

Structure Factor Check

4YSY

Title: CRYSTAL STRUCTURE OF MITOCHONDRIAL RHODOQUINOL-FUMARATE REDU
 ASCARIS SUUM WITH N-[052,4-DICHLOROPHENYL]05METHYL]-2-05TRIFLUO
 BENZAMIDE
 Date: 17-MAR-15
 PDB code: 4YSY

Crystal

Cell parameters:
 a: 124.12 A b: 127.66 A c: 220.74 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

Model

18377 atoms (27 water molecules)
 Number of chains: 31
 Volume not occupied by model: 55.2 %
 $\langle B \rangle$ (for atomic model): 66.0 A²
 $\sigma(B)$: 13.10 A²
 Matthews coefficient: 3.40
 Corresponding solvent % : 63.53

Refinement

Program: REFMAC 5.7.0029
 Nominal resolution range: 20.0 - 3.10 A
 Reported R-factor: 0.183
 Number of reflections used: 58730
 Reported Rfree: 0.24
 Sigma cut-off: N.A.

Structure Factors

Input

Nominal resolution range: 20.0 - 3.10 A
 Reflections in file: 64072
 Unique reflections above 0: 61561
 above 1 σ : 60771
 above 3 σ : 46249
 Reflections > 0: 2511

SFCHECK

Nominal resolution range: 20.0 - 3.10 A
\05max. from input data, min. from author\05
 Used reflections: 61555
 Reflections out of resolution: 6
 Completeness: 96.1 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.061
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.9358 0.9783
 B_{overall} (by Patterson): 50.A²
 Optical resolution: 2.23 A
 Expected opt. resol. for complete data set: 2.23 A
 Estimated minimal error: 0.061 A

Model vs. Structure Factors

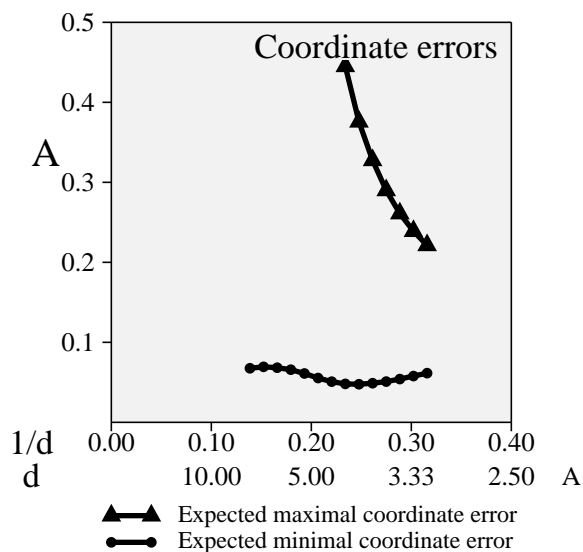
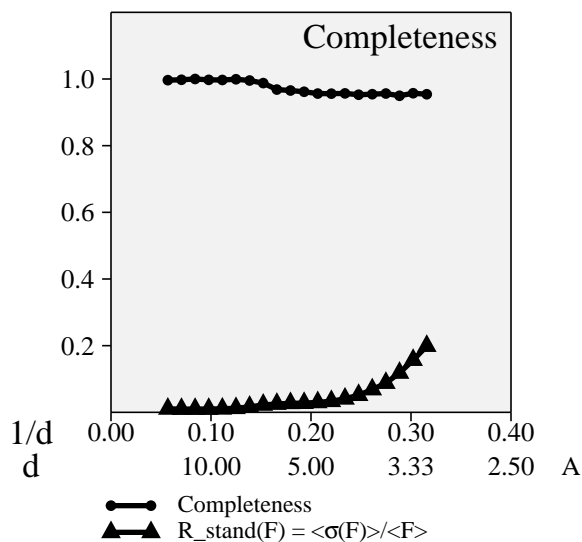
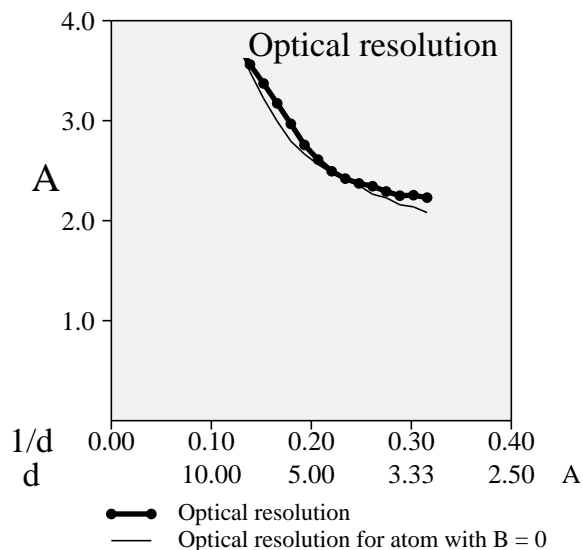
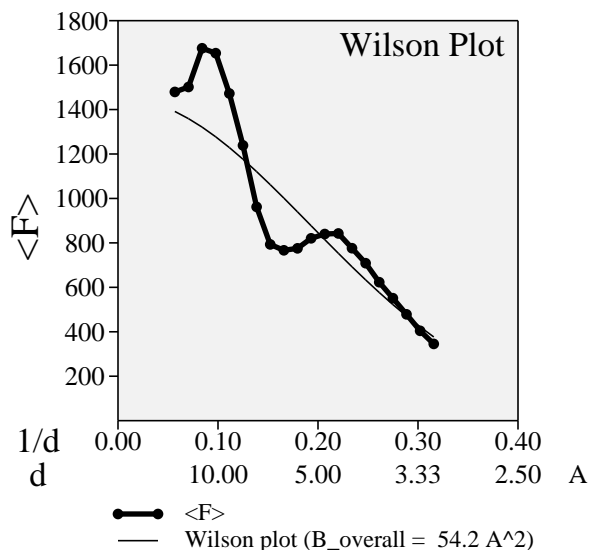
R-factor for all reflections: 0.241
 Correlation factor: 0.855
 R-factor: 0.249
 for $F > 2.0\sigma$
 nom. resolution range: 20.00 - 3.10A
 reflections used: 60765
 Rfree: 0.290
 Nfree: 3094
 R-factor without free-refl.: 0.247
 Non free-reflections: 57671
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.464 A
 Estimated maximal error: 0.221 A
 DPI: 0.408 A

Scaling

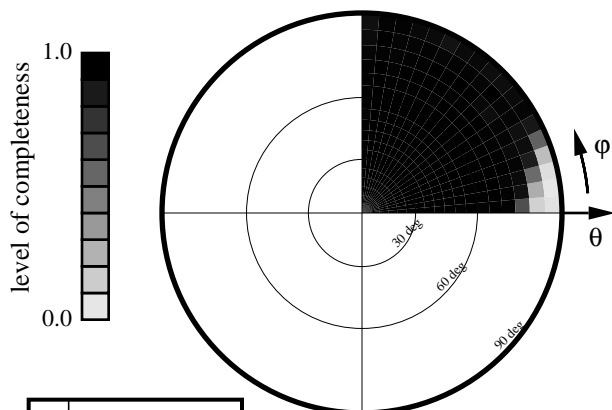
Scale: 0.851
 Bdiff: -8.20
 Anisothermal Scaling (Beta):
 -2.5642 -2.8286 -2.7769 0.0000 0.0000 -0.0000
 Solvent correction - Ks,Bs: 0.335 249.862

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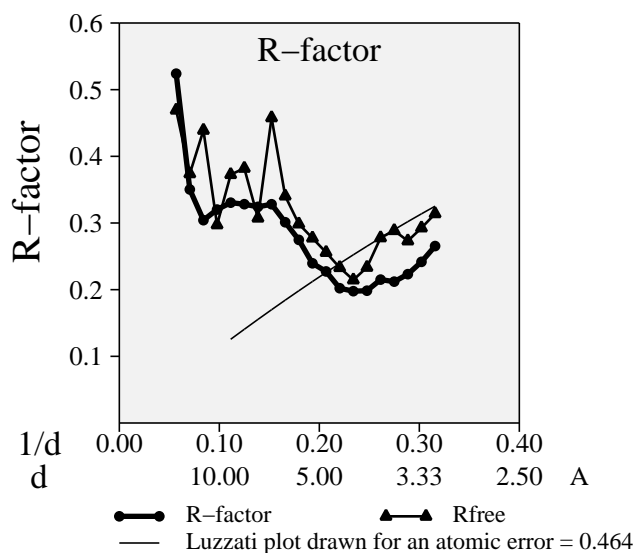


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

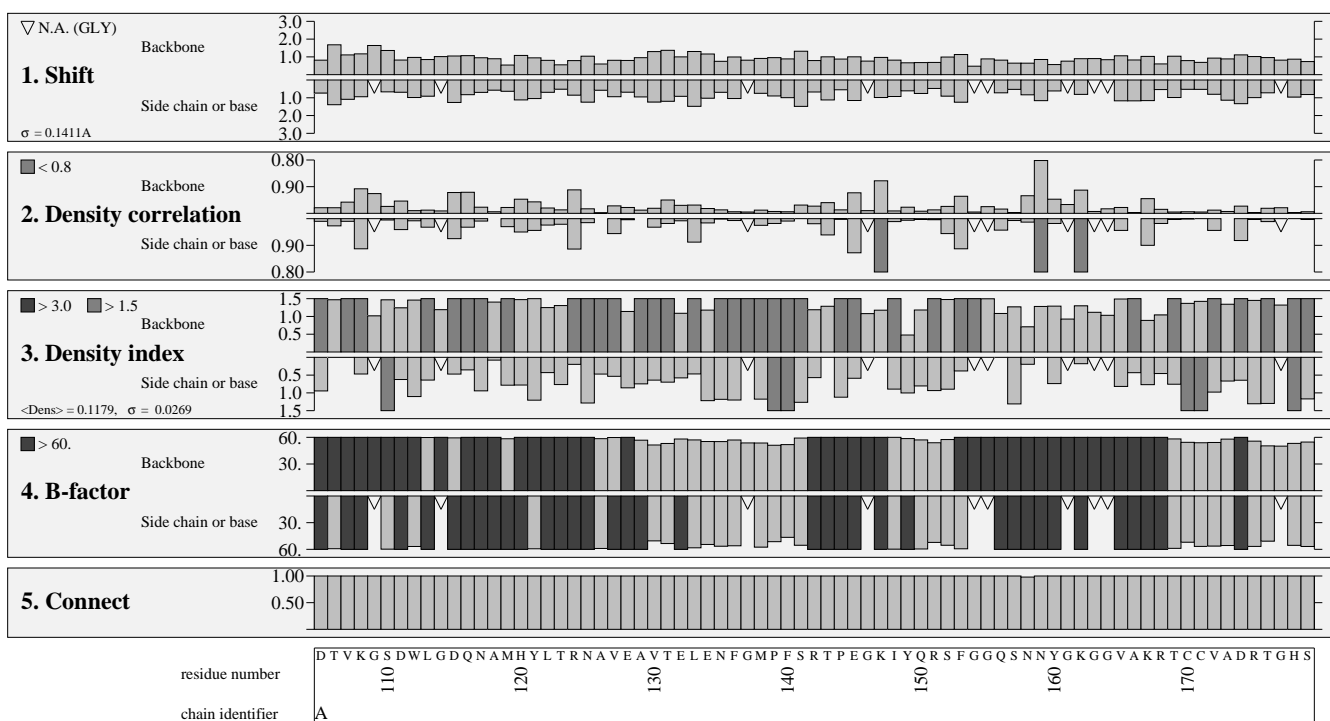
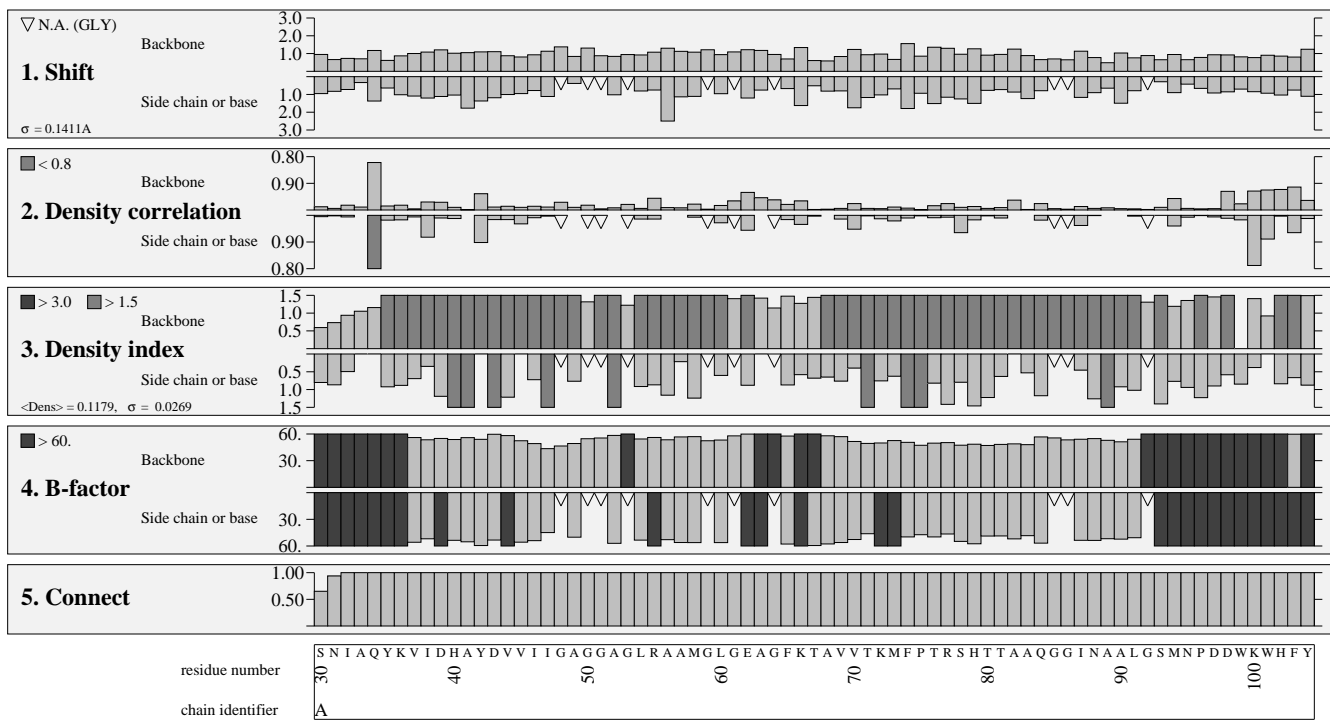
polar coordinates of the crystallographical axes



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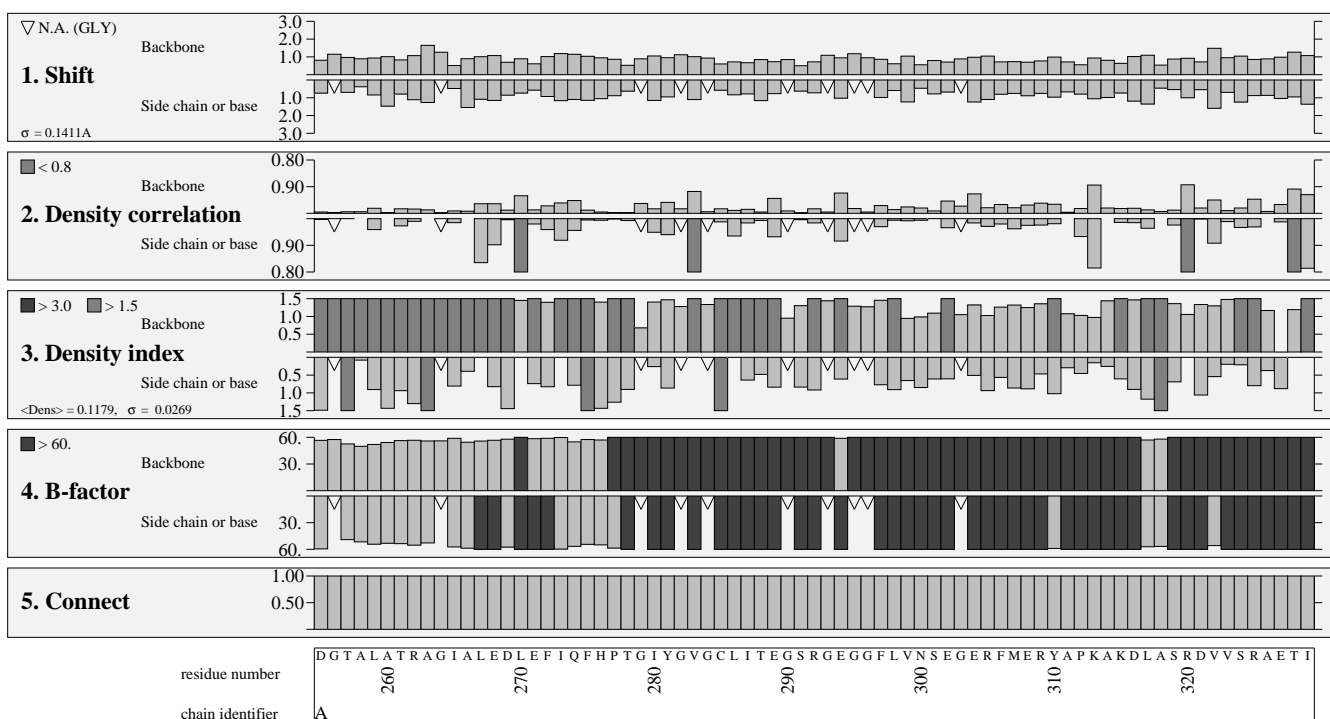
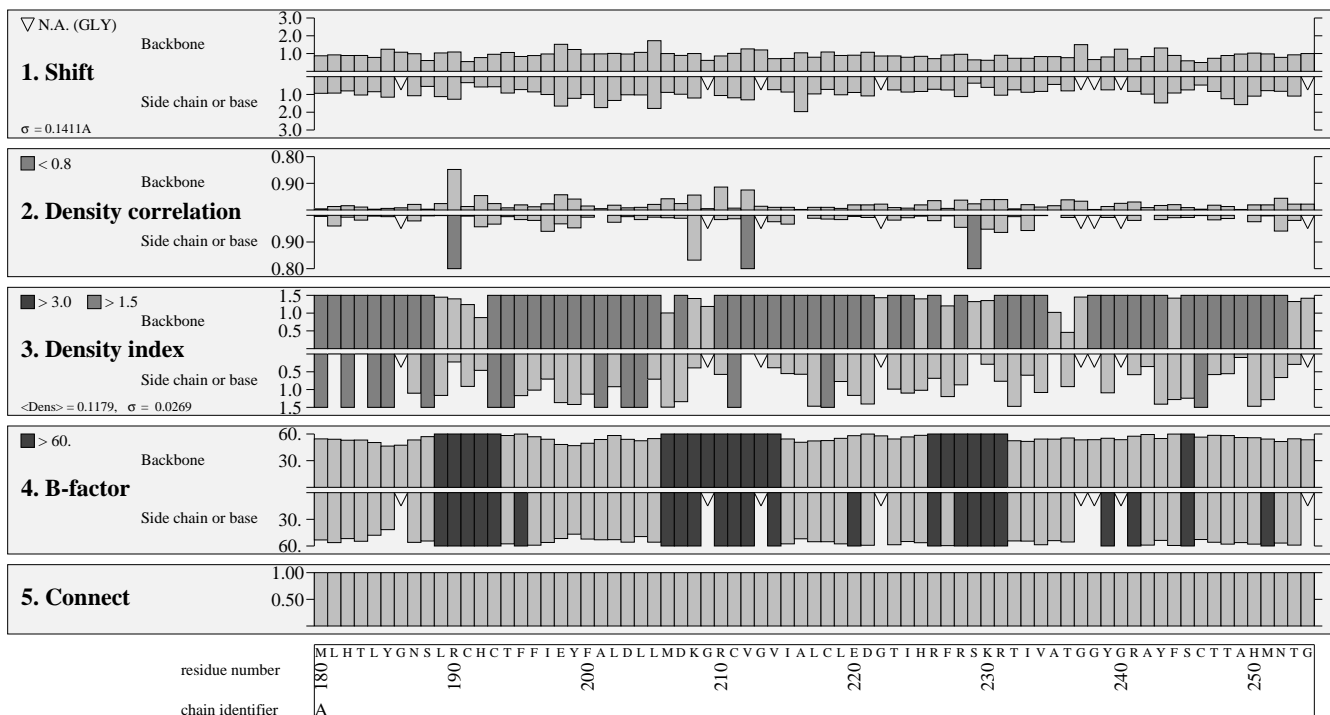
Local estimation



Structure Factor Check

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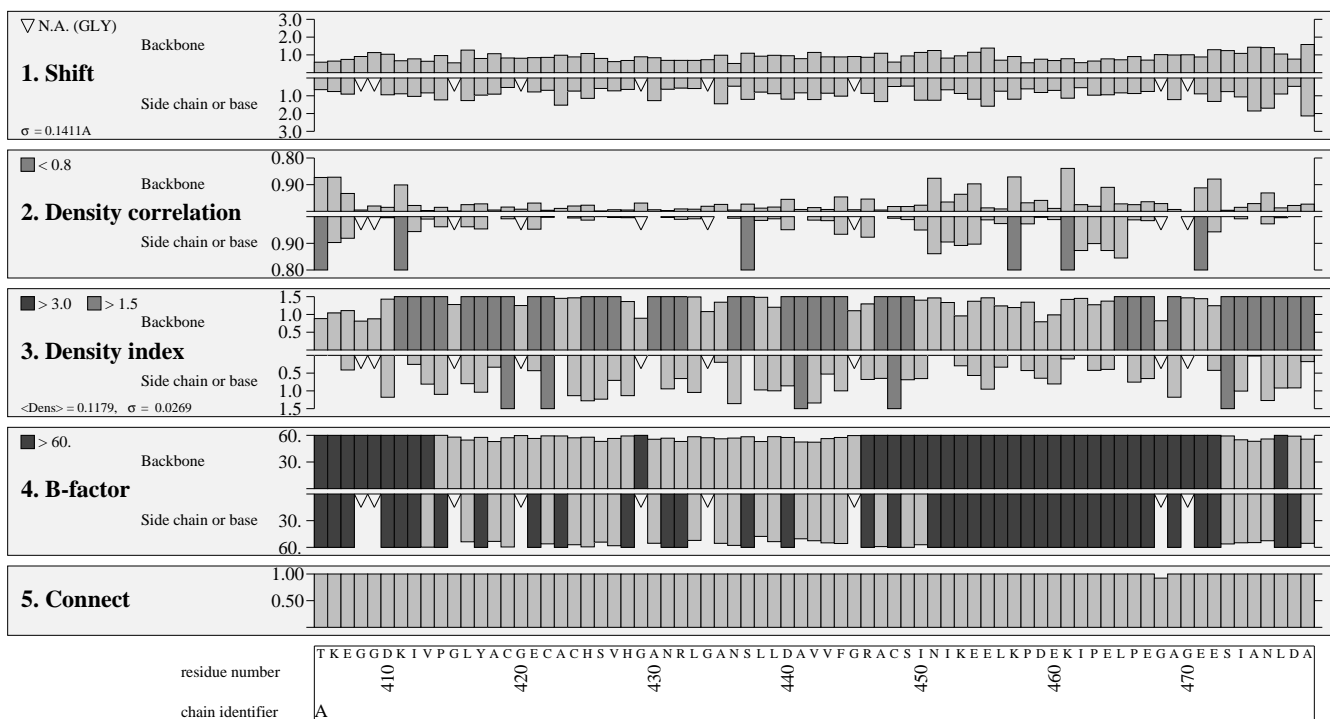
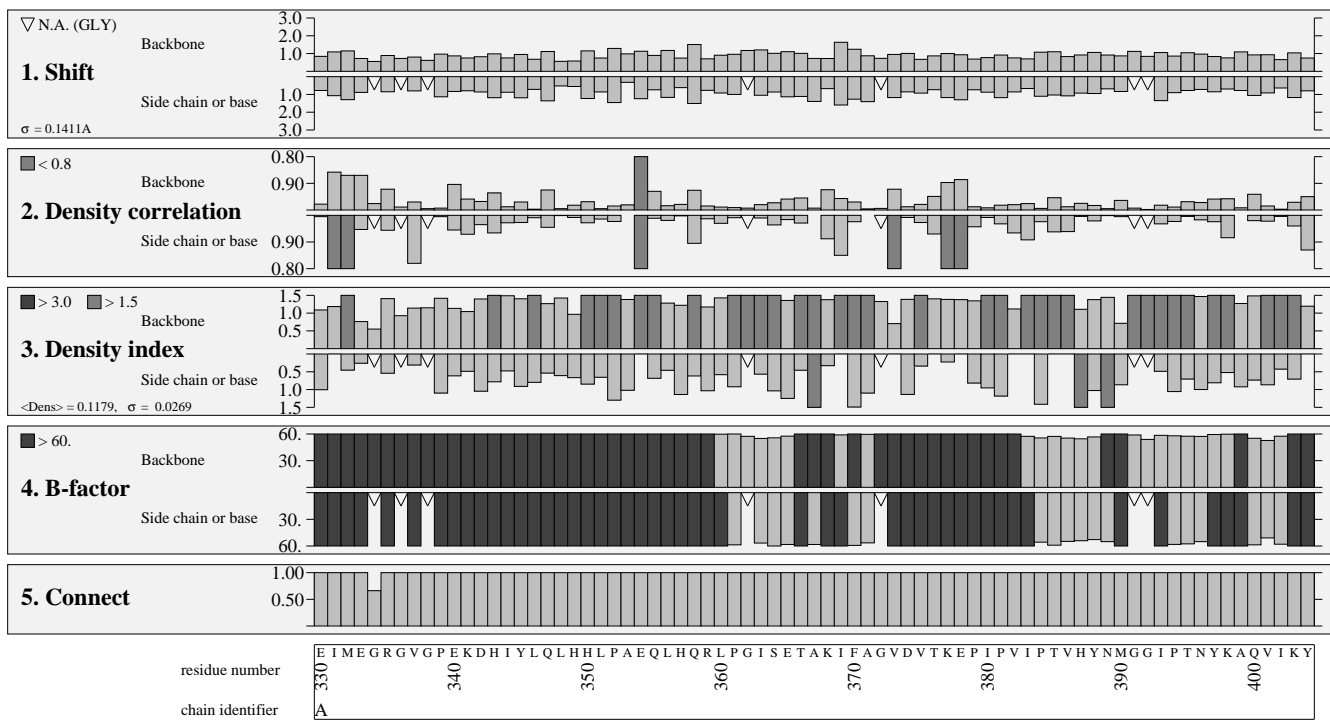
Local estimation (2)



Structure Factor Check

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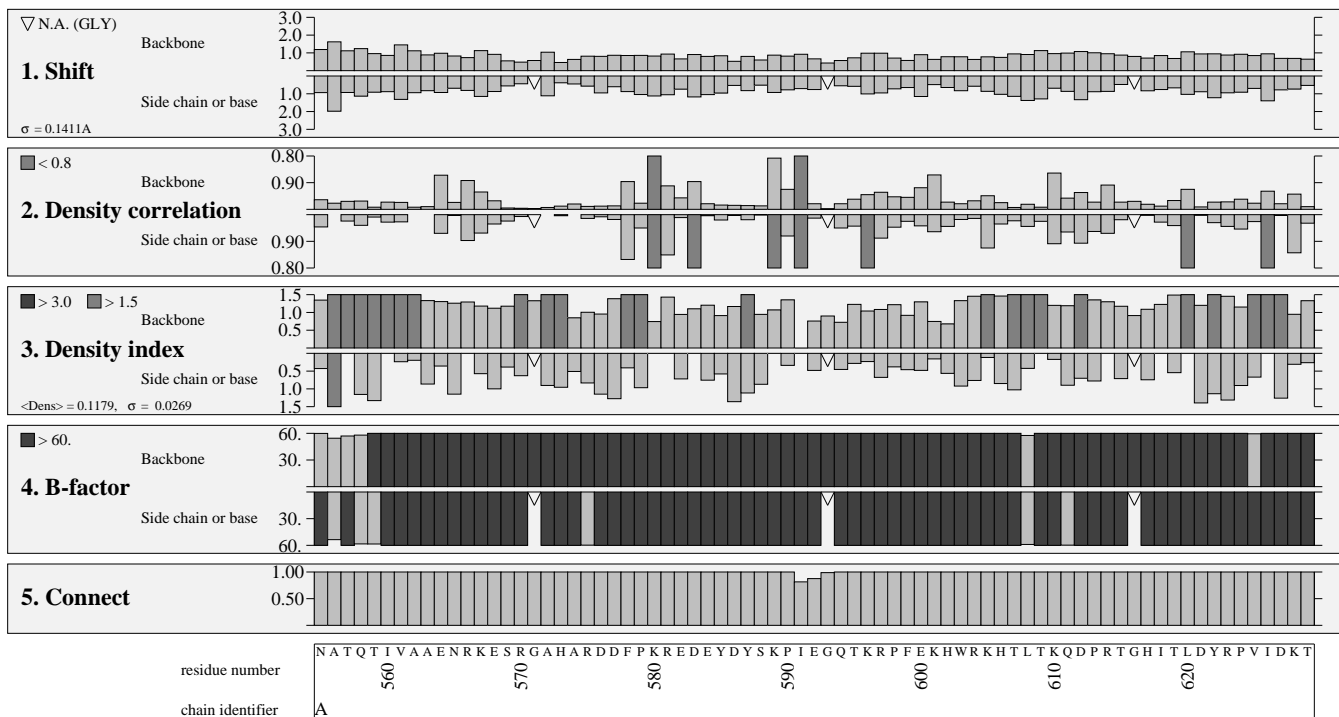
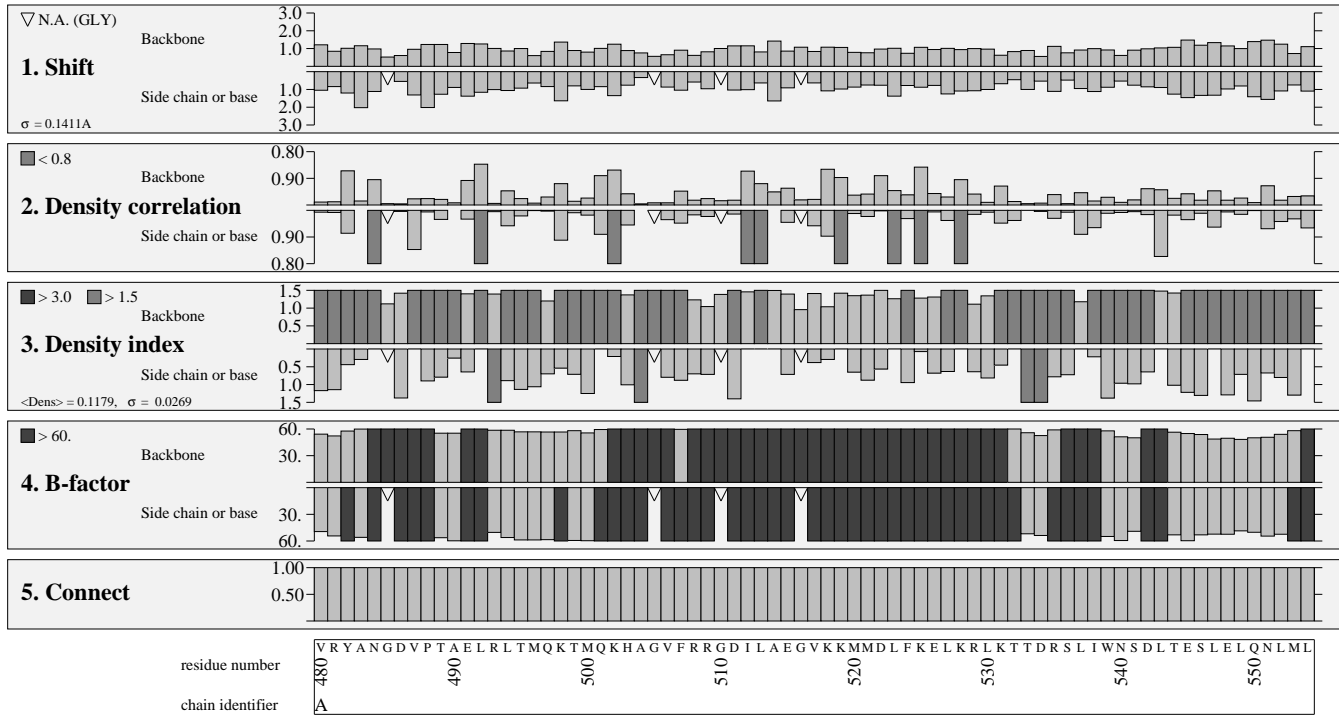
Local estimation (3)



Structure Factor Check

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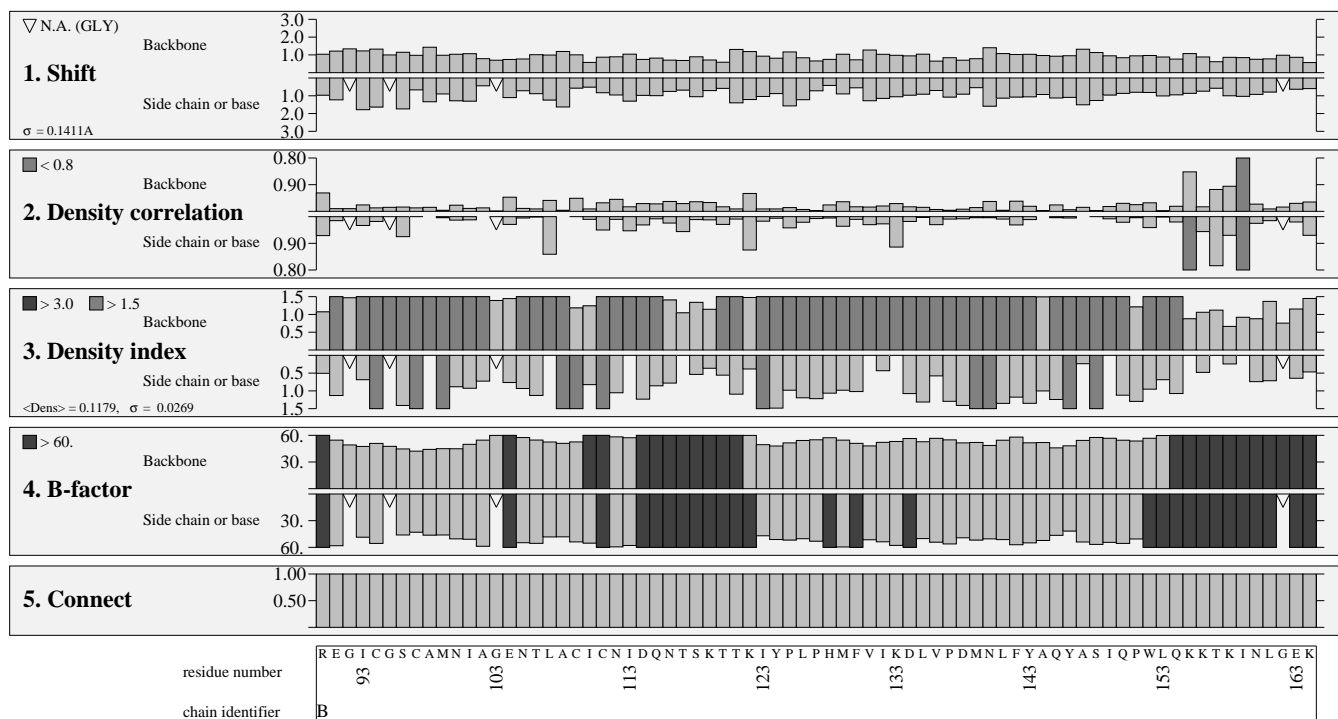
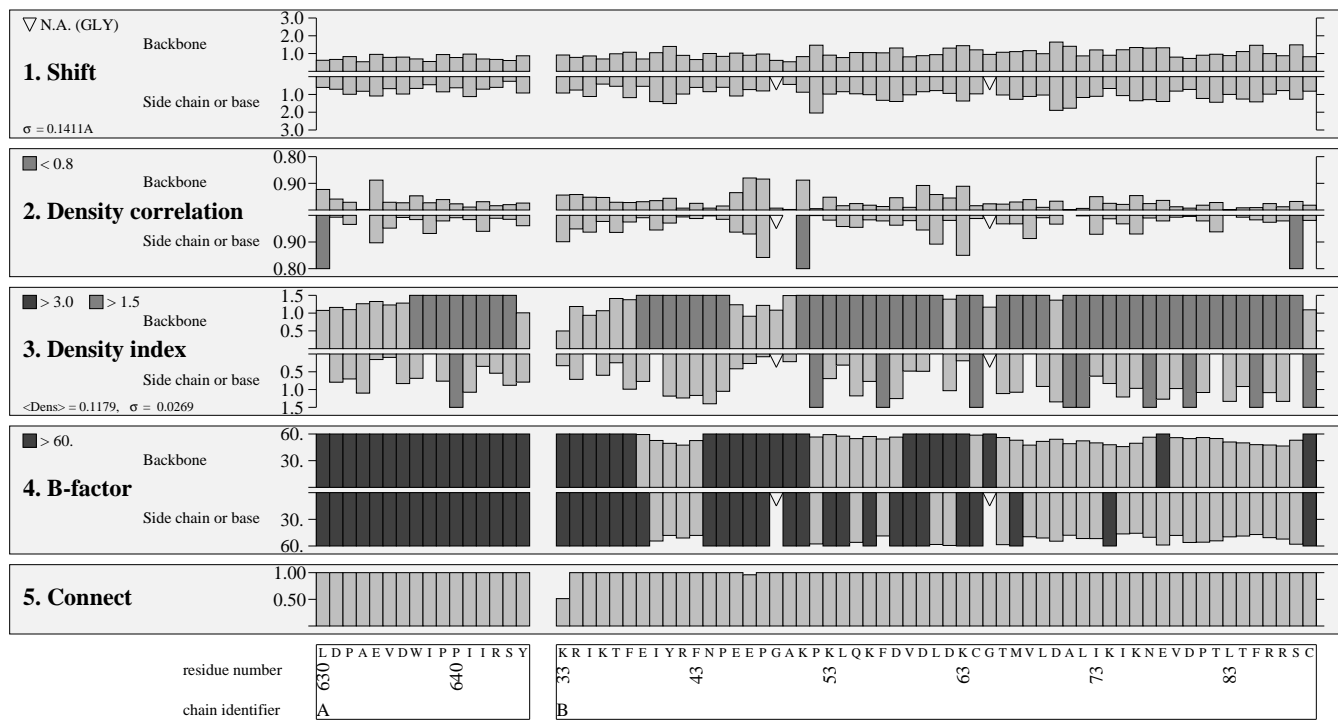
Local estimation (4)



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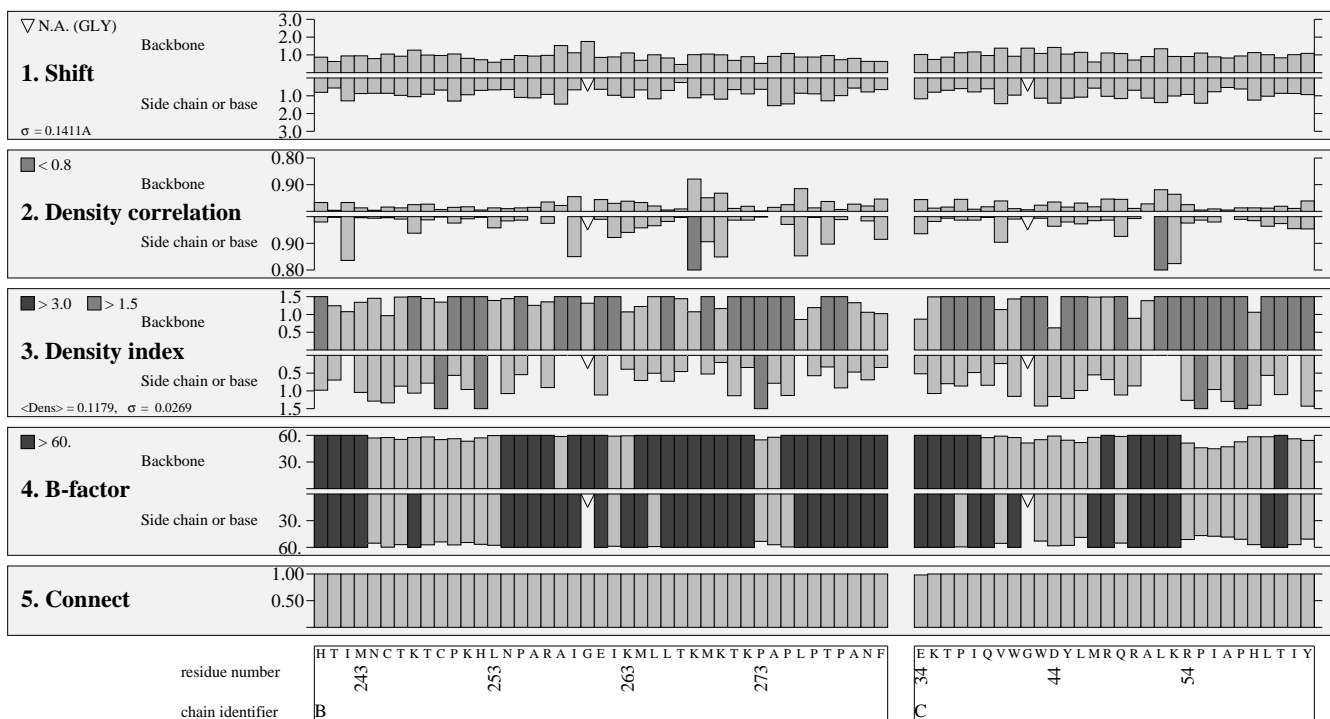
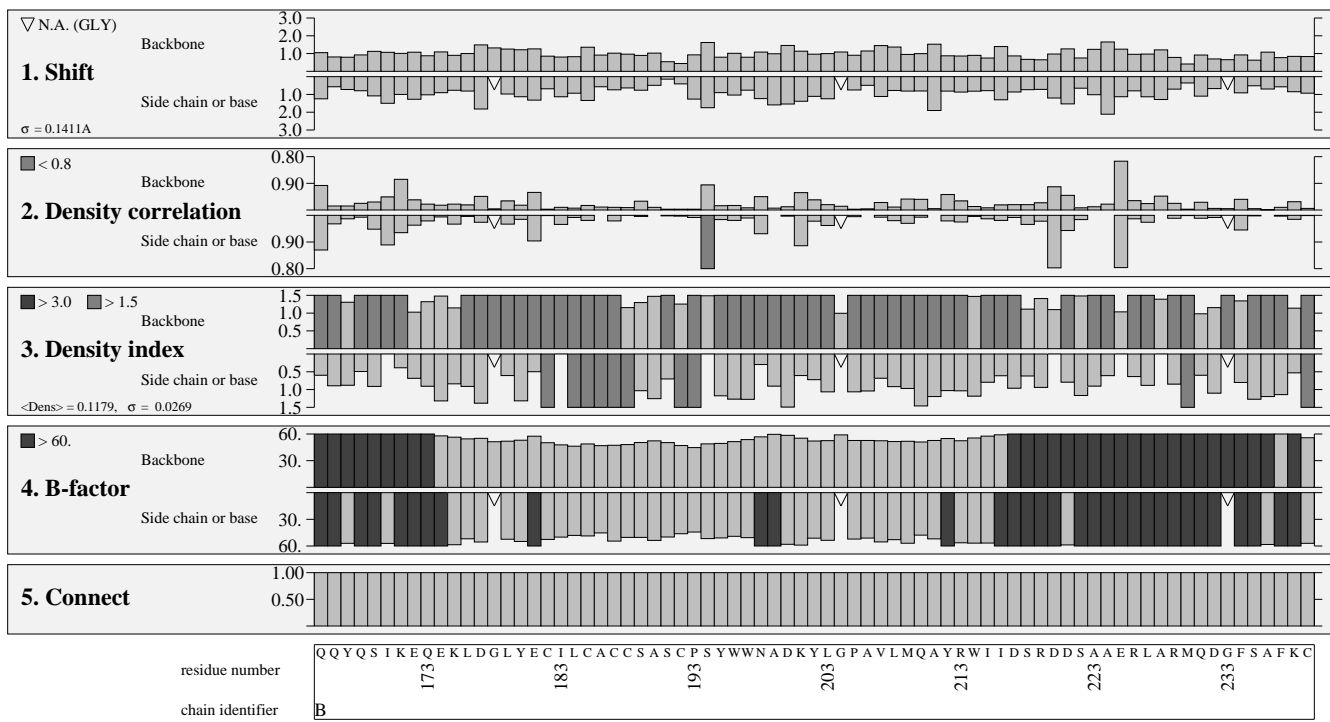
Local estimation (5)



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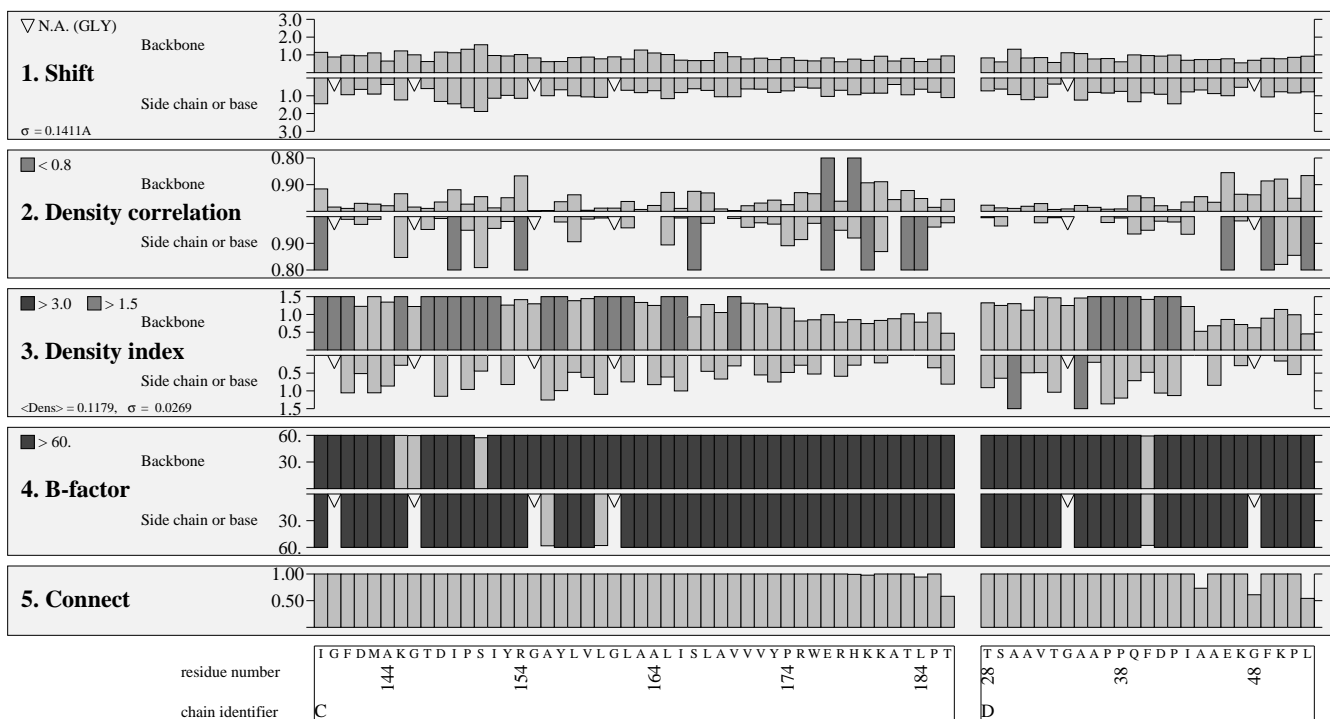
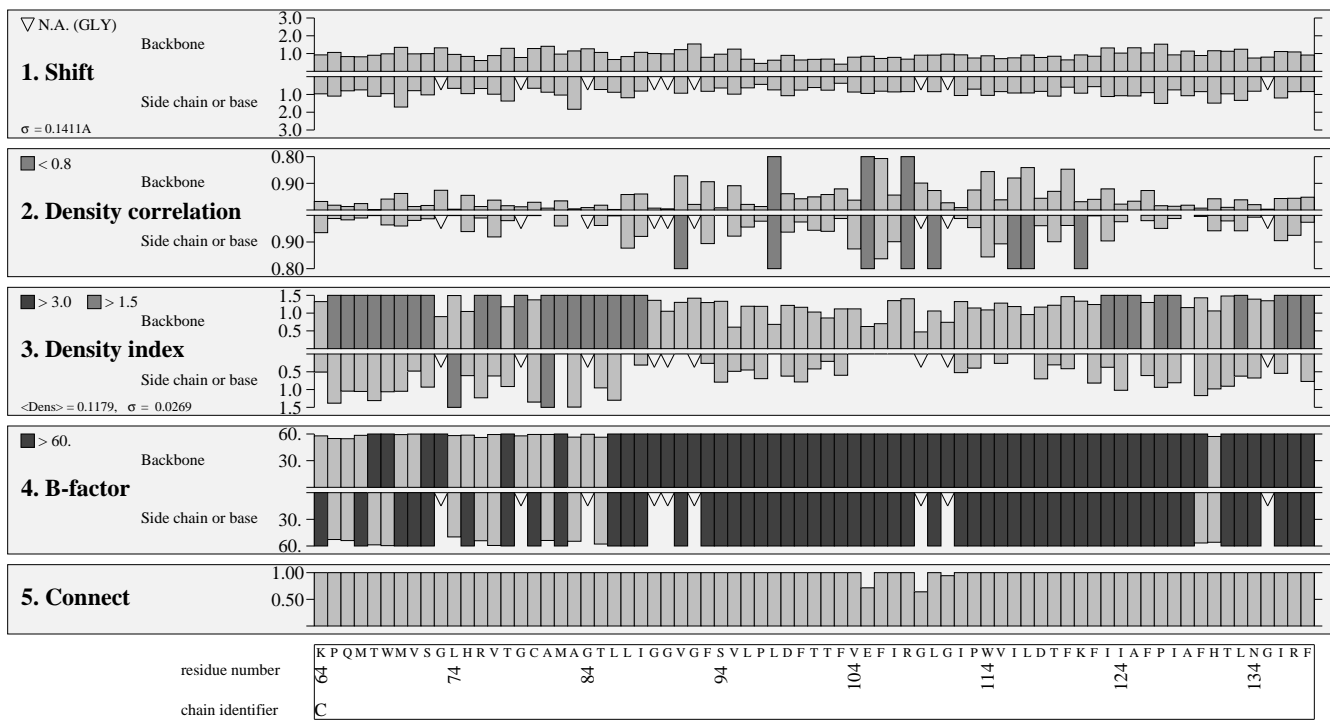
Local estimation (6)



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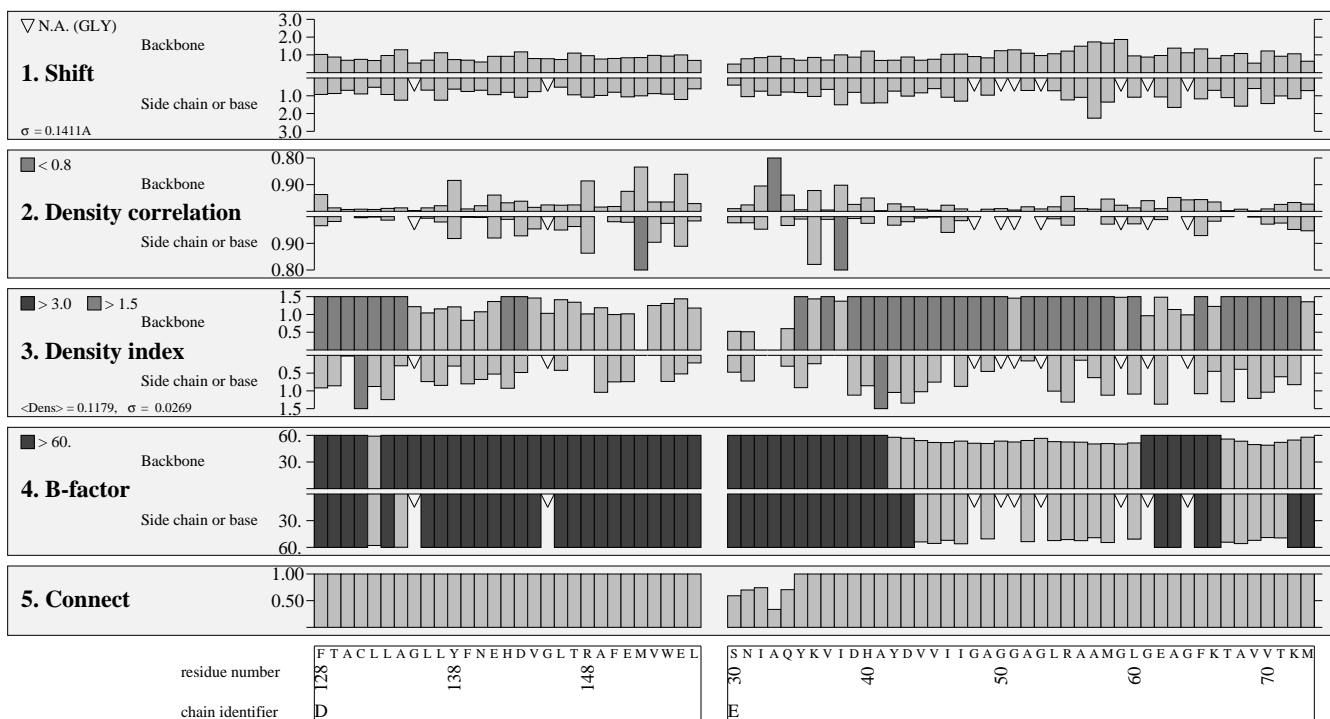
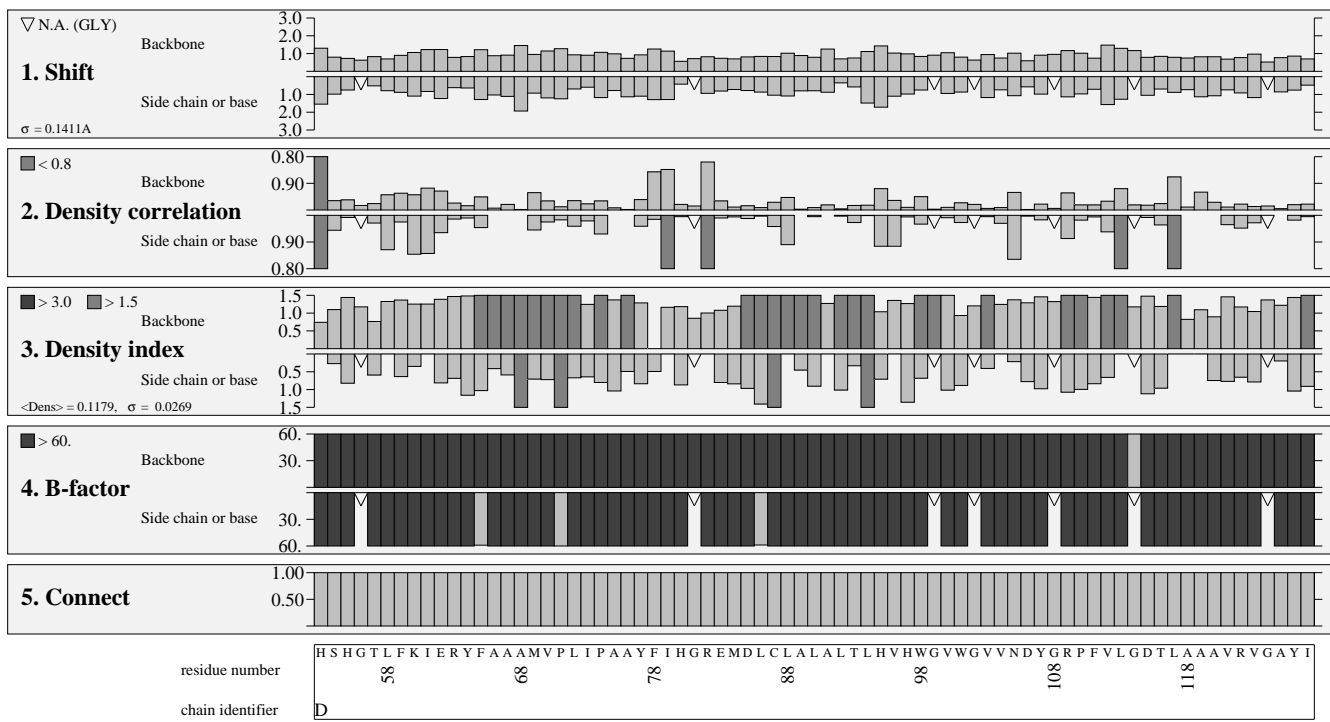
Local estimation (7)



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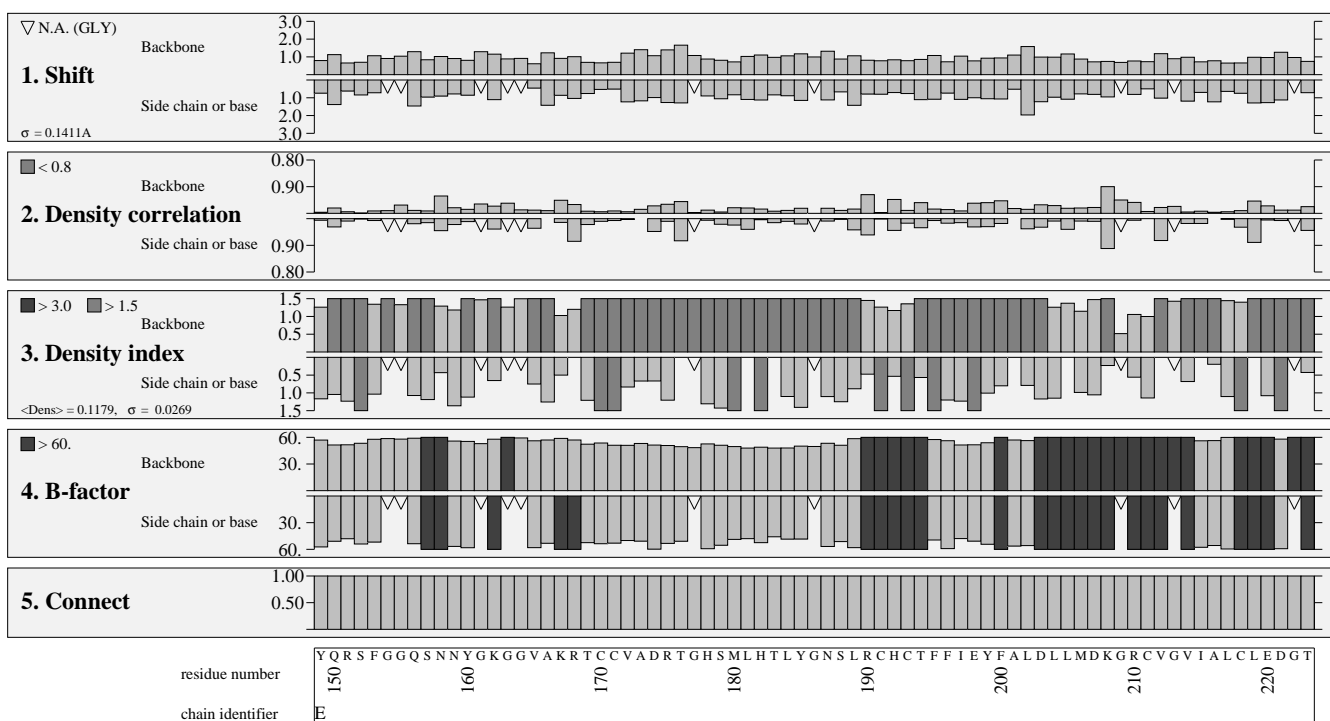
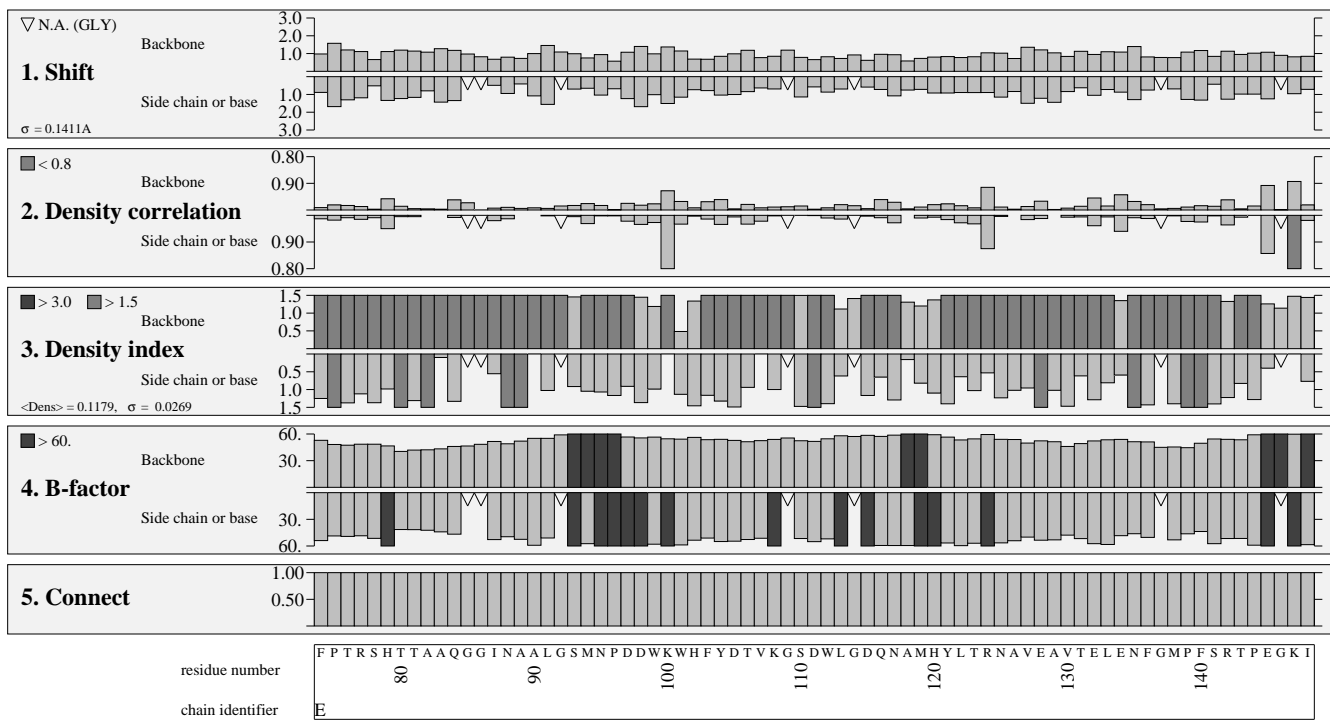
Local estimation (8)



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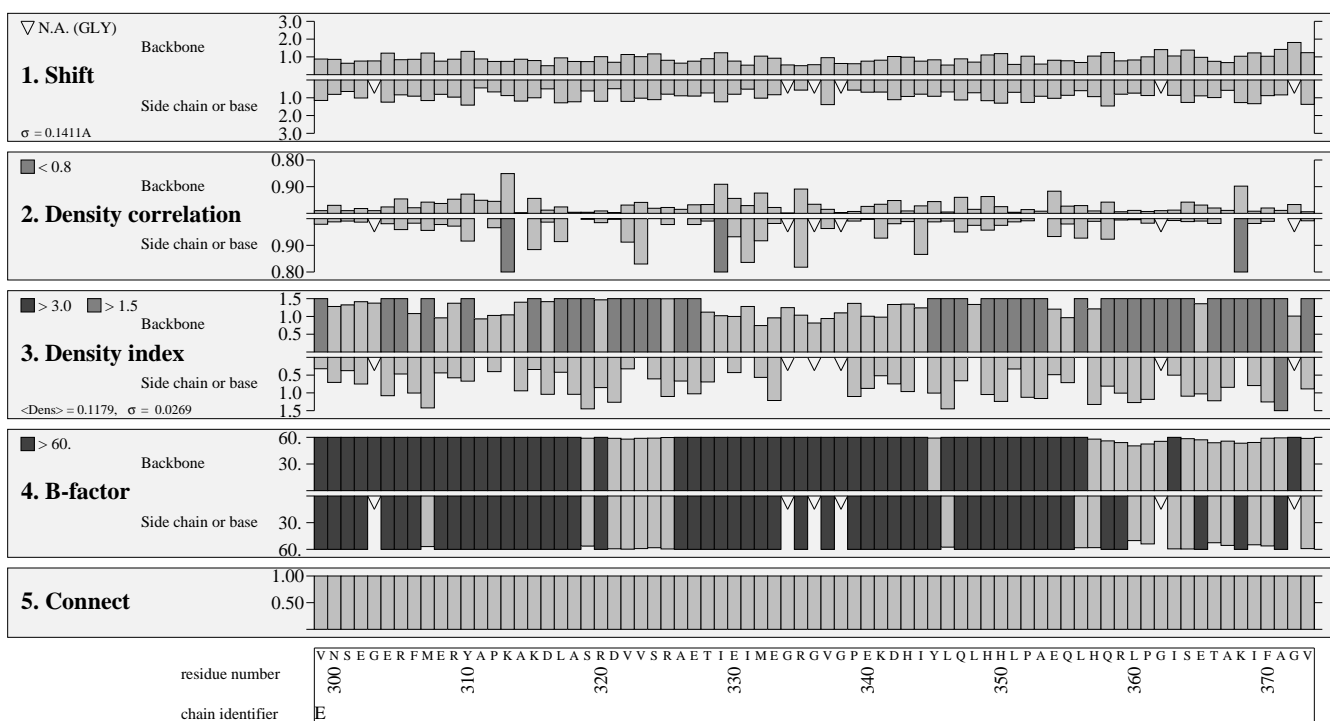
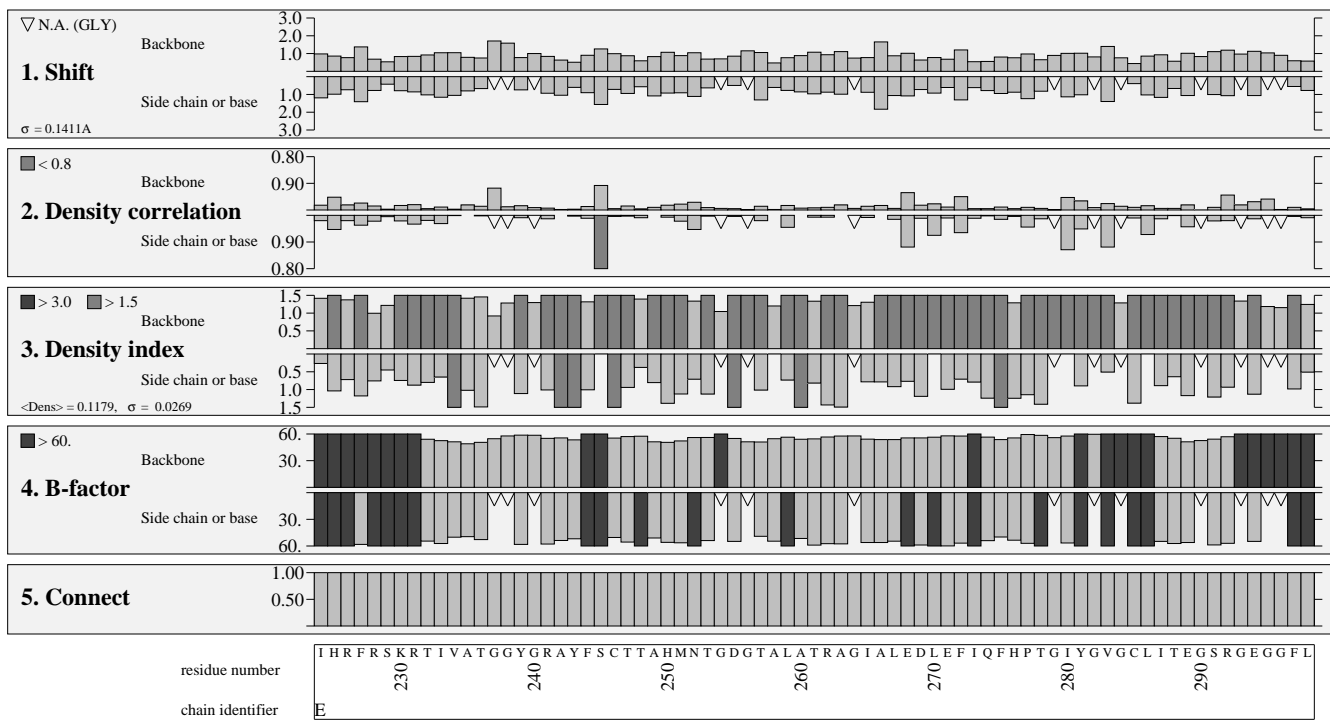
Local estimation (9)



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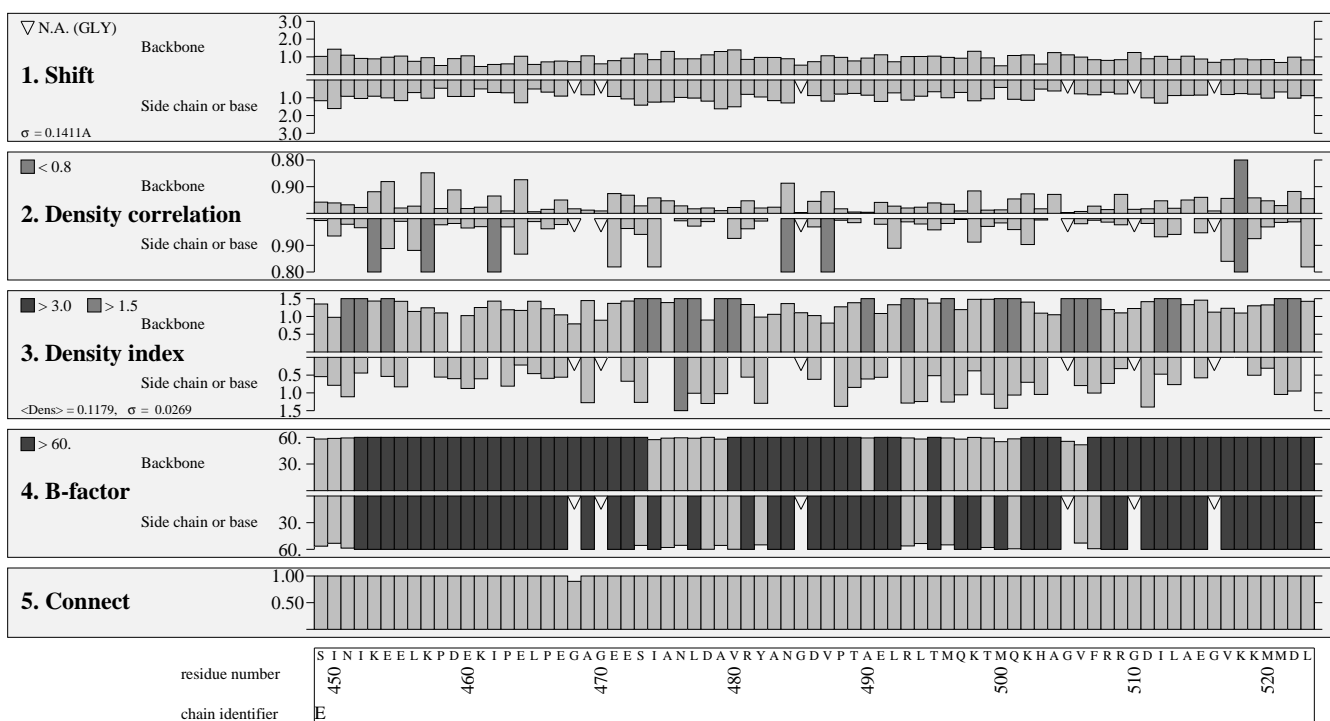
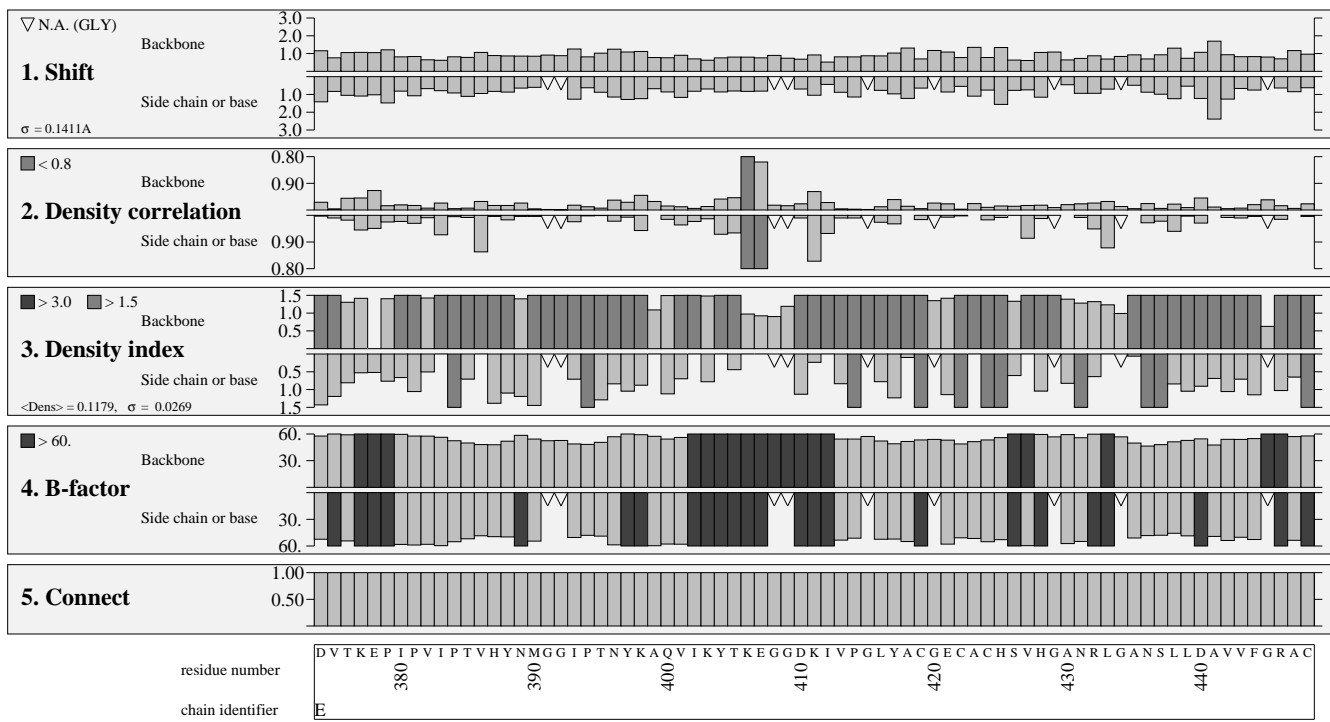
Local estimation (10)



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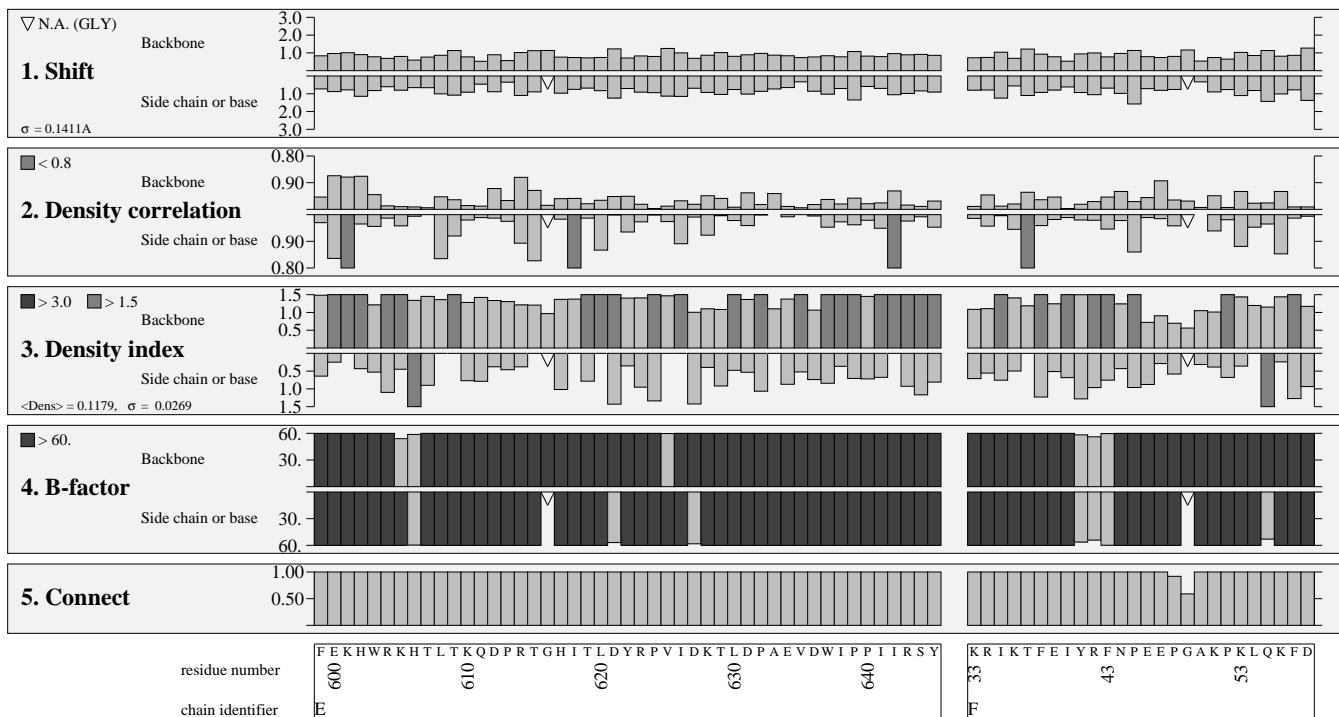
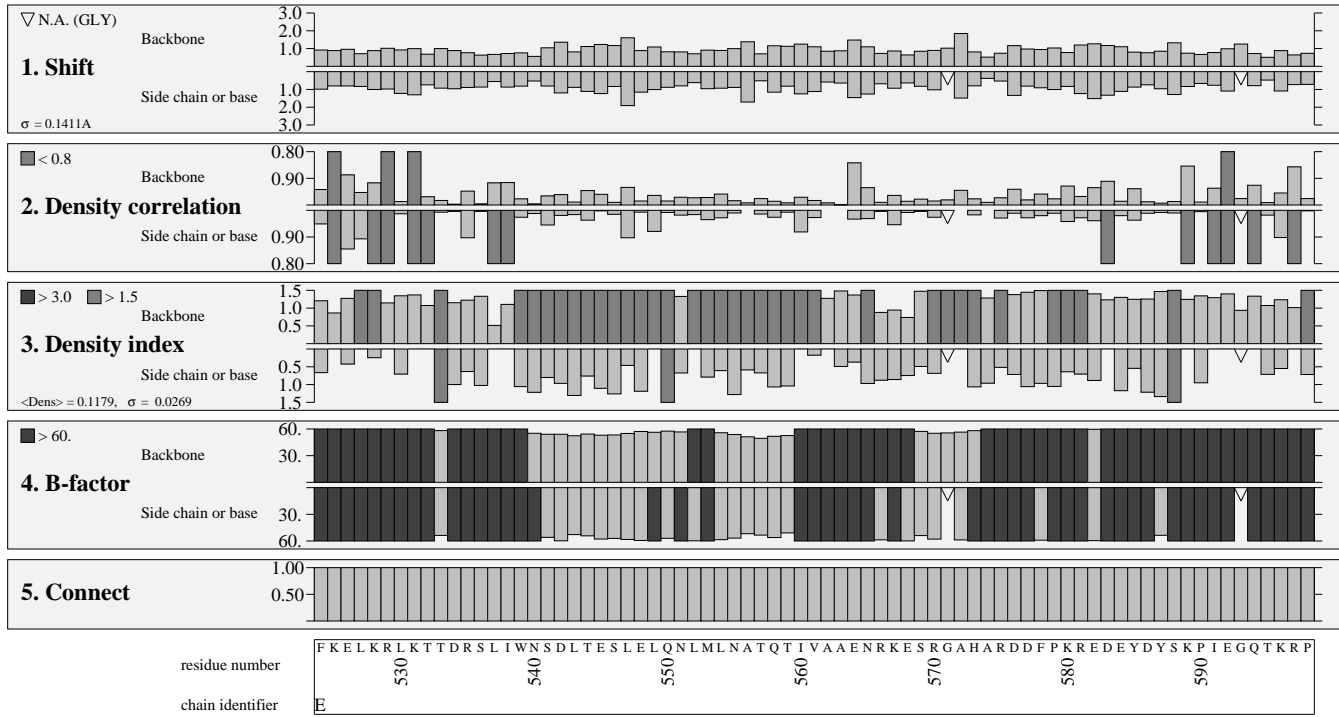
Local estimation (11)



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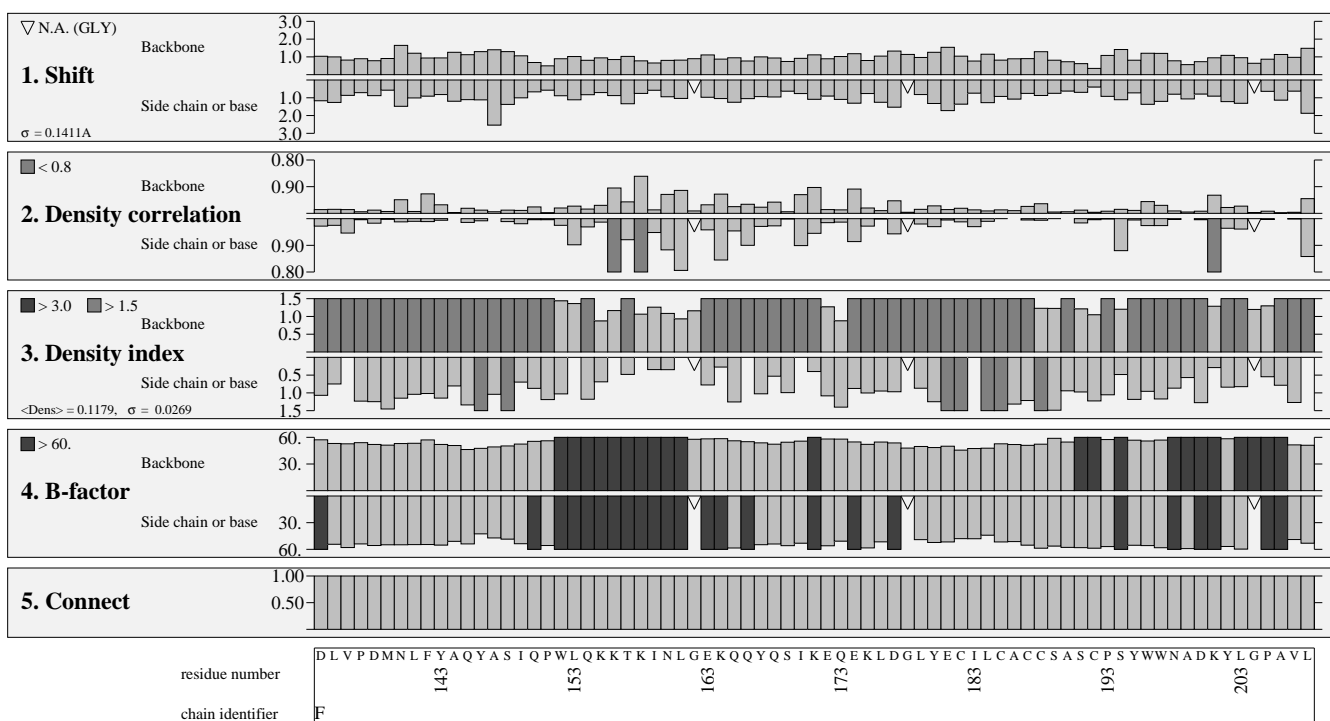
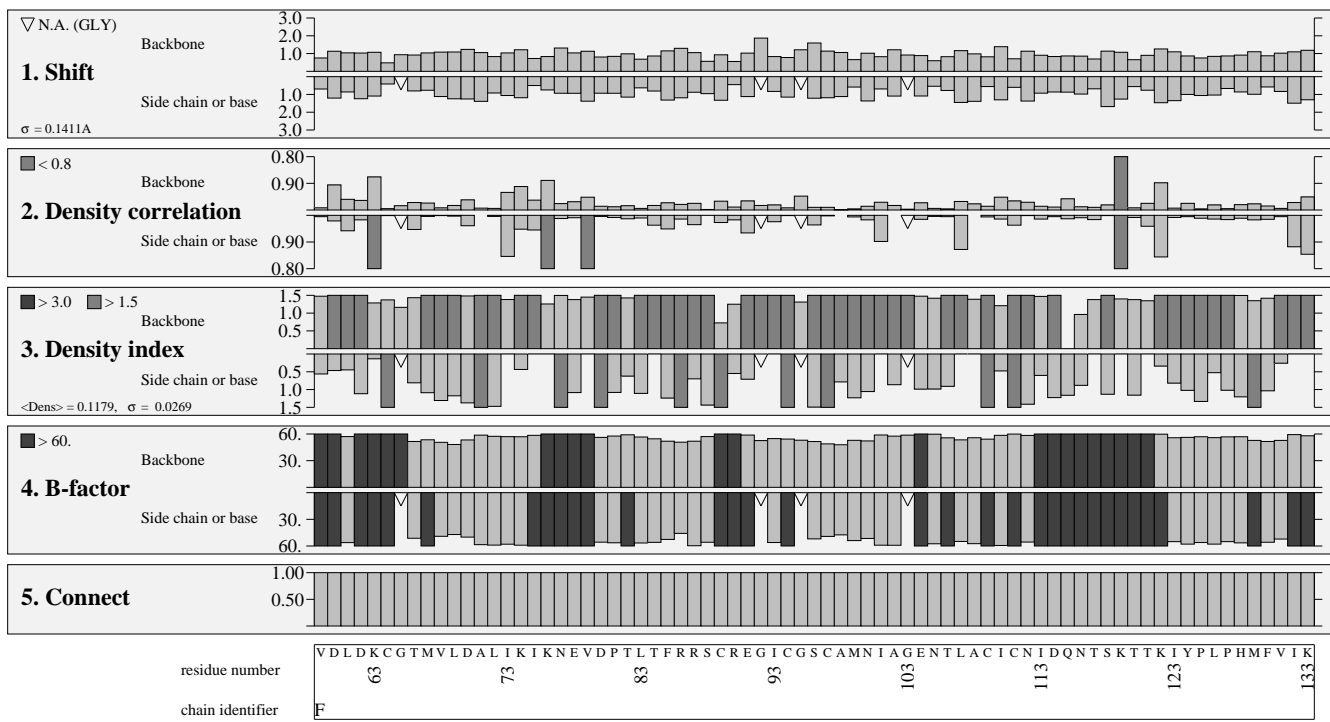
Local estimation (12)



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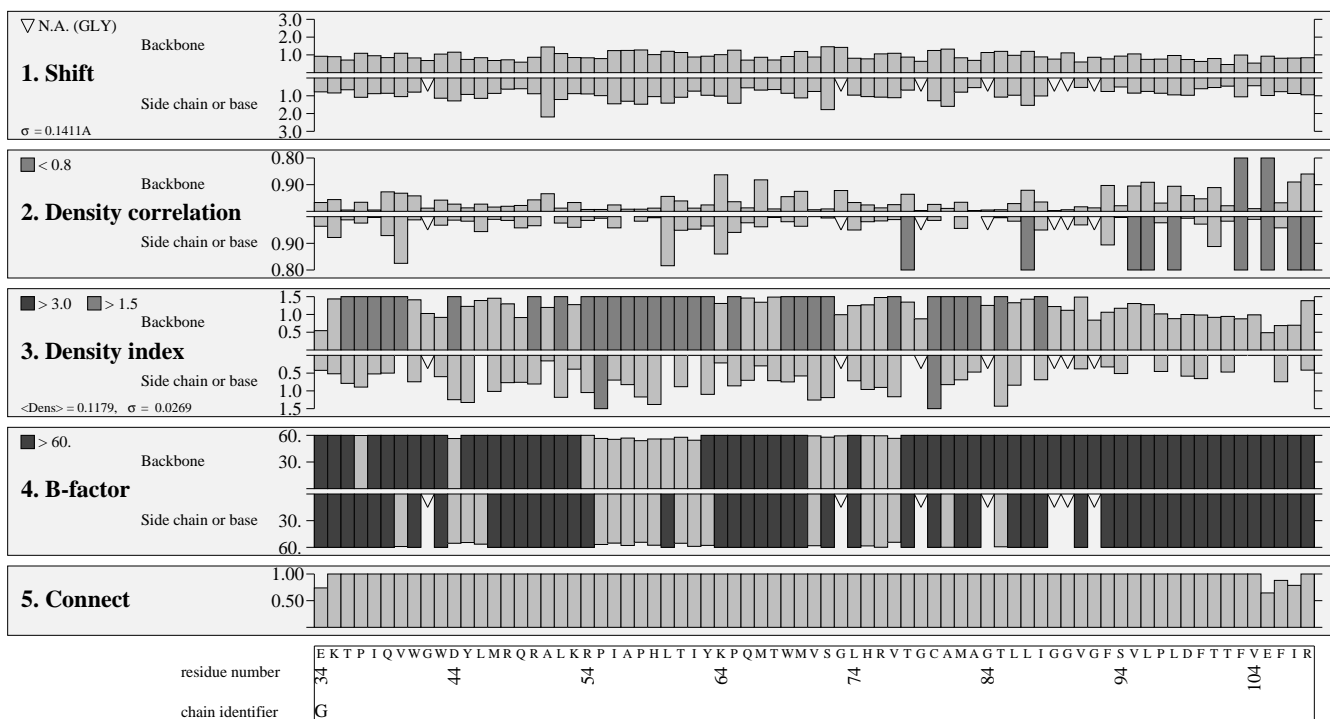
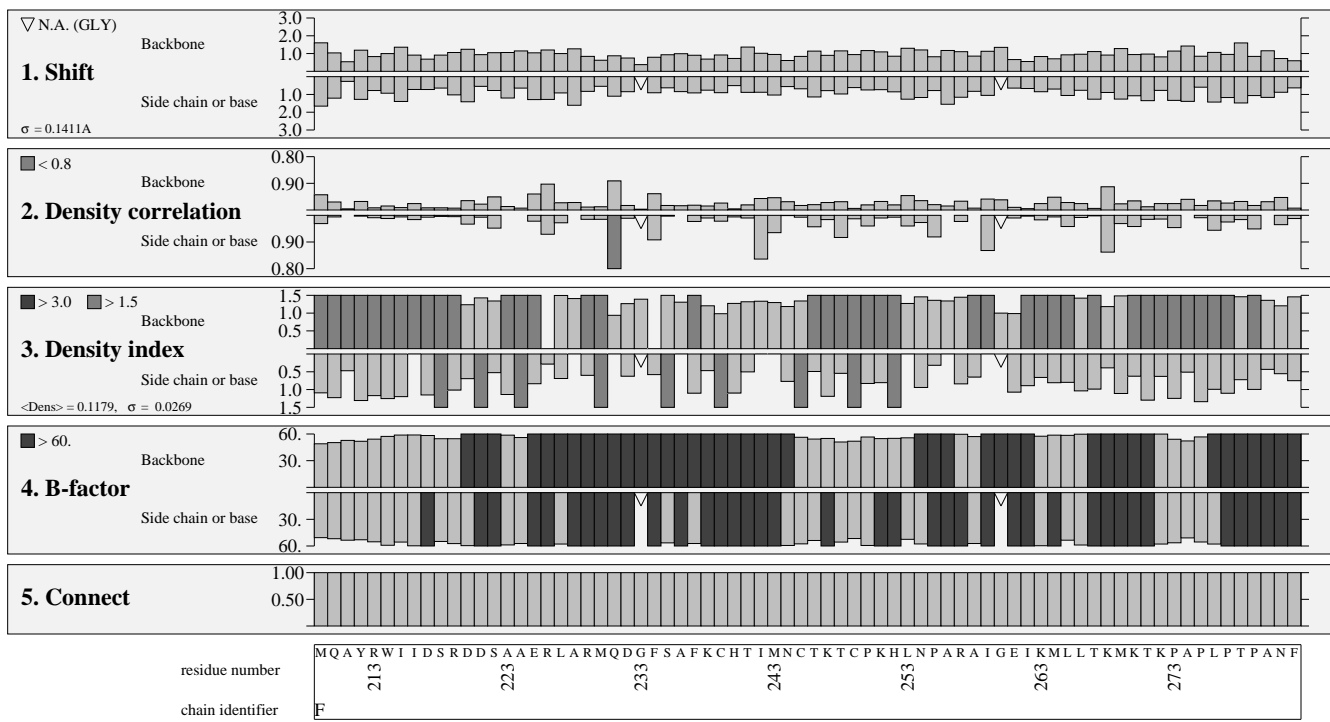
Local estimation (13)



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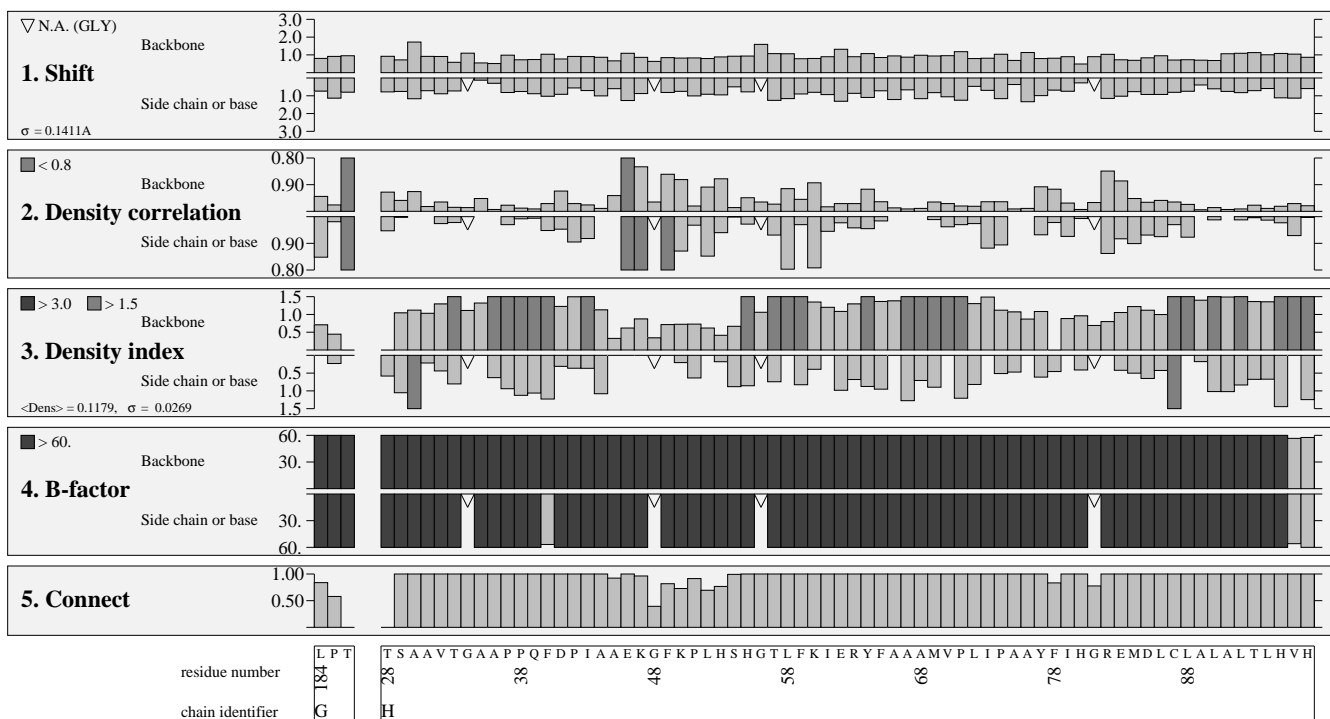
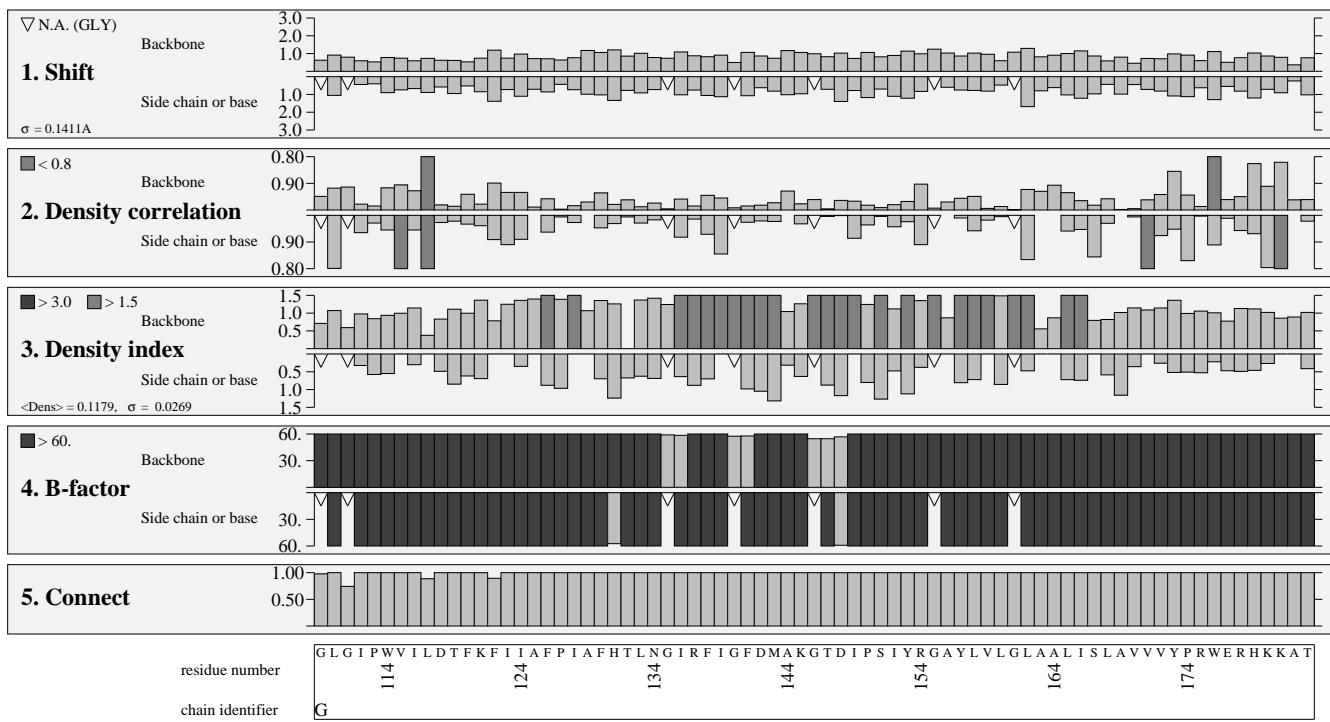
Local estimation (14)



Structure Factor Check

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Local estimation (15)



Structure Factor Check

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Local estimation (16)

