

Structure Factor Check

3VR9

Title: MITOCHONDRIAL RHODOQUINOL-FUMARATE REDUCTASE FROM THE PARASITIC NEMATODE ASCARIS SUUM WITH THE SPECIFIC INHIBITOR FLUTOLANI
 Date: 07-APR-12
 PDB code: 3VR9

Crystal

Cell parameters:
 a: 124.01 Å b: 135.33 Å c: 220.50 Å
 α : 90.00 β : 90.00 γ : 90.00
 Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 47.4 – 3.01 Å
 Reflections in file: 68269
 Unique reflections above 0: 68269
 above 1 σ : 66997
 above 3 σ : 39991

SFCHECK

Nominal resolution range: 47.4 – 3.01 Å
\05max. from input data, min. from author\05
 Used reflections: 68269
 Completeness: 92.0 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.091
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.9408 0.9615
 B_{overall} (by Patterson): 54.Å²
 Optical resolution: 2.25 Å
 Expected opt. resol. for complete data set: 2.25 Å
 Estimated minimal error: 0.089 Å

Model

18262 atoms
 Number of chains: 24
 Volume not occupied by model: 57.5 %
 $\langle B \rangle$ (for atomic model): 82.6 Å²
 $\sigma(B)$: 11.31 Å²
 Matthews coefficient: 3.62
 Corresponding solvent % : 65.74

Model vs. Structure Factors

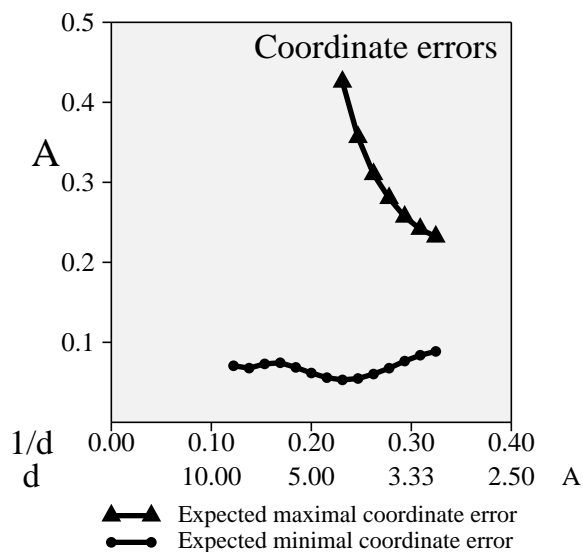
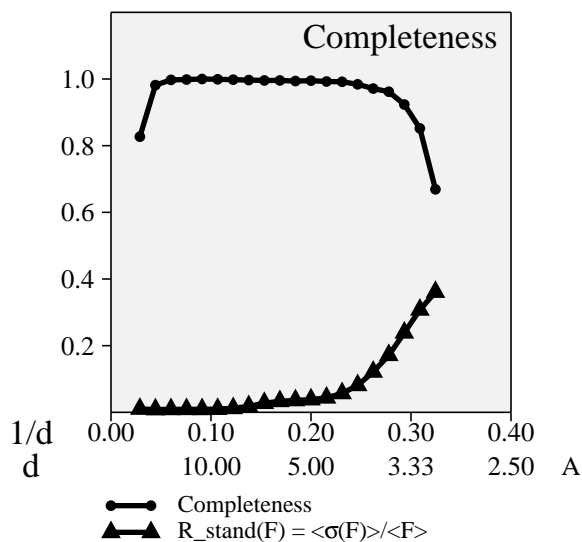
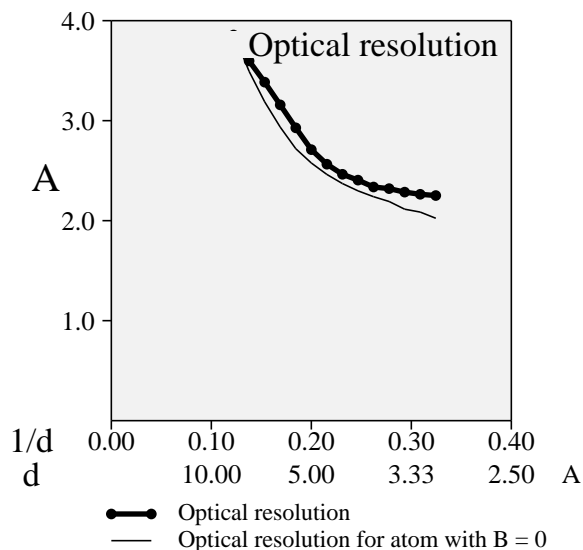
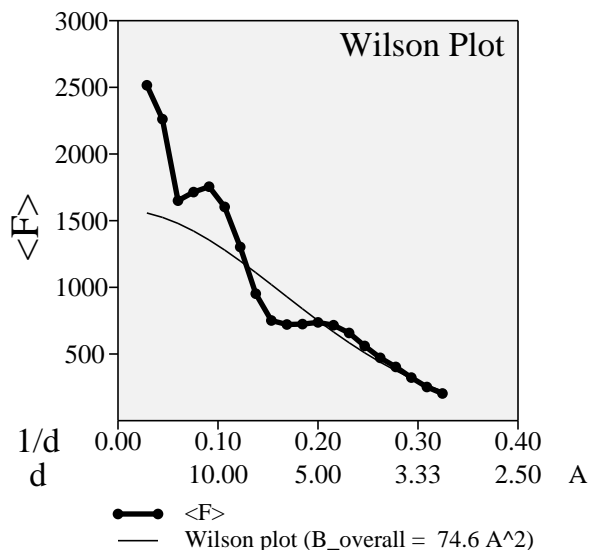
R-factor for all reflections: 0.276
 Correlation factor: 0.848
 R-factor: 0.283
 for $F > 2.0\sigma$
 nom. resolution range: 47.39 – 3.01 Å
 reflections used: 66996
 Rfree: 0.334
 Nfree: 3172
 R-factor without free-refl.: 0.281
 Non free-reflections: 63824
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.546 Å
 Estimated maximal error: 0.232 Å
 DPI: 0.443 Å
Scaling
 Scale: 0.848
 Bdiff: -8.32
 Anisothermal Scaling (Beta):
 1.6306 1.3729 1.1502 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.541 250.096

Refinement

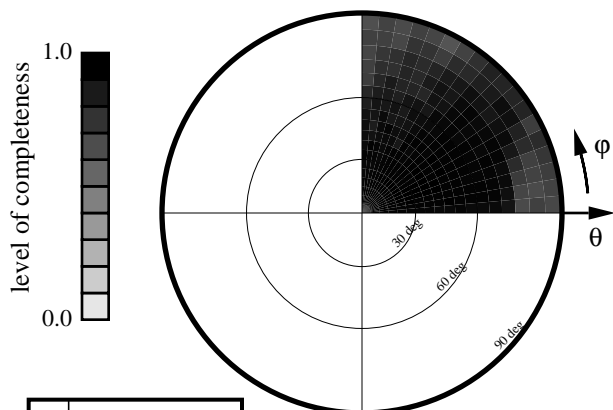
Program: REFMAC 5.5.0109
 Nominal resolution range: 47.4 – 3.01 Å
 Reported R-factor: 0.216
 Number of reflections used: 65024
 Reported Rfree: 0.28
 Sigma cut-off: N.A.

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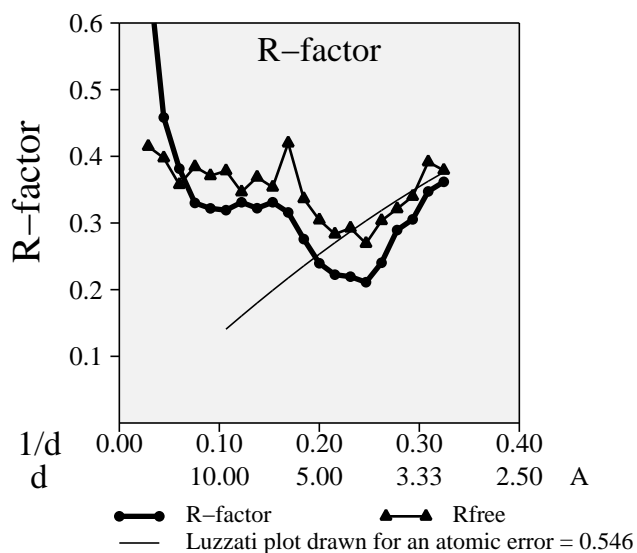


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

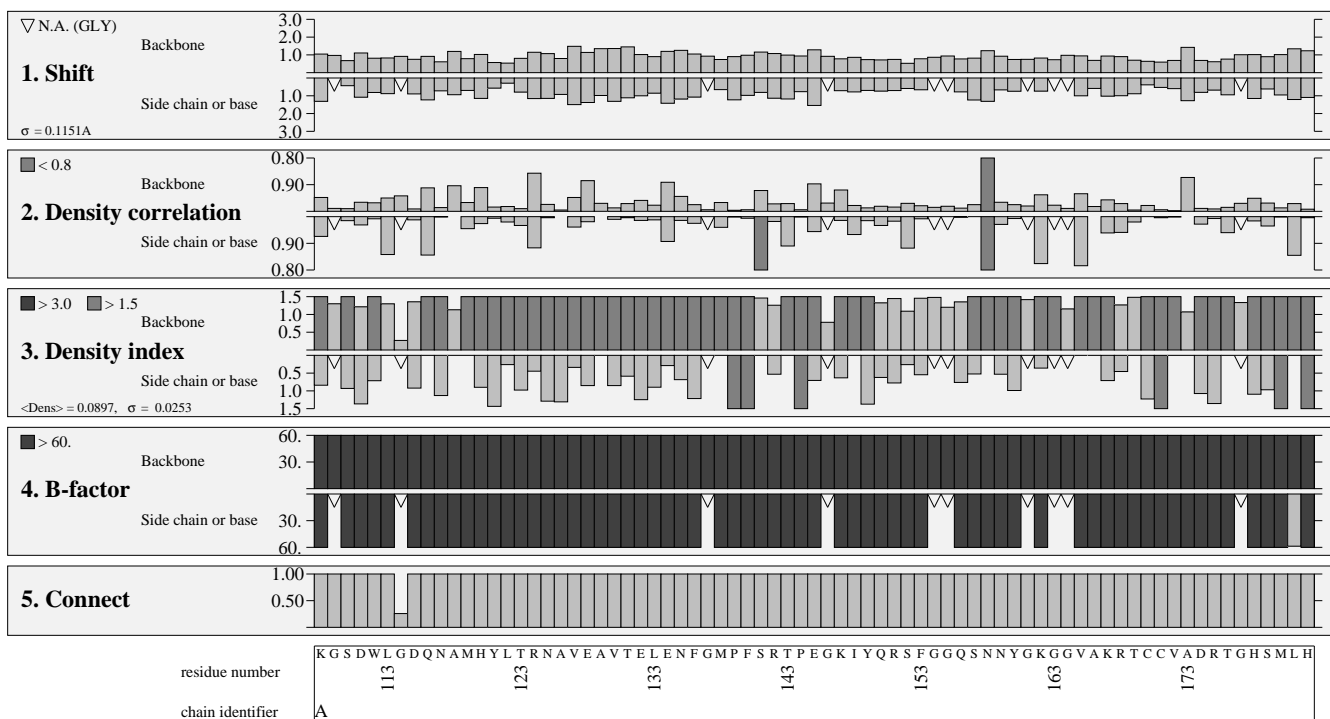
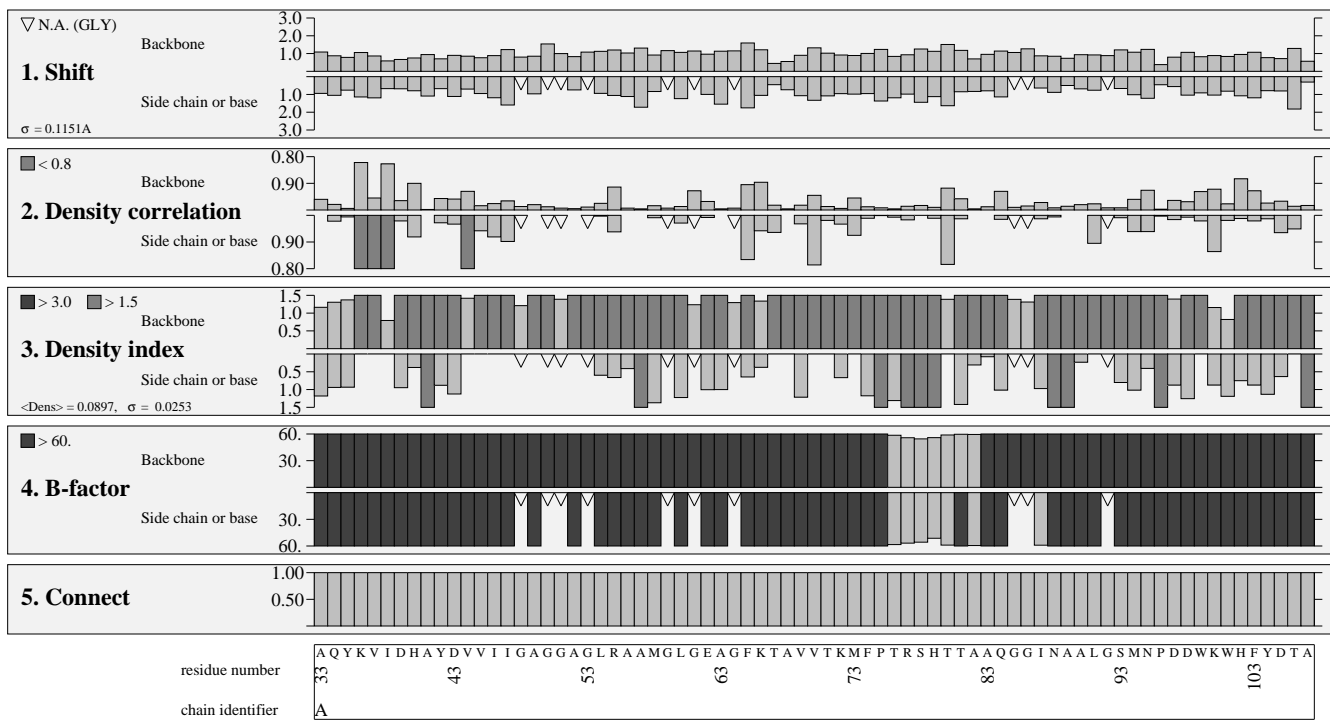
polar coordinates of the crystallographical axes



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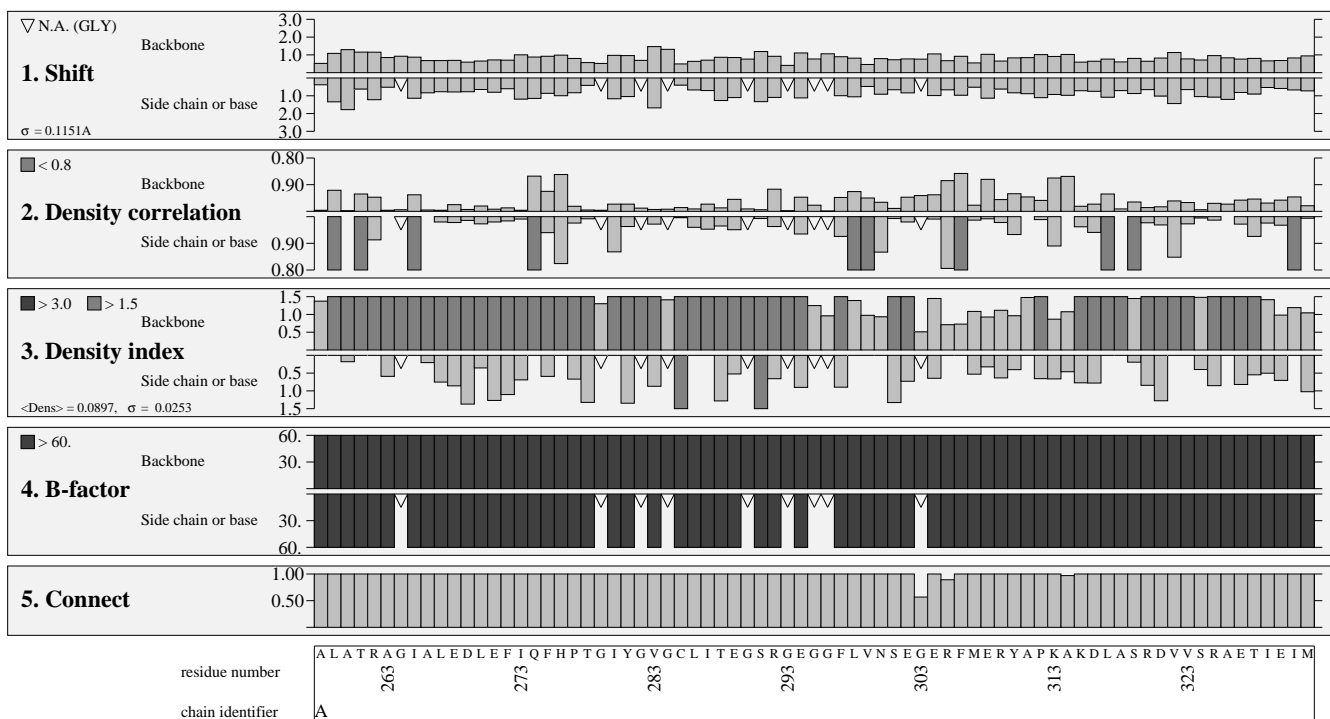
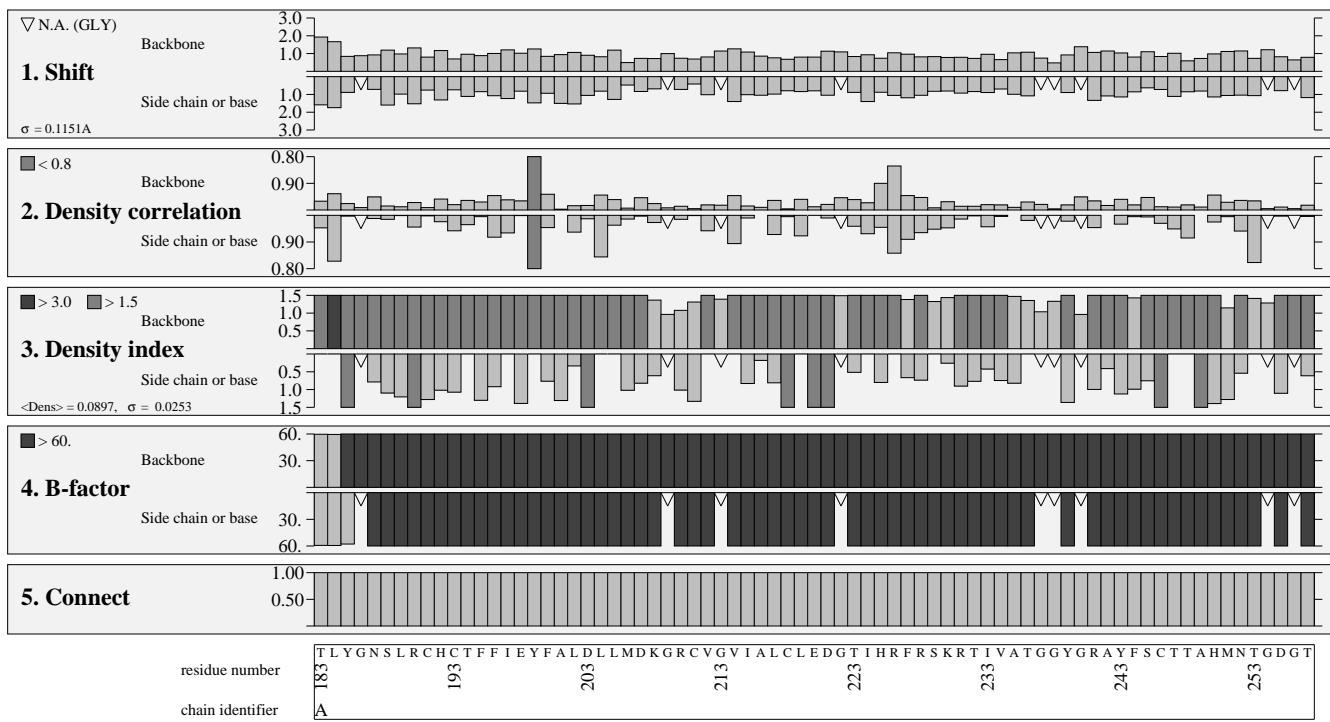
Local estimation



Structure Factor Check

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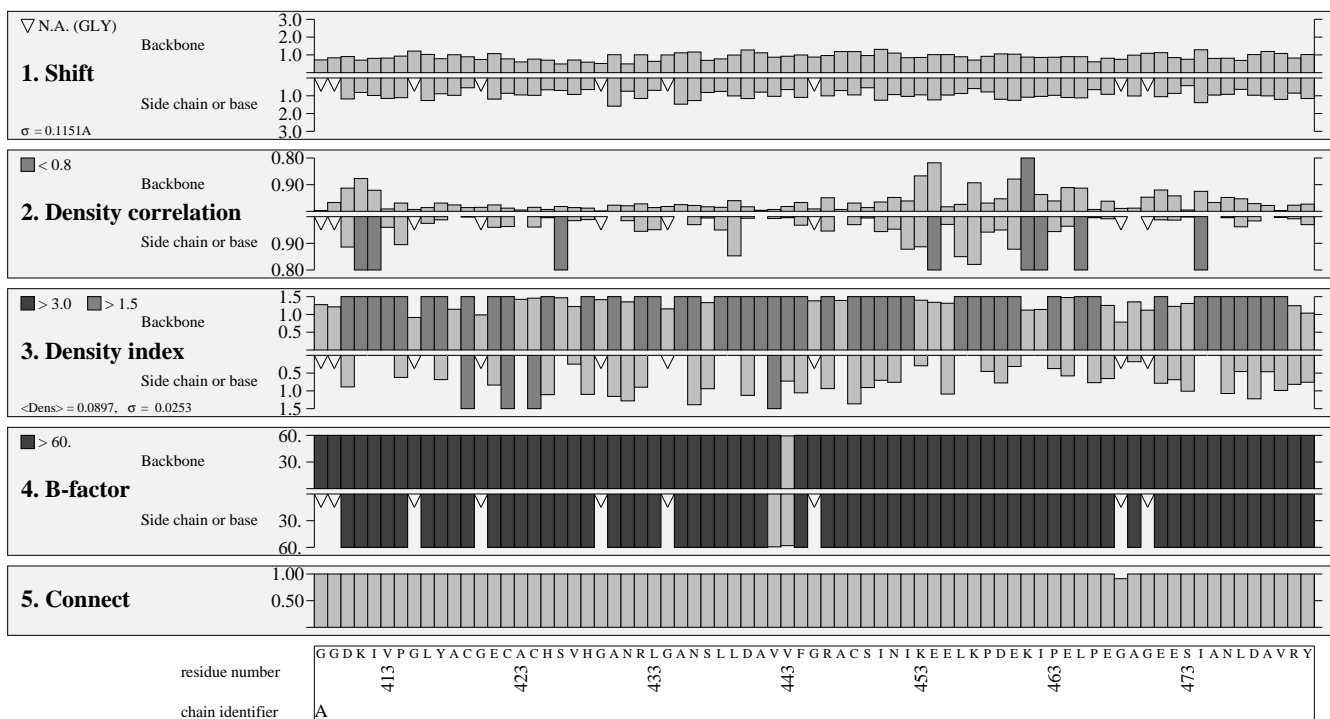
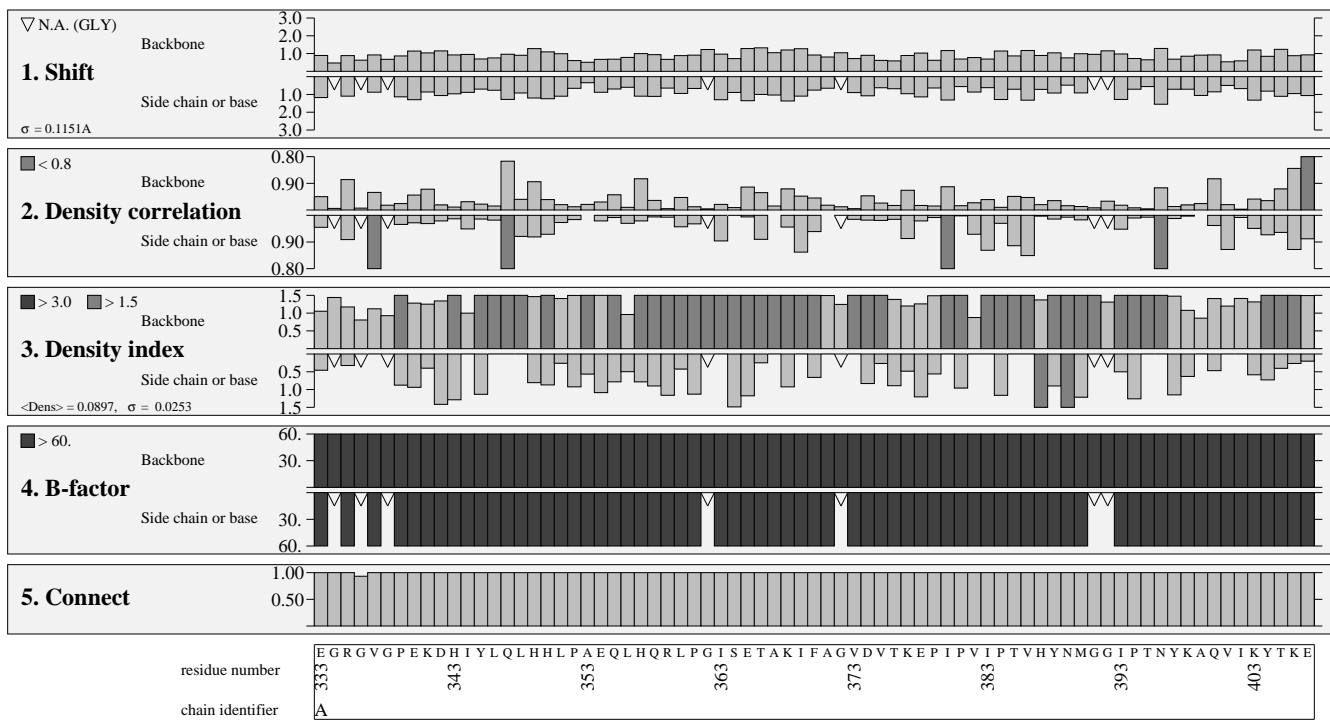
Local estimation (2)



Structure Factor Check

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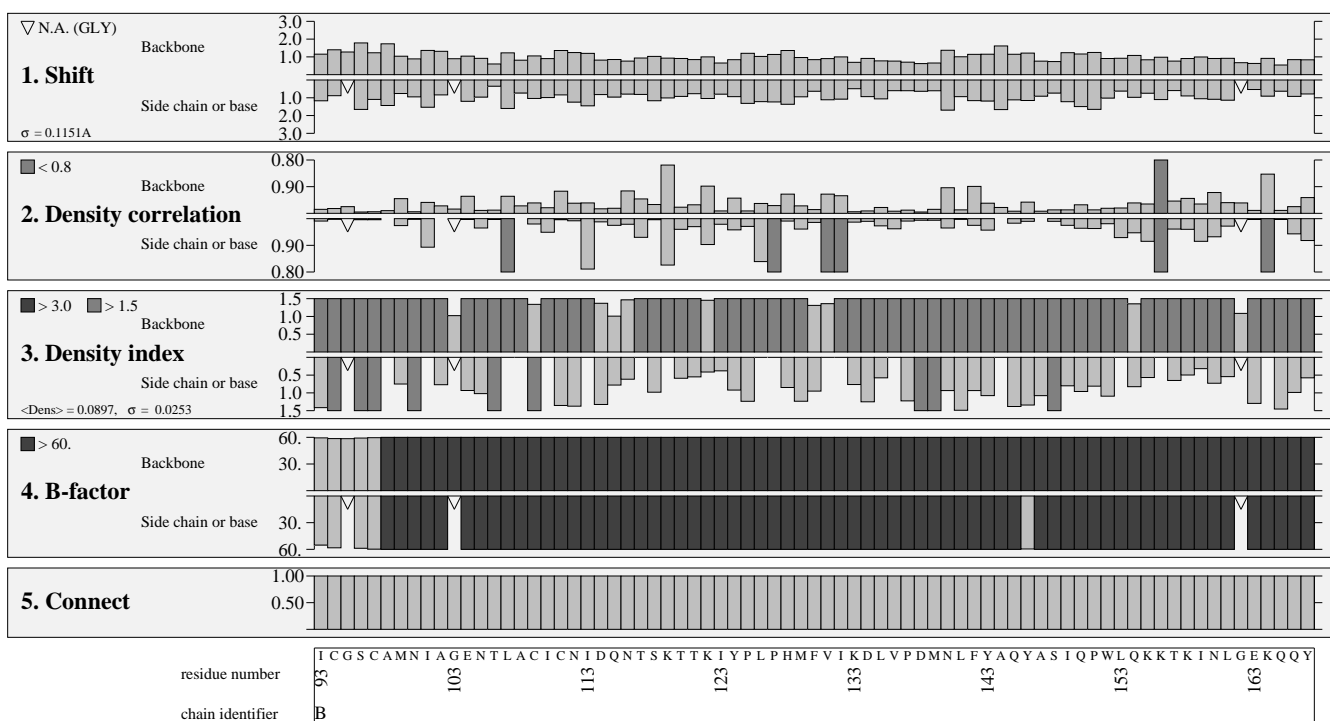
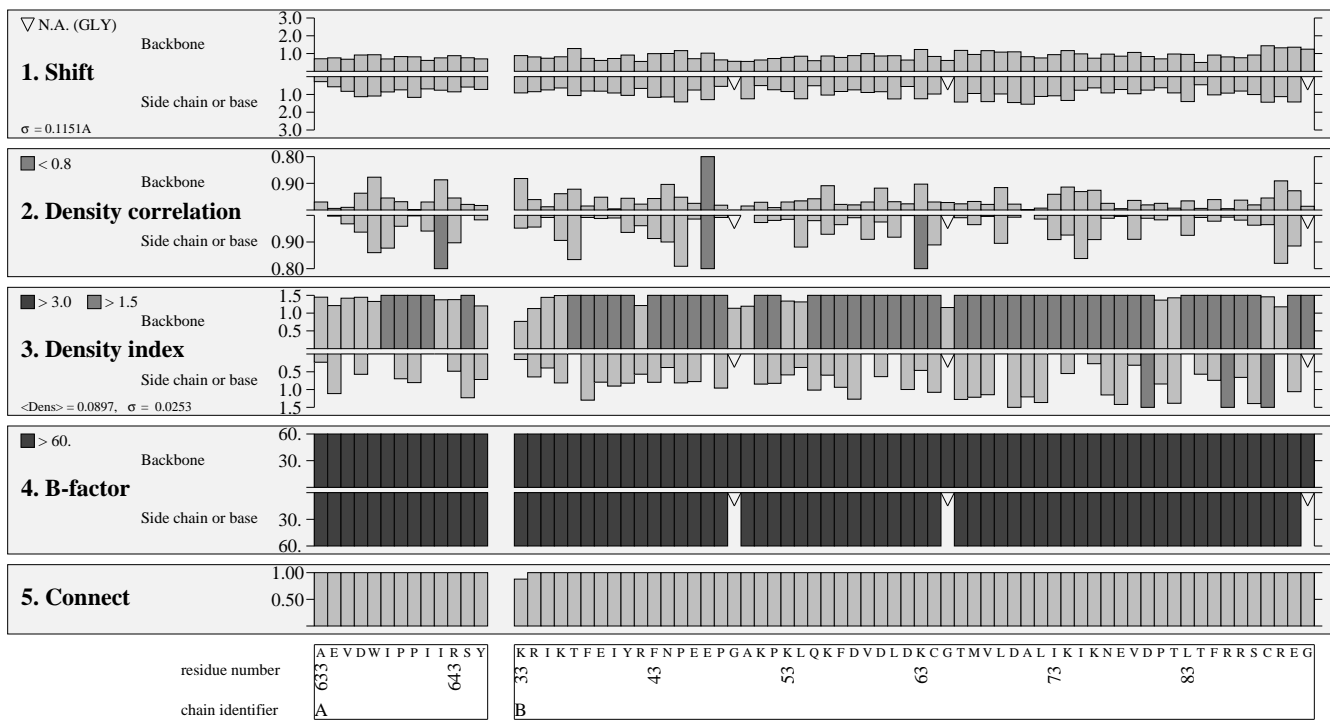
Local estimation (3)



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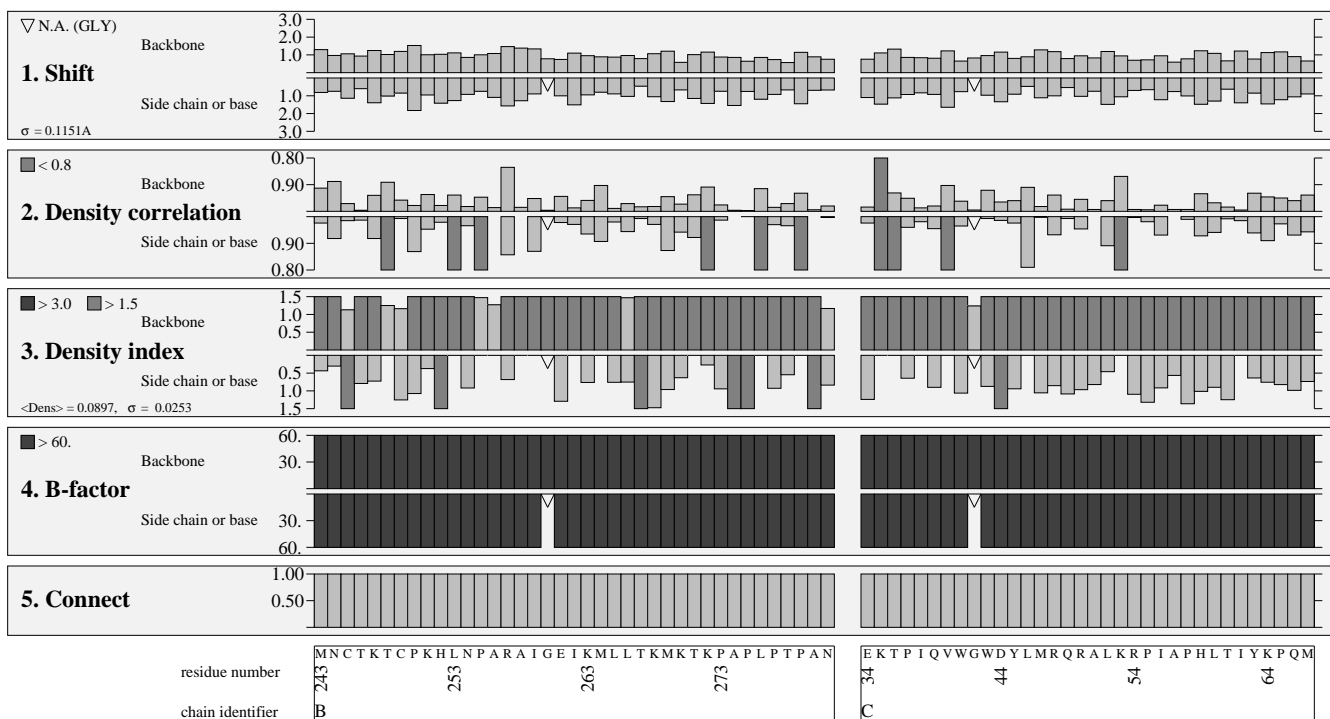
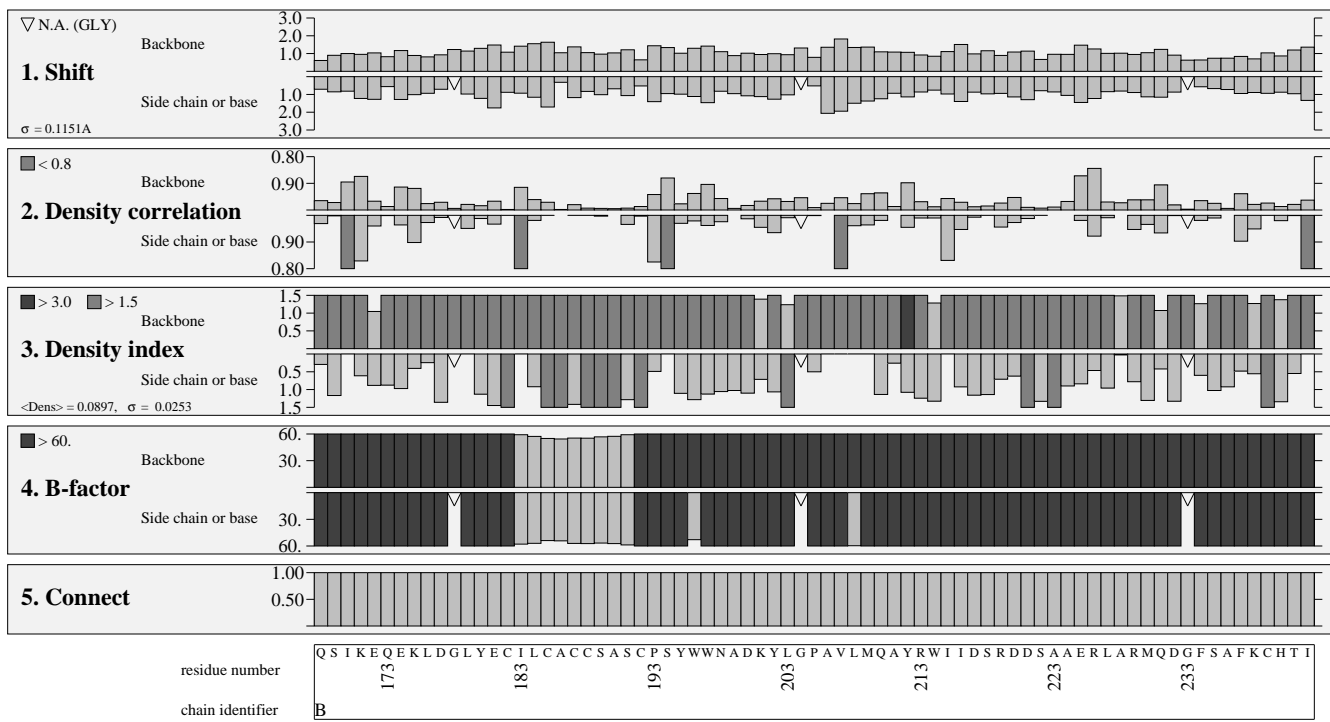
Local estimation (5)



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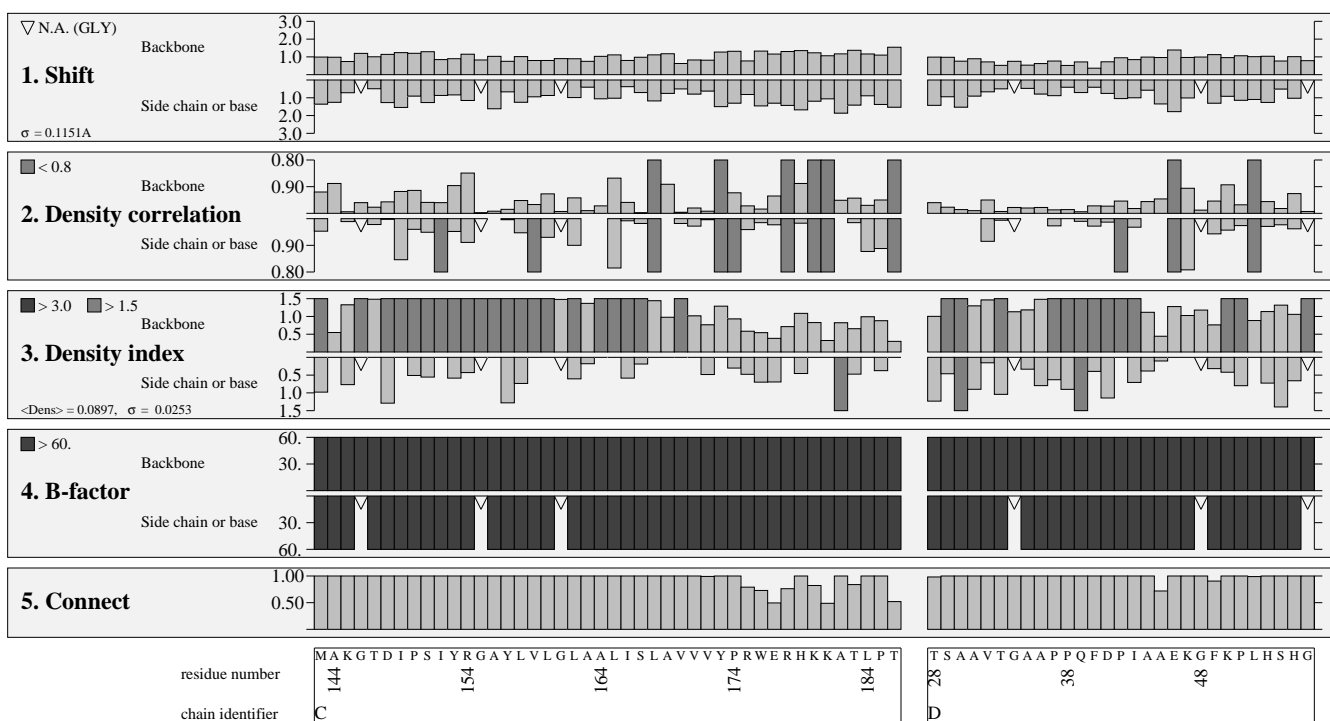
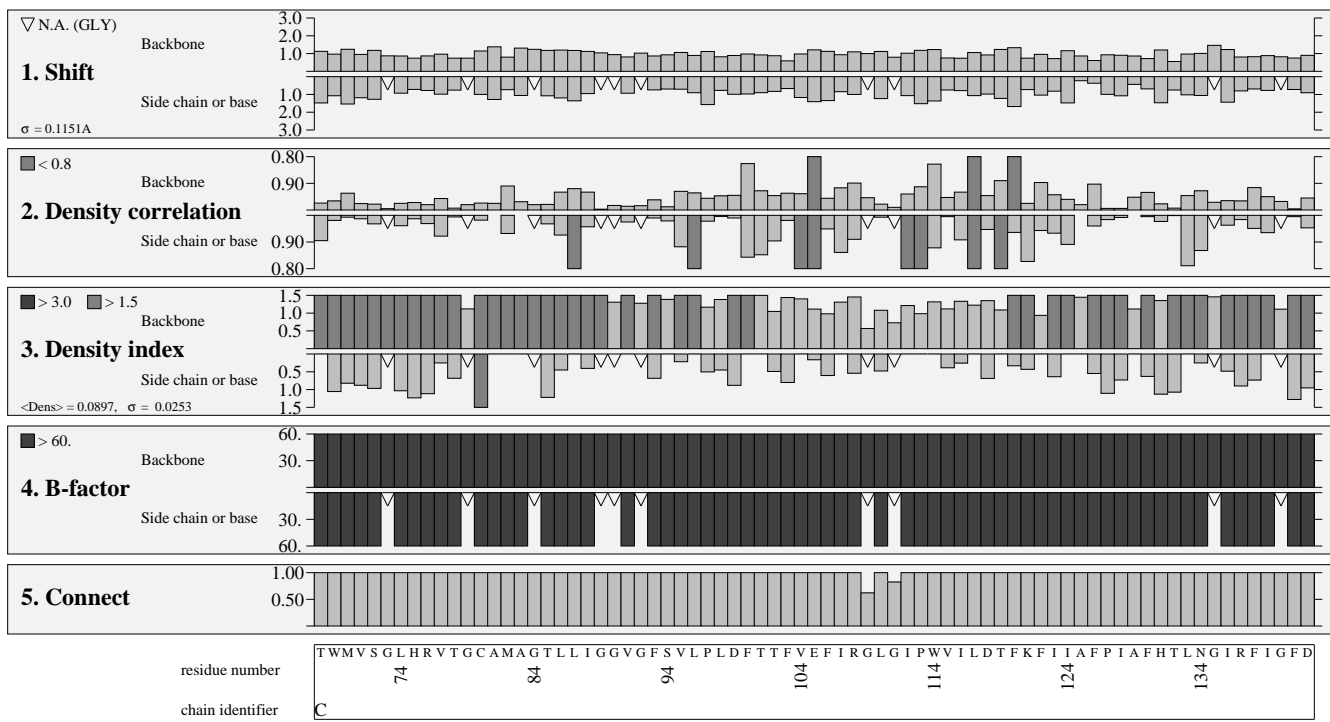
Local estimation (6)



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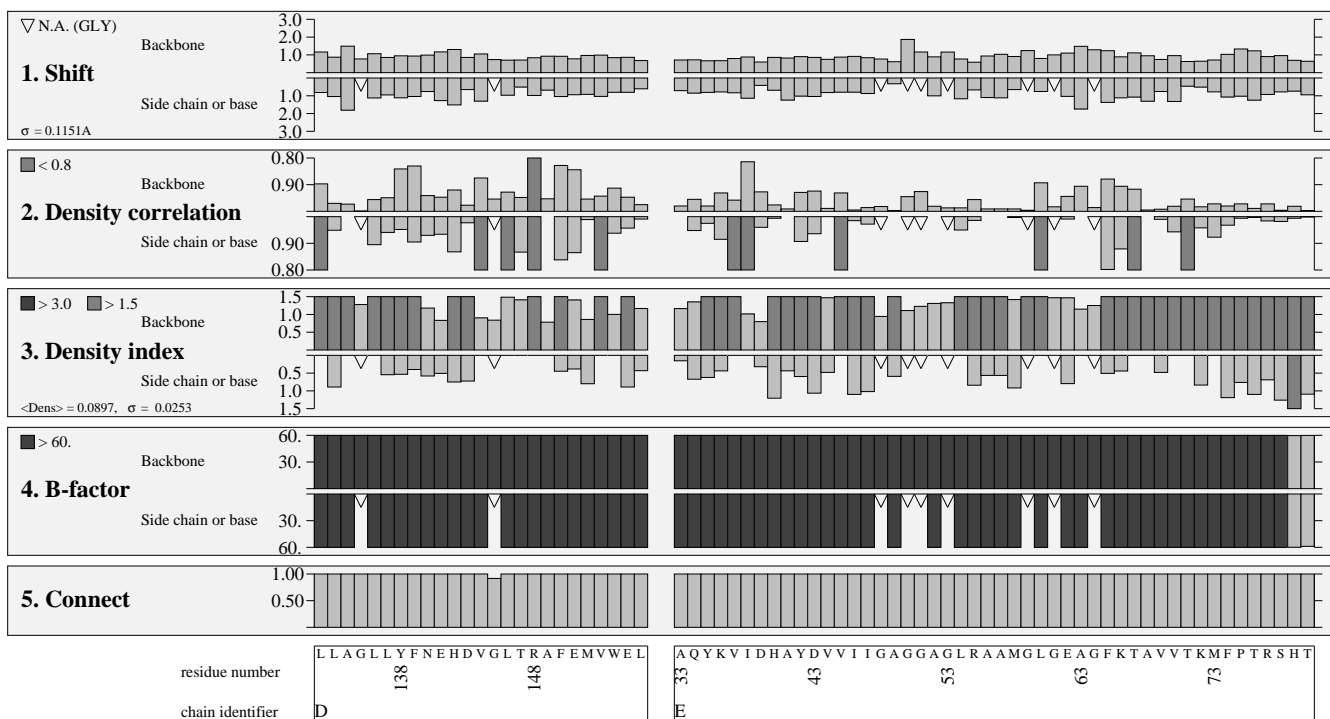
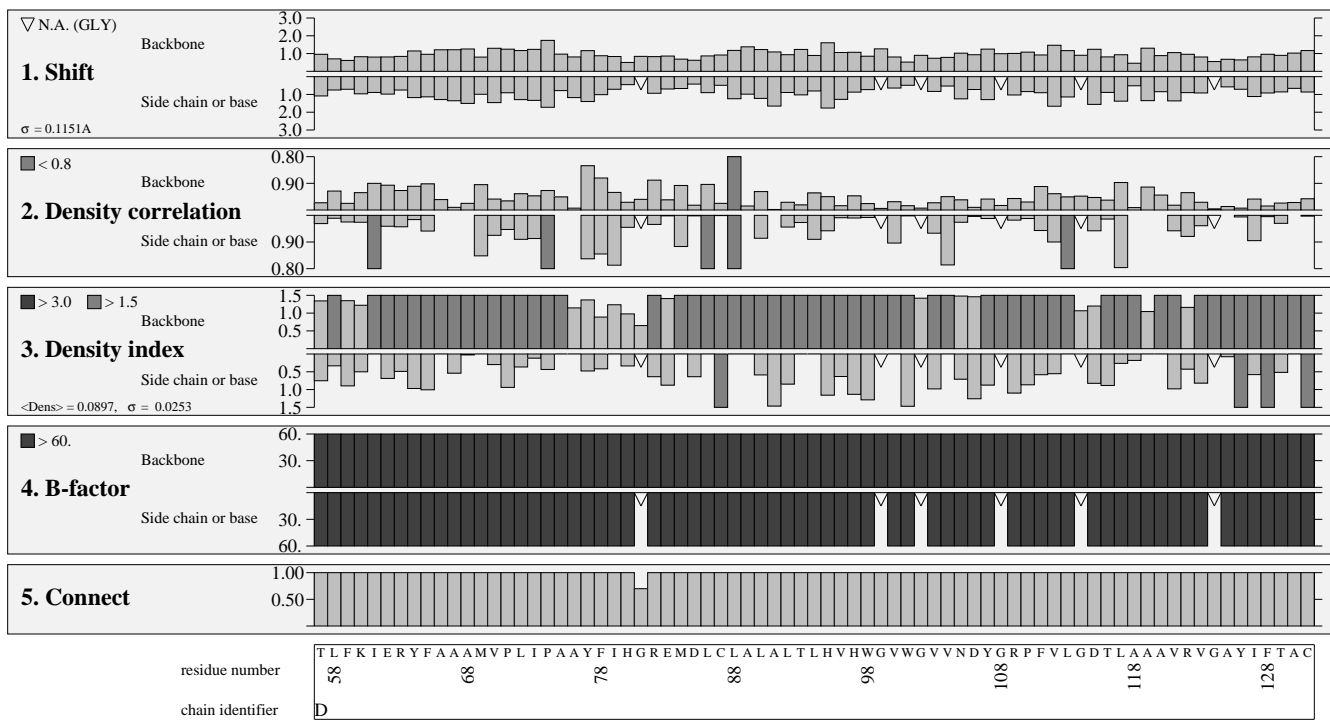
Local estimation (7)



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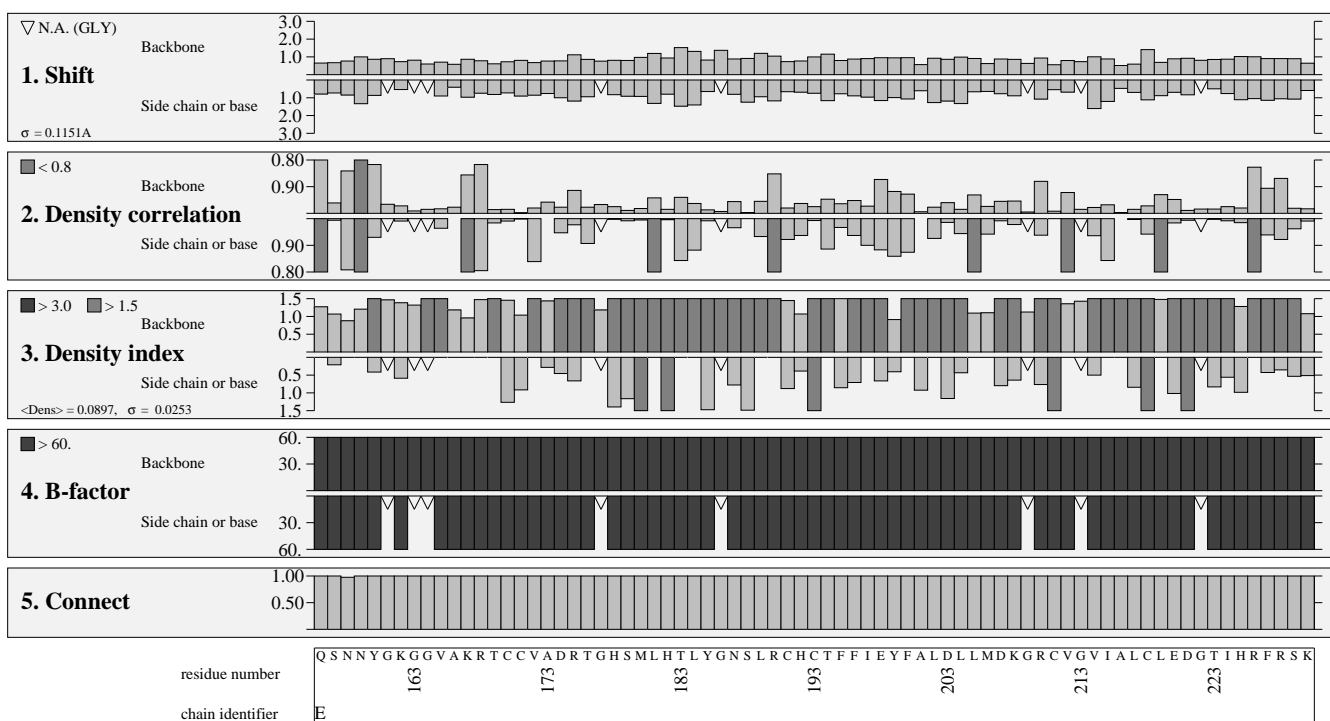
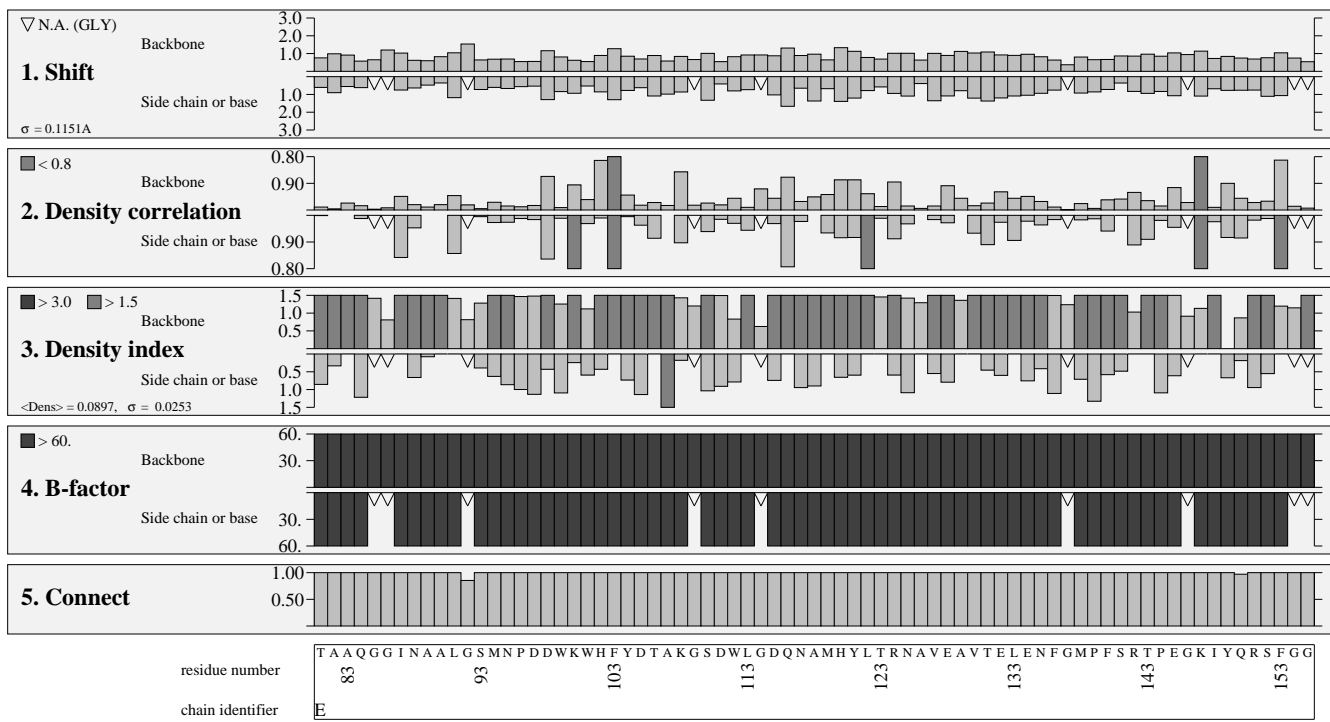
Local estimation (8)



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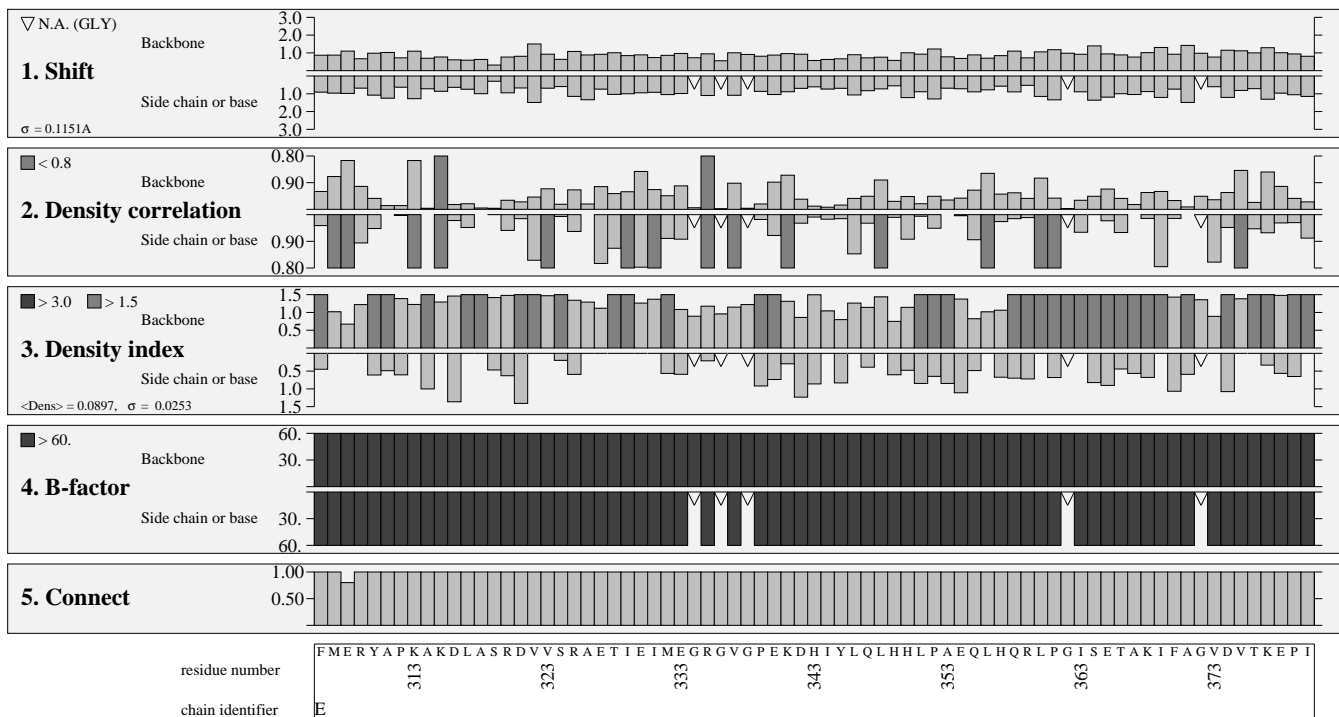
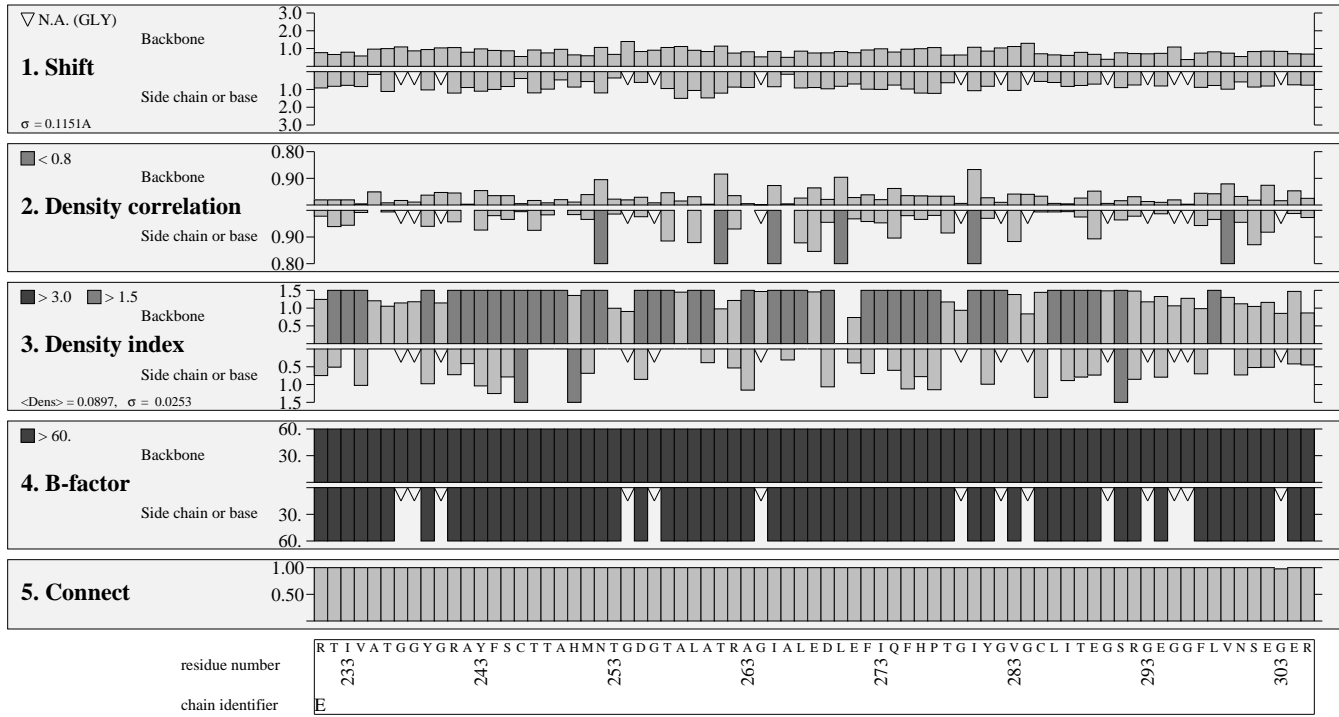
Local estimation (9)



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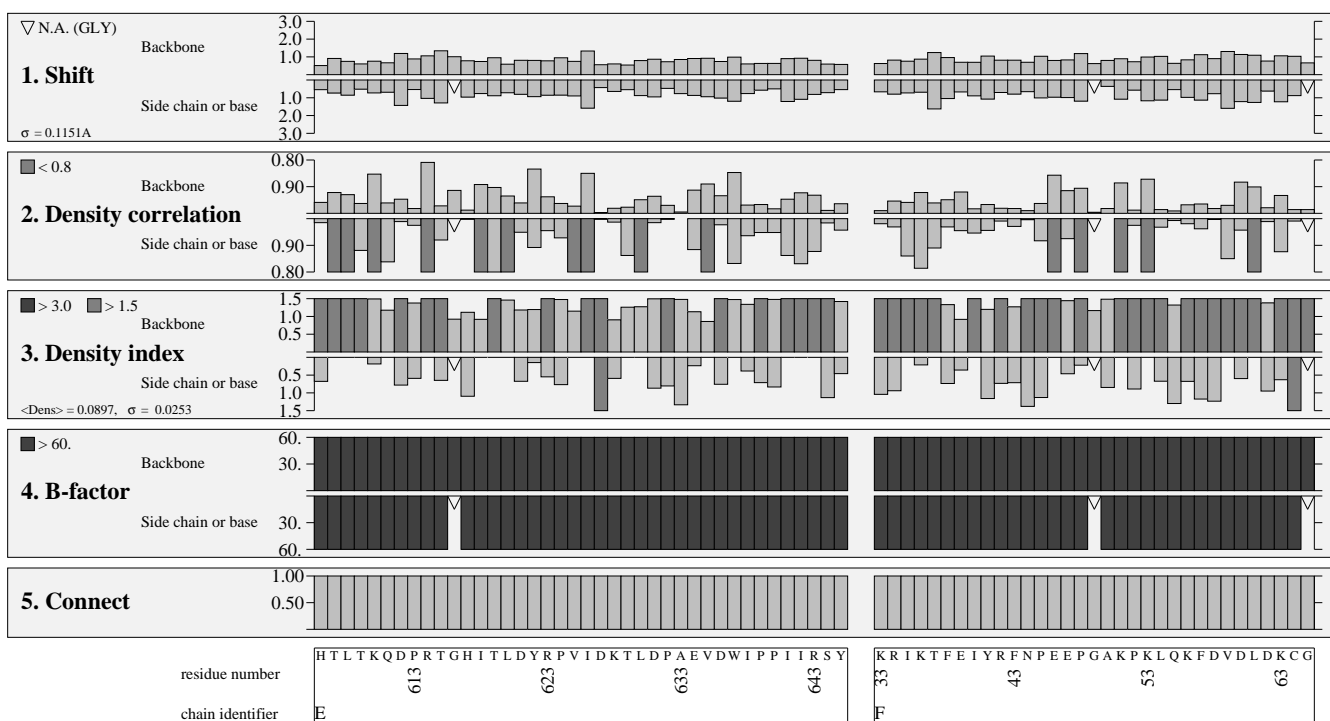
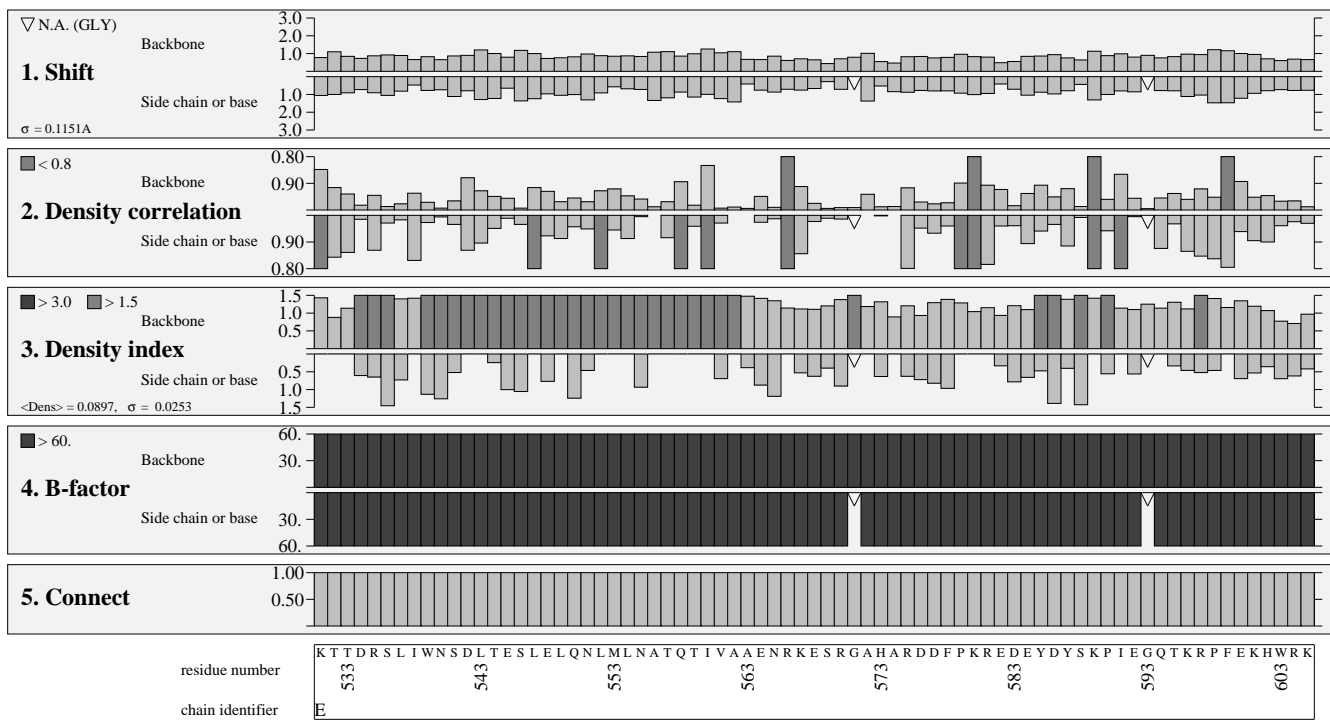
Local estimation (10)



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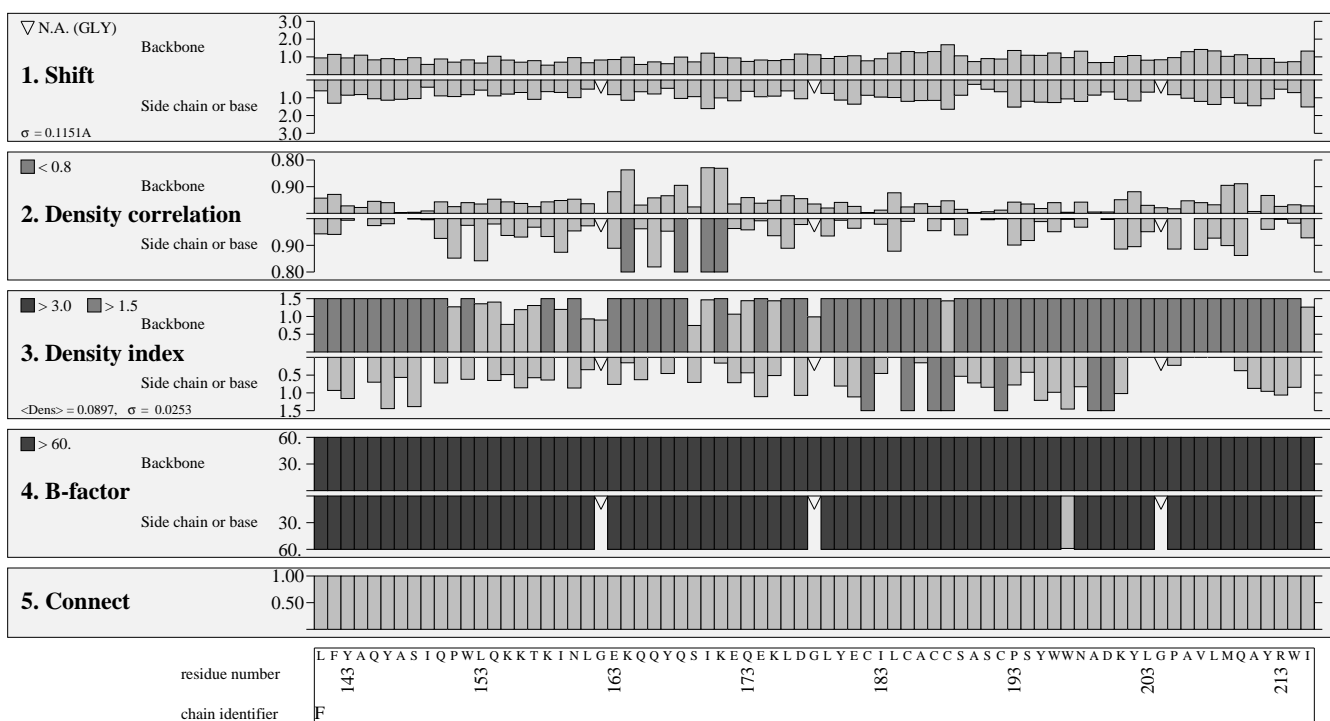
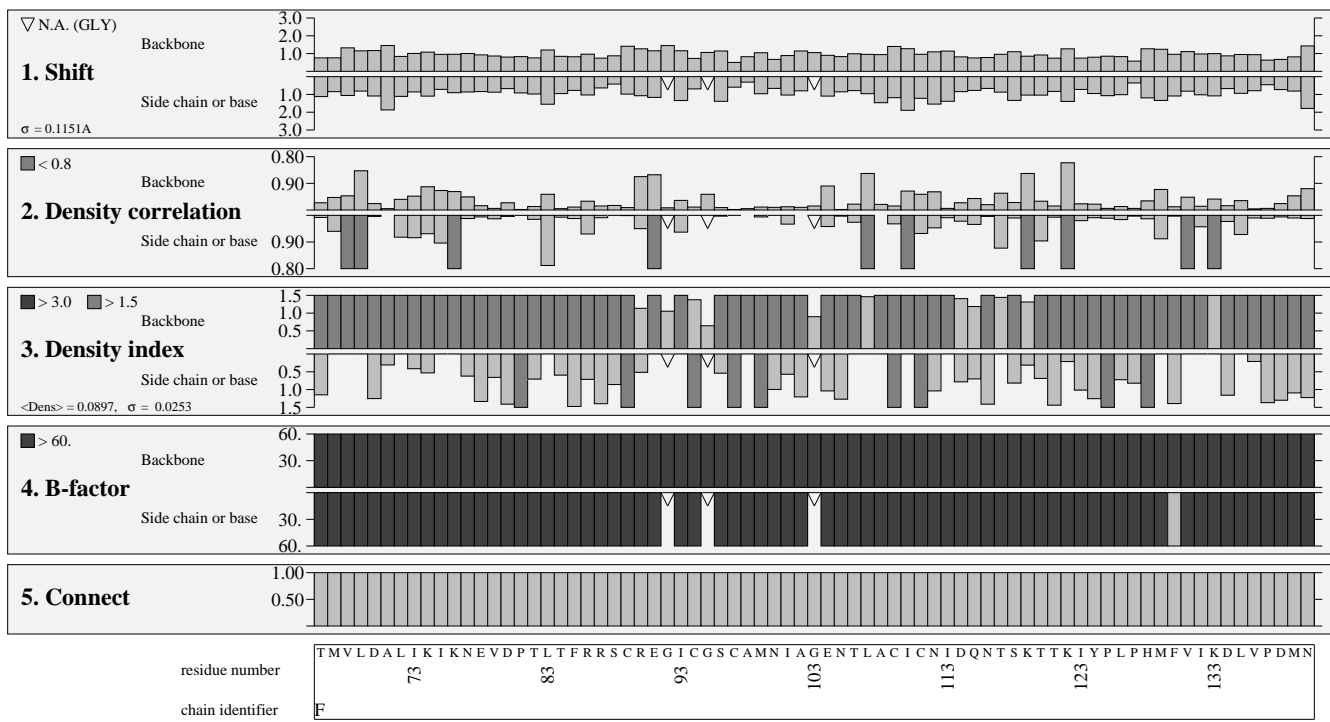
Local estimation (12)



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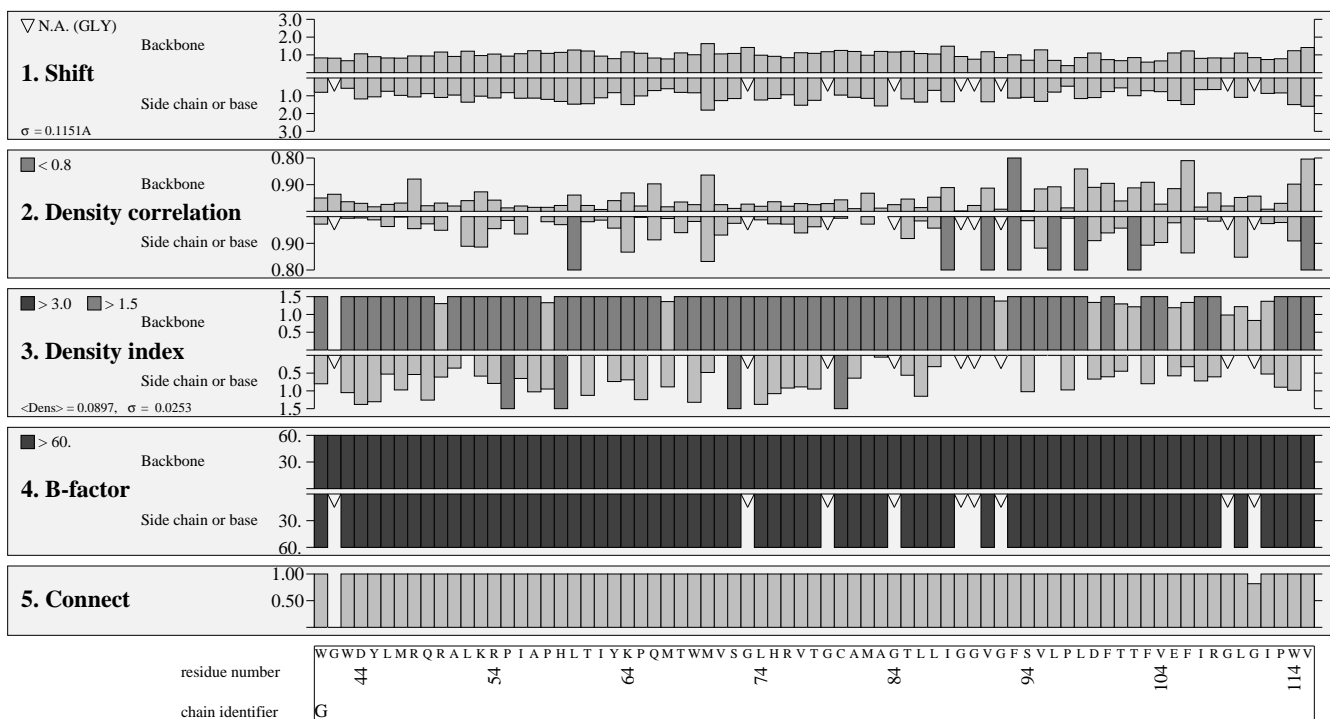
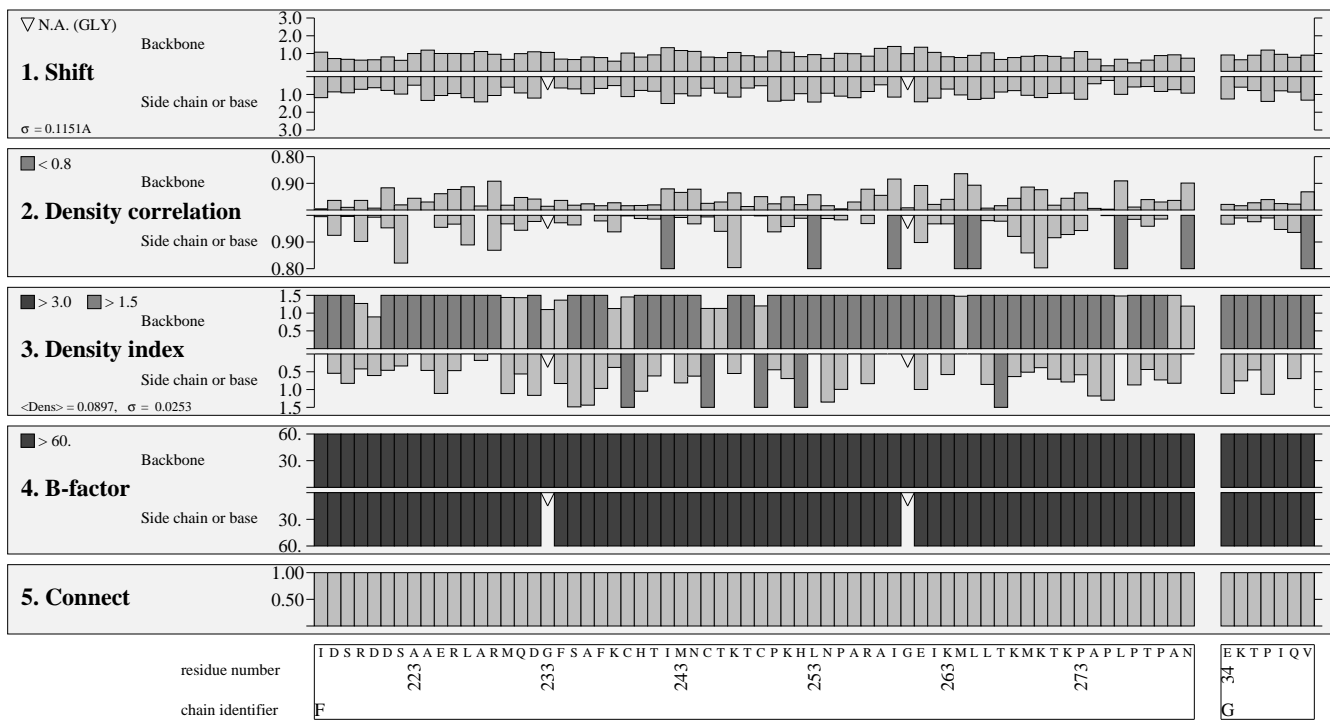
Local estimation (13)



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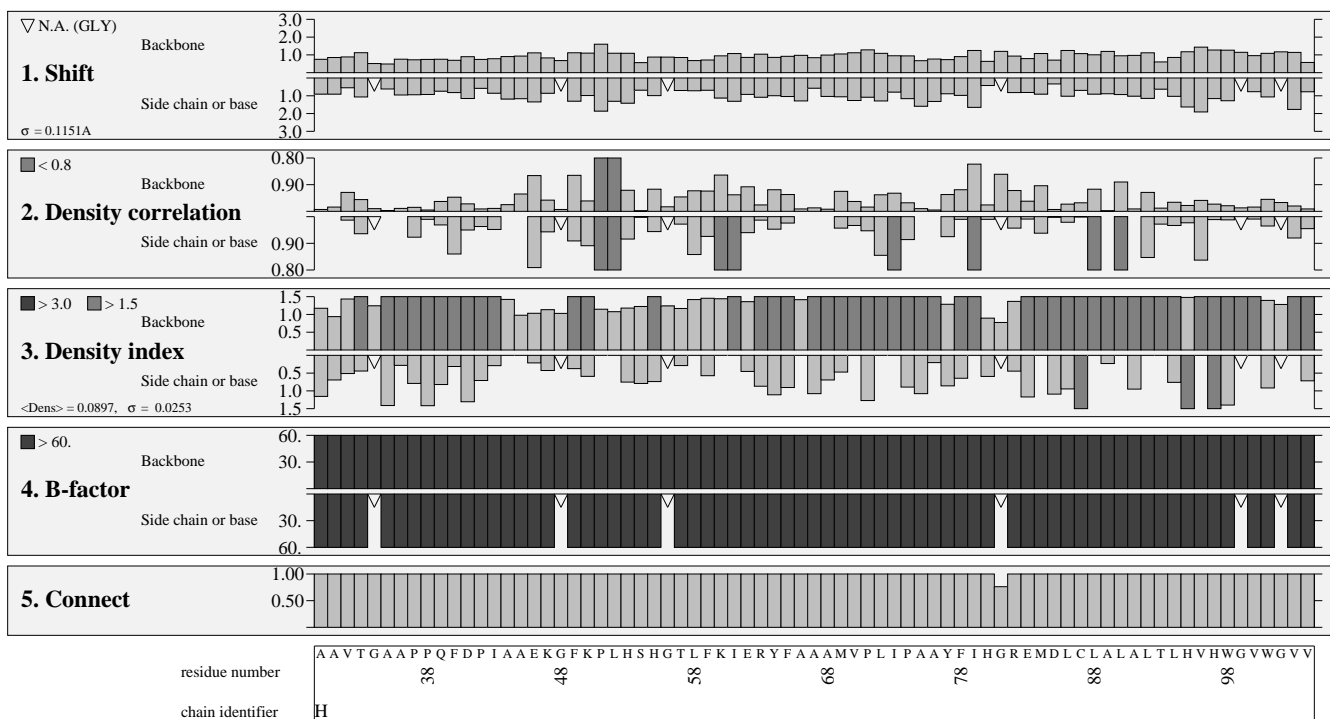
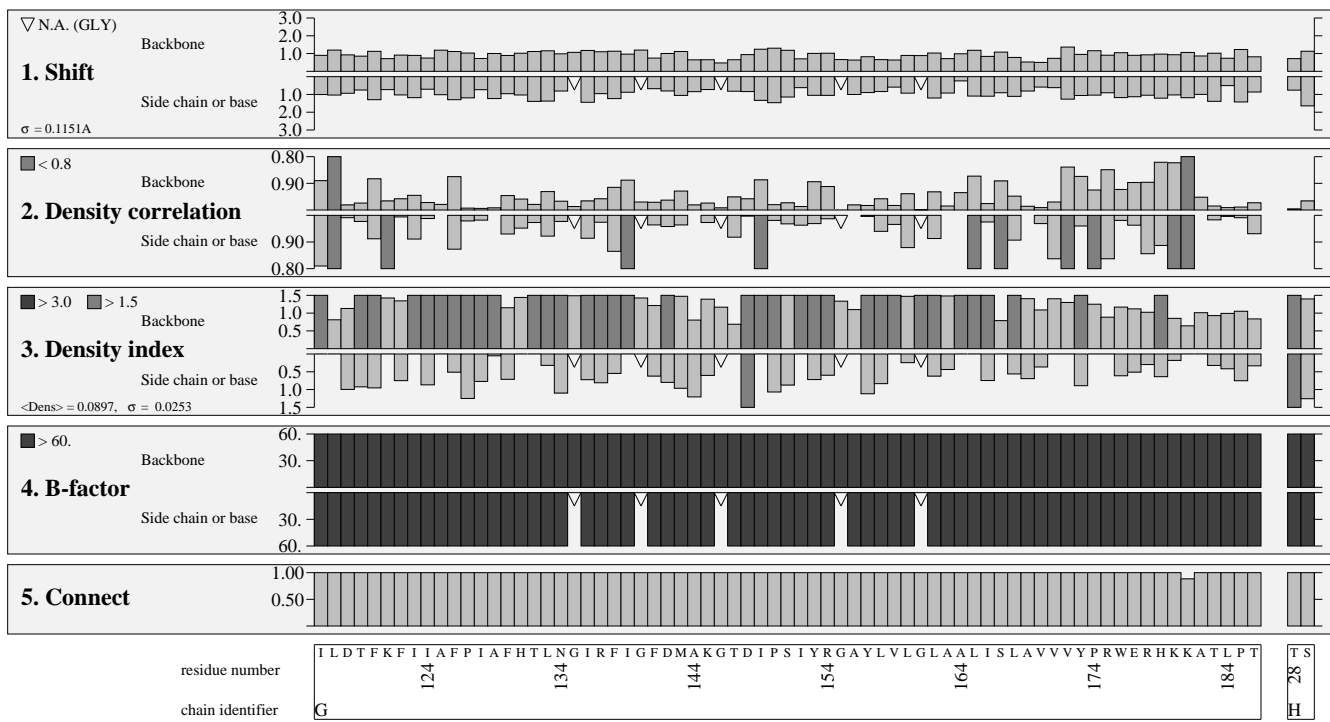
Local estimation (14)



Structure Factor Check

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Local estimation (15)



Structure Factor Check

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Local estimation (16)

