

Structure Factor Check

5C3J

Title: CRYSTAL STRUCTURE OF MITOCHONDRIAL RHODOQUINOL-FUMARATE REDU
 ASCARIS SUUM WITH UBIQUINONE-1
 Date: 17-JUN-15
 PDB code: 5C3J

Crystal

Cell parameters:
 a: 123.75 A b: 126.83 A c: 220.45 A
 α : 90.00 β : 90.00 γ : 90.00
 Space group: P 21 21 21

Model

18342 atoms
 Number of chains: 24
 Volume not occupied by model: 54.8 %
 $\langle B \rangle$ (for atomic model): 51.7 A²
 $\sigma(B)$: 16.46 A²
 Matthews coefficient: 3.37
 Corresponding solvent % : 63.20

Refinement

Program: REFMAC 5.7.0029
 Nominal resolution range: 20.0 - 2.80 A
 Reported R-factor: 0.202
 Number of reflections used: 72671
 Reported Rfree: 0.26
 Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 20.0 - 2.80 A
 Reflections in file: 85744
 Unique reflections above 0: 76331
 above 1 σ : 75108
 above 3 σ : 52541
 Reflections > 0: 9413

SFCHECK

Nominal resolution range: 20.0 - 2.80 A
 \05max. from input data, min. from author\05
 Used reflections: 76330
 Reflections out of resolution: 1
 Completeness: 89.0 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.071
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.9269 0.9929
 B_{overall} (by Patterson): 43.A²
 Optical resolution: 2.04 A
 Expected opt. resol. for complete data set: 2.04 A
 Estimated minimal error: 0.055 A

Model vs. Structure Factors

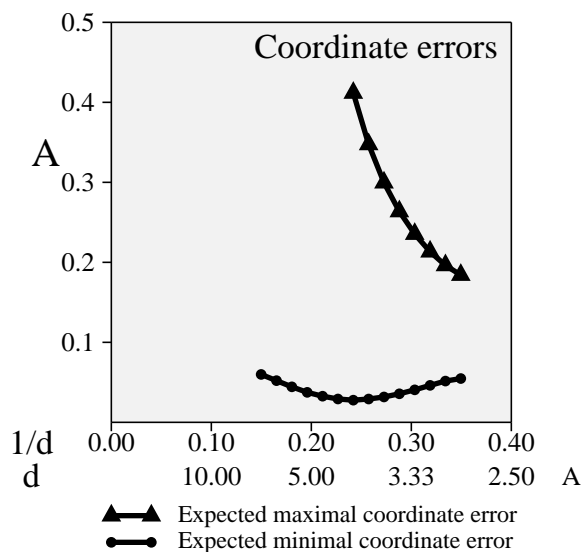
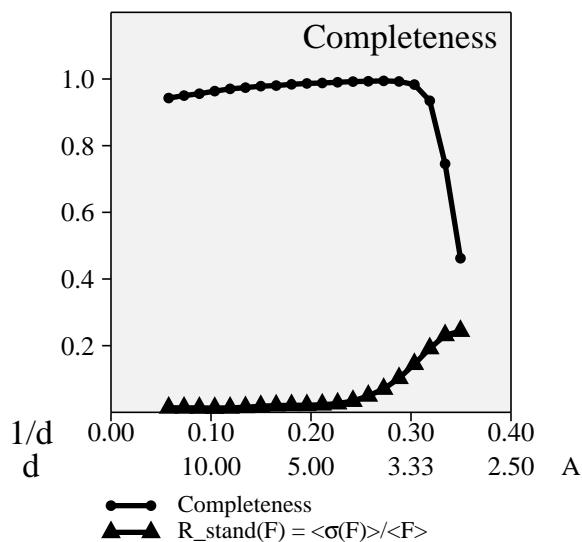
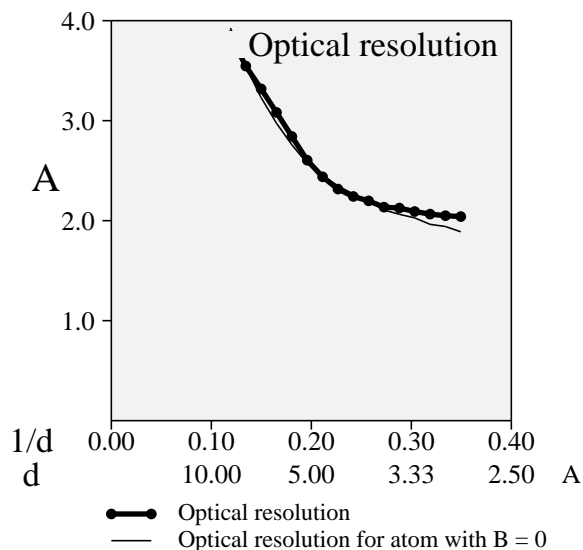
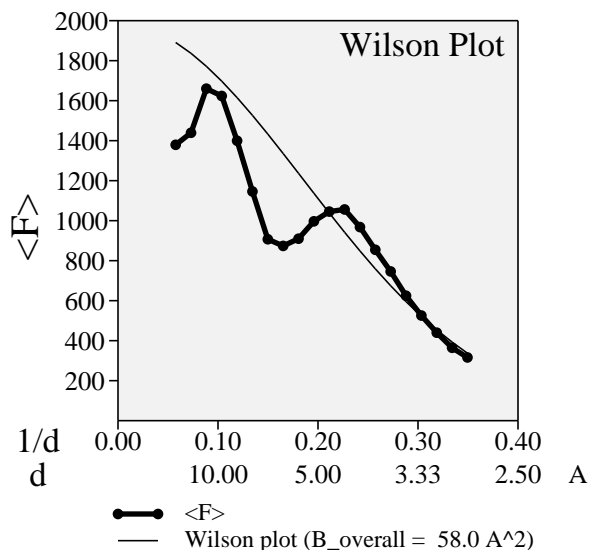
R-factor for all reflections: 0.257
 Correlation factor: 0.862
 R-factor: 0.261
 for $F > 2.0\sigma$
 nom. resolution range: 20.00 - 2.80A
 reflections used: 75106
 Rfree: 0.310
 Nfree: 3771
 R-factor without free-refl.: 0.258
 Non free-reflections: 71335
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.372 A
 Estimated maximal error: 0.184 A
 DPI: 0.371 A

Scaling

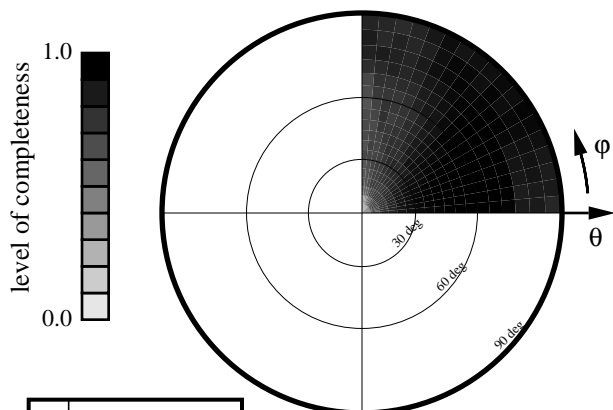
Scale: 0.912
 Bdiff: -5.81
 Anisothermal Scaling (Beta):
 -0.8335 -1.0360 -0.8918 0.0000 -0.0000 0.0000
 Solvent correction - Ks,Bs: 0.569 249.962

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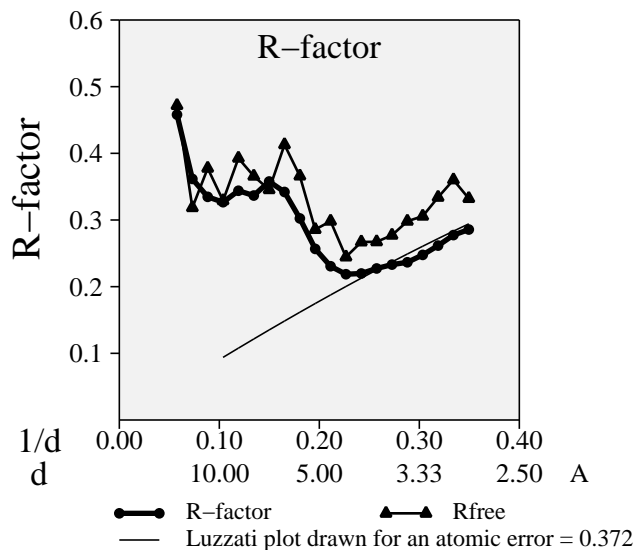


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

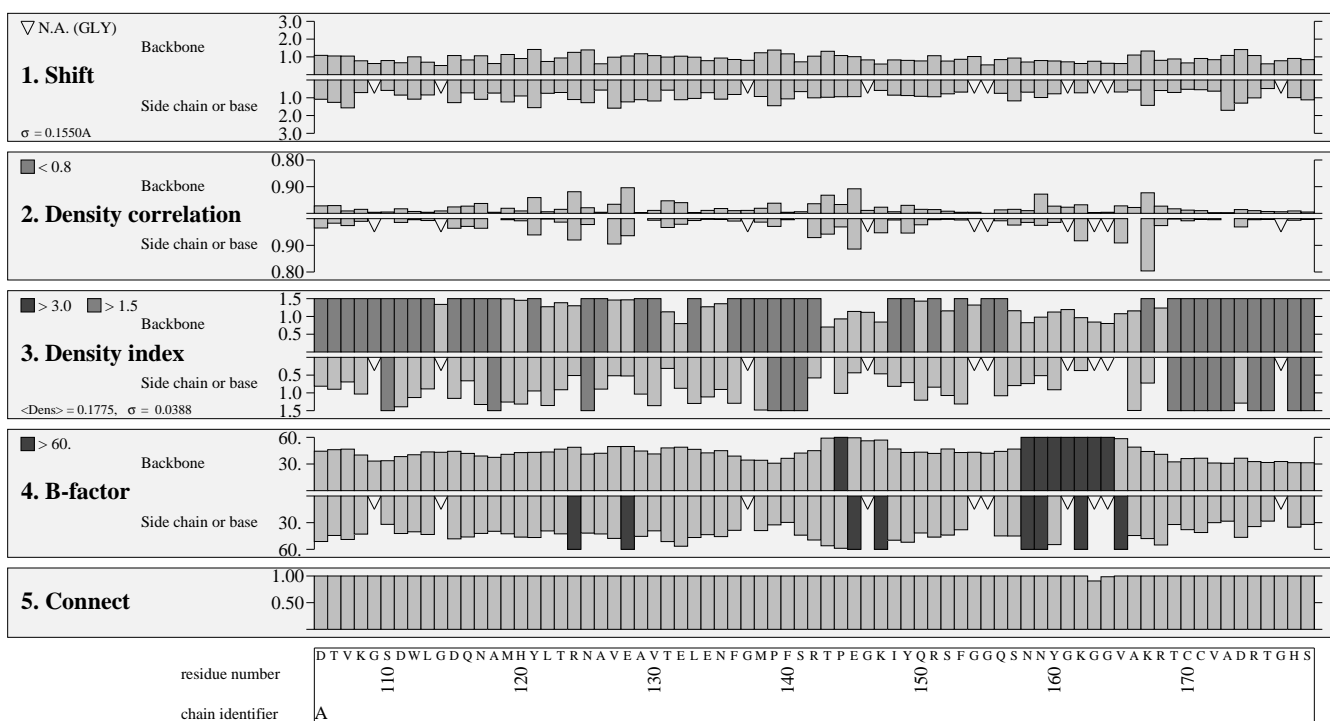
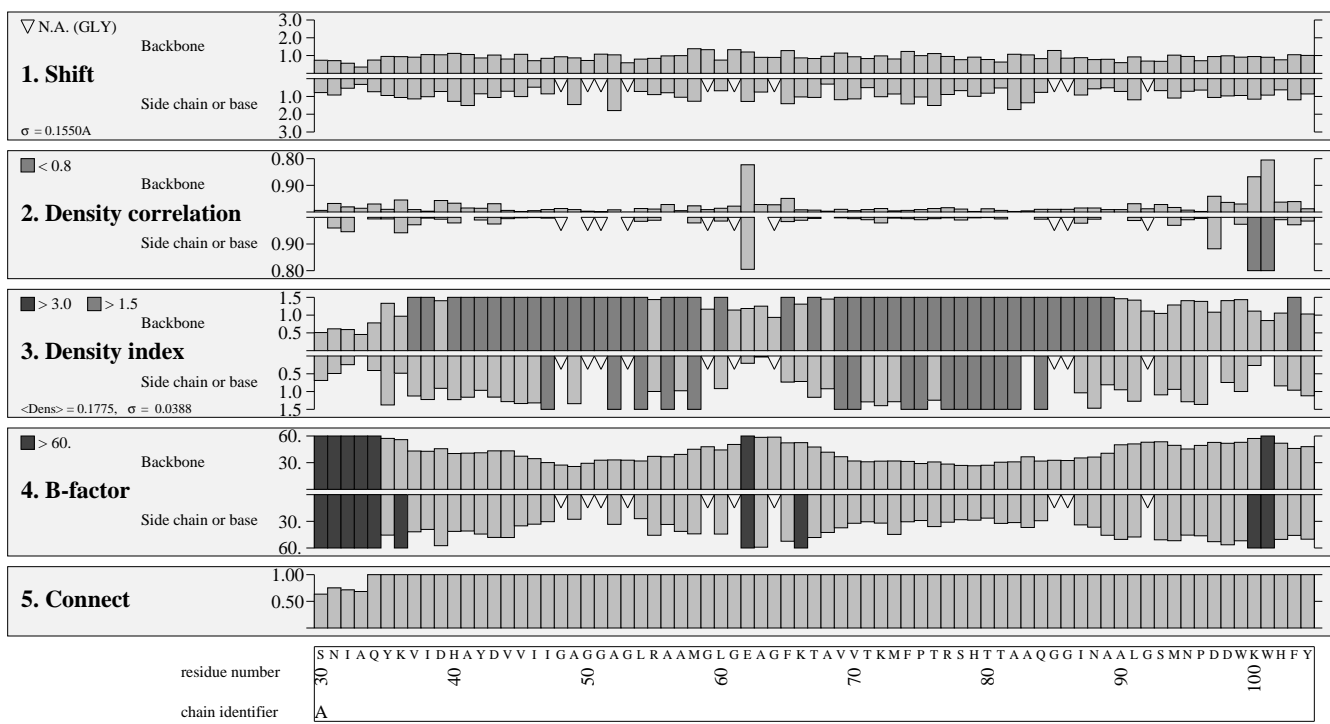
polar coordinates of the crystallographical axes



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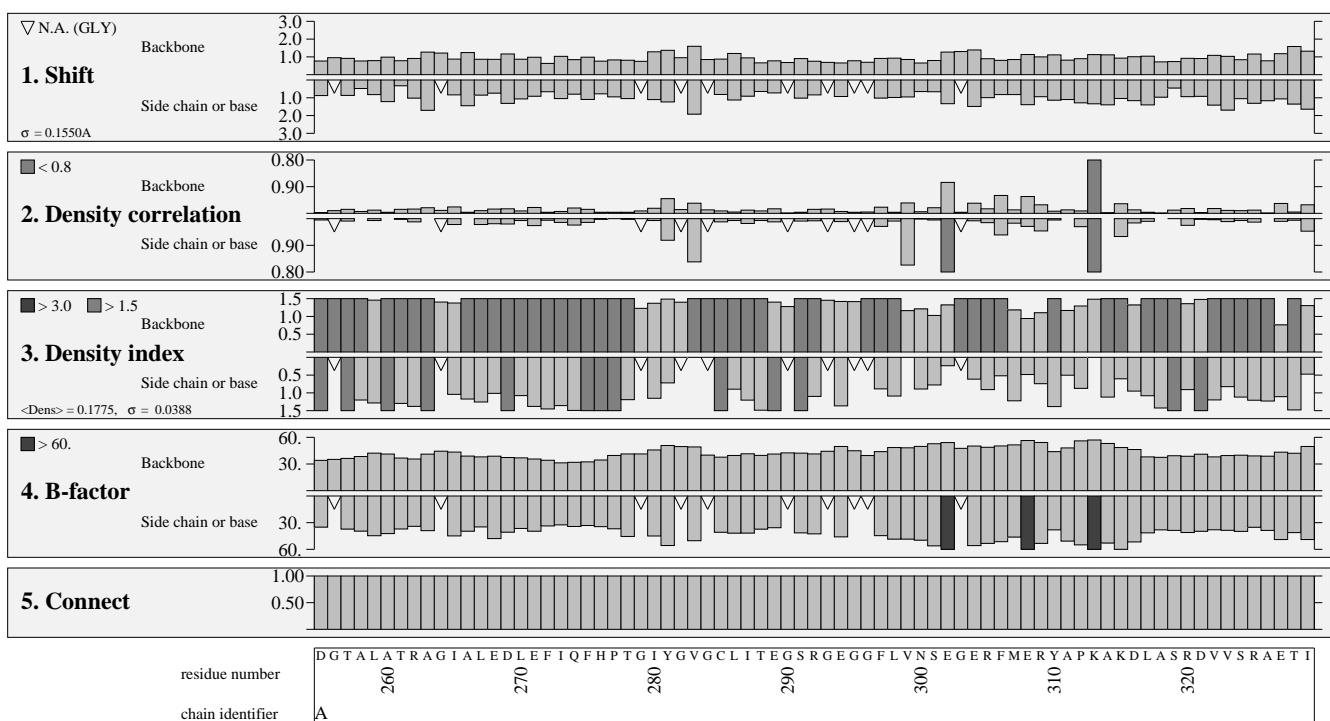
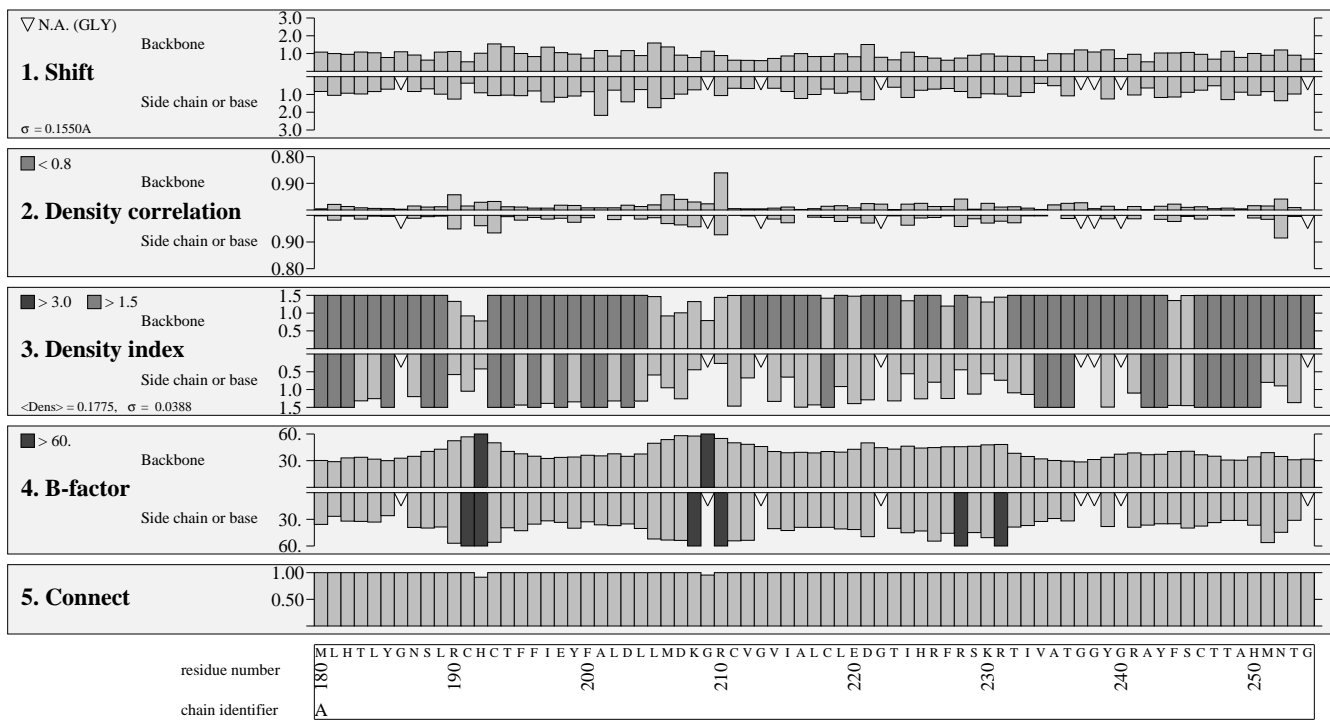
Local estimation



Structure Factor Check

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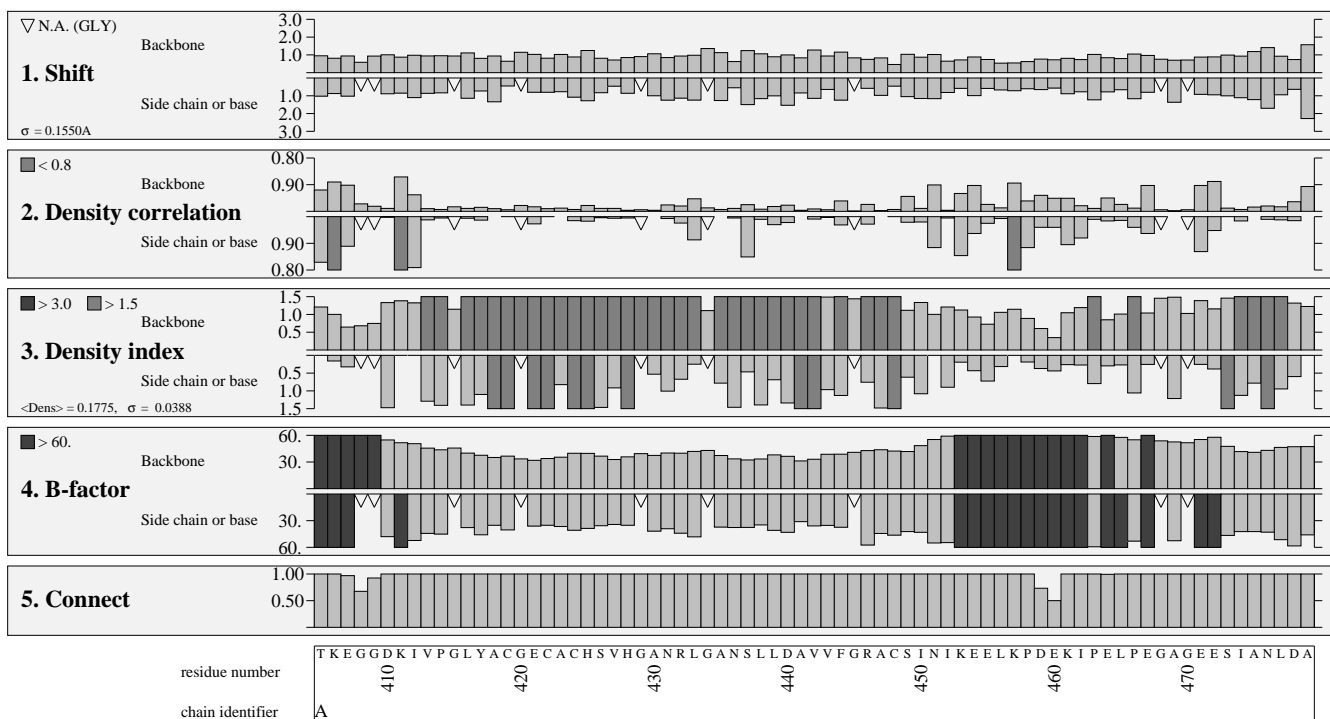
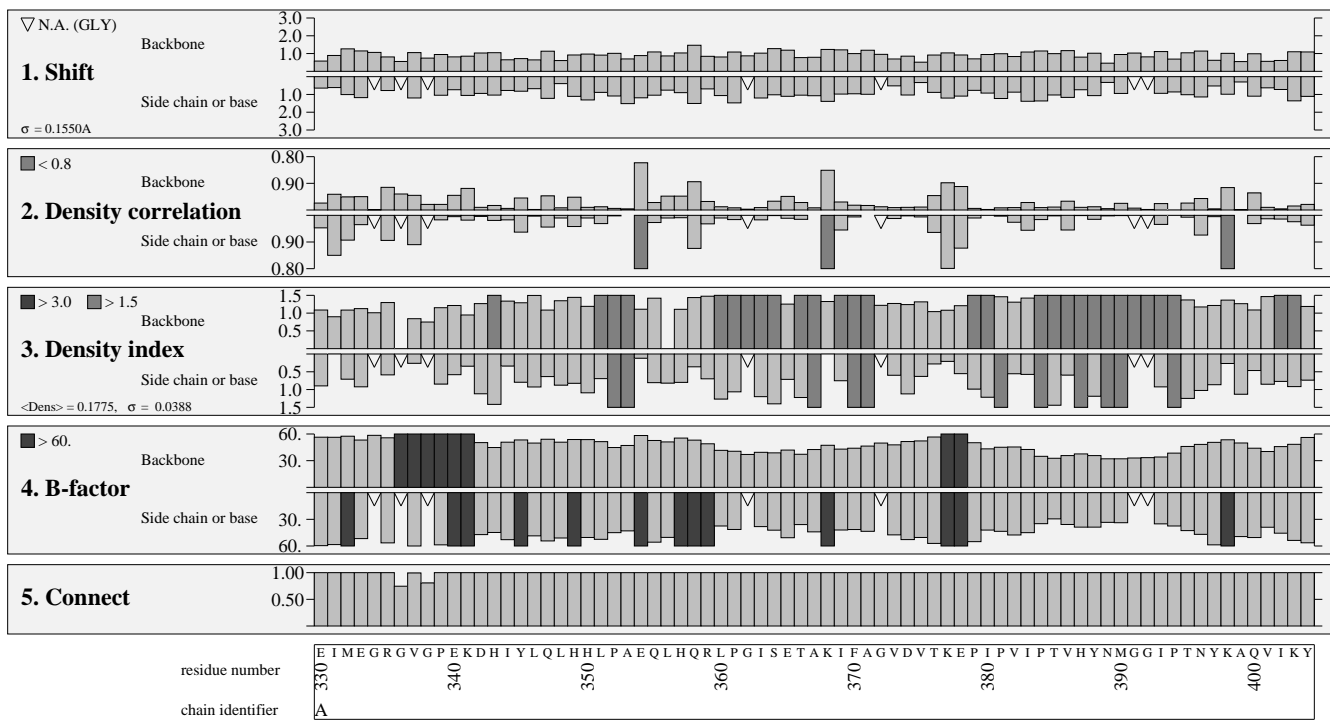
Local estimation (2)



Structure Factor Check

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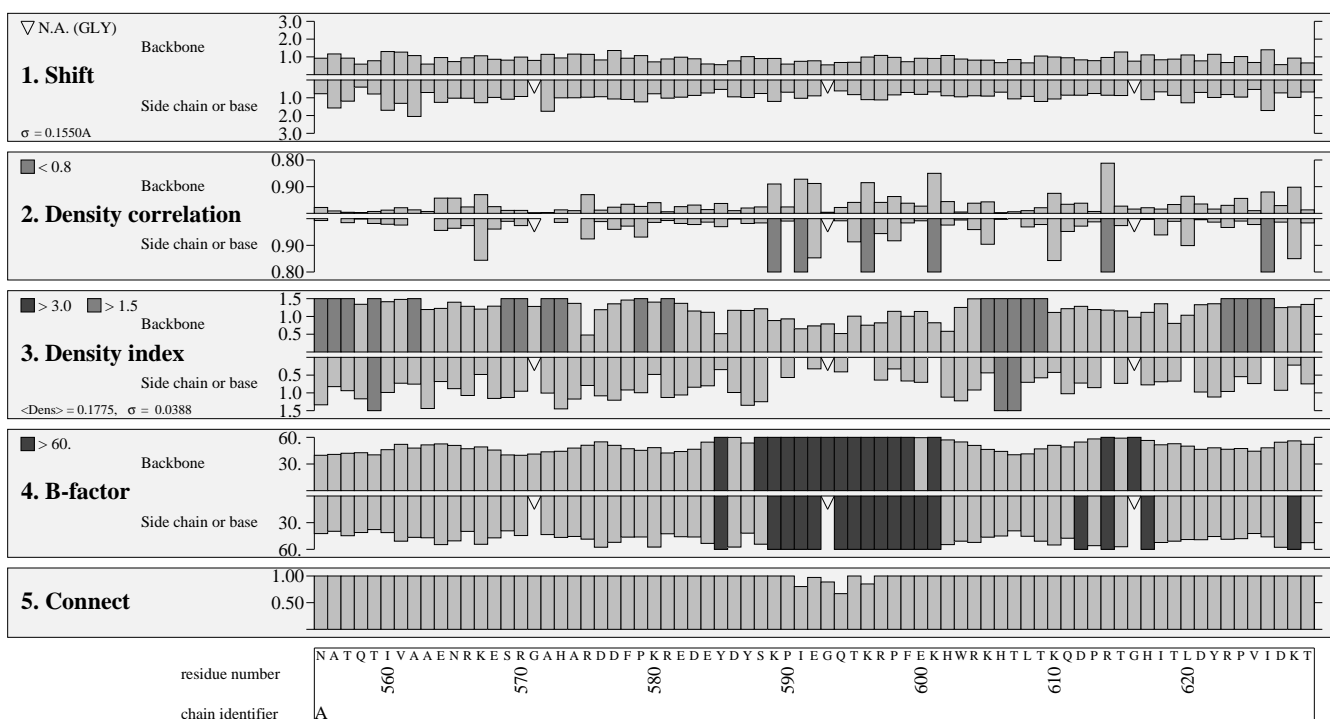
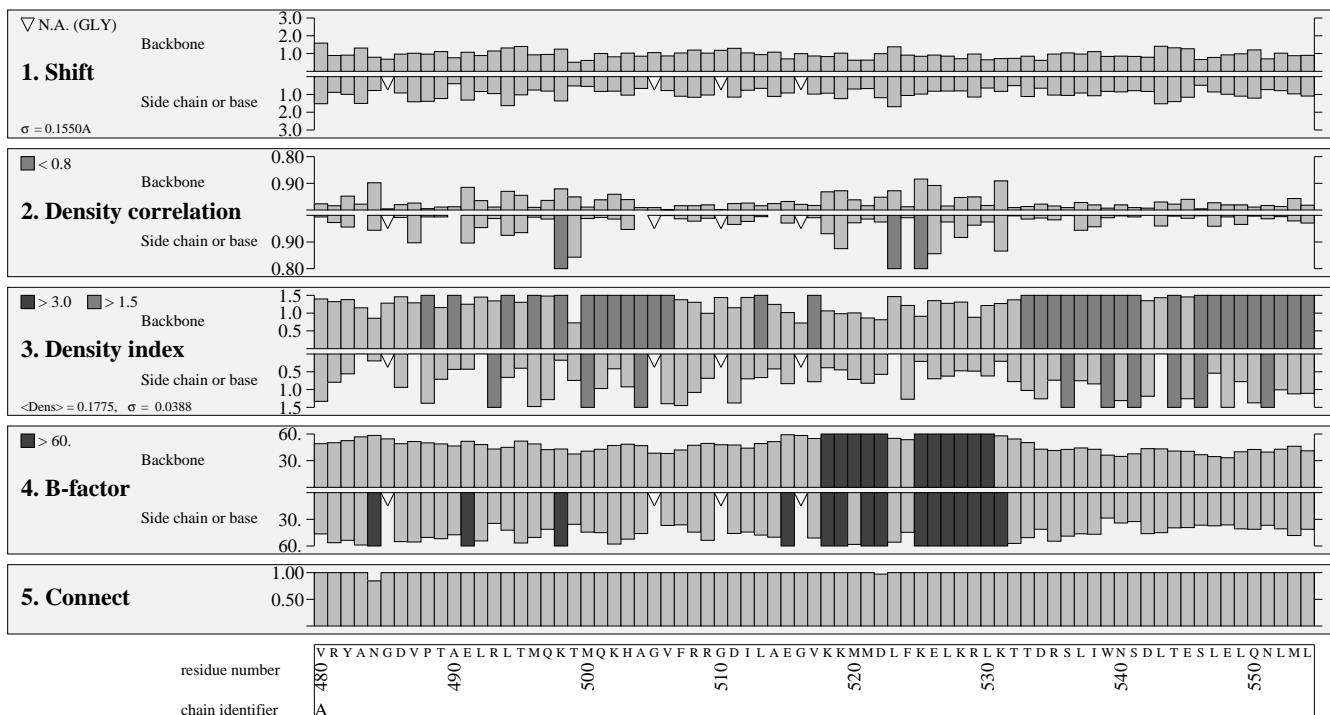
Local estimation (3)



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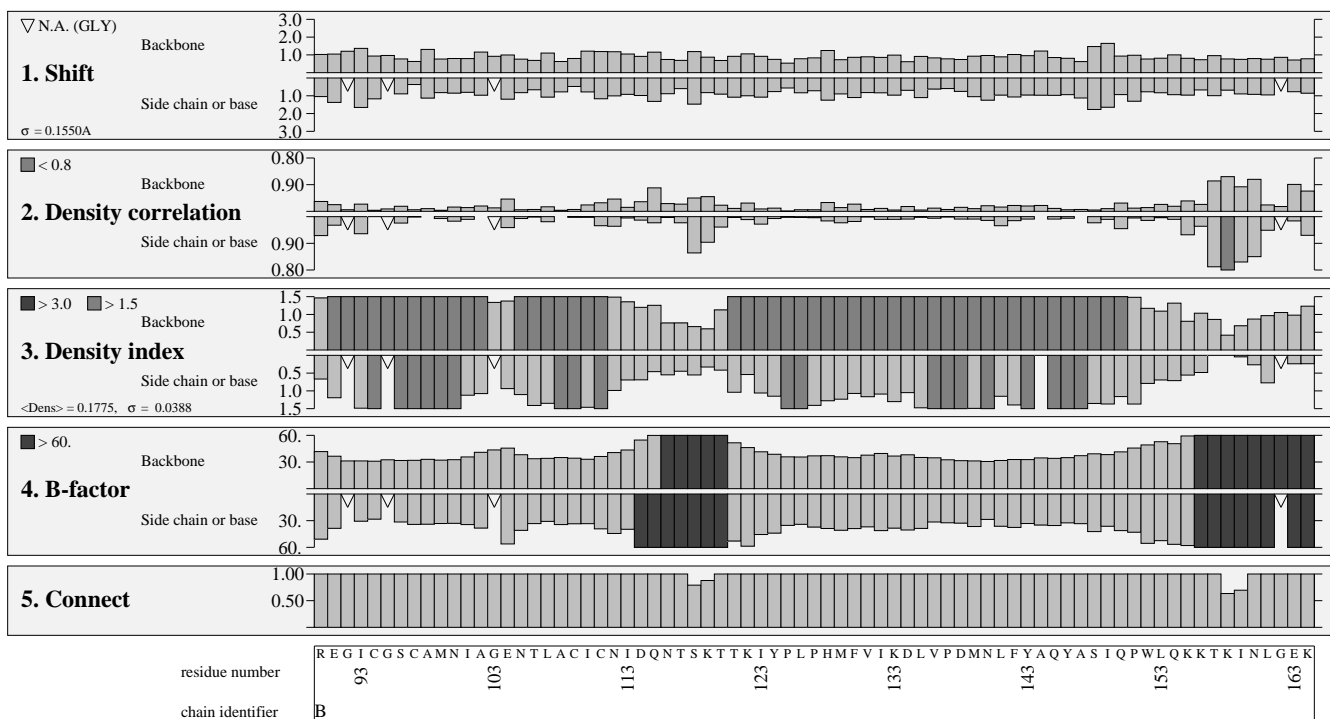
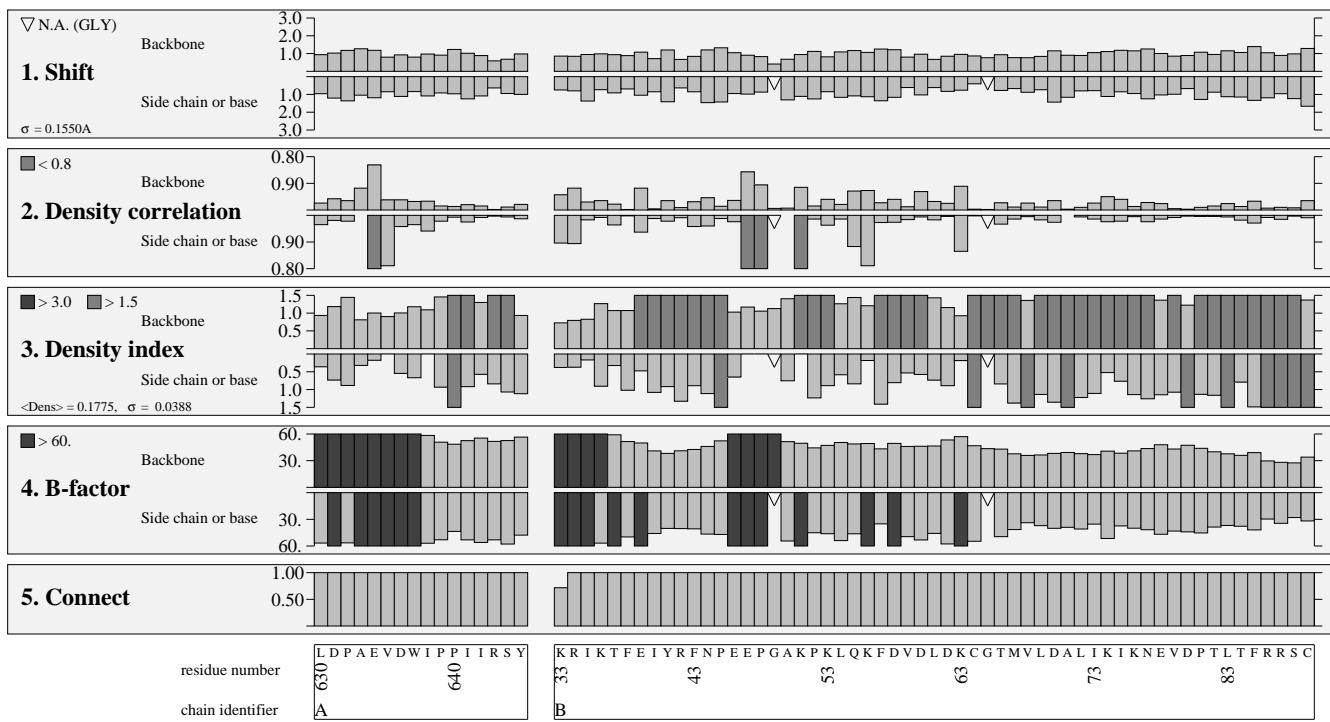
Local estimation (4)



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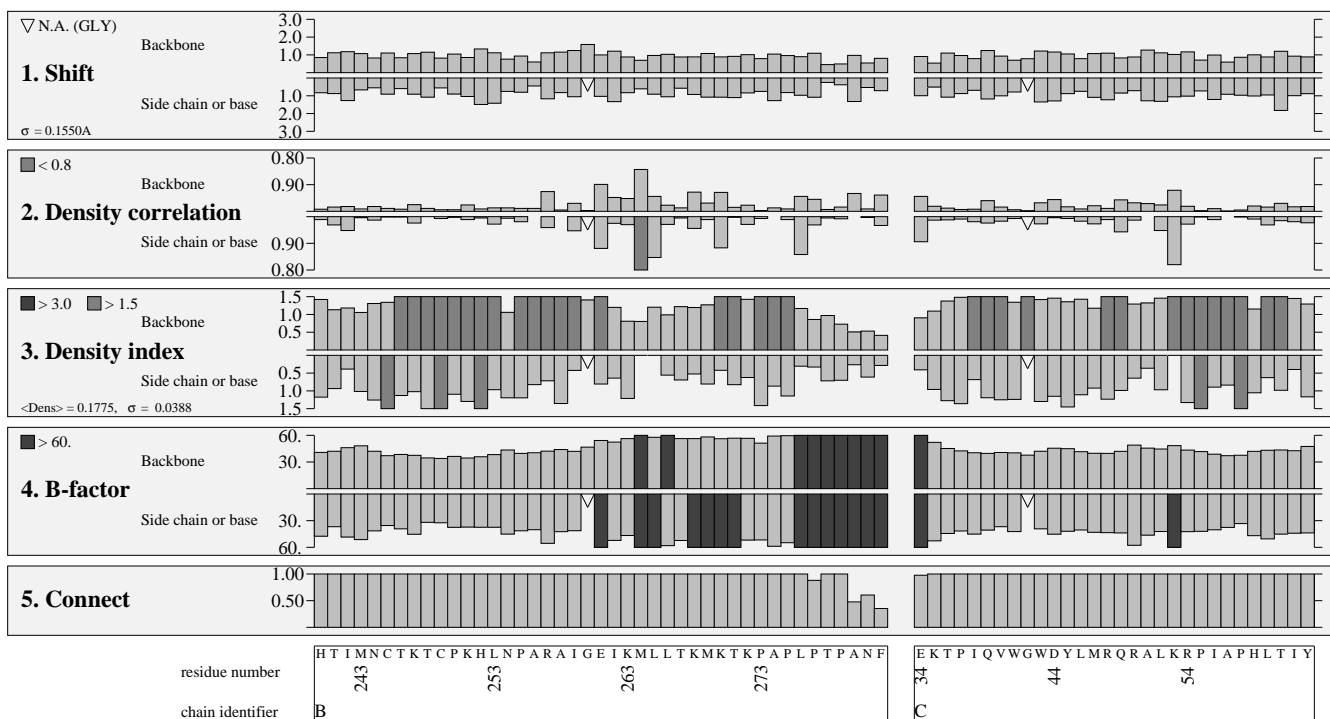
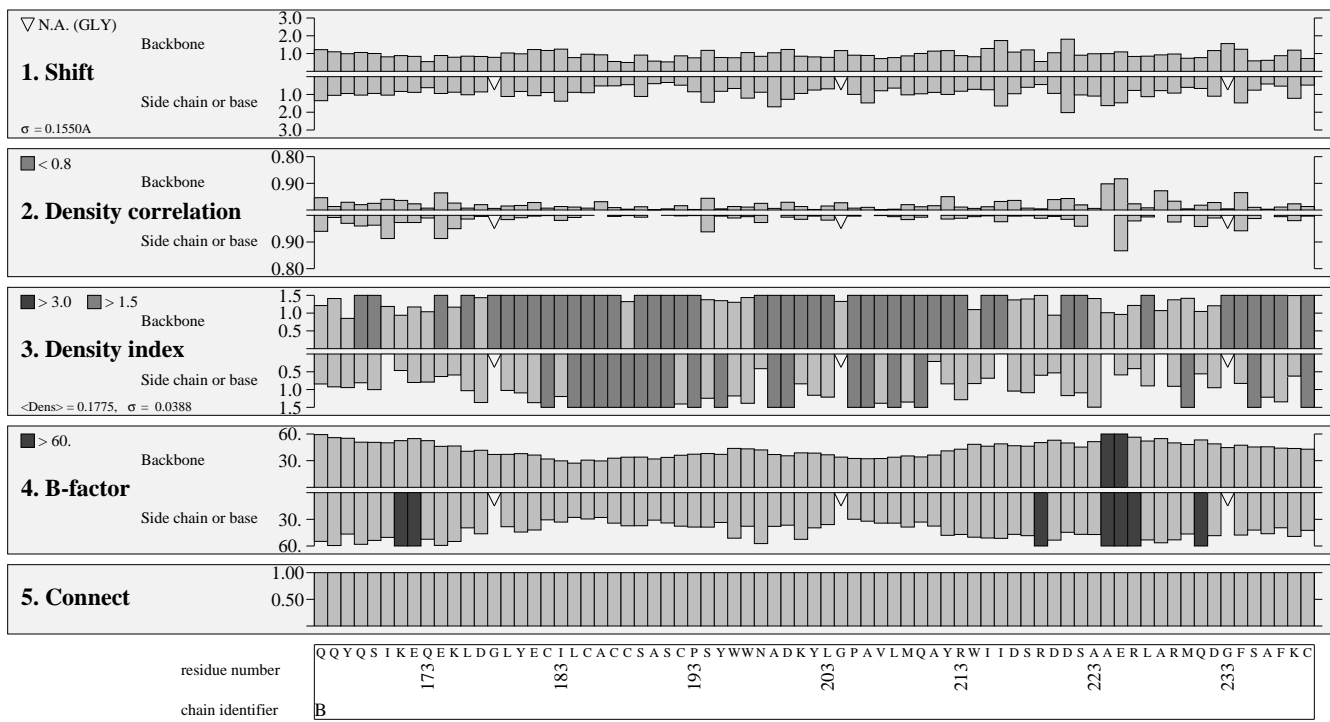
Local estimation (5)



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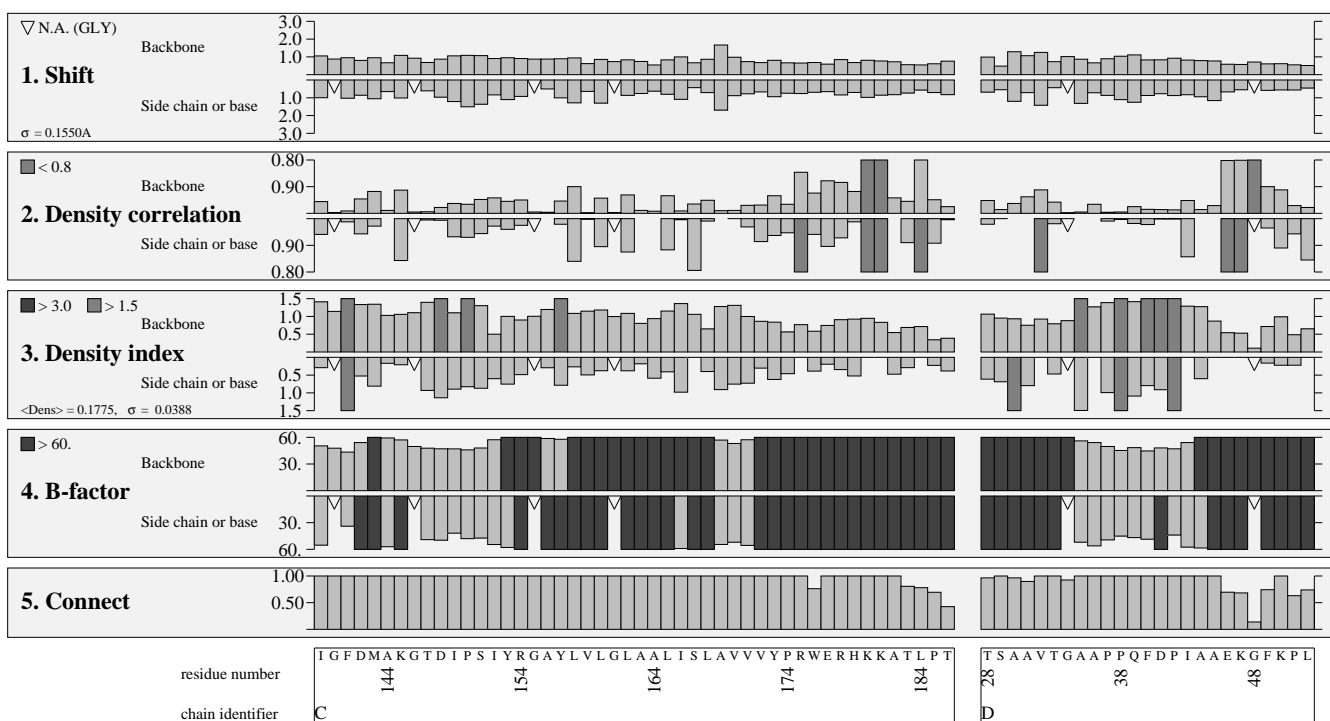
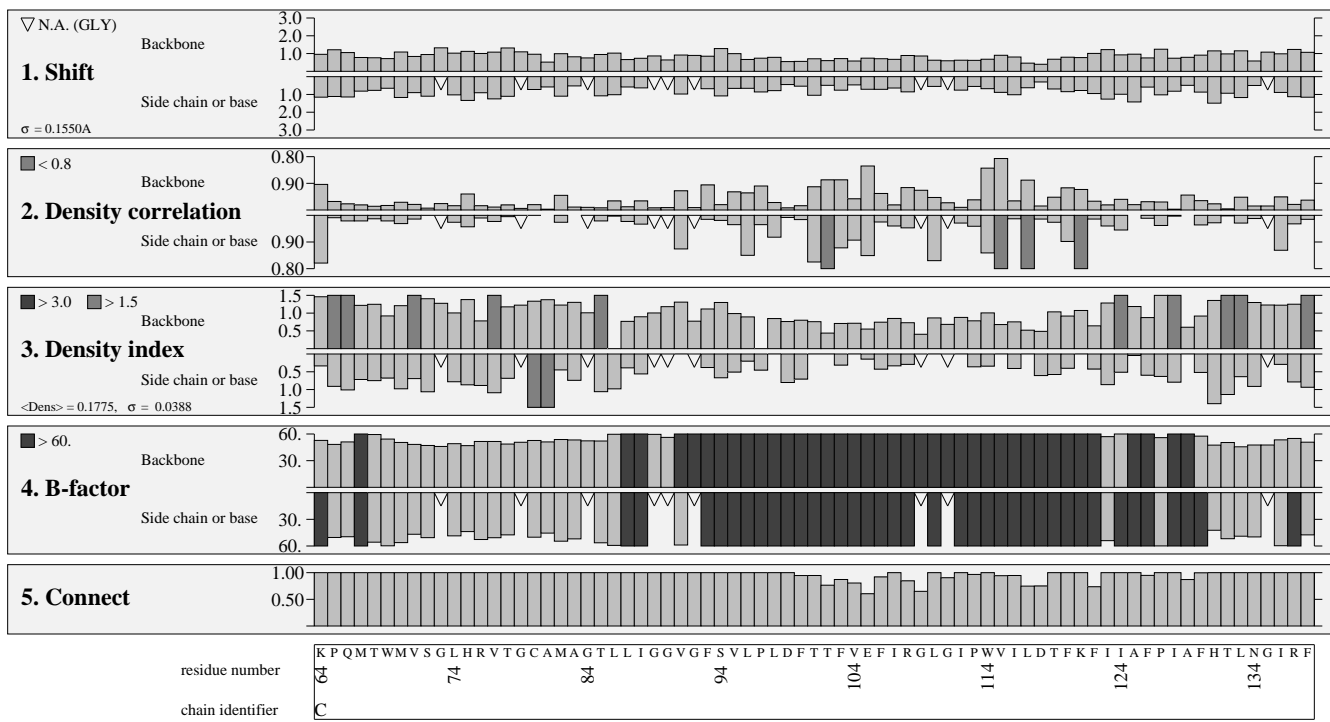
Local estimation (6)



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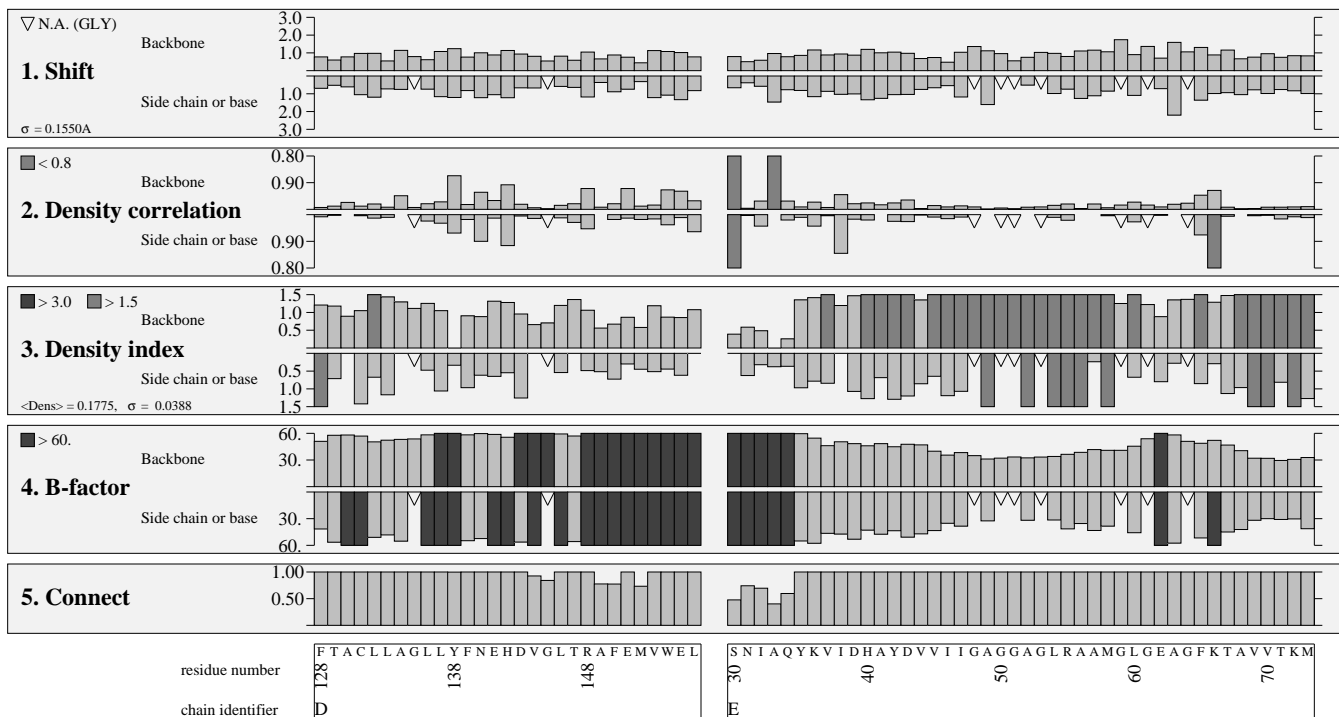
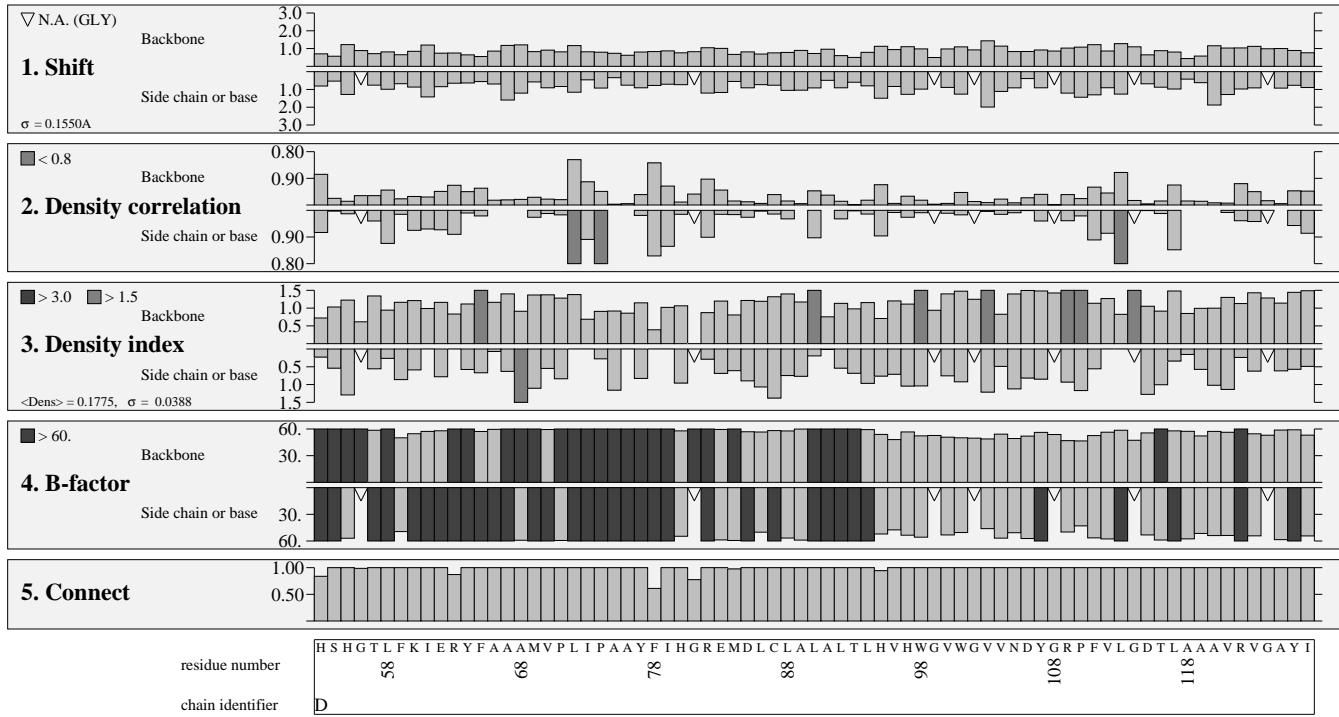
Local estimation (7)



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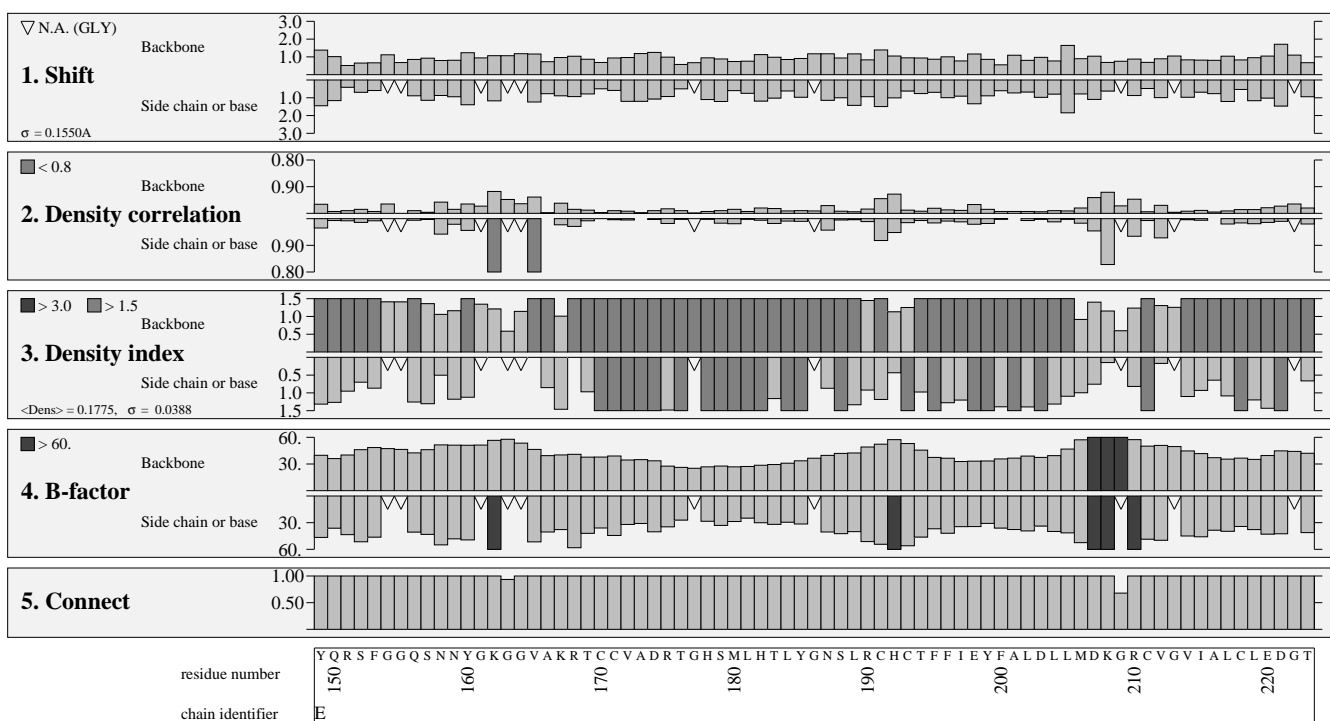
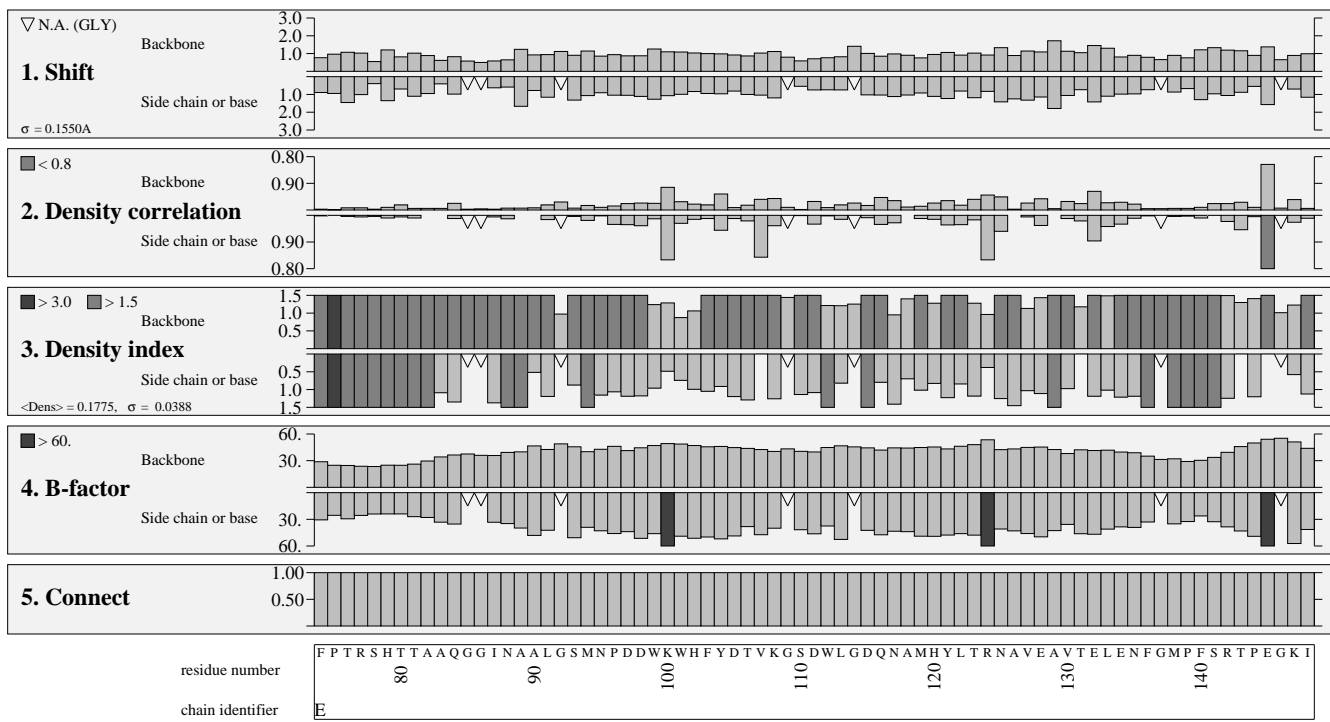
Local estimation (8)



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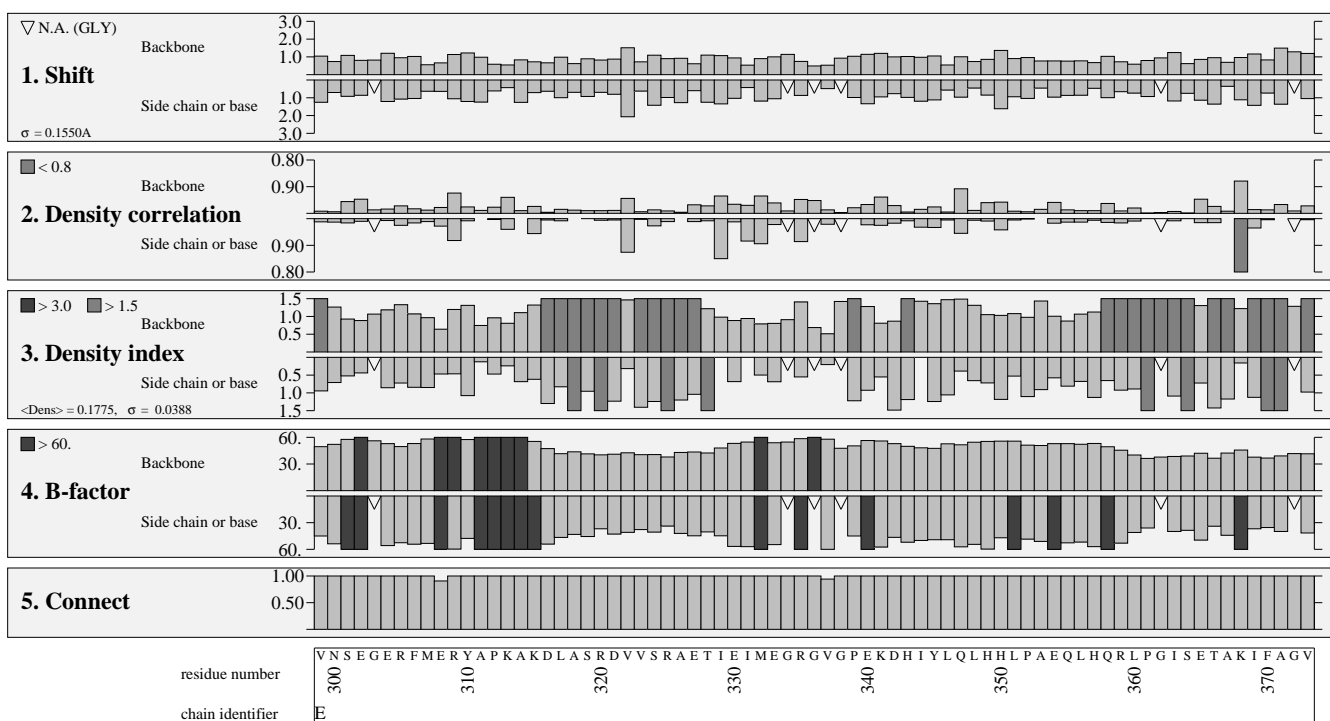
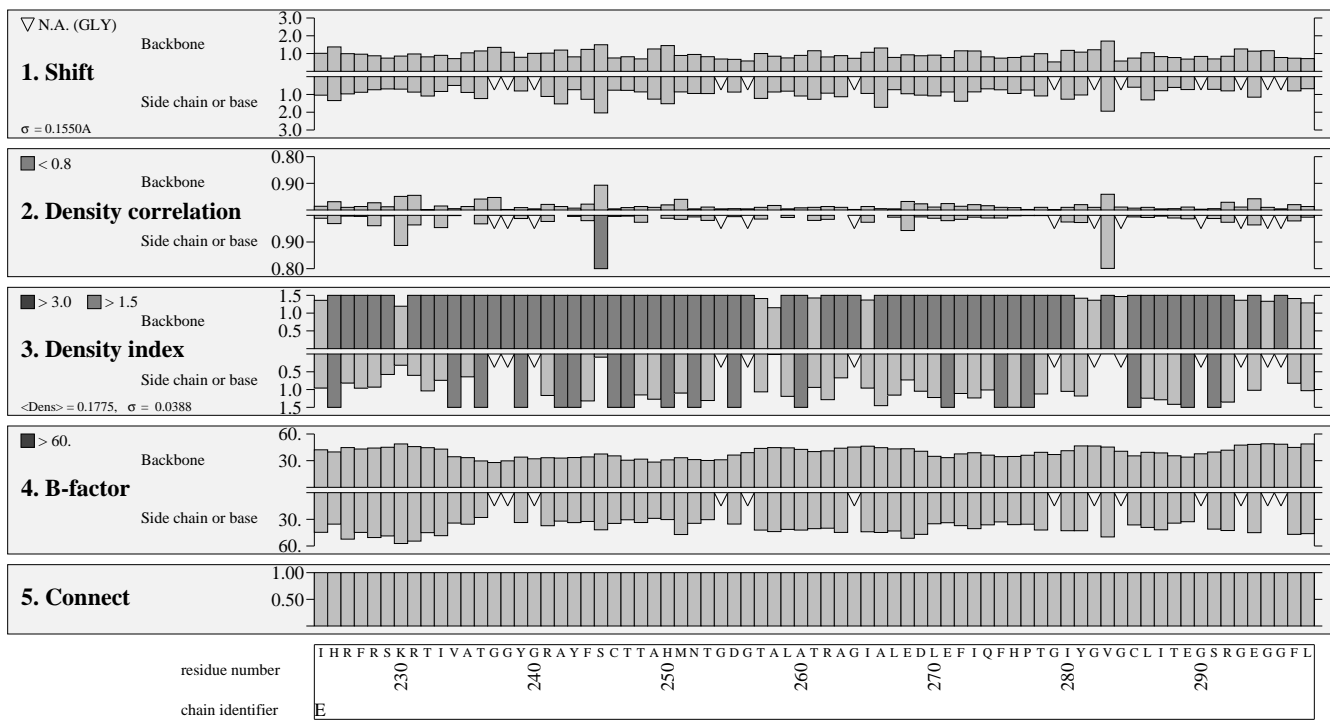
Local estimation (9)



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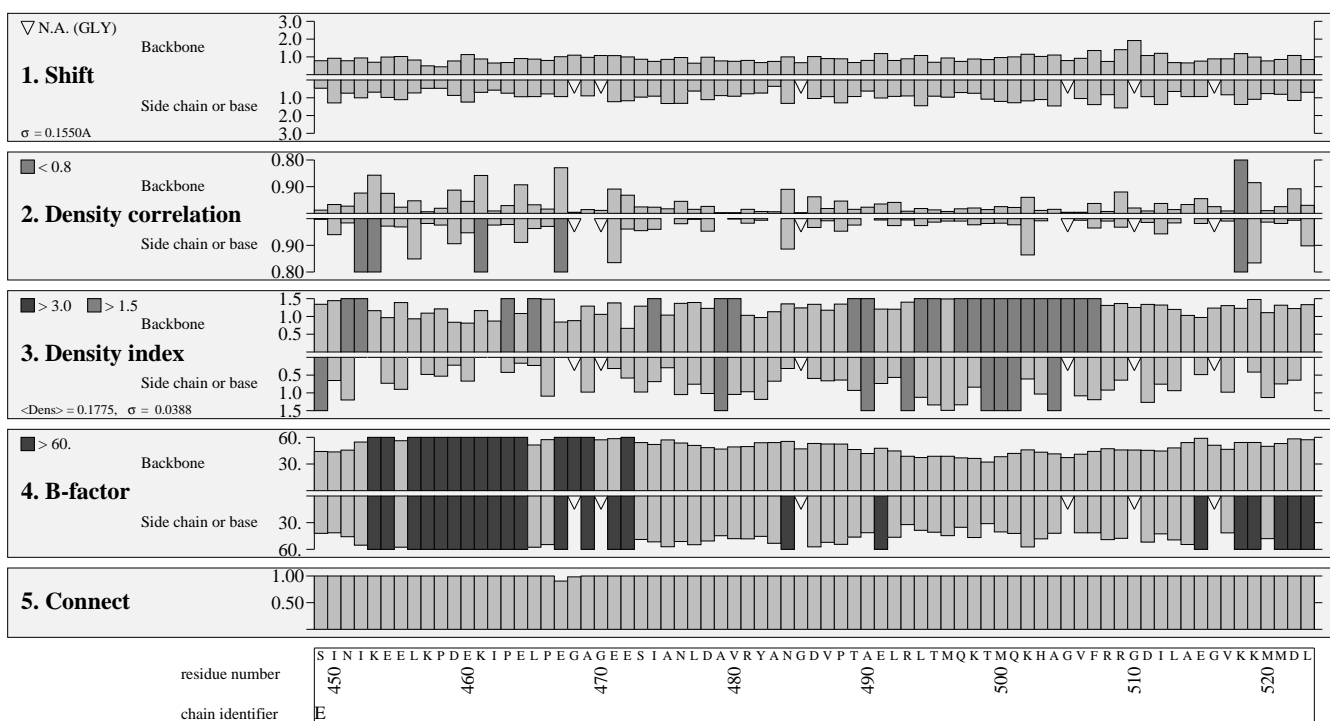
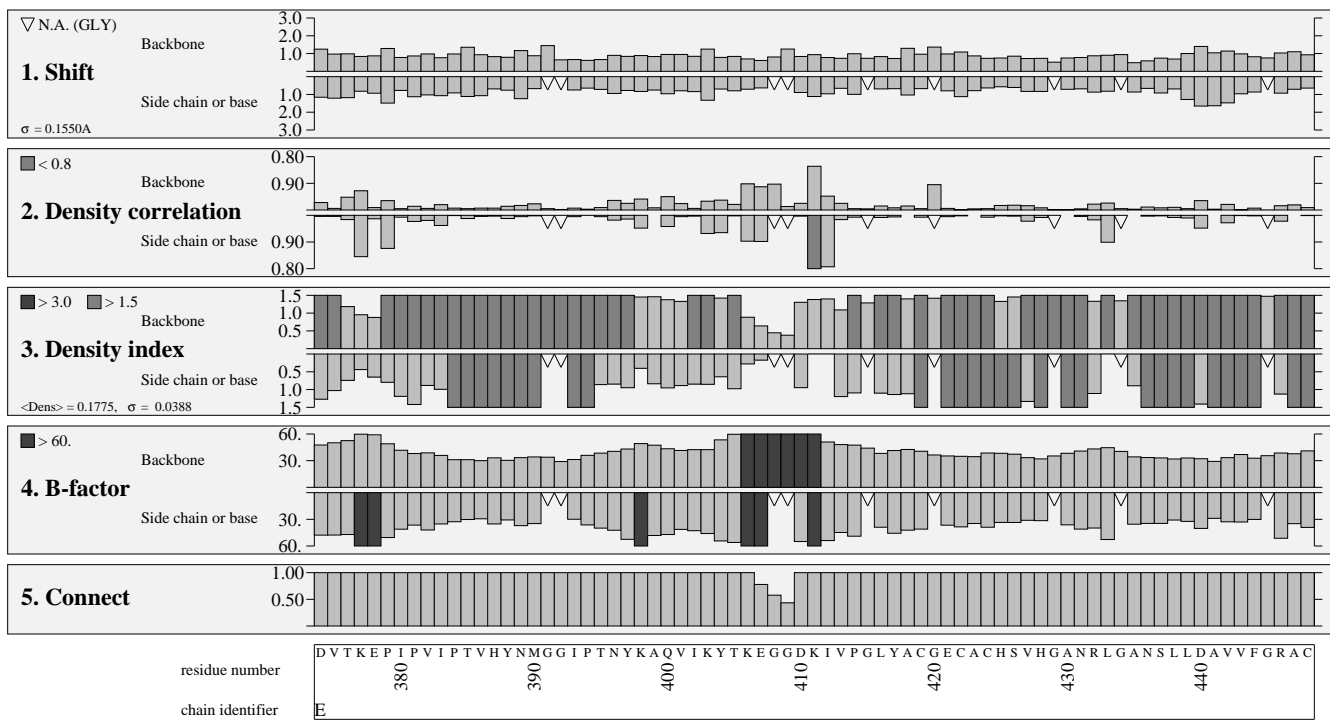
Local estimation (10)



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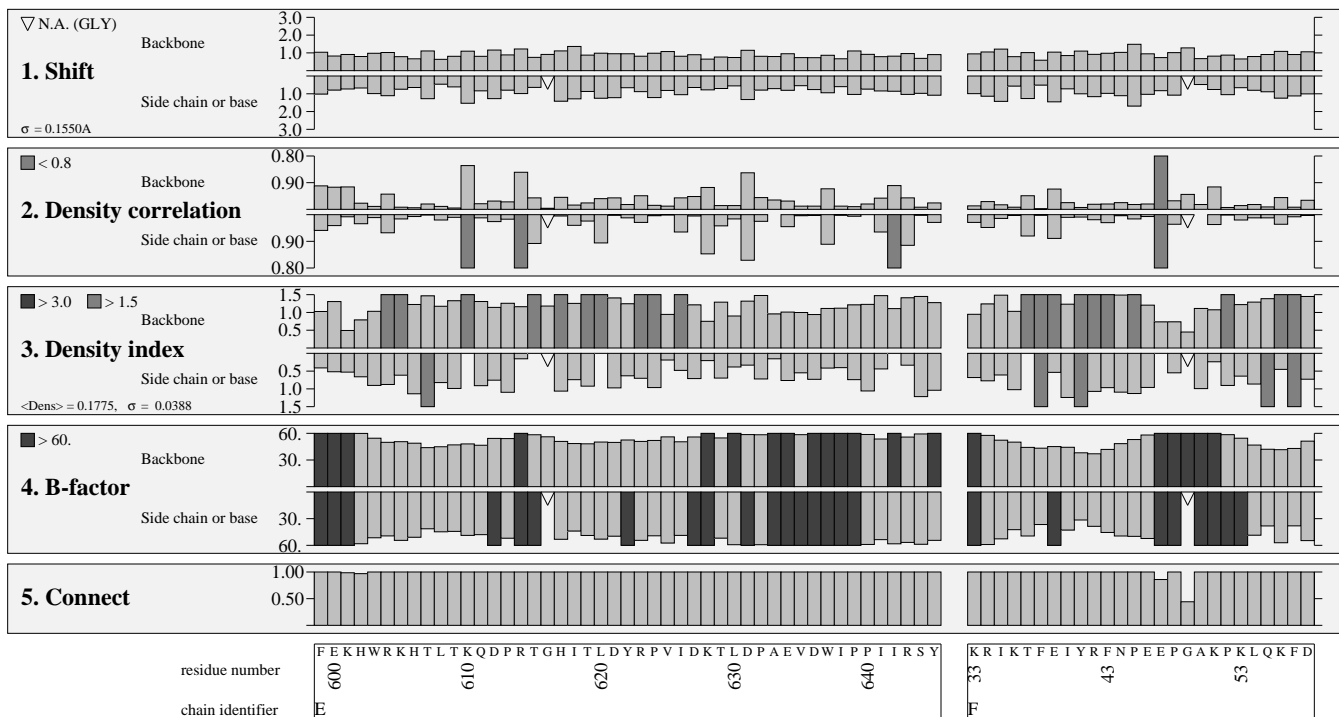
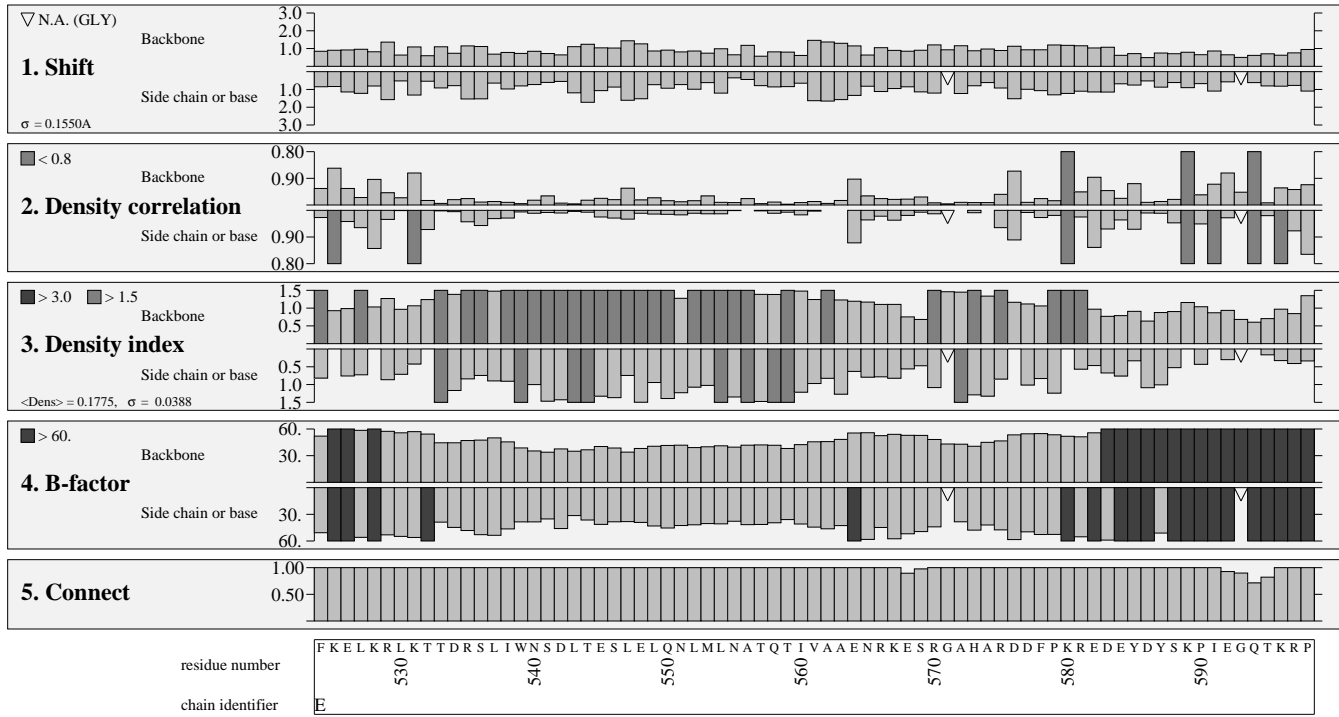
Local estimation (11)



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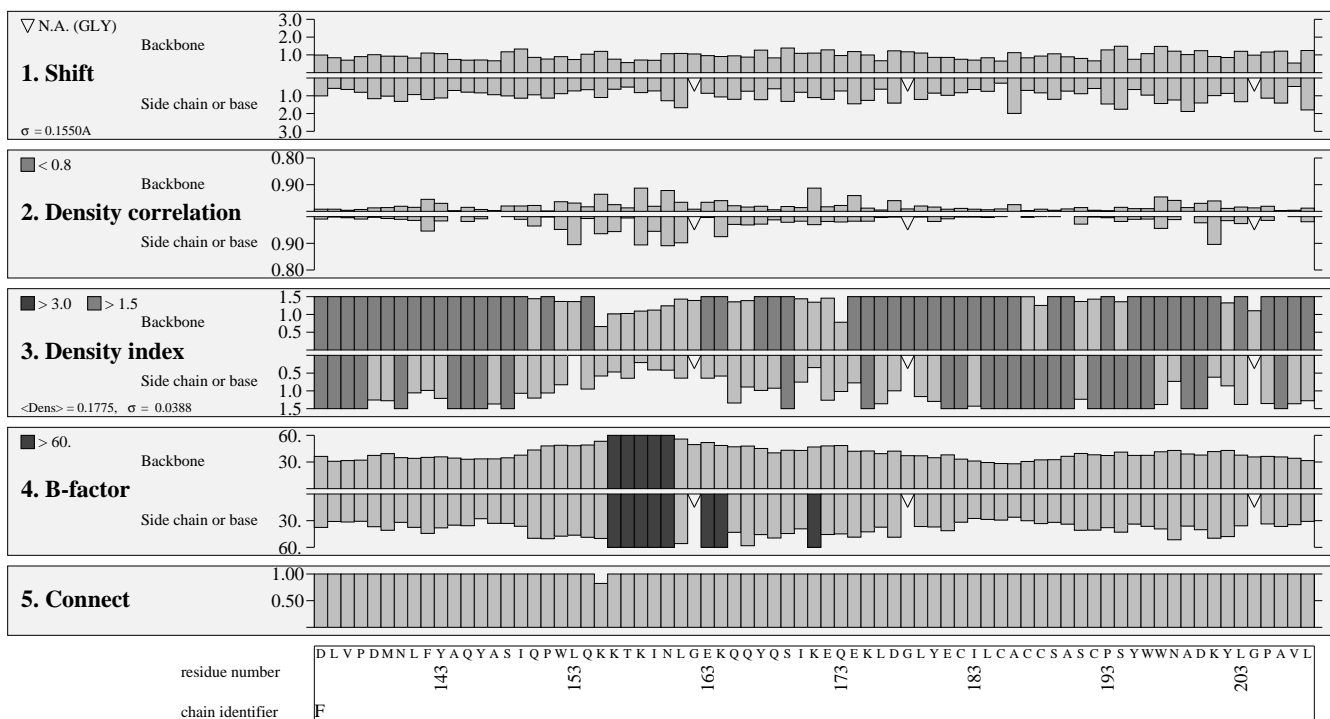
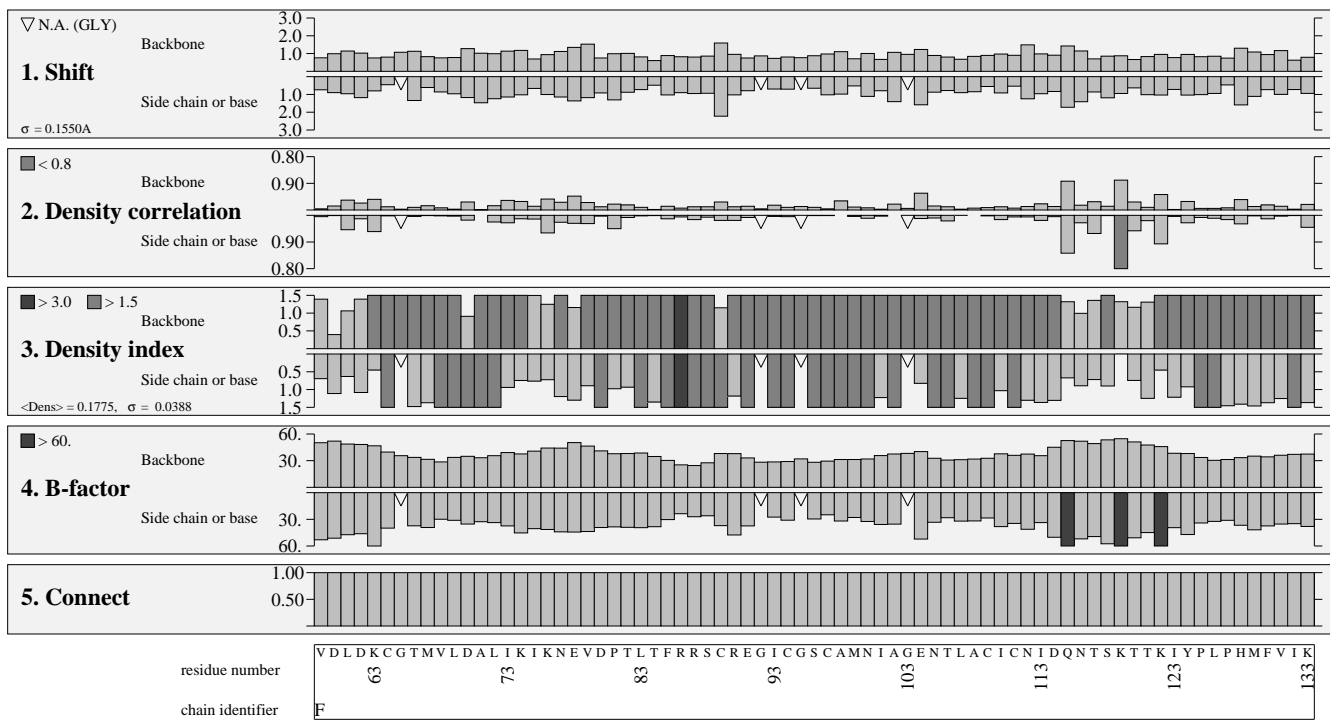
Local estimation (12)



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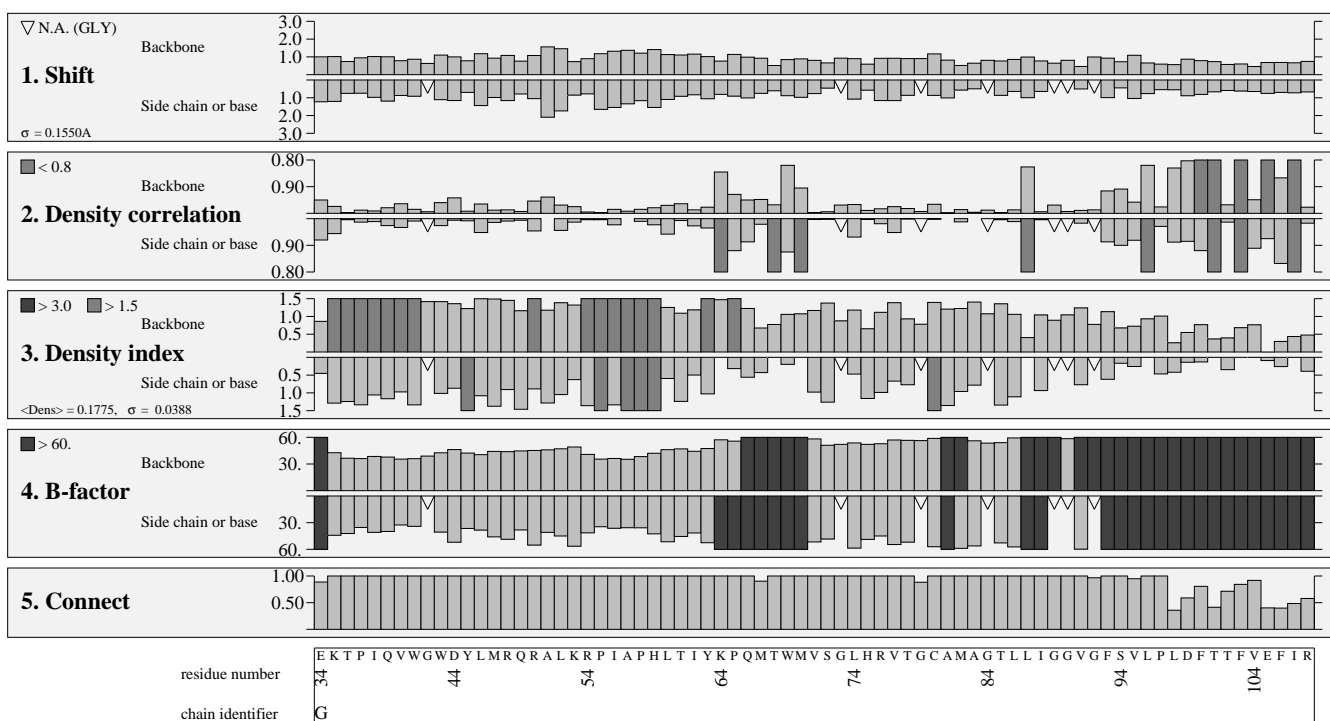
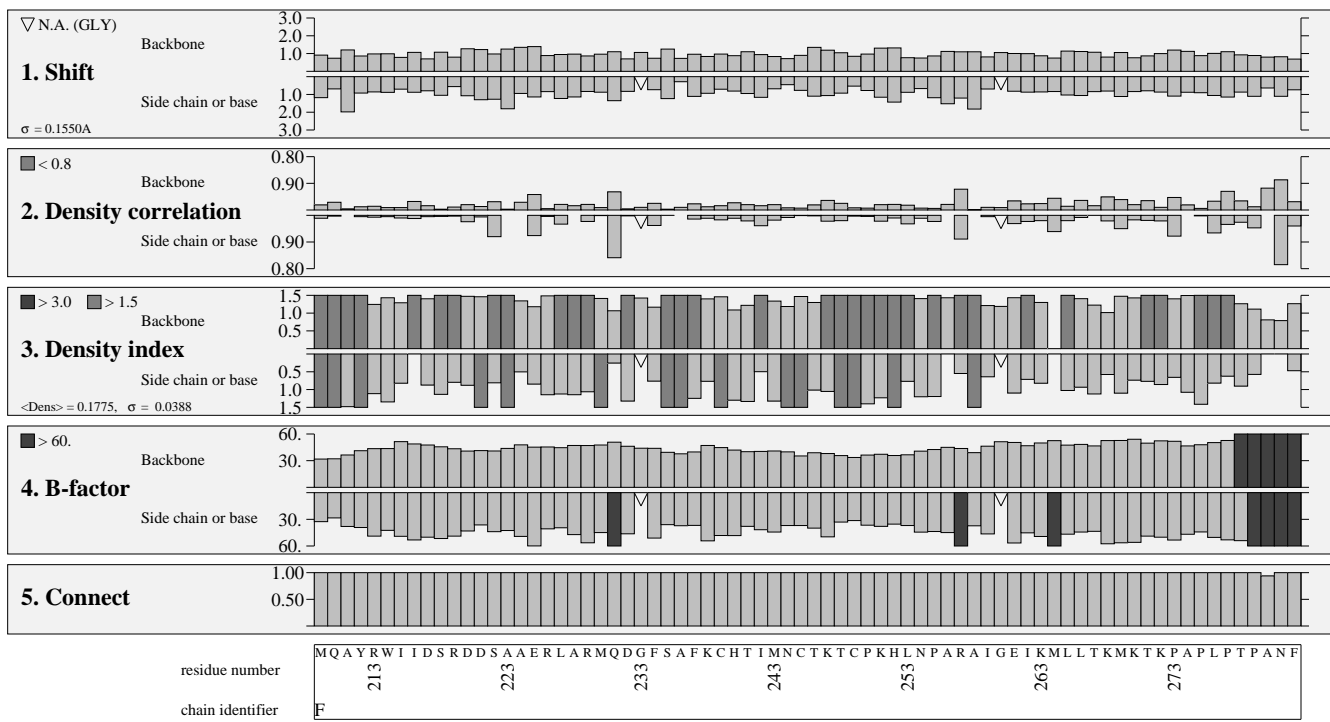
Local estimation (13)



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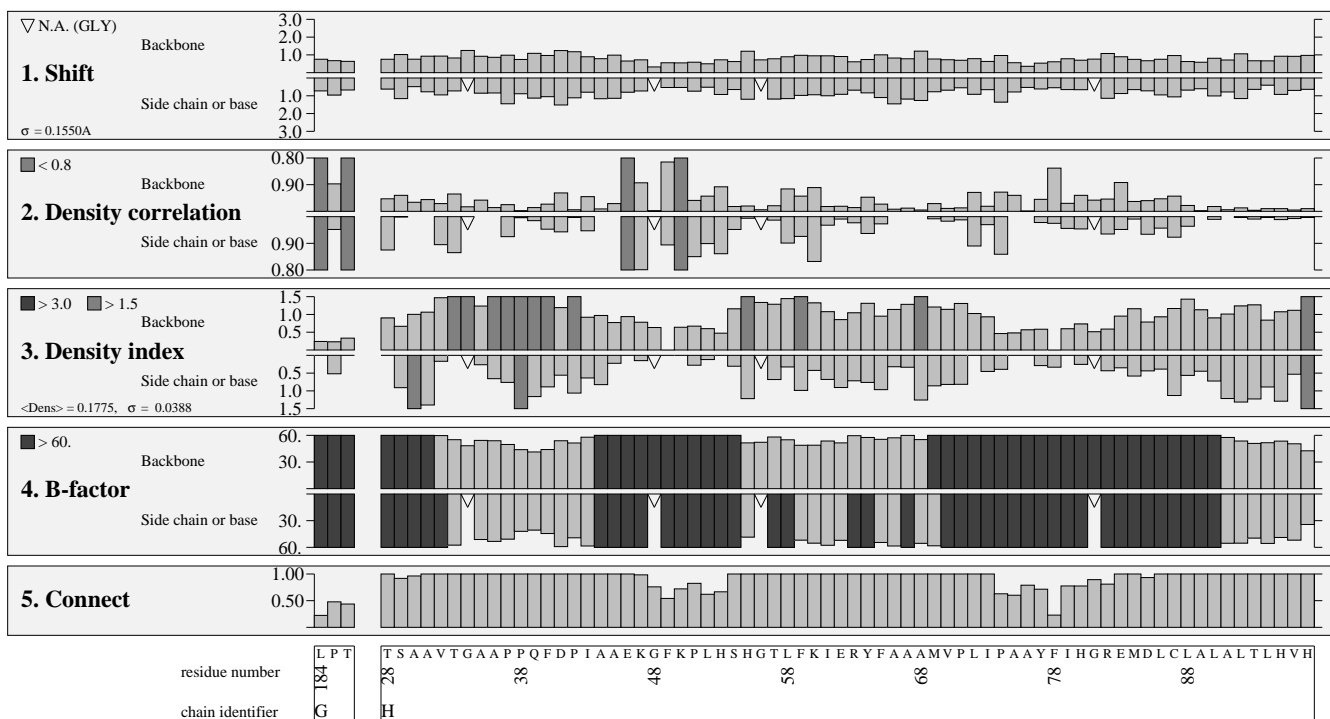
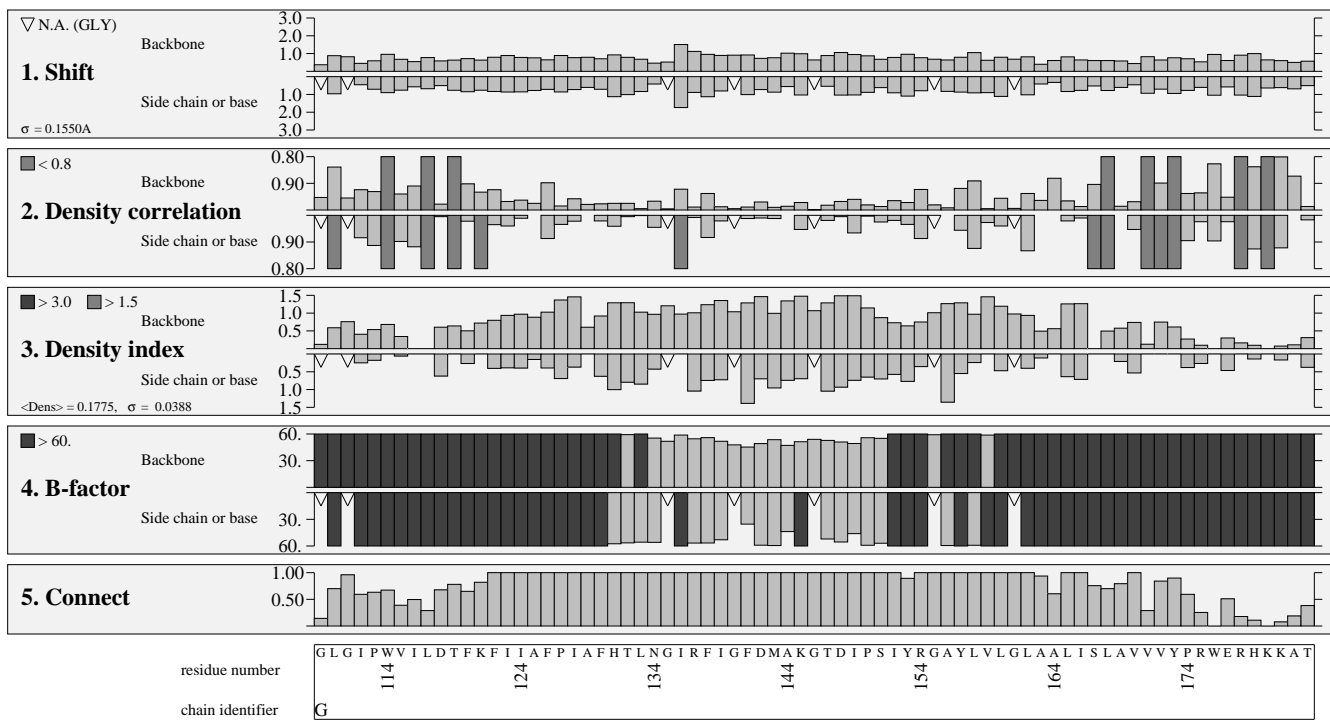
Local estimation (14)



Structure Factor Check

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Local estimation (15)



Structure Factor Check

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Local estimation (16)

