

Structure Factor Check

4YSX

Title: CRYSTAL STRUCTURE OF MITOCHONDRIAL RHODOQUINOL-FUMARATE REDU
 ASCARIS SUUM WITH THE SPECIFIC INHIBITOR NN23
 Date: 17-MAR-15
 PDB code: 4YSX

Crystal

Cell parameters:
 a: 124.20 A b: 127.91 A c: 220.55 A
 α : 90.00 β : 90.00 γ : 90.00
 Space group: P 21 21 21

Model

19103 atoms (721 water molecules)
 Number of chains: 32
 Volume not occupied by model: 53.5 %
 $\langle B \rangle$ (for atomic model): 49.1 A²
 $\sigma(B)$: 13.34 A²
 Matthews coefficient: 3.28
 Corresponding solvent % : 62.15

Refinement

Program: REFMAC 5.7.0029
 Nominal resolution range: 20.0 - 2.25 A
 Reported R-factor: 0.181
 Number of reflections used: 152442
 Reported Rfree: 0.22
 Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 20.0 - 2.25 A
 Reflections in file: 166258
 Unique reflections above 0: 160280
 above 1 σ : 158936
 above 3 σ : 120913
 Reflections > 0: 5978

SFCHECK

Nominal resolution range: 20.0 - 2.25 A
 \05max. from input data, min. from author\05
 Used reflections: 160279
 Reflections out of resolution: 1
 Completeness: 96.4 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.045
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.9323 0.9979
 B_{overall} (by Patterson): 38.A²
 Optical resolution: 1.80 A
 Expected opt. resol. for complete data set: 1.80 A
 Estimated minimal error: 0.020 A

Model vs. Structure Factors

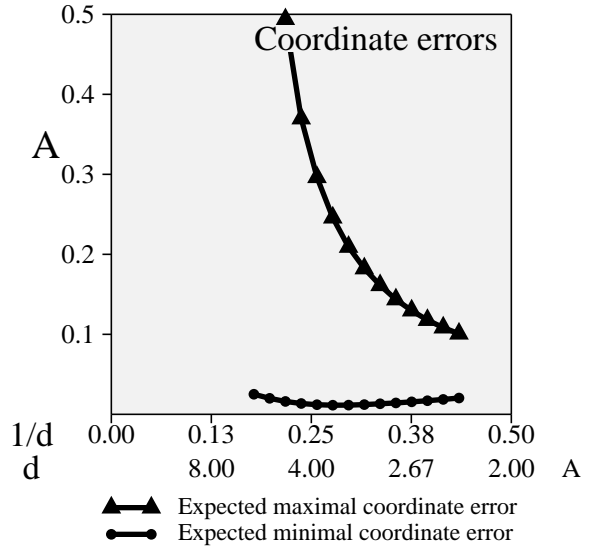
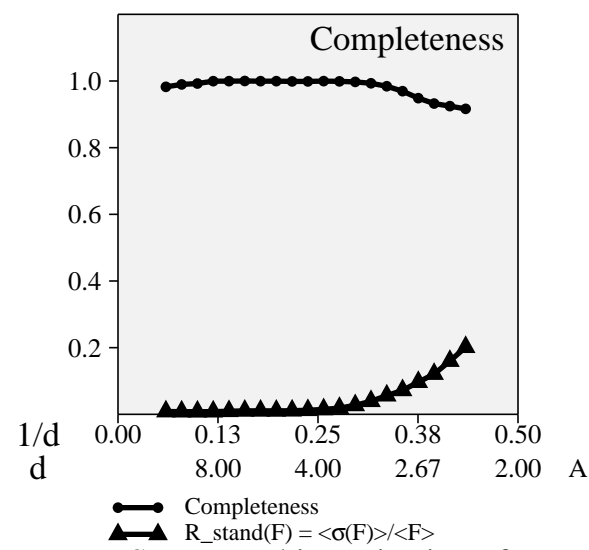
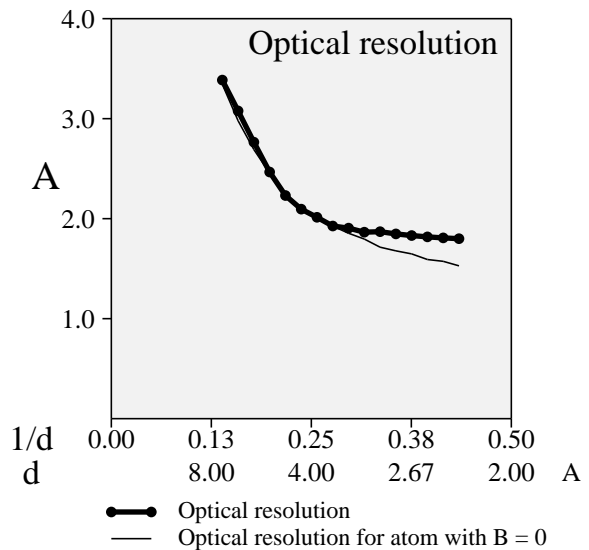
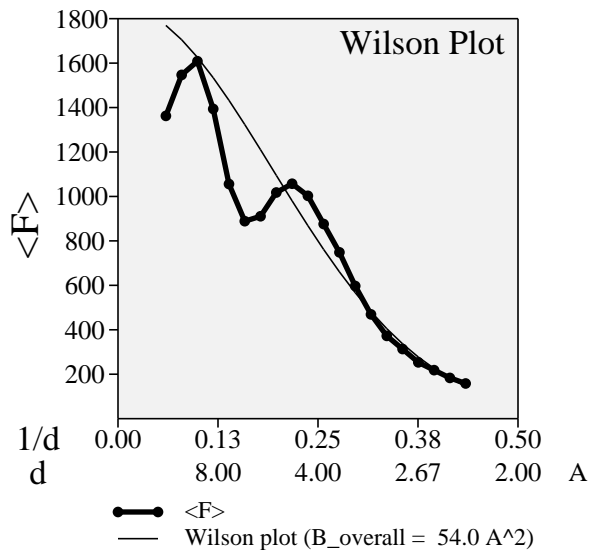
R-factor for all reflections: 0.222
 Correlation factor: 0.926
 R-factor: 0.227
 for $F > 2.0\sigma$
 nom. resolution range: 20.00 - 2.25A
 reflections used: 158928
 Rfree: 0.262
 Nfree: 7994
 R-factor without free-refl.: 0.225
 Non free-reflections: 150934
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.270 A
 Estimated maximal error: 0.101 A
 DPI: 0.174 A

Scaling

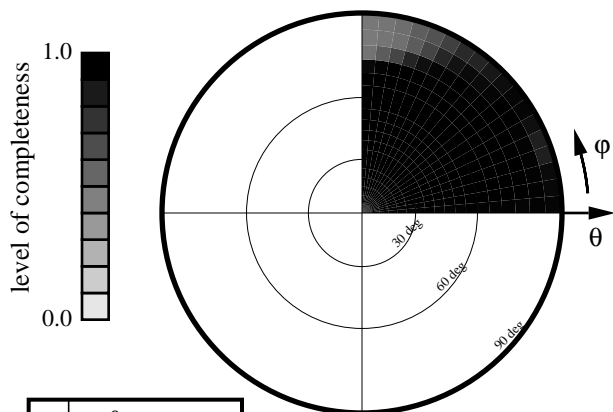
Scale: 0.943
 Bdiff: -3.52
 Anisothermal Scaling (Beta):
 0.4019 0.3287 0.3879 -0.0000 0.0000 -0.0000
 Solvent correction - Ks,Bs: 0.642 250.009

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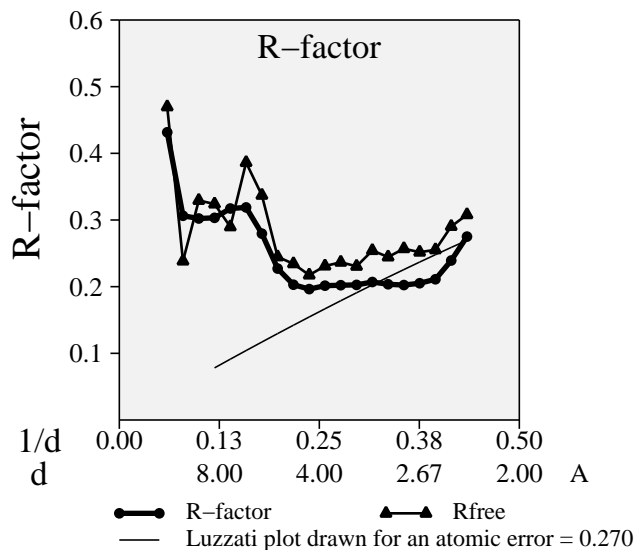


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

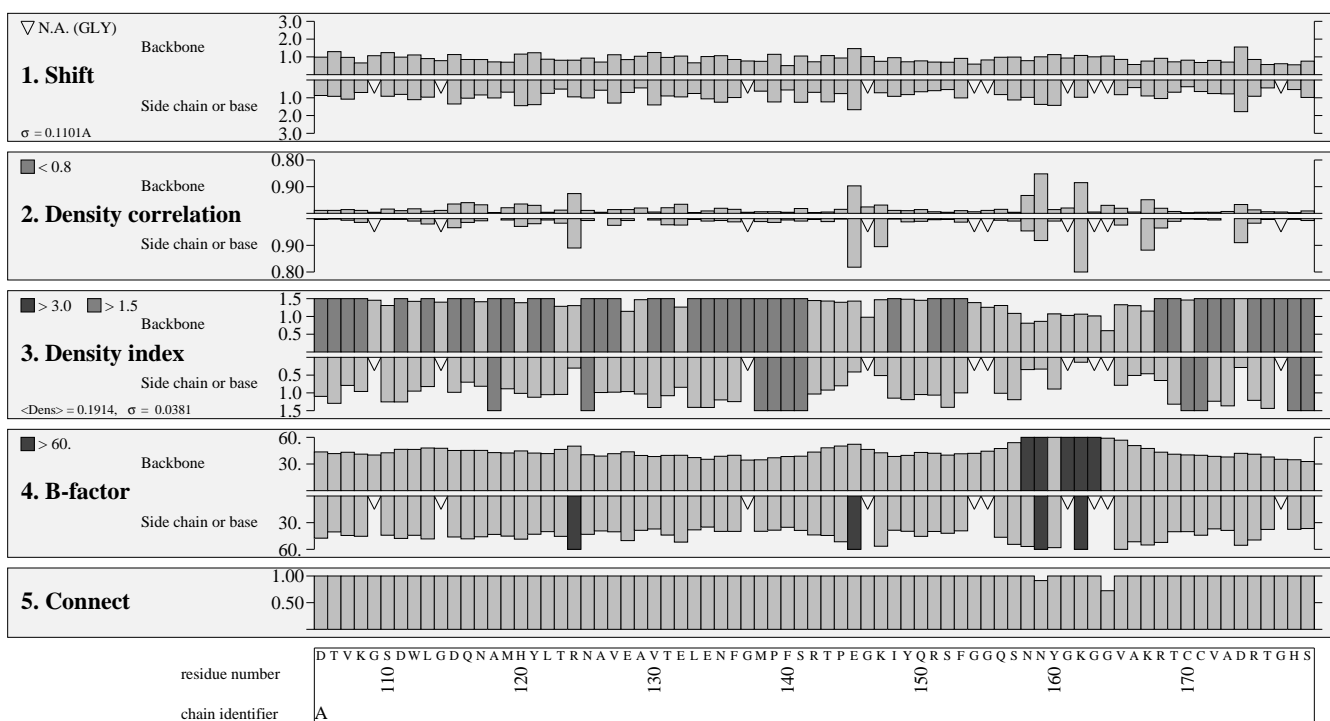
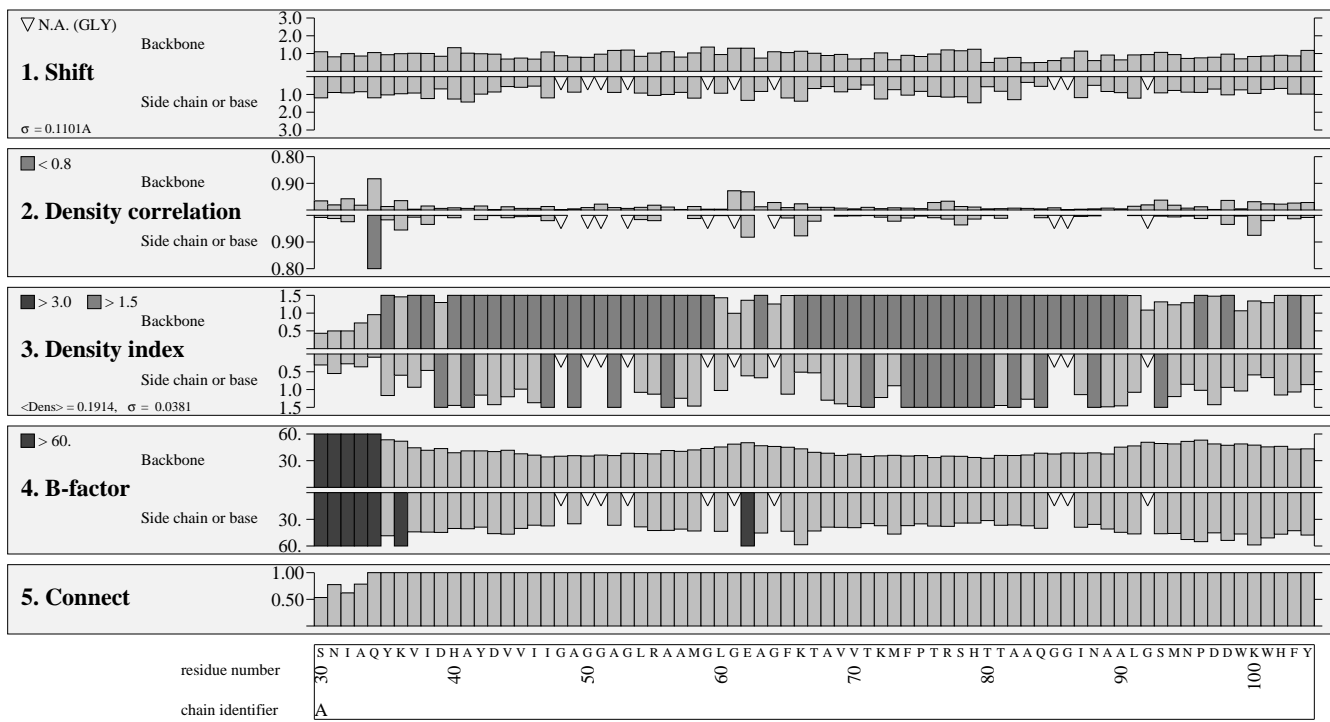
polar coordinates of the crystallographical axes



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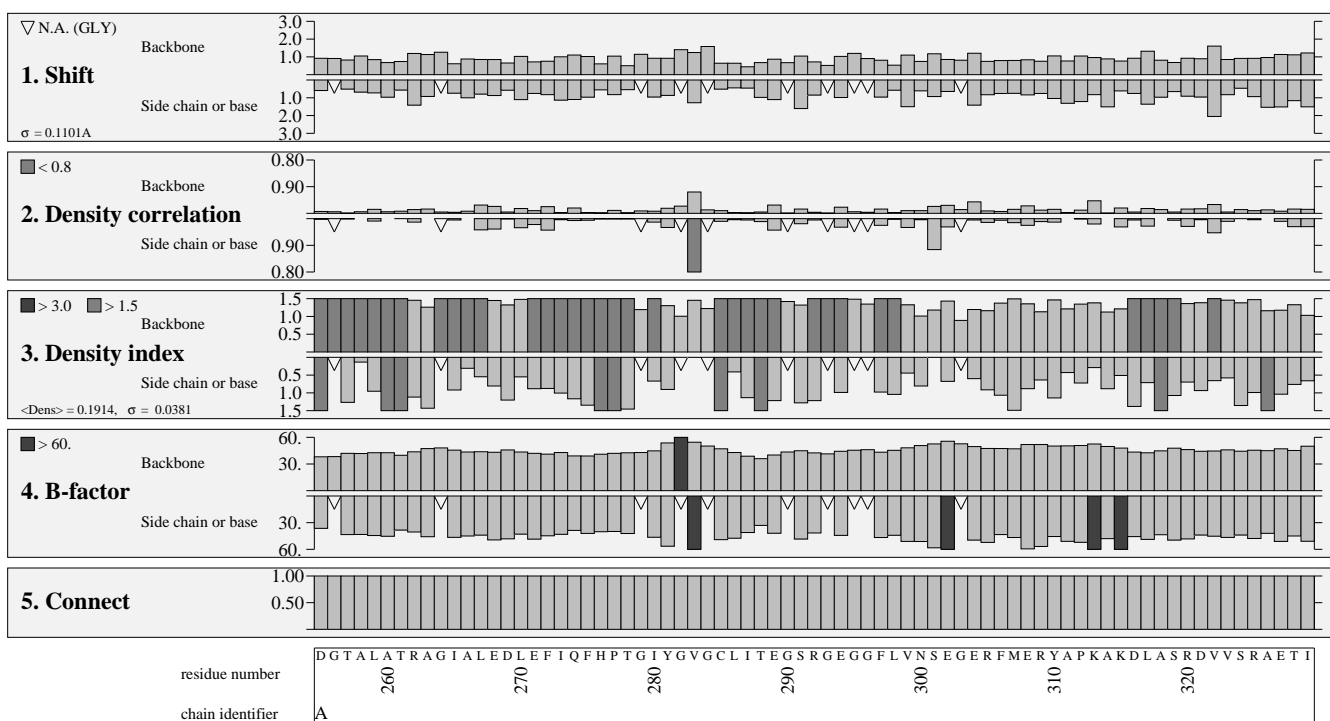
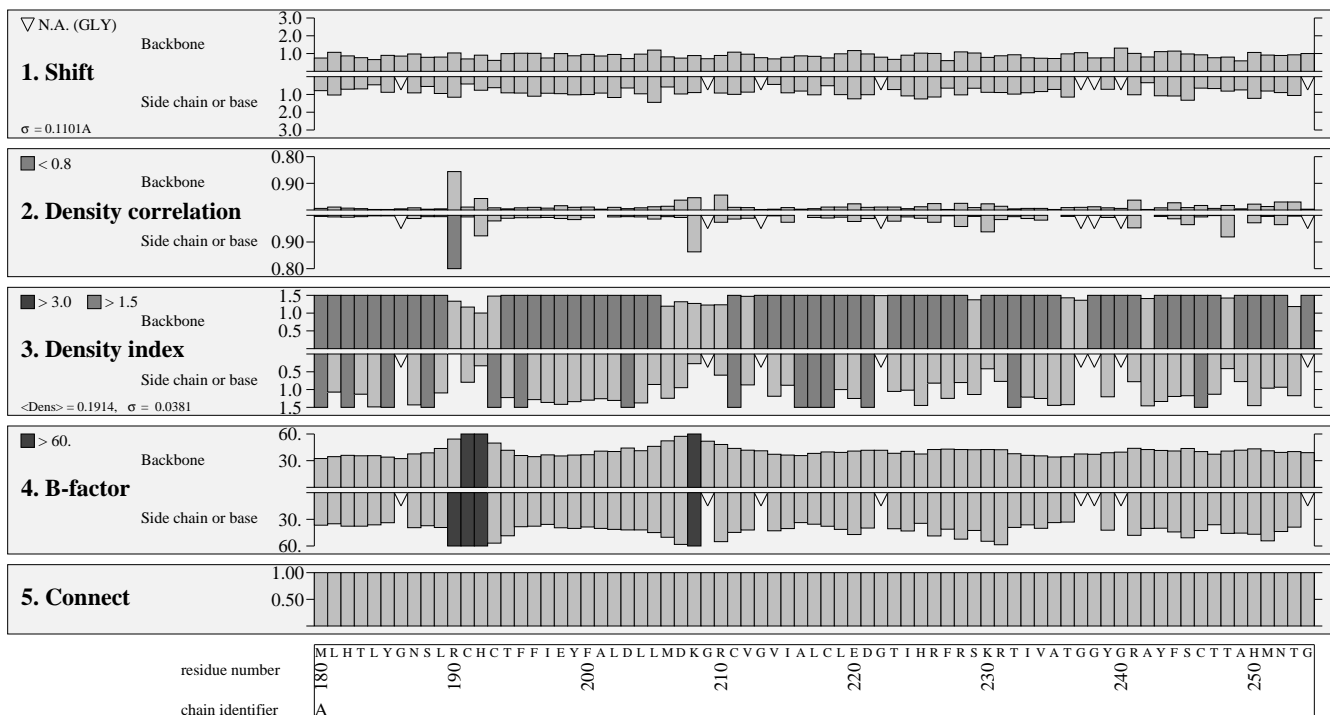
Local estimation



Structure Factor Check

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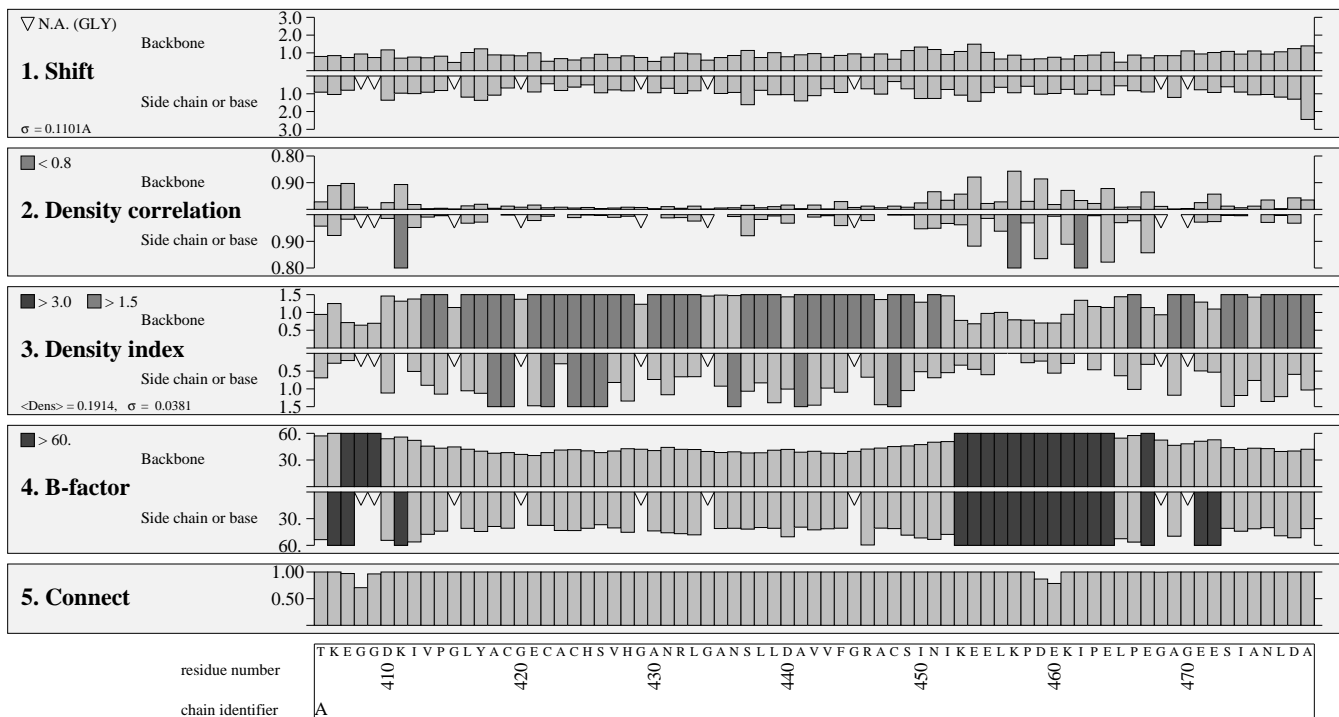
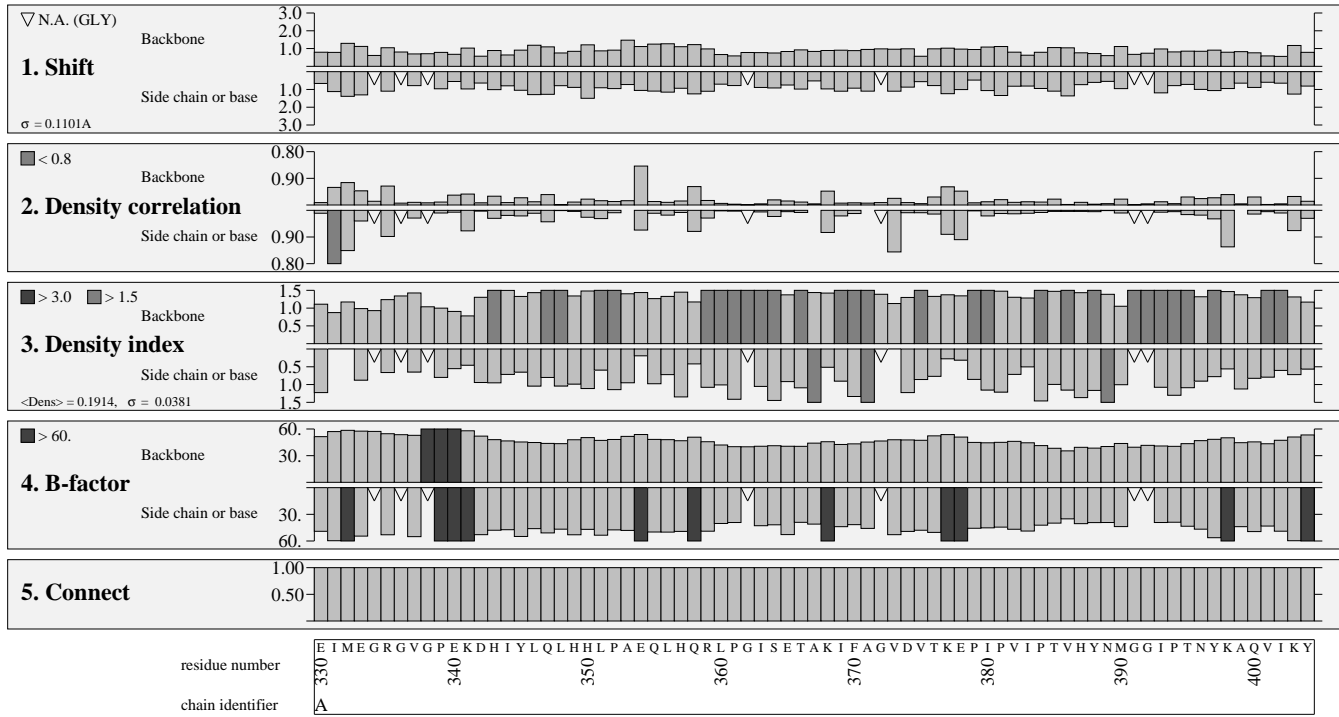
Local estimation (2)



Structure Factor Check

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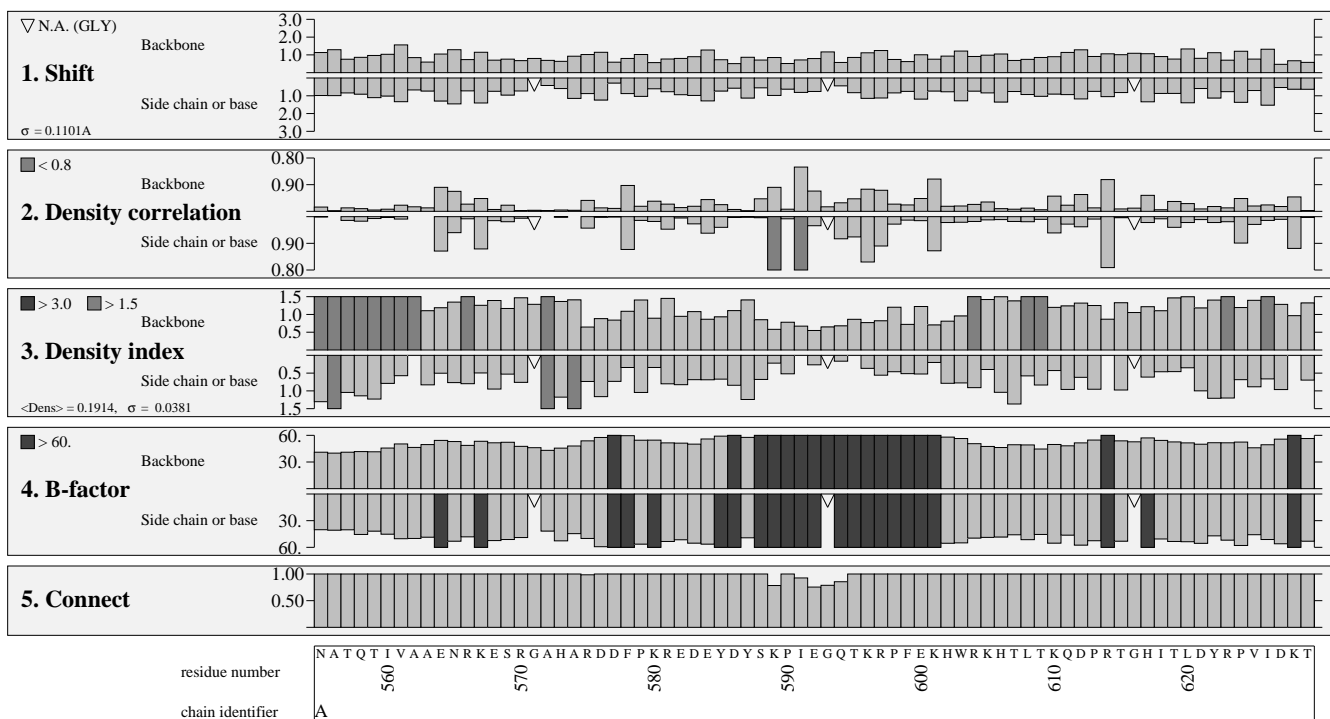
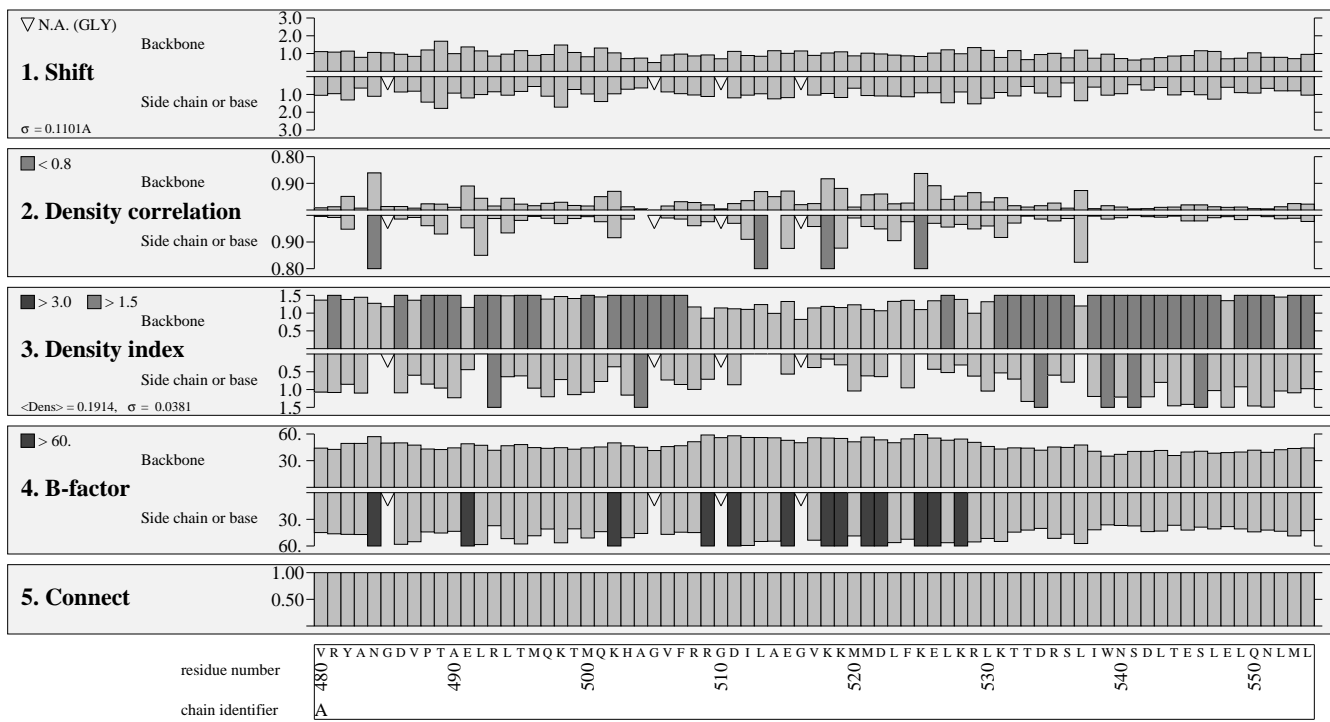
Local estimation (3)



Structure Factor Check

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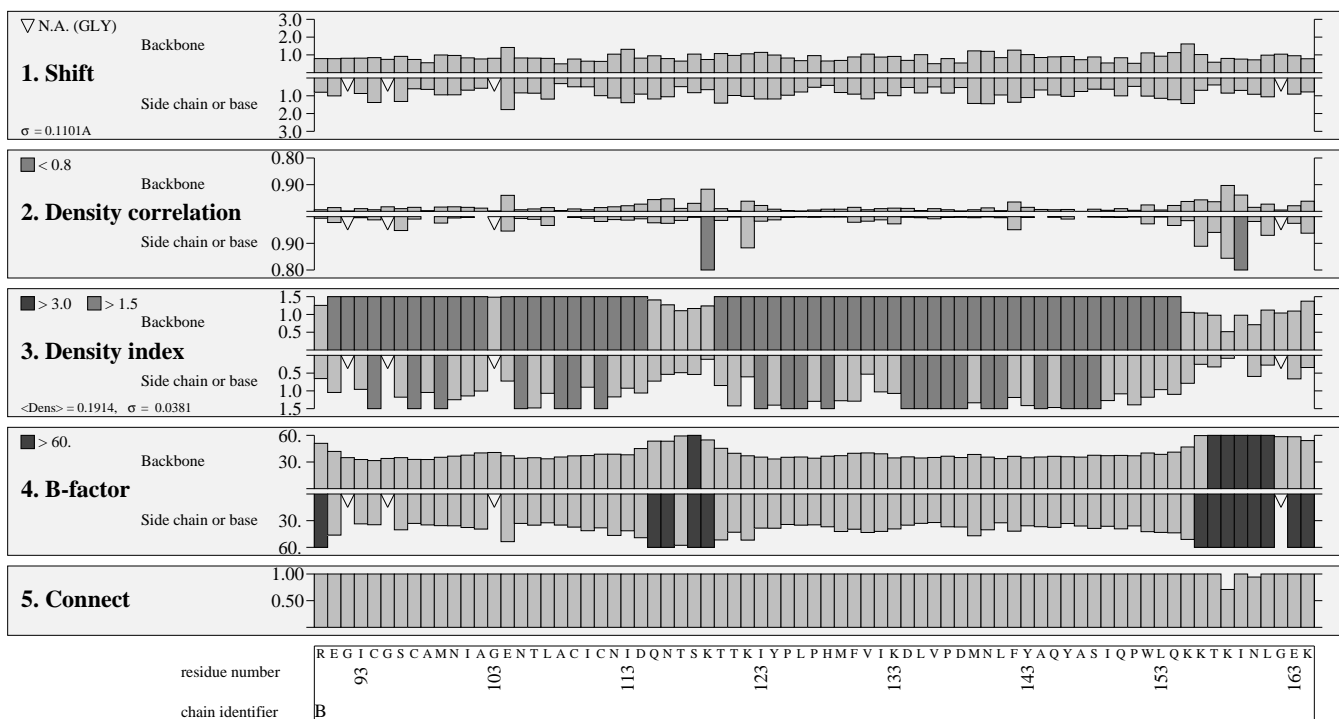
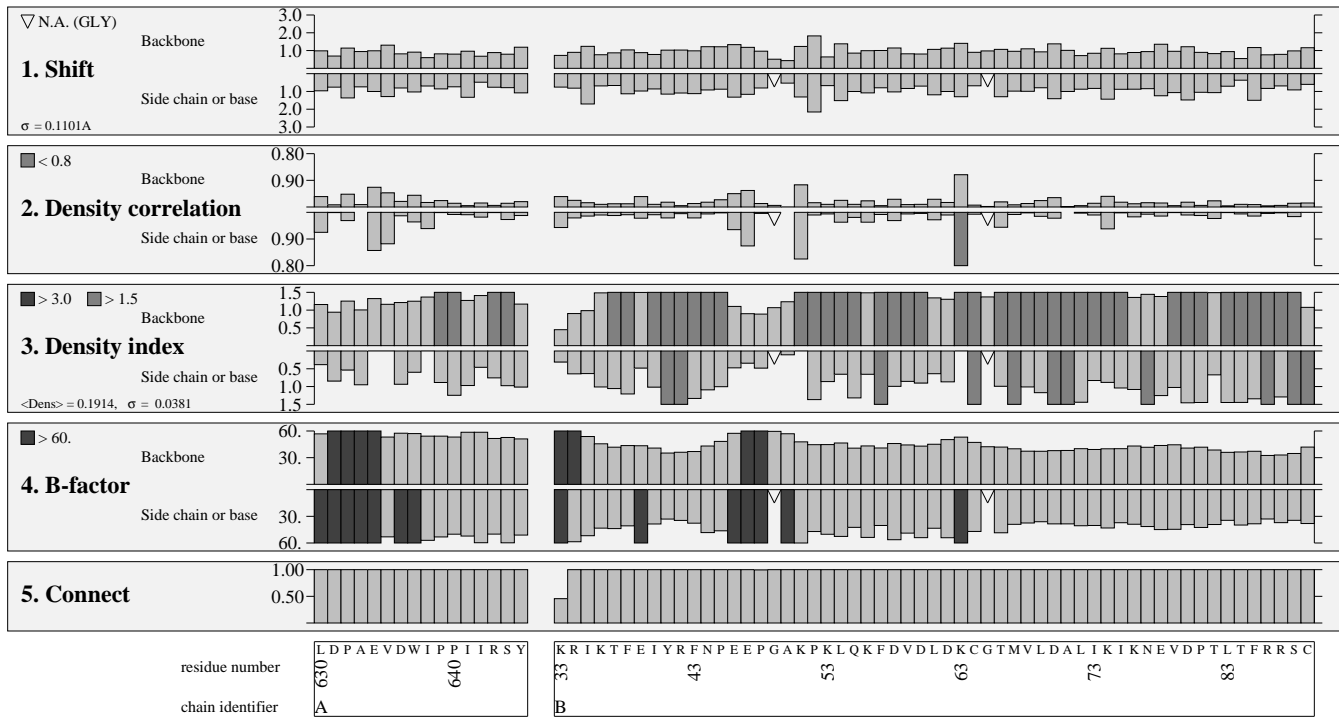
Local estimation (4)



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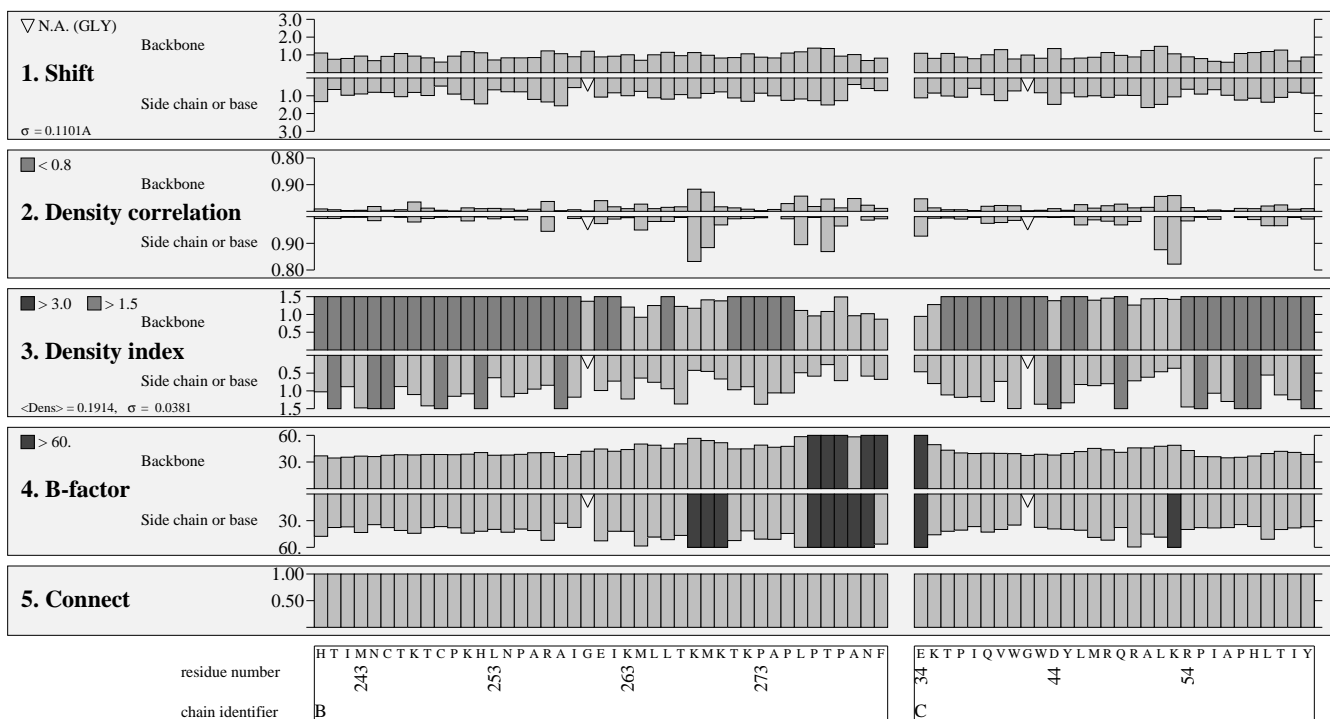
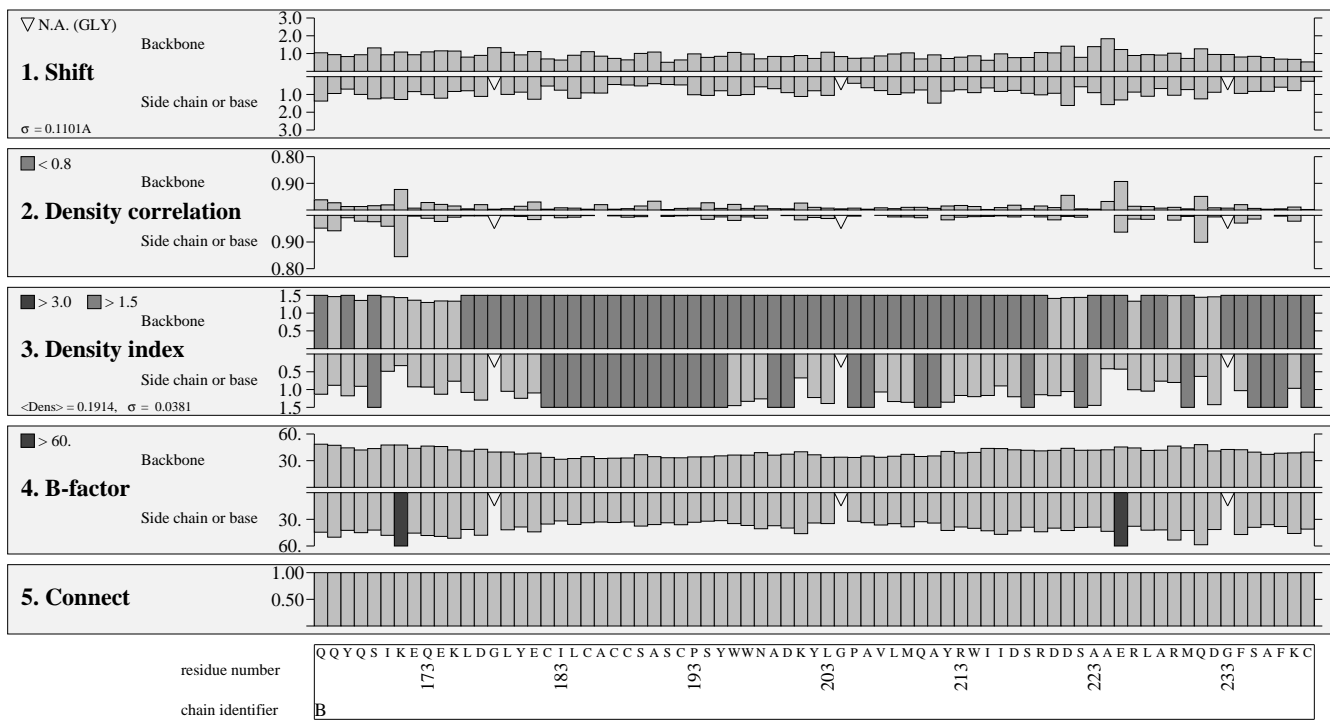
Local estimation (5)



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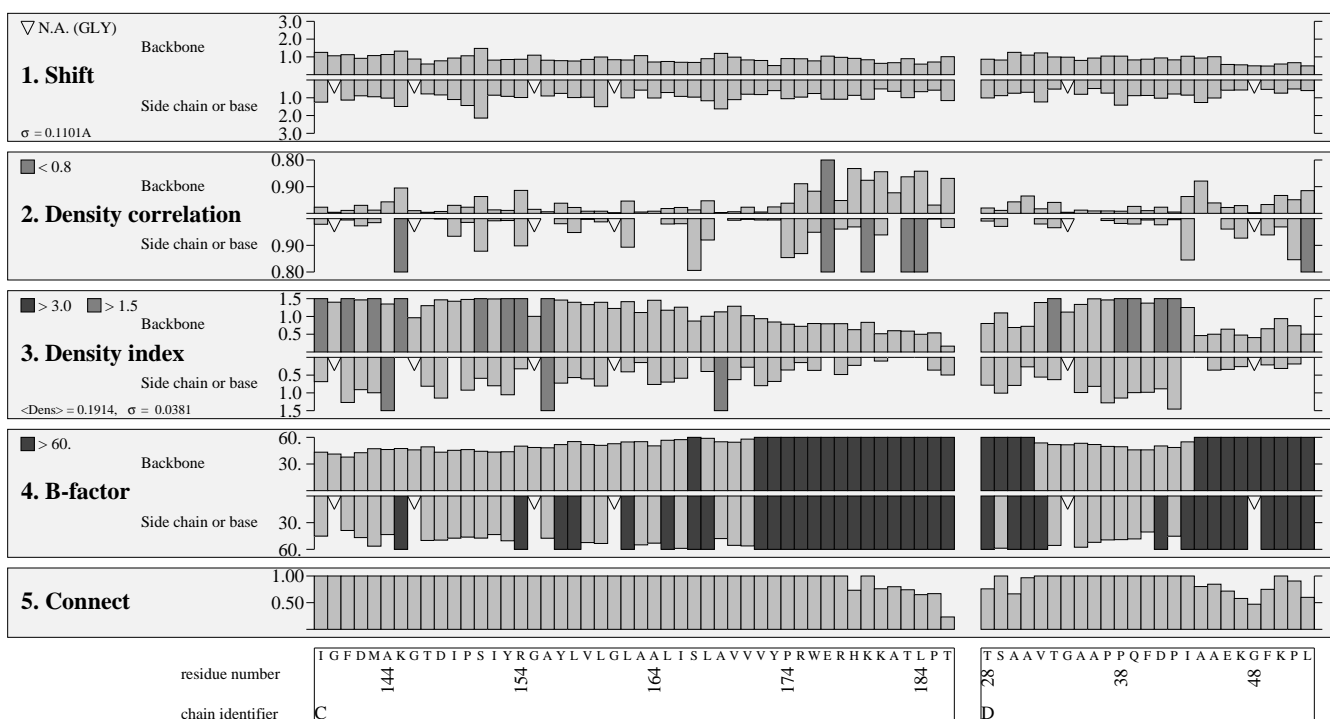
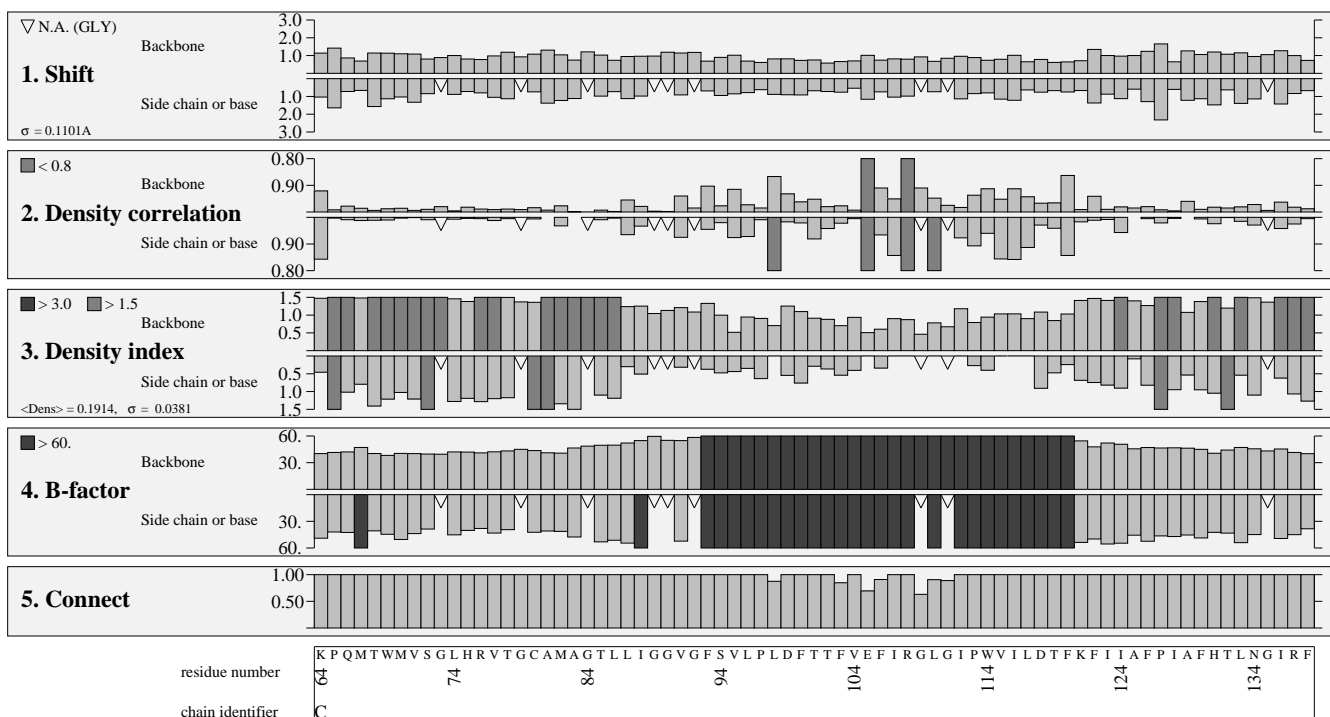
Local estimation (6)



Structure Factor Check

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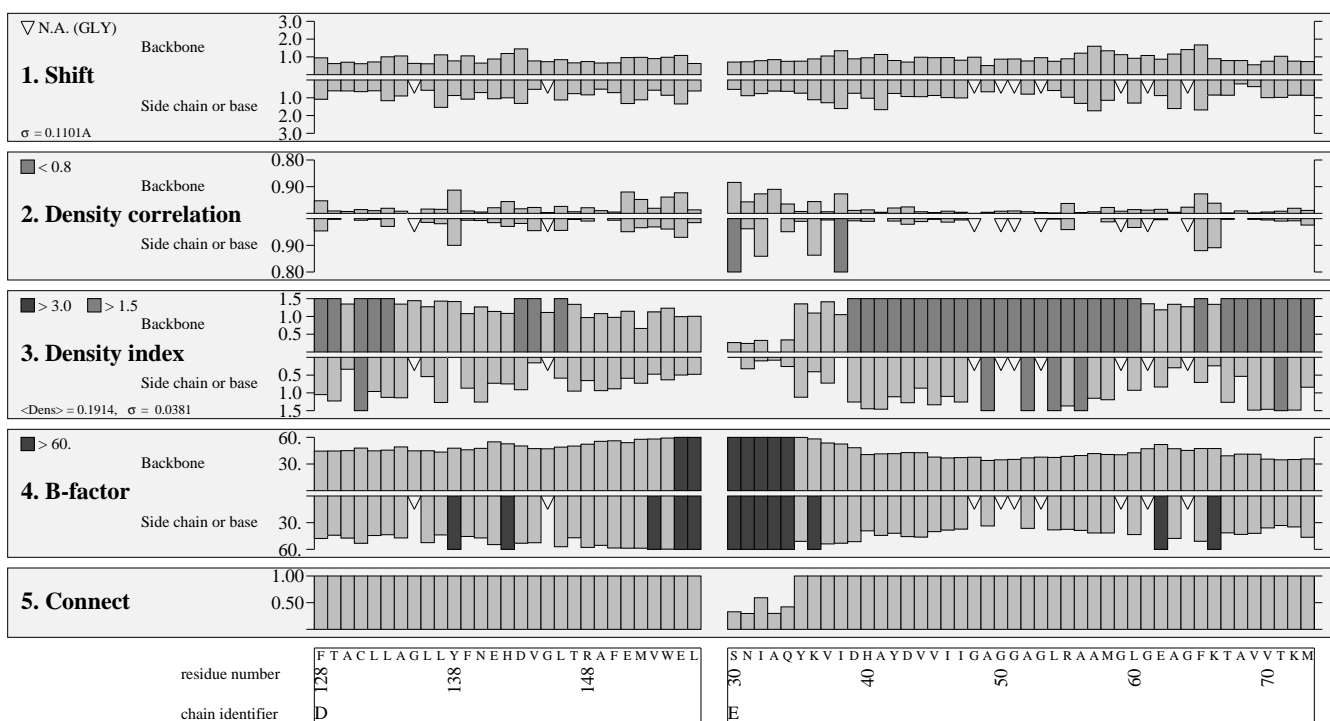
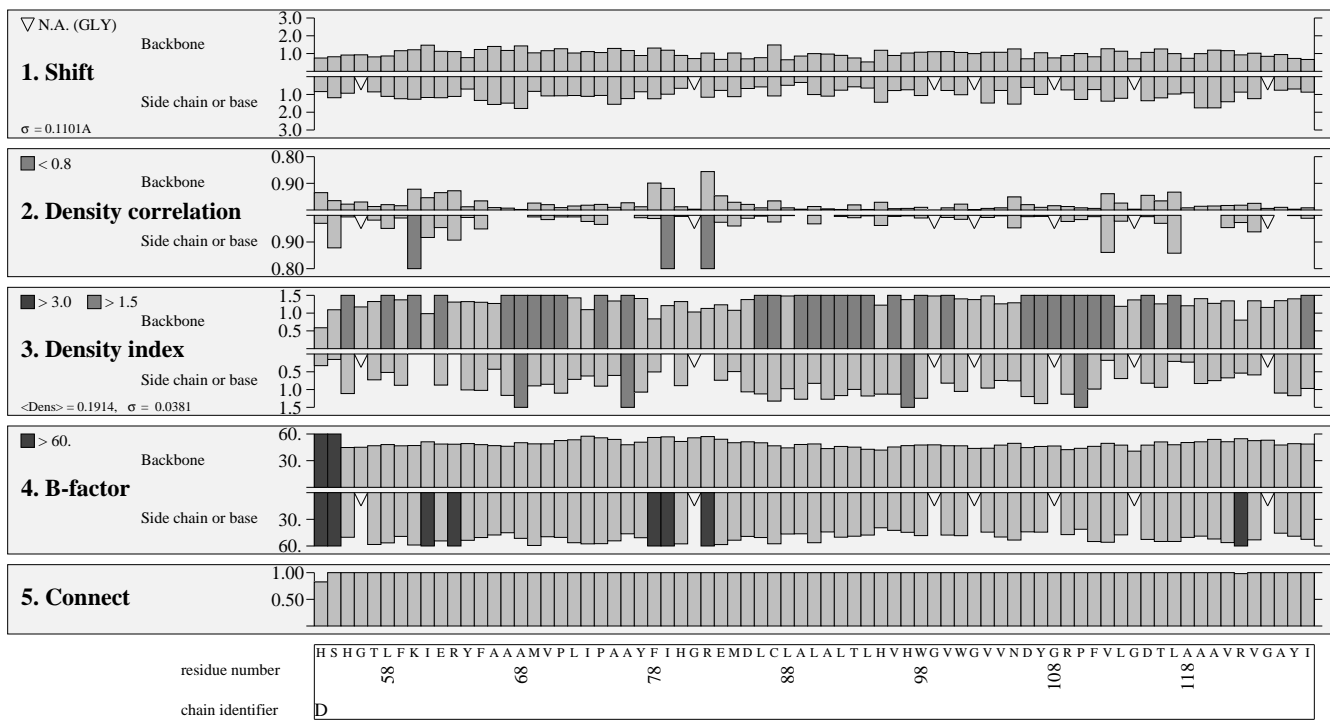
Local estimation (7)



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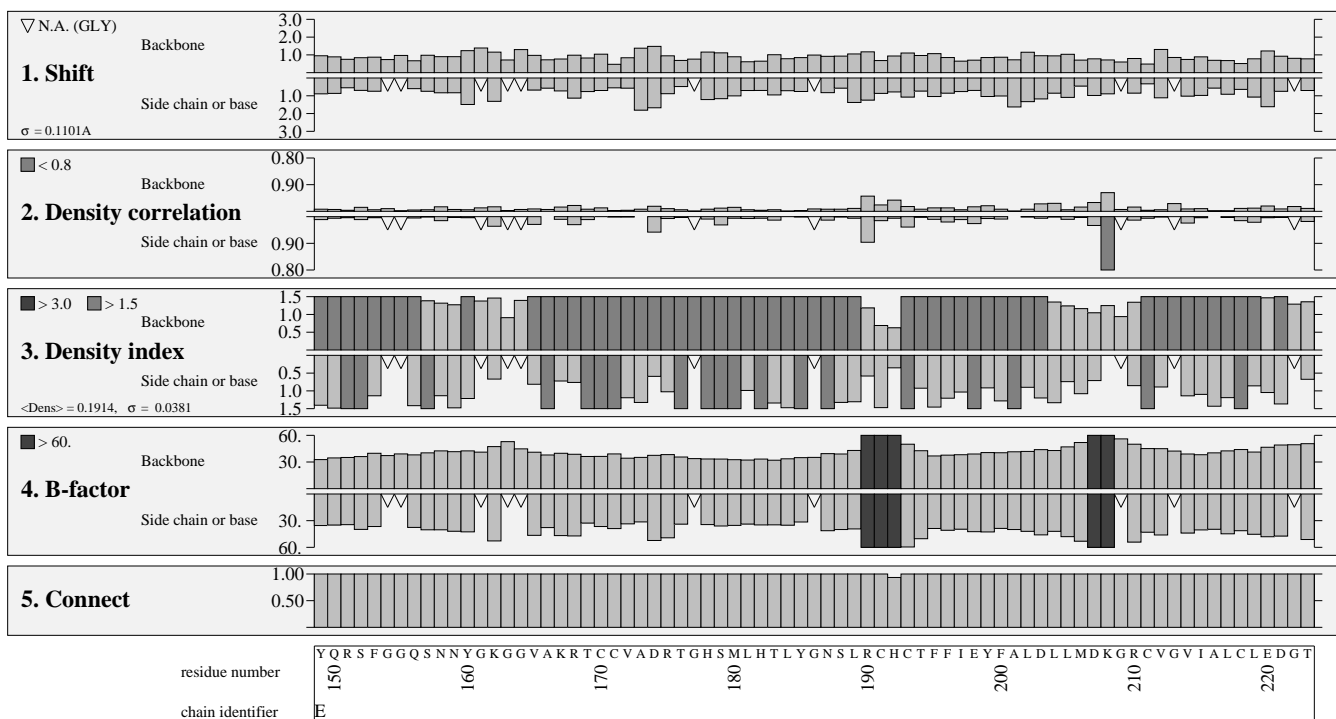
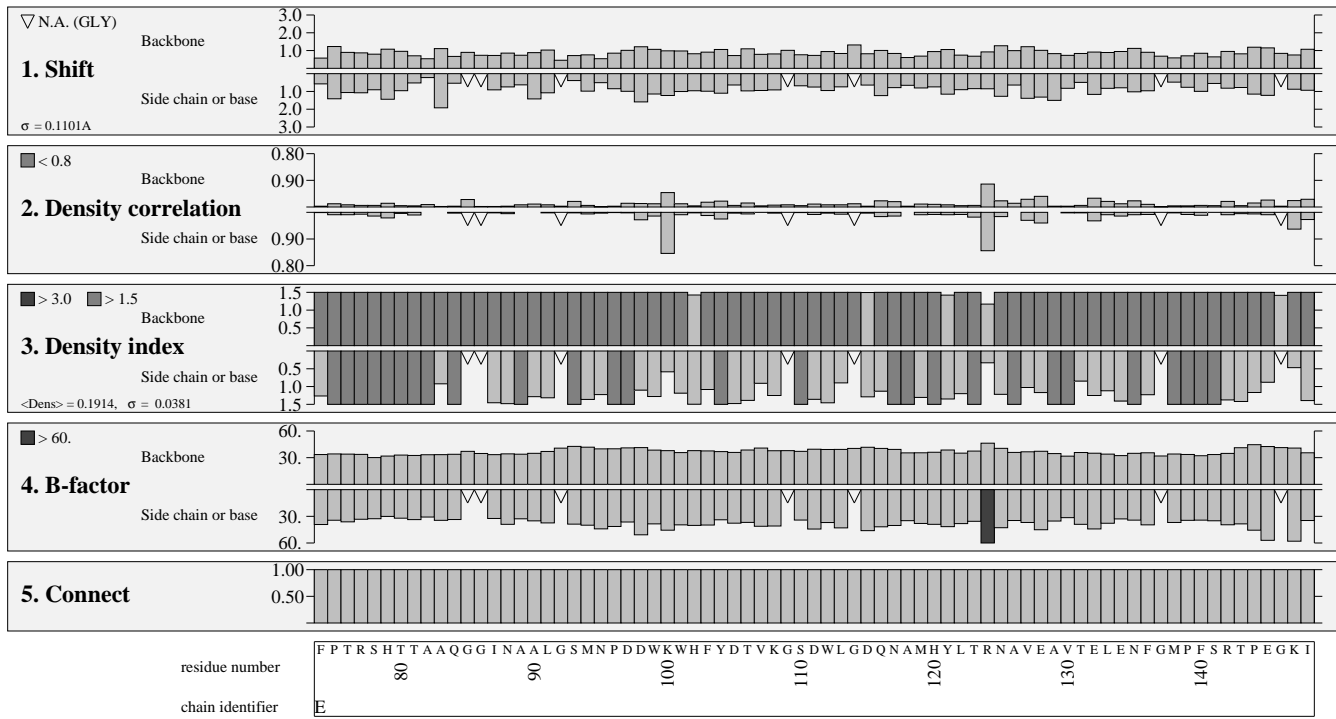
Local estimation (8)



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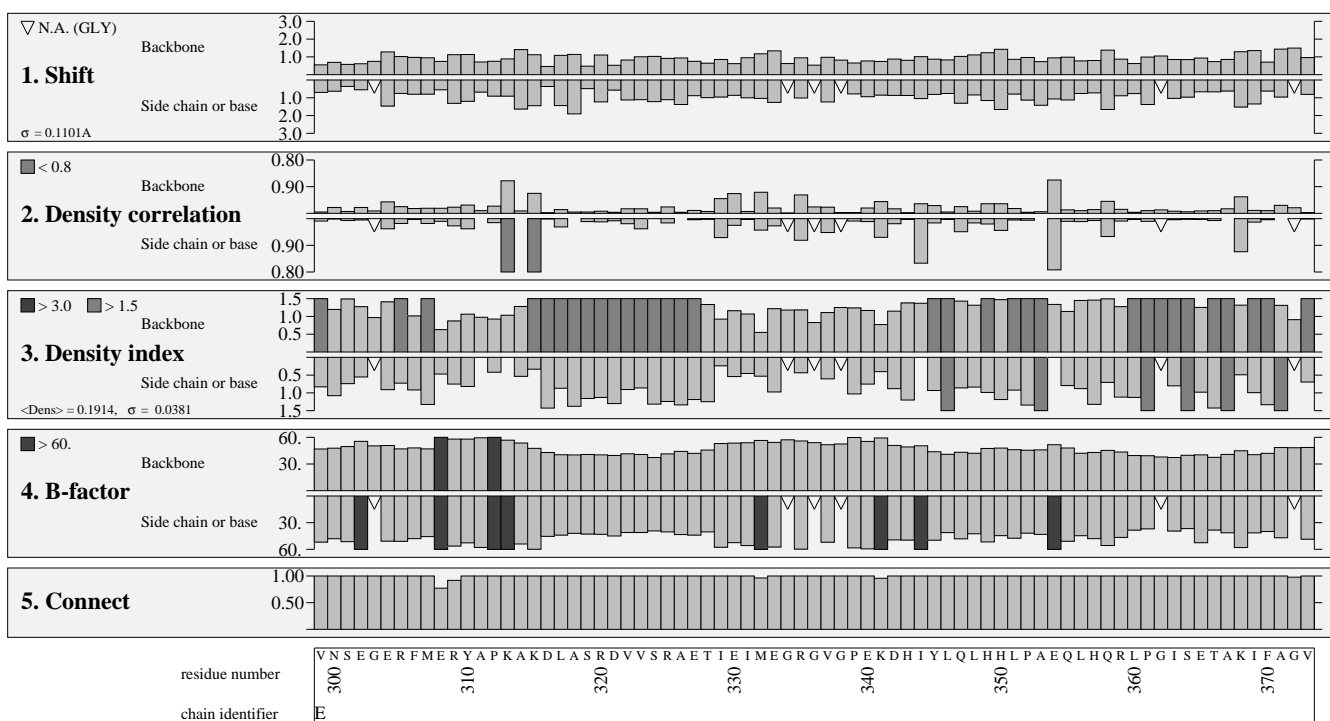
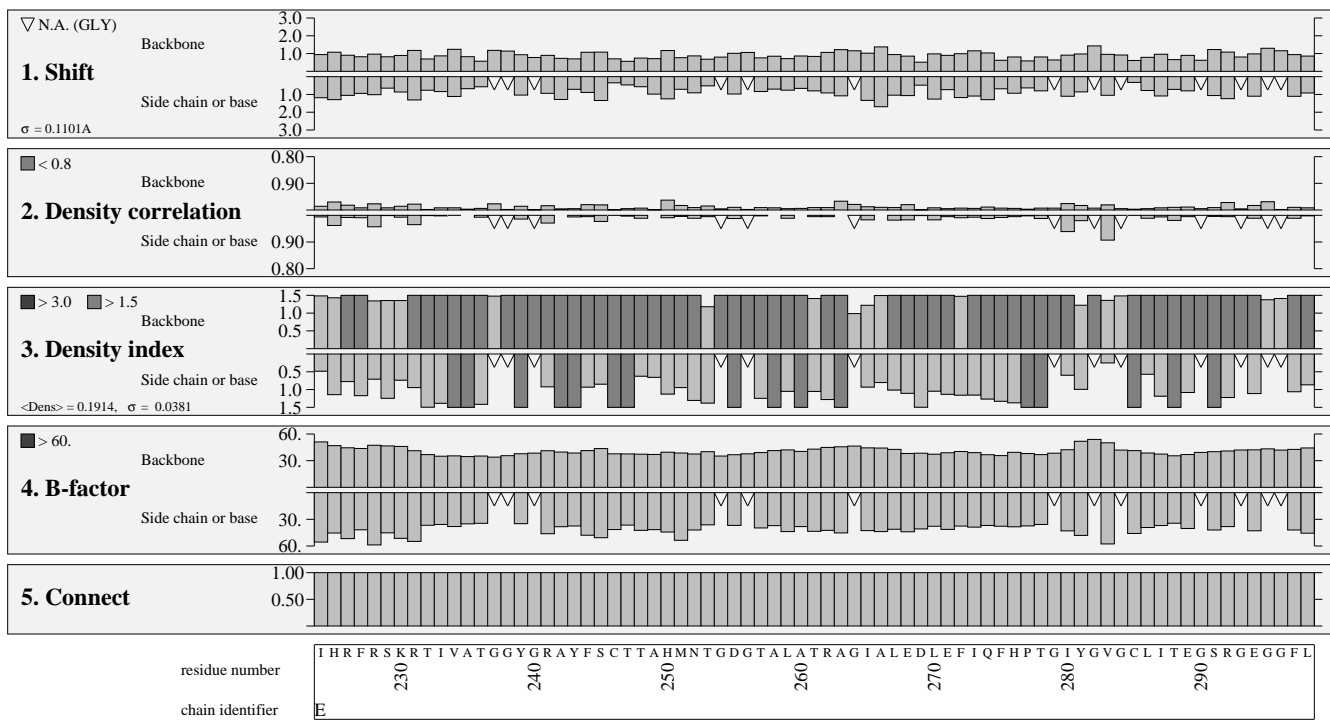
Local estimation (9)



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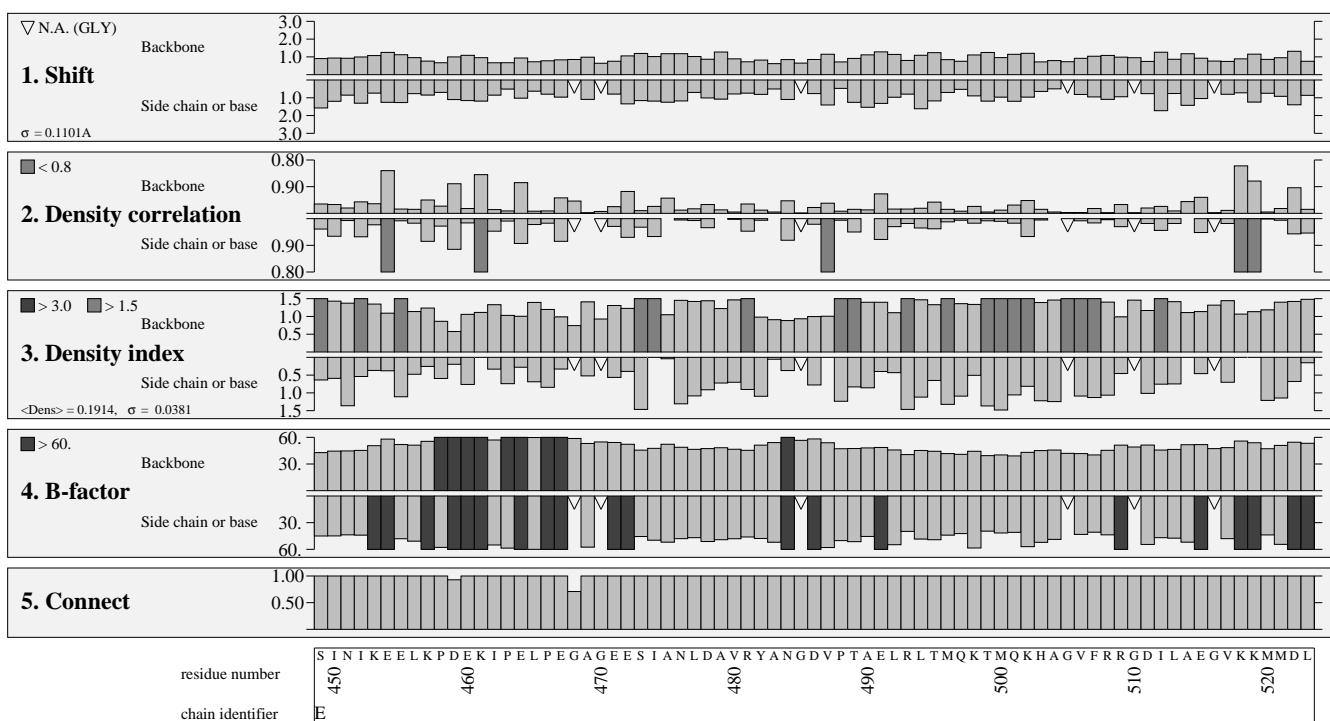
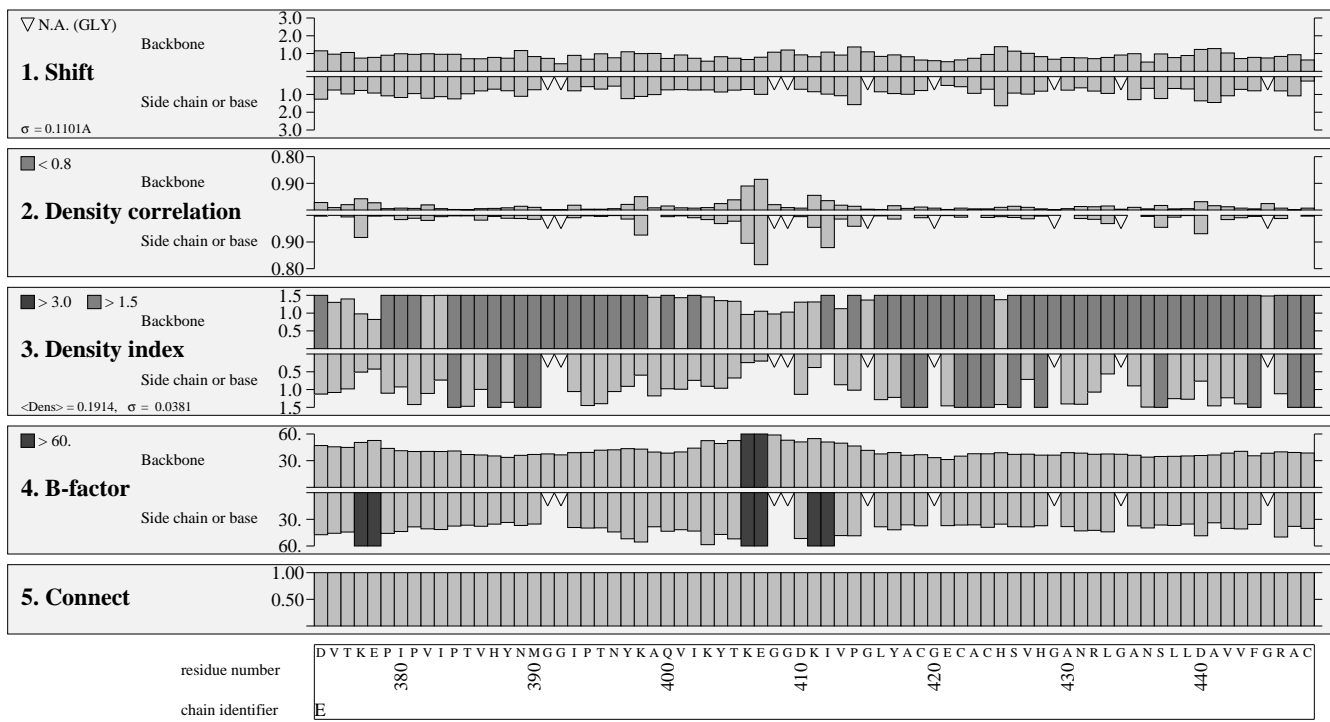
Local estimation (10)



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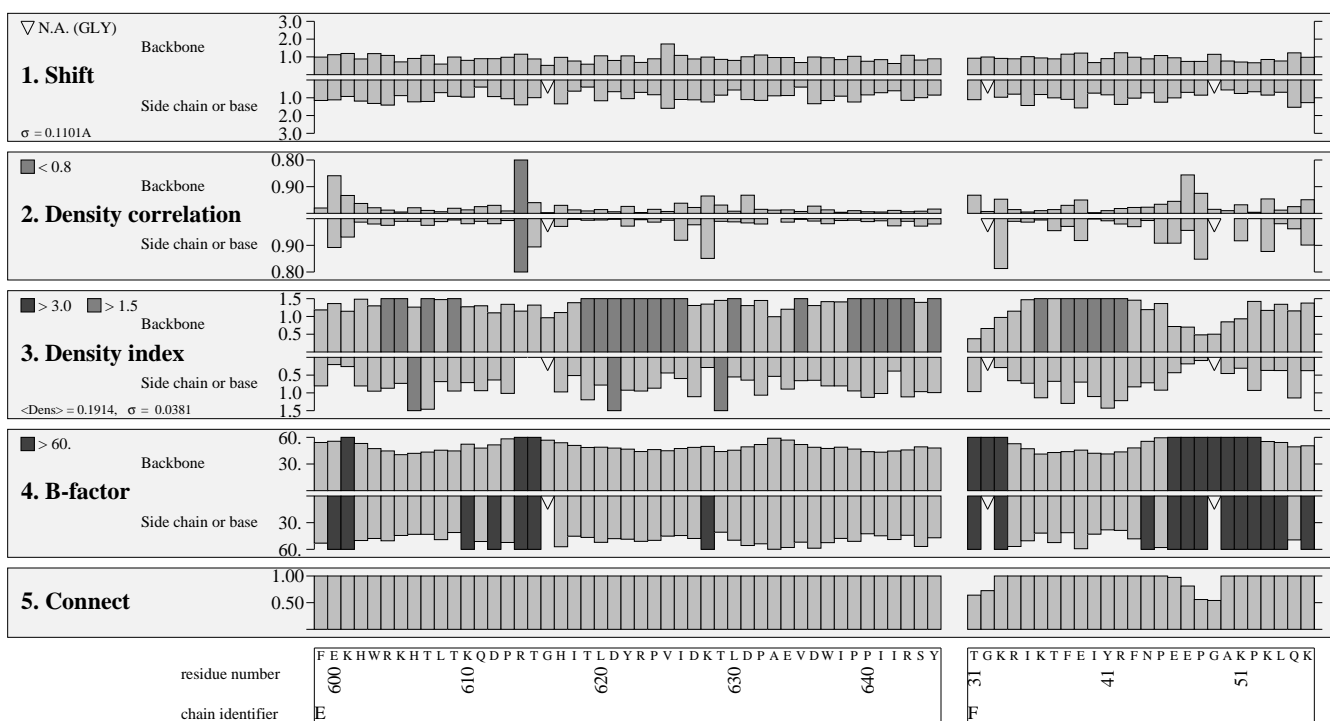
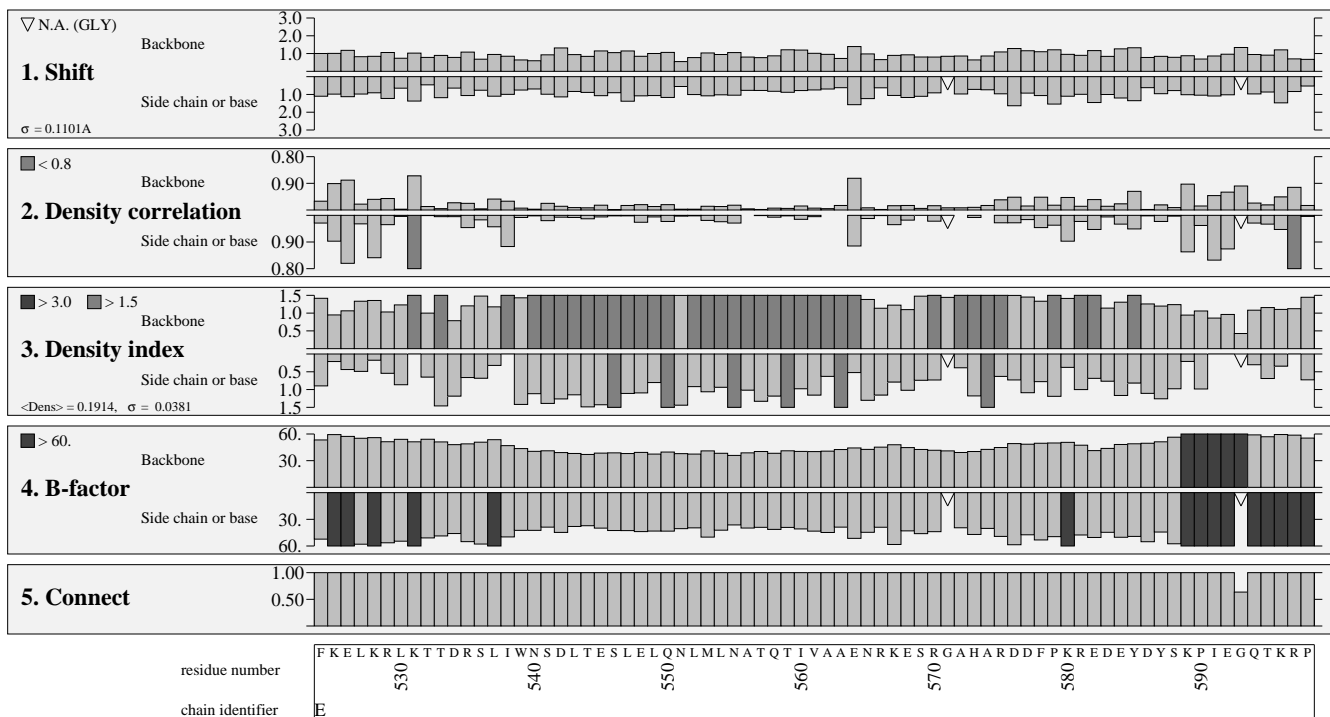
Local estimation (11)



Structure Factor Check

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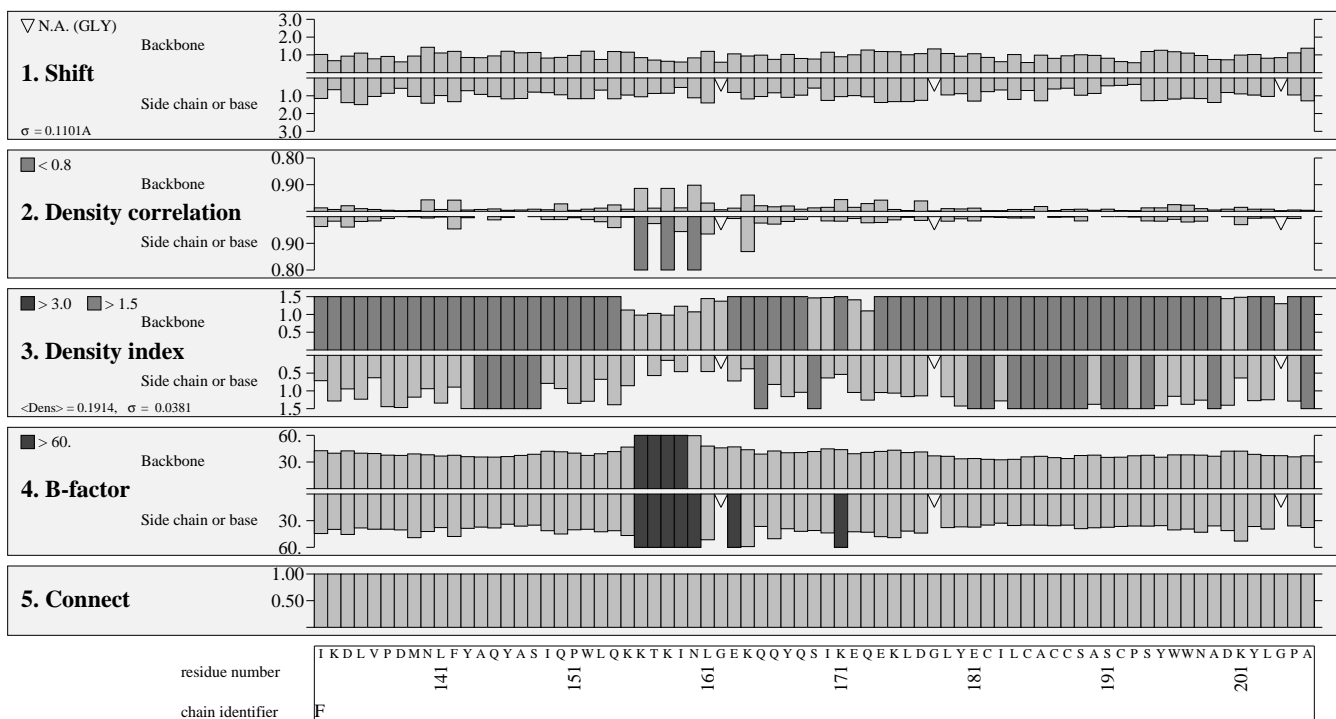
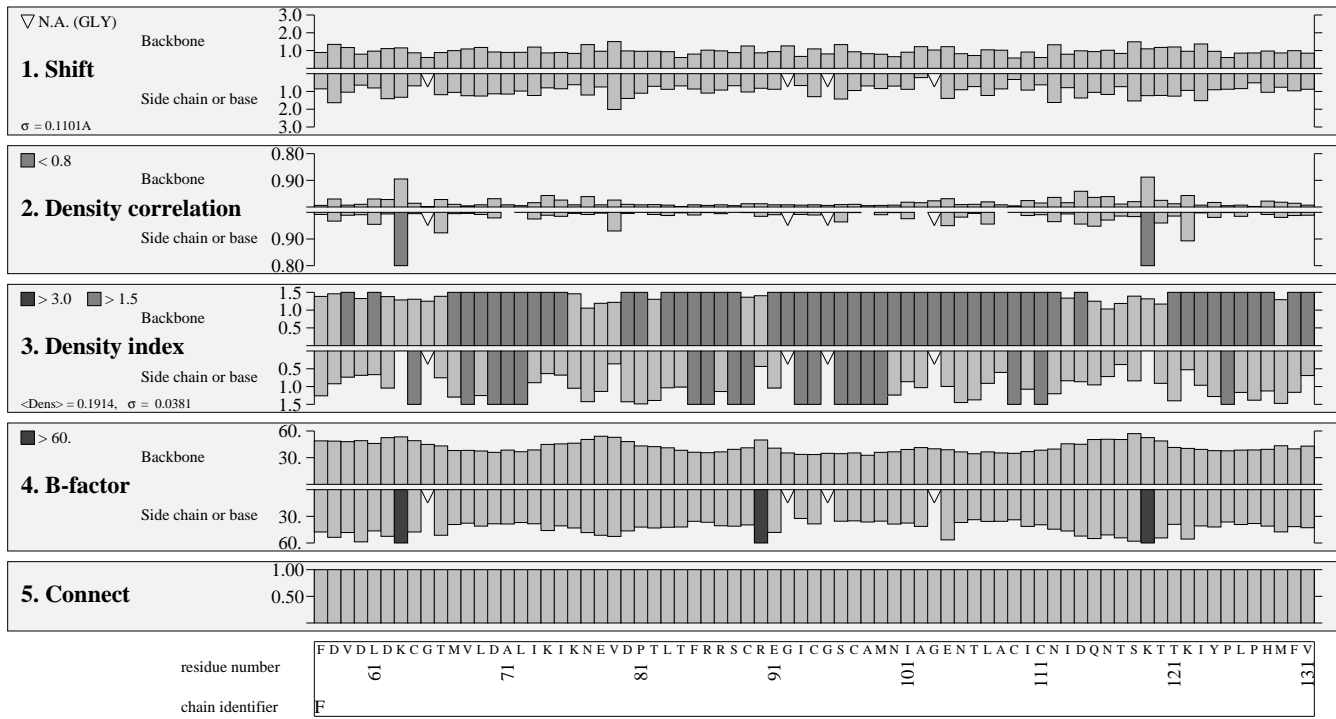
Local estimation (12)



Structure Factor Check

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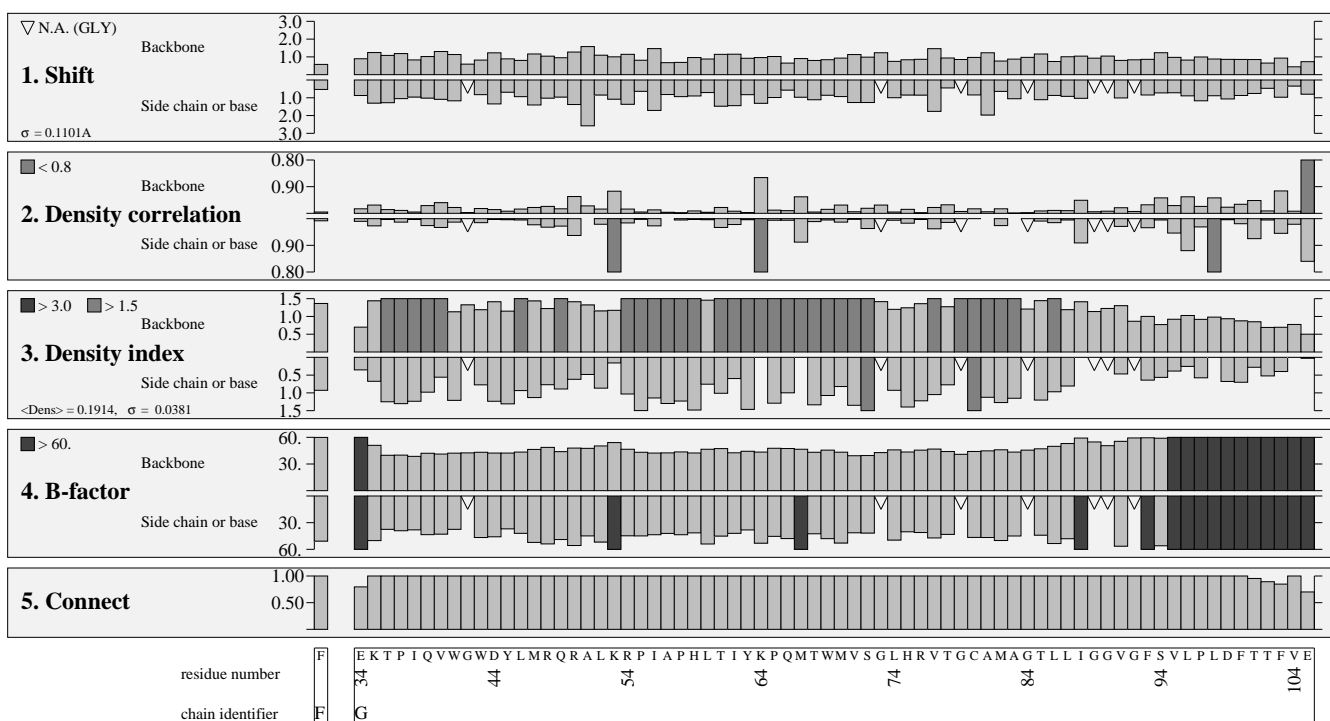
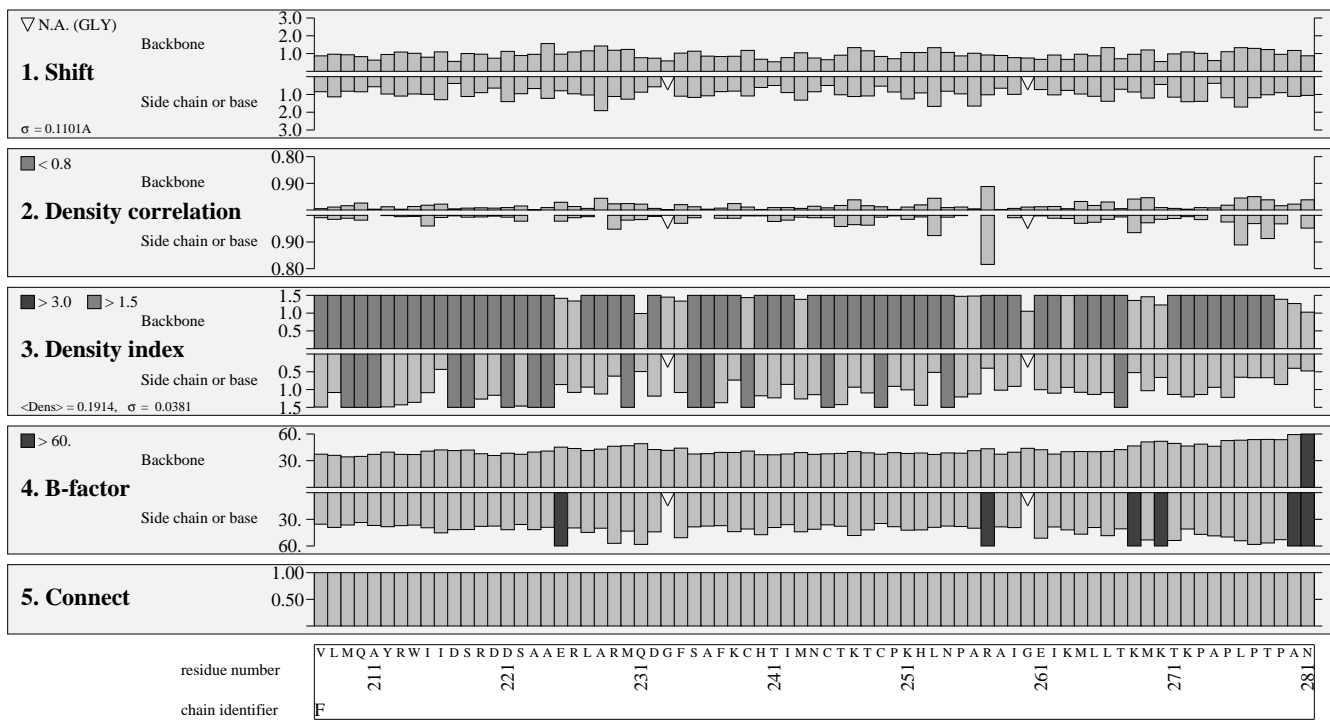
Local estimation (13)



Structure Factor Check

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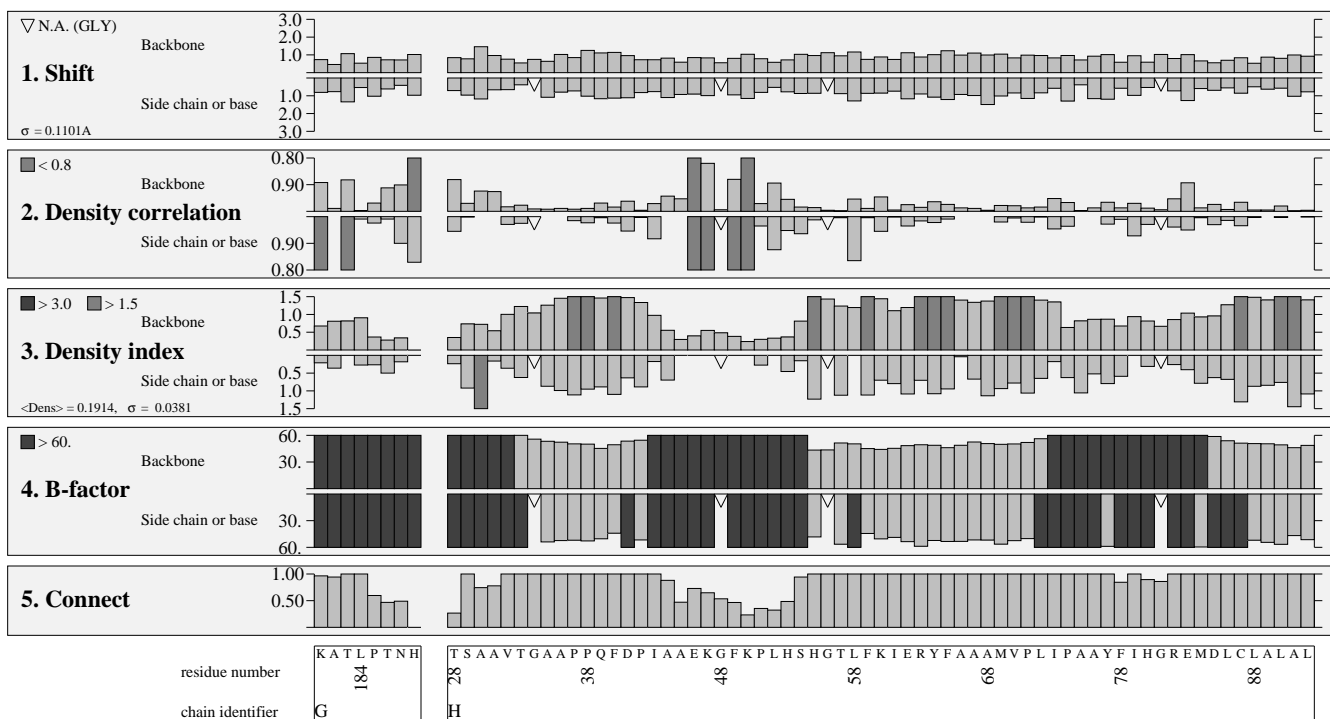
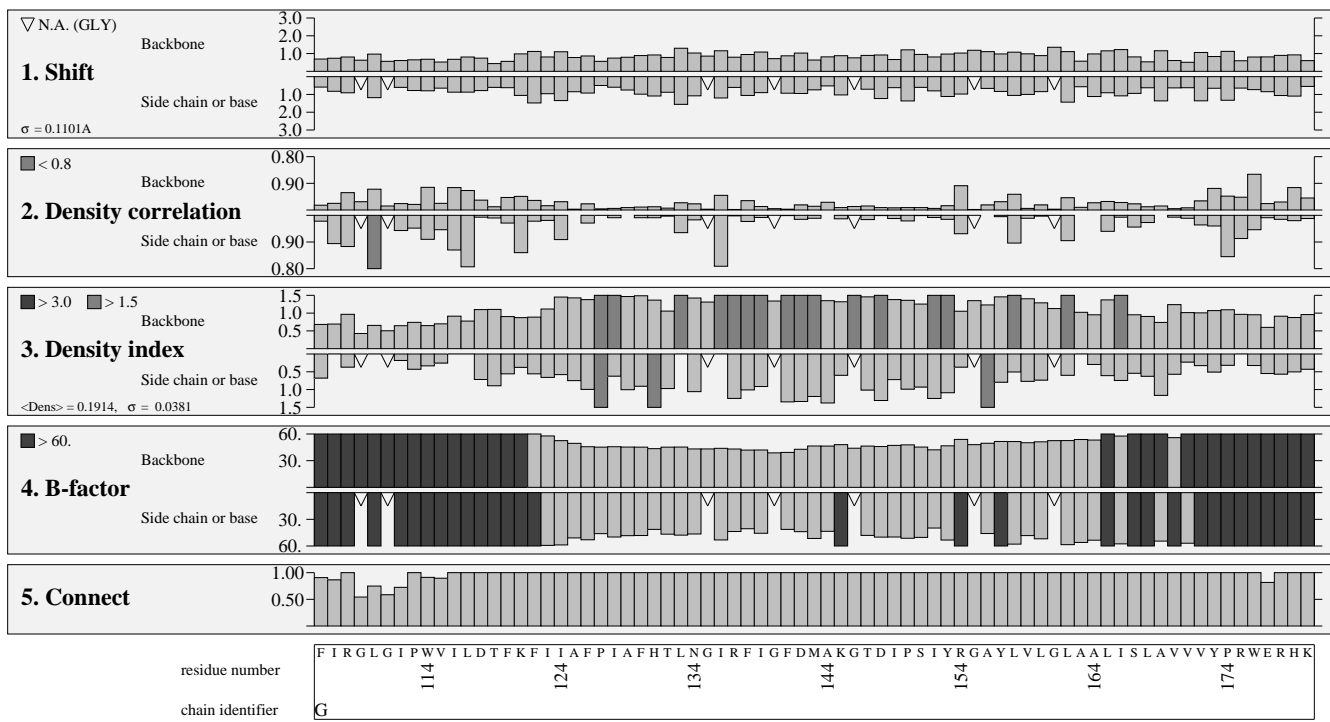
Local estimation (14)



Structure Factor Check

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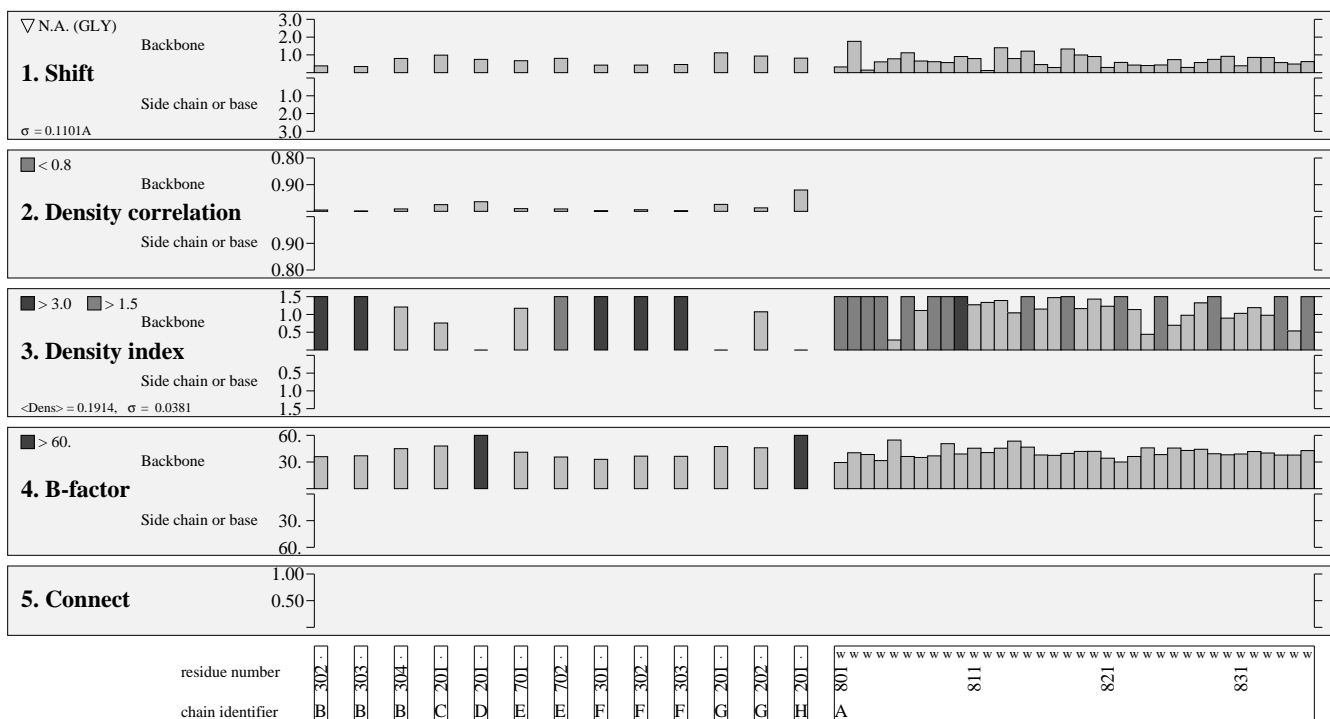
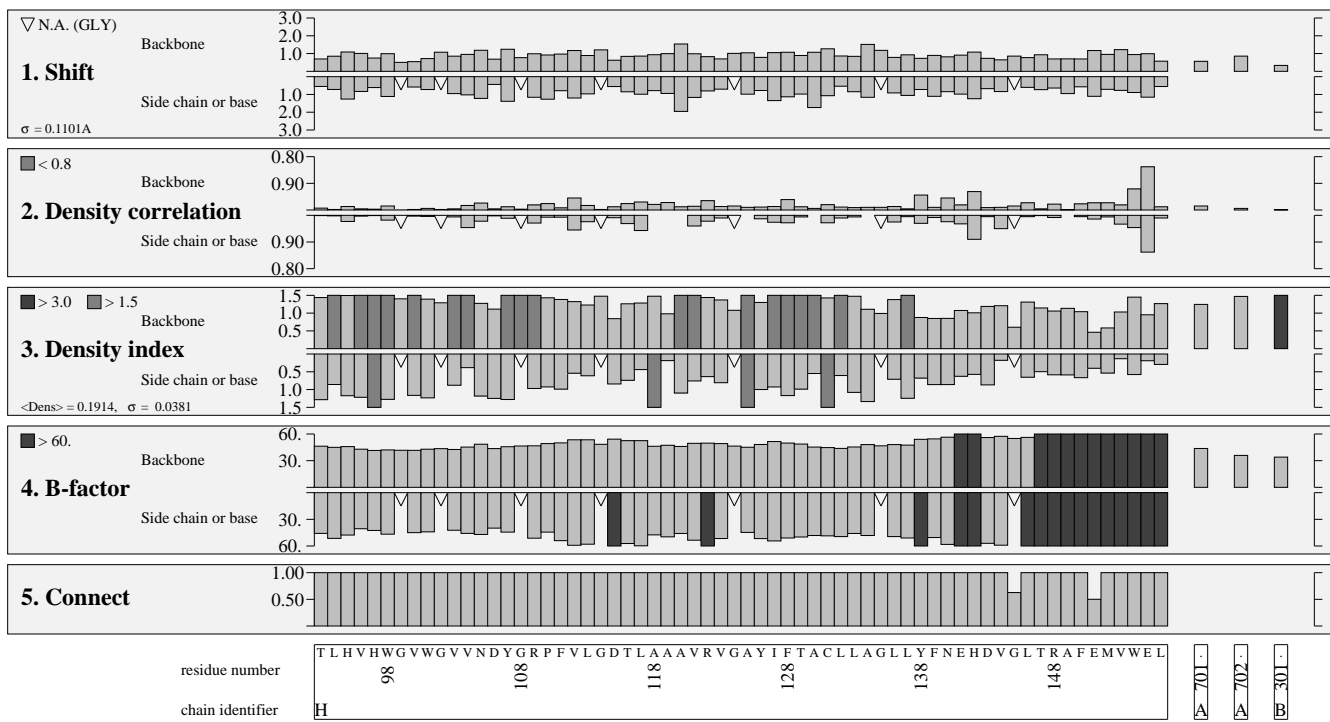
Local estimation (15)



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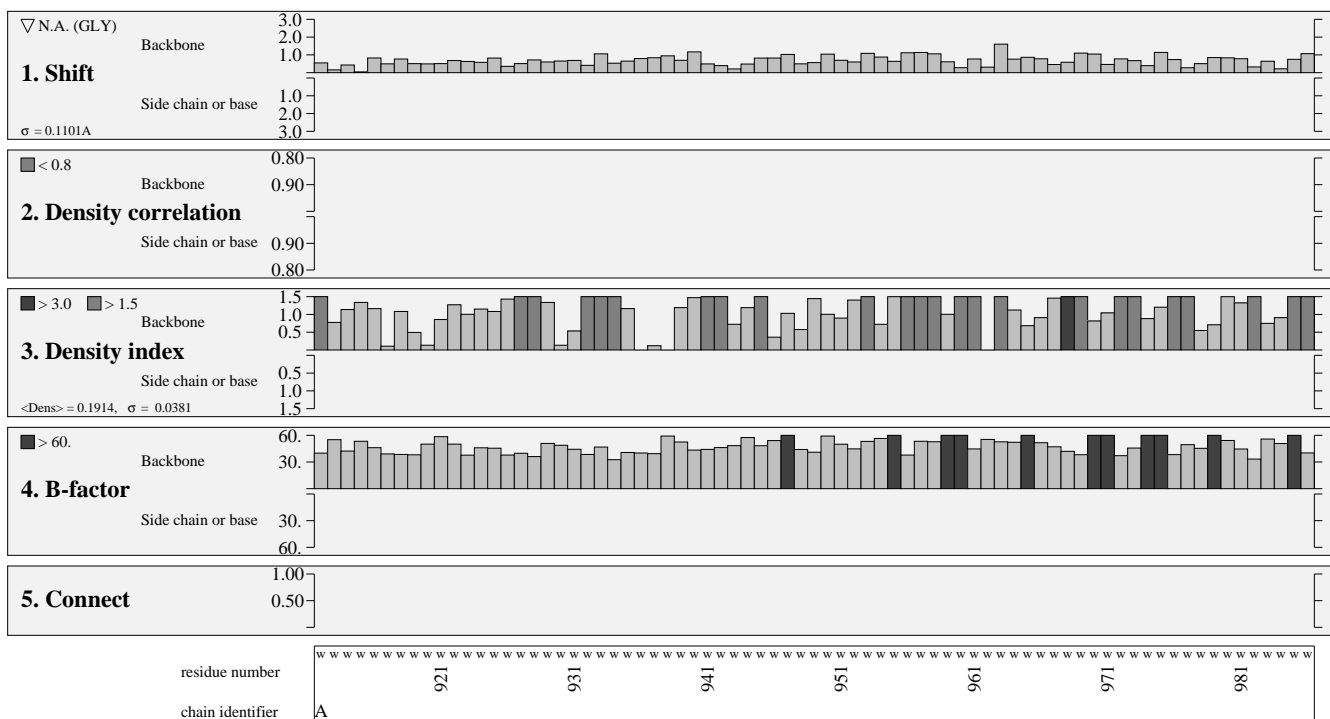
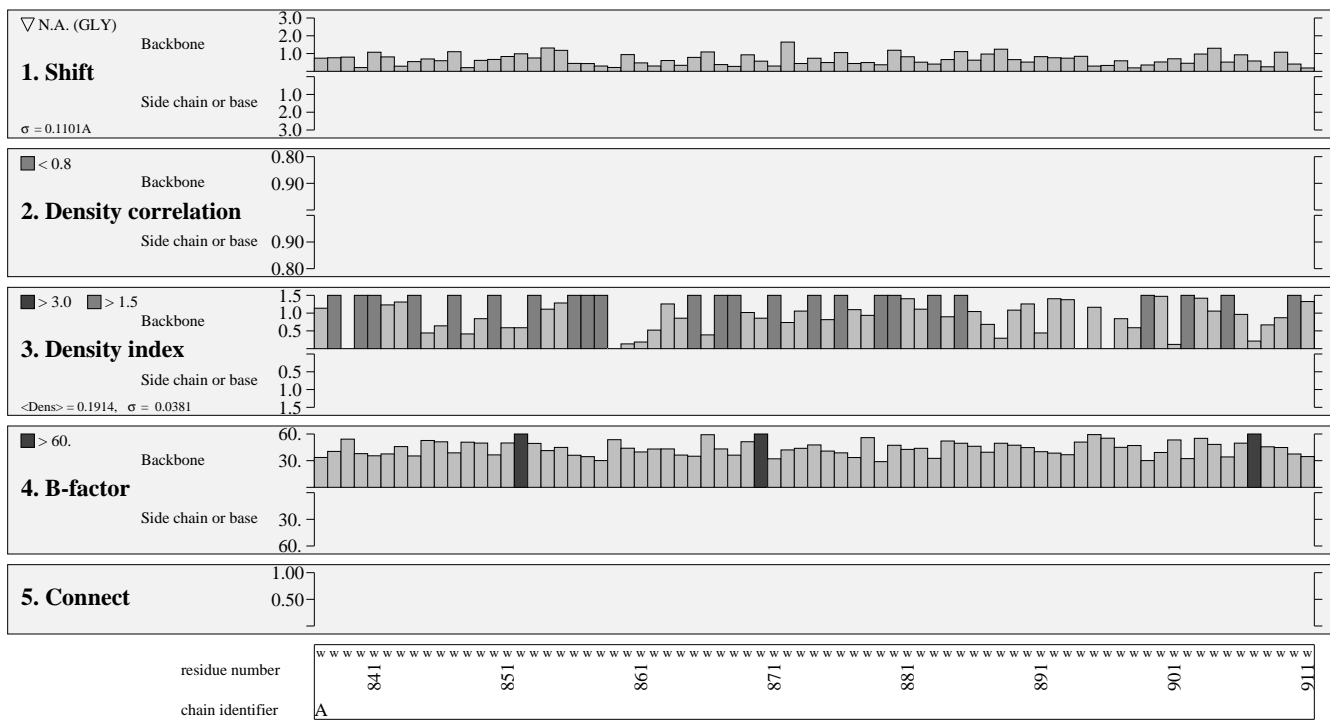
Local estimation (16)



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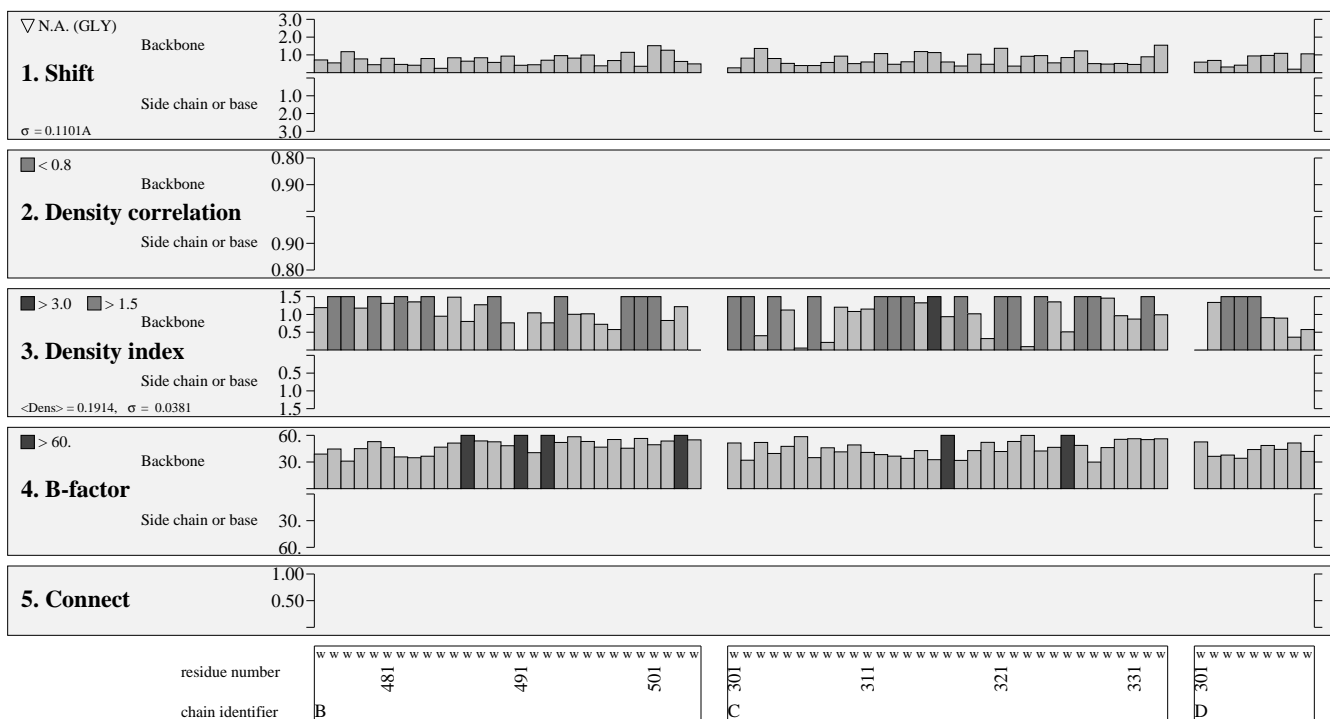
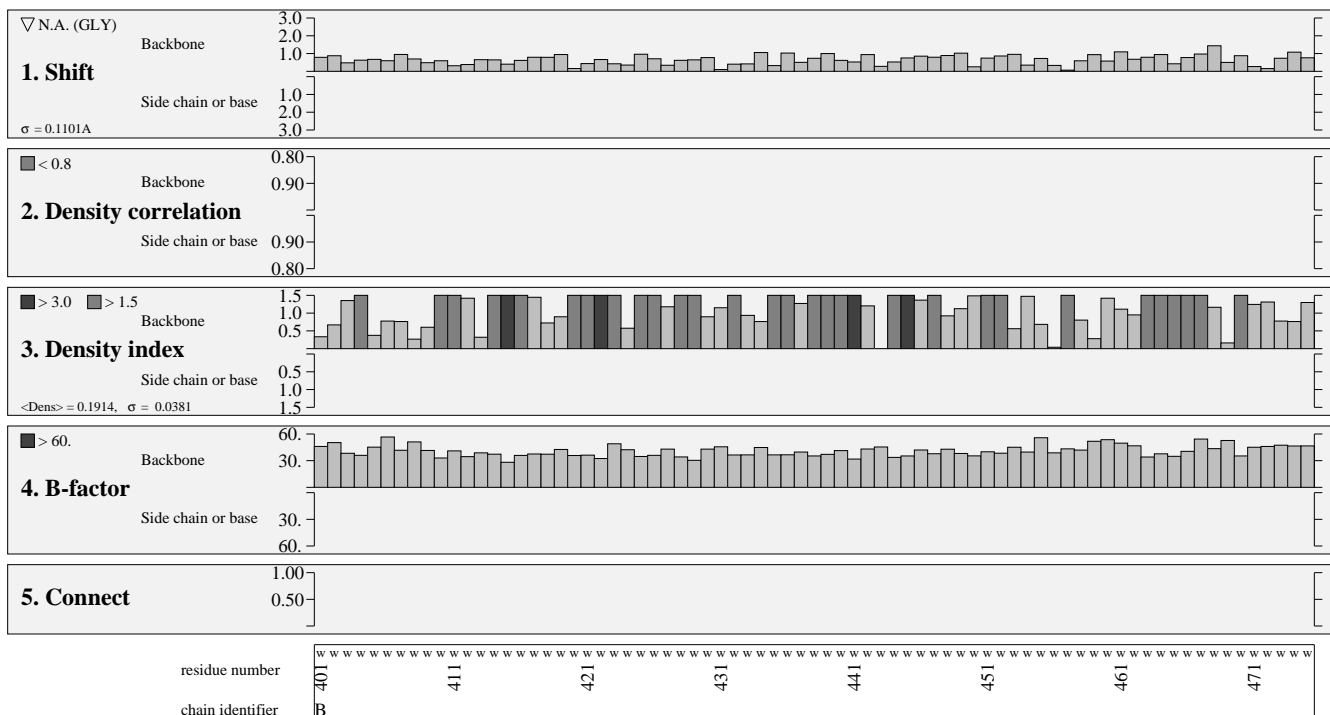
Local estimation (17)



Structure Factor Check

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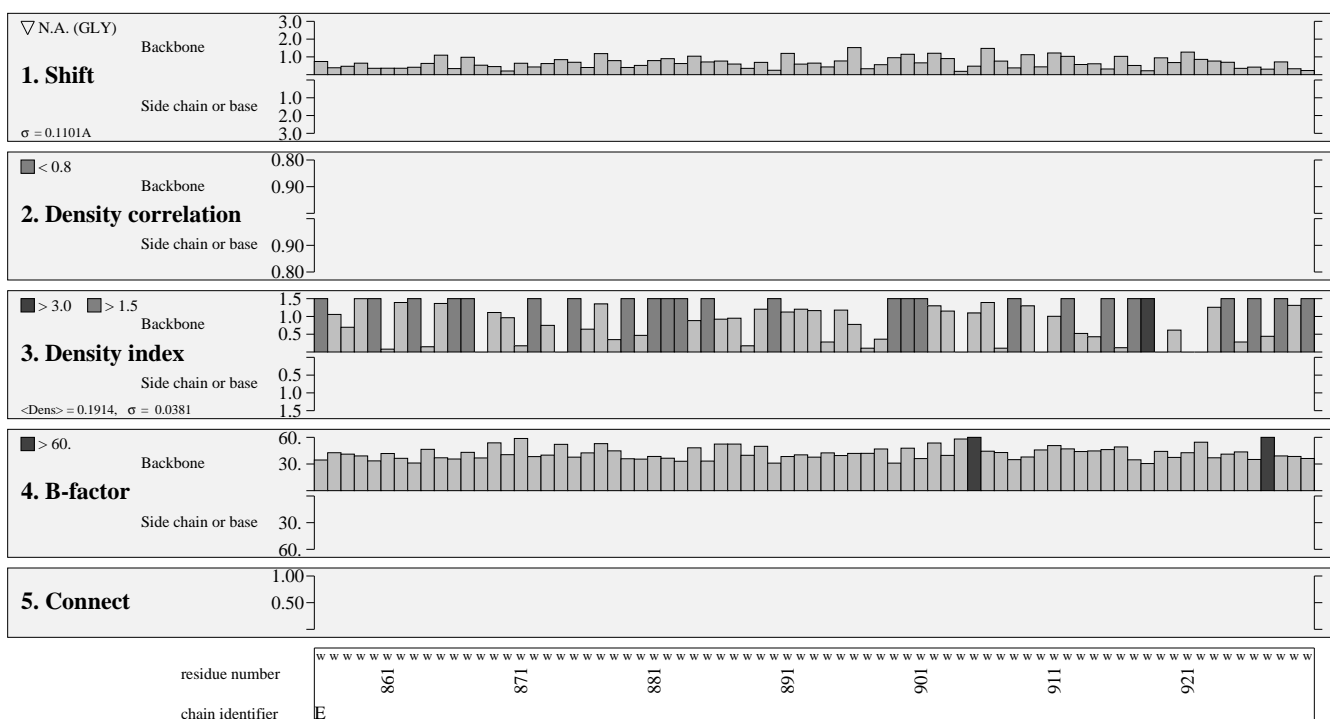
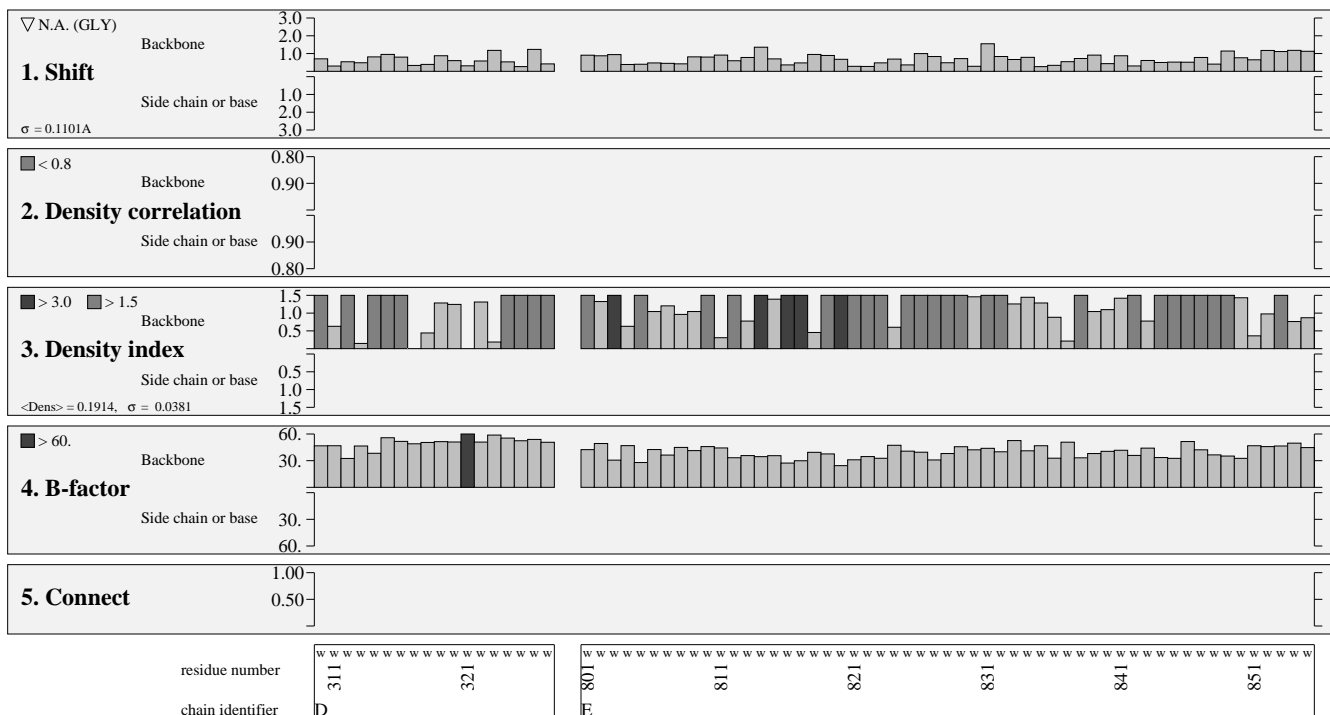
Local estimation (18)



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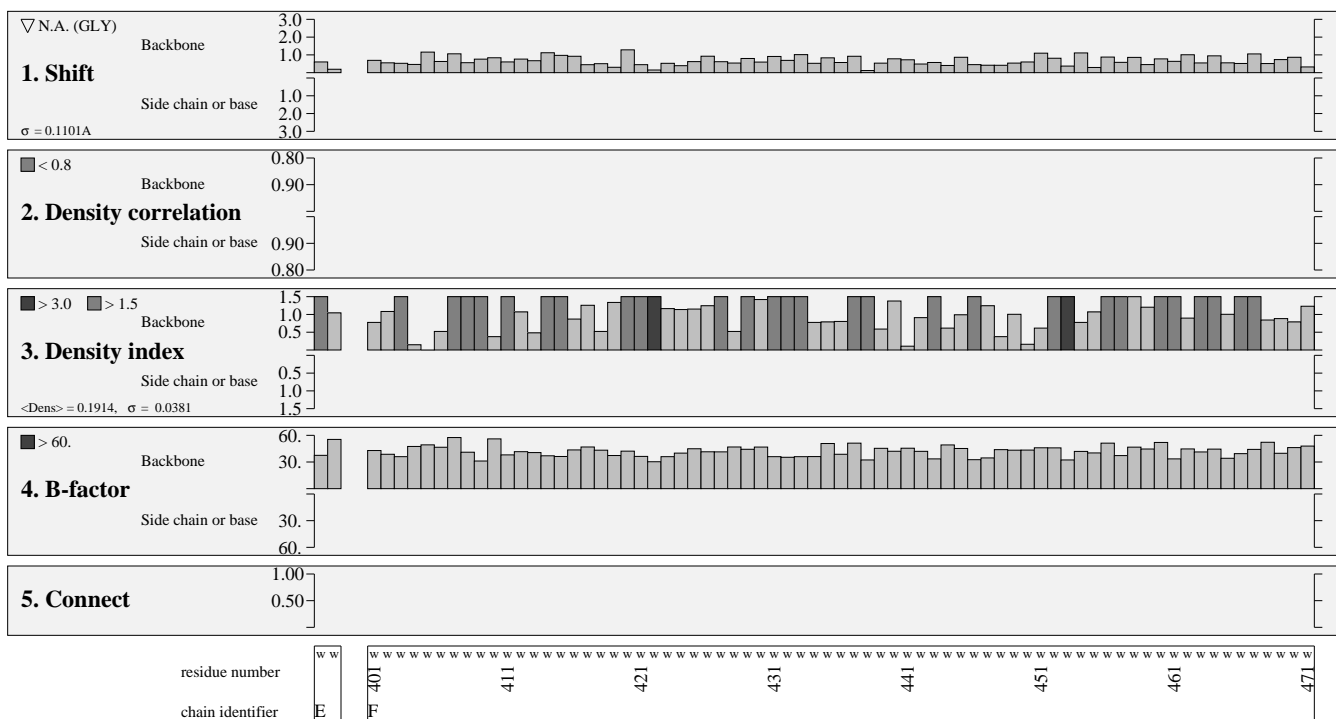
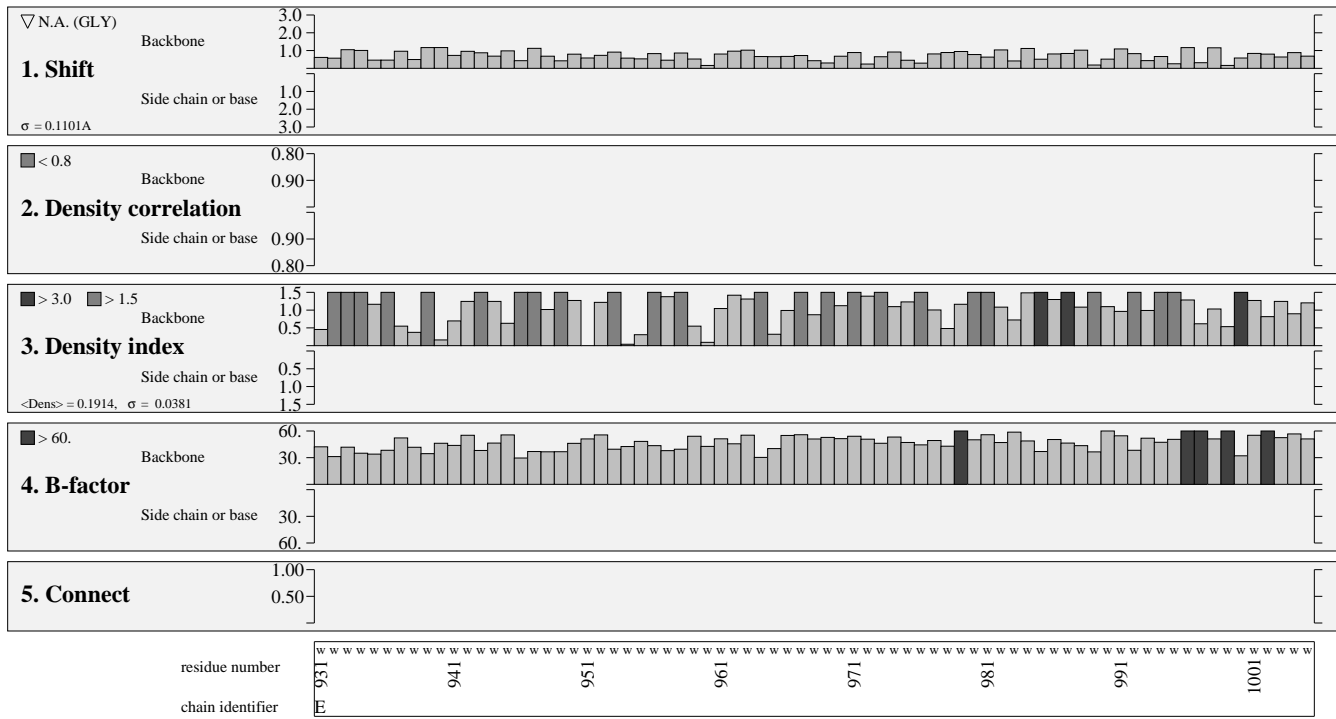
Local estimation (19)



Structure Factor Check

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Local estimation (20)



Structure Factor Check

4YSX

Local estimation (21)

