

Structure Factor Check

3H1K

Title: CHICKEN CYTOCHROME BC1 COMPLEX WITH ZN⁺⁺ AND AN IODINATED
DERIVATIVE OF KRESOXIM-METHYL BOUND
Date: 12-APR-09
PDB code: 3H1K

Crystal

Cell parameters:

a: 171.72 A b: 181.30 A c: 241.29 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 42.6 – 3.48 A
 Reflections in file: 86926
 Unique reflections above 0: 86926
 above 1 σ : 84850
 above 3 σ : 43497

SFCHECK

Nominal resolution range: 42.6 – 3.48 A
\05max. from input data, min. from author\05
 Used reflections: 86926
 Completeness: 89.6 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.099
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.5227 0.6748
 B_{overall} (by Patterson): 63.A²
 Optical resolution: 2.51 A
 Expected opt. resol. for complete data set: 2.51 A
 Estimated minimal error: 0.205 A

Model

32673 atoms (17 water molecules)

Number of chains: 51
 Volume not occupied by model: 62.0 %
 $\langle B \rangle$ (for atomic model): 89.7 A²
 $\sigma(B)$: 14.10 A²
 Matthews coefficient: 4.11
 Corresponding solvent % : 69.80

Model vs. Structure Factors

R-factor for all reflections: 0.315
 Correlation factor: 0.799
 R-factor: 0.313
 for $F > 2.0\sigma$
 nom. resolution range: 18.00 – 3.48A
 reflections used: 84309

Rfree: 0.340
 Nfree: 2500
 R-factor without free-refl.: 0.312
 Non free-reflections: 81809
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.684 A
 Estimated maximal error: 0.539 A
 DPI: 0.628 A

Scaling

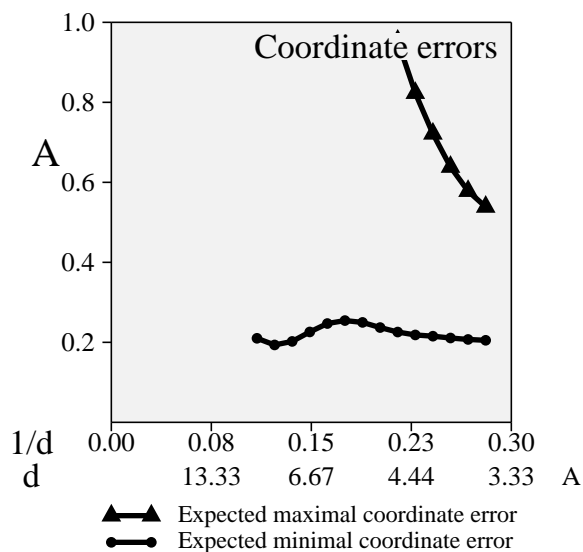
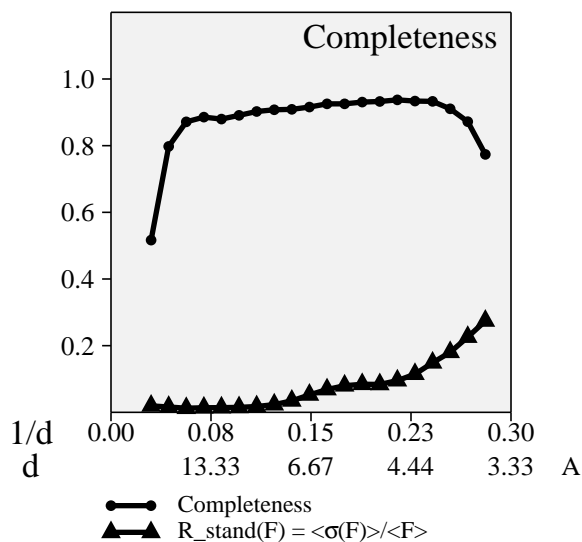
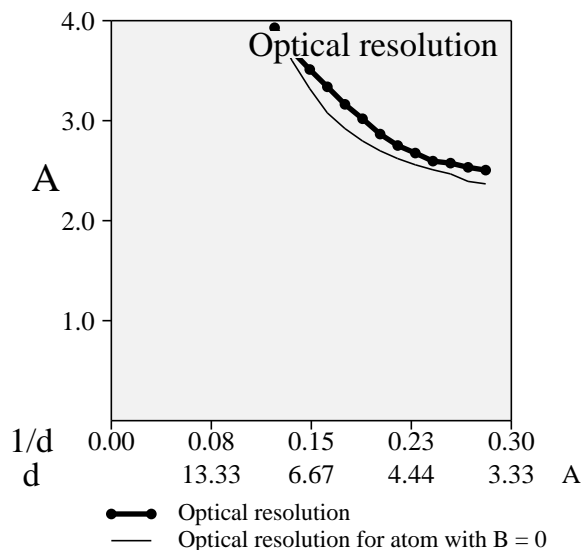
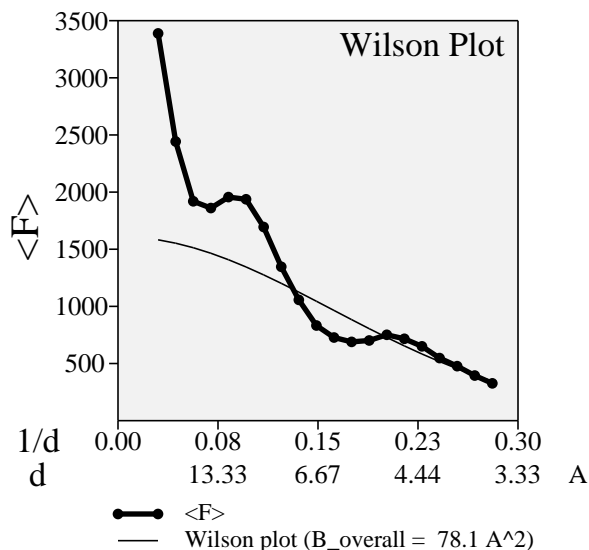
Scale: 0.655
 Bdiff: -8.11
 Anisothermal Scaling (Beta):
 16.0877 -1.3143 4.7514 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.576 250.570

Refinement

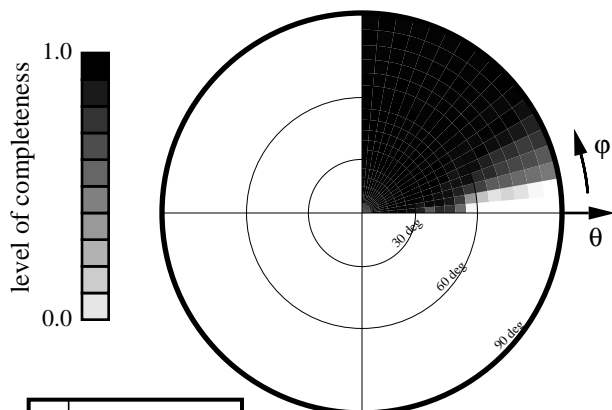
Program: CNS 1.1
 Nominal resolution range: 18.0 – 3.48 A
 Reported nominal resolution: 3.00 A
 Reported R-factor: 0.239
 Number of reflections used: 86369
 Reported Rfree: 0.28
 Sigma cut-off: N.A.

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3H1K

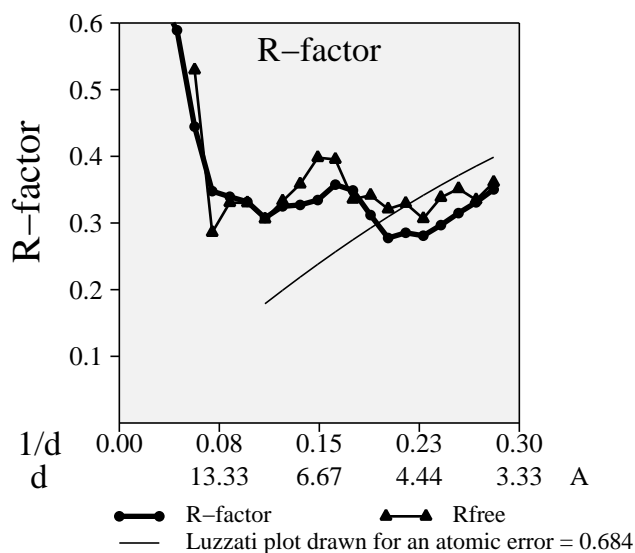


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

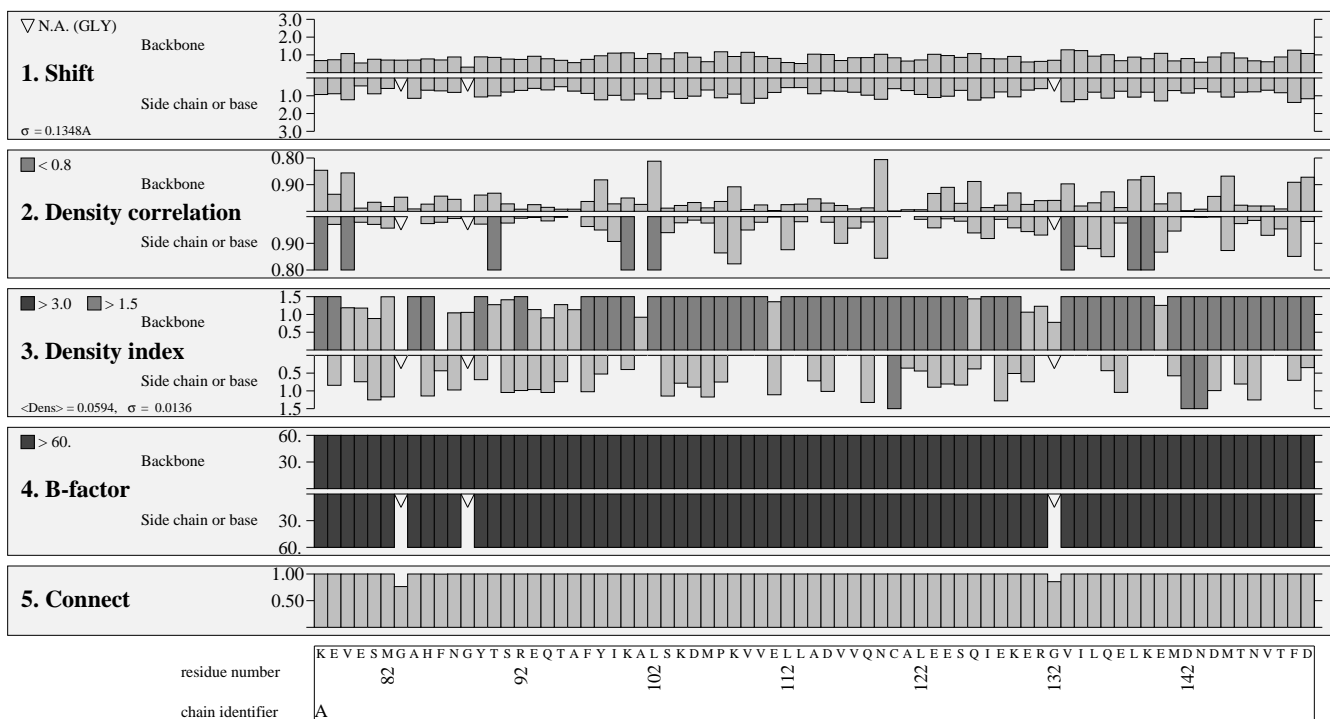
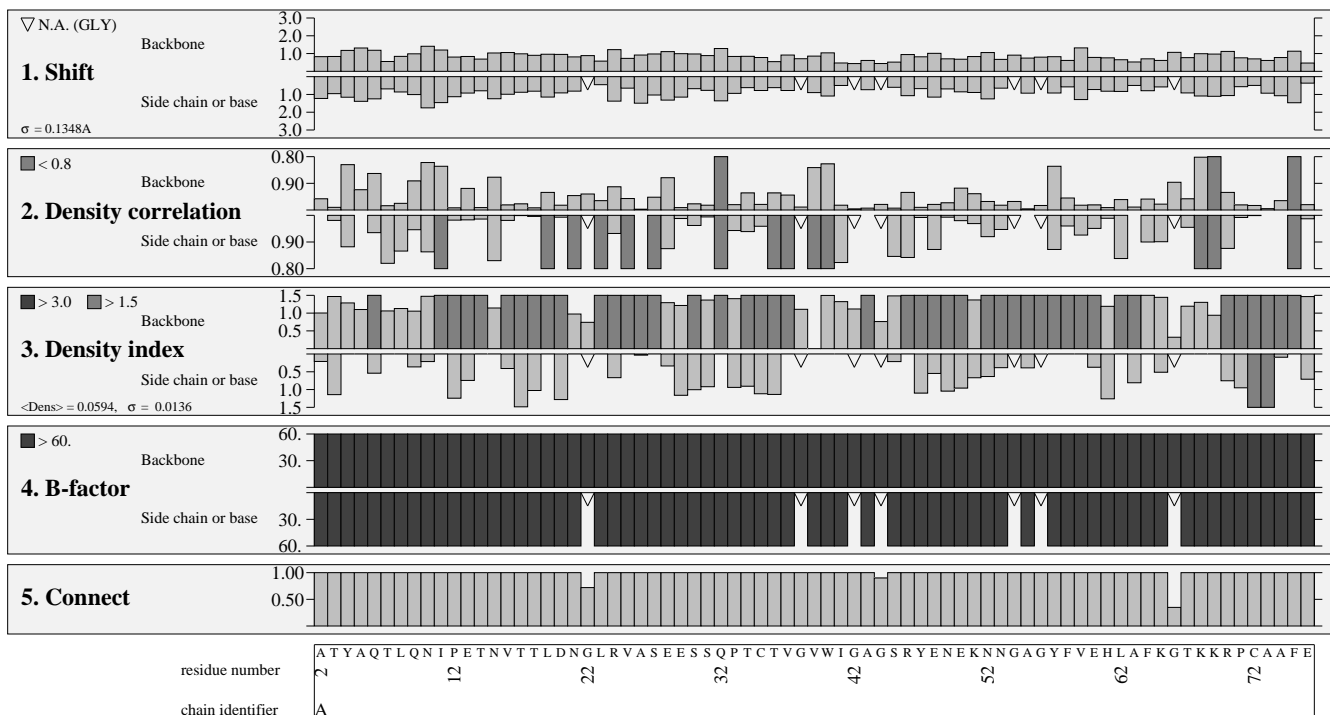
polar coordinates of the crystallographical axes



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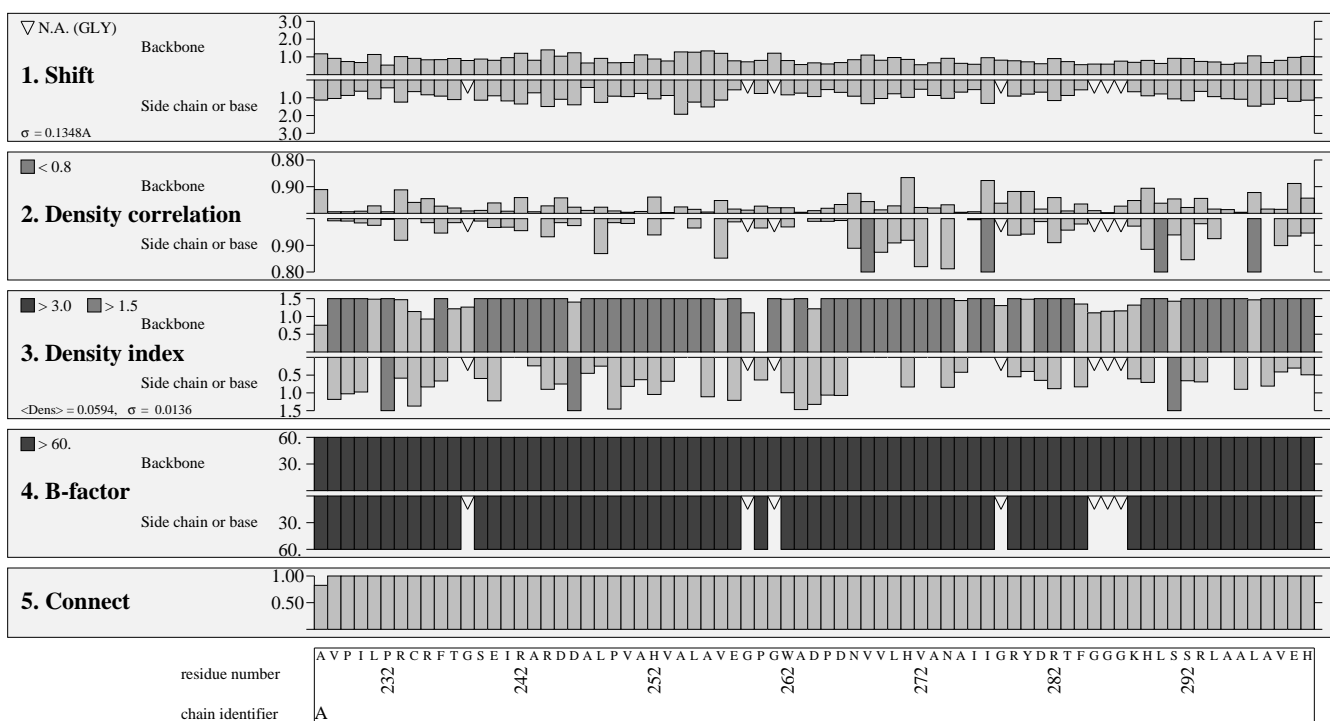
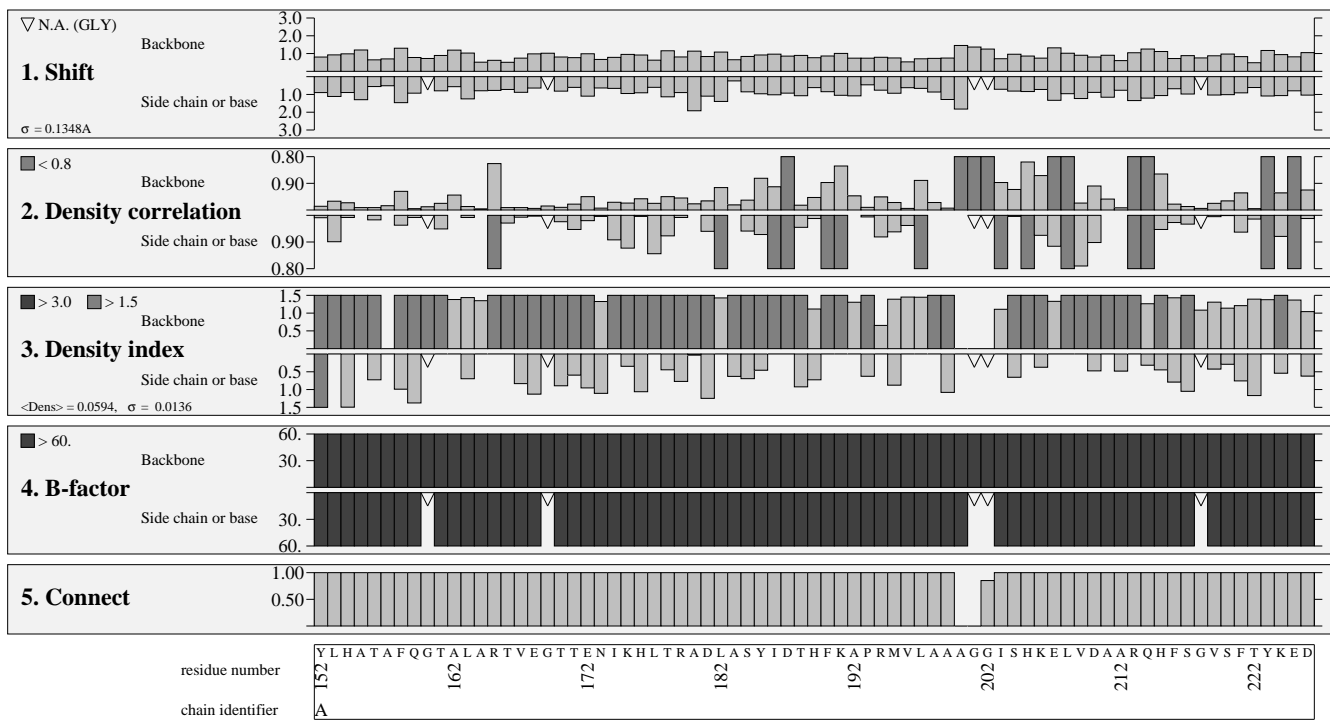
Local estimation



Structure Factor Check

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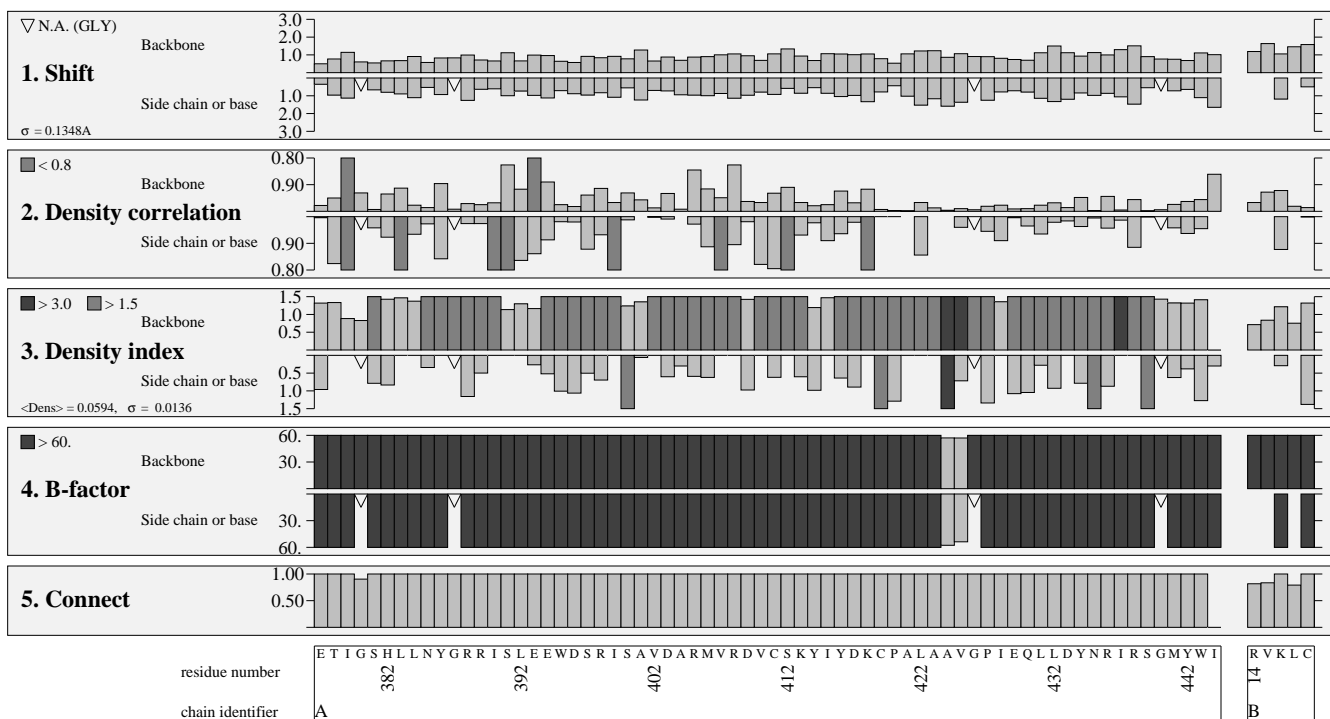
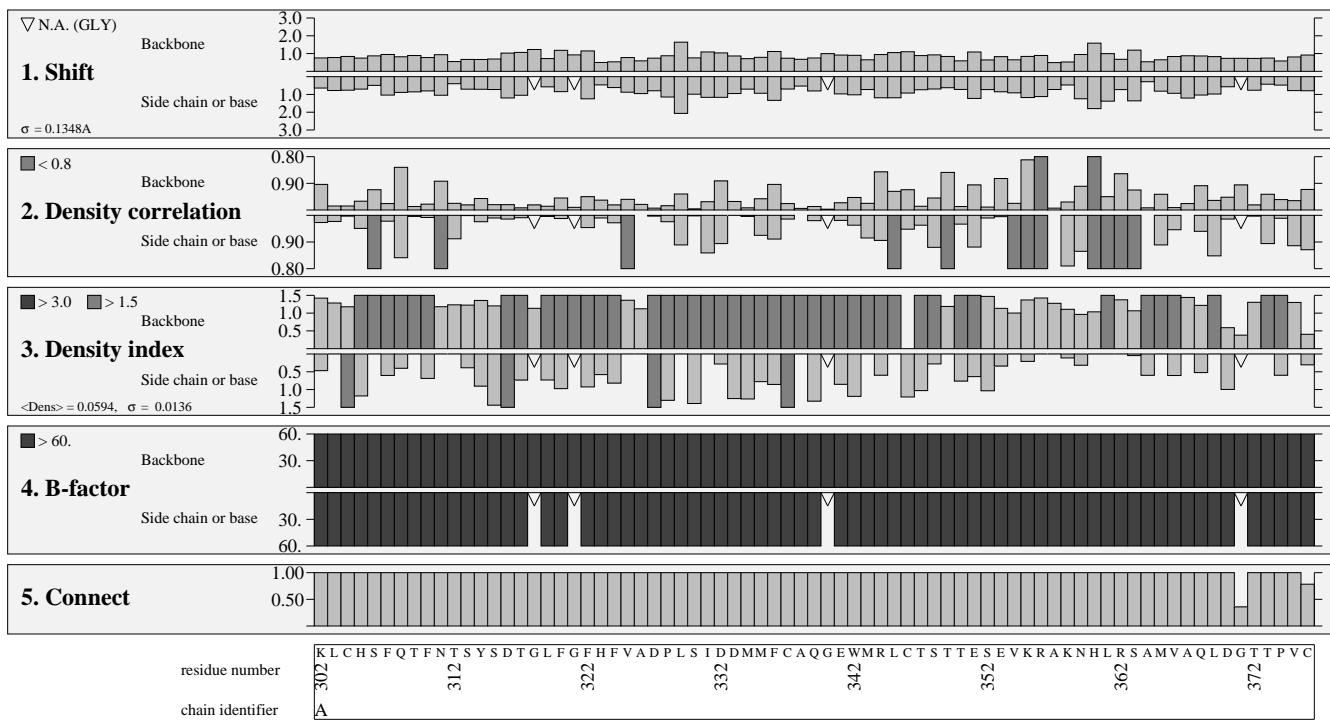
Local estimation (2)



Structure Factor Check

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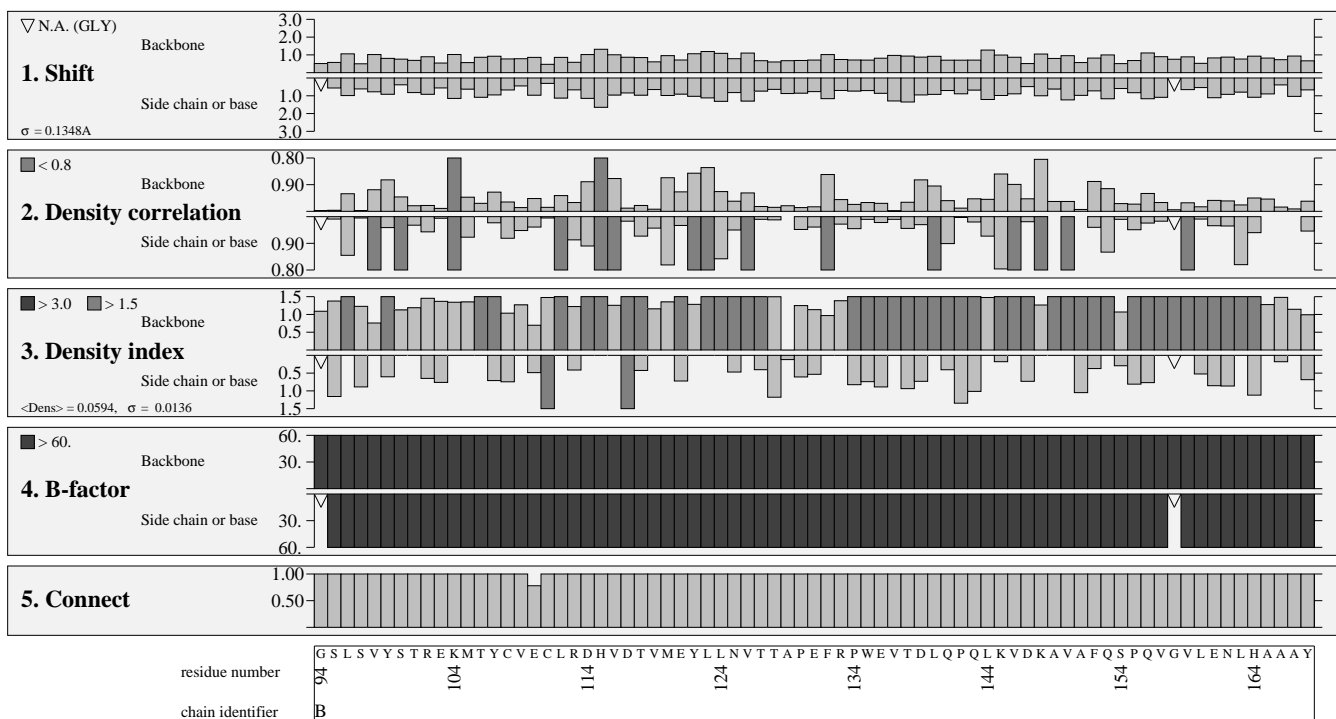
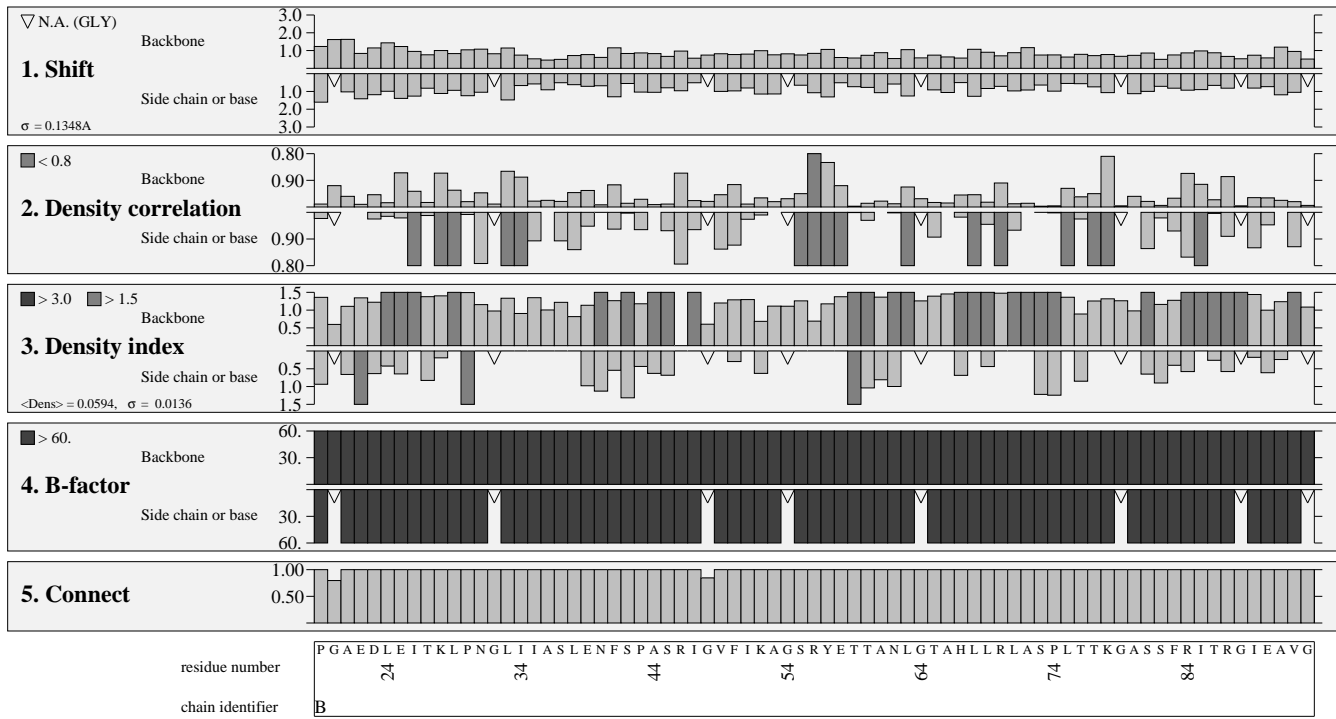
Local estimation (3)



Structure Factor Check

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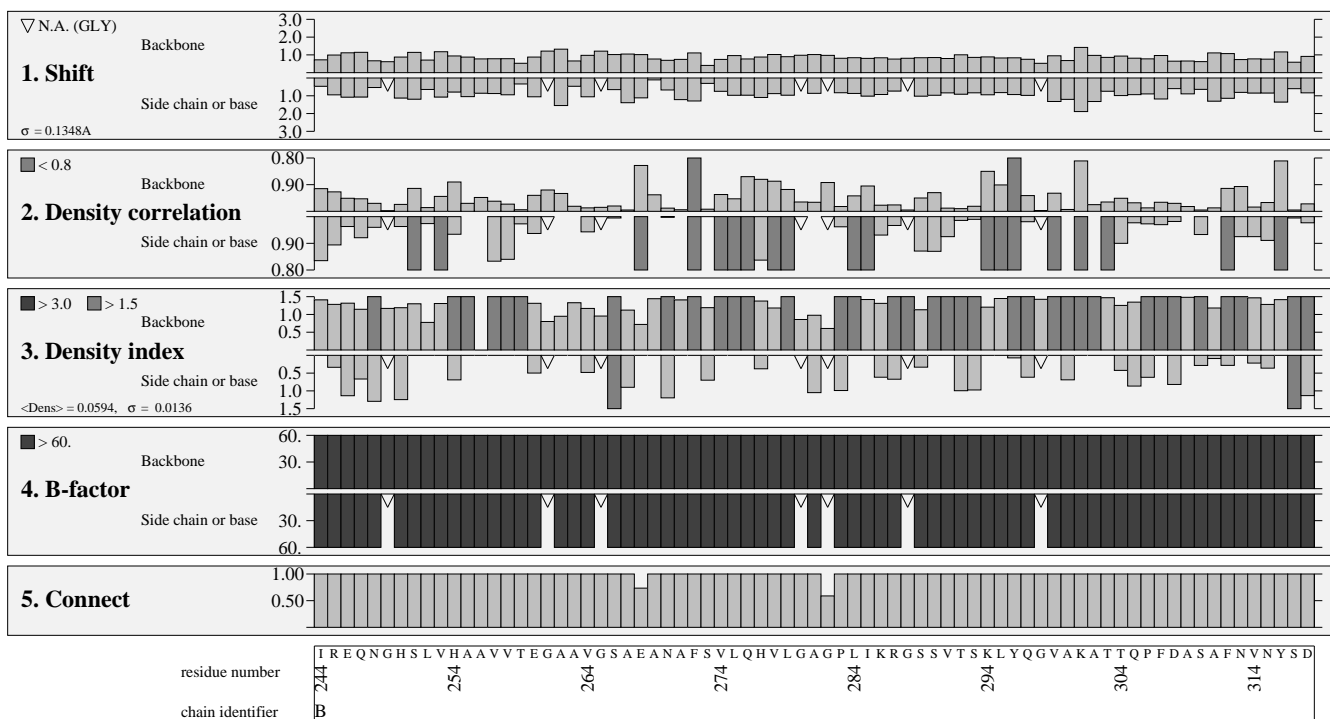
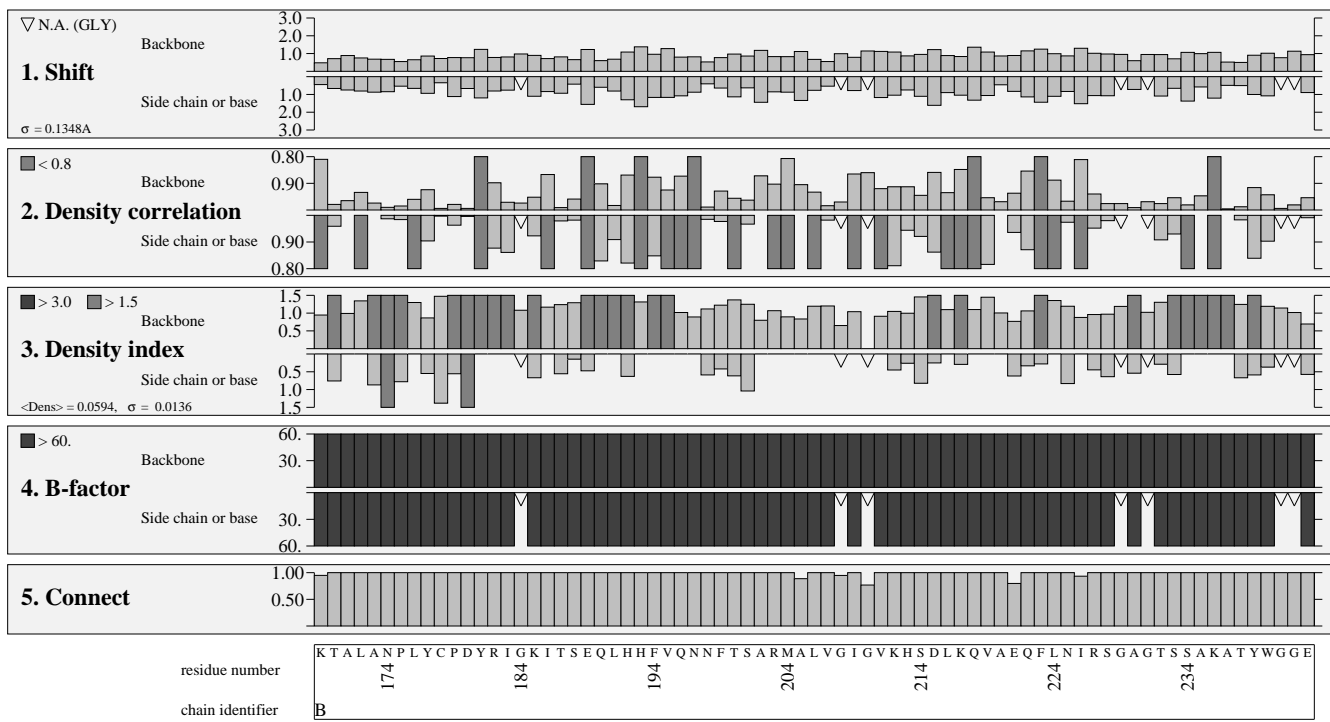
Local estimation (4)



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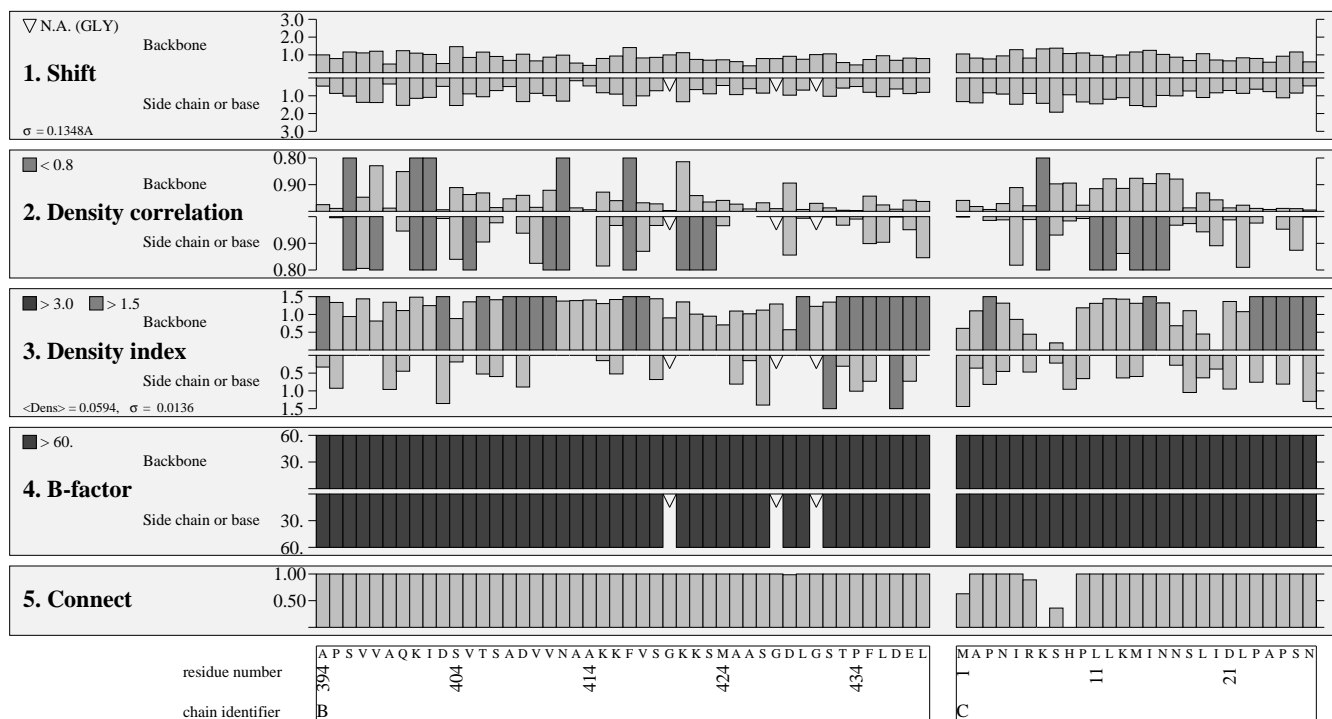
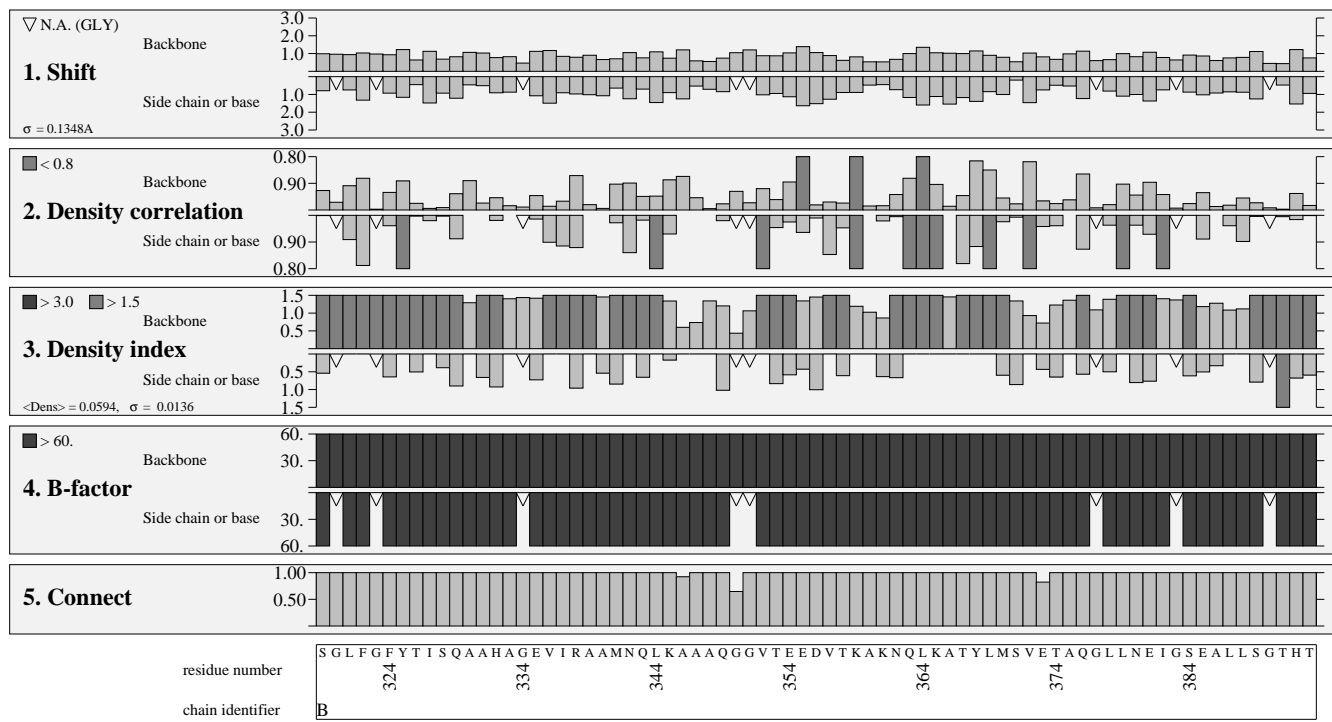
Local estimation (5)



Structure Factor Check

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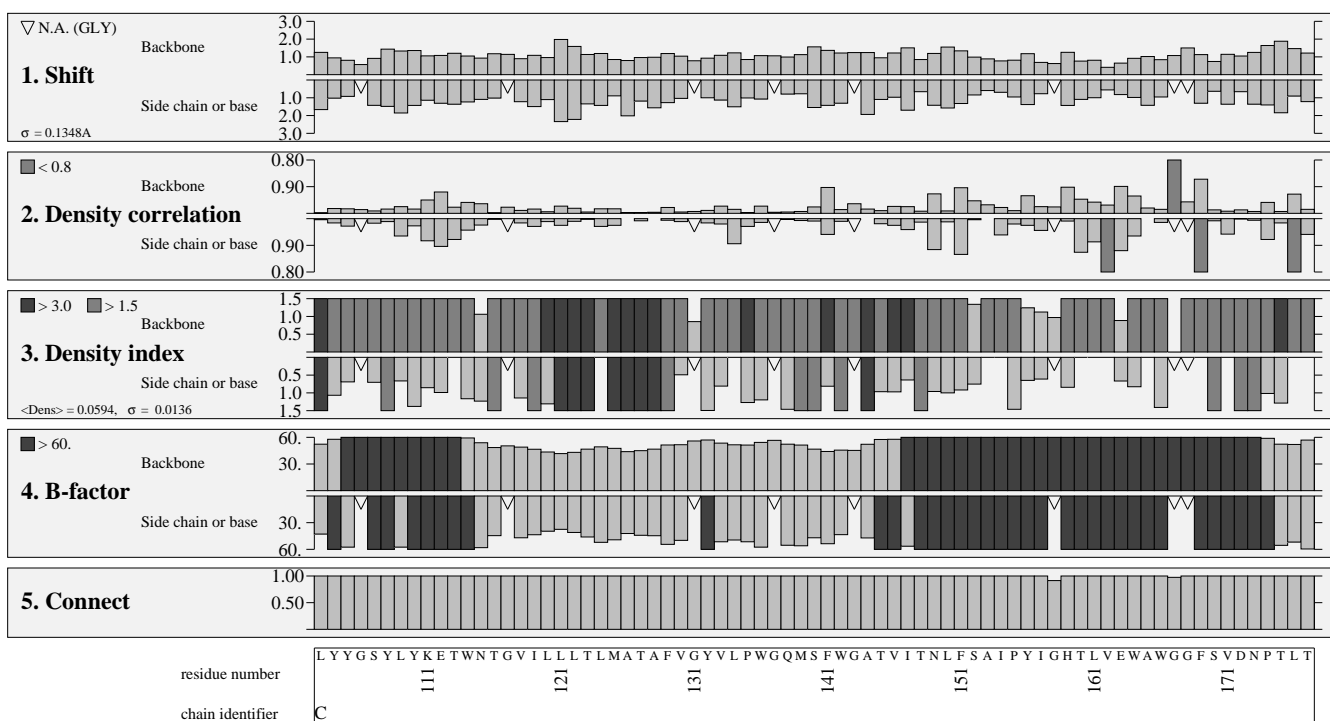
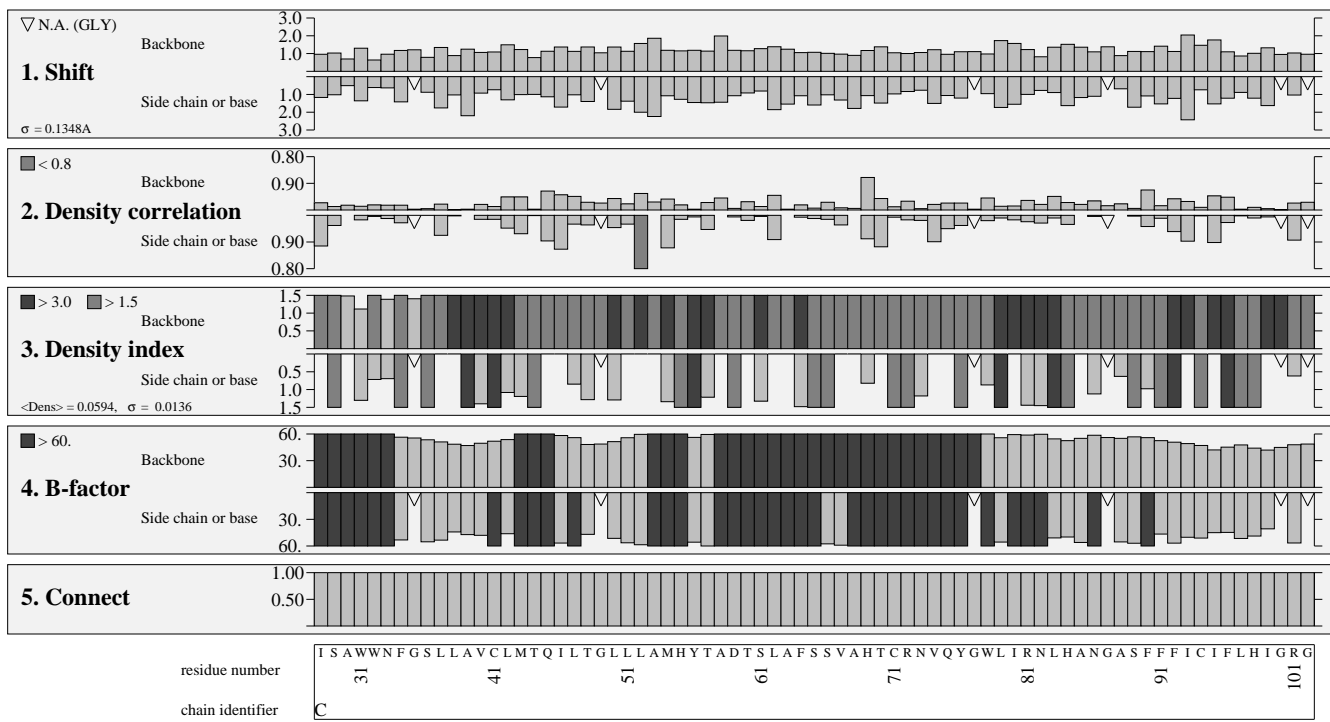
Local estimation (6)



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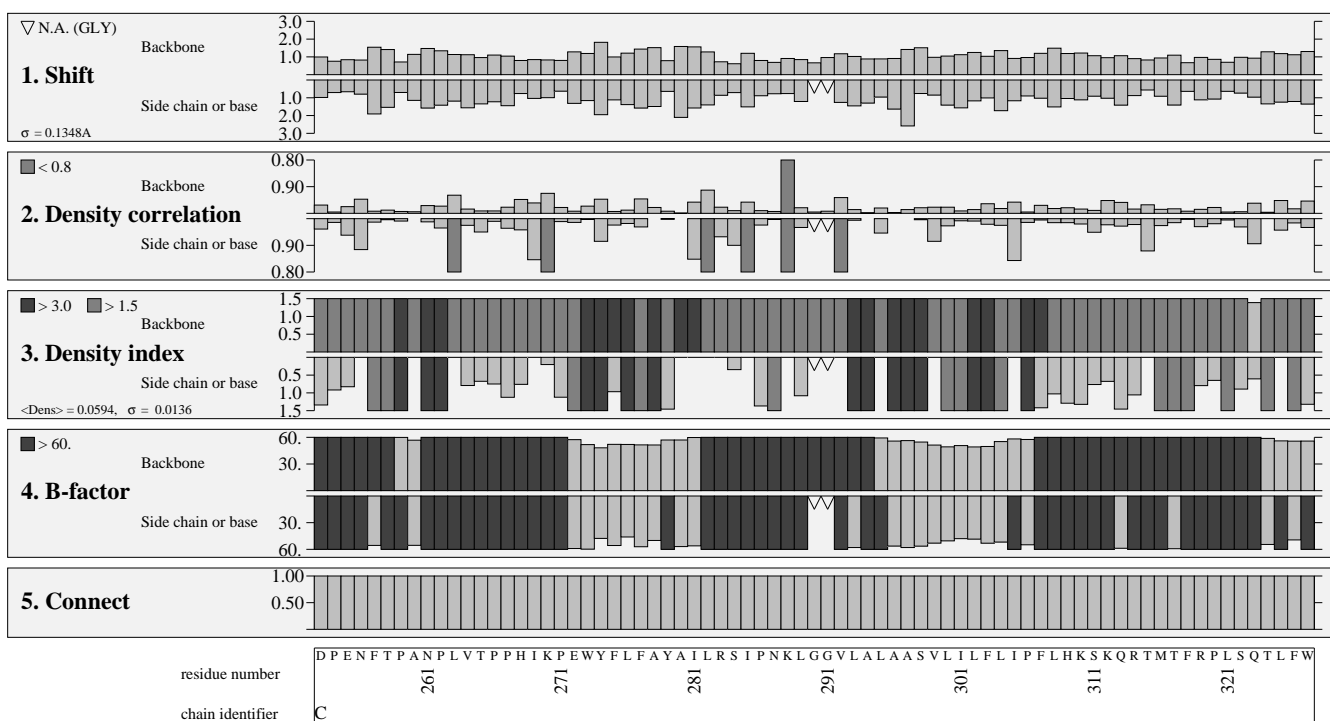
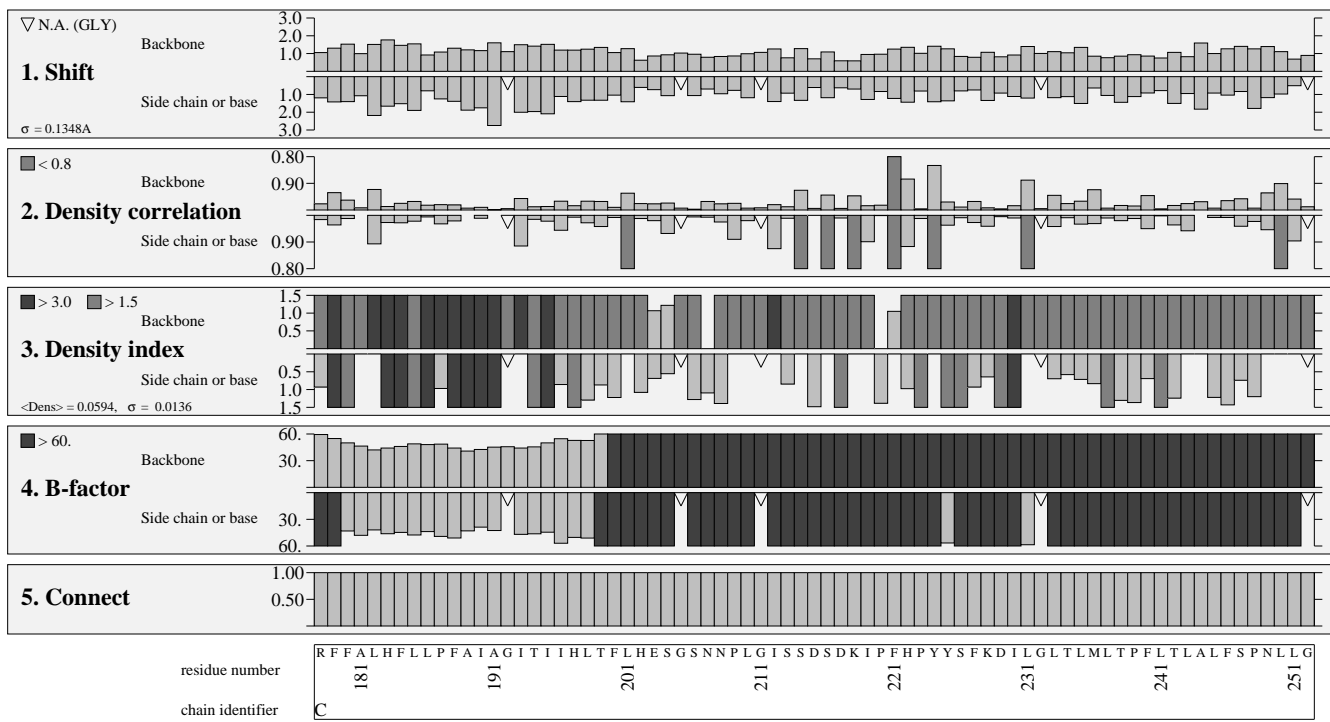
Local estimation (7)



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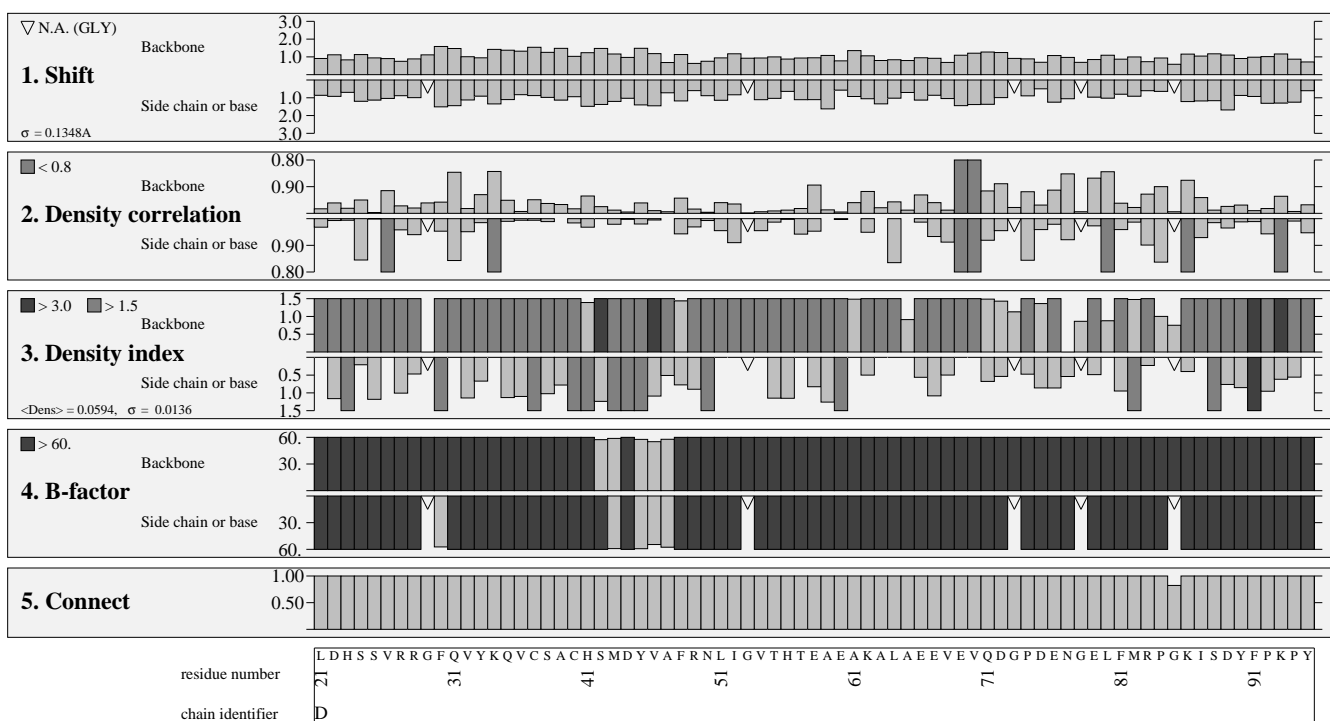
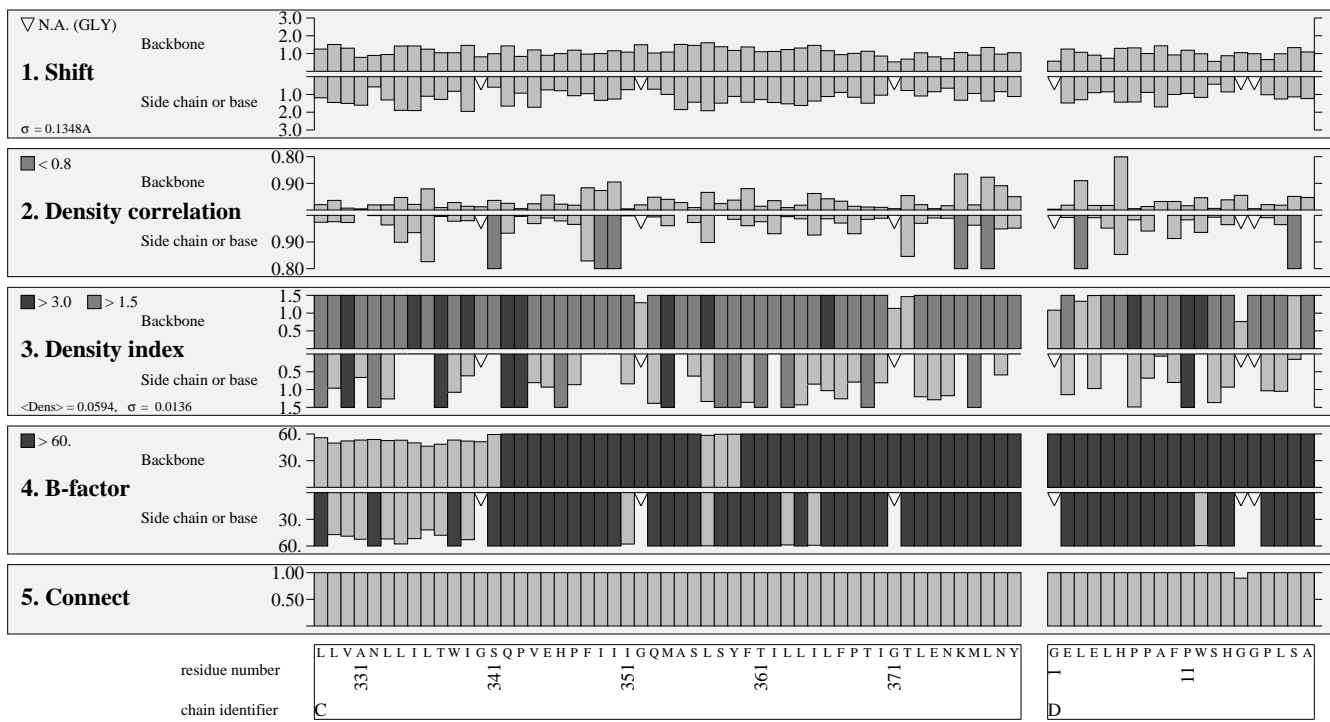
Local estimation (8)



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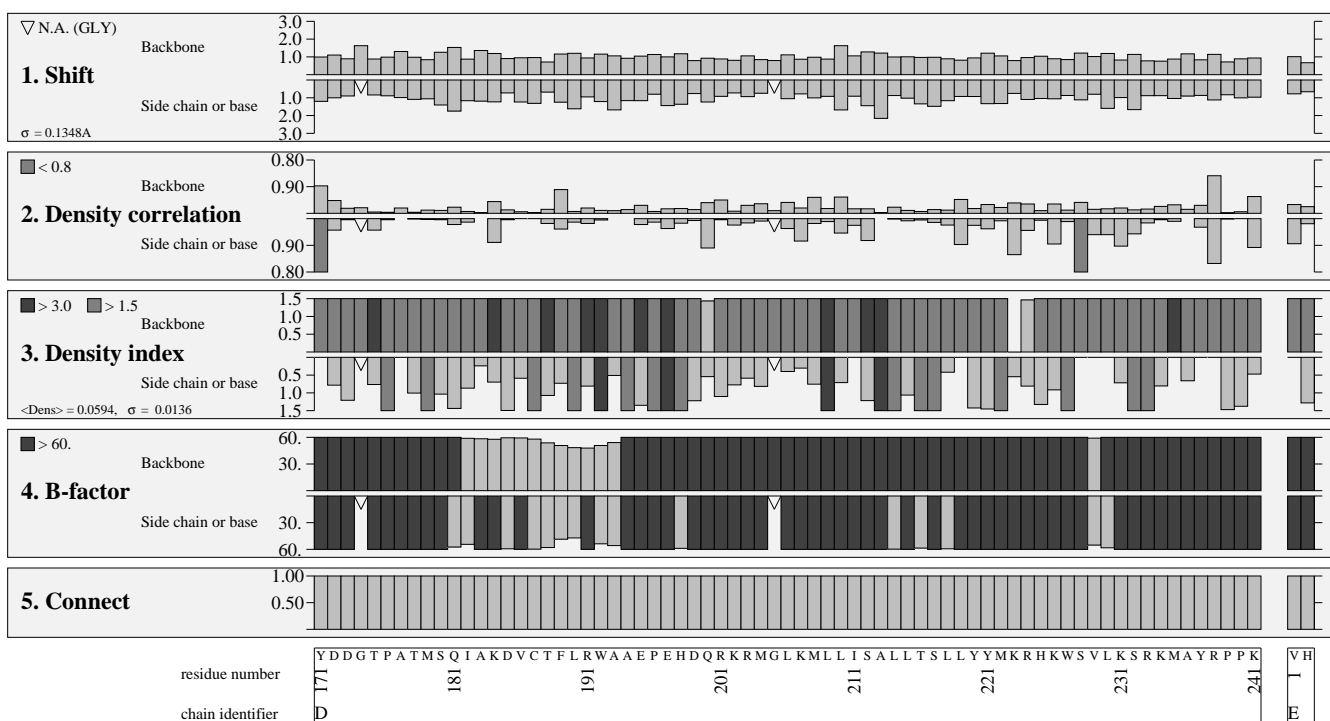
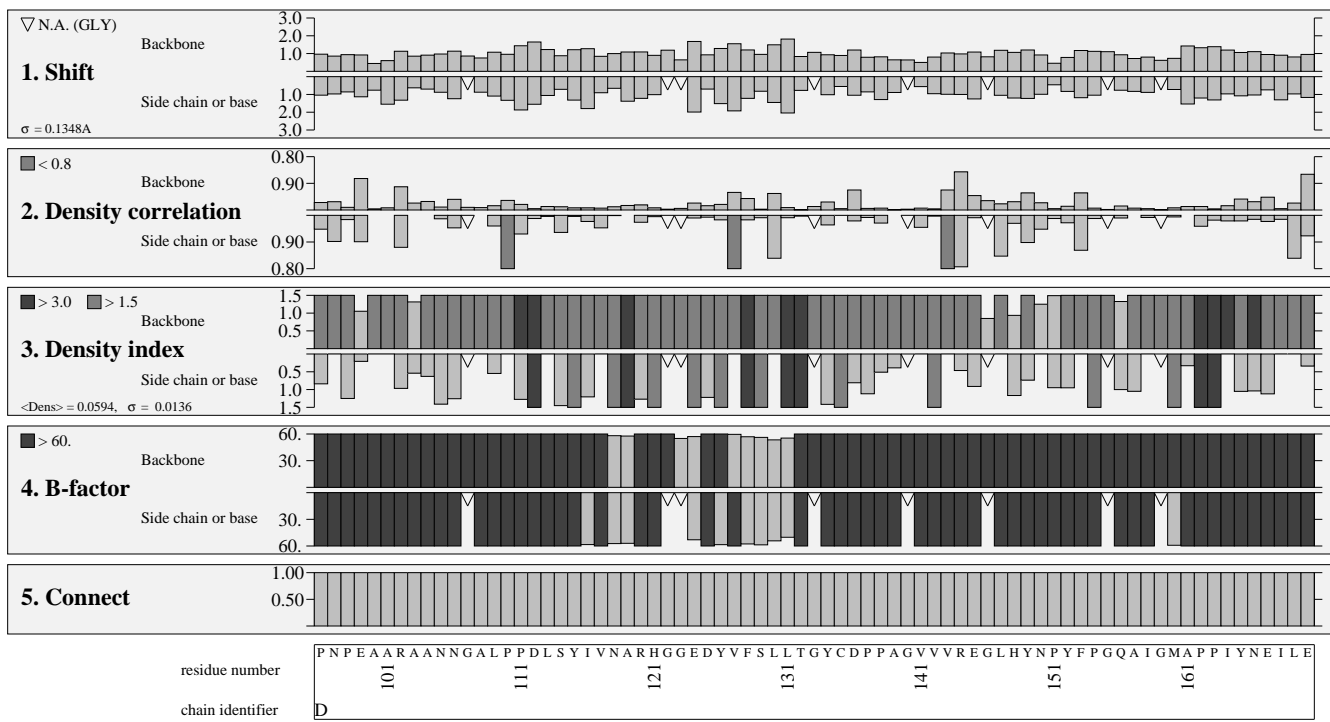
Local estimation (9)



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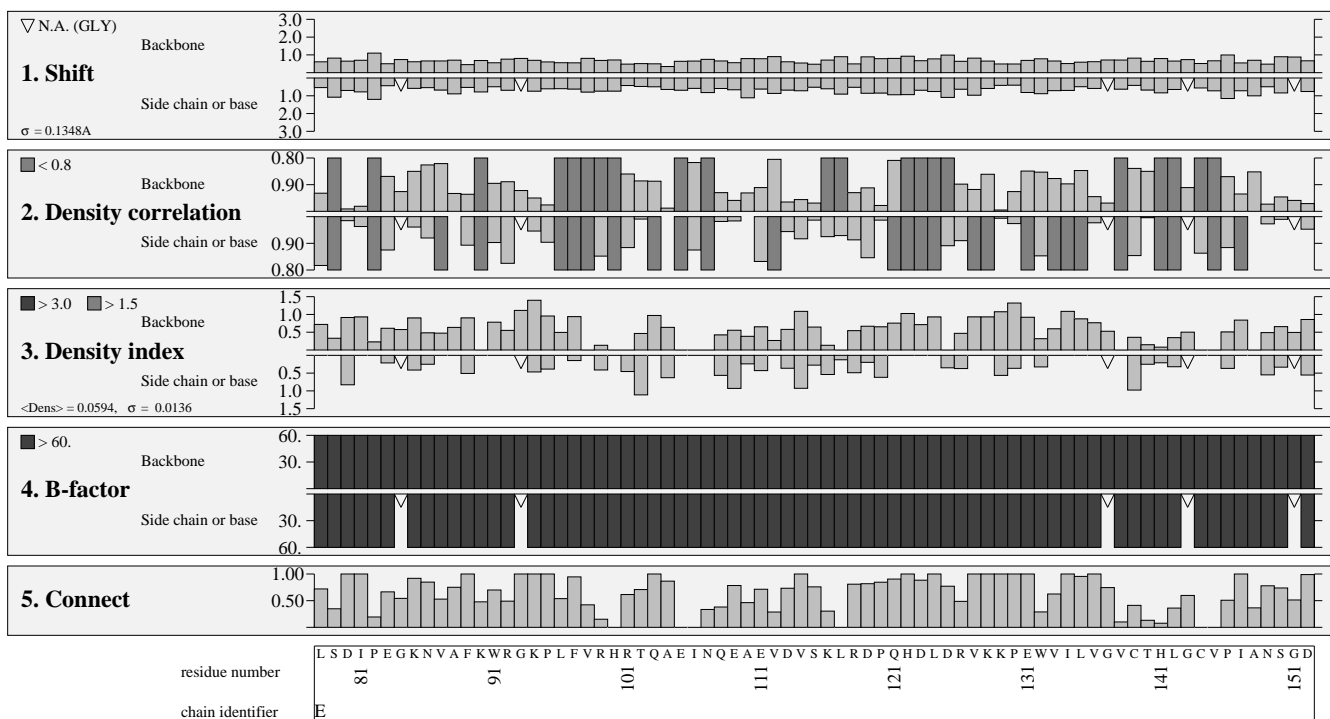
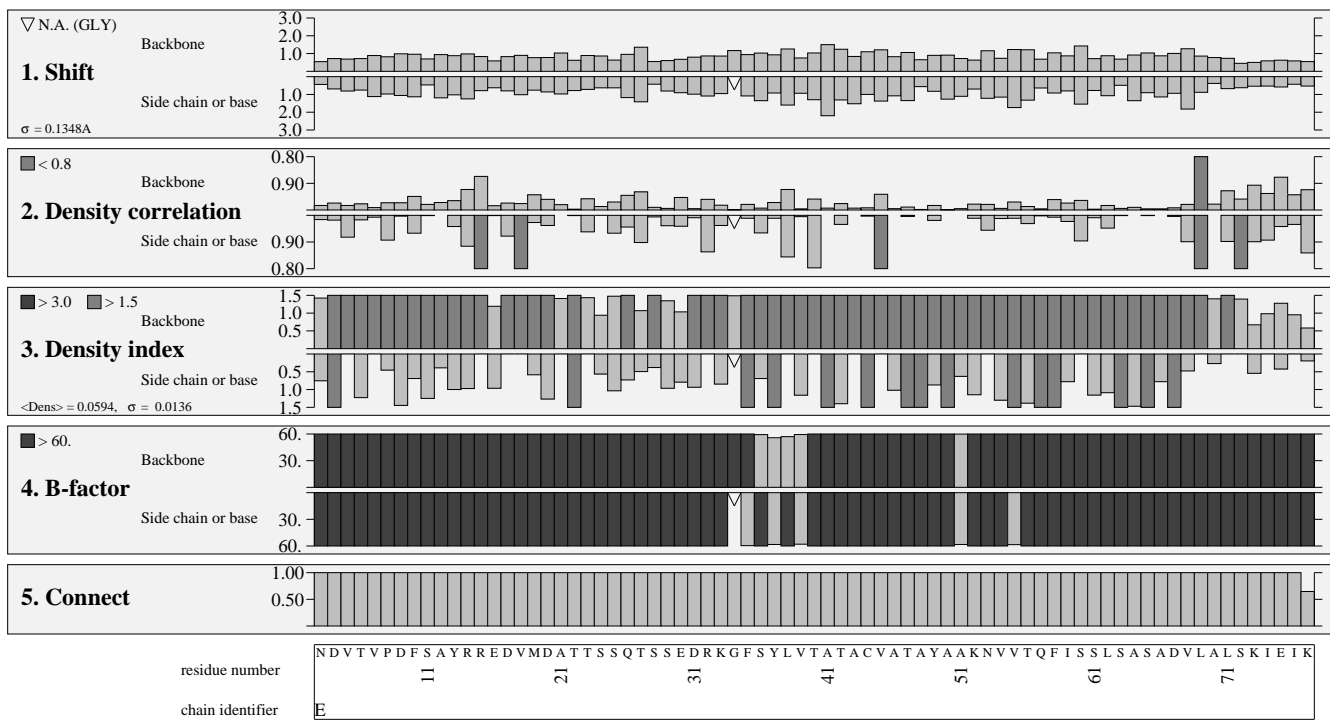
Local estimation (10)



Structure Factor Check

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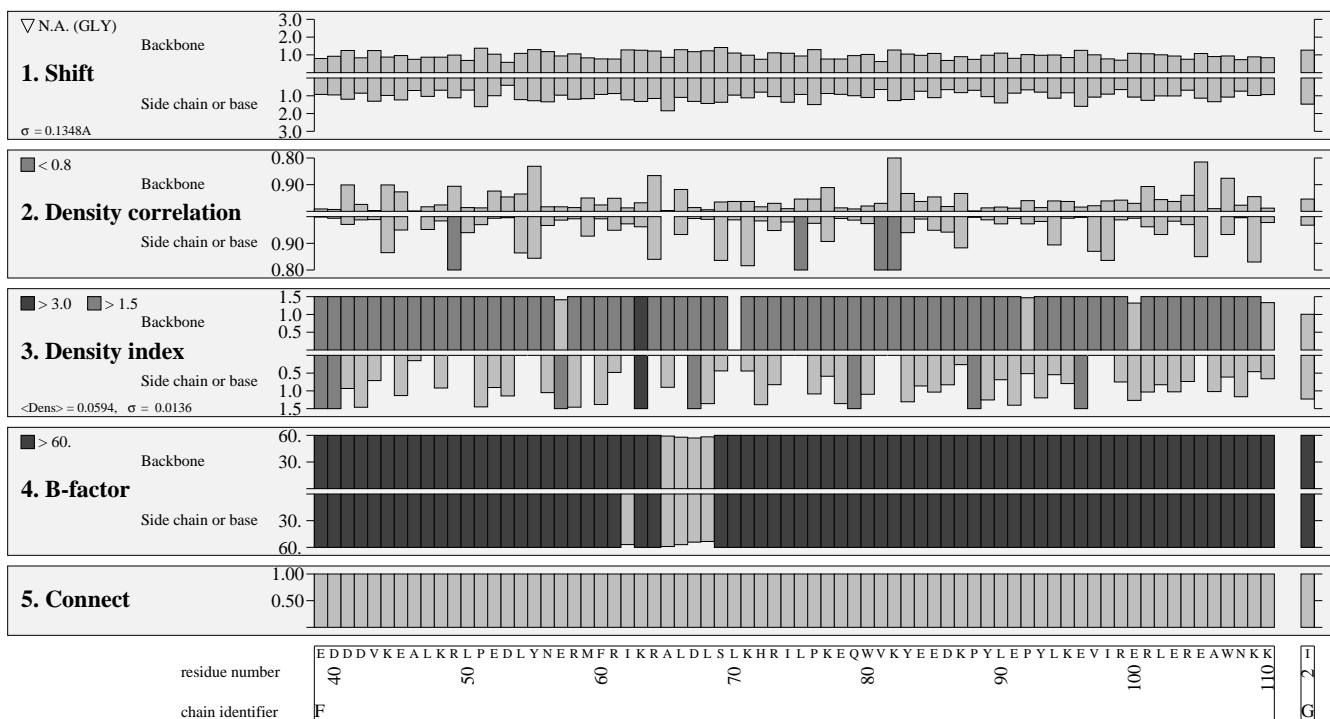
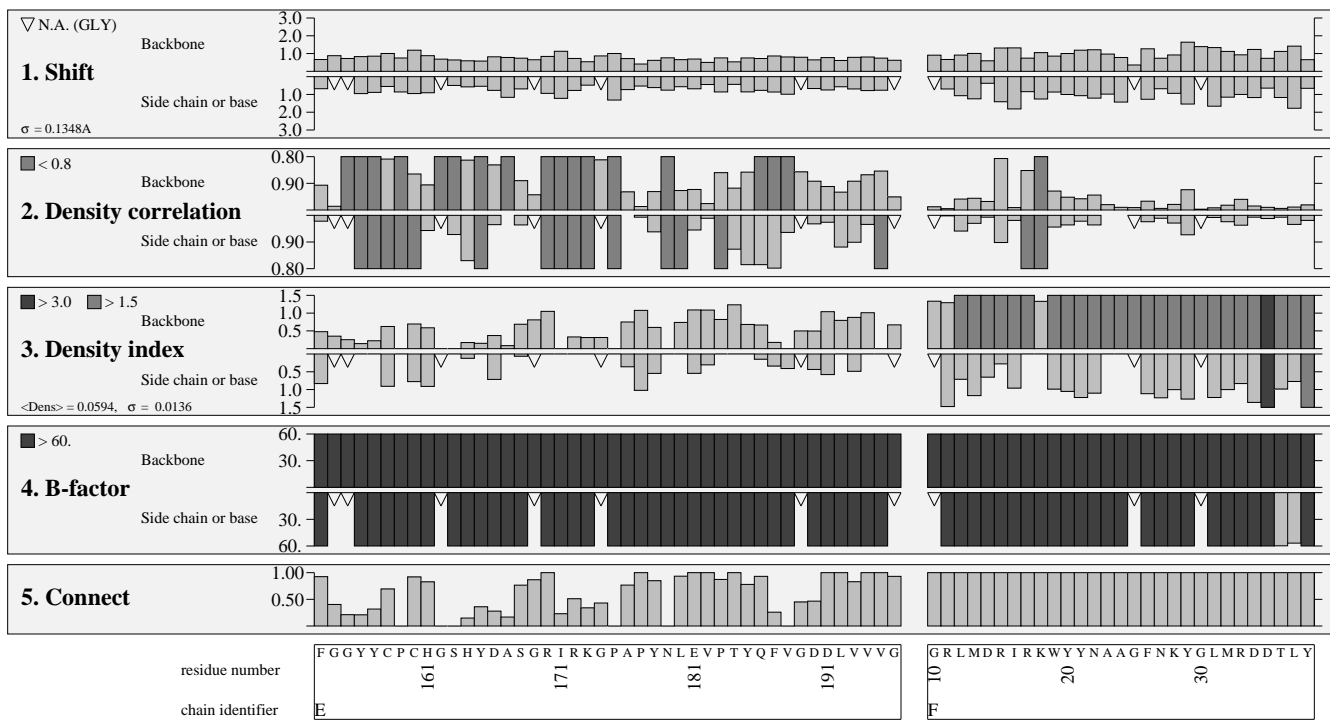
Local estimation (11)



Structure Factor Check

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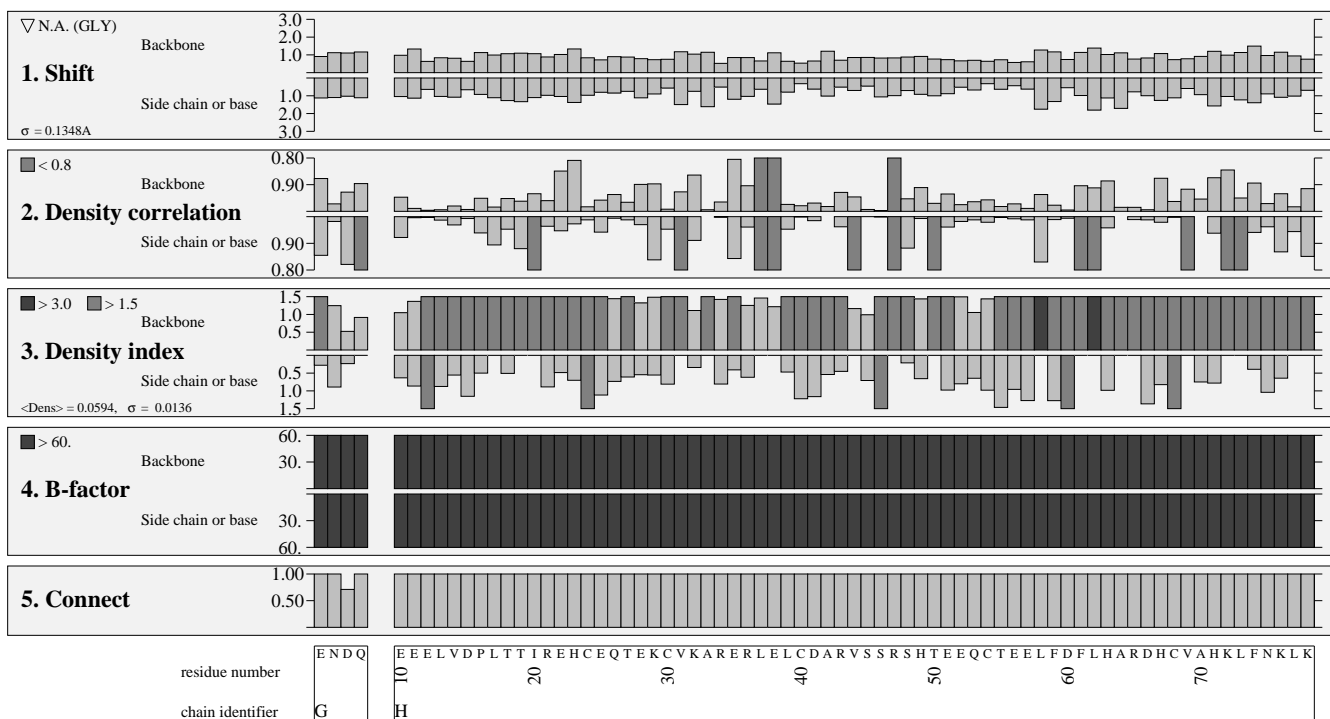
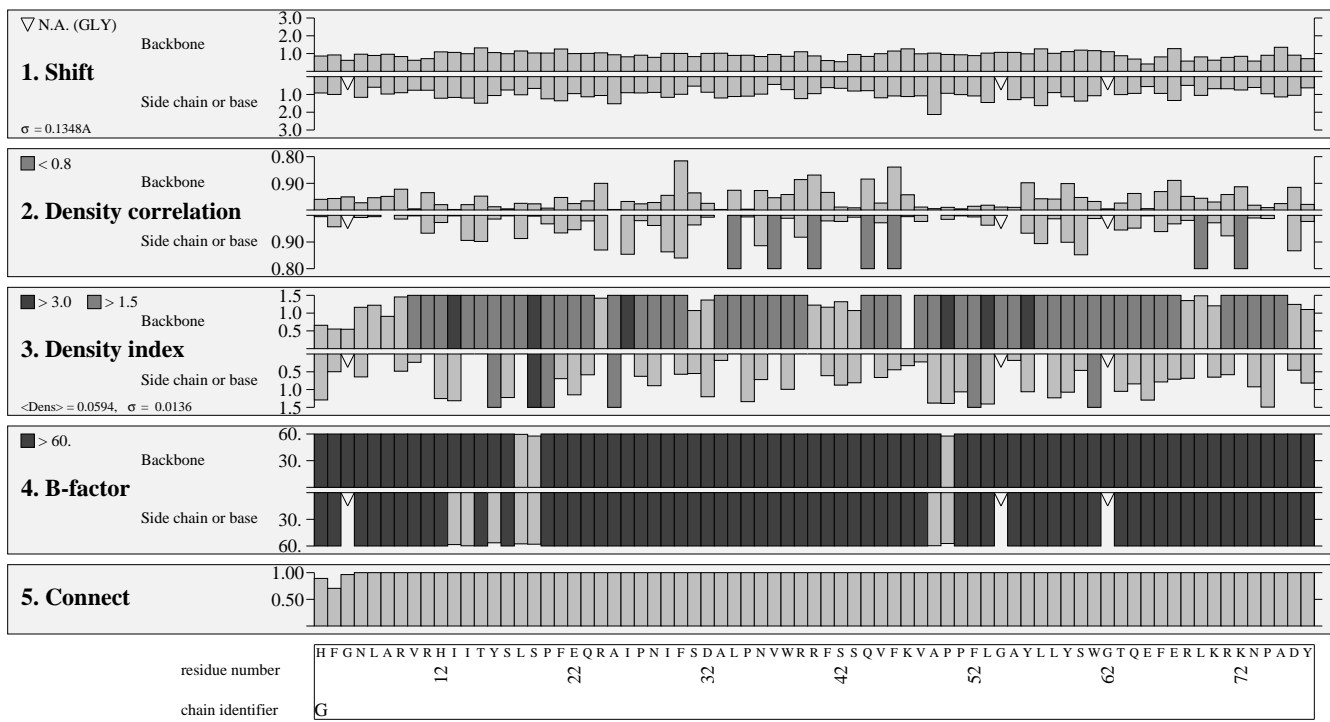
Local estimation (12)



Structure Factor Check

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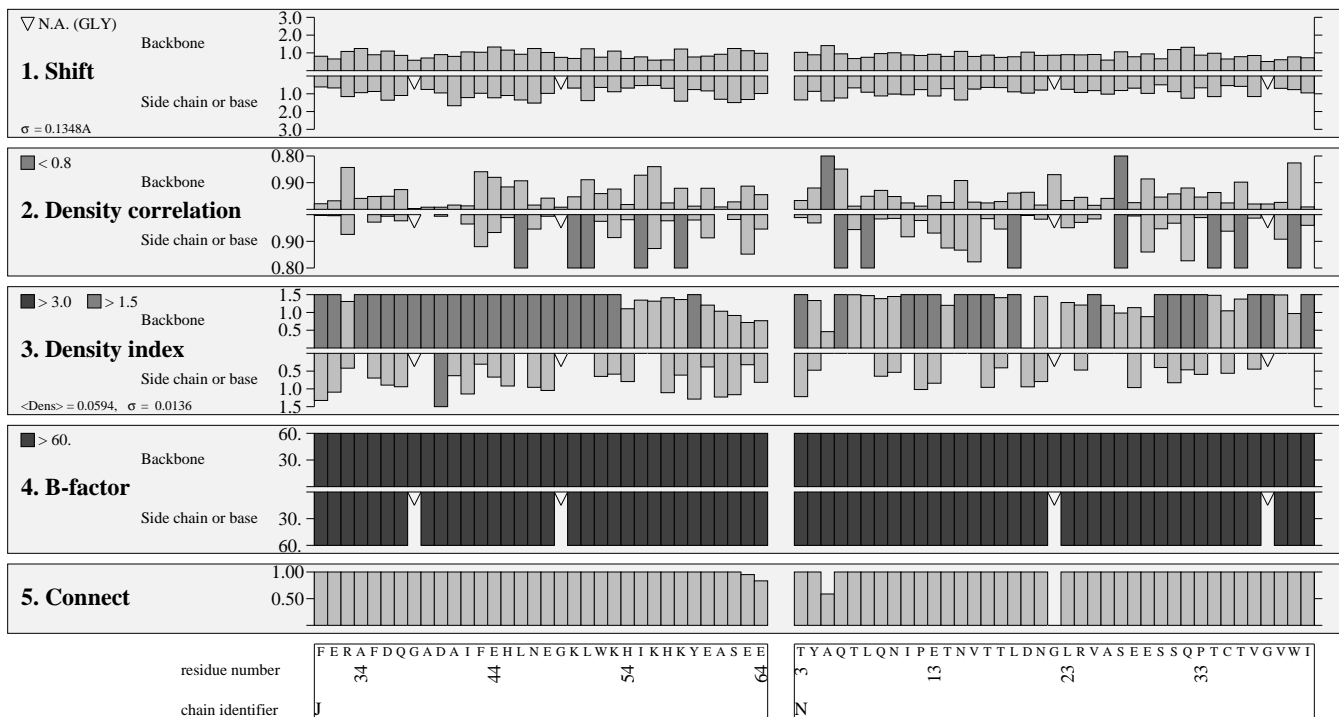
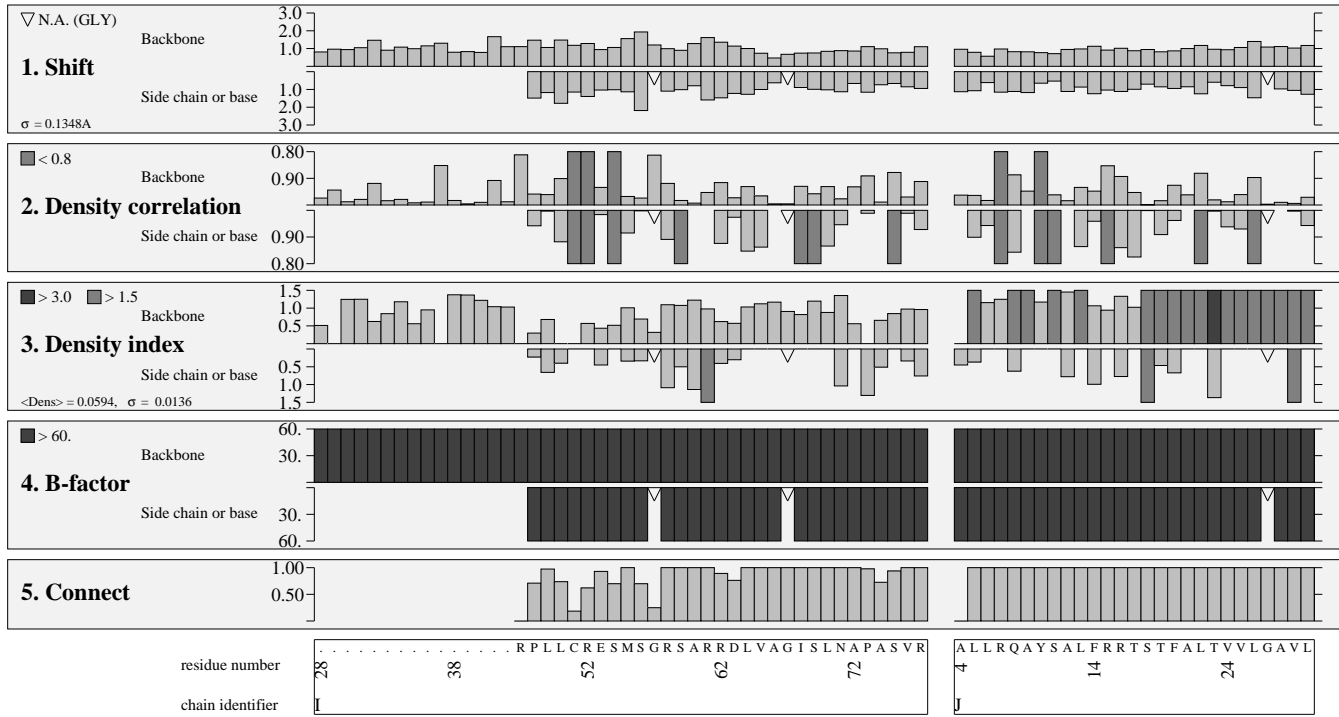
Local estimation (13)



Structure Factor Check

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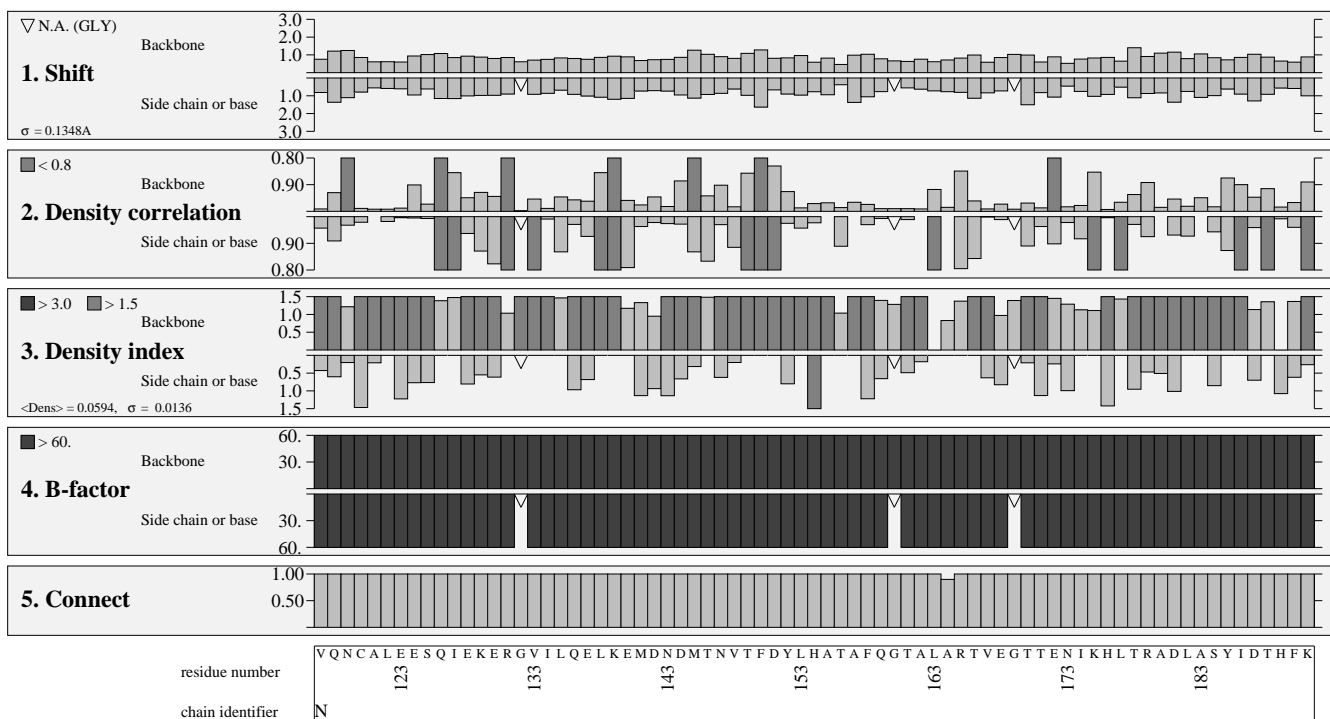
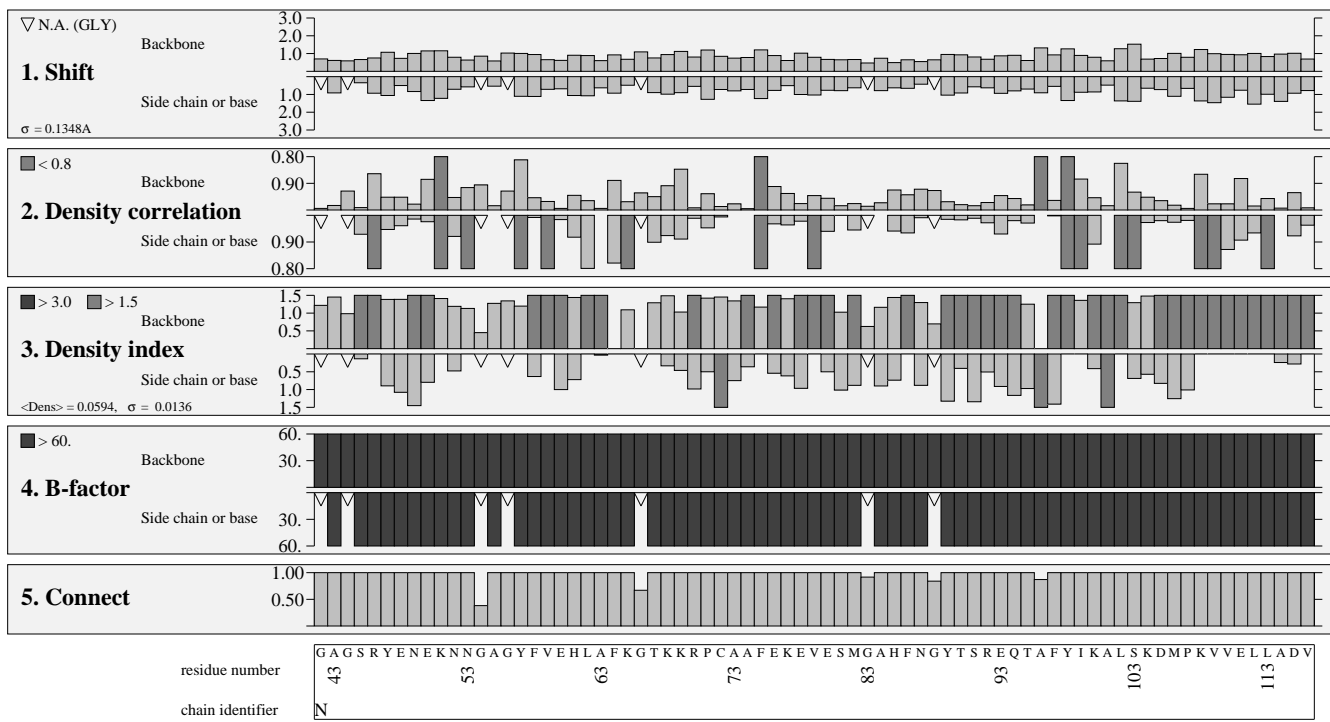
Local estimation (14)



Structure Factor Check

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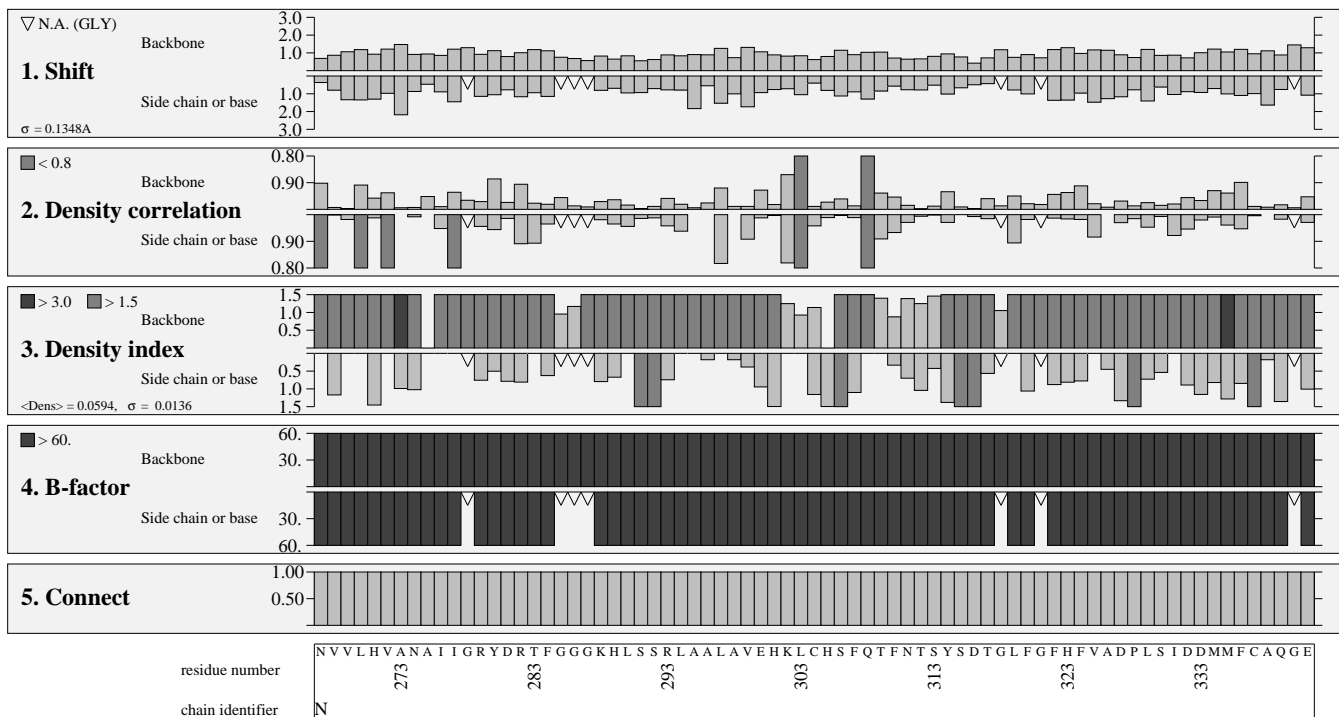
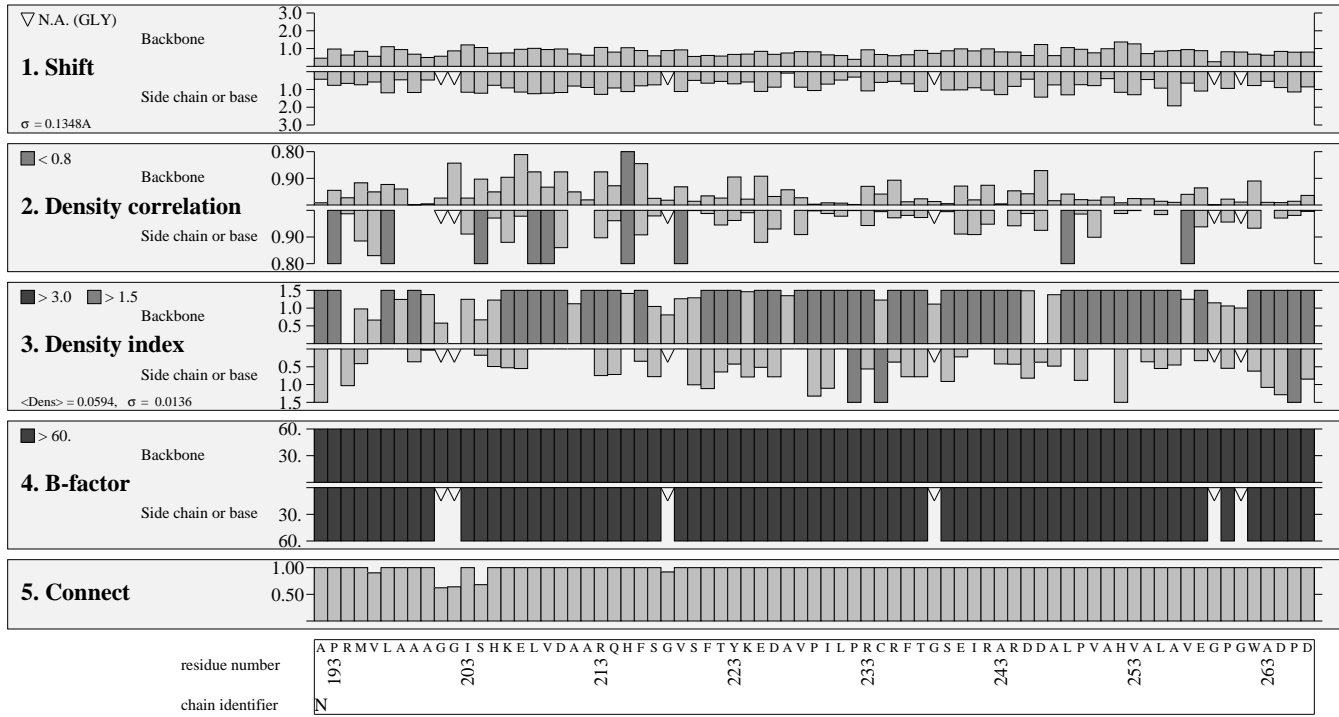
Local estimation (15)



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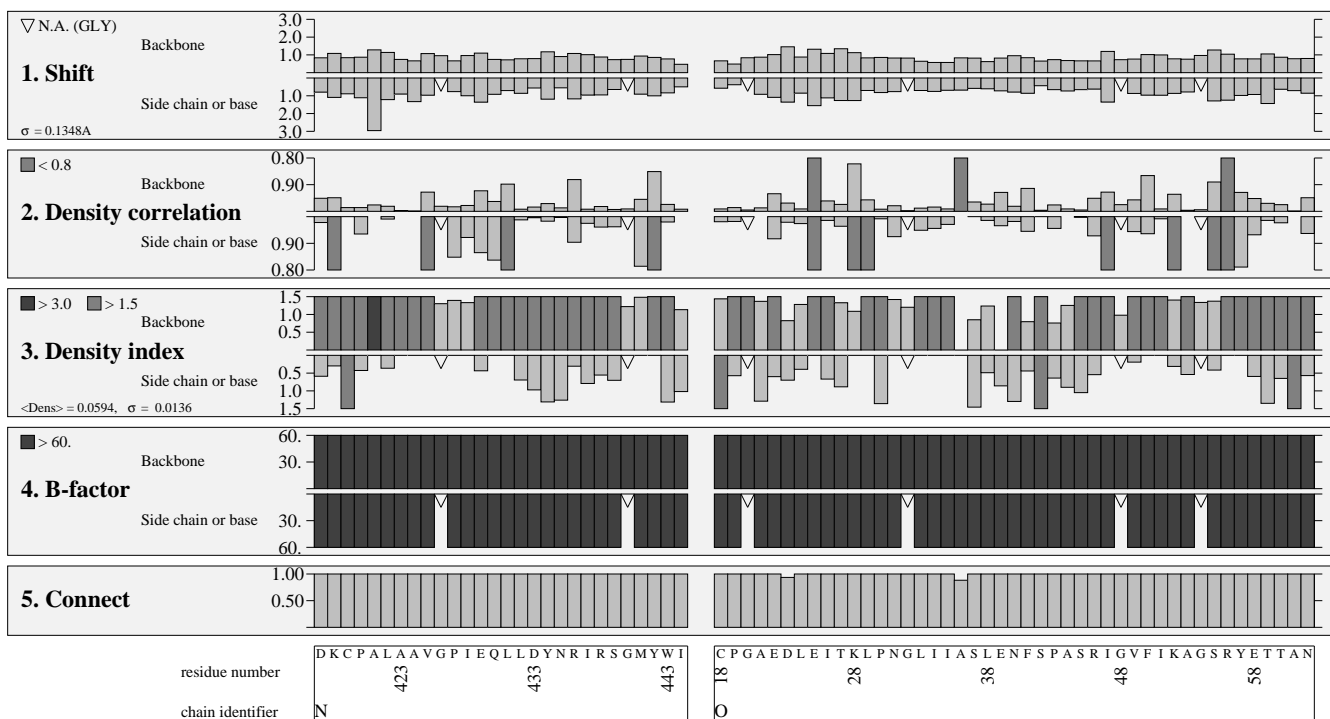
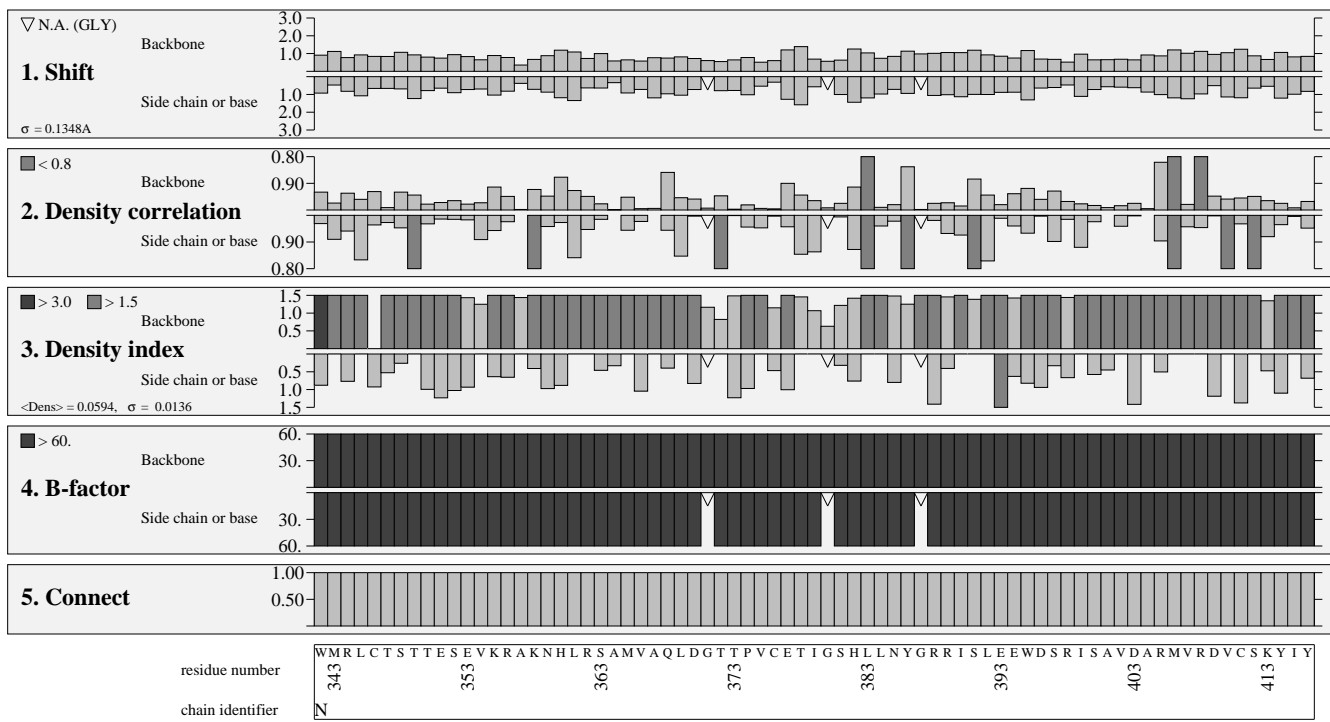
Local estimation (16)



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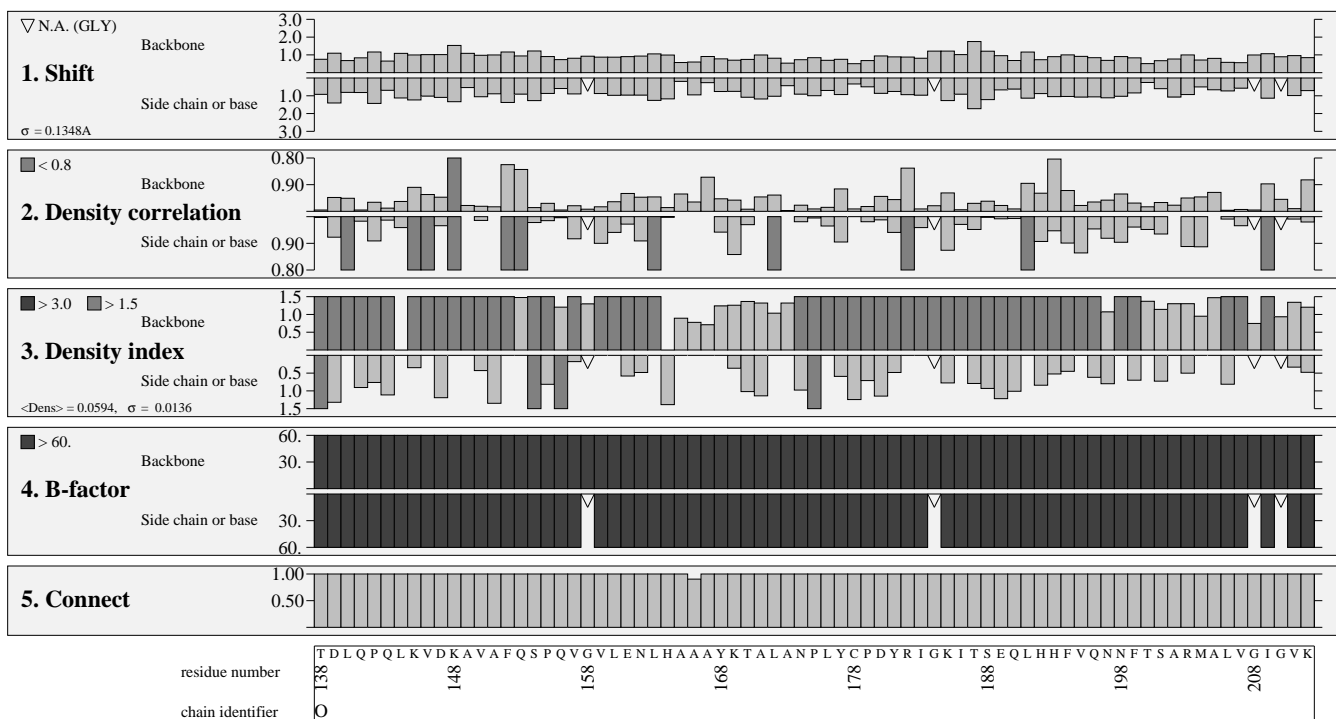
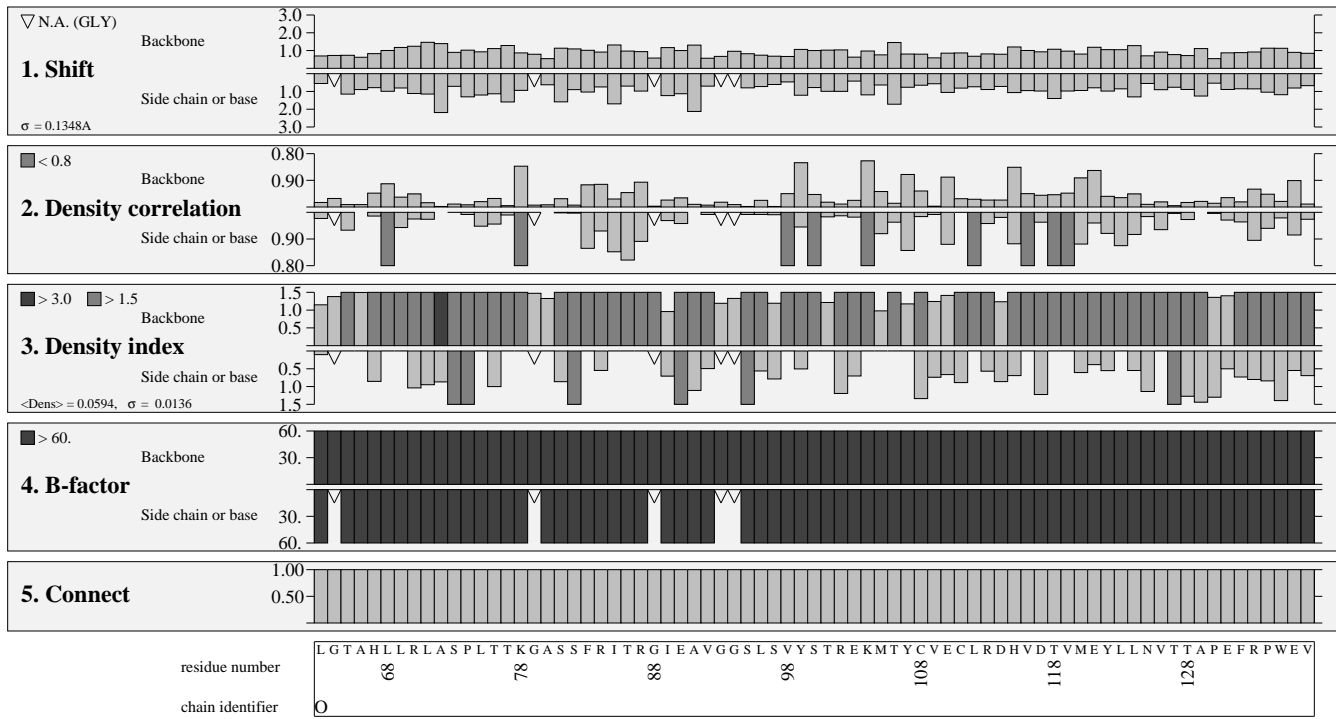
Local estimation (17)



Structure Factor Check

3H1K

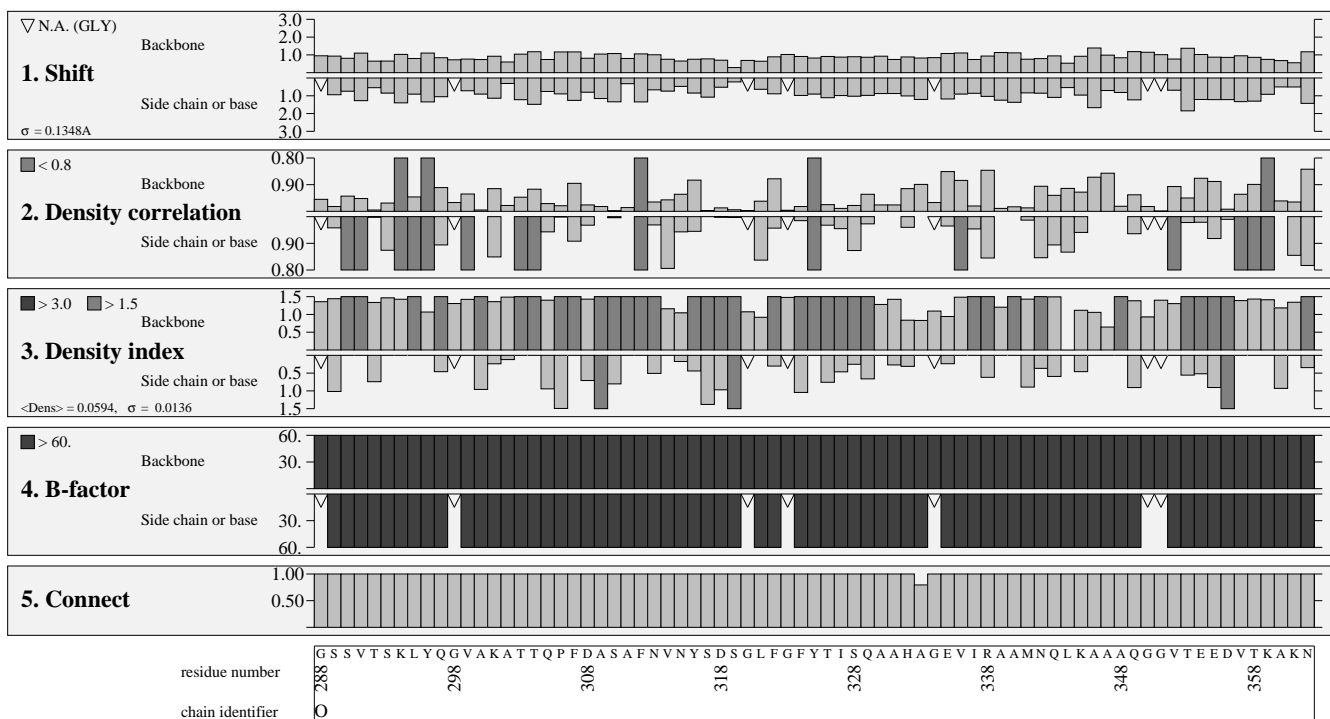
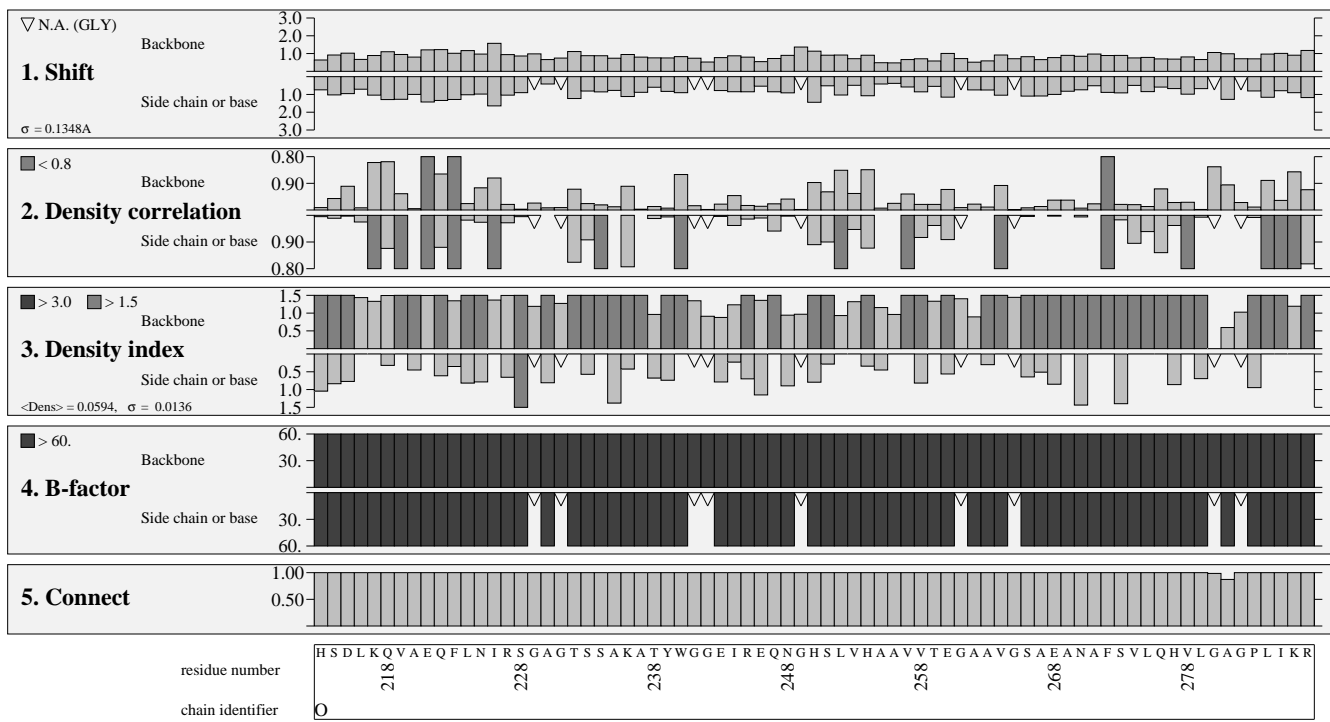
Local estimation (18)



Structure Factor Check

3H1K

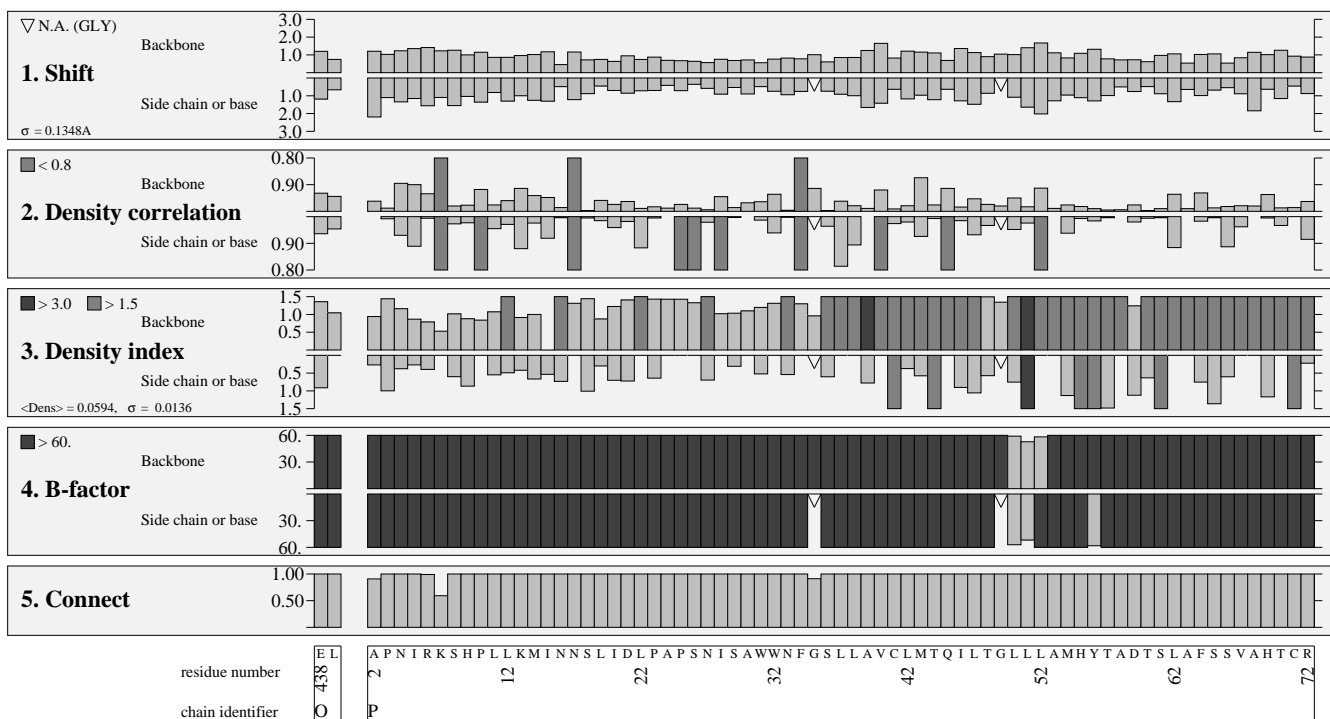
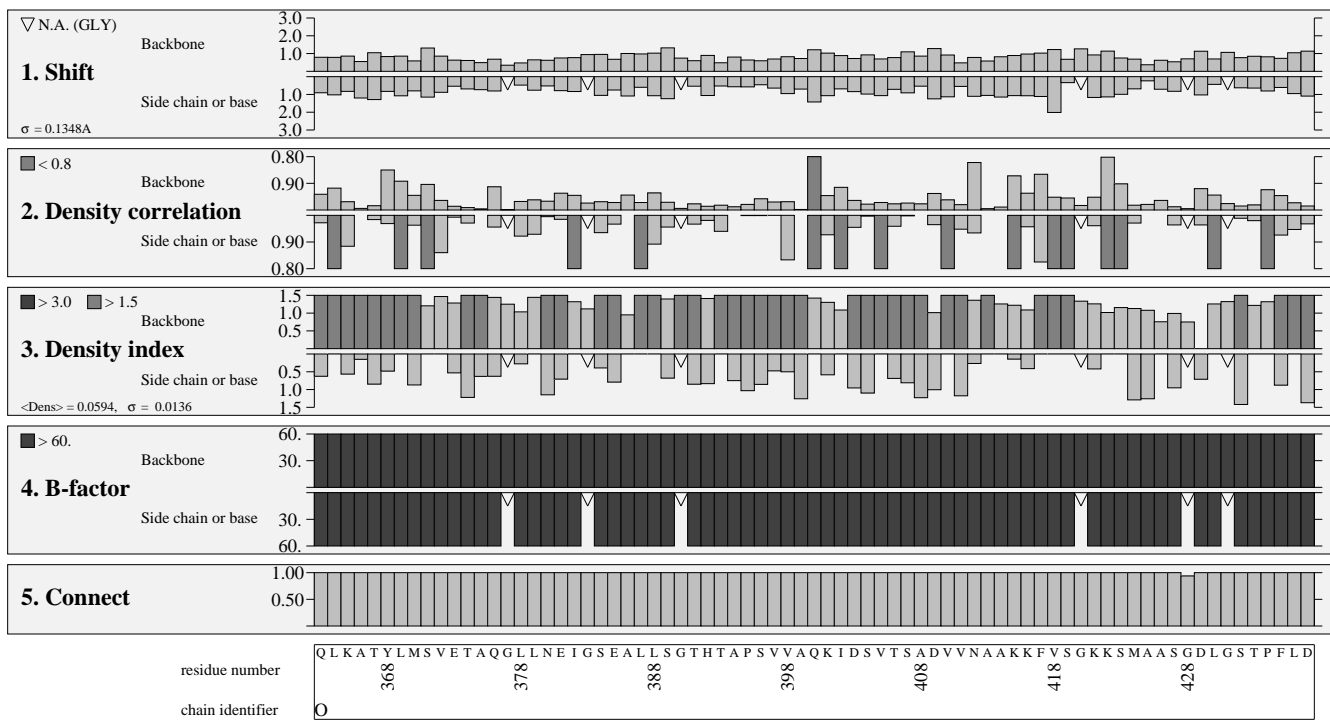
Local estimation (19)



Structure Factor Check

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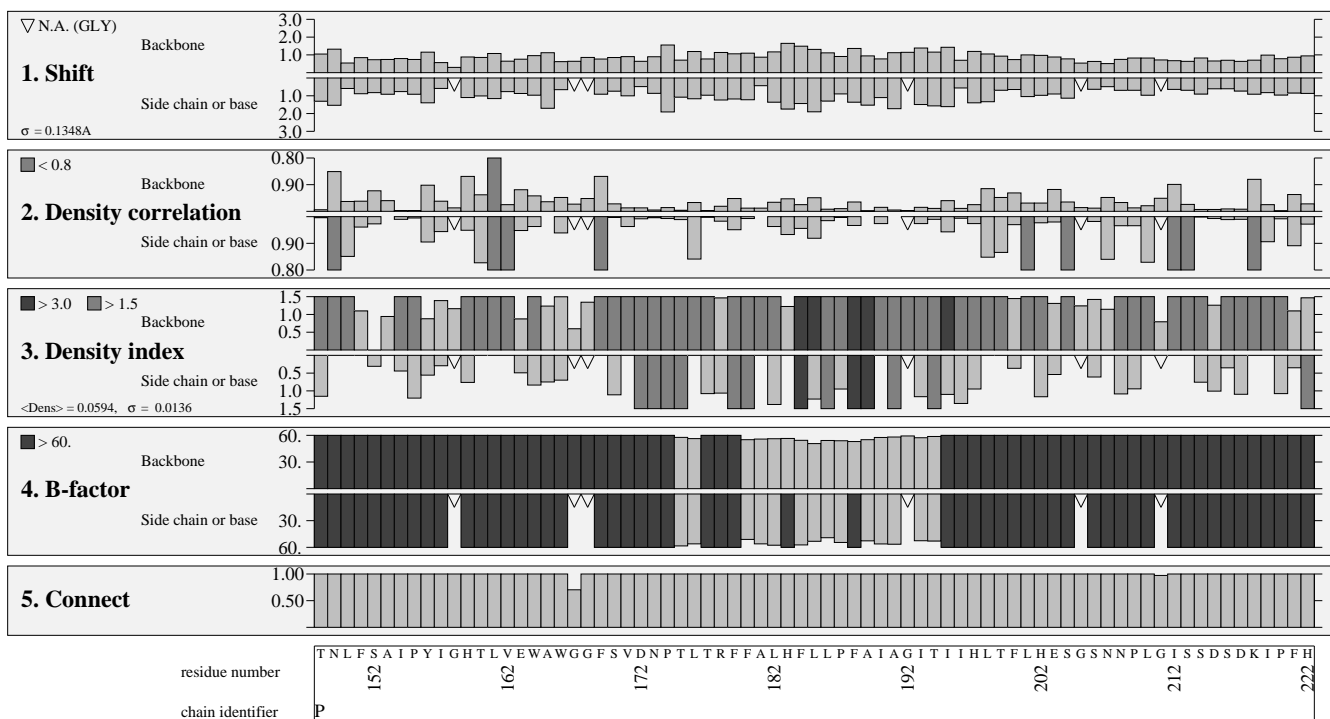
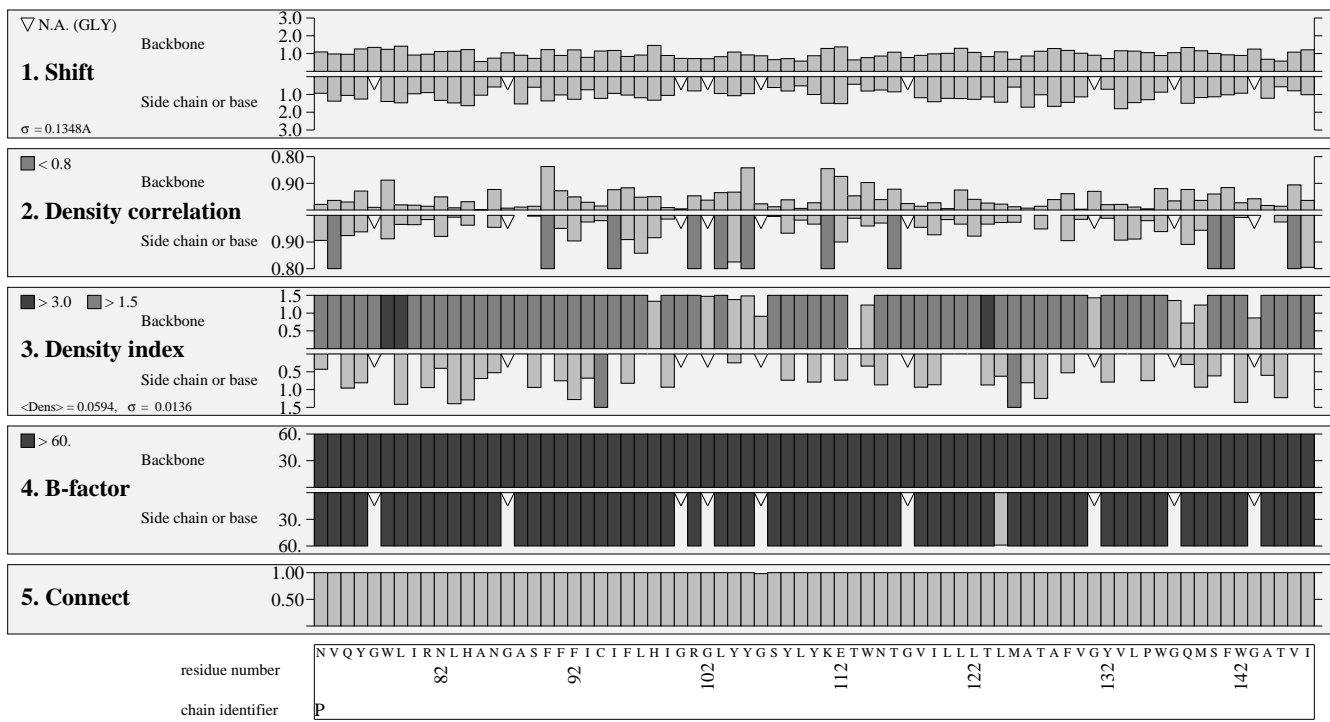
Local estimation (20)



Structure Factor Check

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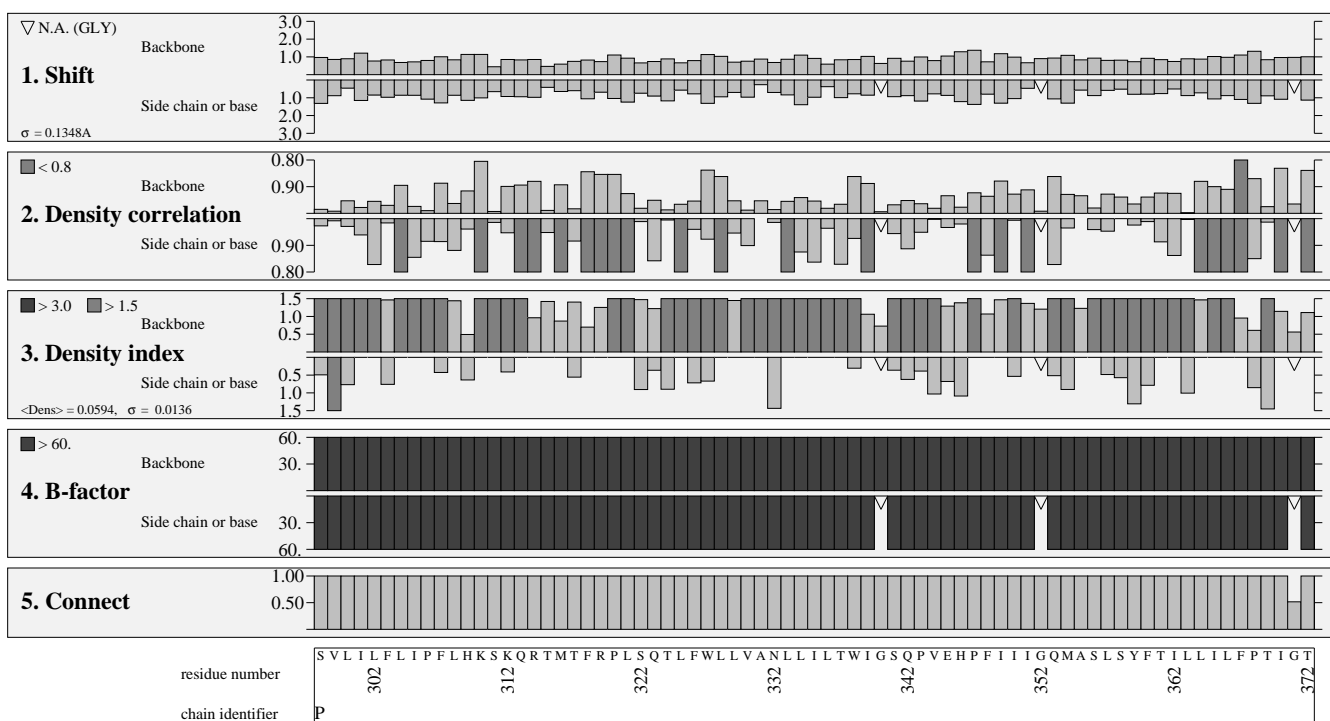
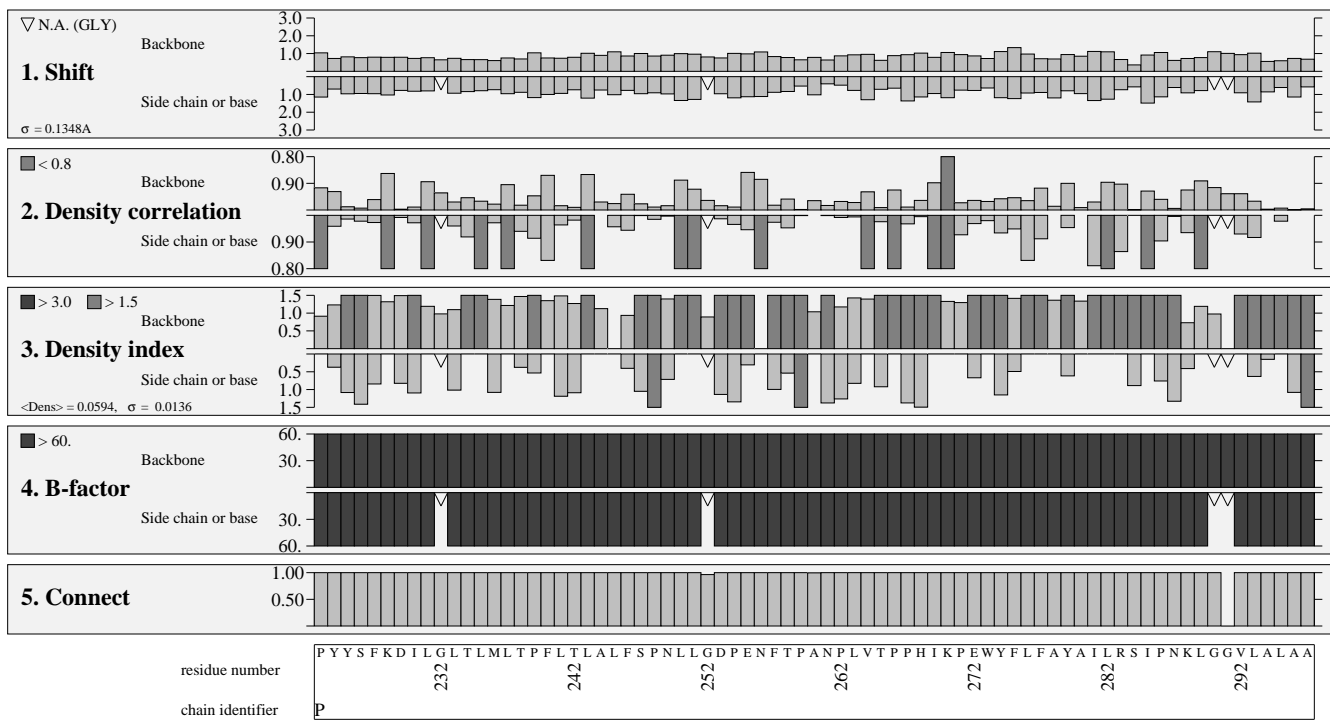
Local estimation (21)



Structure Factor Check

3H1K

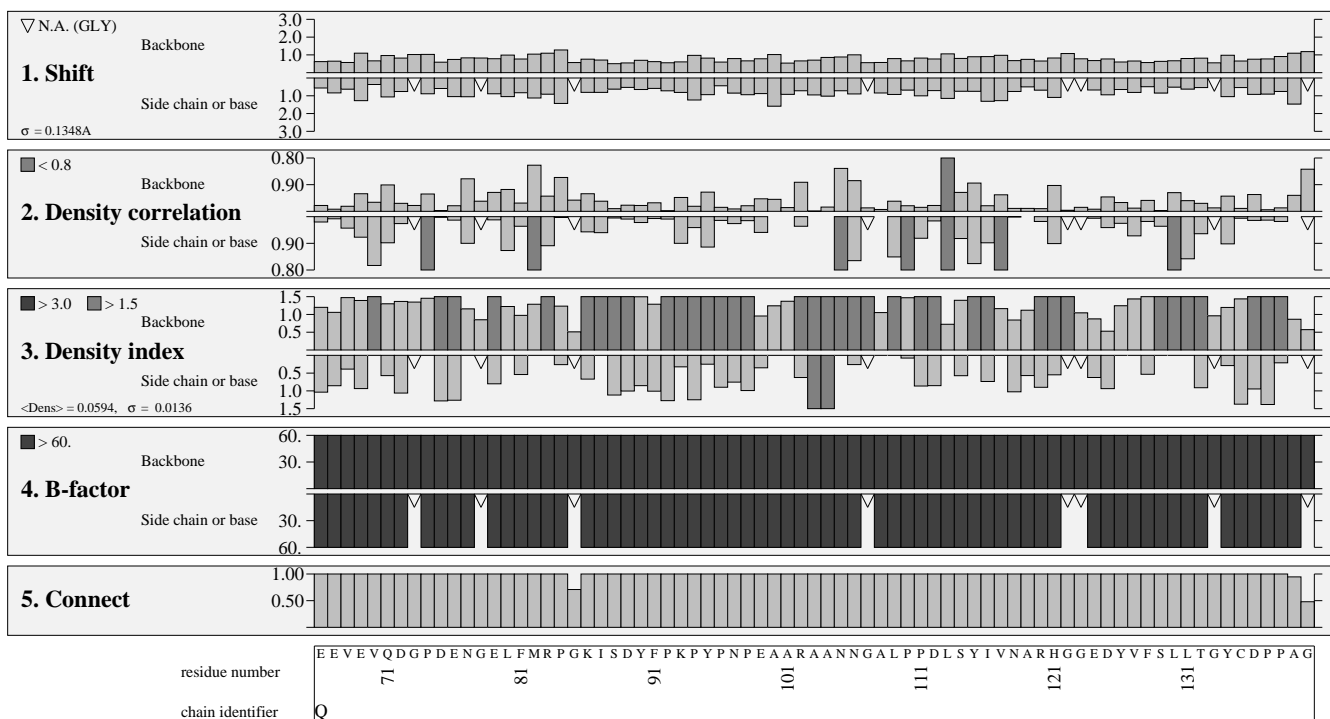
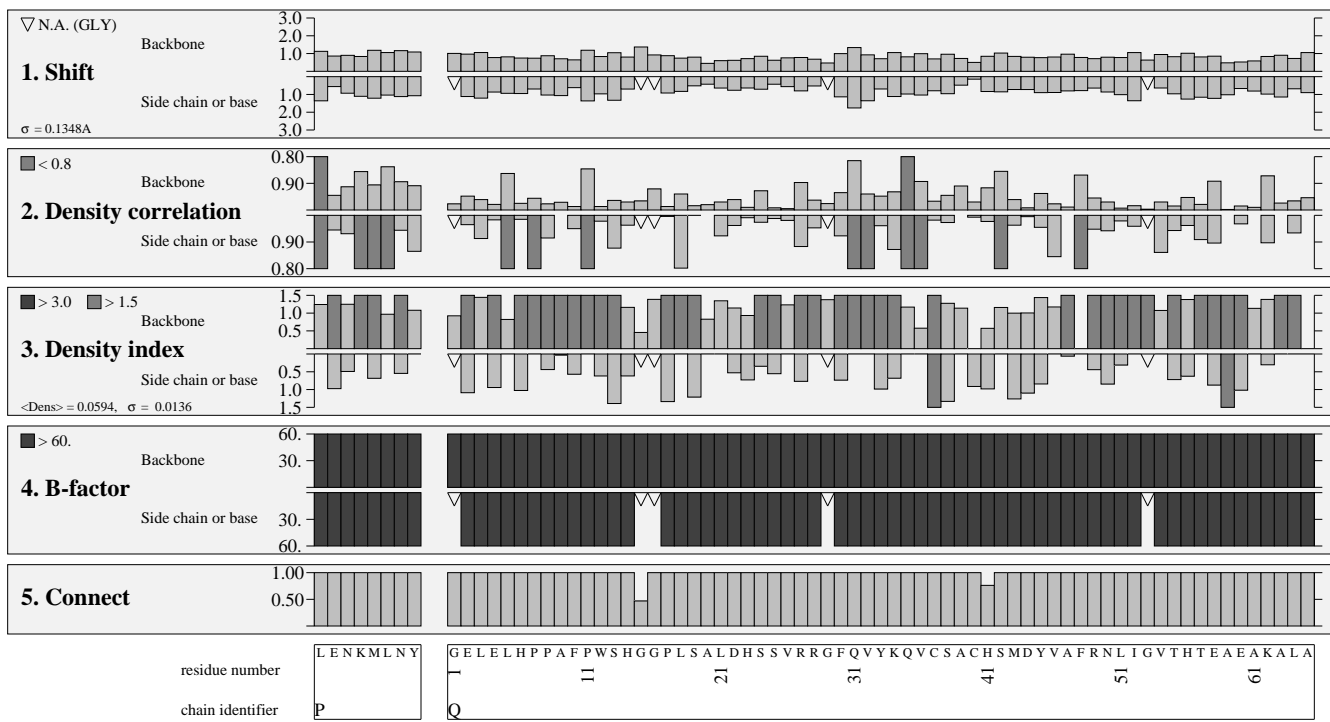
Local estimation (22)



Structure Factor Check

3H1K

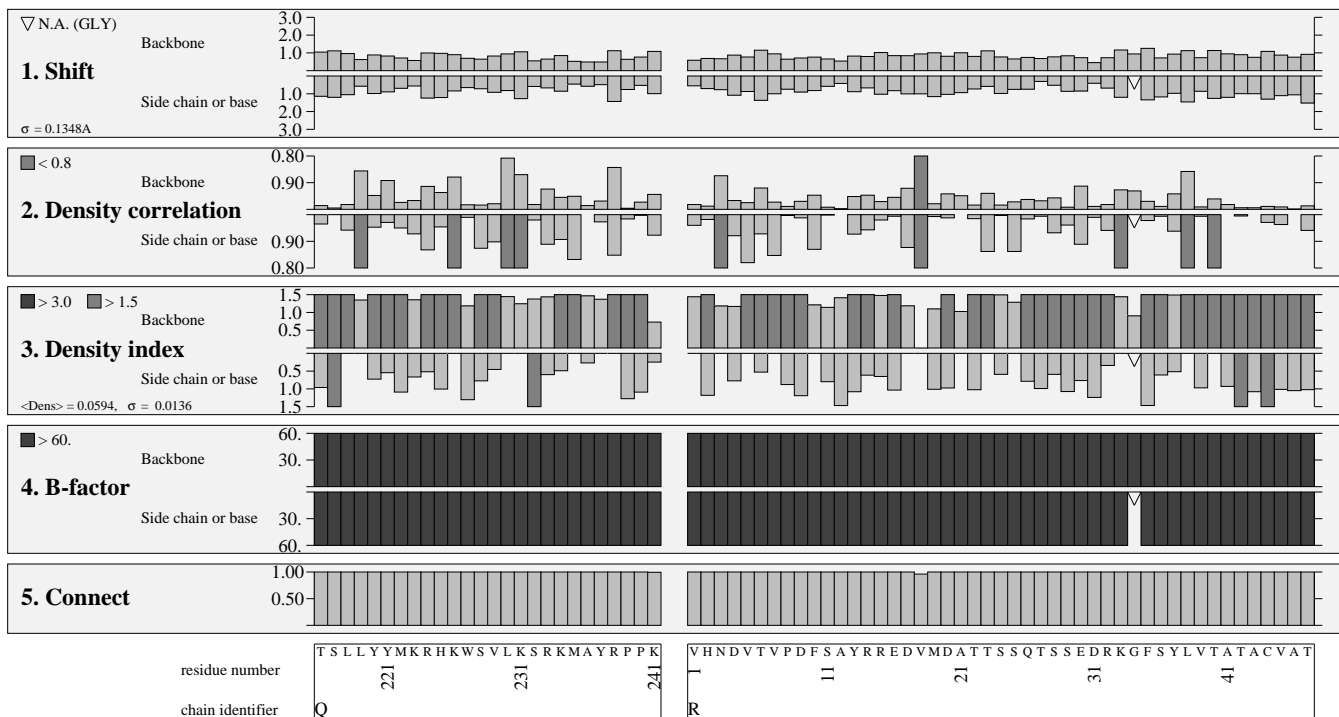
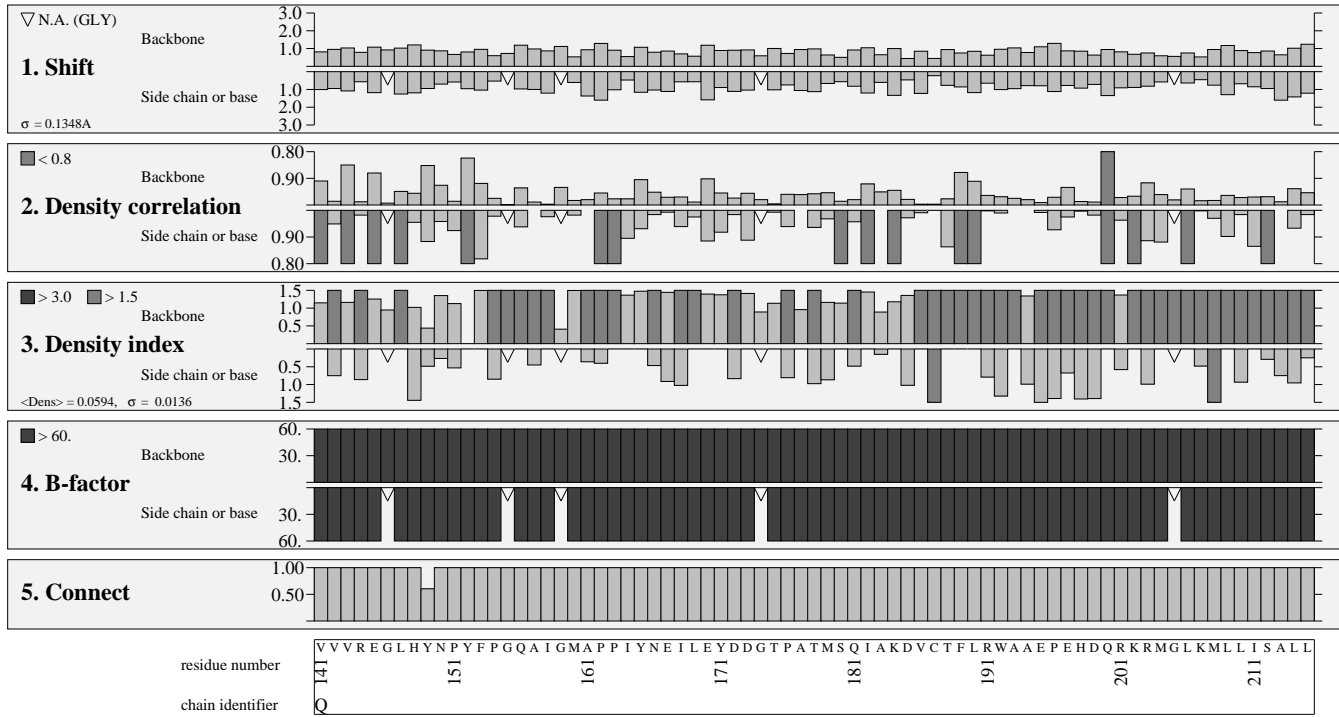
Local estimation (23)



Structure Factor Check

3H1K

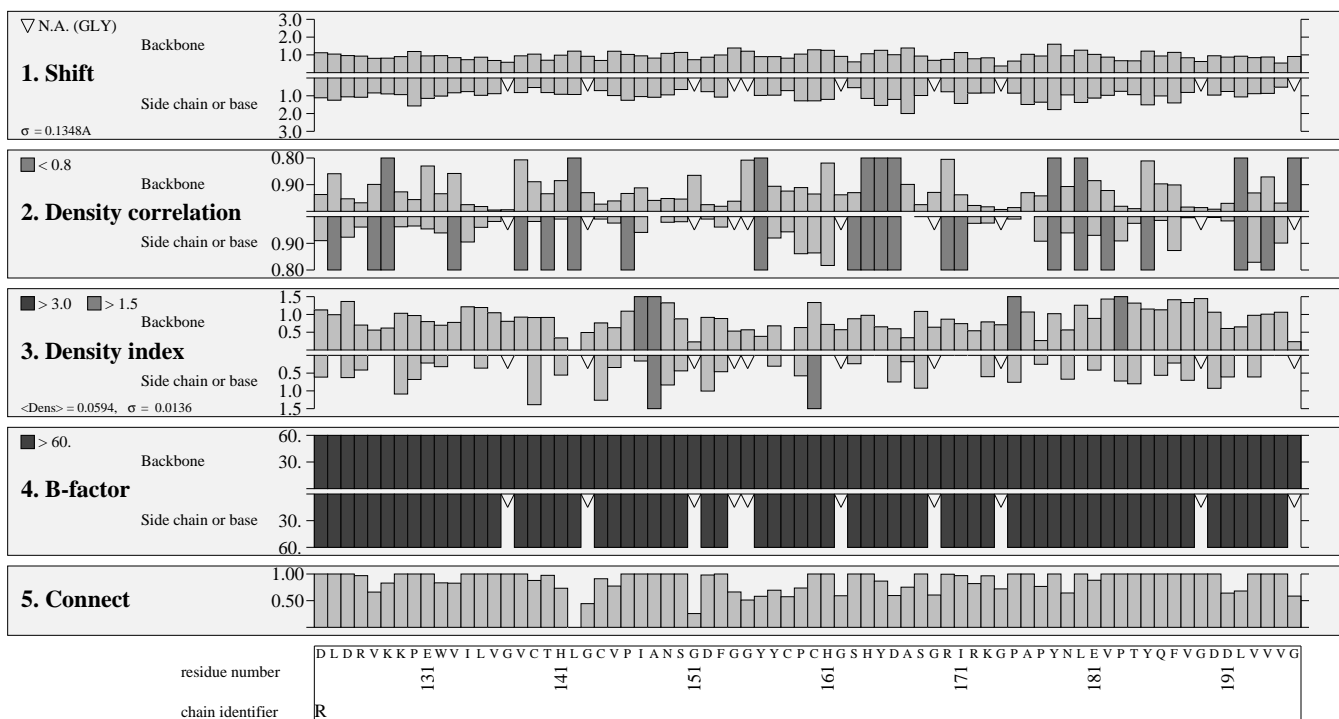
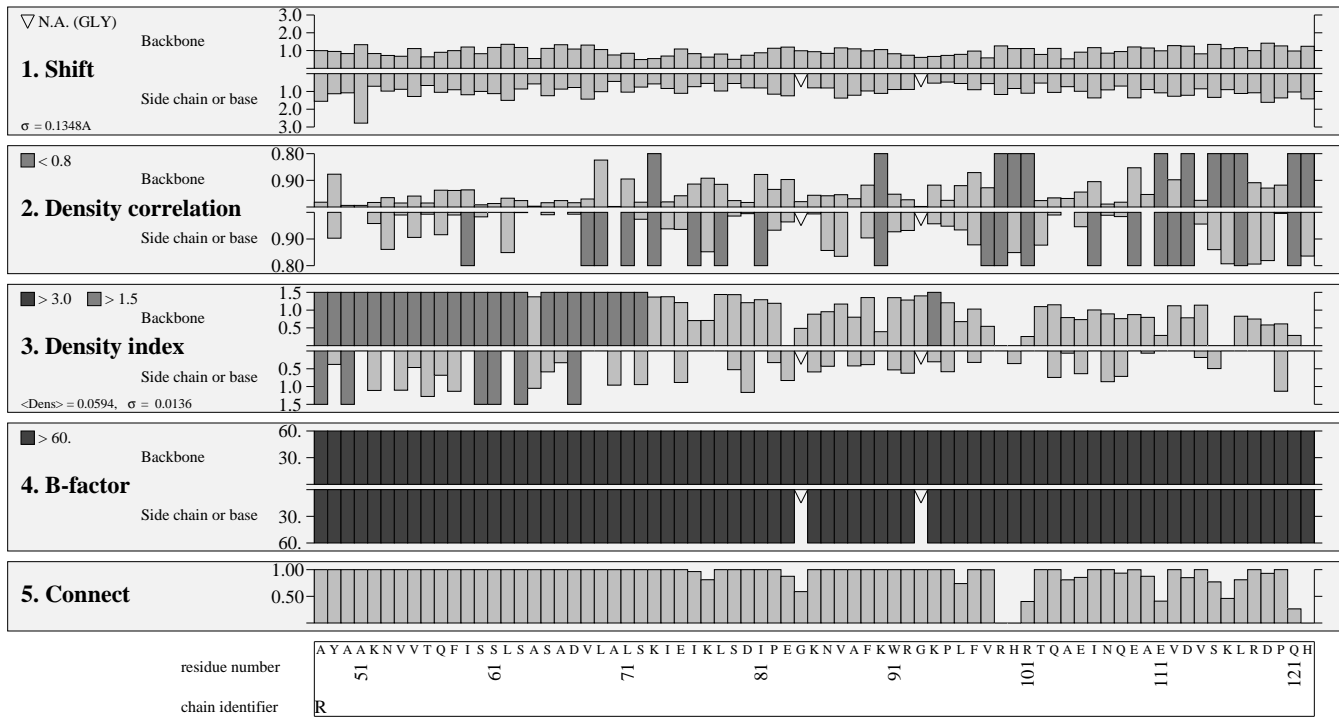
Local estimation (24)



Structure Factor Check

3H1K

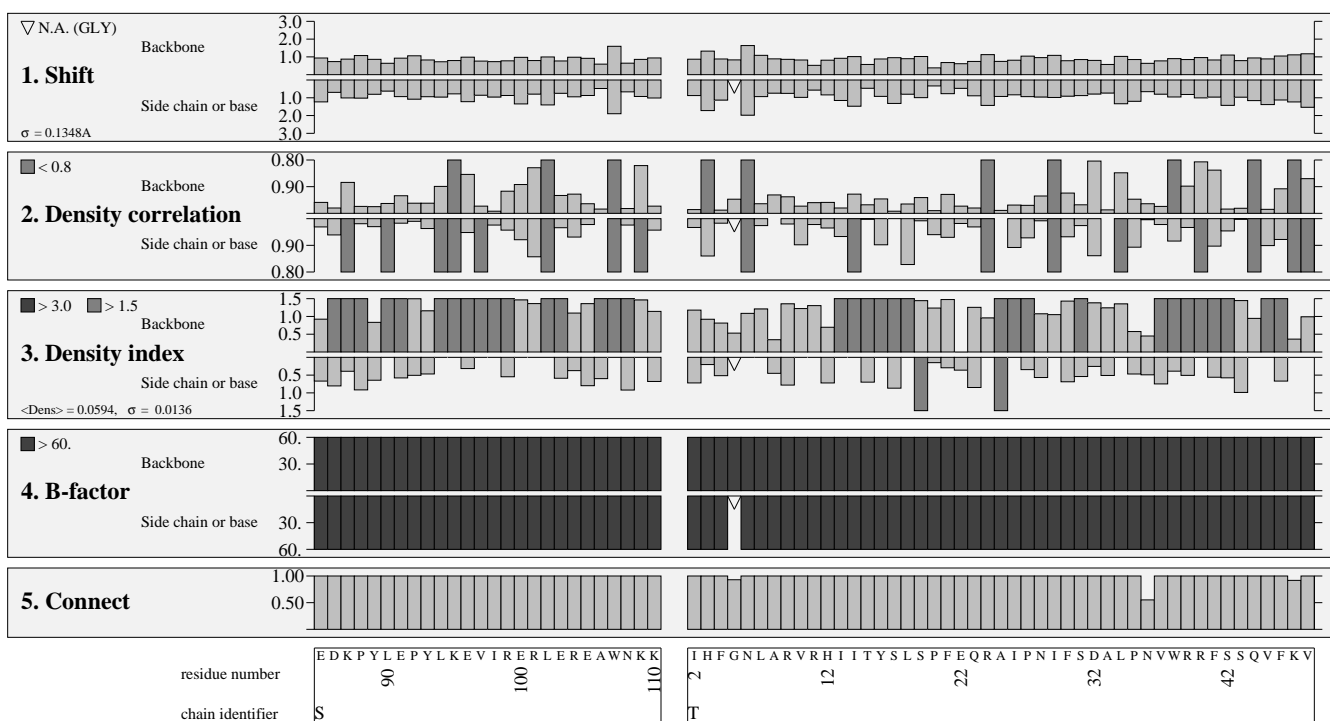
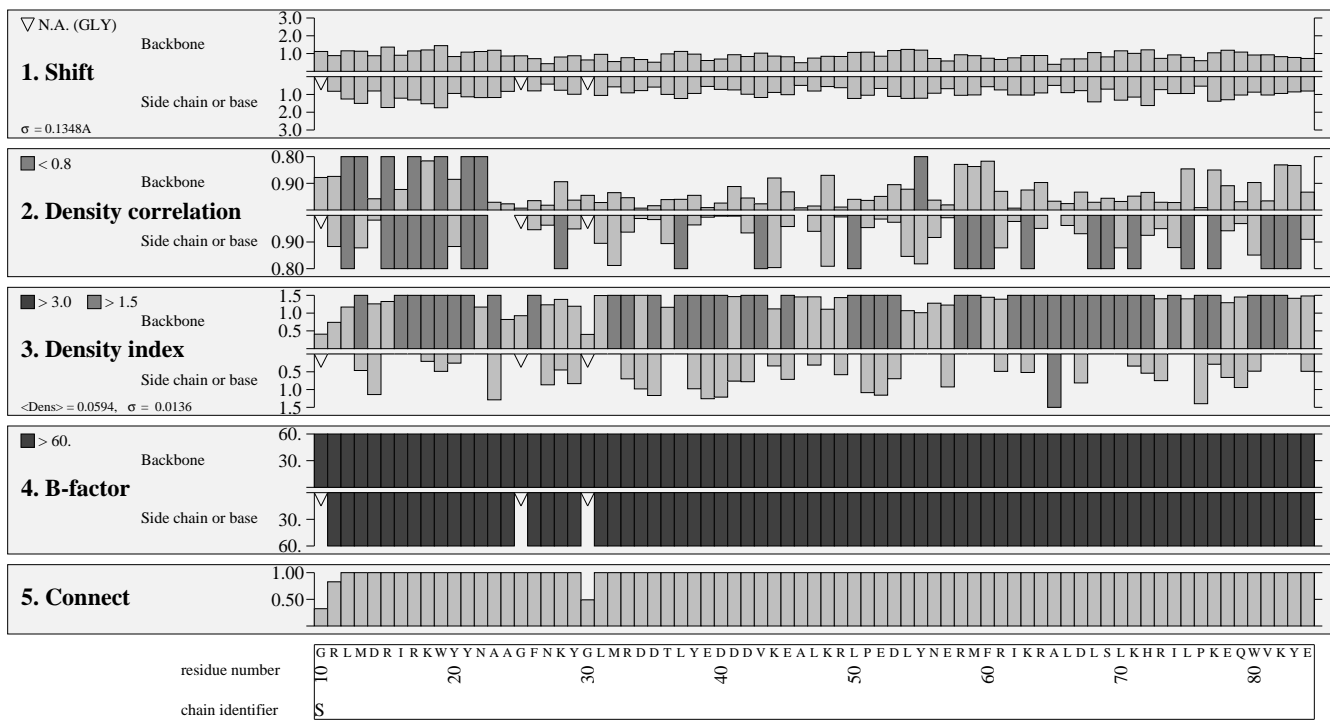
Local estimation (25)



Structure Factor Check

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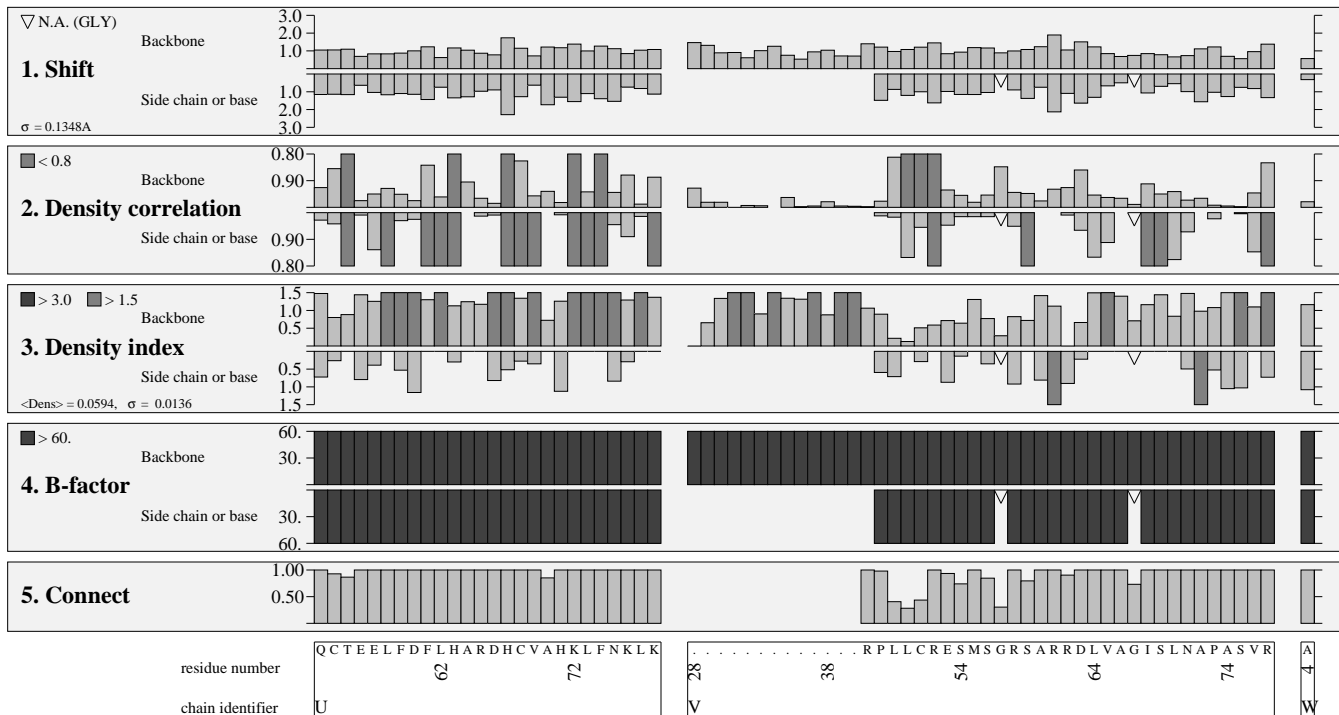
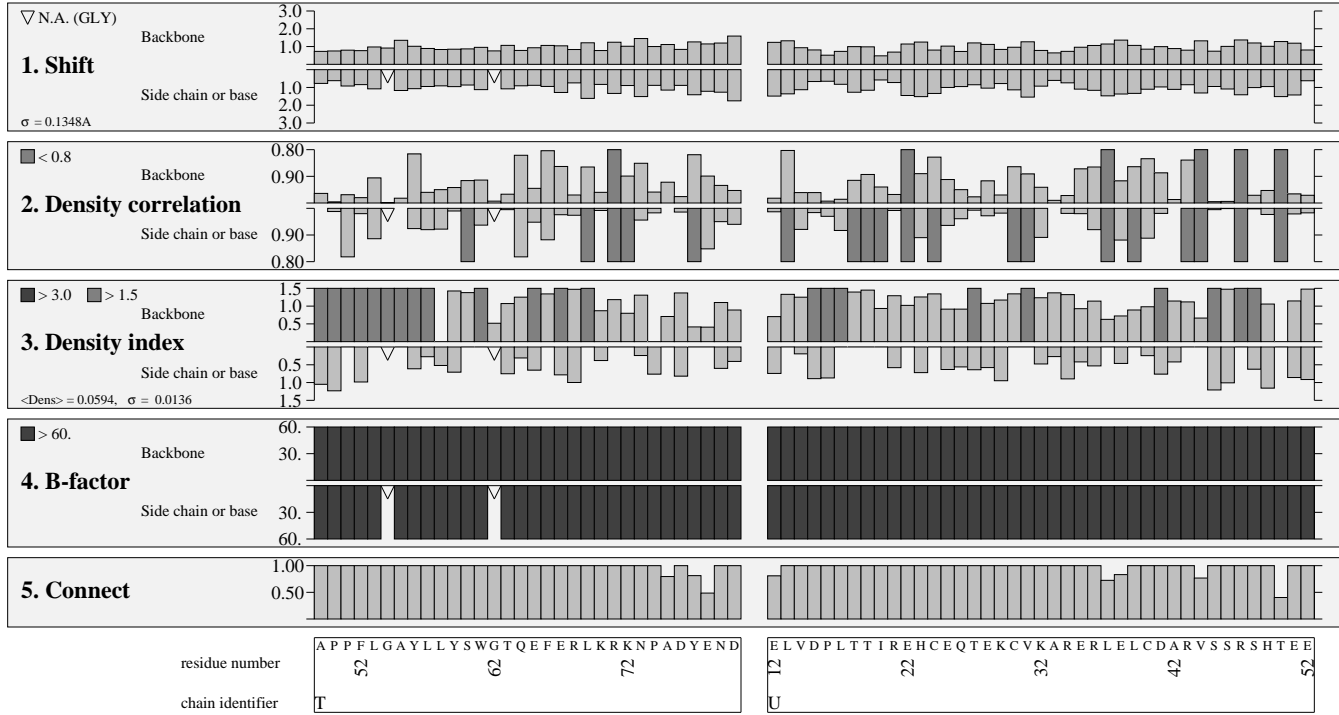
Local estimation (26)



Structure Factor Check

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Local estimation (27)



Structure Factor Check

3H1K

Local estimation (28)

