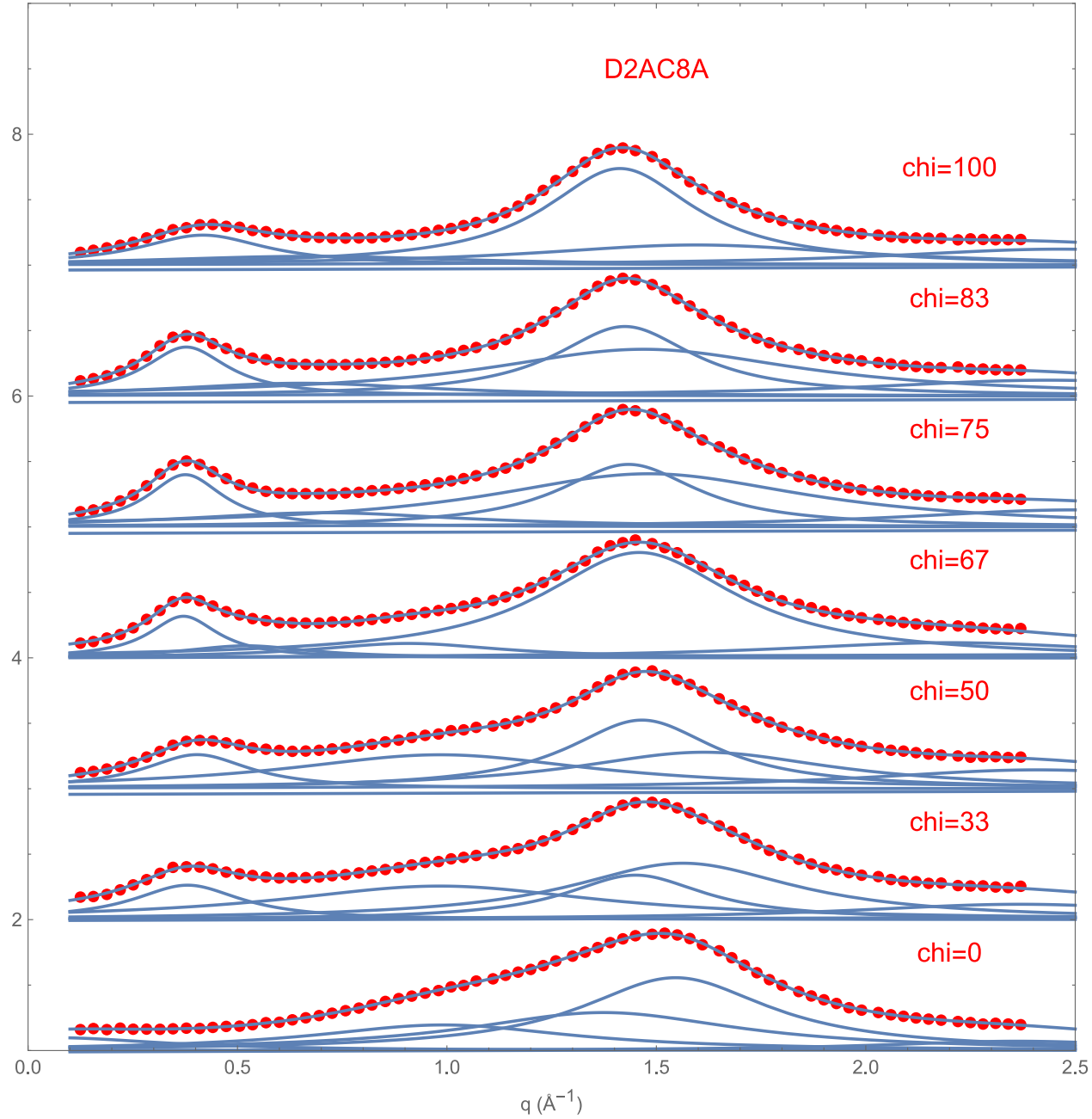
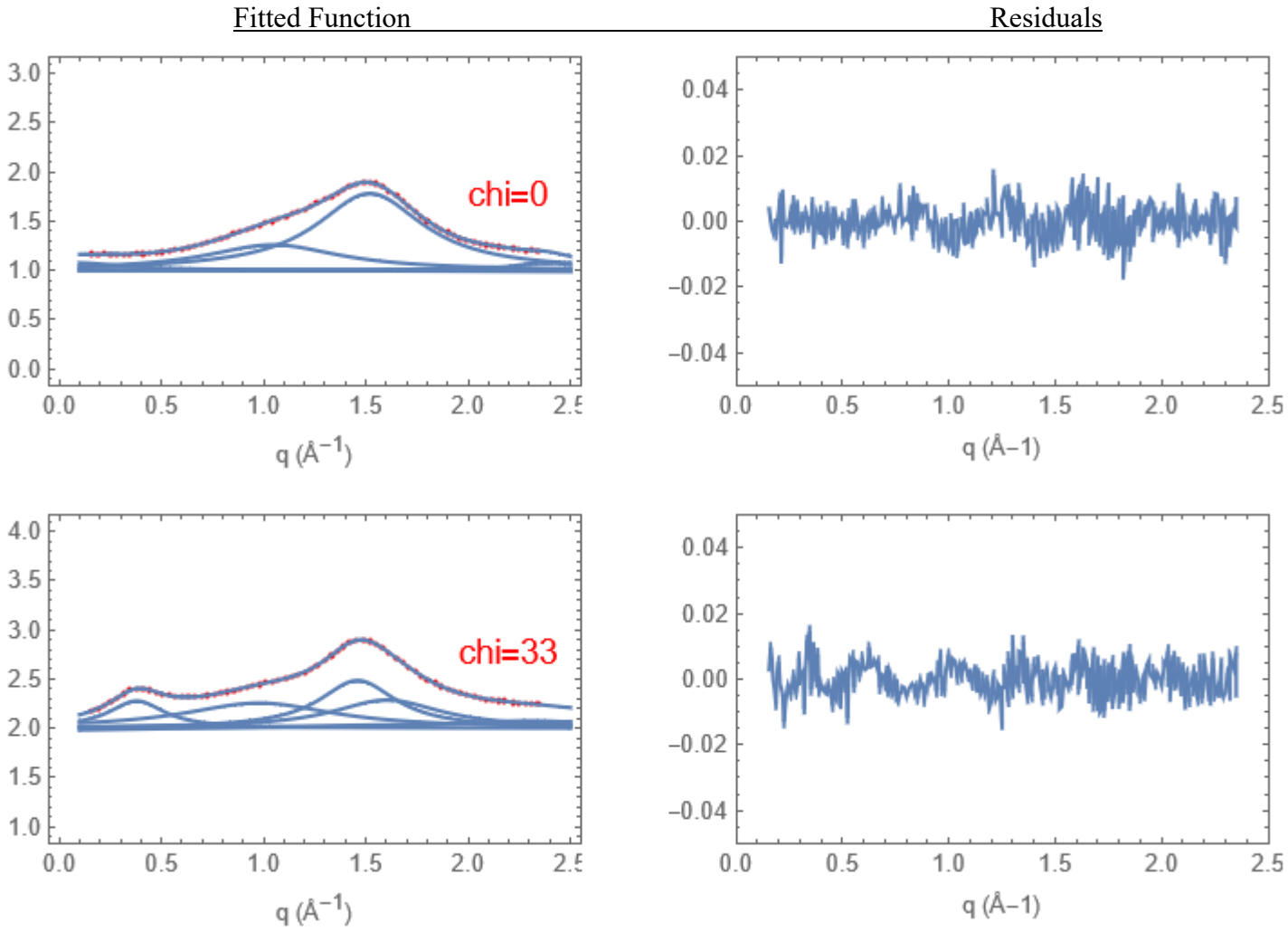
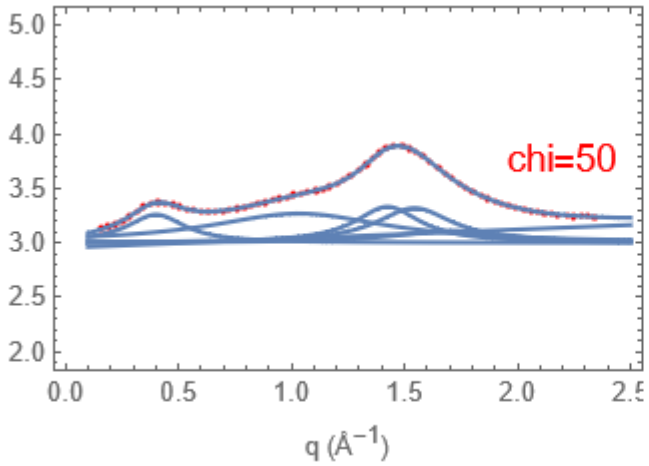
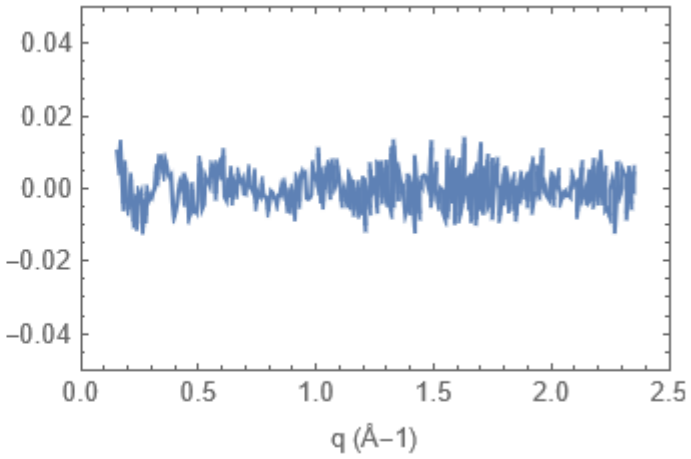
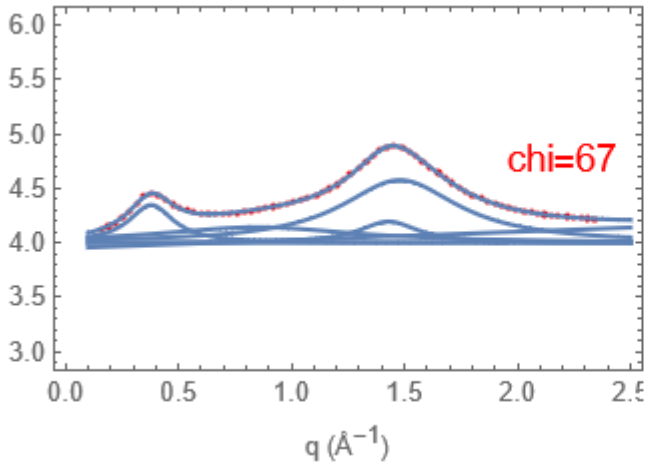


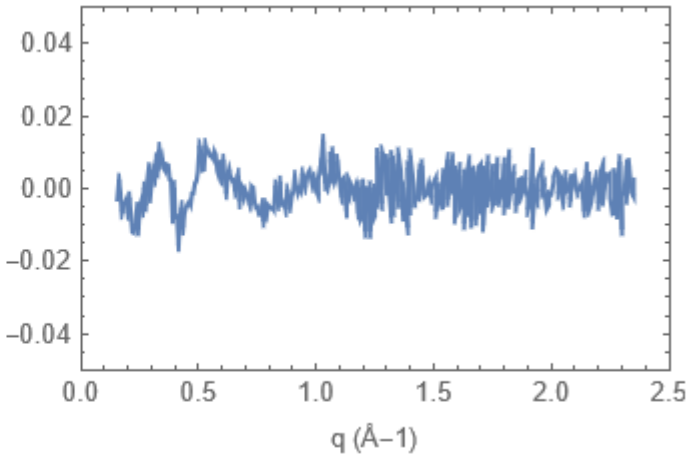
Figure S.26: Fitting functions and residuals for D2A C8A

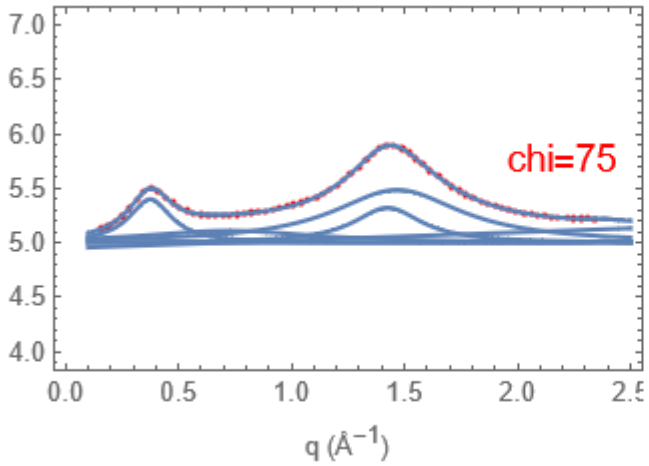


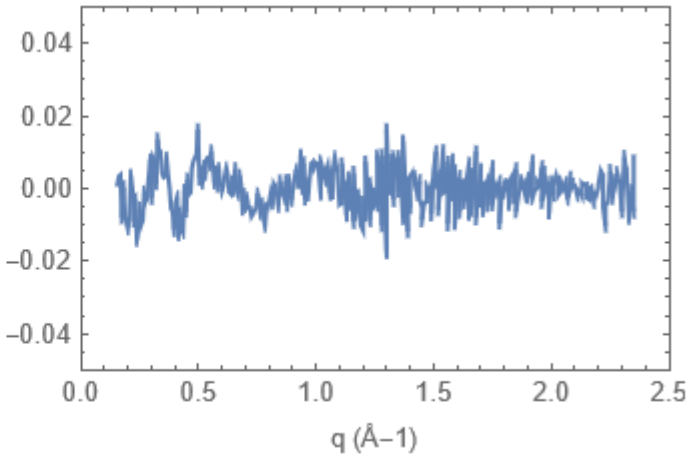

chi=50
q (Å$^{-1}$)

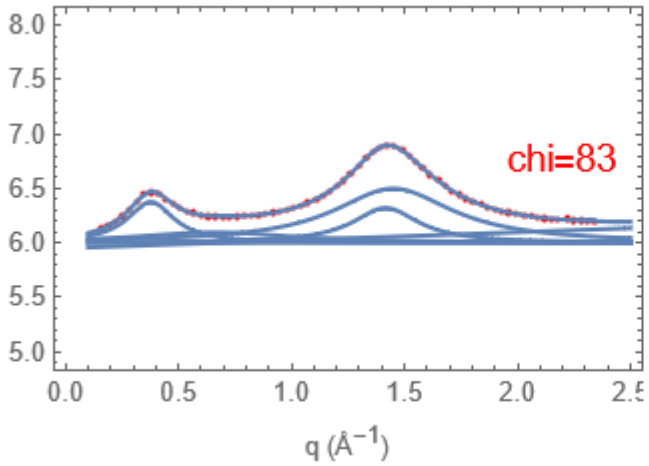

q (Å–1)

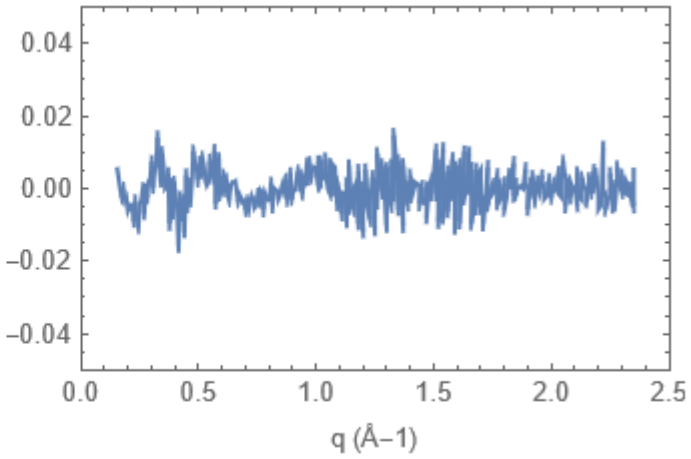

chi=67
q (Å$^{-1}$)

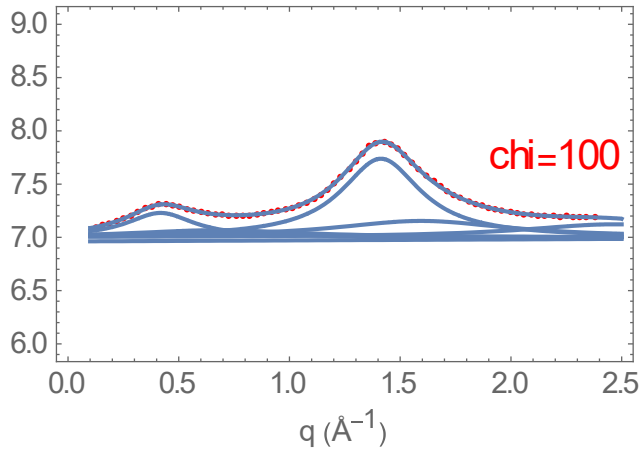

q (Å–1)

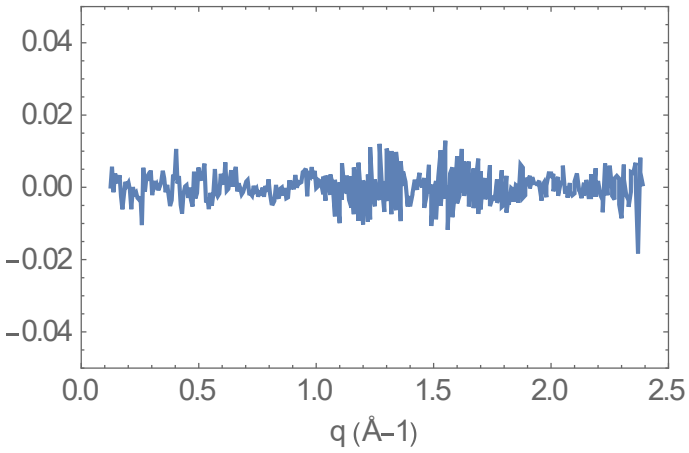

chi=75
q (Å$^{-1}$)


q (Å−1)


chi=83
q (Å$^{-1}$)


q (Å−1)


chi=100
9.0
8.5
8.0
7.5
7.0
6.5
6.0
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
2.5
q (Å–1)

## S.4: Fitting Information for Mixtures Presented in Figure 6

**M18A C8A**

### Table S.28: Local Structure Peaks for M18A C8A

| | M18AC8A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=75 | 0.318451 | 0.069415 |
| chi=83 | 0.332883 | 0.080044 |
| chi=100 | 0.41763 | 0.185602 |

### Table S.29: Fitting Parameters for M18A C8A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.0222 | 0.00999 | 0.318 | 0.0694 | 0.00244 | 1.4 | 0.155 | 0.0101 | 1.47 | 0.3 | 0.0403 | 2.25 | 0.3 | 0.00545 | 0.398 | 0.111 | 0.00227 |
| 1.02 | 0.00999 | 0.333 | 0.08 | 0.00247 | 1.41 | 0.182 | 0.0181 | 1.48 | 0.329 | 0.0339 | 2.36 | 0.5 | 0.0174 | 0.415 | 0.135 | 0.00326 |
| 1.96 | 0.00948 | 0.418 | 0.186 | 0.0079 | 0.674 | 0.466 | 0.0146 | 2.46 | 0.498 | 0.0303 | 1.41 | 0.218 | 0.0351 | 1.59 | 0.479 | 0.0353 |

Figure S.27: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for M18A C8A

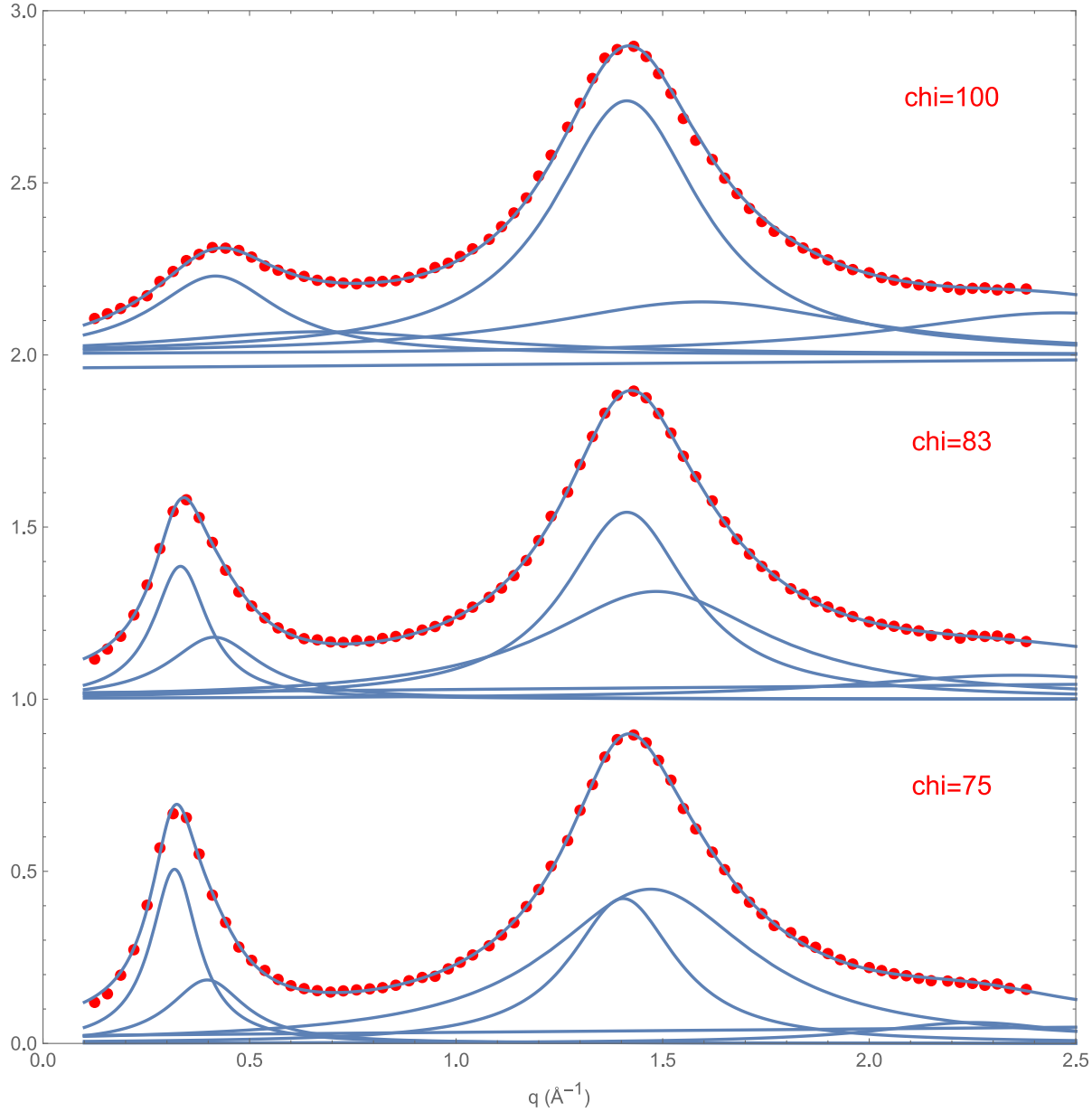
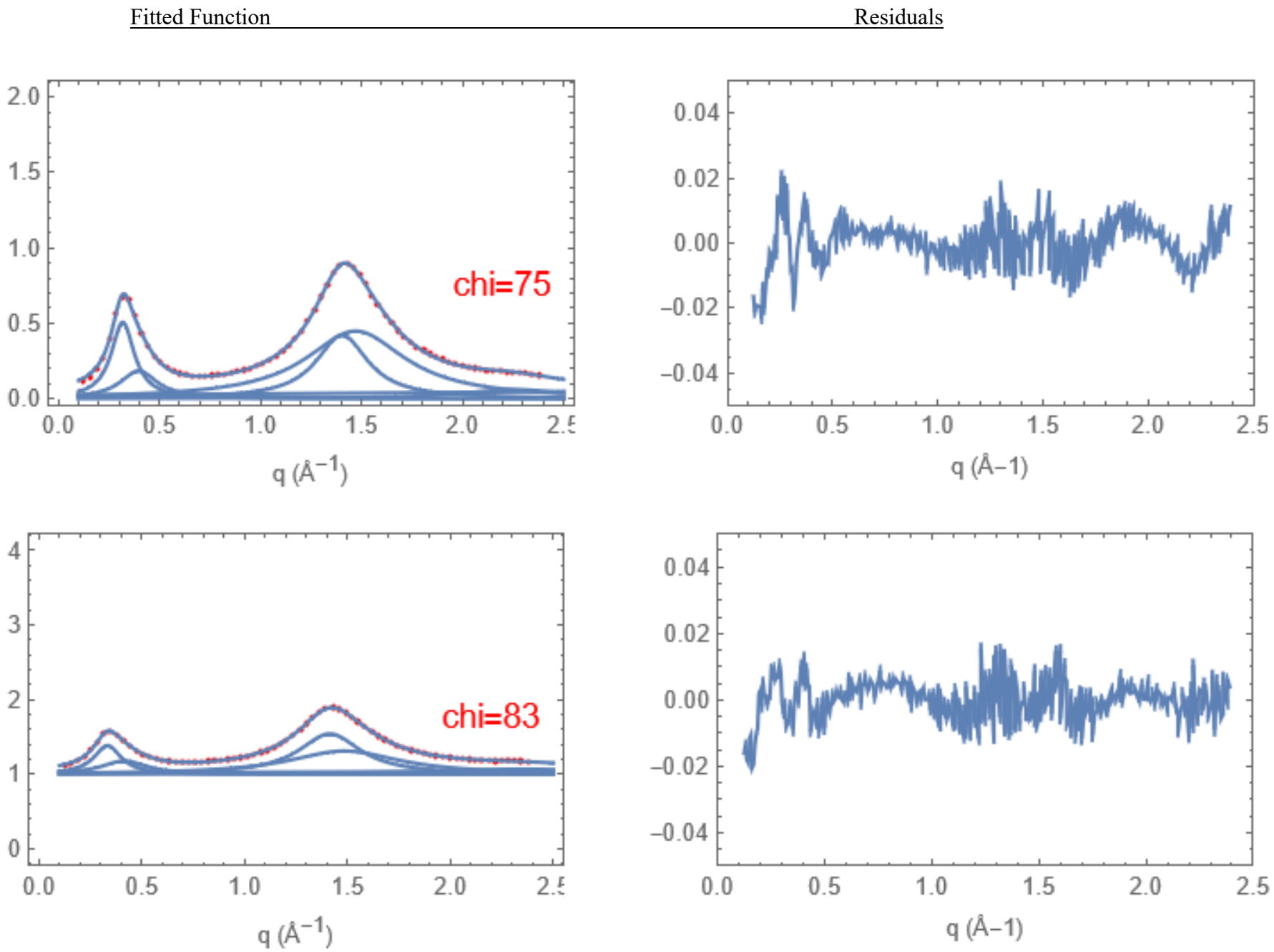
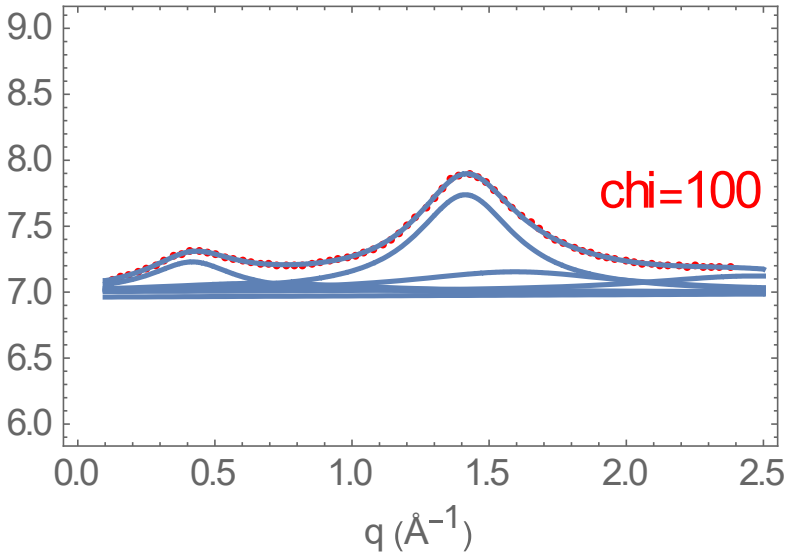
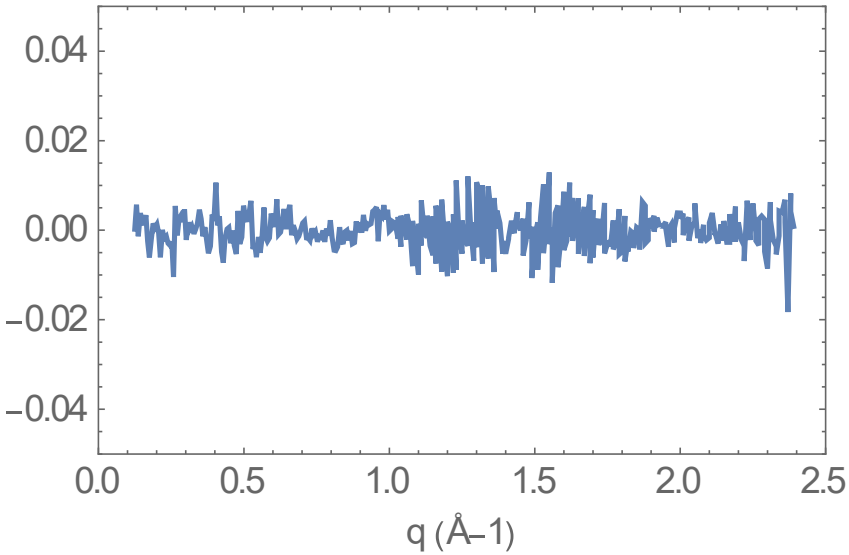


Figure S.28: Fitting functions and residuals for M18A C8A




9.0
8.5
8.0
7.5
7.0
6.5
6.0
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)
chi=100


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
2.5
q (Å–1)

## S.5: Fitting Information for Mixtures Presented in Figure 7

**T6A HCyc**

### Table S.30: Local Structure Peaks for T6a HCyc

| | T6AHCYC | | |
|---|---|---|---|
| | q (Å^-1) | w (Å^-1) | D |
| 0 | 0 | 0 | |
| chi=33 | 0.516731 | 0.141115 | 12.15948 |
| chi=50 | 0.501485 | 0.12816 | 12.52915 |
| chi=67 | 0.514674 | 0.100444 | 12.20808 |
| chi=75 | 0.512741 | 0.102592 | 12.2541 |
| chi=83 | 0.560425 | 0.186199 | 11.21146 |

### Table S.31: Fitting Parameters for T6a HCyc

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | | | | | | | |
| 2.05 | 0.015 | -0.301 | 0.0934 | 0.0205 | 0.517 | 0.141 | 0.00234 | 1.34 | 0.188 | 0.0198 | 0.657 | 0.123 | 0.000907 | 1.49 | 0.323 | 0.0322 |
| 3.05 | 0.015 | 0.501 | 0.128 | 0.00377 | 0.631 | 0.105 | 0.000814 | 1.33 | 0.173 | 0.0187 | 0.119 | 0.173 | 0.00237 | 1.53 | 0.347 | 0.0334 |
| 4.01 | -0.015 | 0.515 | 0.1 | 0.00373 | 0.668 | 0.146 | 0.00205 | 1.31 | 0.172 | 0.0199 | 1.57 | 0.344 | 0.0376 | 2.36 | 0.5 | 0.0315 |
| 5.01 | -0.015 | 0.513 | 0.103 | 0.00366 | 0.666 | 0.152 | 0.00224 | 1.31 | 0.171 | 0.02 | 1.56 | 0.35 | 0.037 | 2.37 | 0.5 | 0.0319 |
| 6 | 0.00289 | 0.56 | 0.186 | 0.00722 | 2.48 | 0.497 | 0.0228 | 1.23 | 0.118 | 0.00337 | 1.33 | 0.162 | 0.0133 | 1.56 | 0.442 | 0.0487 |

Figure S.29: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T6A HCyc

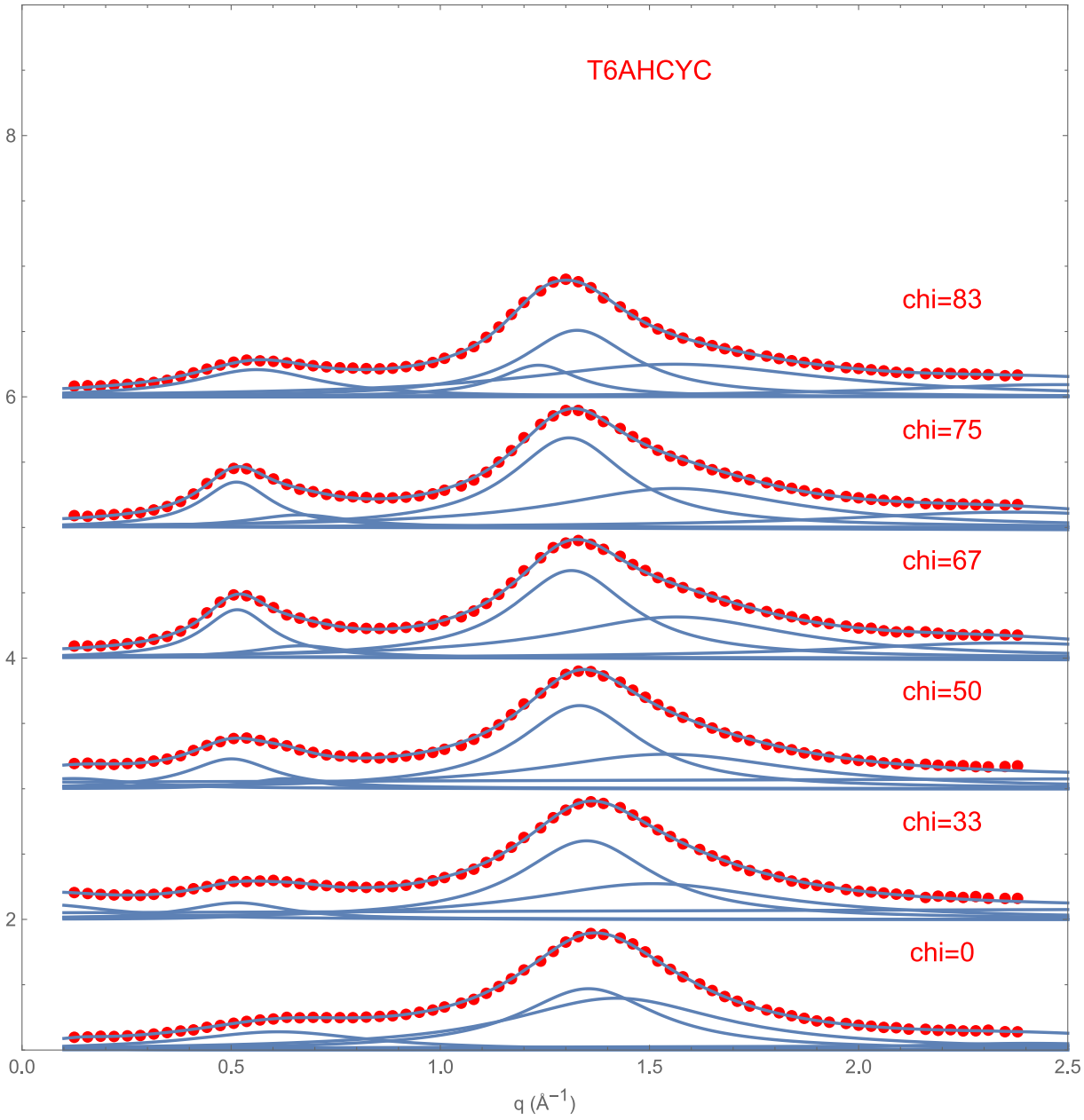
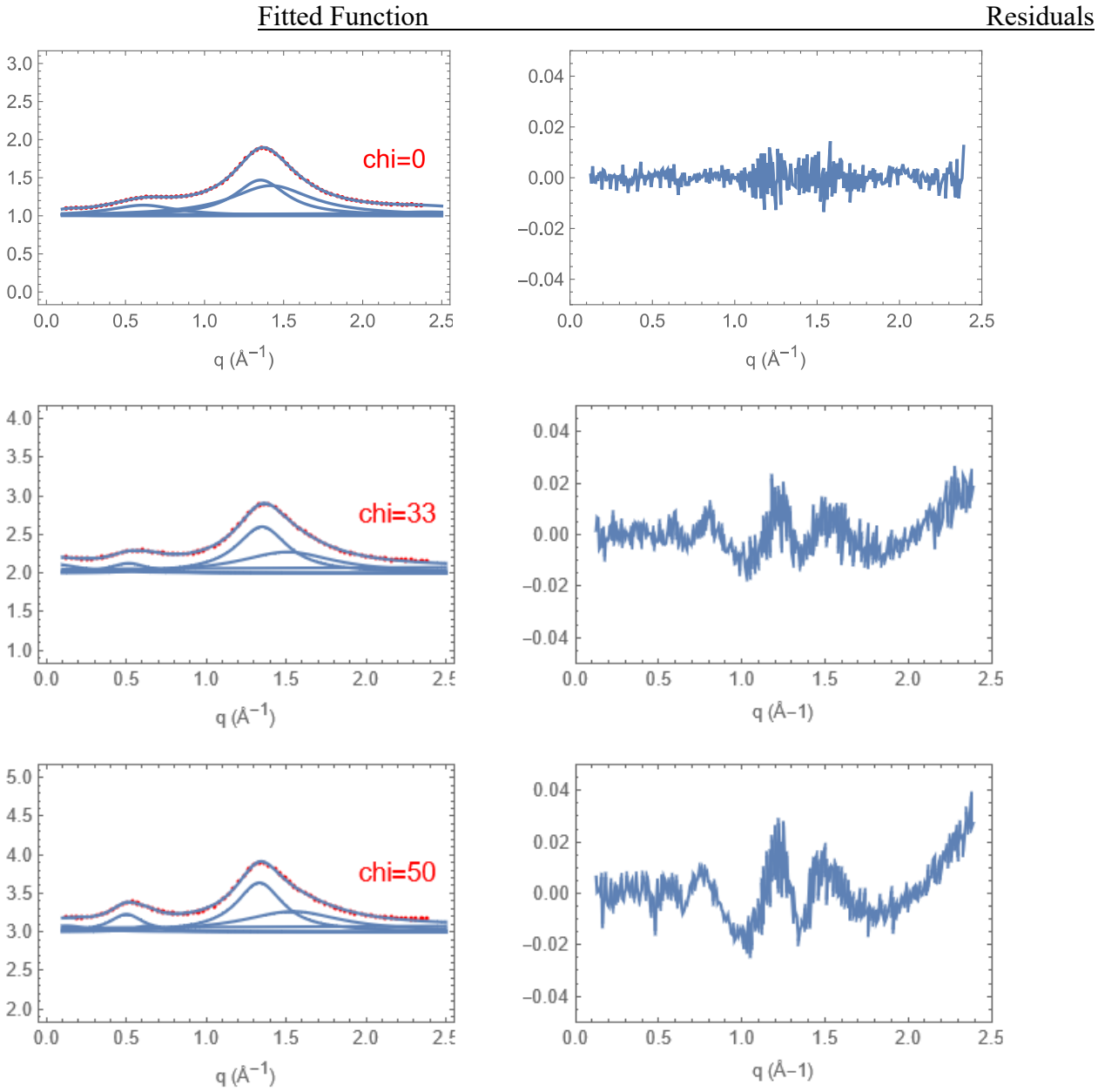
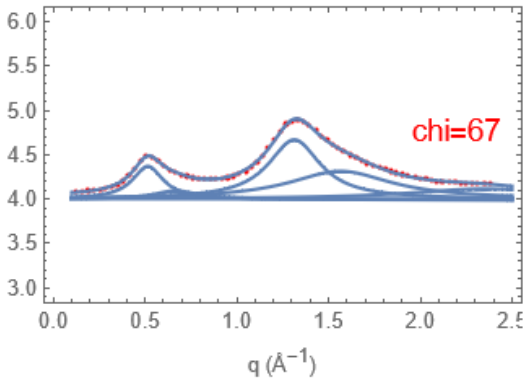
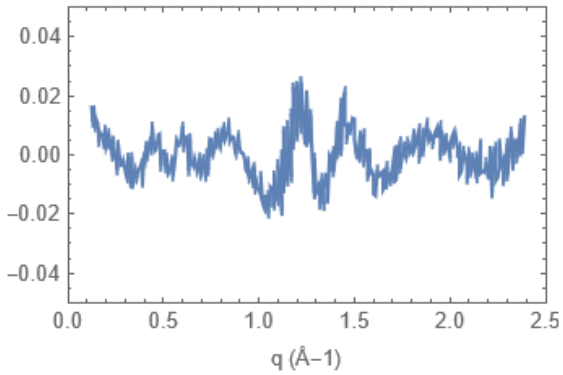
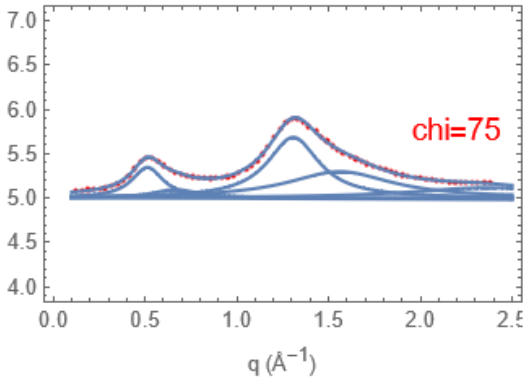


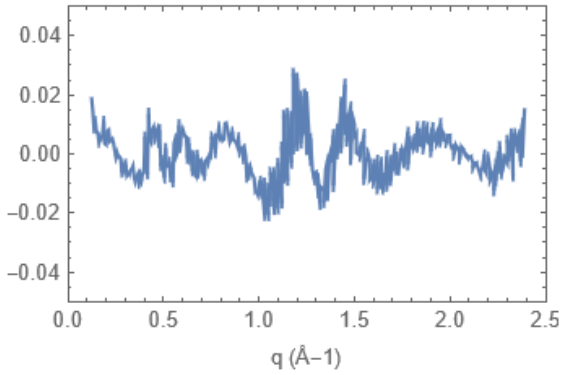
Figure S.30: Fitting functions and residuals for T6A HCyc

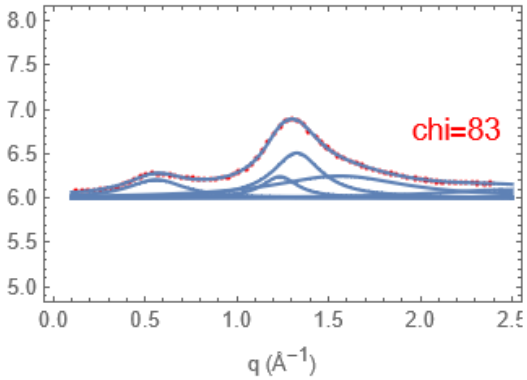


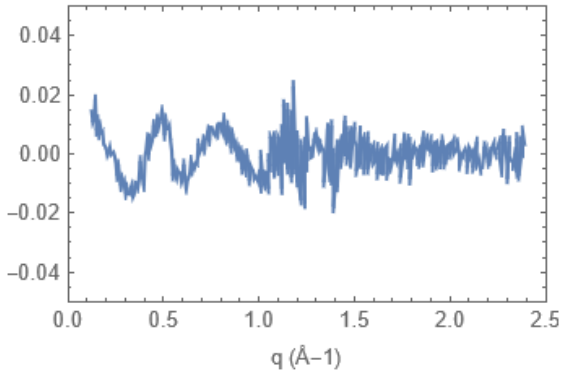

chi=67
q (Å$^{-1}$)


q (Å−1)


chi=75
q (Å$^{-1}$)


q (Å−1)


chi=83
q (Å$^{-1}$)


q (Å−1)

## Table S.32: Local Structure Peaks for T6A HBz

| | T6AHBz | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | 0.613009 | 0.260993 |
| chi=33 | 0.53251 | 0.226206 |
| chi=50 | 0.518535 | 0.173511 |
| chi=67 | 0.527031 | 0.114658 |

## Table S.33: Fitting Parameters for T2A C6A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.011 | 0.00886 | 0.142 | 0.0693 | 8.99E-05 | 0.613 | 0.261 | 0.00948 | 1.35 | 0.2 | 0.0187 | 1.42 | 0.312 | 0.0385 | 2.41 | 0.387 | 0.0076 |
| 0.981 | 0.00984 | 0.000547 | 0.0758 | 0.00679 | 0.533 | 0.226 | 0.00993 | 1.35 | 0.219 | 0.0209 | 1.51 | 0.334 | 0.0384 | 2.5 | 0.499 | 0.0188 |
| 1.97 | 0.00991 | 0.00437 | 0.119 | 0.00987 | 0.519 | 0.174 | 0.0101 | 1.35 | 0.223 | 0.0235 | 1.53 | 0.329 | 0.054 | 2.52 | 0.5 | 0.0261 |
| 3.03 | 0.0095 | 1.38 | 0.212 | 0.0177 | 0.527 | 0.115 | 0.0065 | 1.24 | 0.161 | 0.00297 | 1.58 | 0.302 | 0.0481 | 2.39 | 0.263 | 0.00372 |

Figure S.31: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T6A HBz

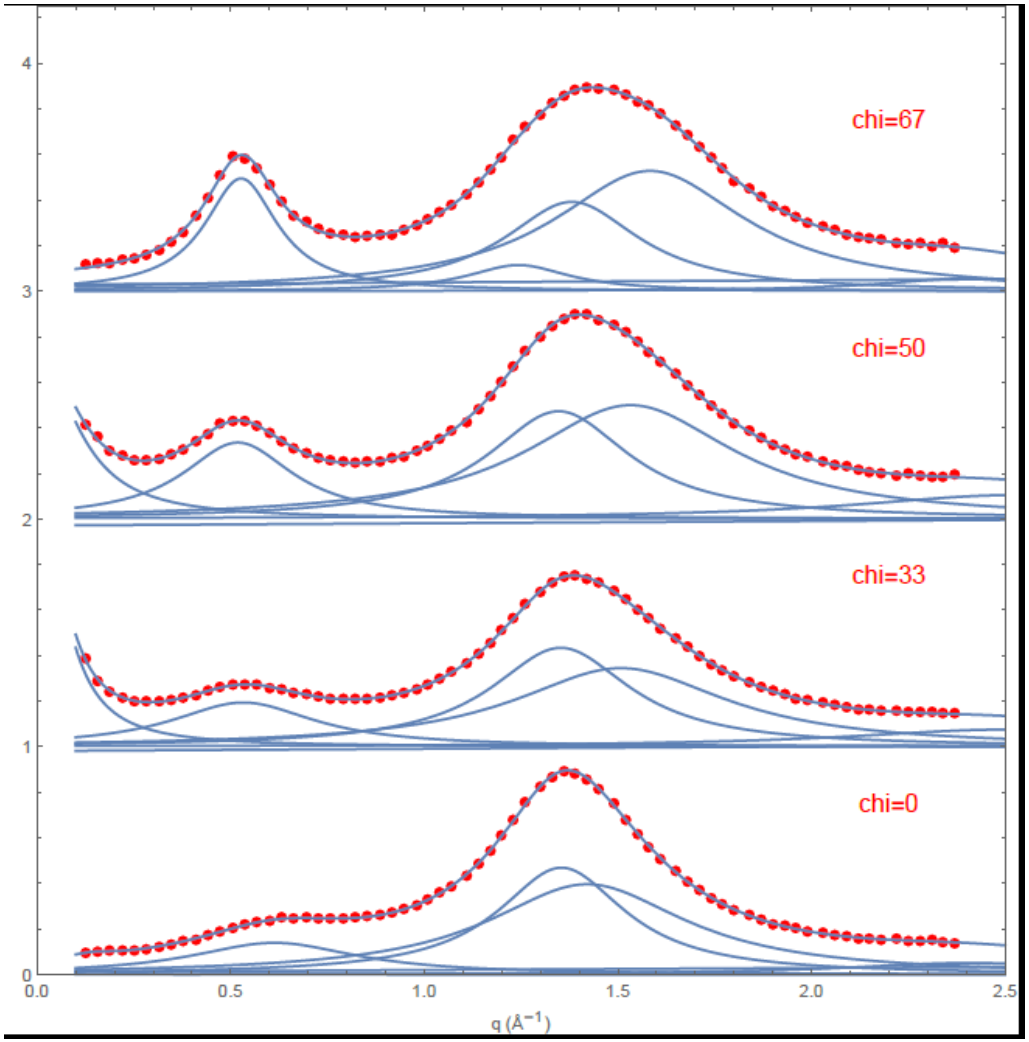
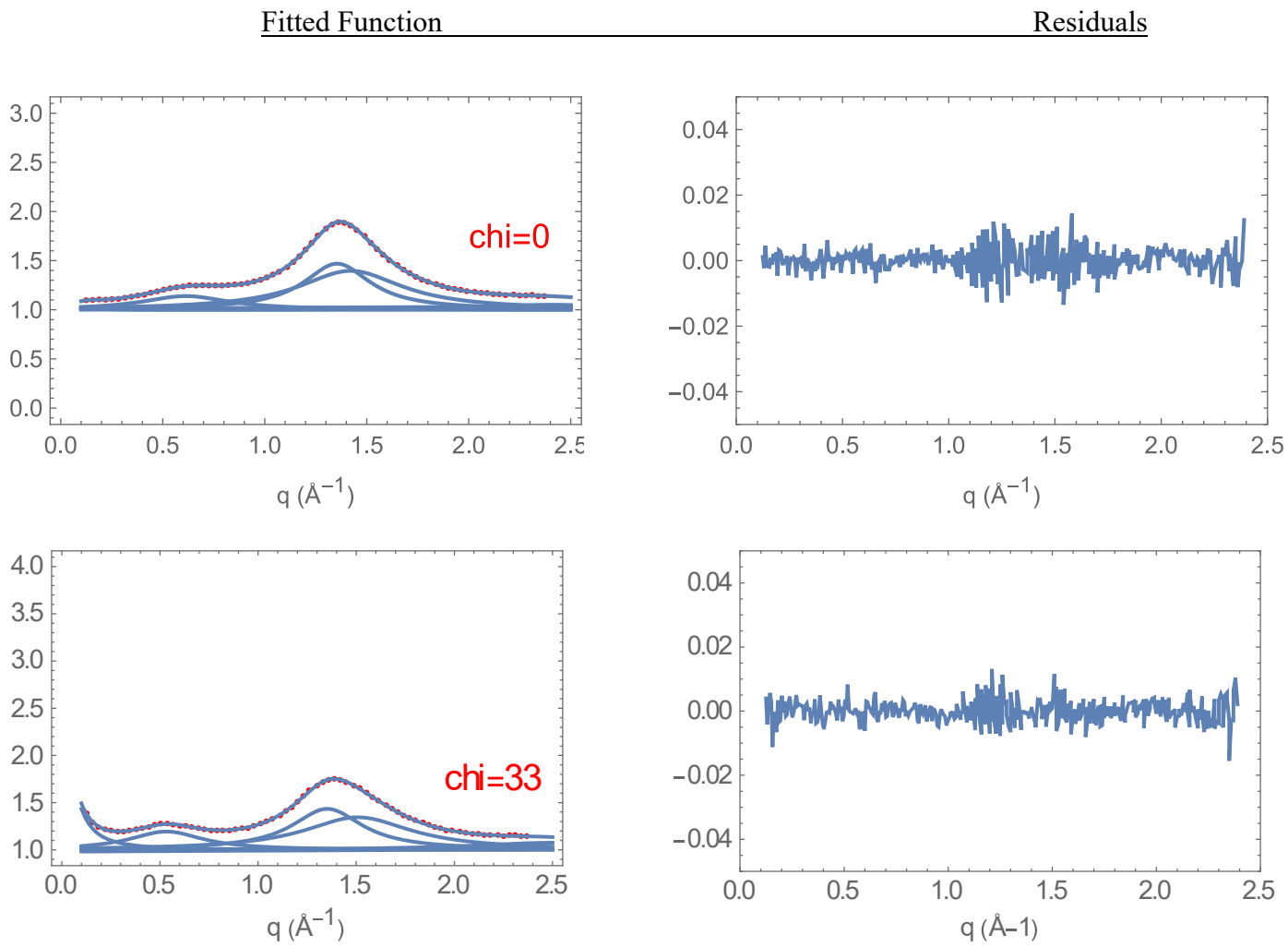
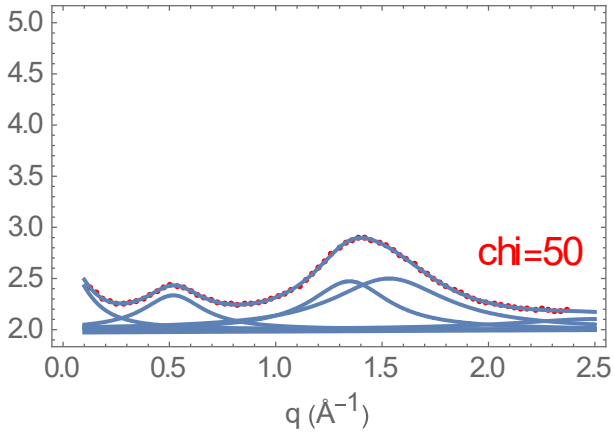
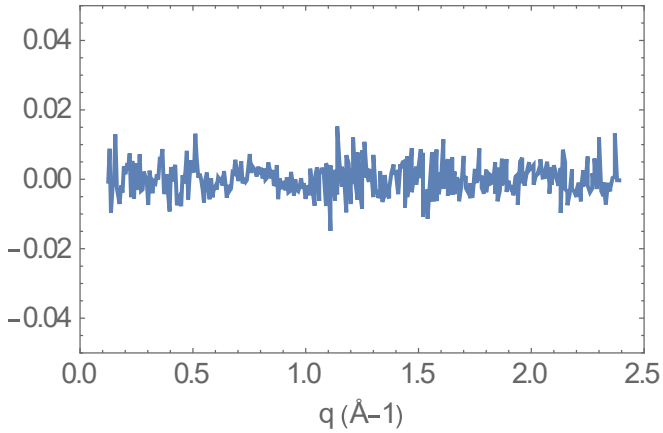
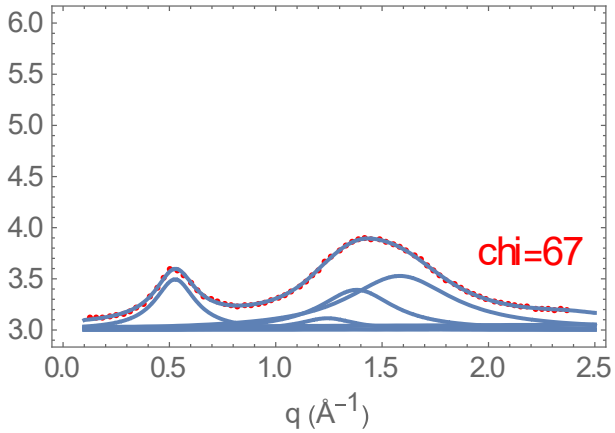


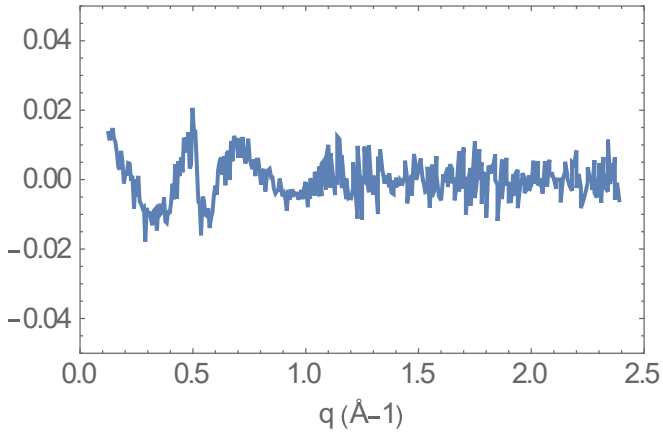
Figure S.32: Fitting functions and residuals for T6A HBz




chi=50
q (Å$^{-1}$)


q (Å–1)


chi=67
q (Å$^{-1}$)


q (Å–1)

## Table S.34: Local Structure Peaks for T6A HSa

| | T6AHSa | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | 0.613009 | 0.260993 |
| chi=33 | 0.516897 | 0.179139 |
| chi=50 | 0.517378 | 0.108299 |
| chi=67 | 0.520673 | 0.110168 |

## Table S.35: Fitting Parameters for T6A HSa

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0.011 | 0.00886 | 0.142 | 0.0693 | 8.99E-05 | 0.613 | 0.261 | 0.00948 | 1.35 | 0.2 | 0.0187 | 1.42 | 0.312 | 0.0385 | 2.41 | 0.387 | 0.0076 |
| 0.986 | 0.0098 | 0.00853 | 0.108 | 0.00829 | 0.517 | 0.179 | 0.0116 | 1.35 | 0.213 | 0.0229 | 1.53 | 0.336 | 0.05 | 2.55 | 0.499 | 0.0227 |
| 2.01 | -0.00998 | 0.626 | 0.169 | 0.00262 | 0.517 | 0.108 | 0.00557 | 1.35 | 0.215 | 0.0214 | 2.55 | 0.5 | 0.0298 | 1.56 | 0.336 | 0.0603 |
| 3.01 | -0.00997 | 0.636 | 0.167 | 0.00234 | 0.521 | 0.11 | 0.00504 | 1.35 | 0.308 | 0.047 | 2.44 | 0.362 | 0.015 | 1.61 | 0.298 | 0.0474 |

Figure S.33: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T6A HSa

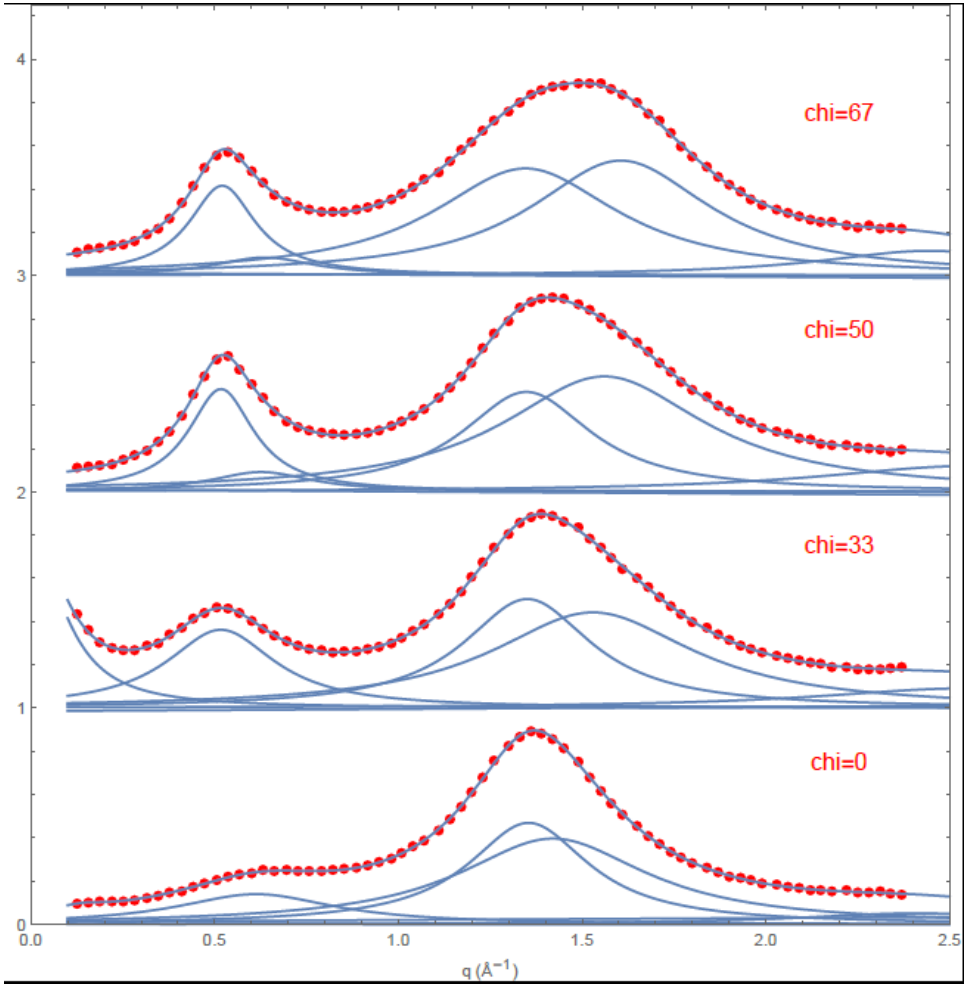
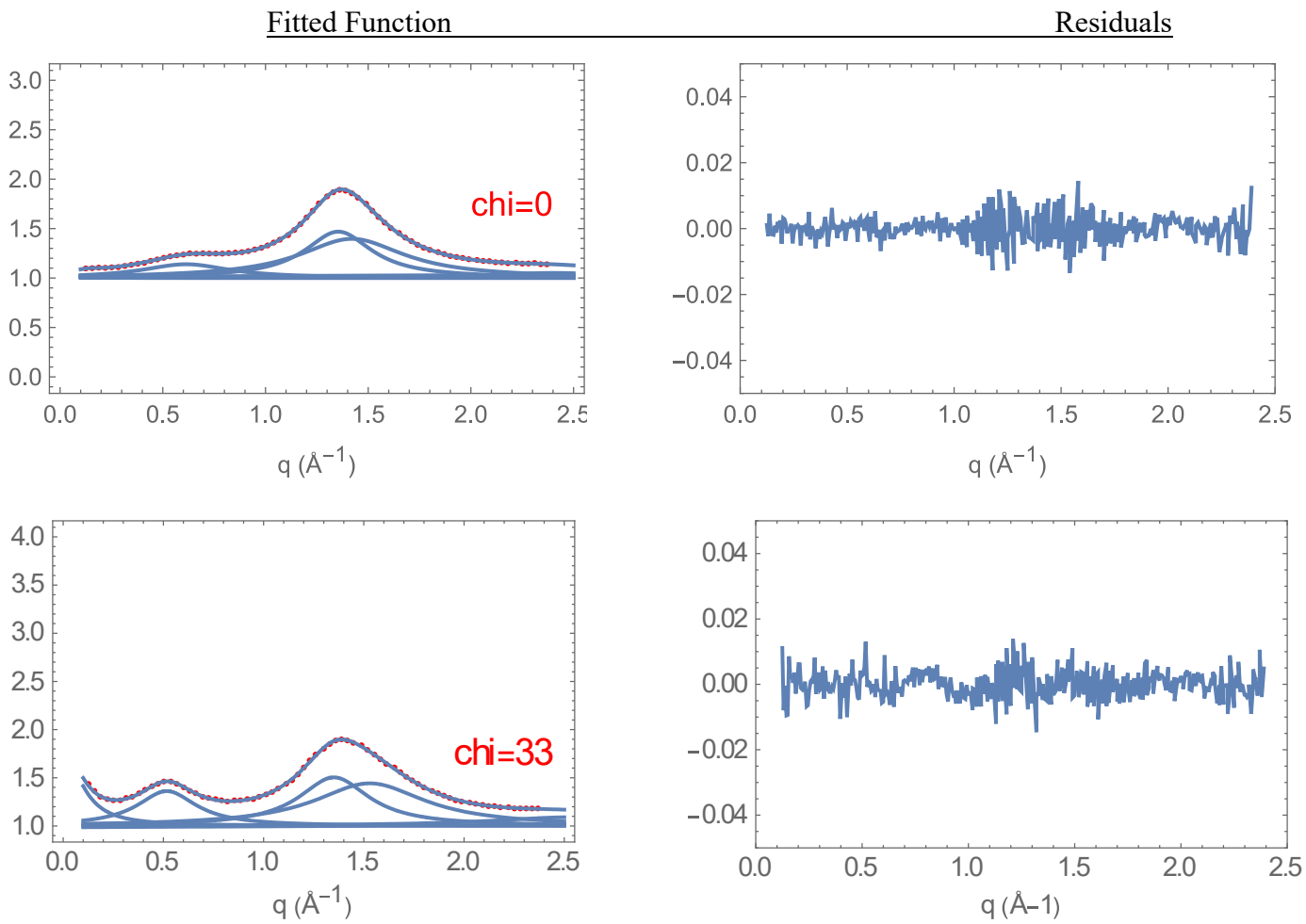
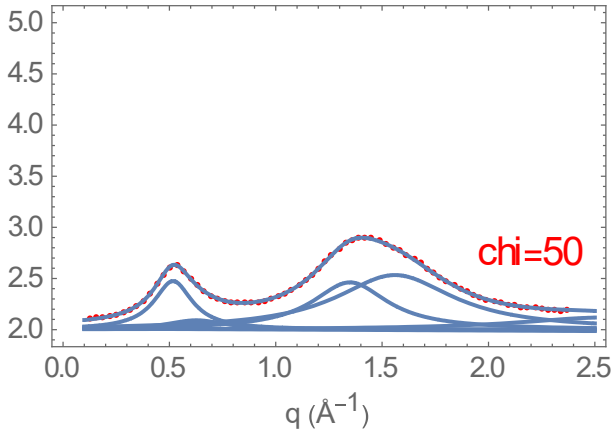
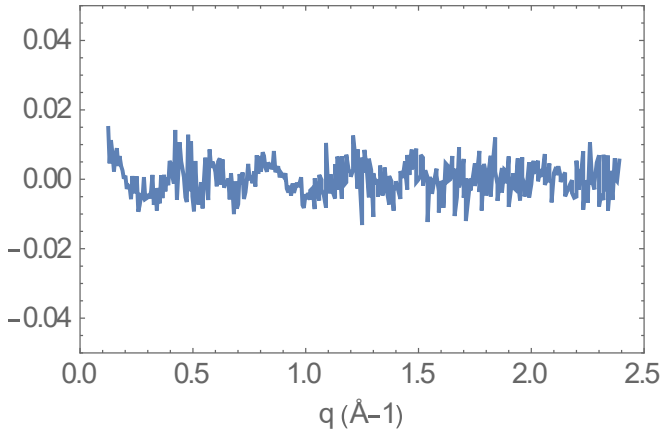
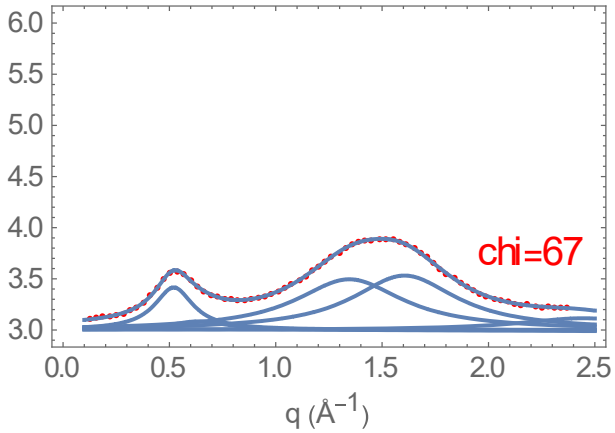


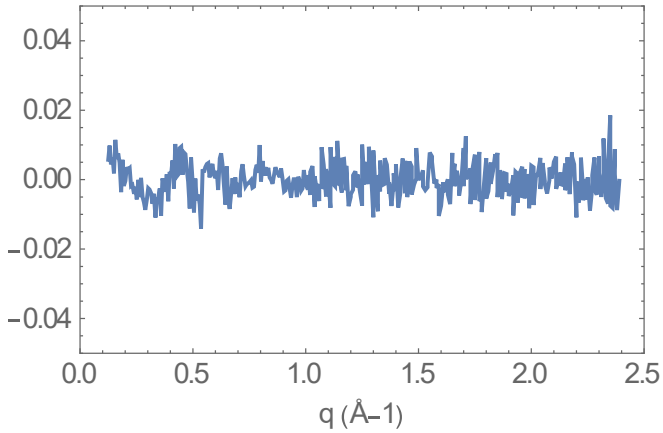
Figure S.34: Fitting functions and residuals for T6A HSa




chi=50
q (Å$^{-1}$)


q (Å–1)


chi=67
q (Å$^{-1}$)


q (Å–1)

## S.6: Fitting Information for Mixtures Presented in Figure 8

**T2OH C8A**

### Table S.36: Local Structure Peaks for T2OH C8A

| | T2OHC8A | |
|---|---|---|
| | q (Å^-1) | w (Å^-1) |
| chi=0 | 0 | 0 |
| chi=33 | 0.314138 | 0.180562 |
| chi=50 | 0.28027 | 0.045717 |
| chi=67 | 0.284711 | 0.044336 |
| chi=75 | 0.290773 | 0.052285 |
| chi=83 | 0.29214 | 0.065702 |
| chi=100 | 0.41763 | 0.185602 |

### Table S.37: Fitting Parameters for T2A C6A

| a | b | $q_{01}$ | $w_1$ | $A_1$ | $q_{02}$ | $w_2$ | $A_2$ | $q_{03}$ | $w_3$ | $A_3$ | $q_{04}$ | $w_4$ | $A_4$ | $q_{05}$ | $w_5$ | $A_5$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.00995 | 0.138 | 0.0583 | 6.11E-05 | 1.17 | 0.16 | 0.0106 | 1.36 | 0.436 | 0.0788 | 1.74 | 0.308 | 0.0387 | 2.44 | 0.493 | 0.0358 |
| 1.95 | 0.00994 | 0.314 | 0.079 | 0.00491 | 0.439 | 0.181 | 0.00348 | 1.26 | 0.255 | 0.0265 | 1.6 | 0.448 | 0.118 | 2.43 | 0.415 | 0.0242 |
| 2.95 | 0.00995 | 0.28 | 0.0457 | 0.00185 | 0.462 | 0.285 | 0.00414 | 1.4 | 0.336 | 0.0301 | 1.73 | 0.499 | 0.0162 | 2.45 | 0.493 | 0.0138 |
| 3.95 | 0.00999 | 0.285 | 0.0443 | 0.00174 | 0.428 | 0.2 | 0.00216 | 0.8 | 0.19 | 0.000776 | 2.17 | 0.5 | 0.0179 | 1.43 | 0.315 | 0.0307 |
| 4.95 | 0.00998 | 0.291 | 0.0523 | 0.00239 | 0.467 | 0.259 | 0.00377 | 1.5 | 0.5 | 0.0499 | 2.43 | 0.487 | 0.0156 | 1.41 | 0.206 | 0.00964 |
| 5.95 | 0.00999 | 0.292 | 0.0657 | 0.00363 | 0.457 | 0.272 | 0.00539 | 1.41 | 0.209 | 0.0156 | 2.45 | 0.5 | 0.0214 | 1.51 | 0.5 | 0.0562 |
| 6.96 | 0.00948 | 0.418 | 0.186 | 0.0079 | 0.674 | 0.466 | 0.0146 | 2.46 | 0.498 | 0.0303 | 1.41 | 0.218 | 0.0351 | 1.59 | 0.479 | 0.0353 |

Figure S.35: Fitting functions (blue) and raw data (red, 1/5$^{th}$ of points shown) for T2OH C8A

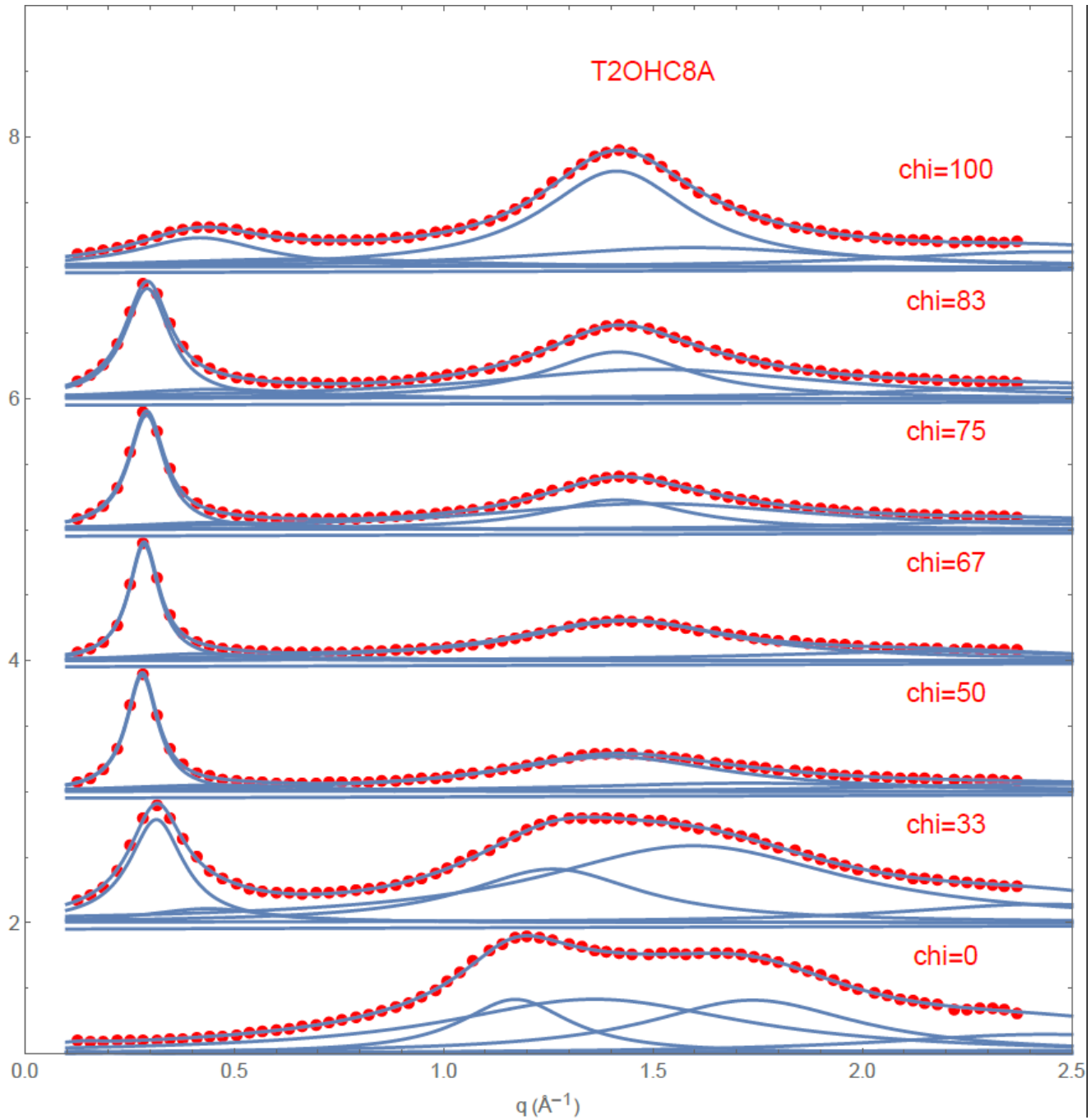
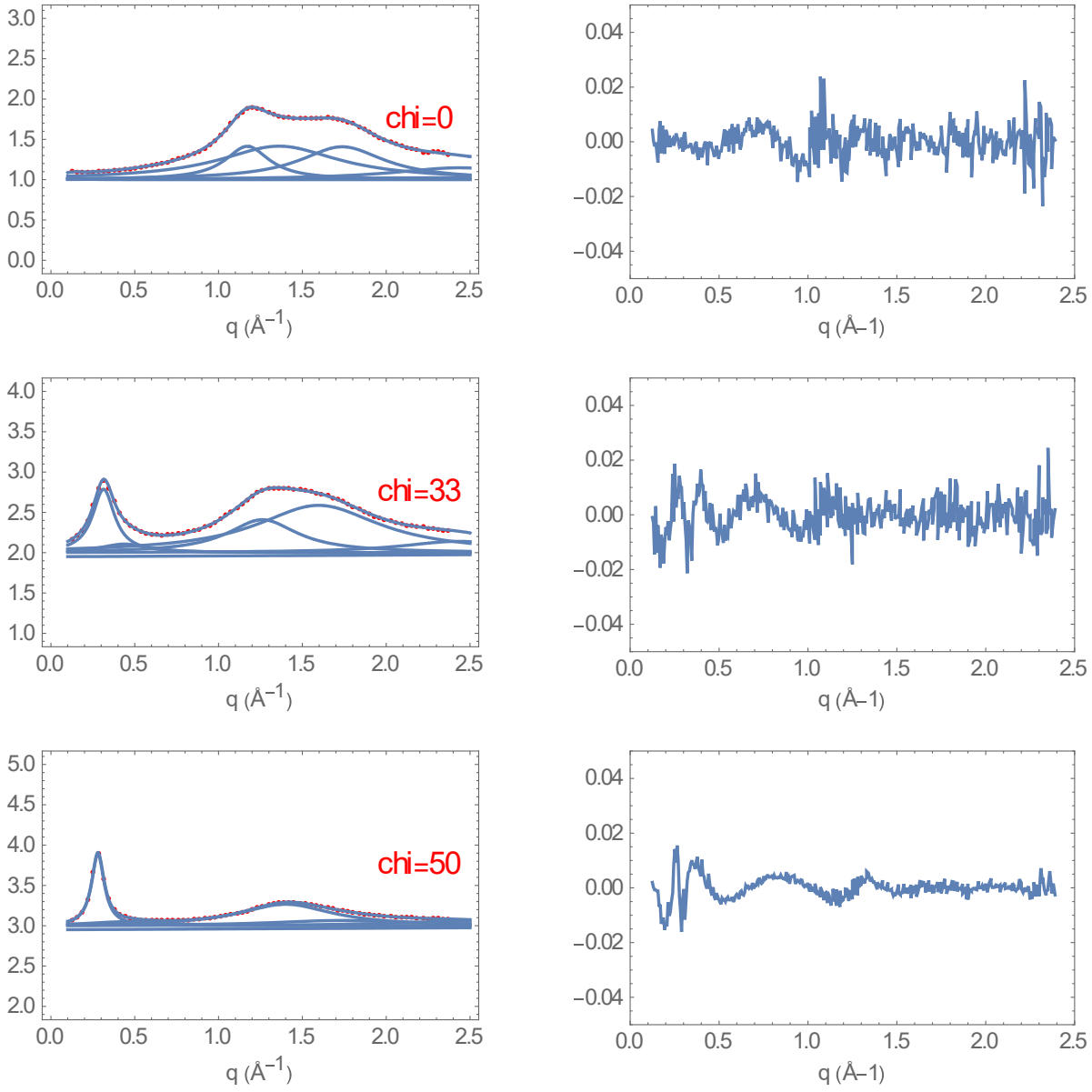
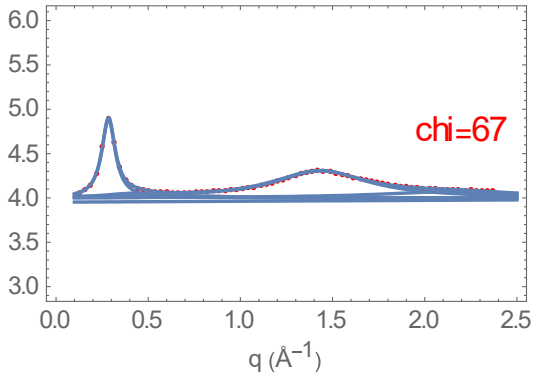
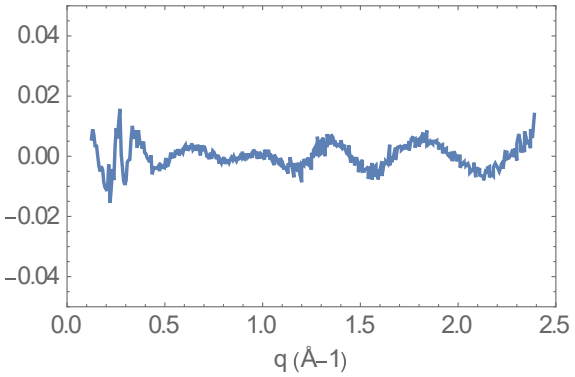
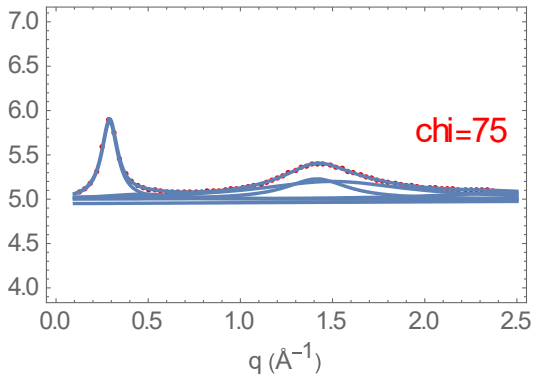


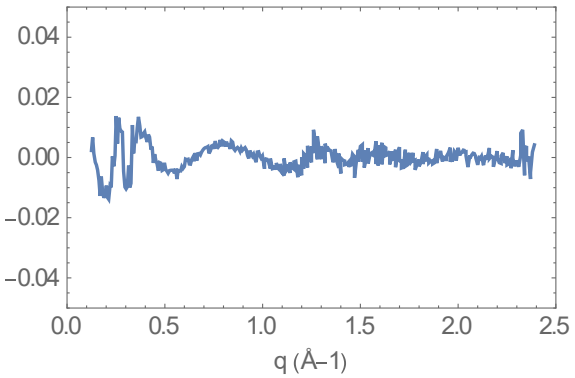
Figure S.36: Fitting functions and residuals for T2OH C8A

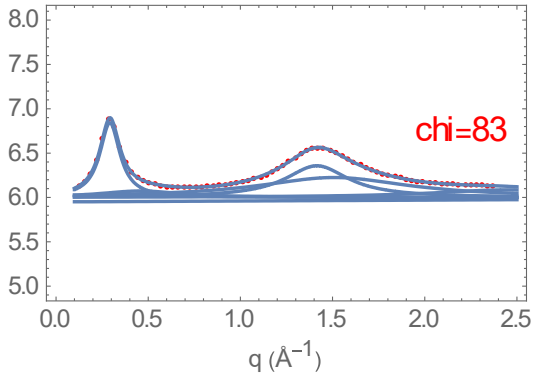


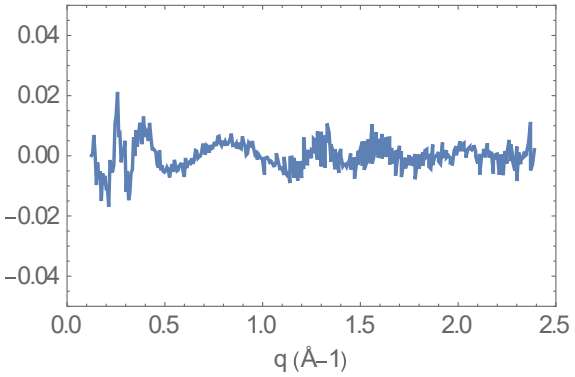

chi=67
q (Å$^{-1}$)

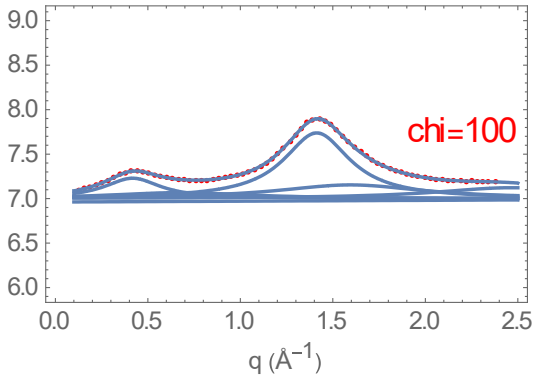

q (Å–1)

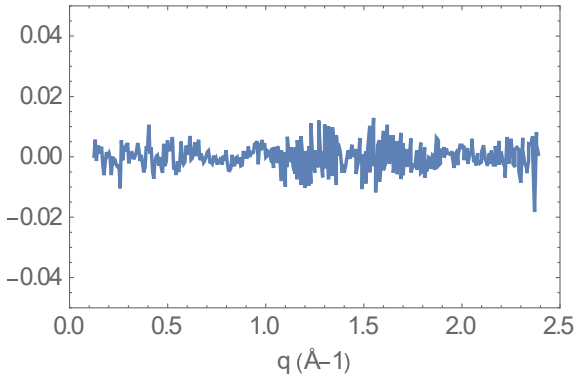

chi=75
q (Å$^{-1}$)


q (Å–1)


chi=83
q (Å$^{-1}$)


q (Å–1)


chi=100
9.0
8.5
8.0
7.5
7.0
6.5
6.0
0.0
0.5
1.0
1.5
2.0
2.5
q (Å$^{-1}$)


0.04
0.02
0.00
−0.02
−0.04
0.0
0.5
1.0
1.5
2.0
2.5
q (Å−1)

# S.7: Figures for Low-Q SAXS Analysis

## Figure S.37: Log-log plots of low-q scattering for compositions showing evidence of structure in this regime

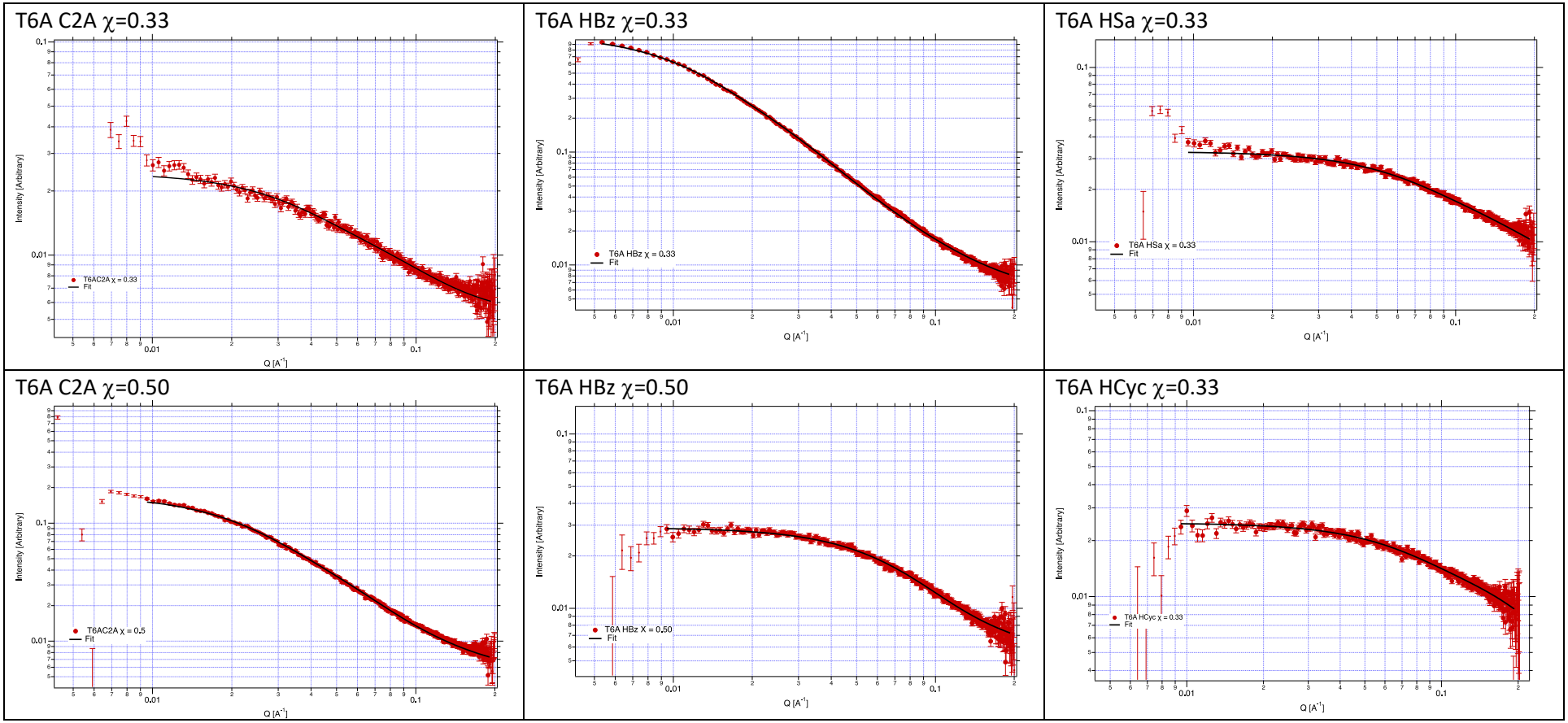


Figure S.38: Low-q scattering for T6A HCyc $\chi$=0.5; structure insufficient to allow fitting to estimate lengthscale.