

Structure Factor Check

4YT0

Title: CRYSTAL STRUCTURE OF MITOCHONDRIAL RHODOQUINOL-FUMARATE REDU
 ASCARIS SUUM WITH 2-METHYL-N-[3-(5-METHYLETHOXY)PHENYL]BENZ
 Date: 17-MAR-15
 PDB code: 4YT0

Crystal

Cell parameters:

a: 122.80 A b: 123.39 A c: 219.00 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Number of NCS-operators: 2
 NC-symmetry only for information

Structure Factors

Input

Nominal resolution range: 19.9 – 3.65 A
 Reflections in file: 37265
 Unique reflections above 0: 33241
 above 1 σ : 32649
 above 3 σ : 21595
 Reflections > 0: 4024

SF CHECK

Nominal resolution range: 19.9 – 3.66 A
\05max. from input data, min. from author\05
 Used reflections: 33209
 Reflections out of resolution: 32
 Completeness: 89.4 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.105
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.5236 1.0000 0.9265
 B_{overall} (by Patterson): 55. A²
 Optical resolution: 2.49 A
 Expected opt. resol. for complete data set: 2.49 A
 Estimated minimal error: 0.215 A

Model

18236 atoms
 Number of chains: 22
 Volume not occupied by model: 53.3 %
 $\langle B \rangle$ (for atomic model): 58.9 A²
 $\sigma(B)$: 16.09 A²
 Matthews coefficient: 3.25
 Corresponding solvent % : 61.85

Model vs. Structure Factors

R-factor for all reflections: 0.258
 Correlation factor: 0.794
 R-factor: 0.266
 for $F > 2.0\sigma$
 nom. resolution range: 20.00 – 3.66A
 reflections used: 32616
 Rfree: 0.321
 Nfree: 1615
 R-factor without free-refl.: 0.263
 Non free-reflections: 31001
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.615 A
 Estimated maximal error: 0.410 A
 DPI: 0.736 A

Refinement

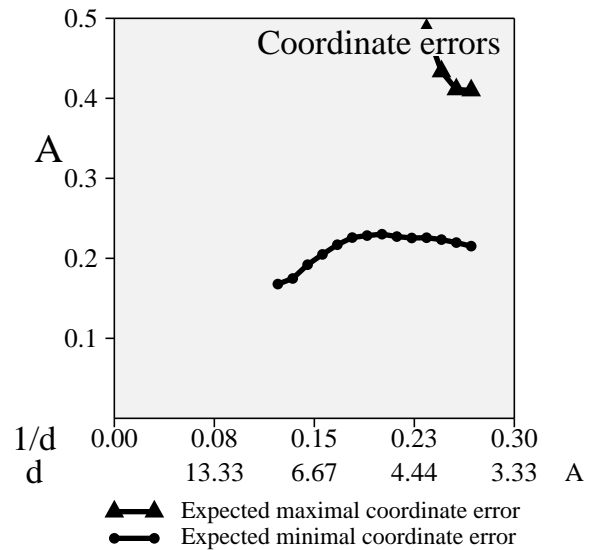
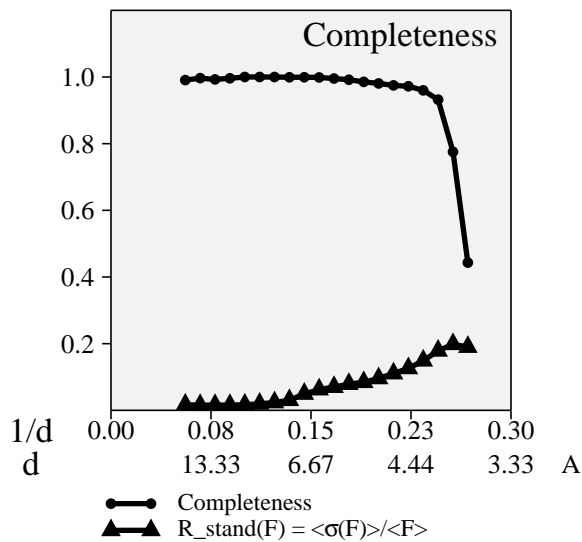
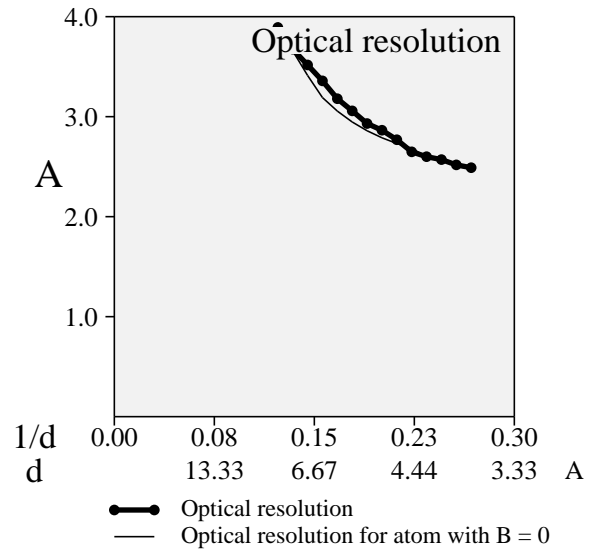
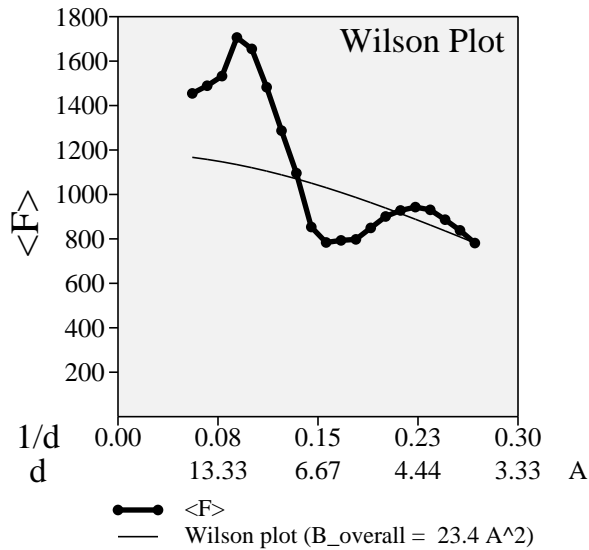
Program: REFMAC 5.7.0029
 Nominal resolution range: 20.0 – 3.66 A
 Reported R-factor: 0.193
 Number of reflections used: 31772
 Reported Rfree: 0.26
 Sigma cut-off: N.A.

Scaling

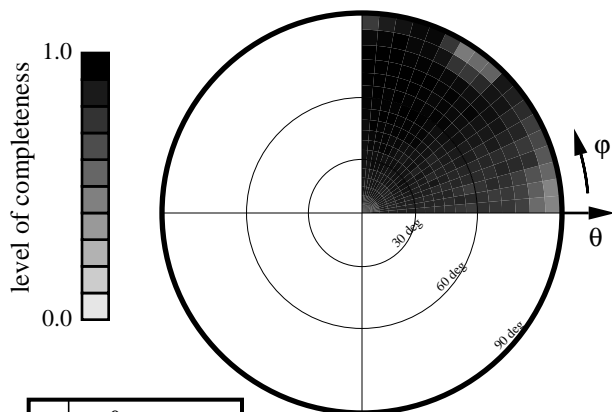
Scale: 0.840
 Bdiff: -8.96
 Anisothermal Scaling (Beta):
 -5.8118 -5.1721 -5.4138 0.0000 -0.0000 0.0000
 Solvent correction – Ks,Bs: 0.244 249.623

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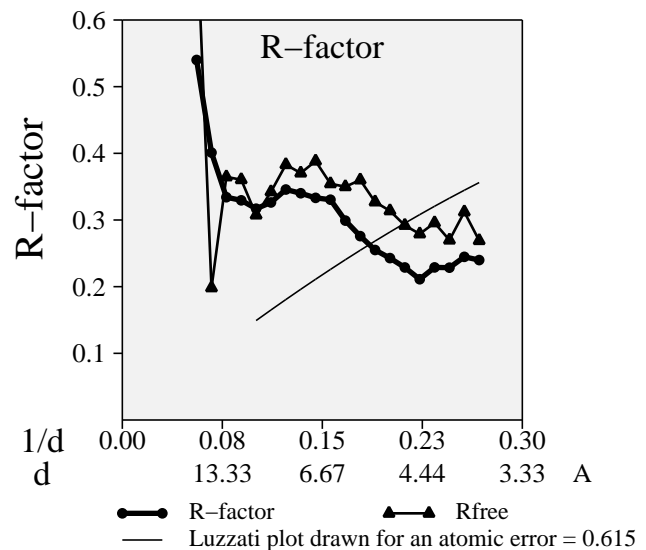


Stereographic projection of the averaged radial completeness



| | θ | ϕ |
|---|----------|--------|
| h | 90.00 | 0.00 |
| k | 90.00 | 90.00 |
| l | 0.00 | 0.00 |

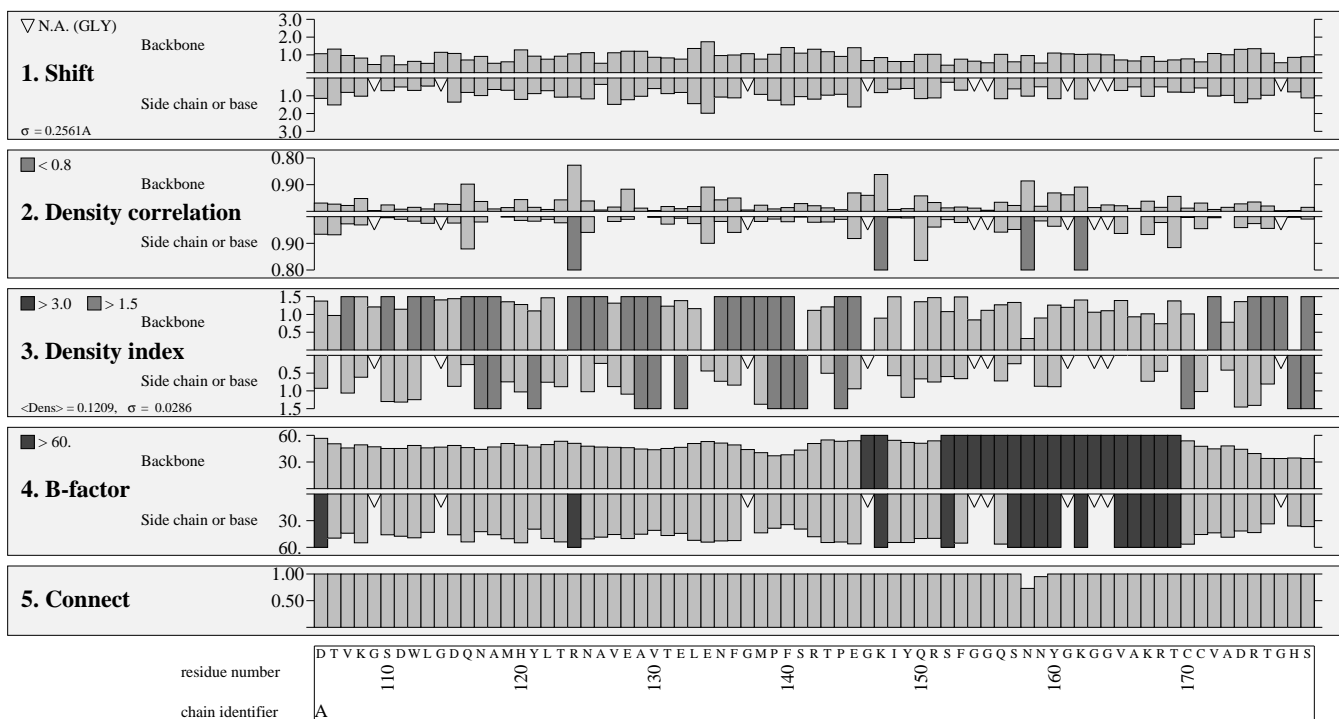
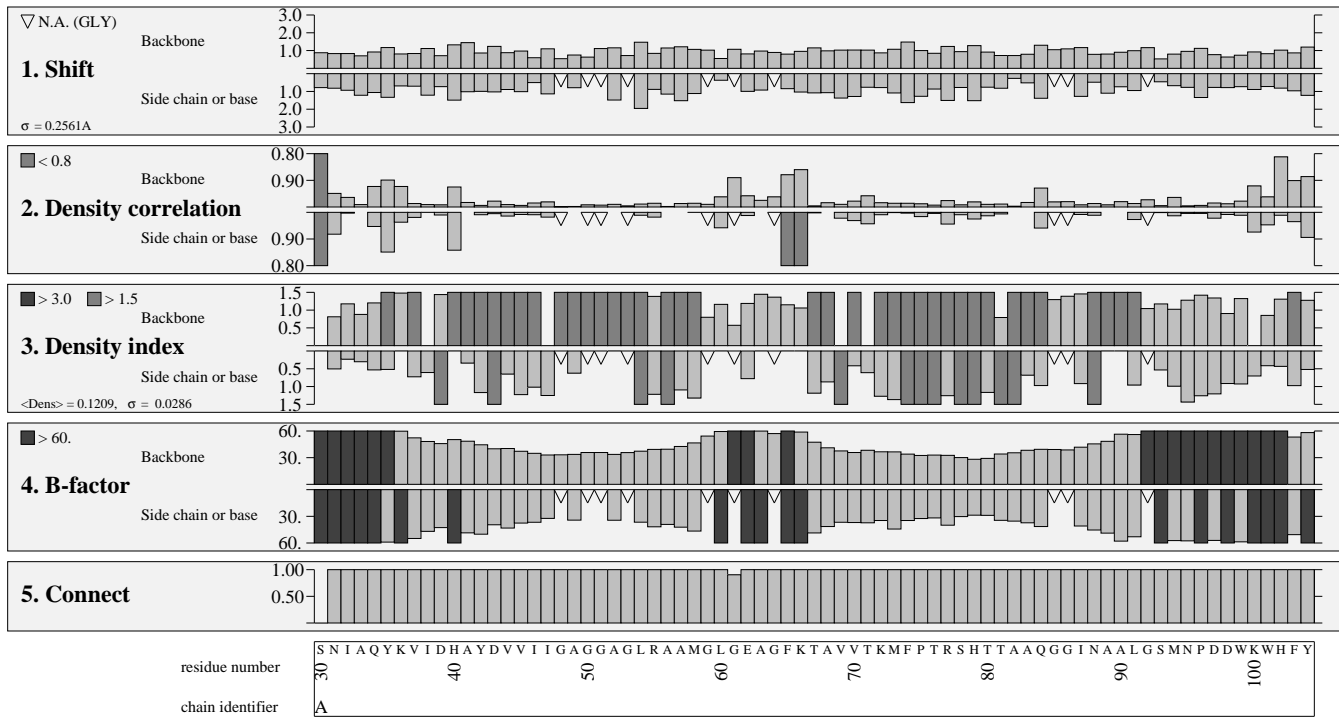
polar coordinates of the crystallographical axes



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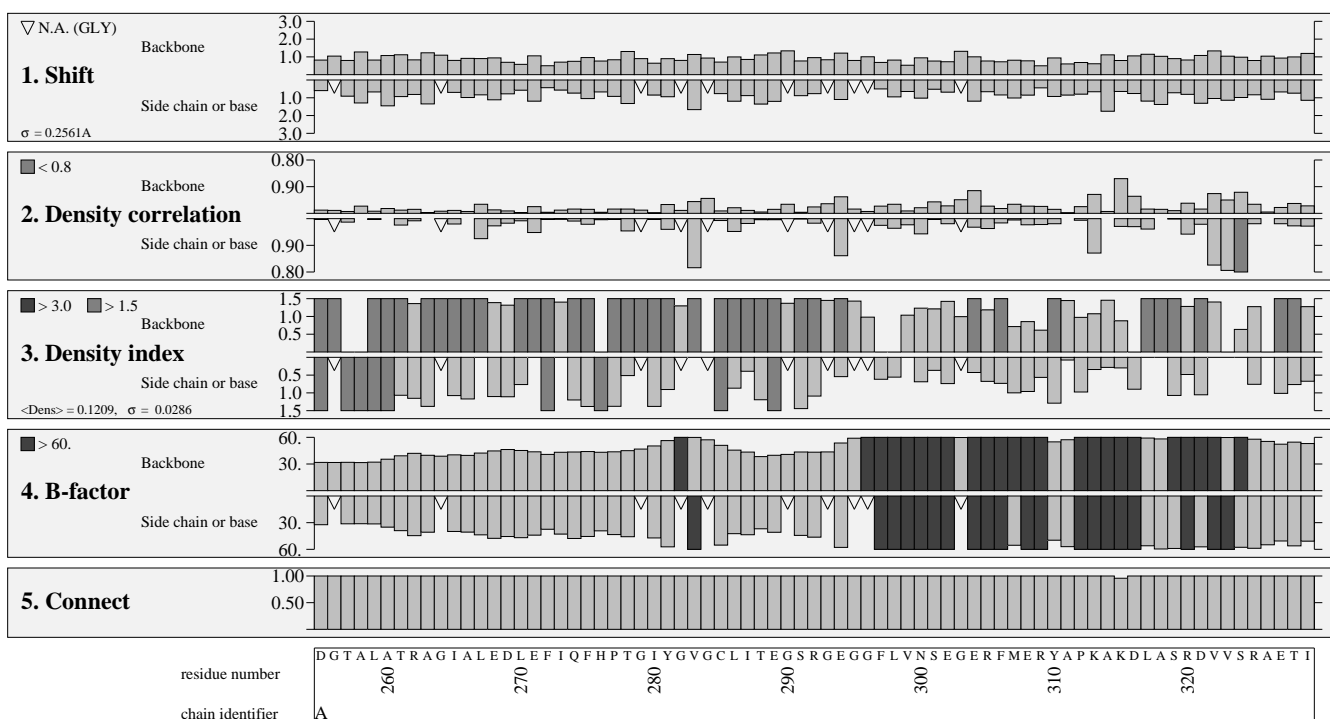
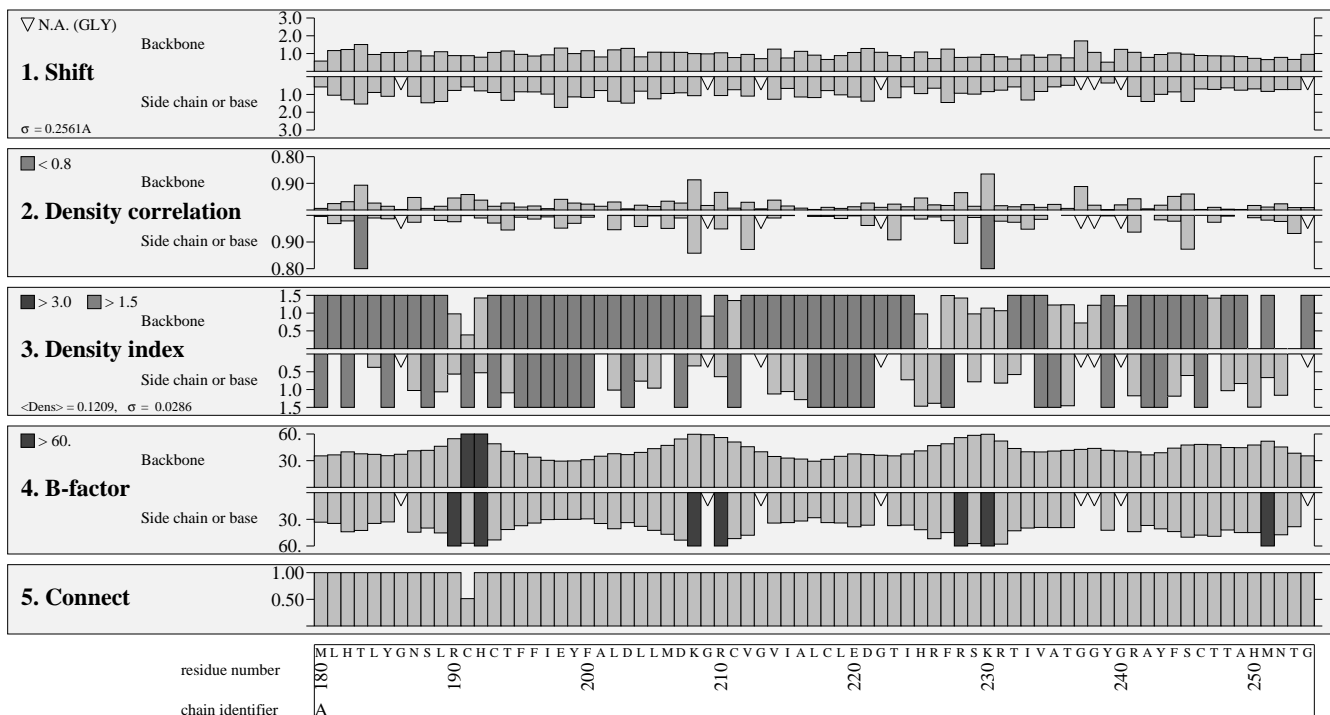
Local estimation



Structure Factor Check

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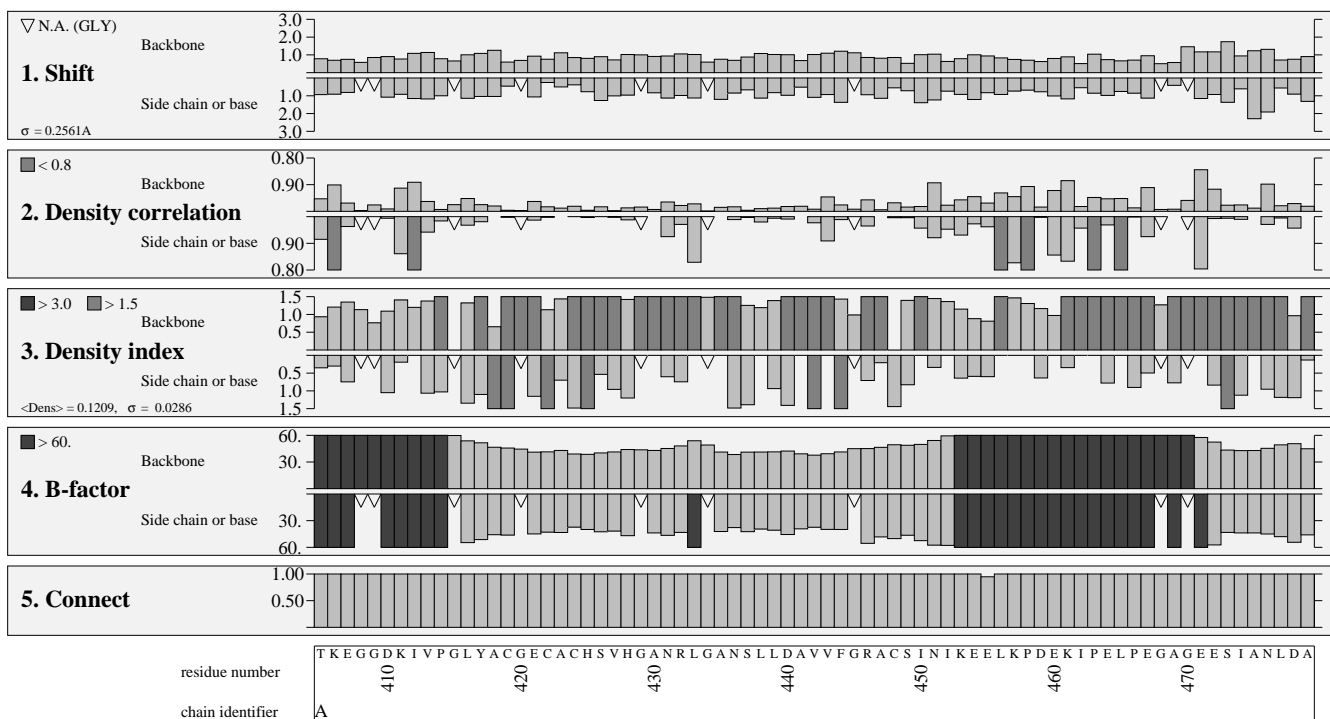
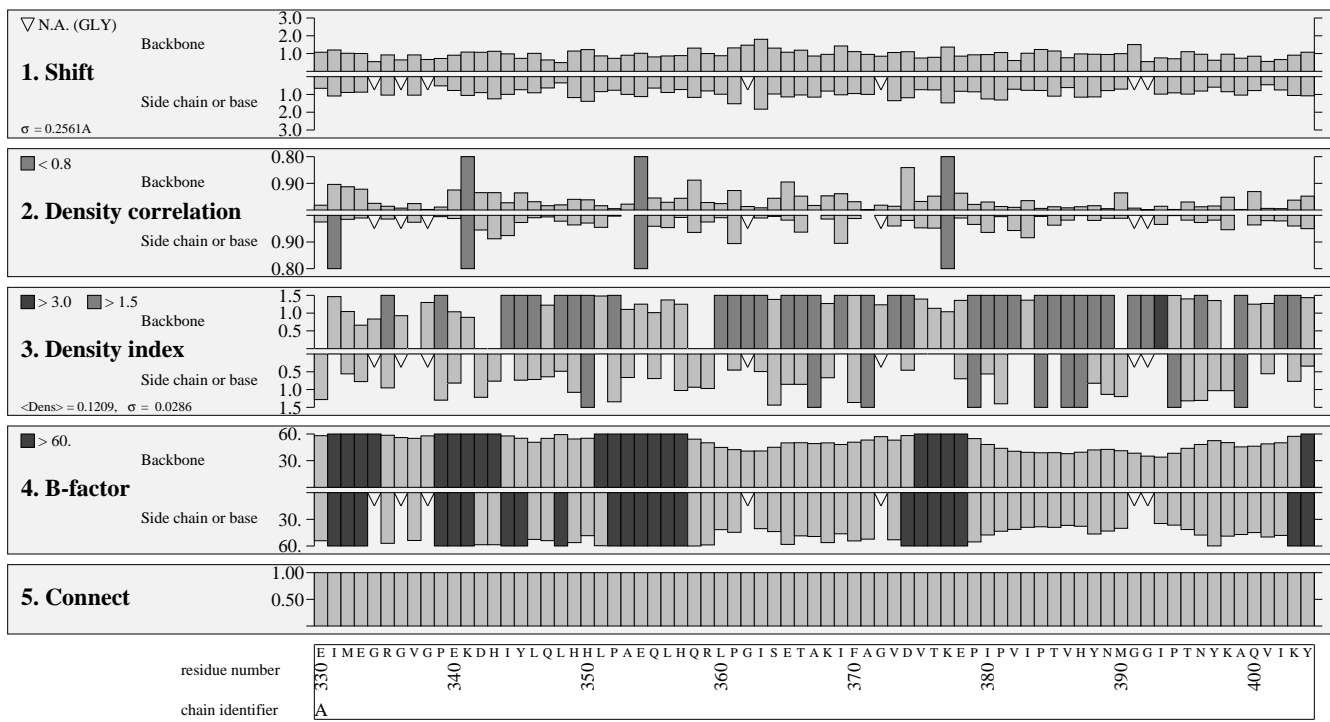
Local estimation (2)



Structure Factor Check

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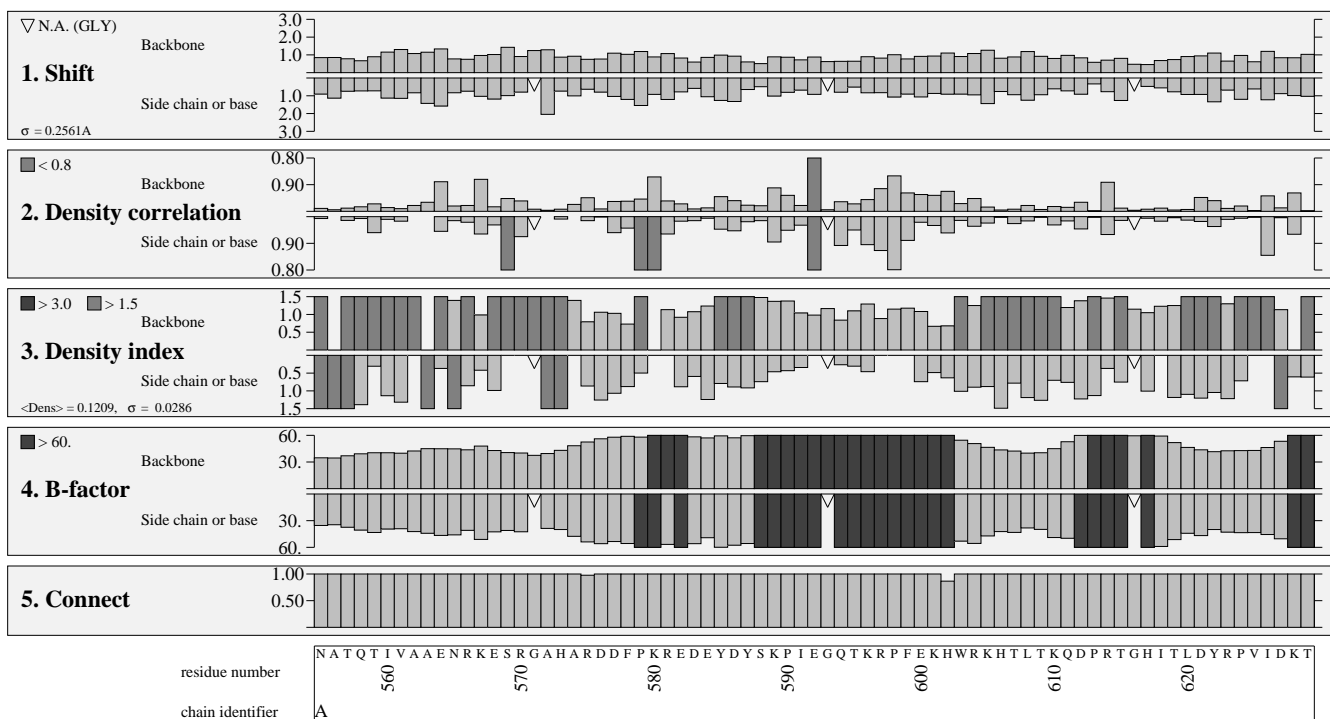
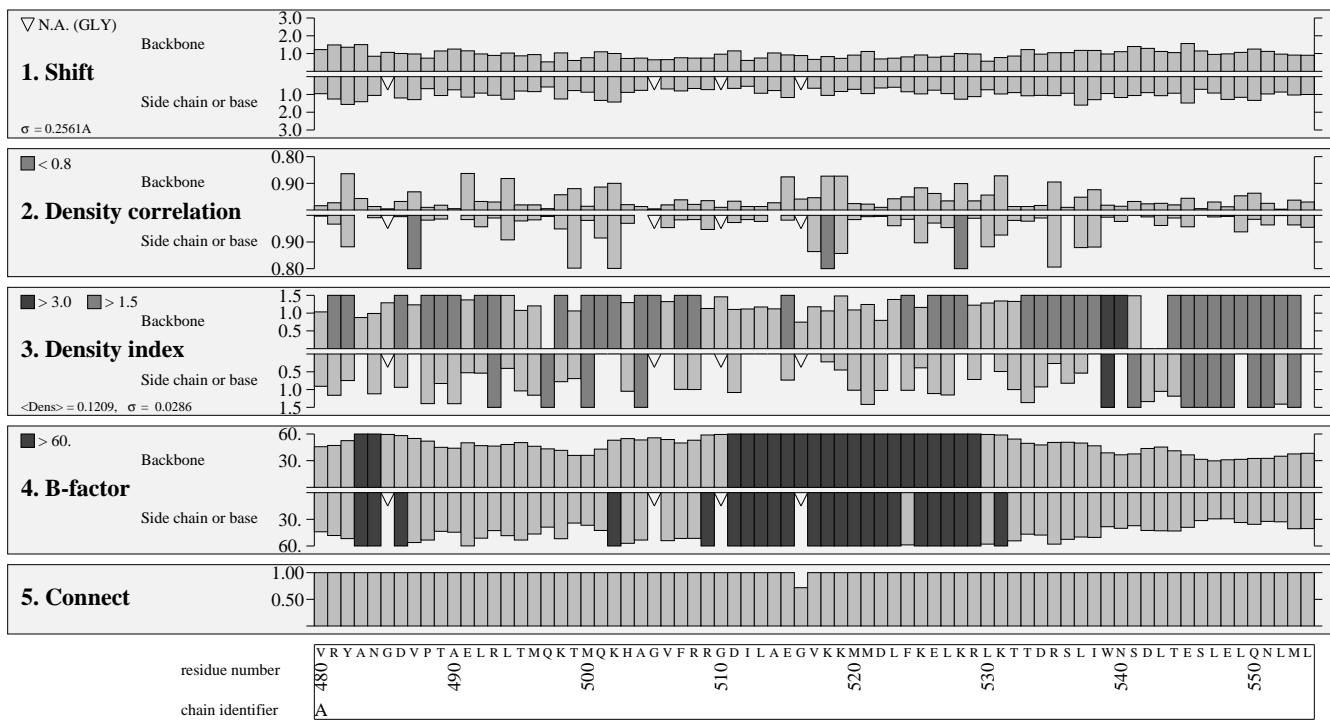
Local estimation (3)



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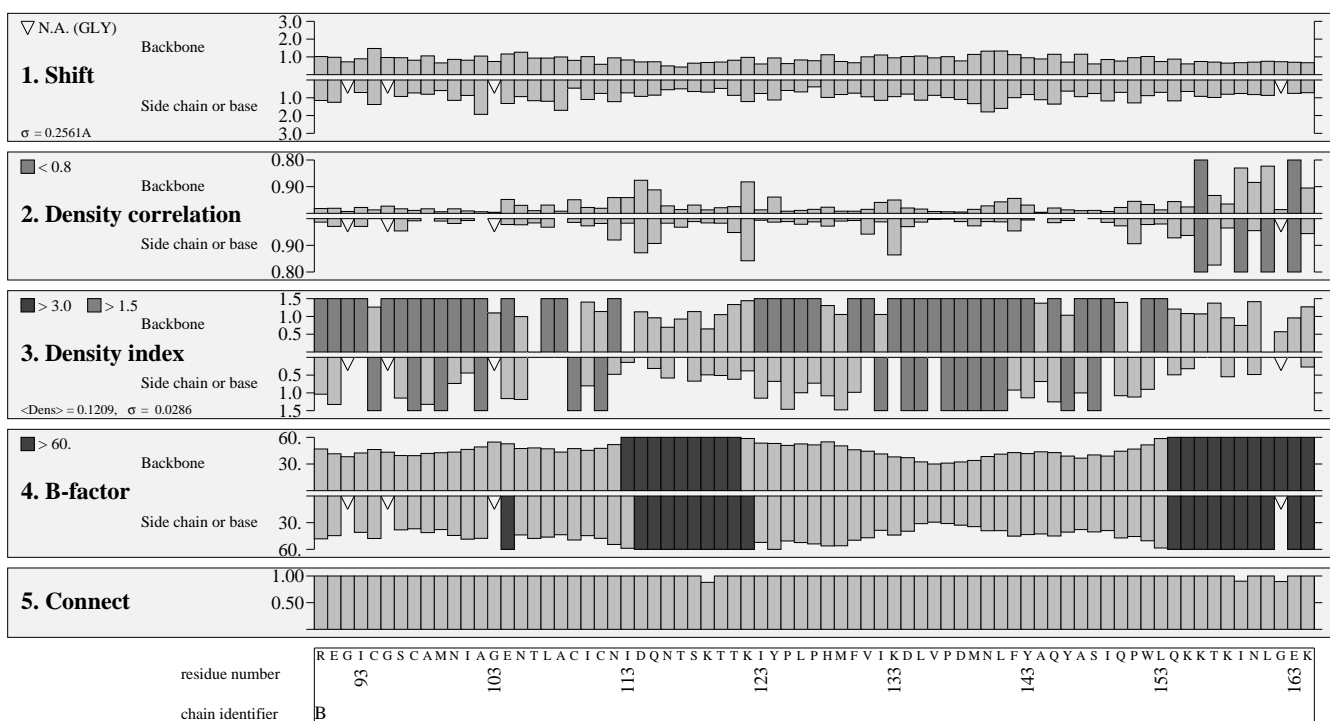
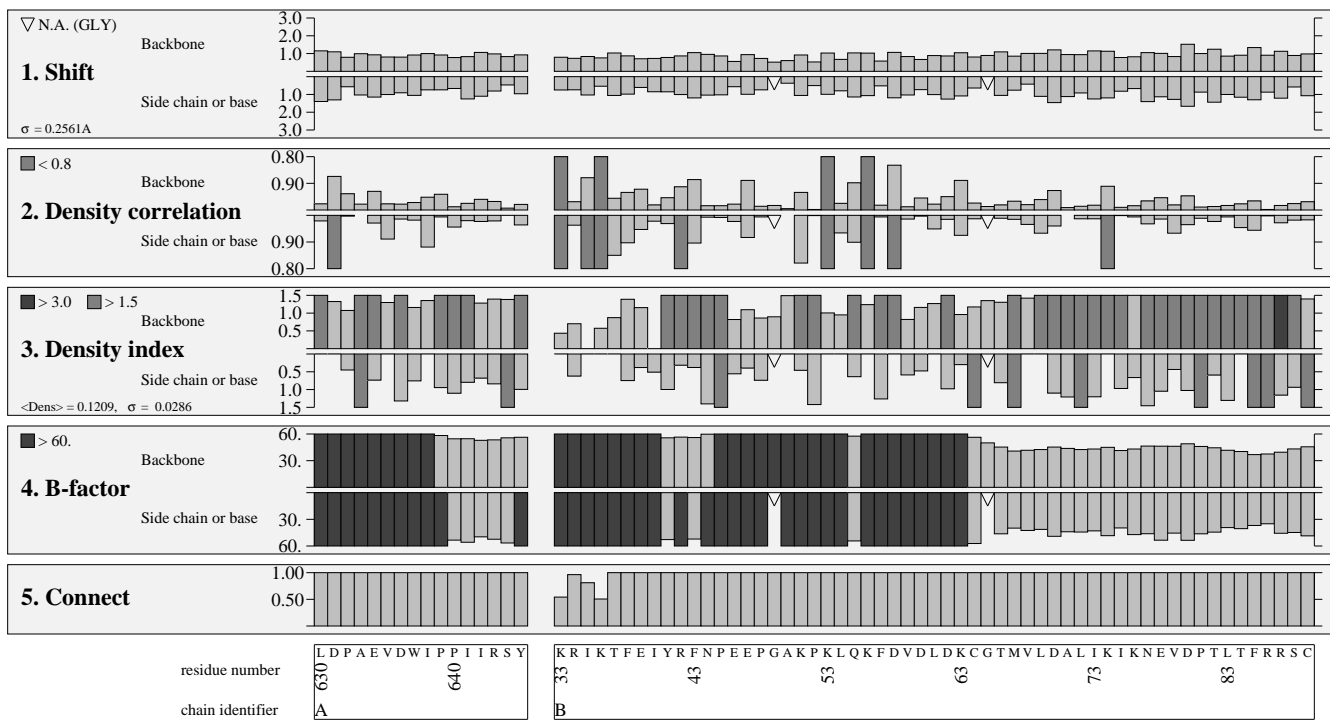
Local estimation (4)



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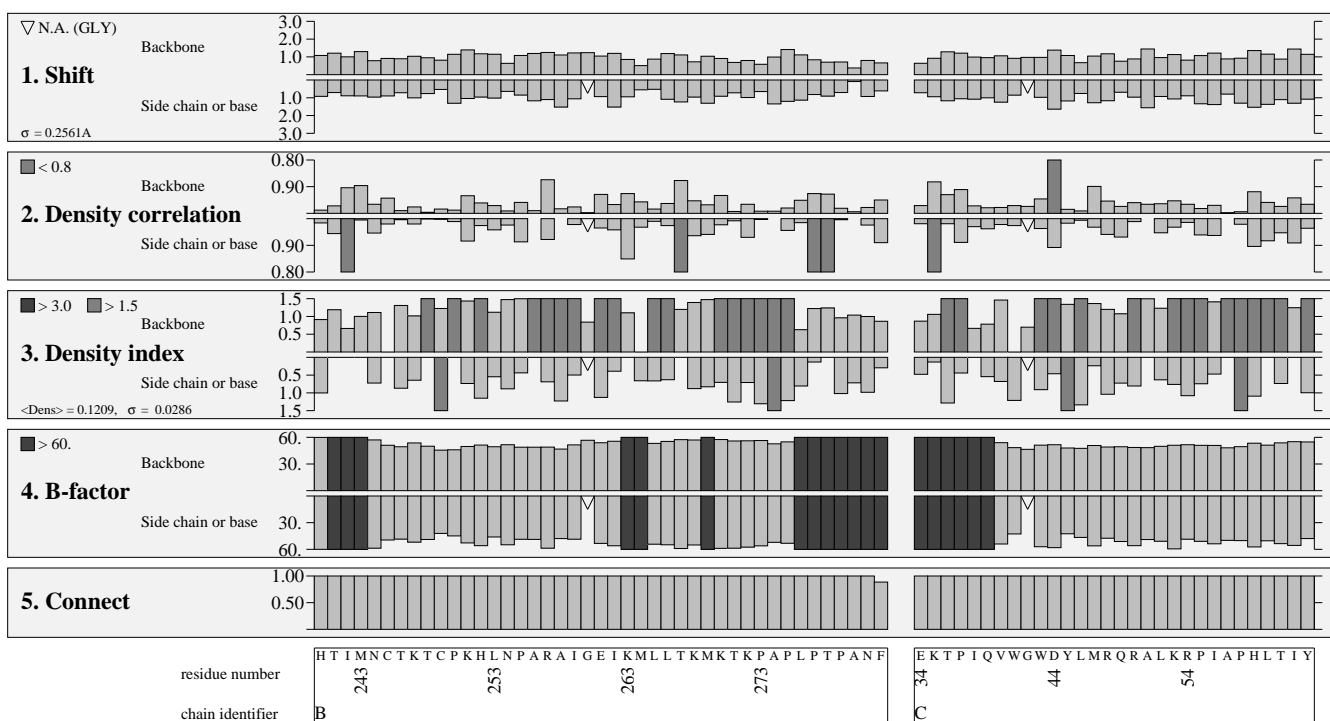
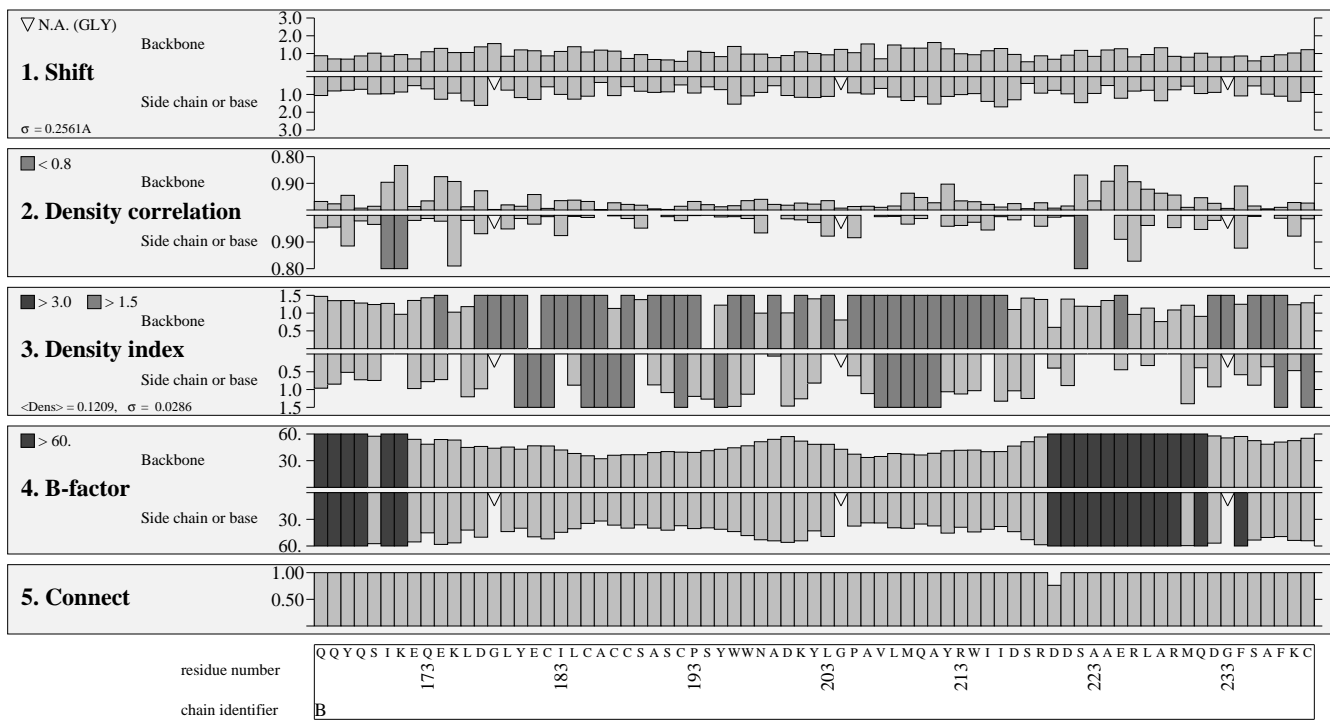
Local estimation (5)



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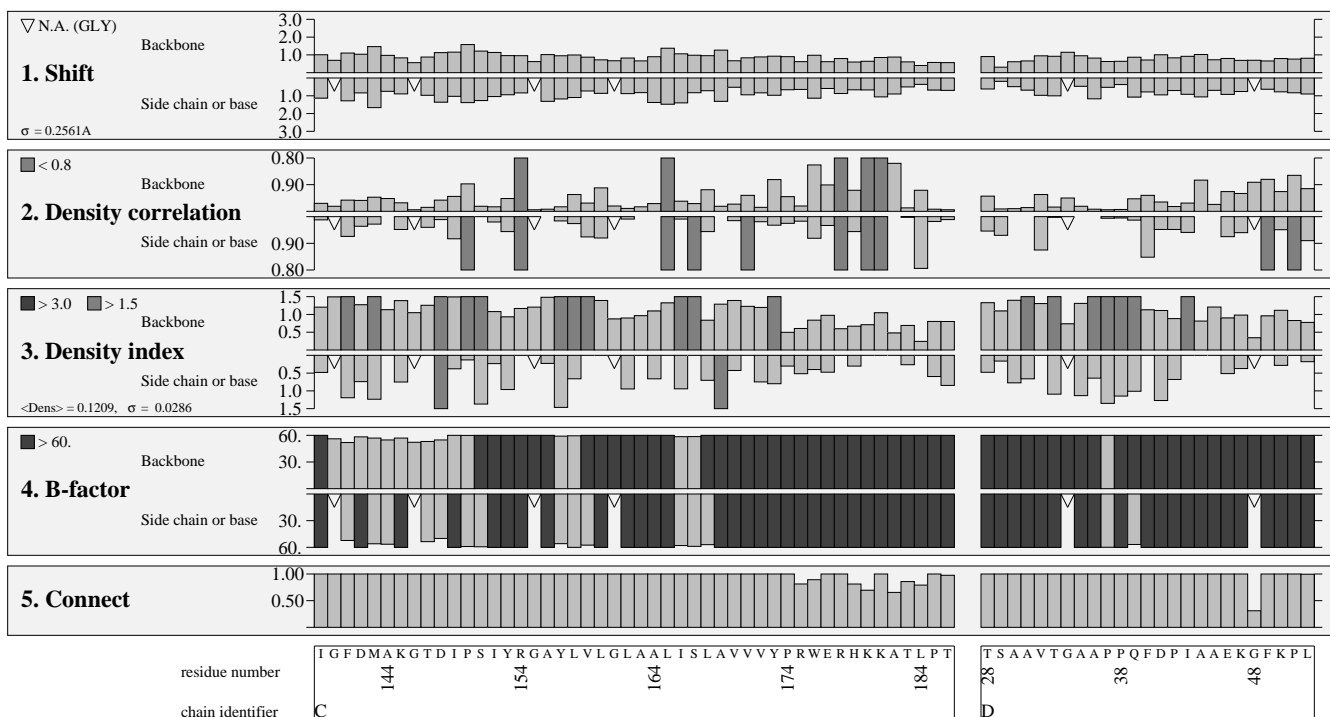
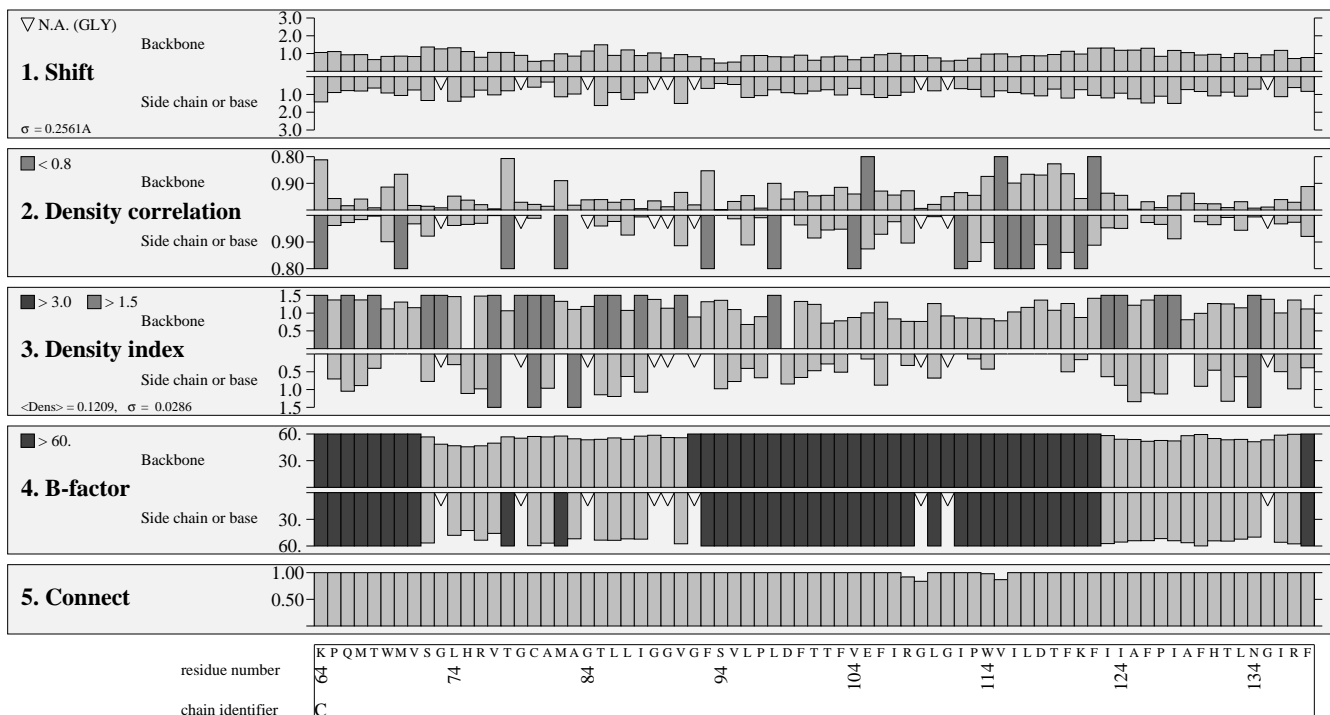
Local estimation (6)



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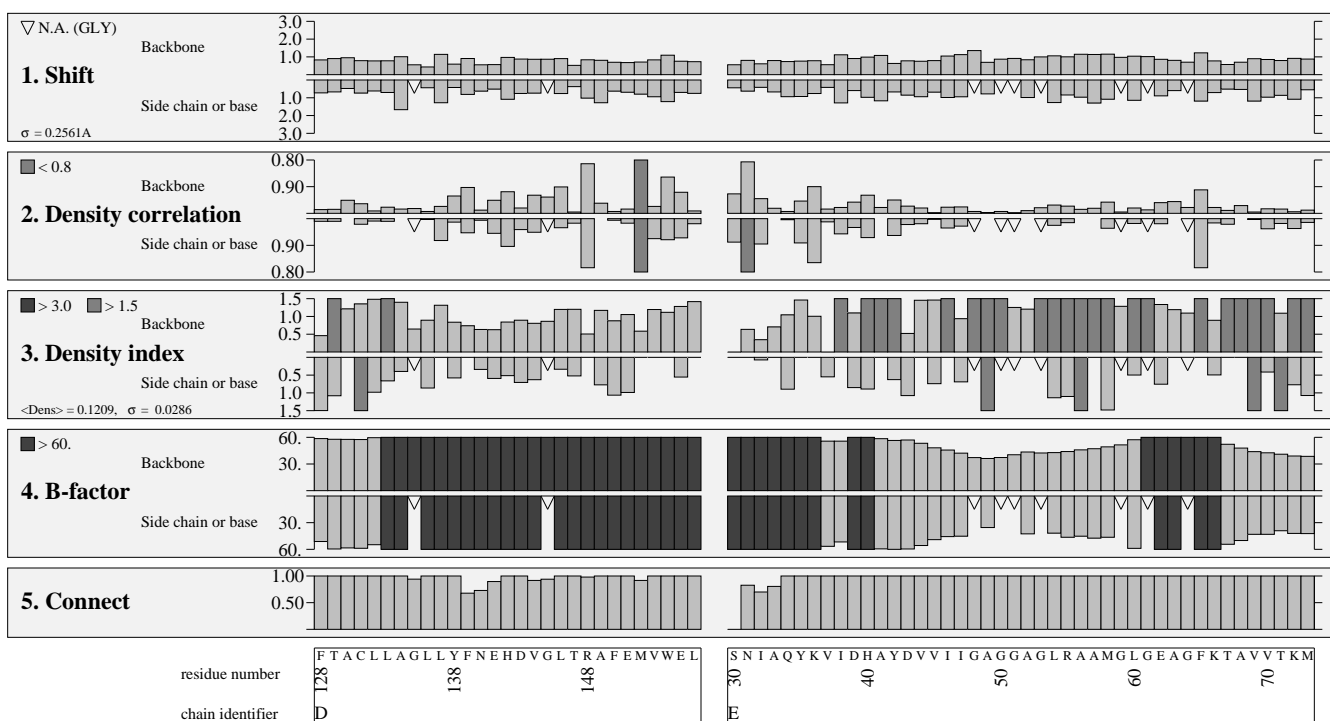
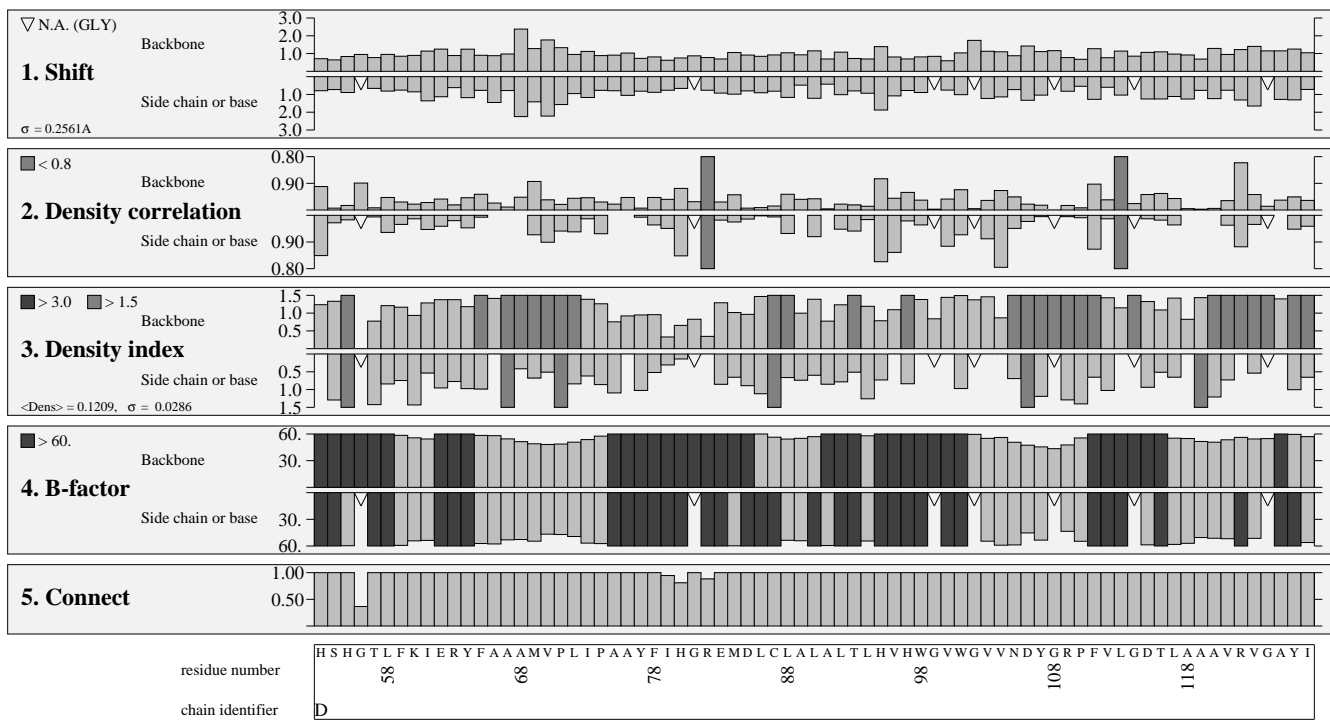
Local estimation (7)



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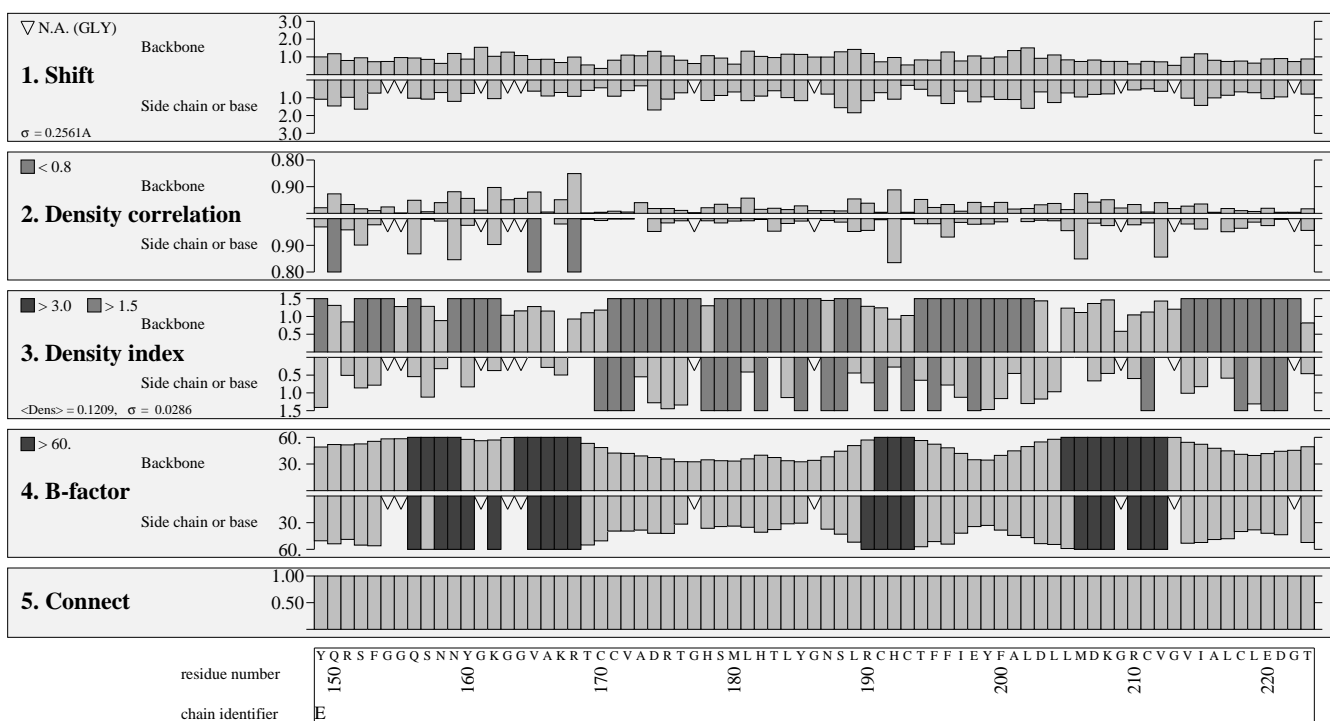
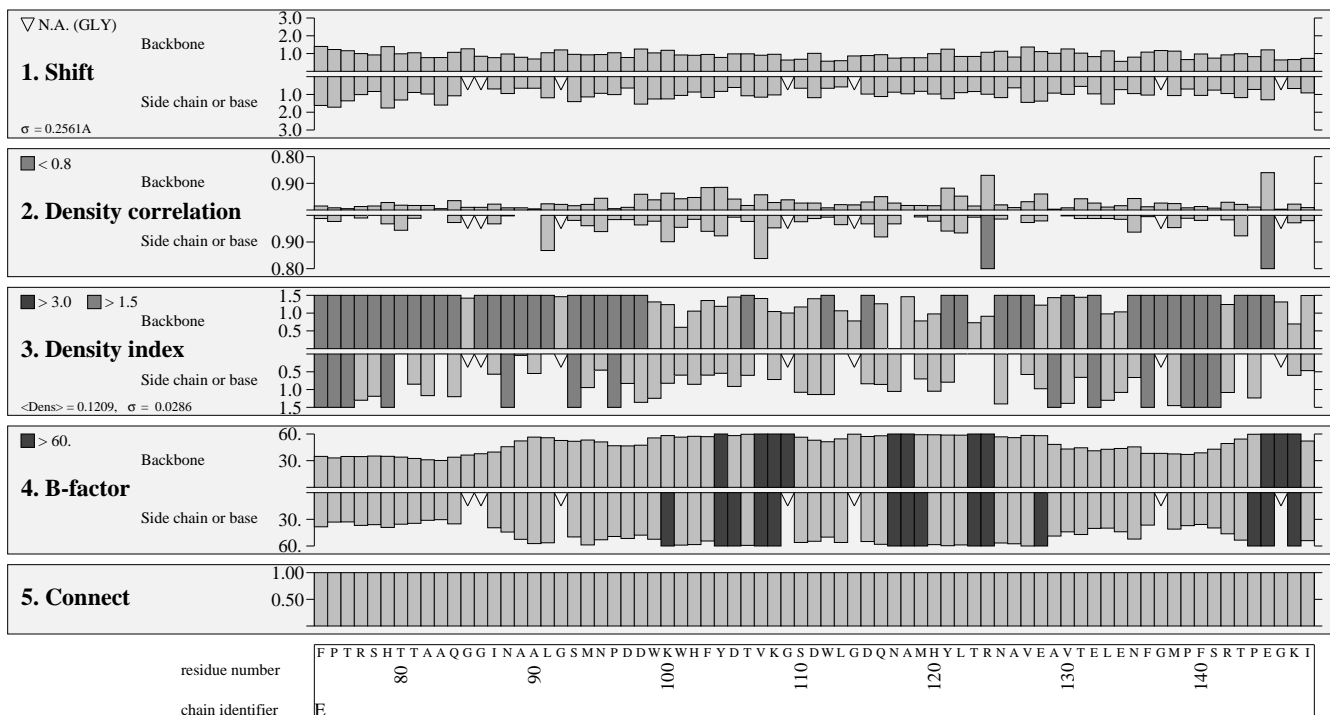
Local estimation (8)



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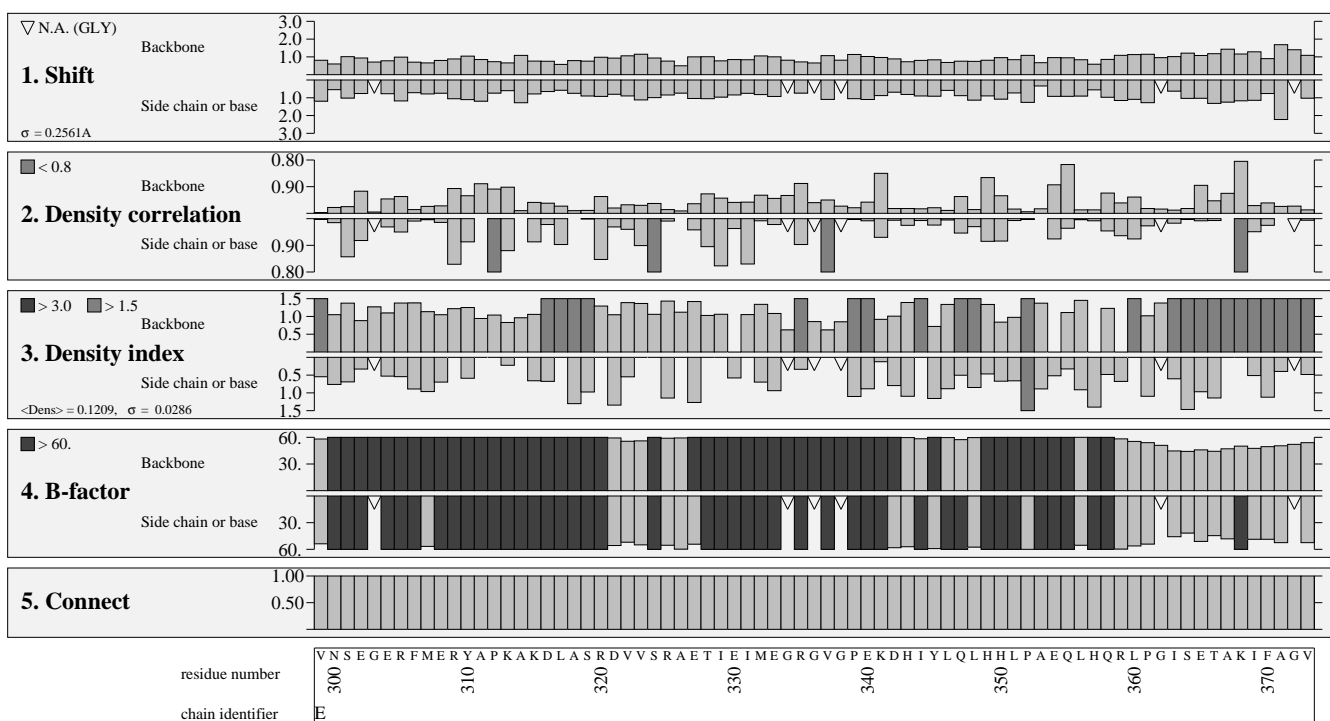
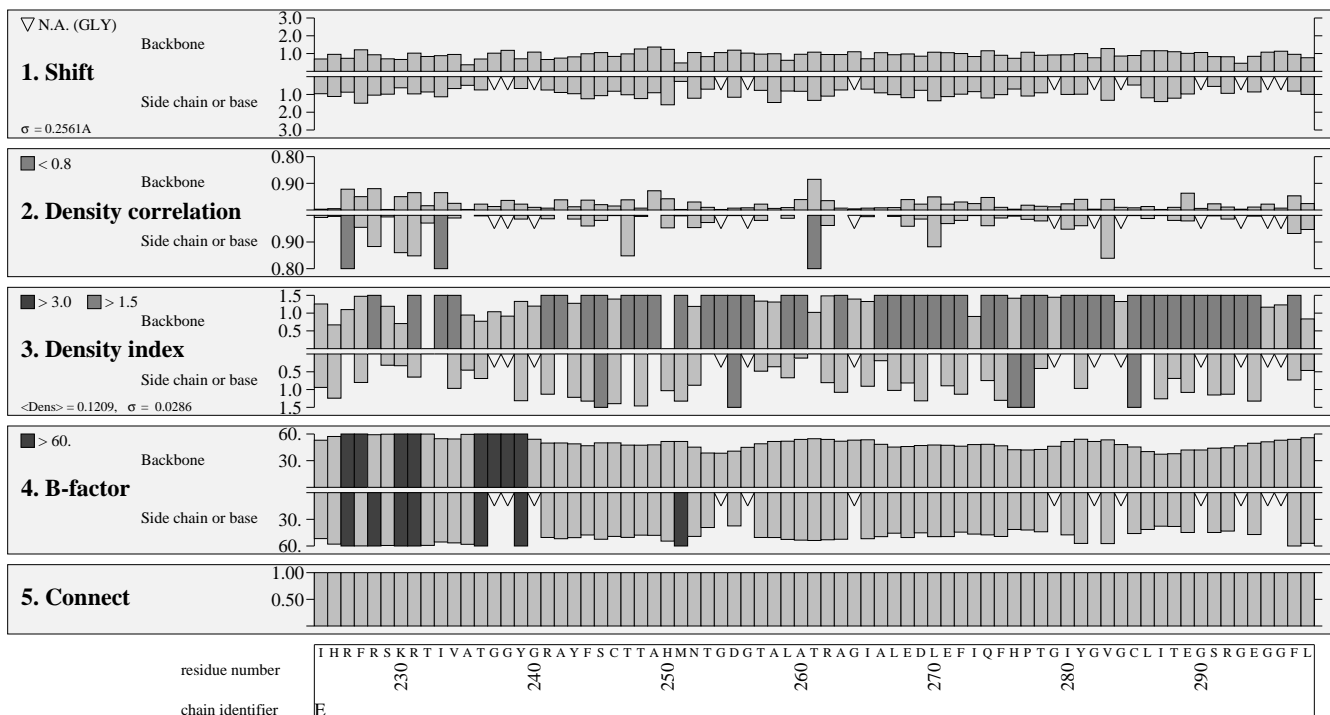
Local estimation (9)



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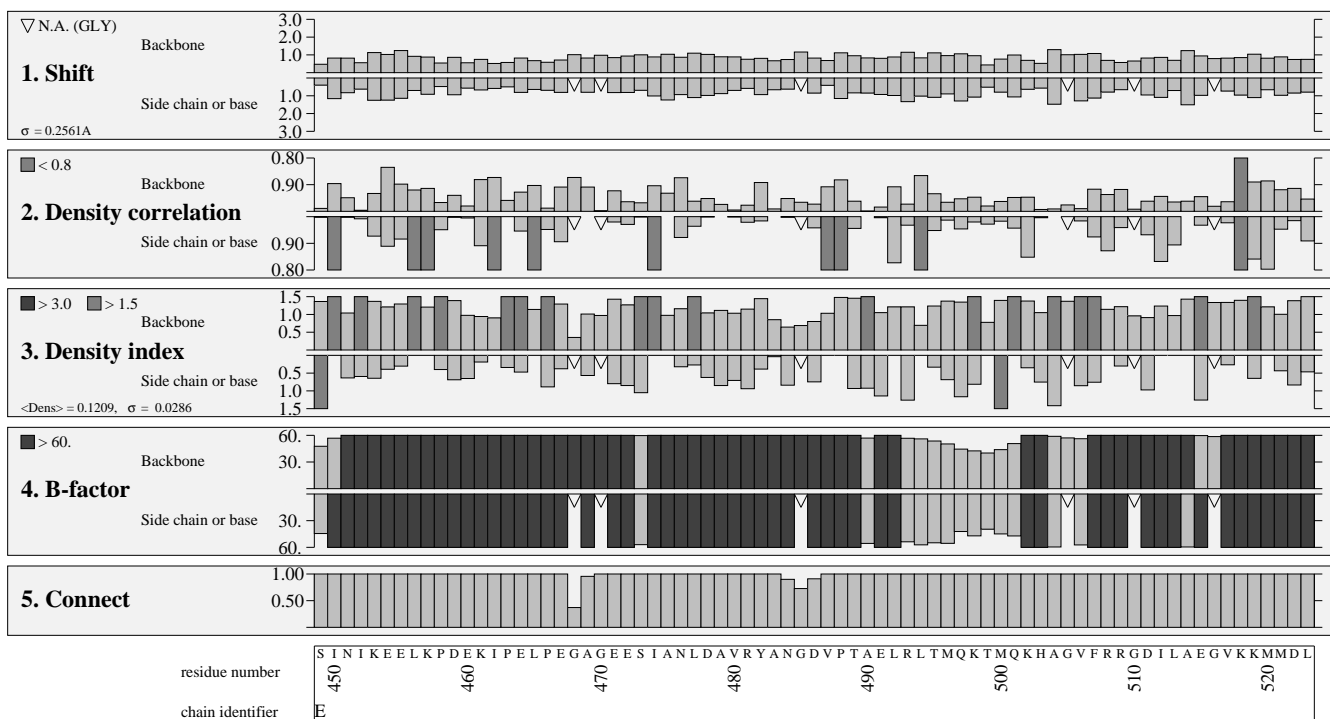
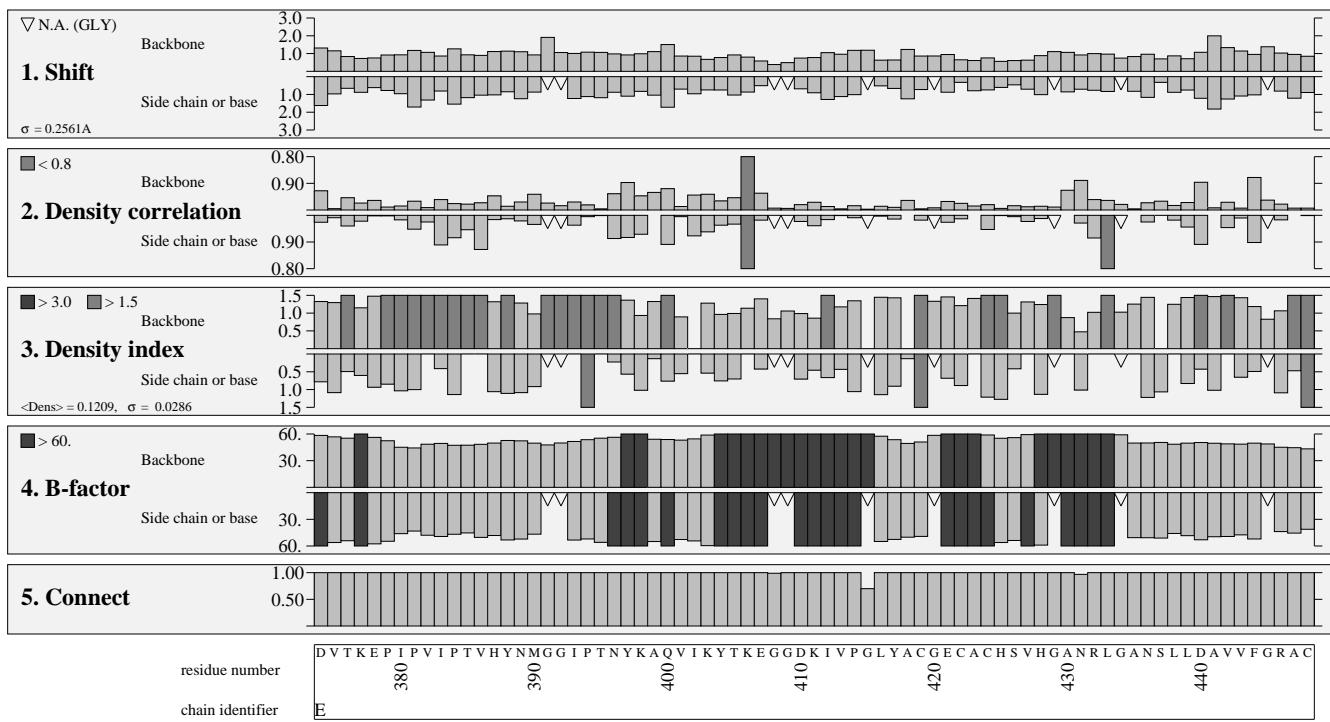
Local estimation (10)



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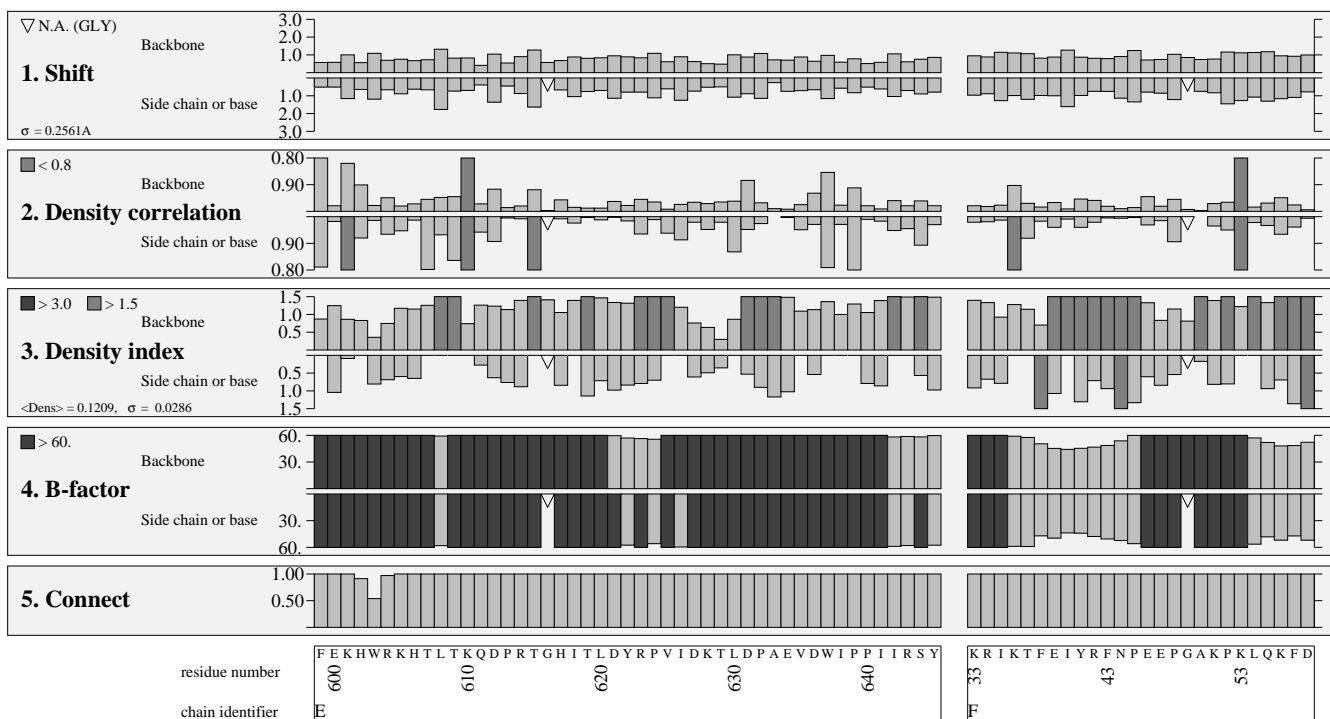
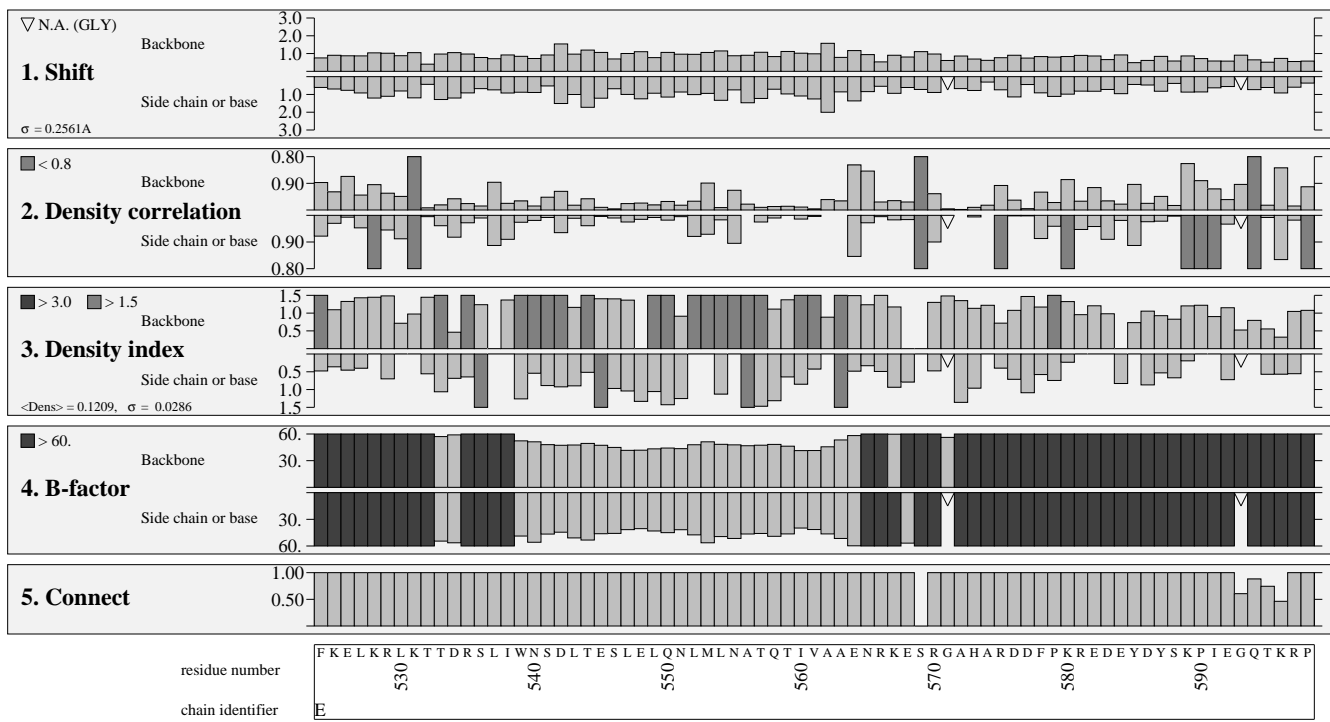
Local estimation (11)



Structure Factor Check

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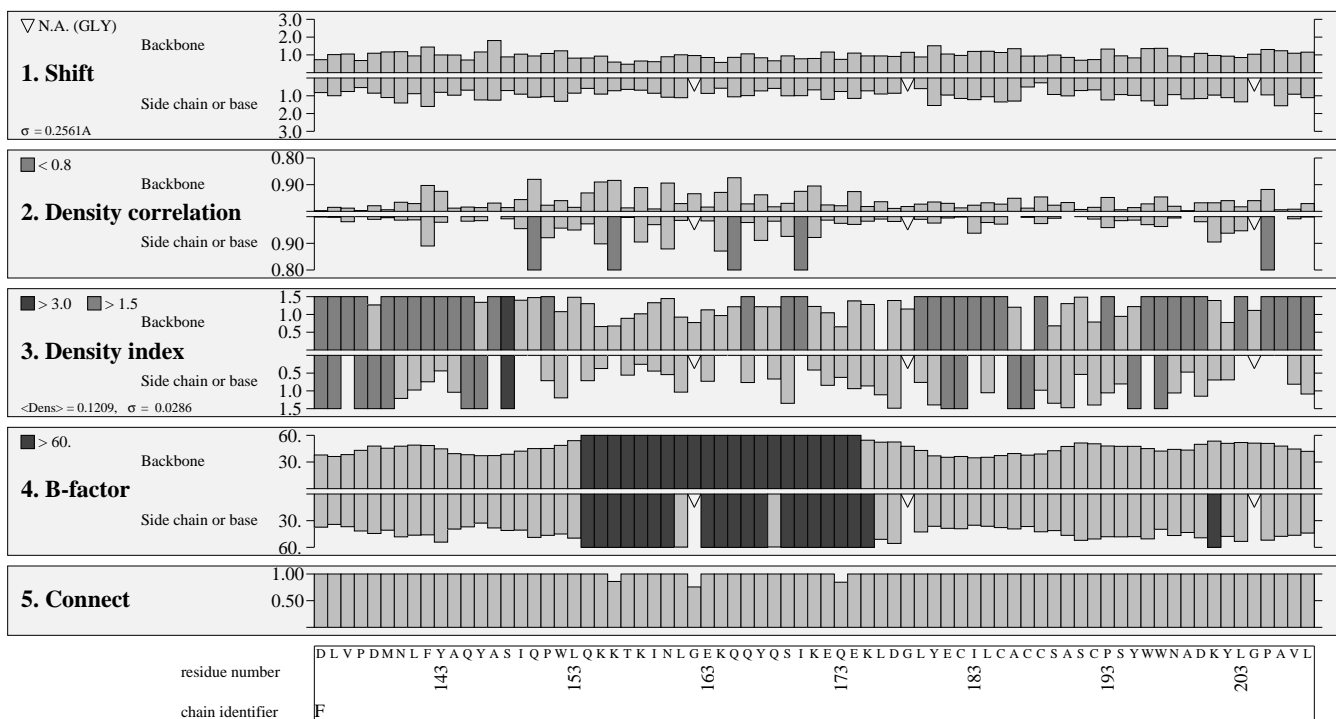
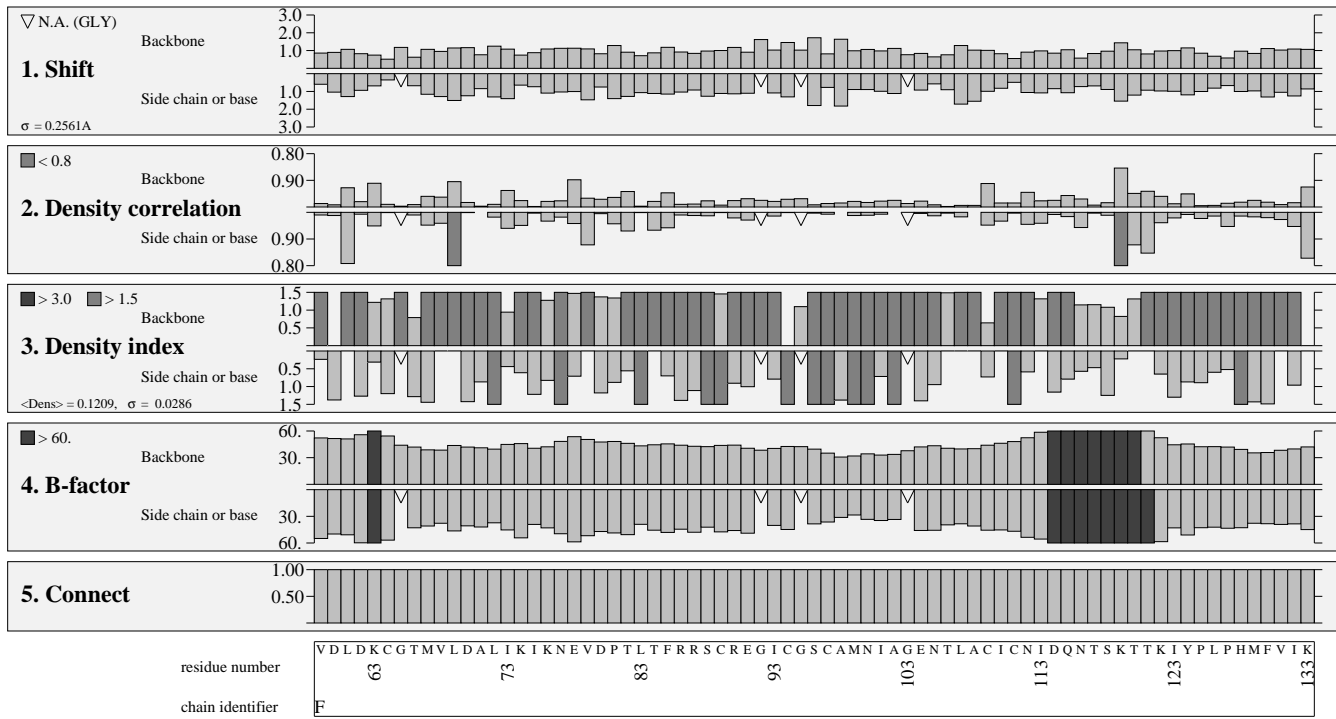
Local estimation (12)



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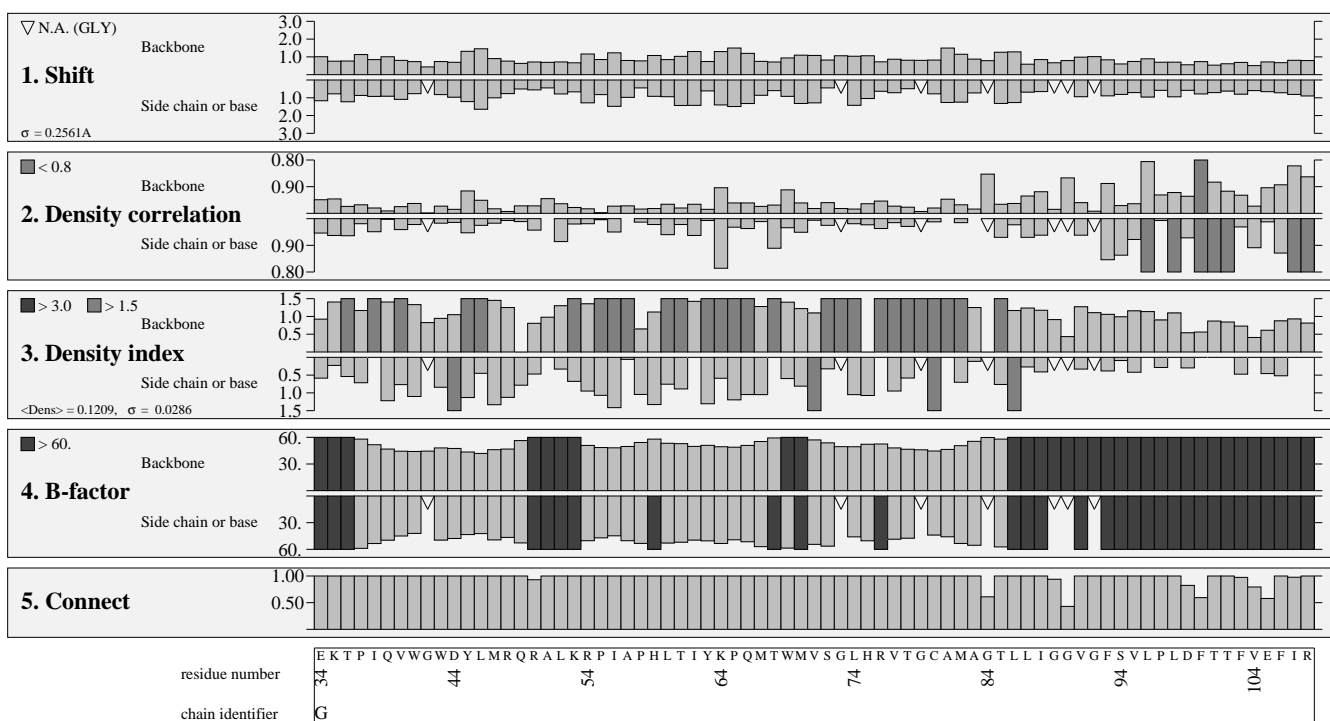
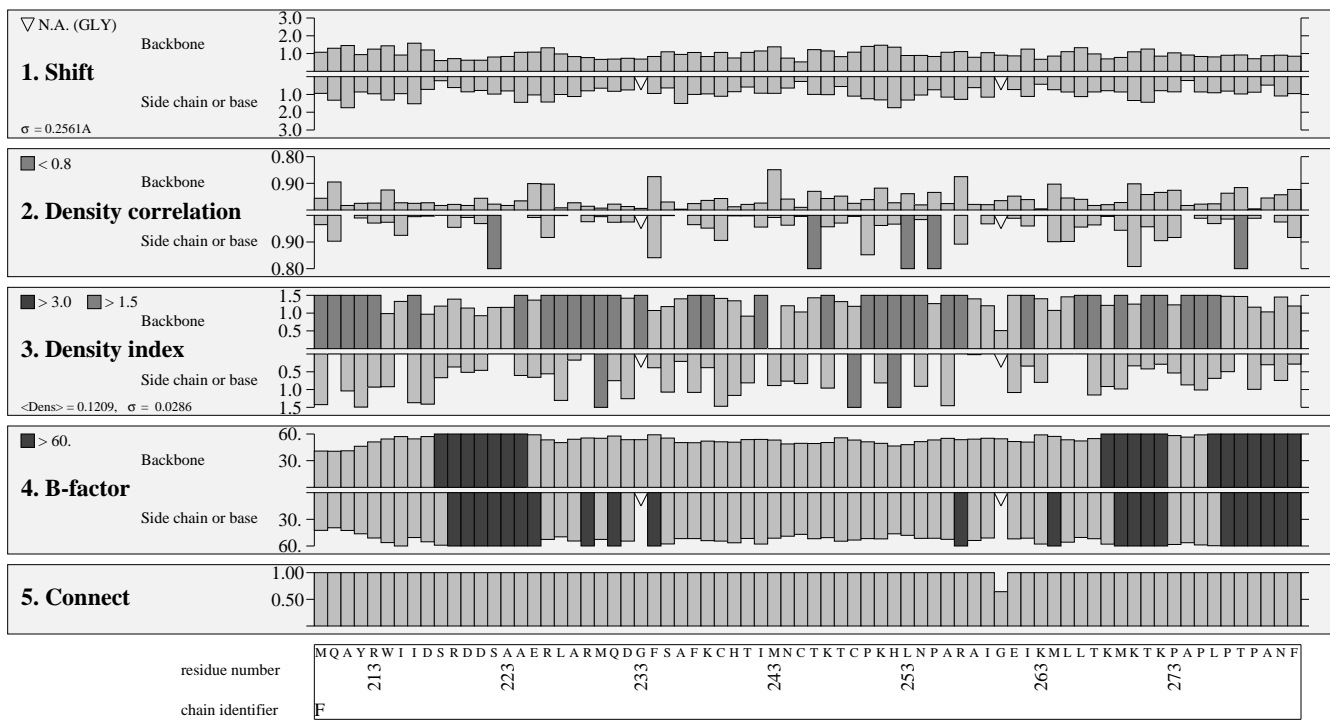
Local estimation (13)



Structure Factor Check

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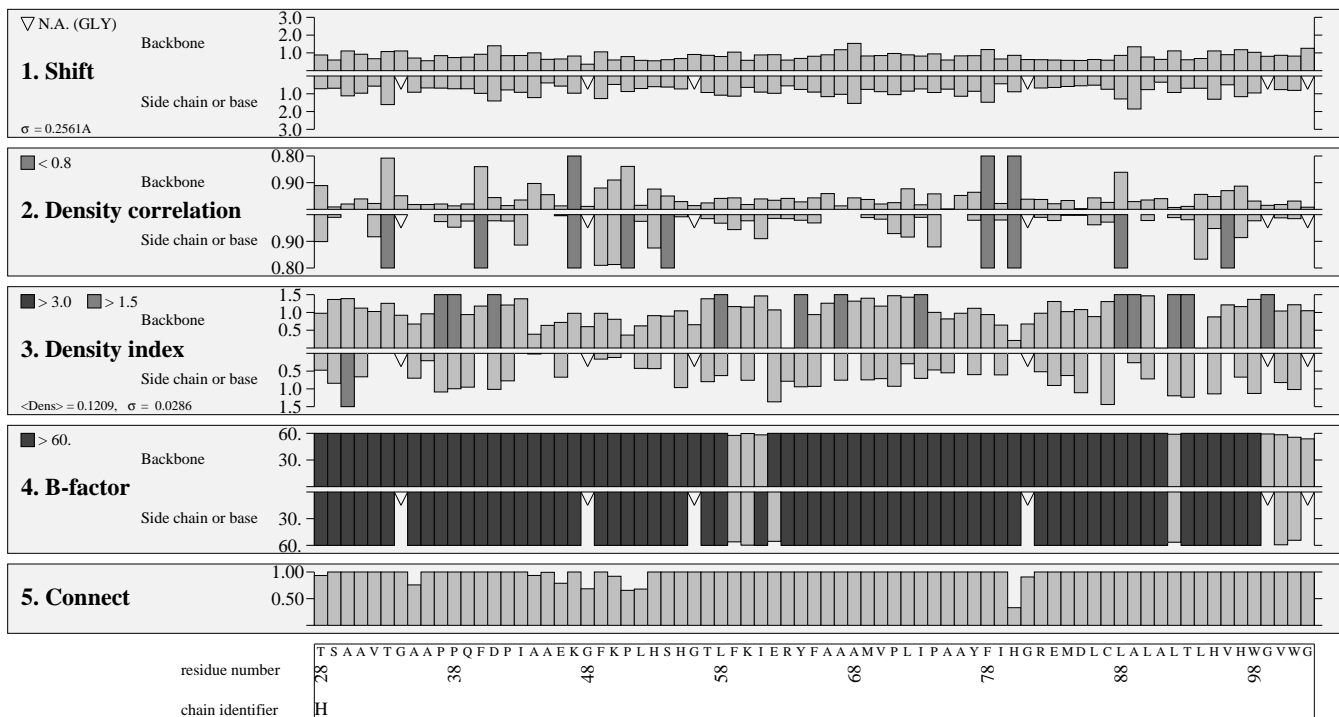
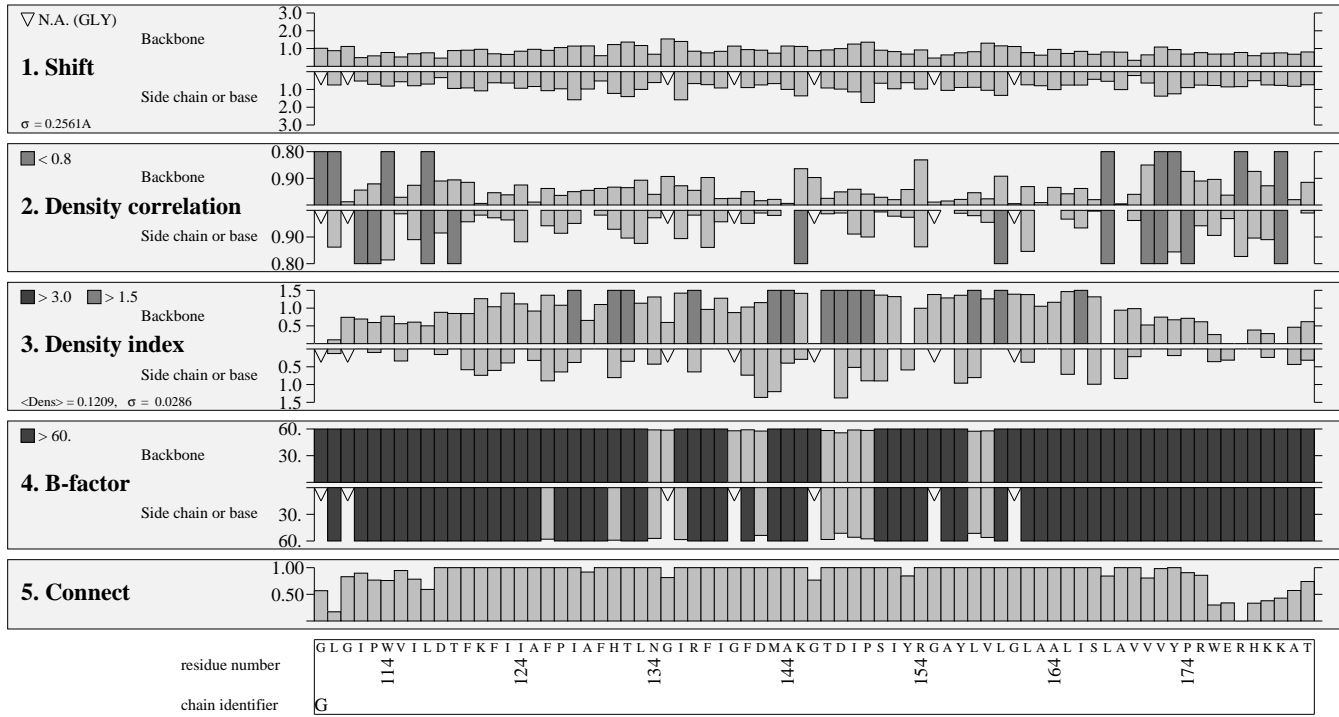
Local estimation (14)



Structure Factor Check

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Local estimation (15)



Structure Factor Check

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Local estimation (16)

