

Structure Factor Check

4YTM

Title: CRYSTAL STRUCTURE OF MITOCHONDRIAL RHODOQUINOL-FUMARATE REDU
 ASCARIS SUUM WITH N-BIPHENYL-3-YL-2-(O5TRIFLUOROMETHYL)O5BENZAM
 Date: 18-MAR-15
 PDB code: 4YTM

Crystal

Cell parameters:

a: 123.65 A b: 126.43 A c: 220.87 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: 20.0 – 3.40 A
 Reflections in file: 48088
 Unique reflections above 0: 45652
 above 1 σ : 45042
 above 3 σ : 35677
 Reflections > 0: 2436

SFCHECK

Nominal resolution range: 20.0 – 3.40 A
\05max. from input data, min. from author\05
 Used reflections: 45652
 Completeness: 94.9 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.095
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.8714 0.8620 1.0000
 B_{overall} (by Patterson): 54. A²
 Optical resolution: 2.39 A
 Expected opt. resol. for complete data set: 2.39 A
 Estimated minimal error: 0.140 A

Model

18300 atoms
 Number of chains: 23
 Volume not occupied by model: 54.5 %
 $\langle B \rangle$ (for atomic model): 76.8 A²
 $\sigma(B)$: 15.16 A²
 Matthews coefficient: 3.37
 Corresponding solvent % : 63.21

Model vs. Structure Factors

R-factor for all reflections: 0.254
 Correlation factor: 0.829
 R-factor: 0.263
 for $F > 2.0\sigma$
 nom. resolution range: 20.00 – 3.40A
 reflections used: 45039

Rfree: 0.314
 Nfree: 2302
 R-factor without free-refl.: 0.260
 Non free-reflections: 42737
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.546 A
 Estimated maximal error: 0.288 A
 DPI: 0.536 A

Scaling

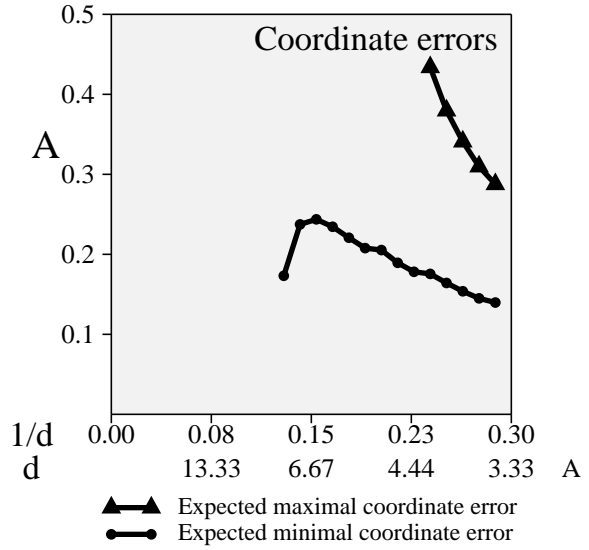
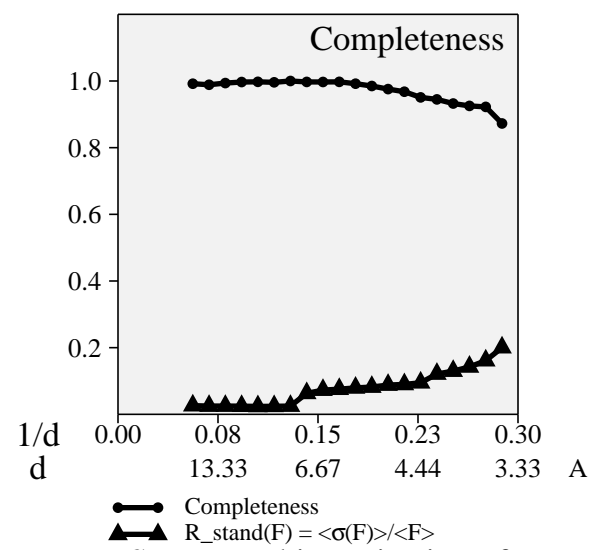
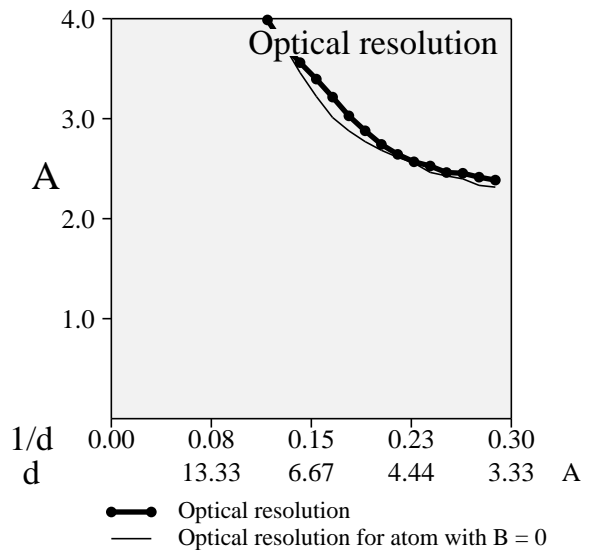
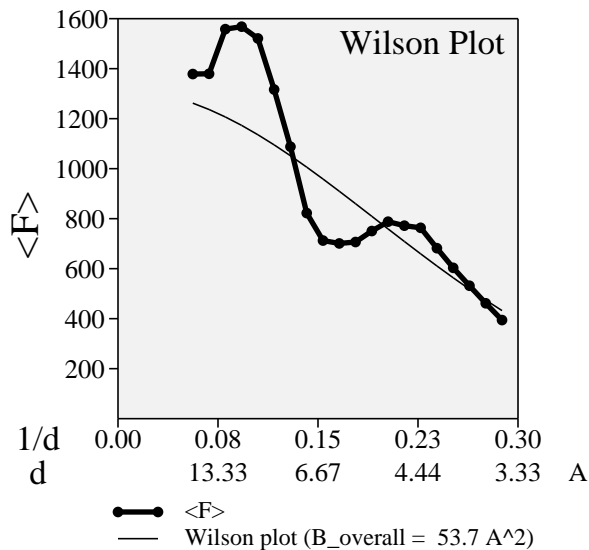
Scale: 0.836
 Bdiff: -7.48
 Anisothermal Scaling (Beta):
 -3.7125 -3.6078 -3.0758 -0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.335 249.778

Refinement

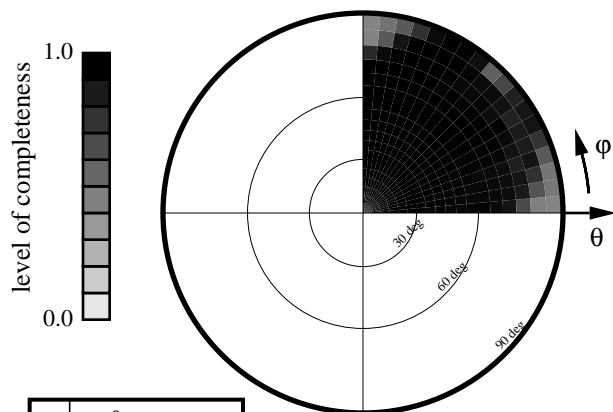
Program: REFMAC 5.7.0029
 Nominal resolution range: 20.0 – 3.40 A
 Reported R-factor: 0.178
 Number of reflections used: 43572
 Reported Rfree: 0.25
 Sigma cut-off: N.A.

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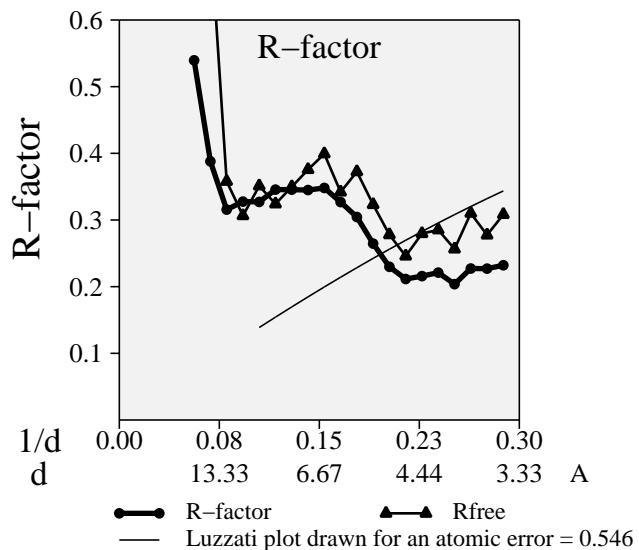


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

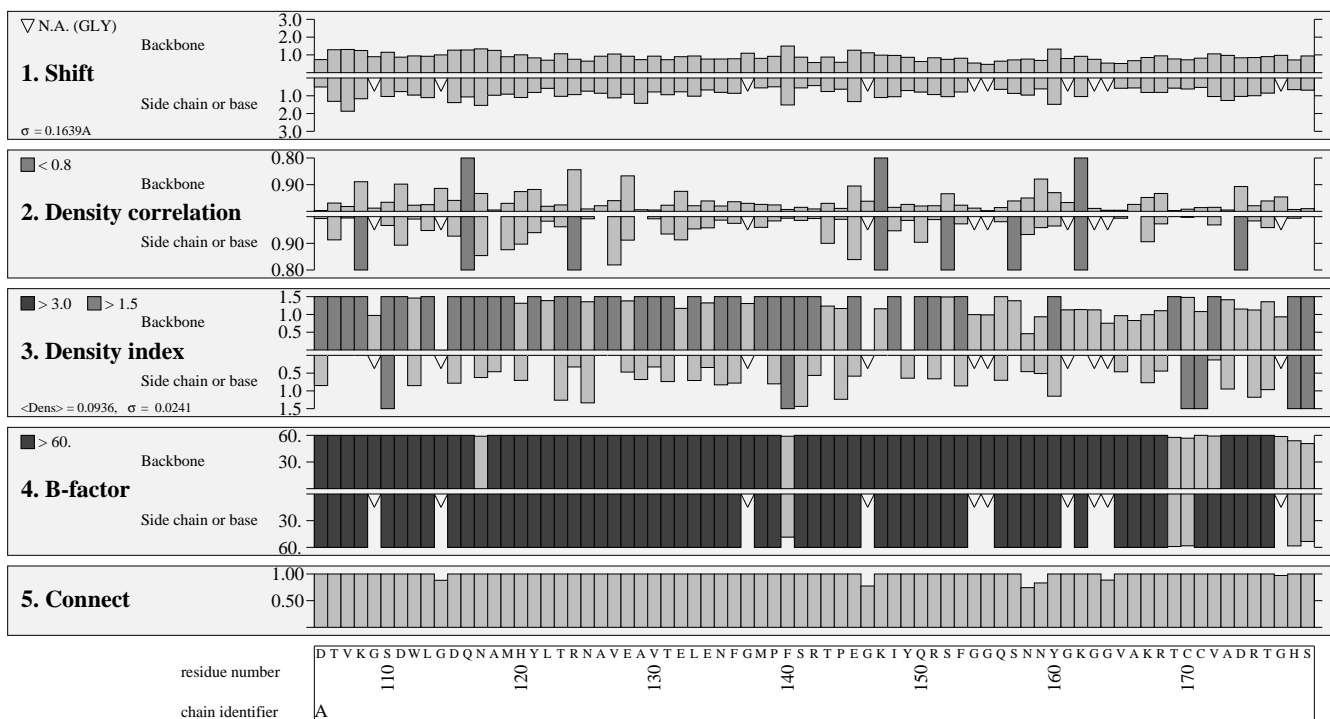
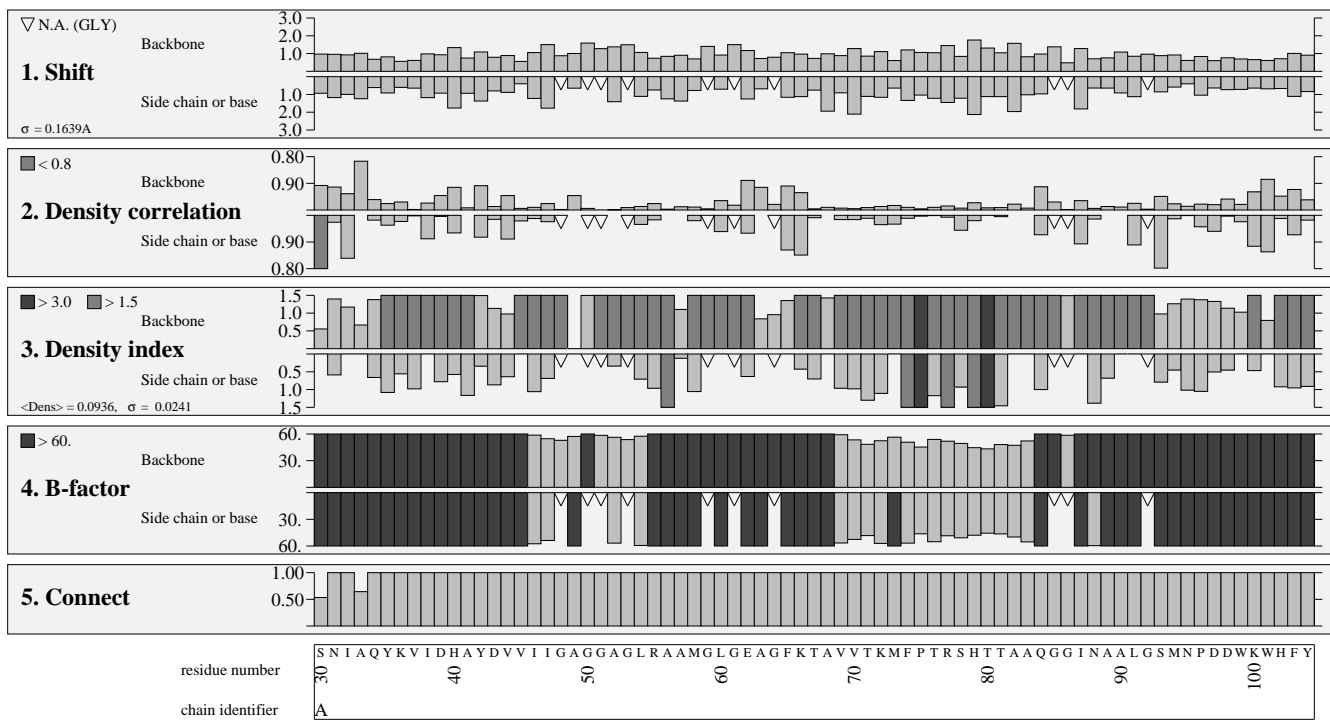
polar coordinates of the crystallographical axes



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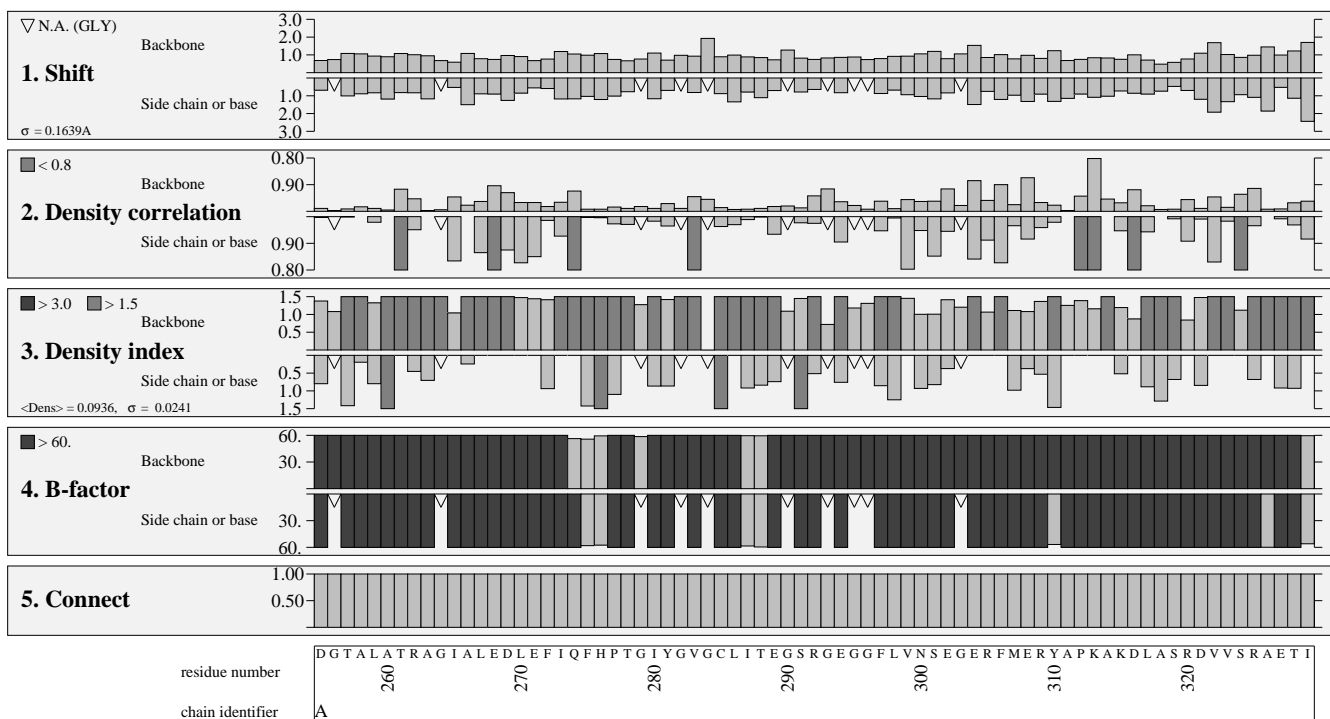
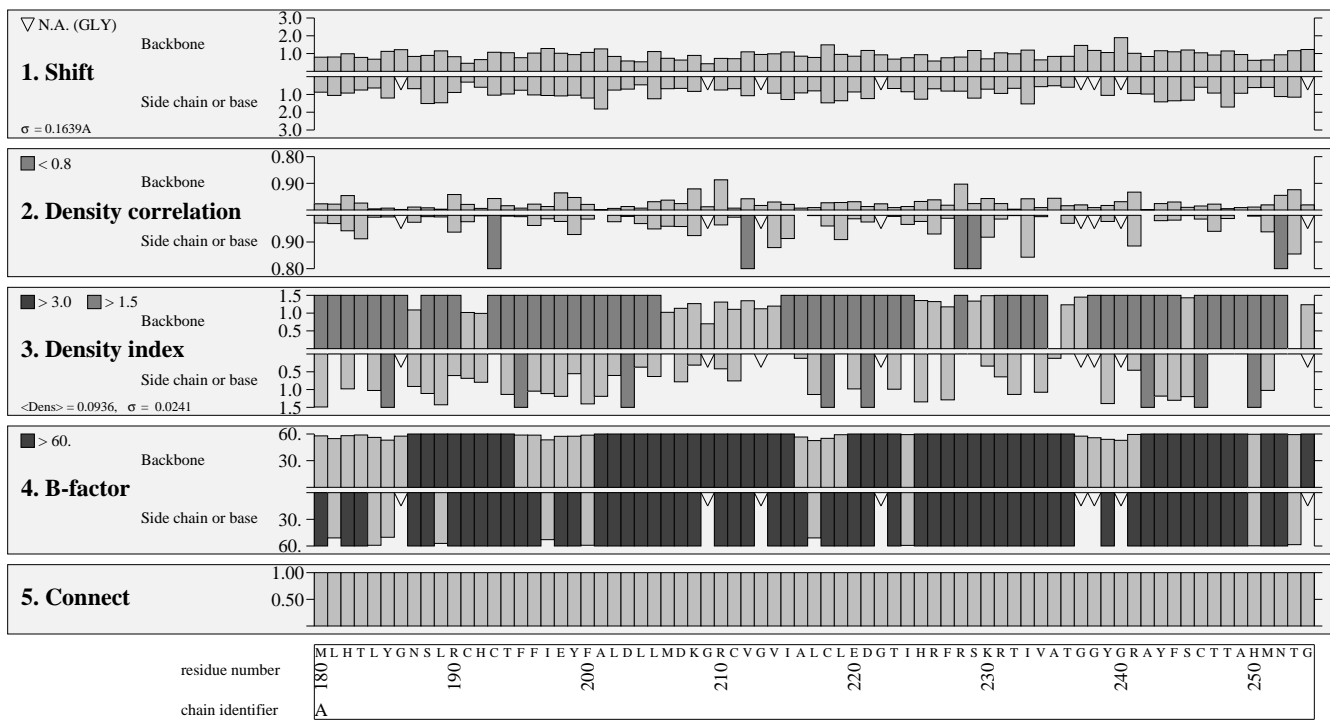
Local estimation



Structure Factor Check

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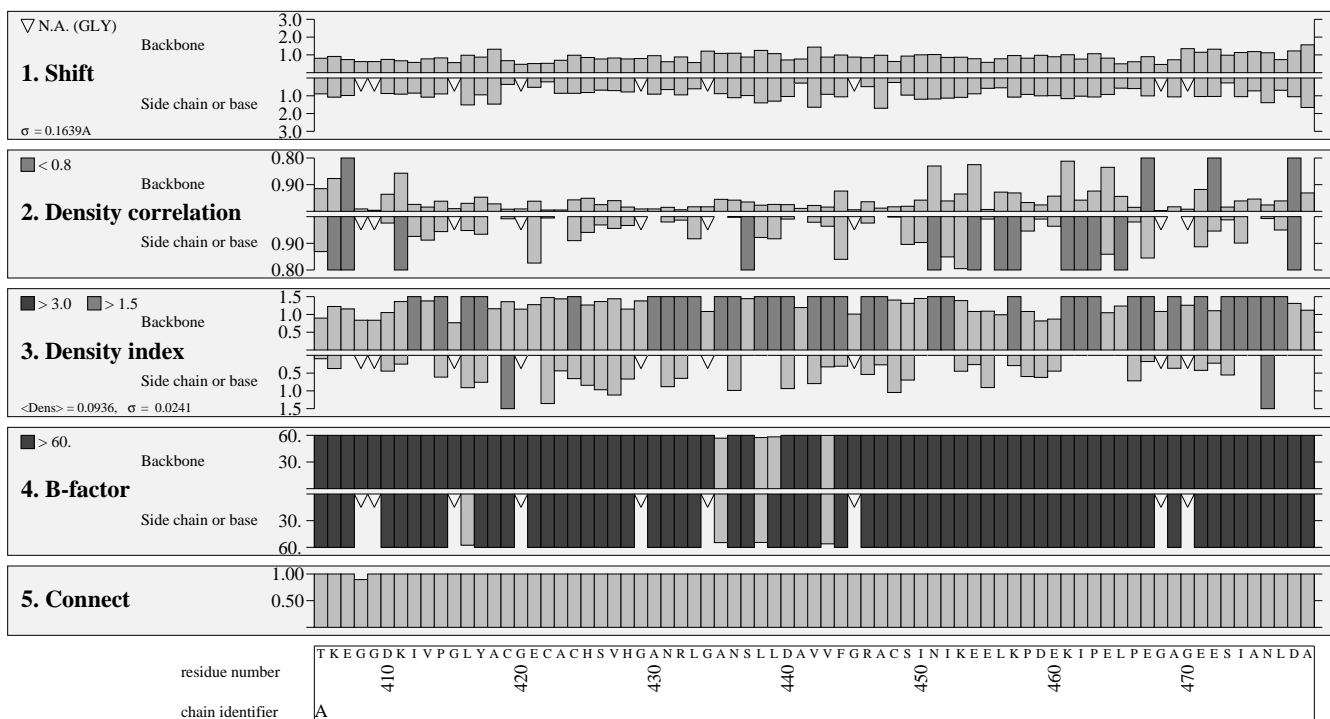
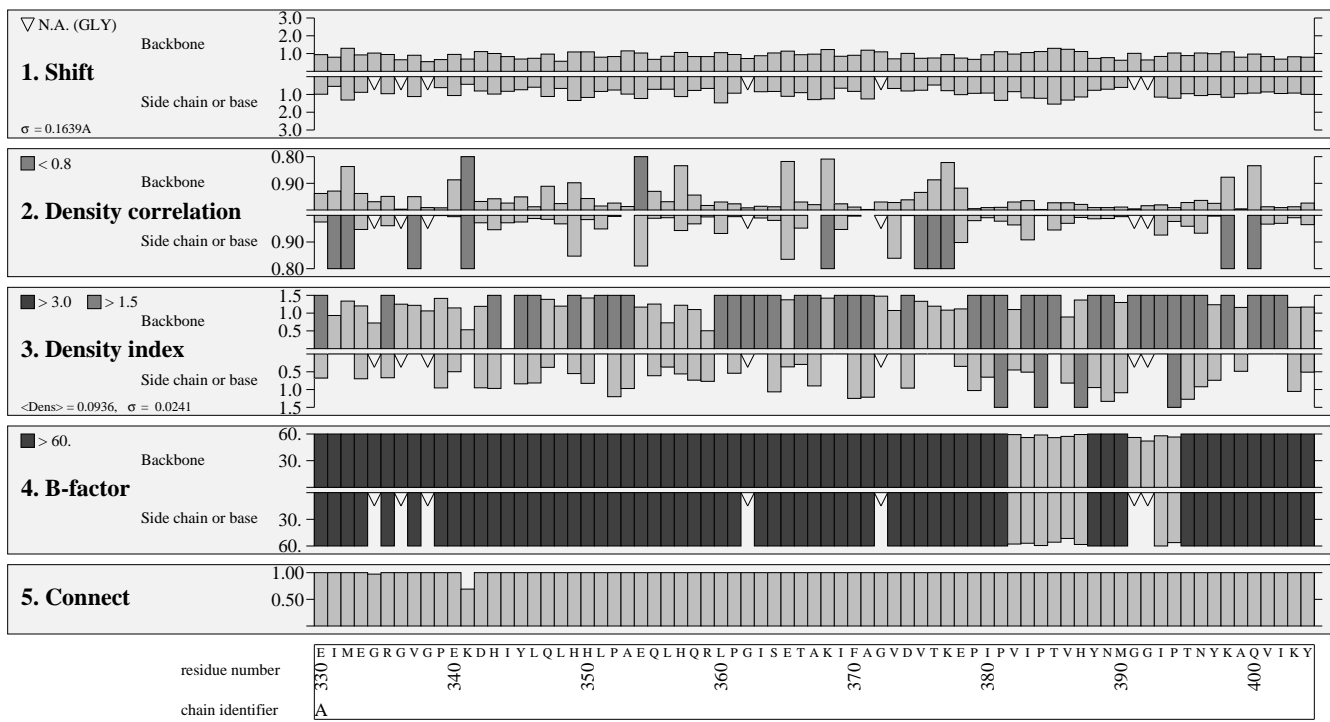
Local estimation (2)



Structure Factor Check

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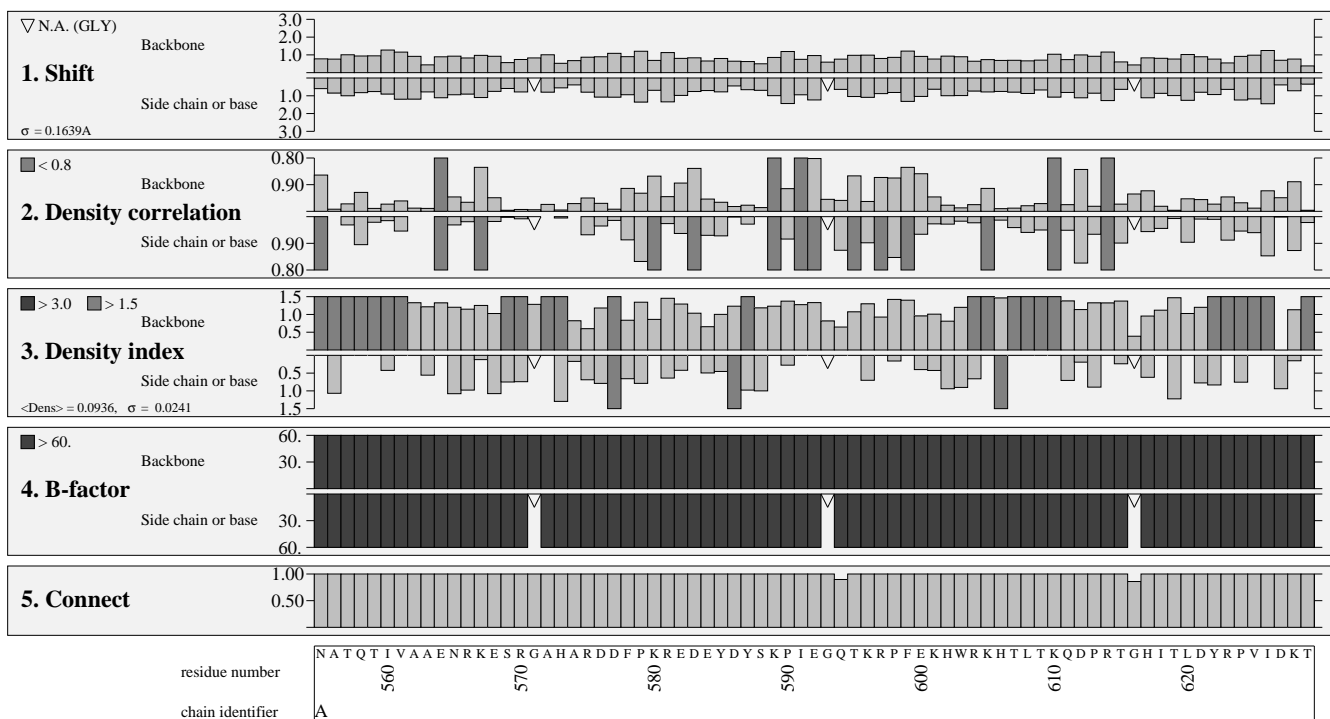
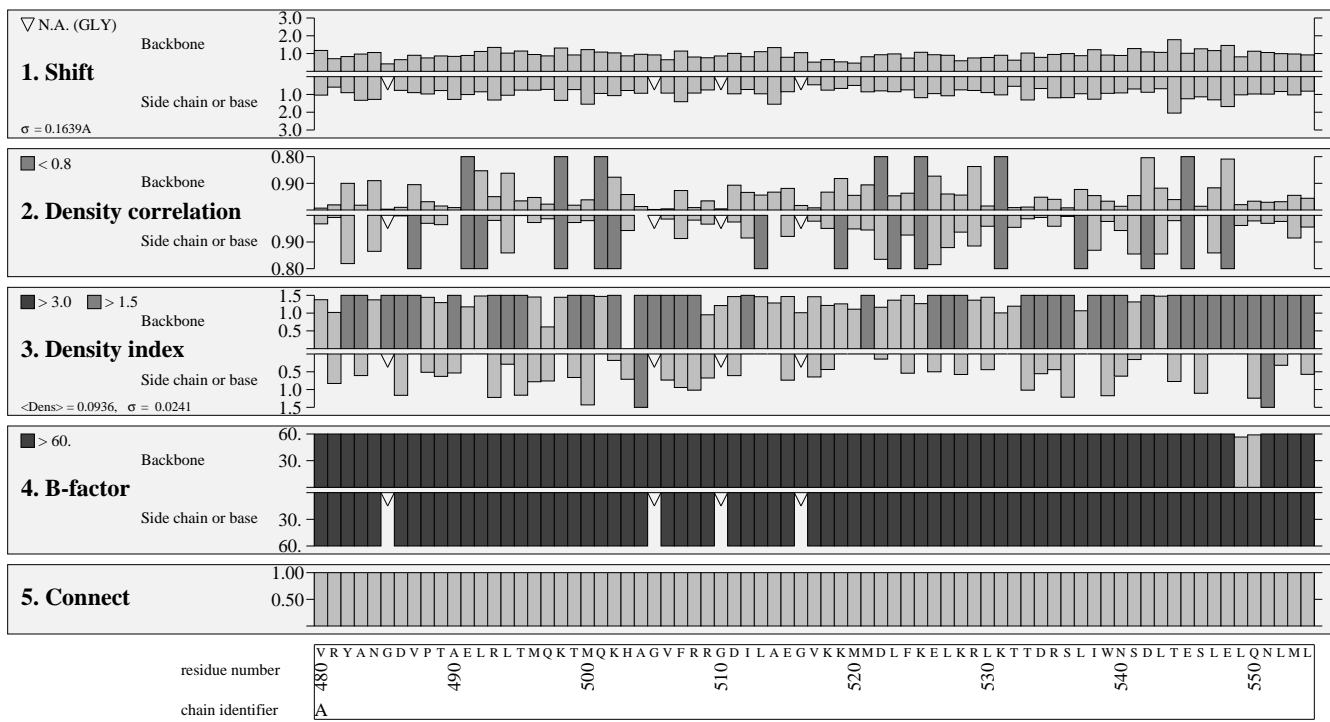
Local estimation (3)



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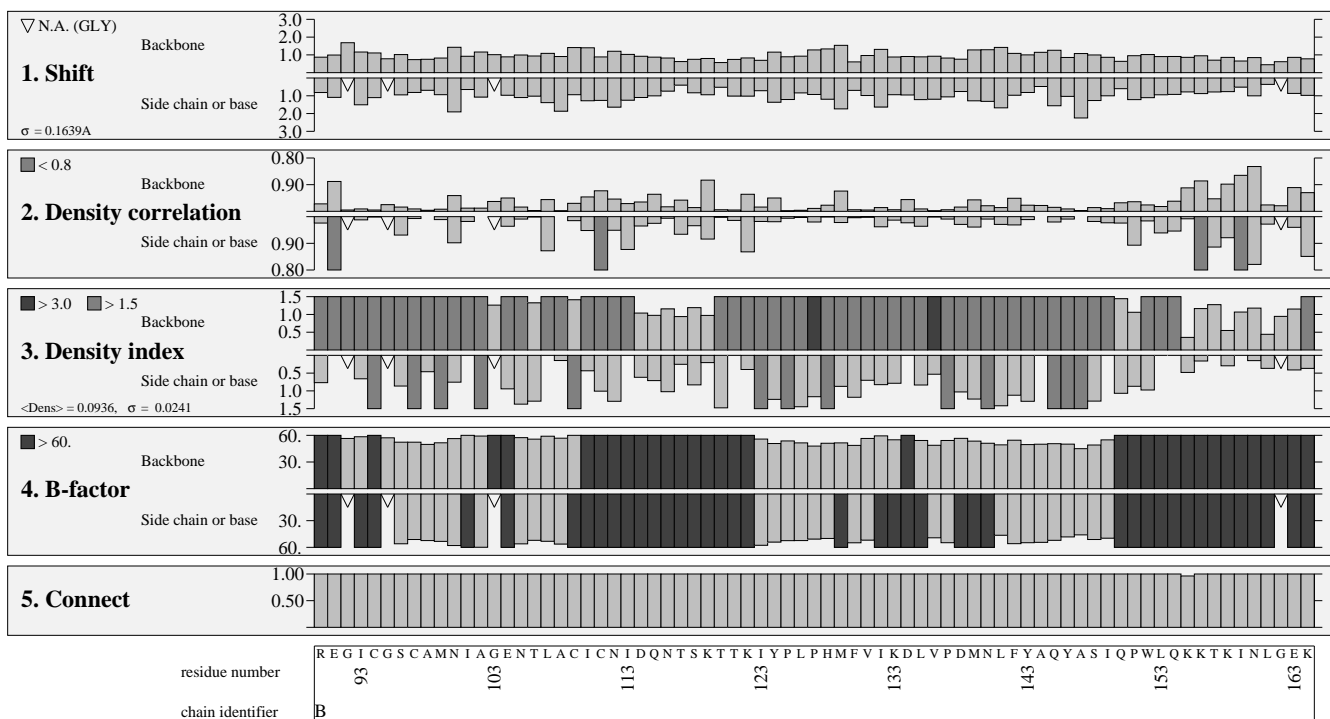
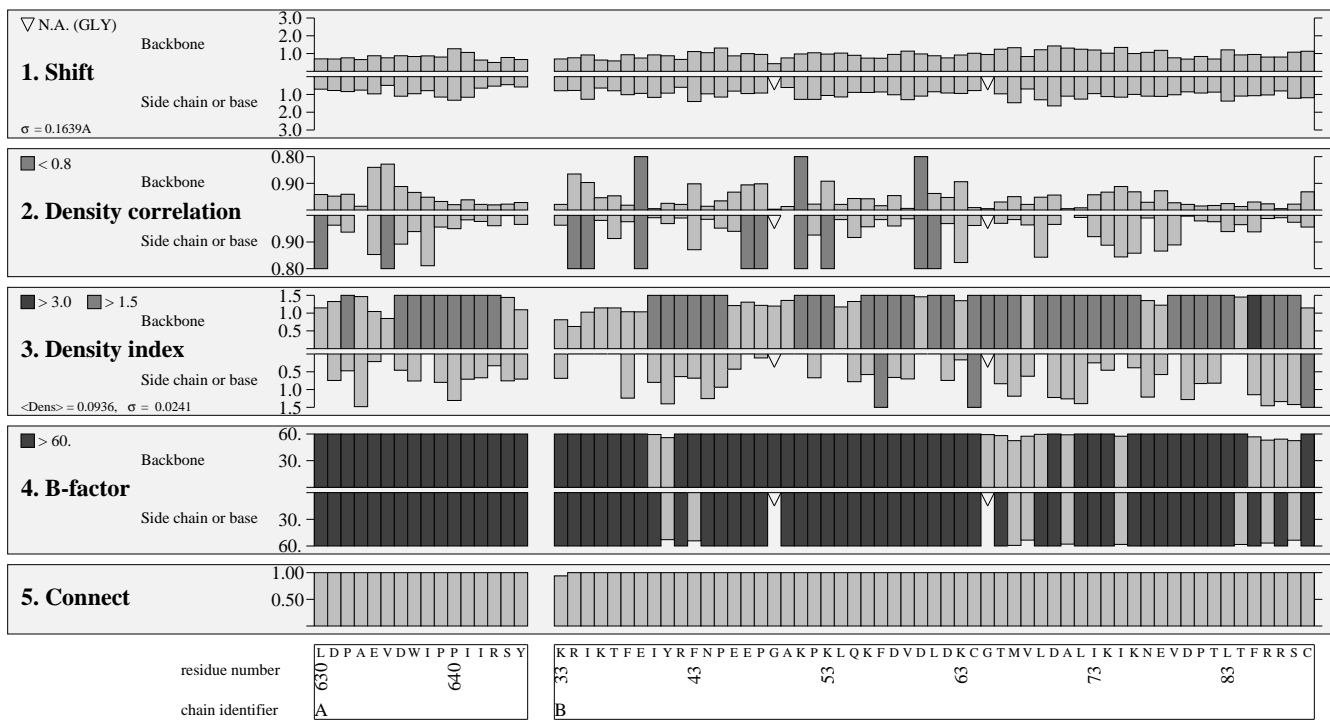
Local estimation (4)



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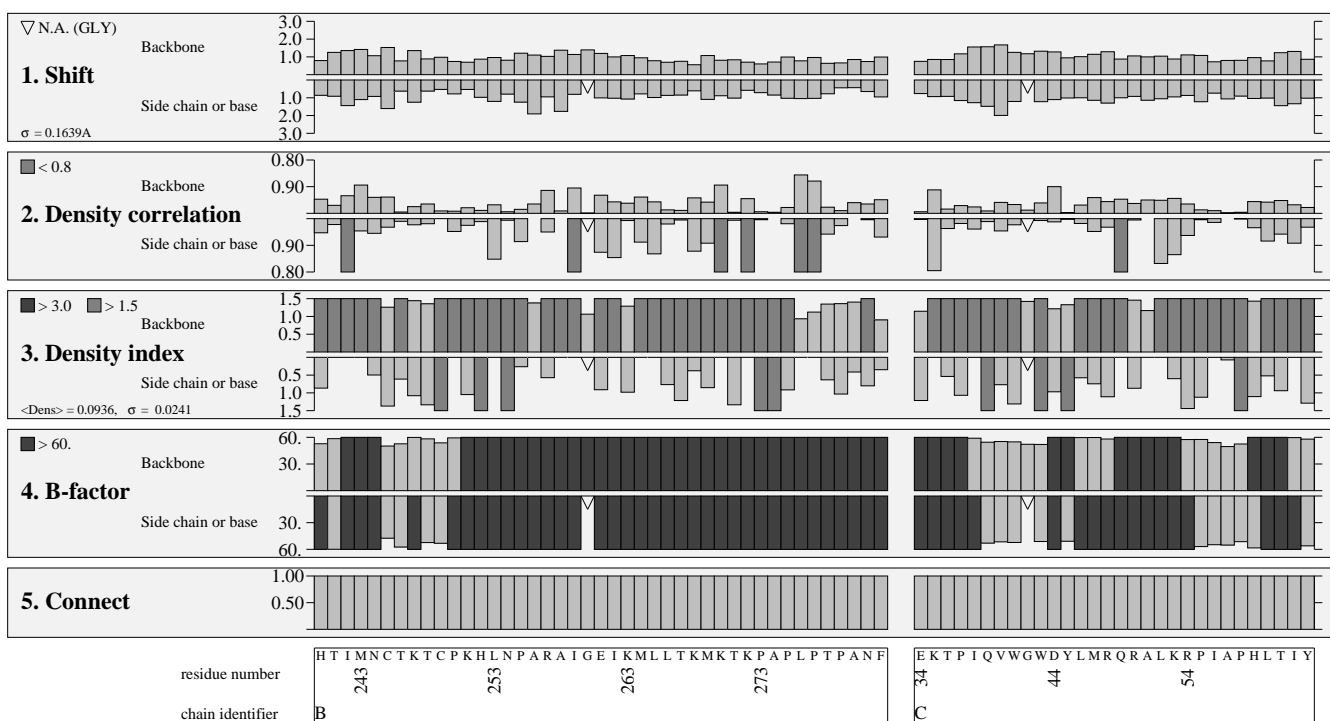
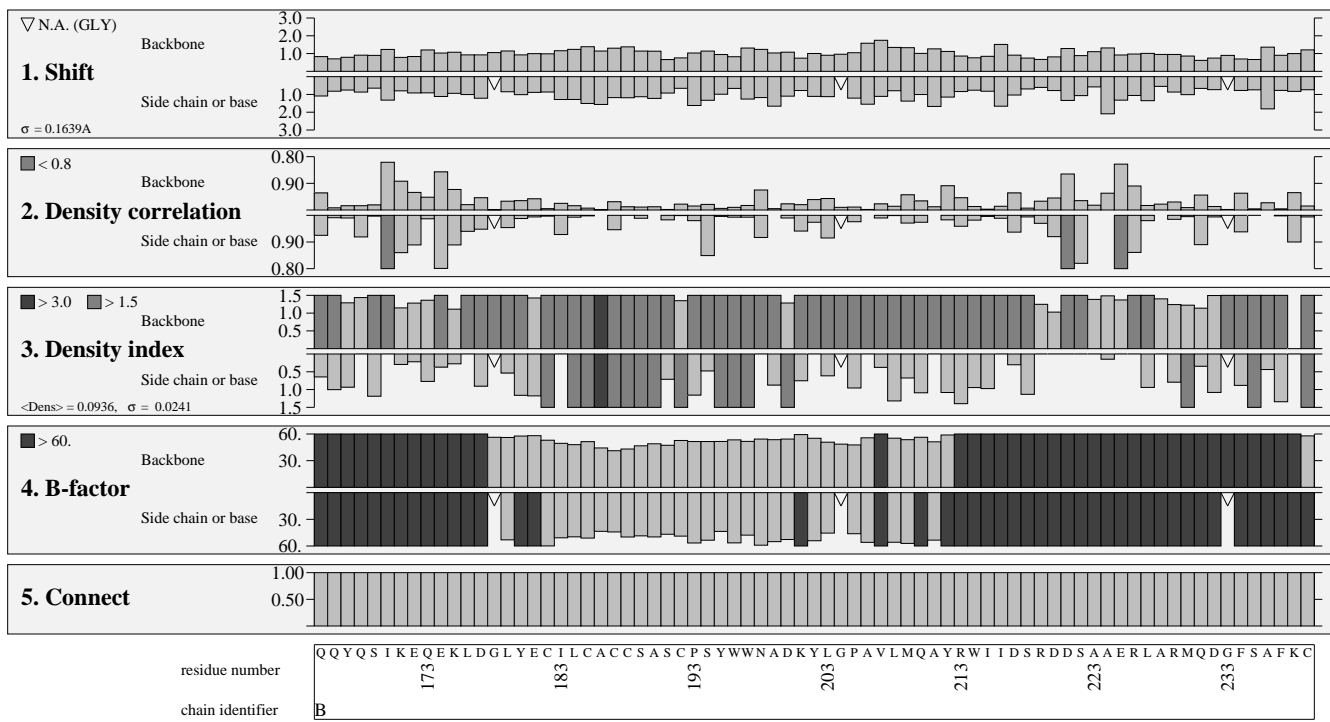
Local estimation (5)



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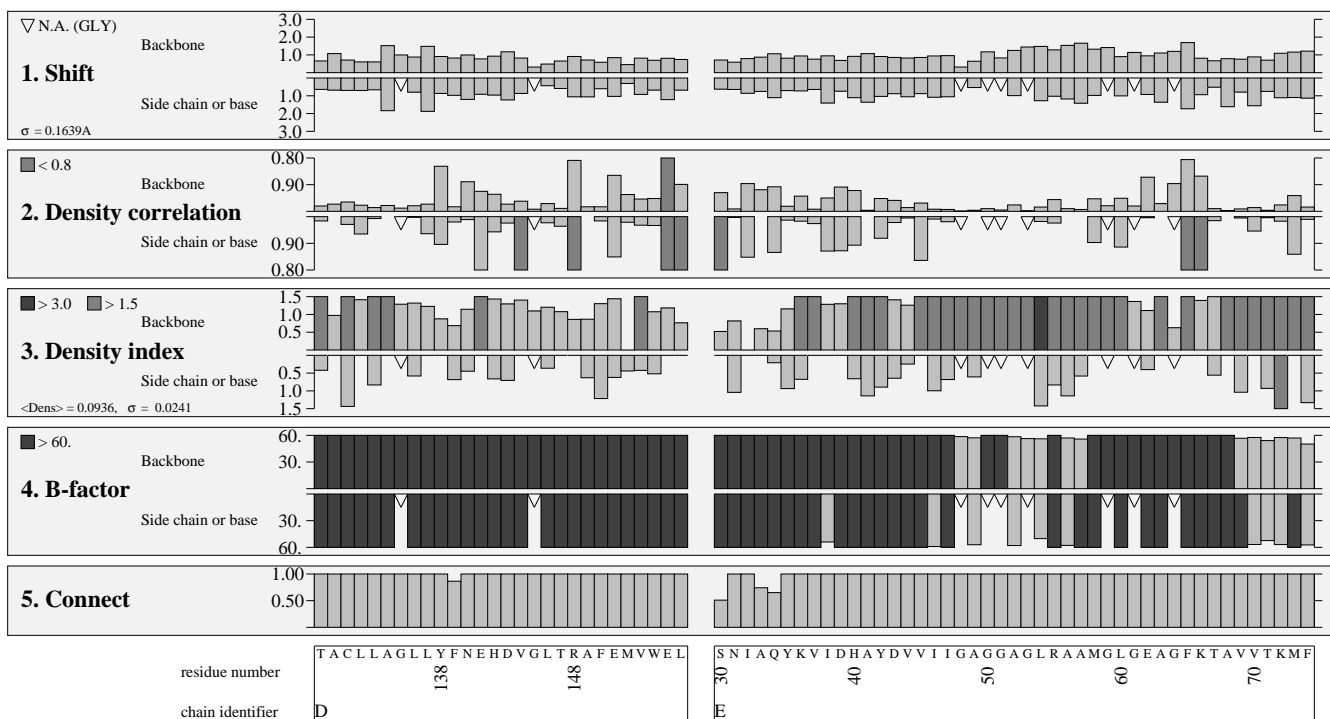
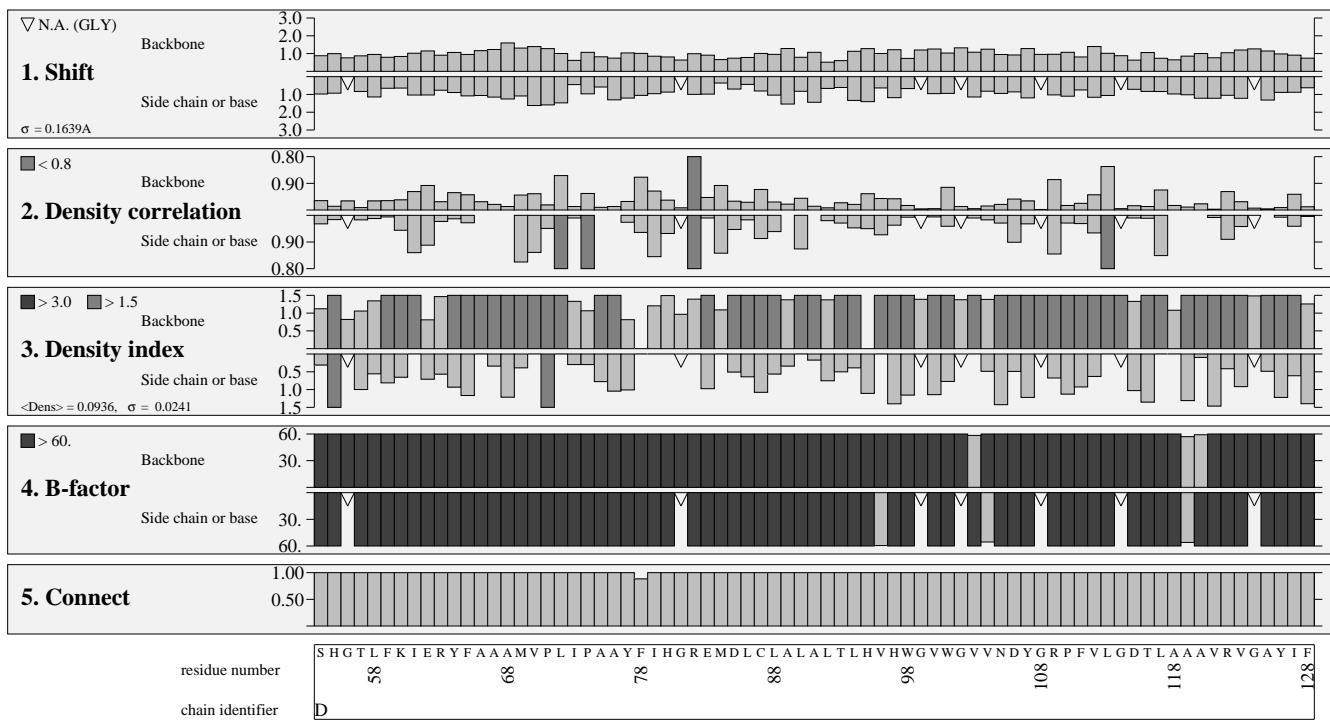
Local estimation (6)



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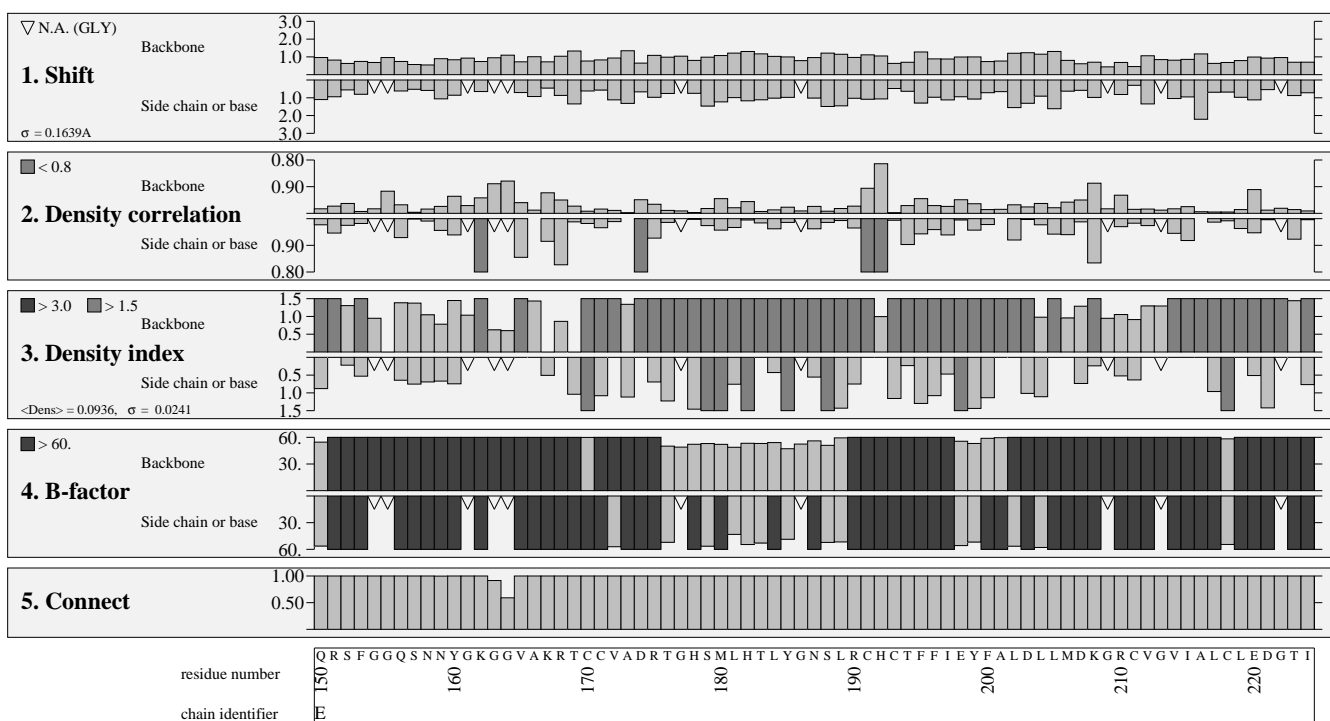
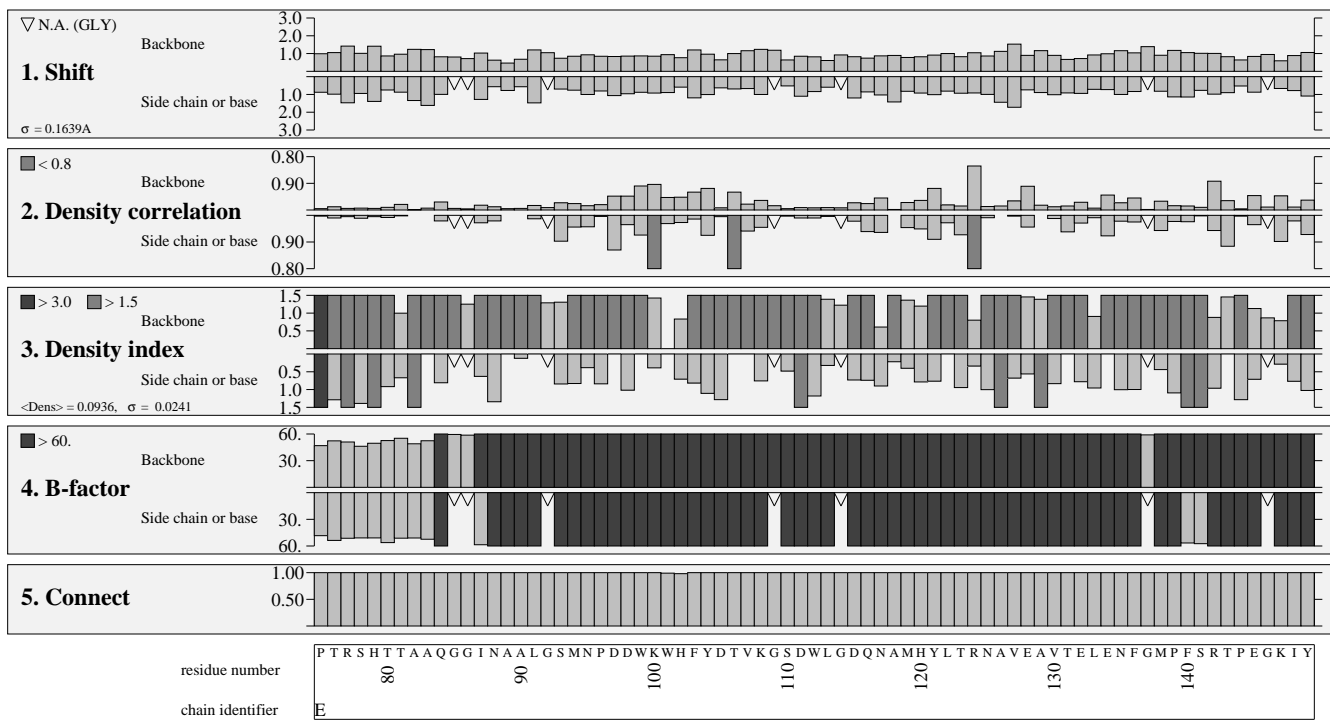
Local estimation (8)



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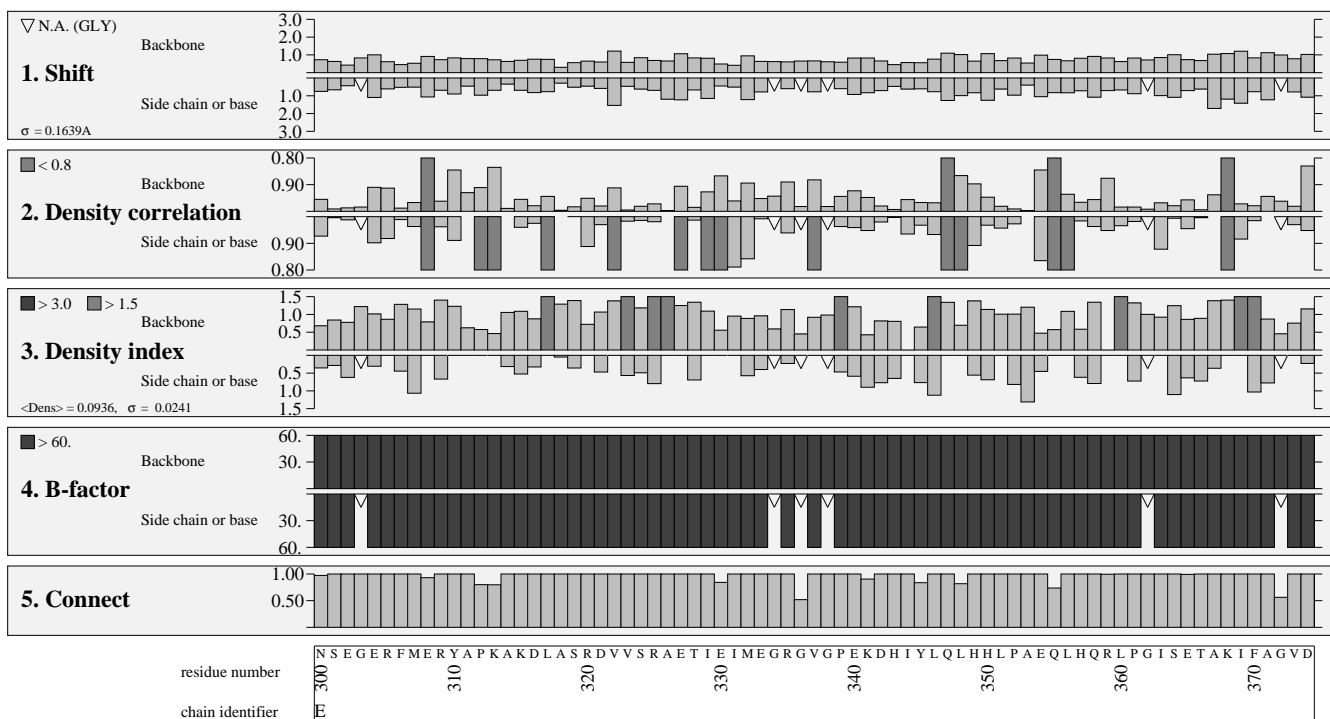
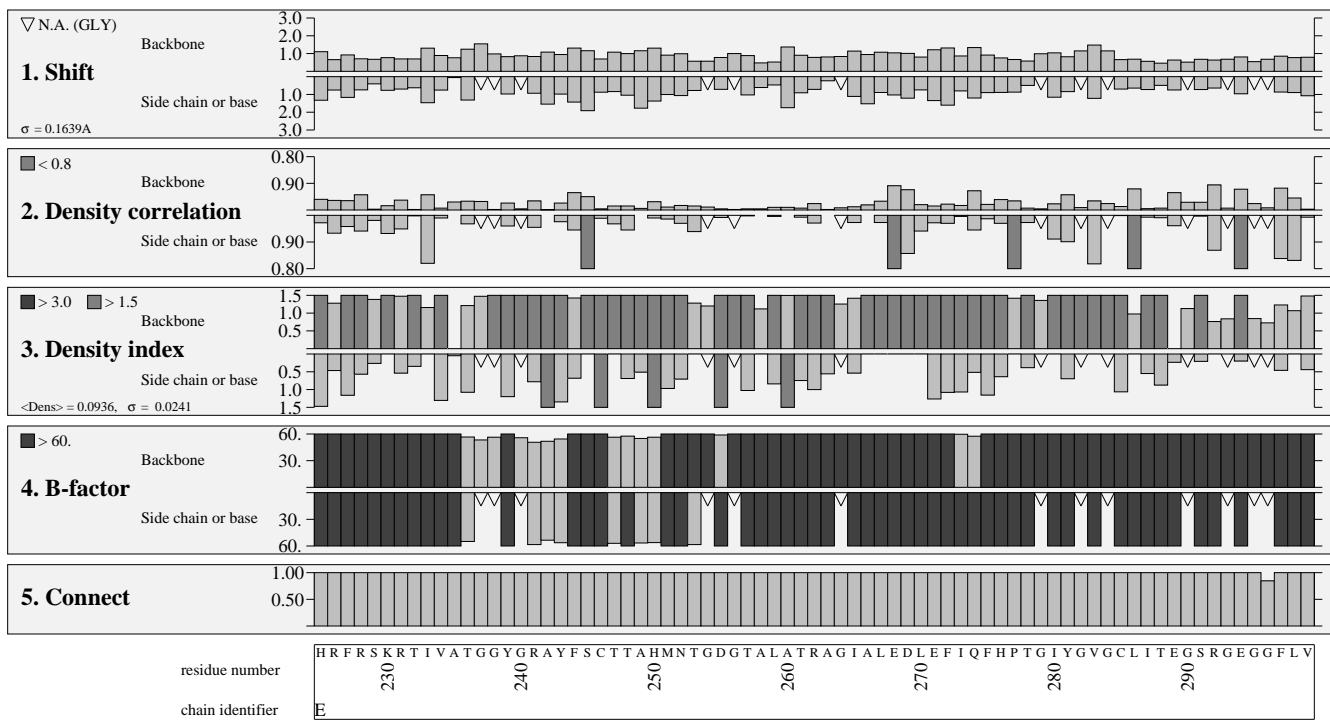
Local estimation (9)



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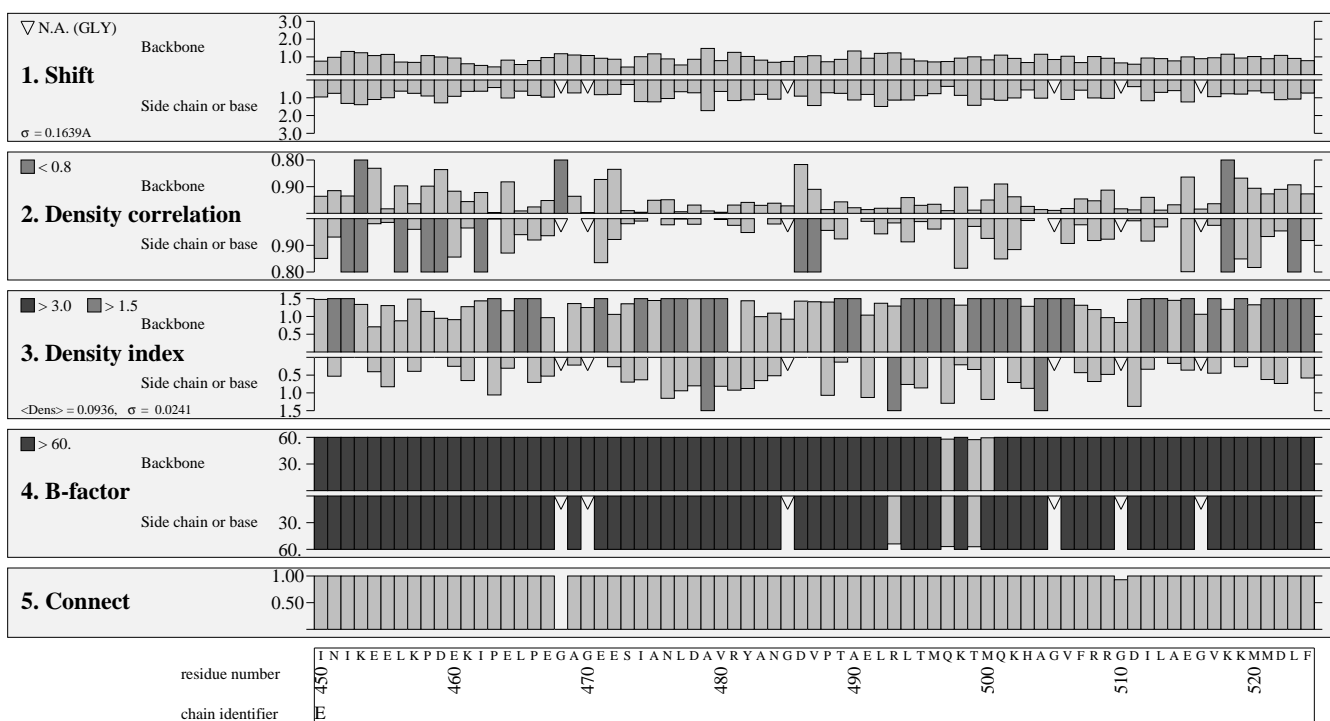
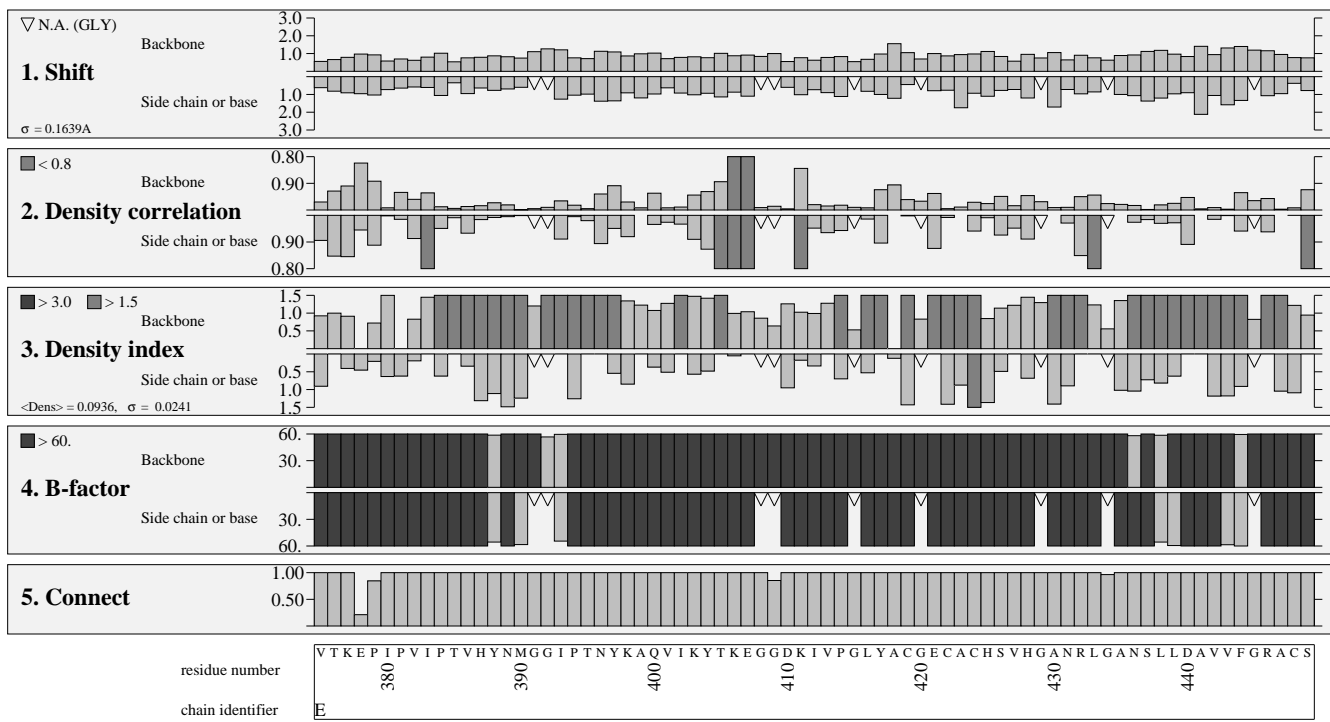
Local estimation (10)



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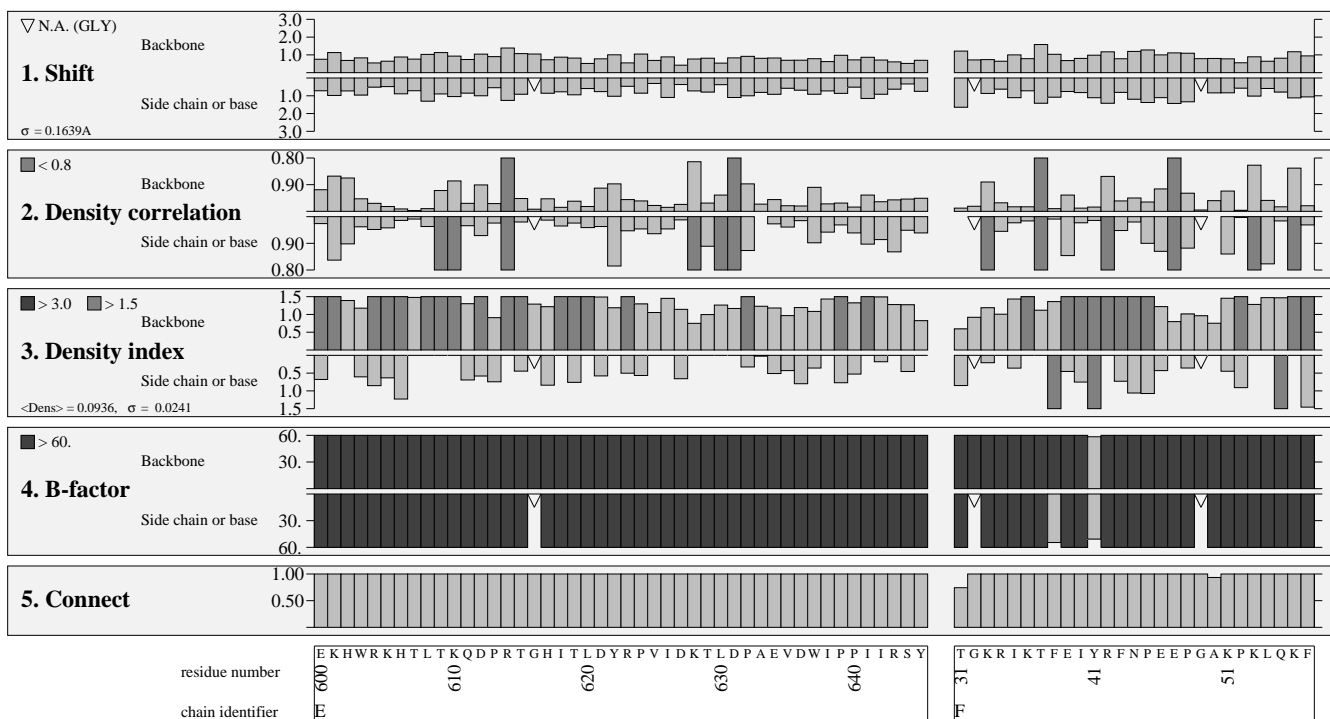
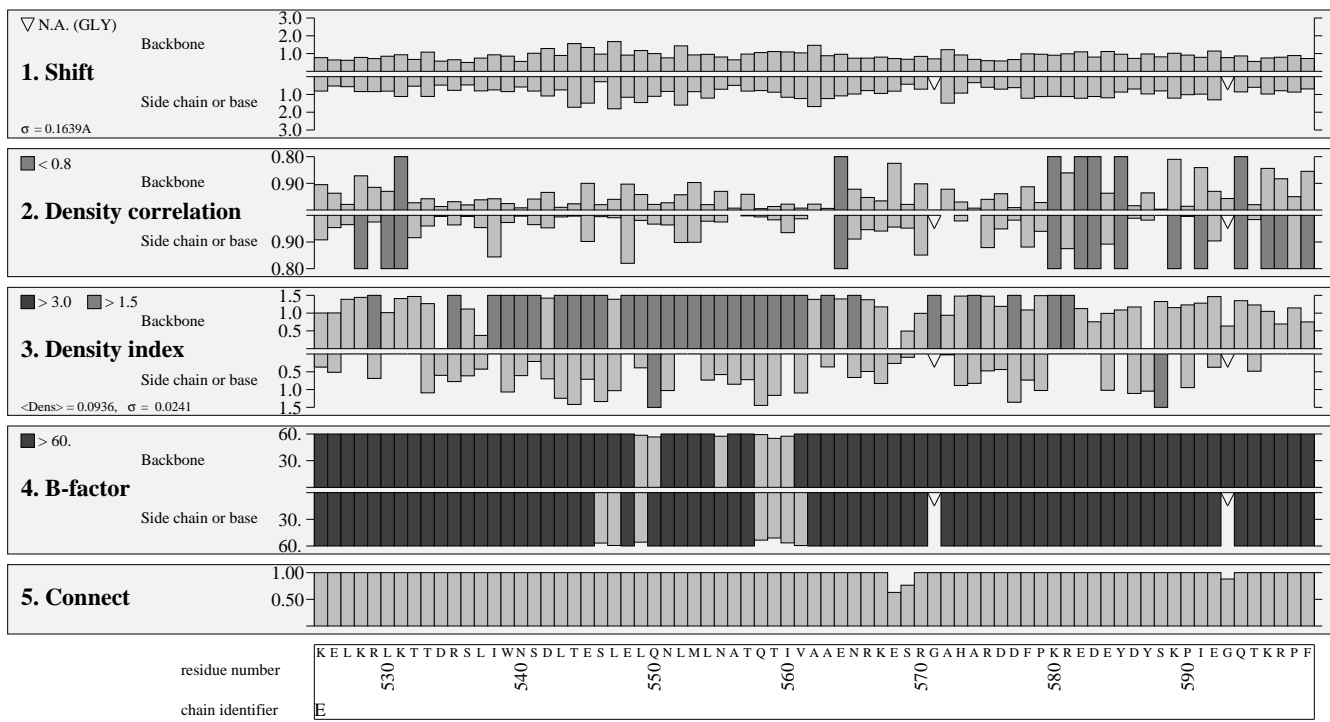
Local estimation (11)



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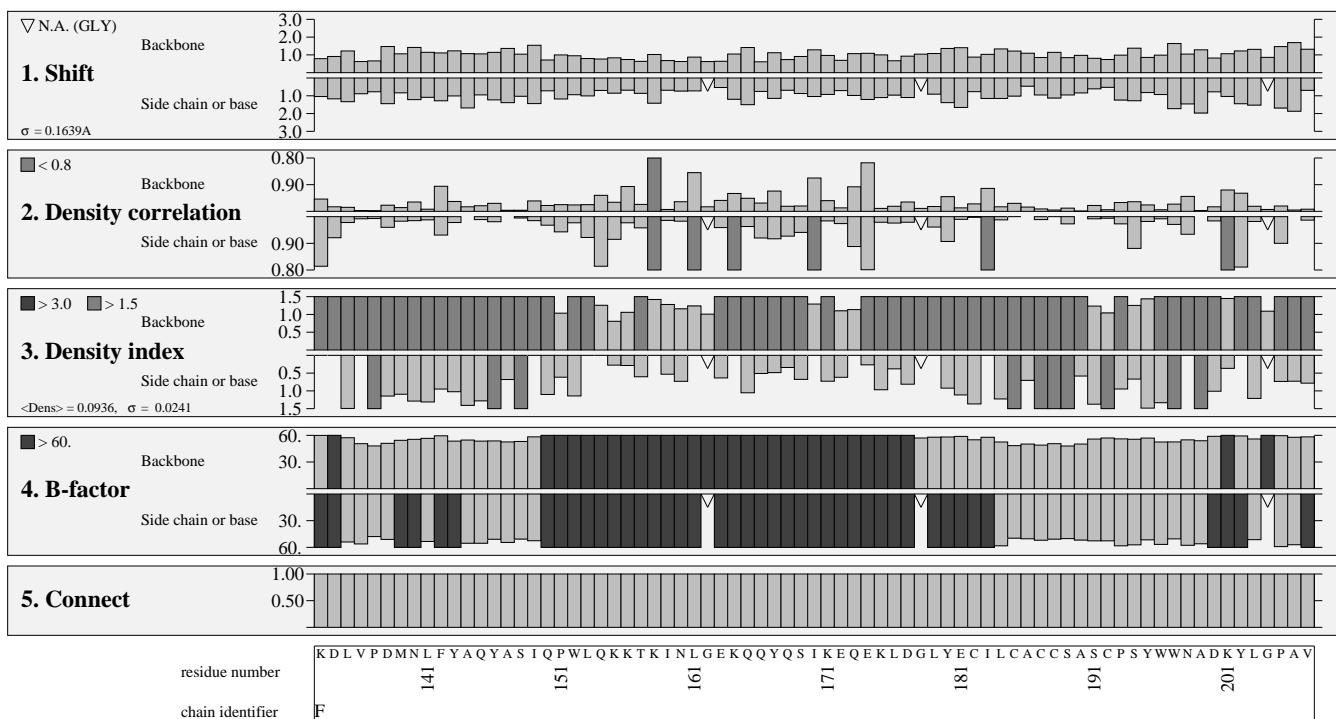
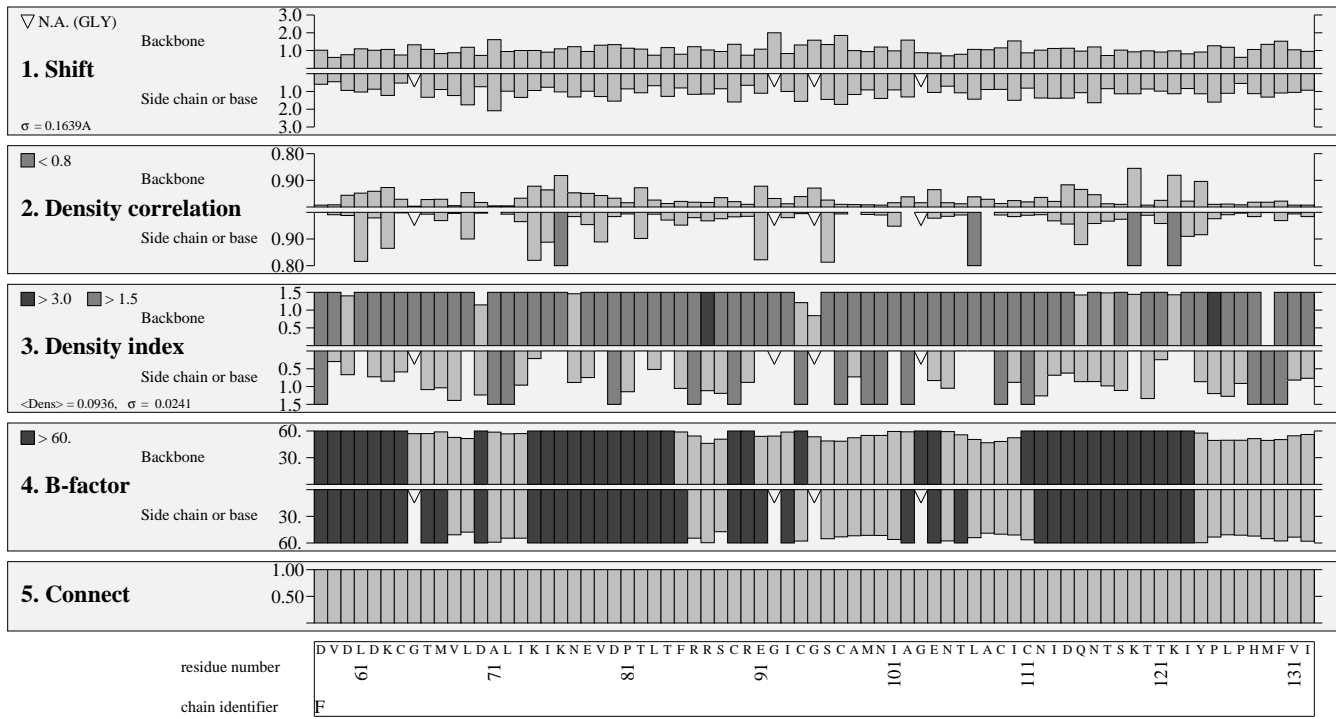
Local estimation (12)



Structure Factor Check

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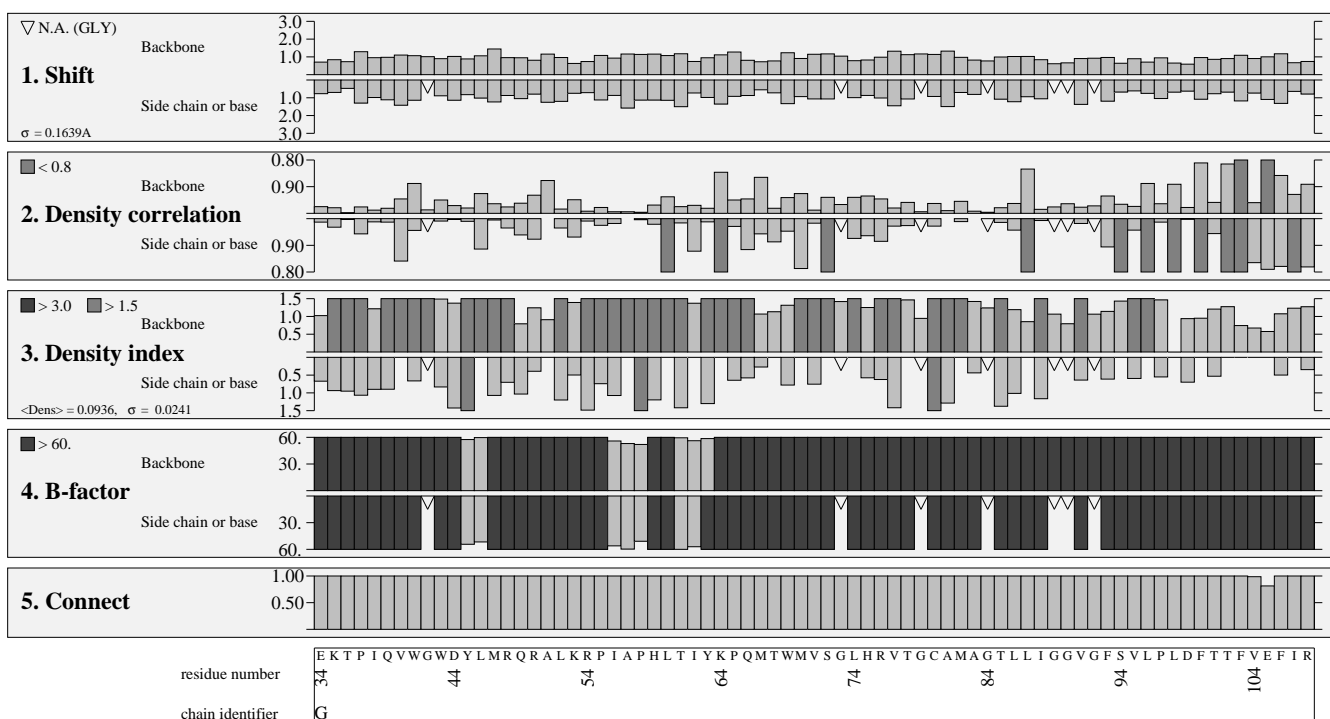
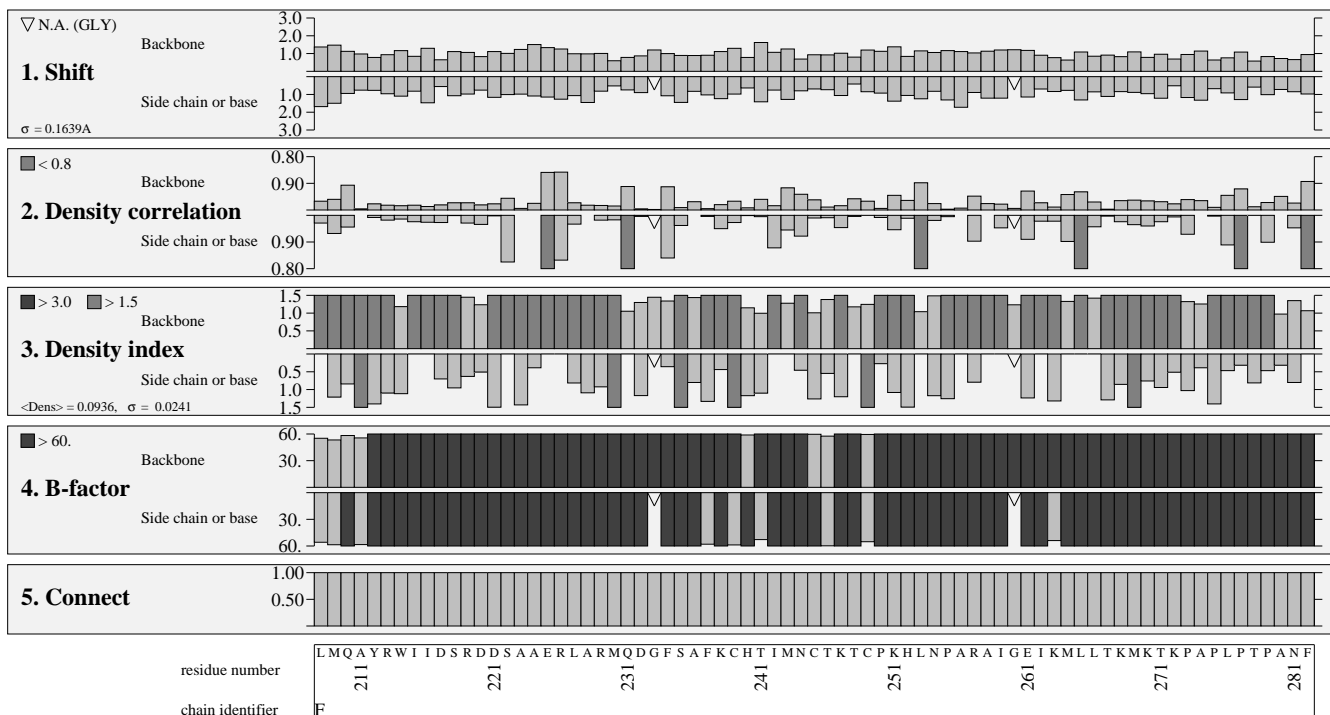
Local estimation (13)



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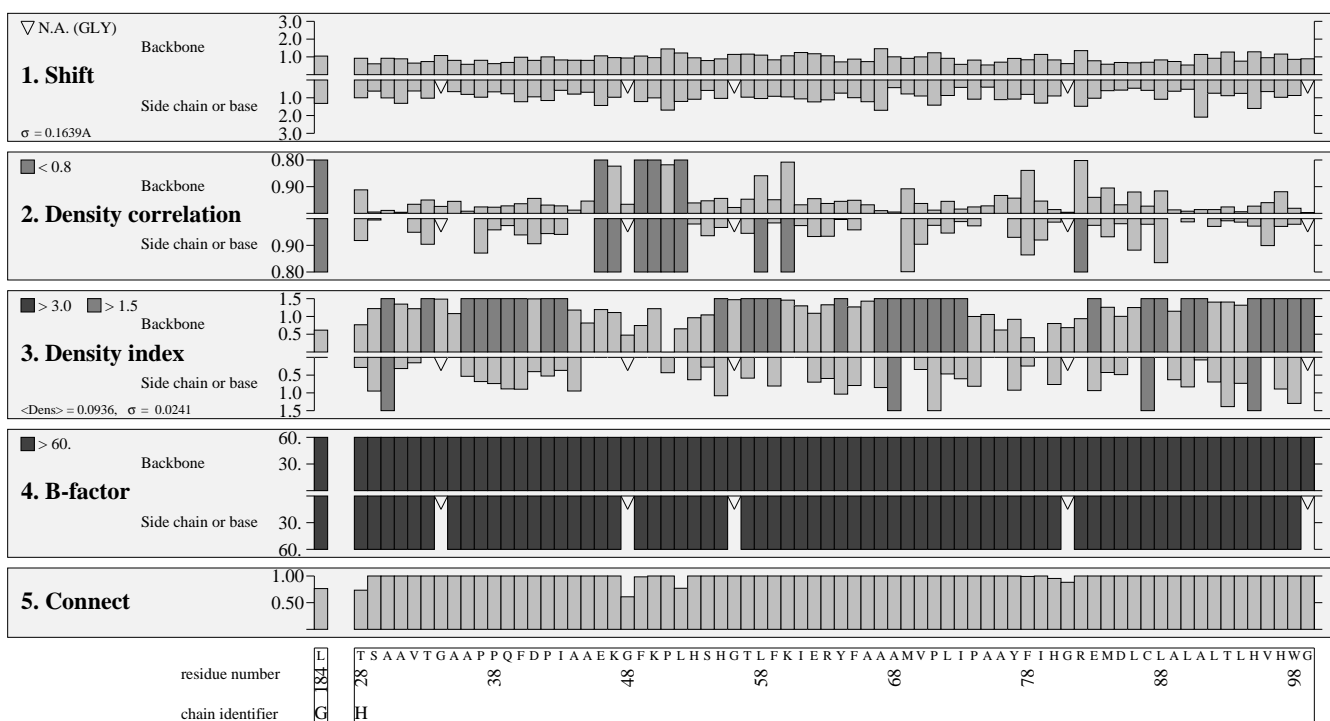
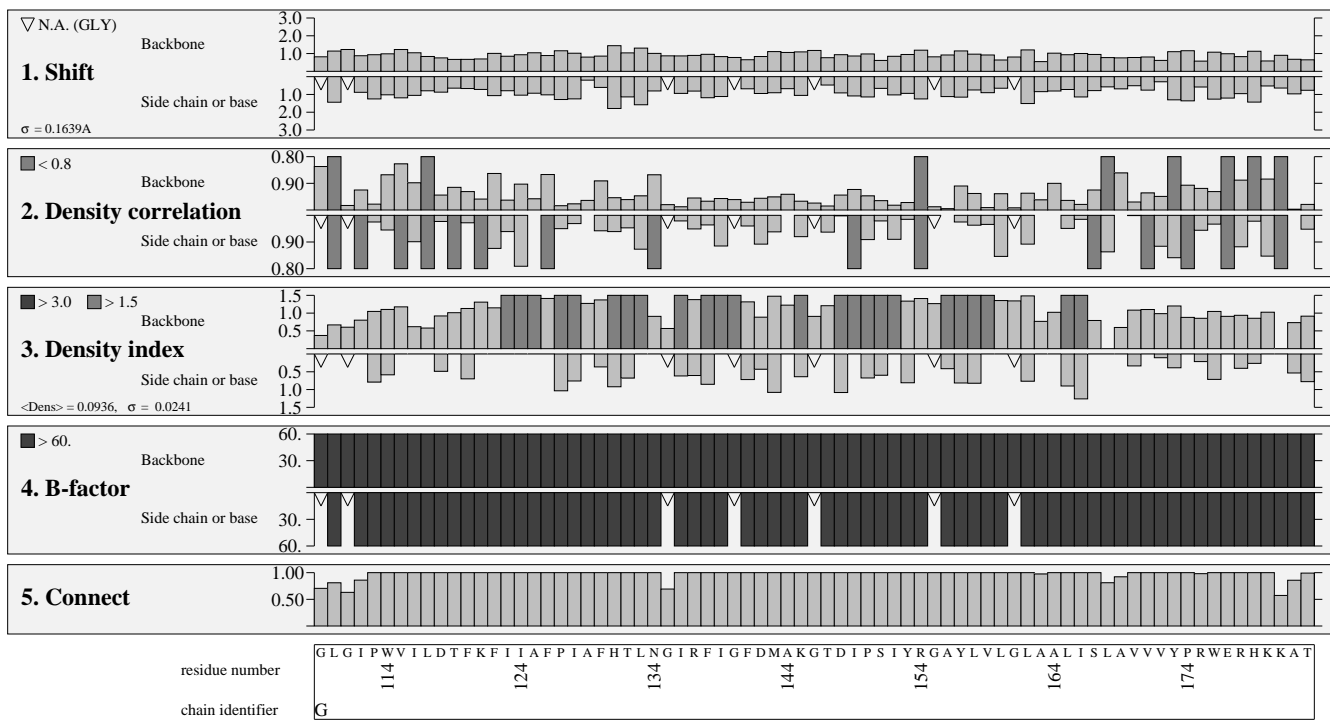
Local estimation (14)



Structure Factor Check

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Local estimation (15)



Structure Factor Check

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Local estimation (16)

