

Structure Factor Check

5C2T

Title: CRYSTAL STRUCTURE OF MITOCHONDRIAL RHODOQUINOL-FUMARATE REDU
ASCARIS SUUM WITH RHODOQUINONE-2
Date: 16-JUN-15
PDB code: 5C2T

Crystal

Cell parameters:

a: 122.81 A b: 123.63 A c: 219.81 A
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Structure Factors

Input

Nominal resolution range: 20.0 – 2.75 A
 Reflections in file: 86937
 Unique reflections above 0: 82006
 above 1 σ : 80795
 above 3 σ : 59040
 Reflections > 0: 4931

SFCHECK

Nominal resolution range: 20.0 – 2.75 A
\05max. from input data, min. from author\05
 Used reflections: 82006
 Completeness: 94.1 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.063
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 0.9209 1.0000 0.9962
 B_{overall} (by Patterson): 42. A²
 Optical resolution: 2.01 A
 Expected opt. resol. for complete data set: 2.01 A
 Estimated minimal error: 0.061 A

Model

18467 atoms (106 water molecules)
 Number of chains: 32
 Volume not occupied by model: 52.7 %
 $\langle B \rangle$ (for atomic model): 50.2 A²
 $\sigma(B)$: 17.06 A²
 Matthews coefficient: 3.23
 Corresponding solvent % : 61.59

Model vs. Structure Factors

R-factor for all reflections: 0.248
 Correlation factor: 0.871
 R-factor: 0.253
 for $F > 2.0\sigma$
 nom. resolution range: 20.00 – 2.75A
 reflections used: 80793

Rfree: 0.301
 Nfree: 4049
 R-factor without free-refl.: 0.251
 Non free-reflections: 76744
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.342 A
 Estimated maximal error: 0.176 A
 DPI: 0.336 A

Scaling

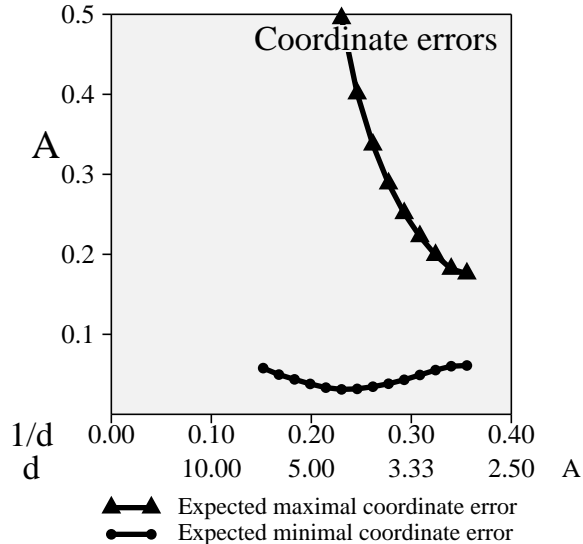
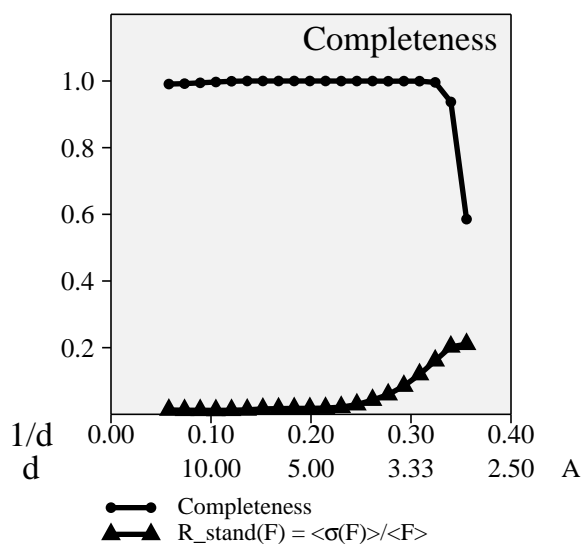
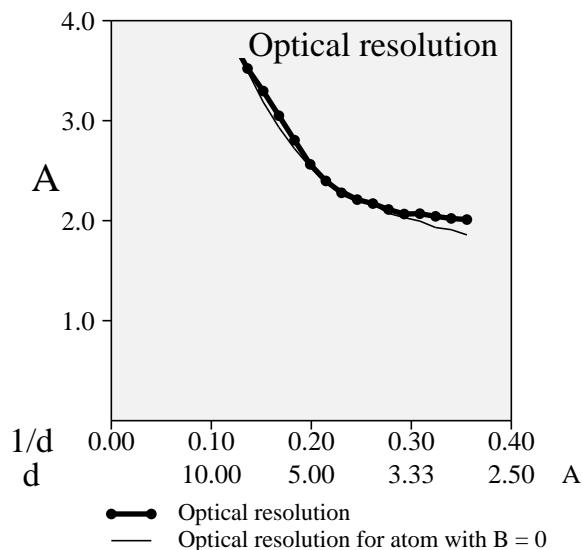
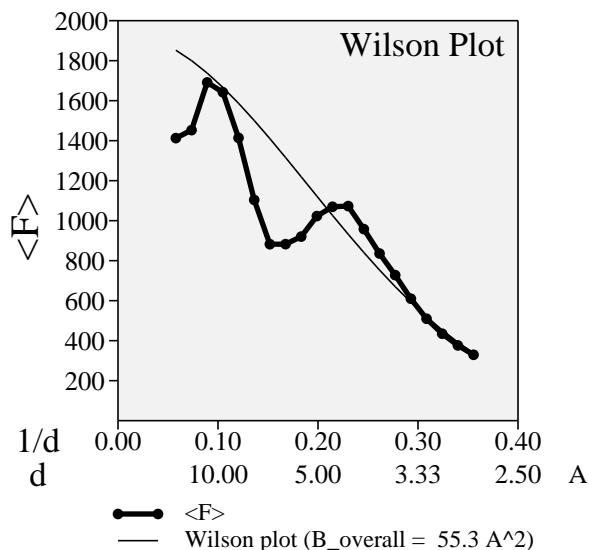
Scale: 0.914
 Bdiff: -5.25
 Anisothermal Scaling (Beta):
 -0.6273 -0.4422 -0.4335 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.586 249.981

Refinement

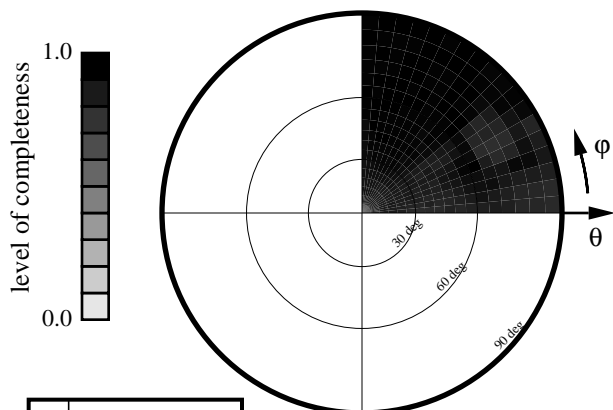
Program: REFMAC 5.7.0029
 Nominal resolution range: 20.0 – 2.75 A
 Reported R-factor: 0.196
 Number of reflections used: 78102
 Reported Rfree: 0.25
 Sigma cut-off: N.A.

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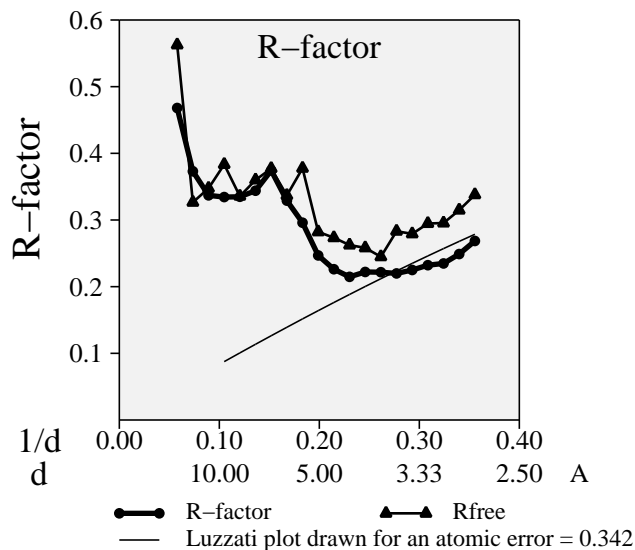


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

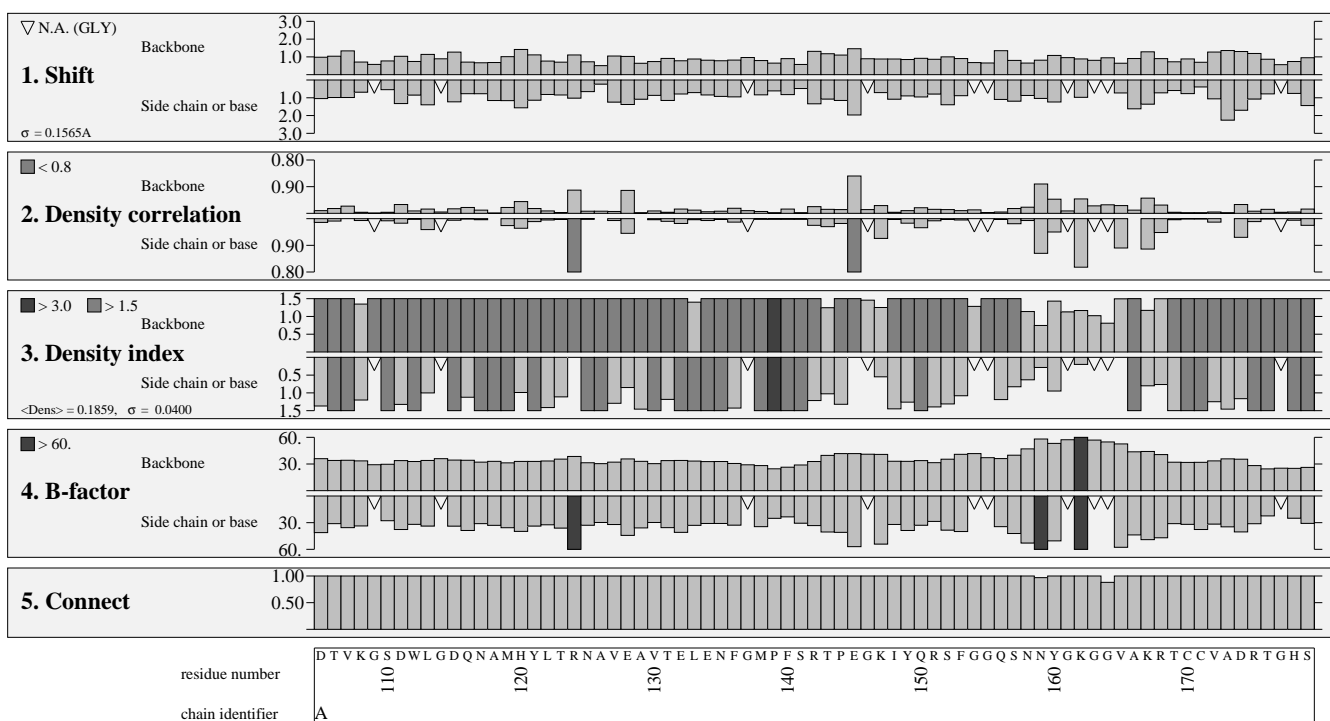
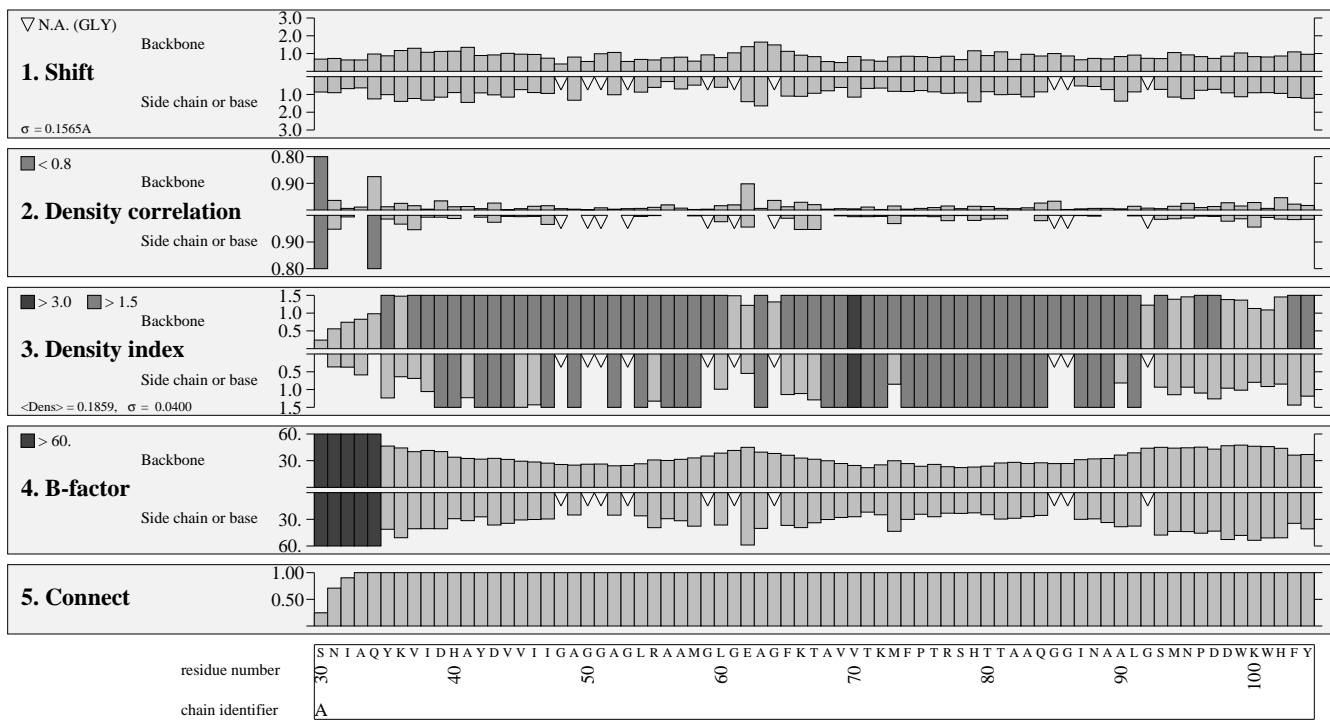
polar coordinates of the crystallographical axes



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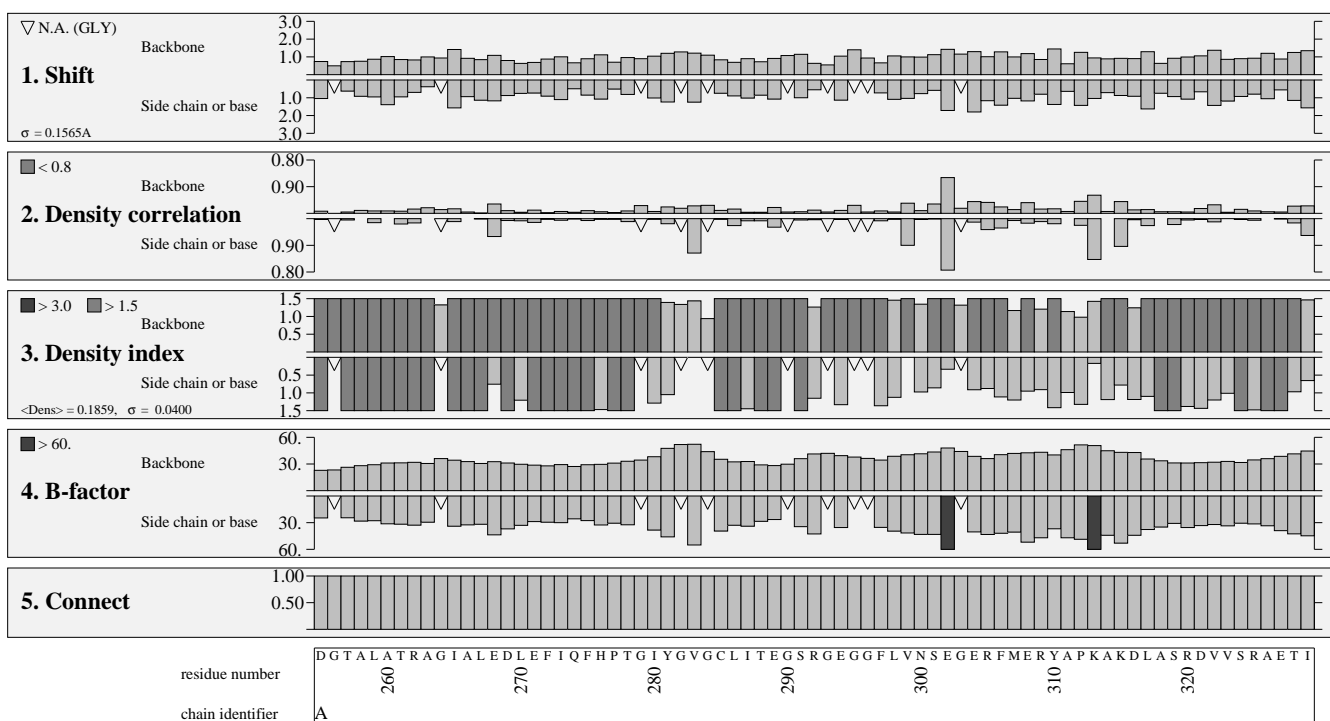
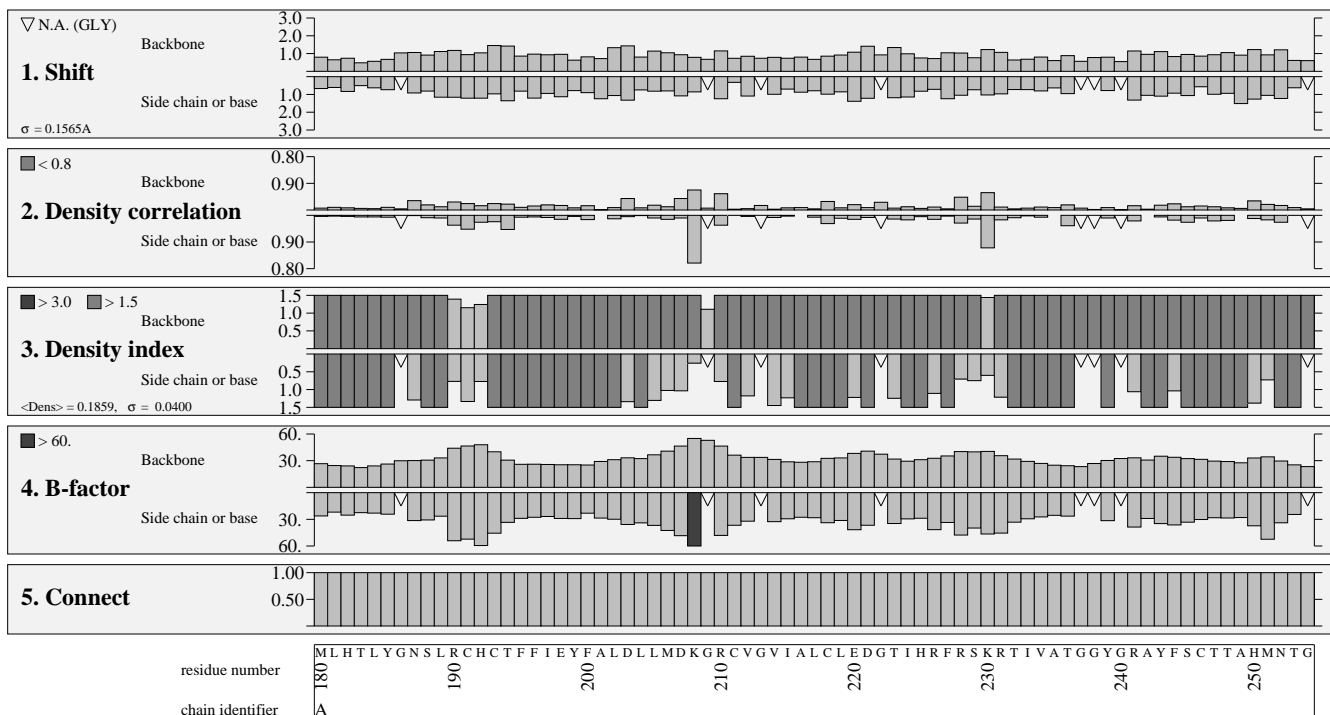
Local estimation



Structure Factor Check

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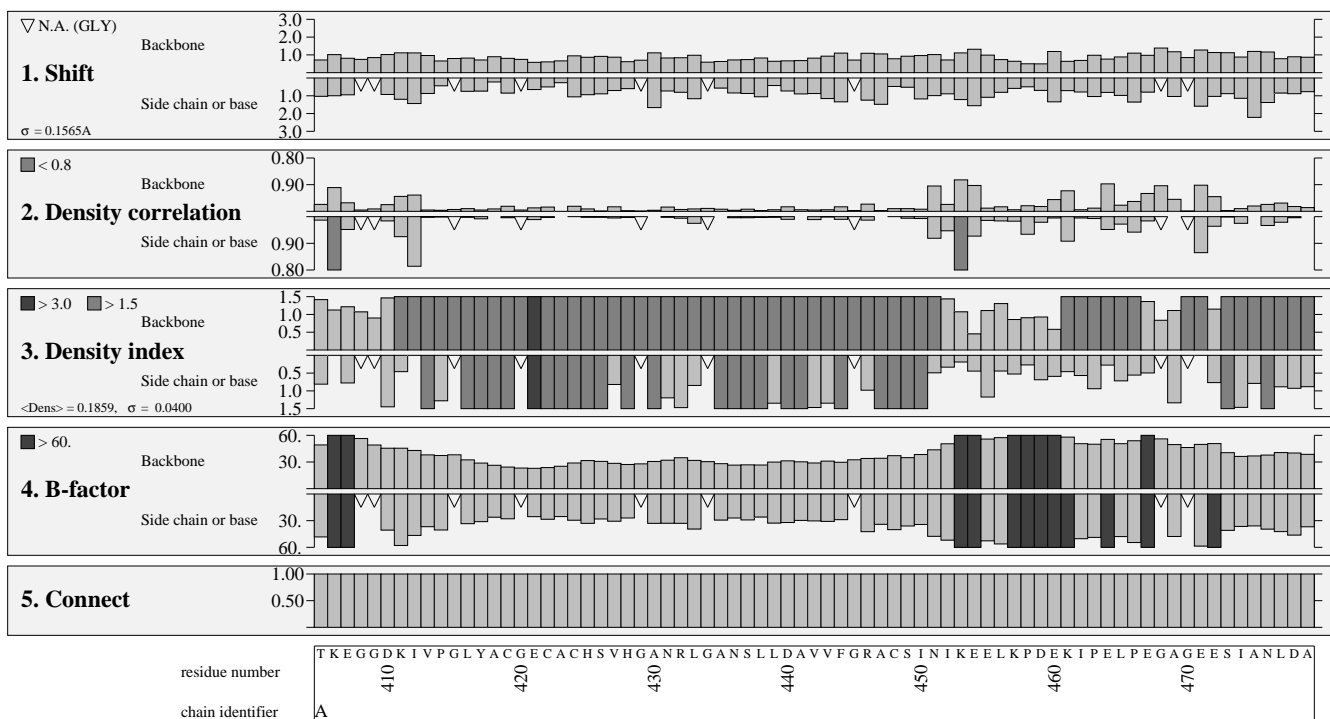
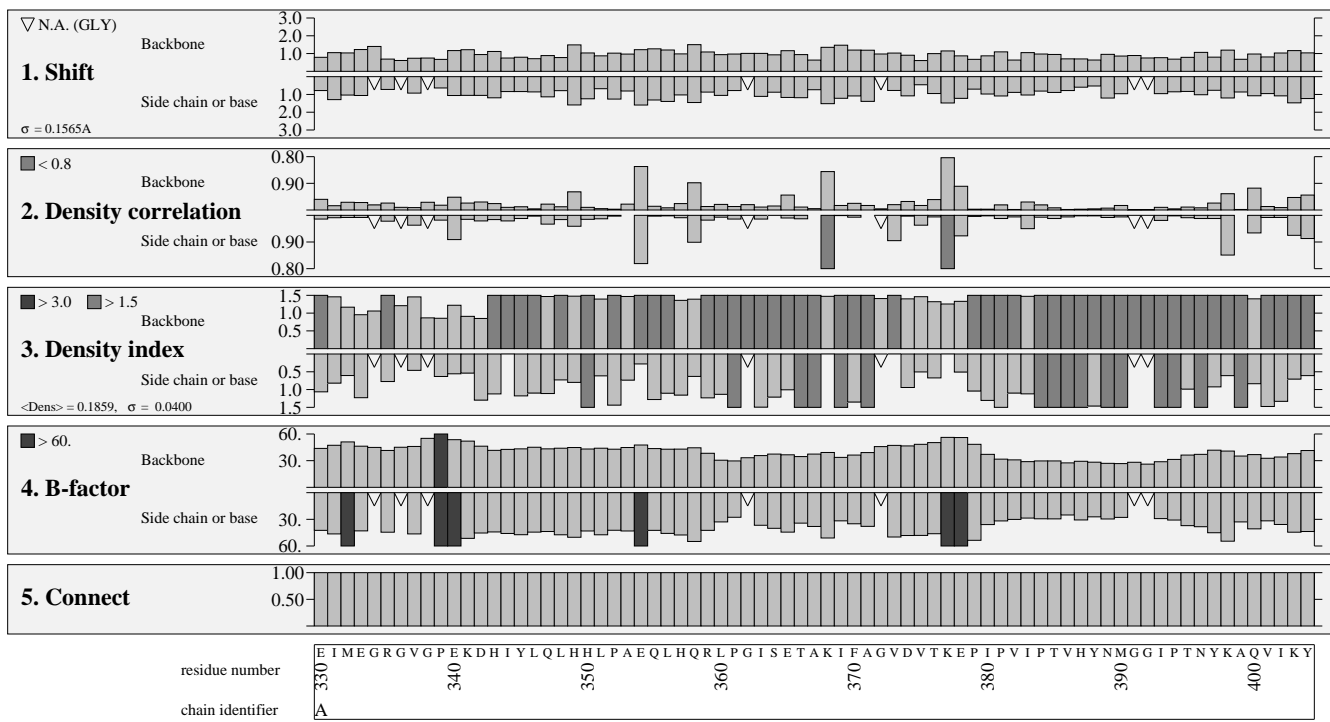
Local estimation (2)



Structure Factor Check

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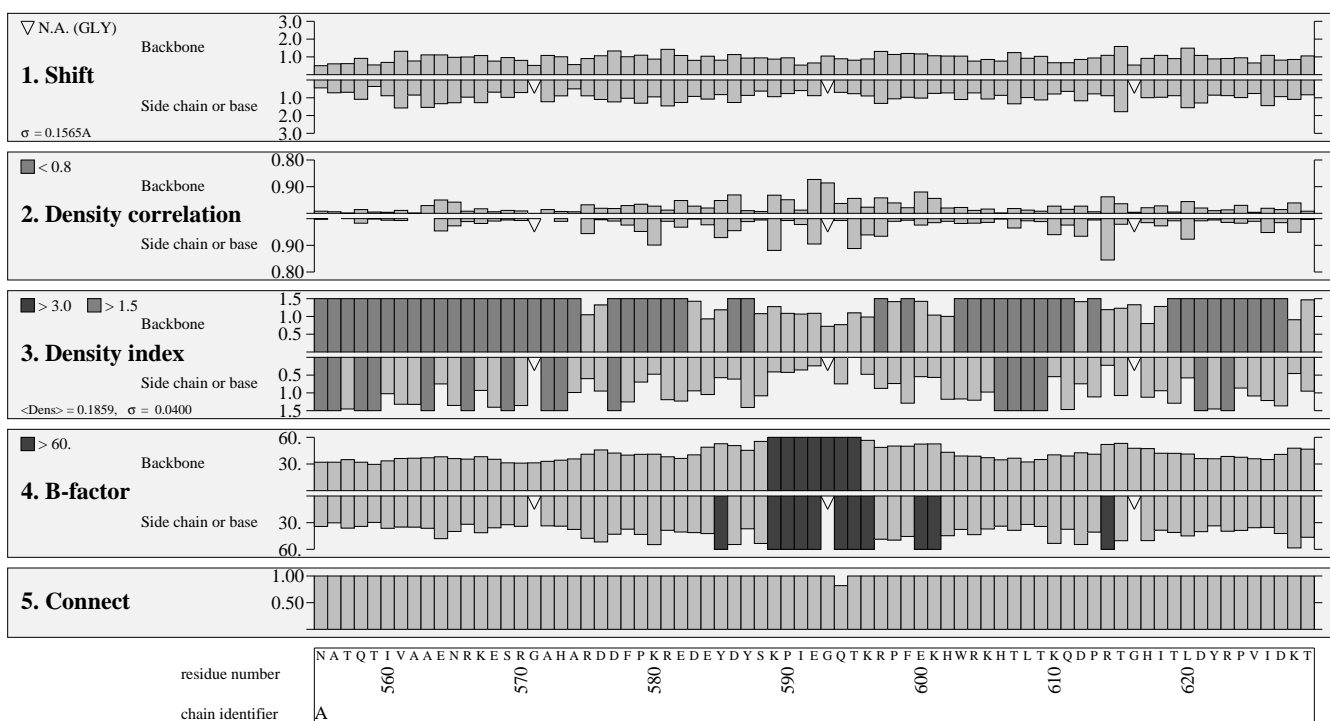
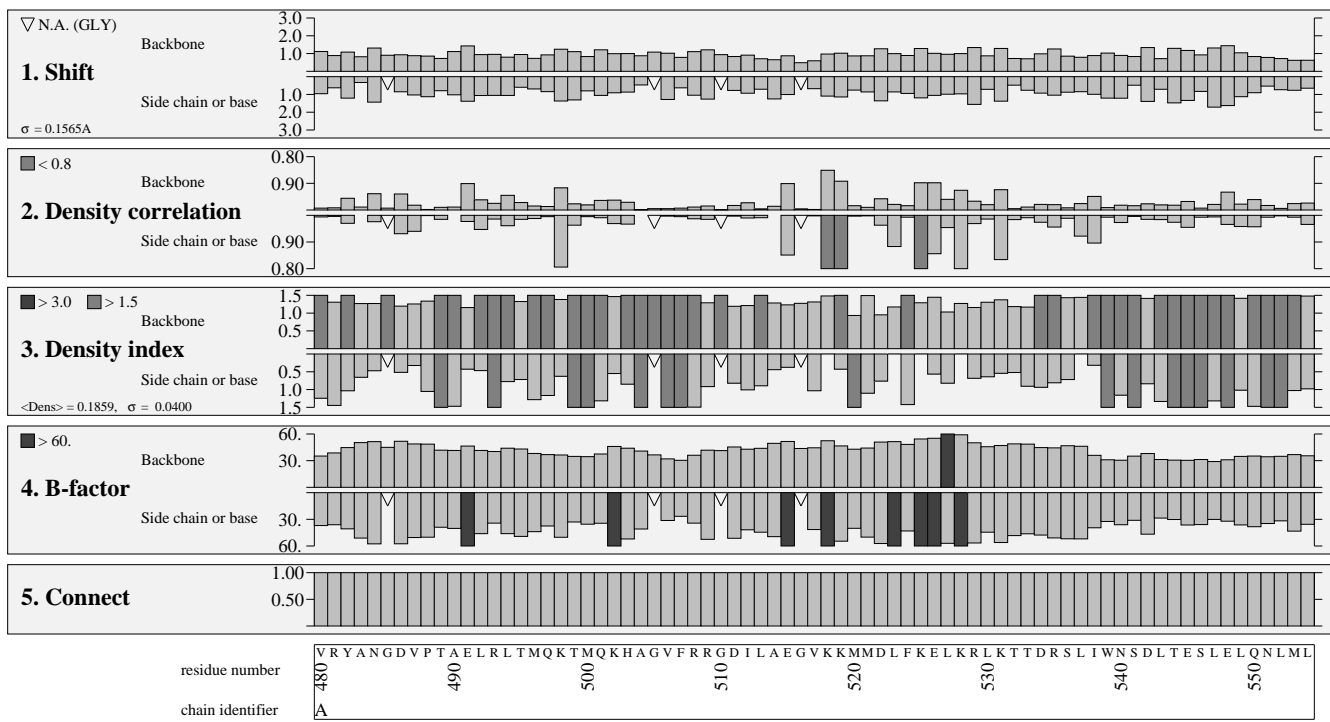
Local estimation (3)



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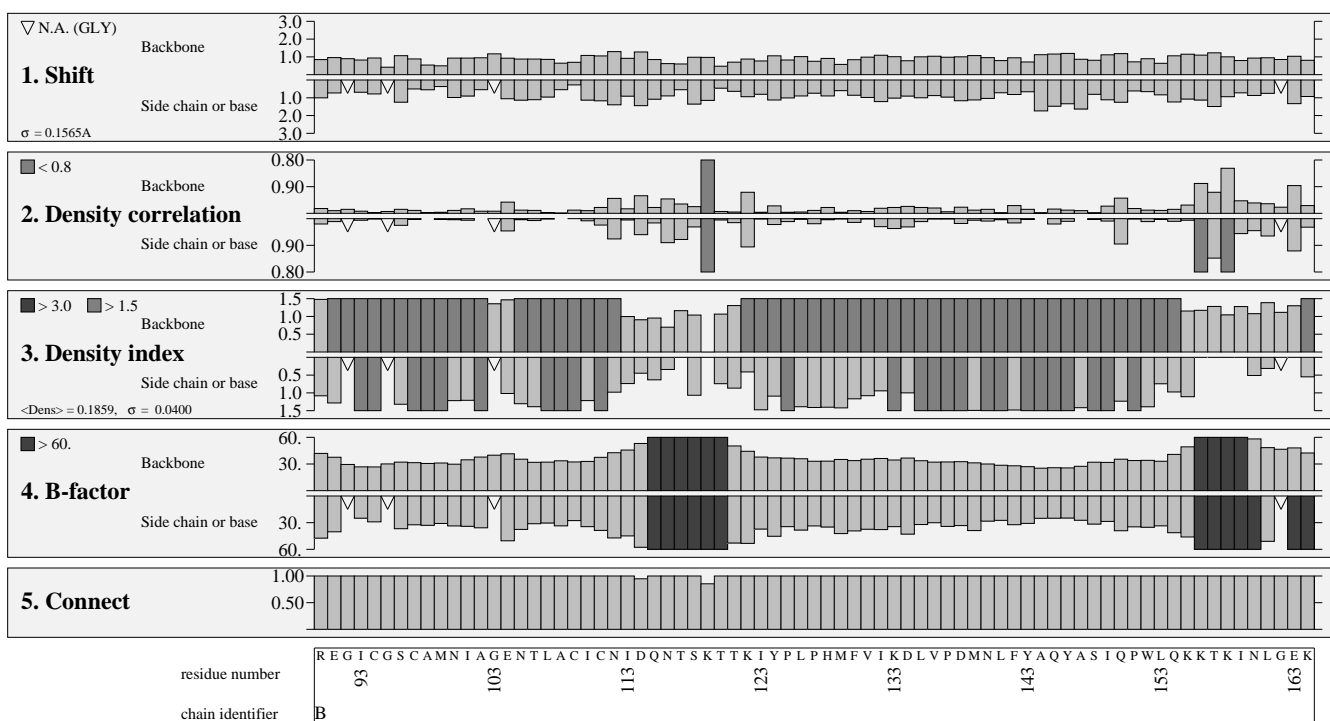
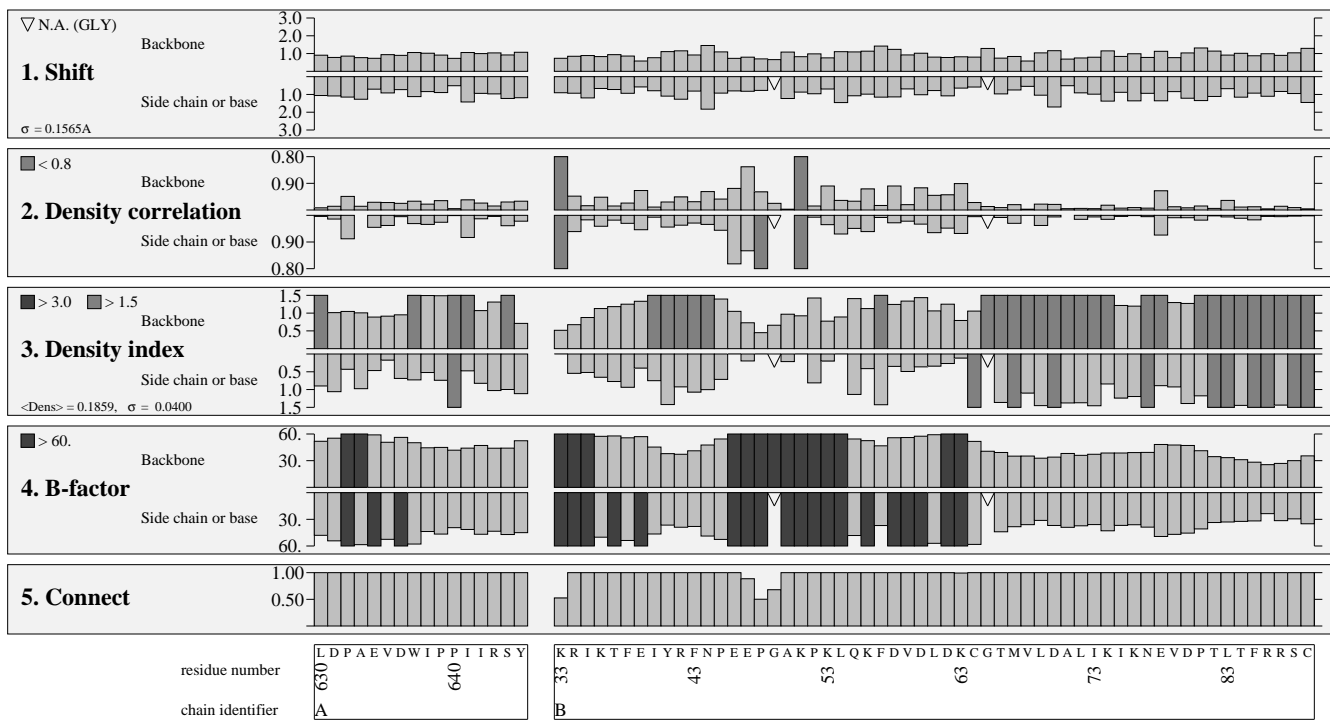
Local estimation (4)



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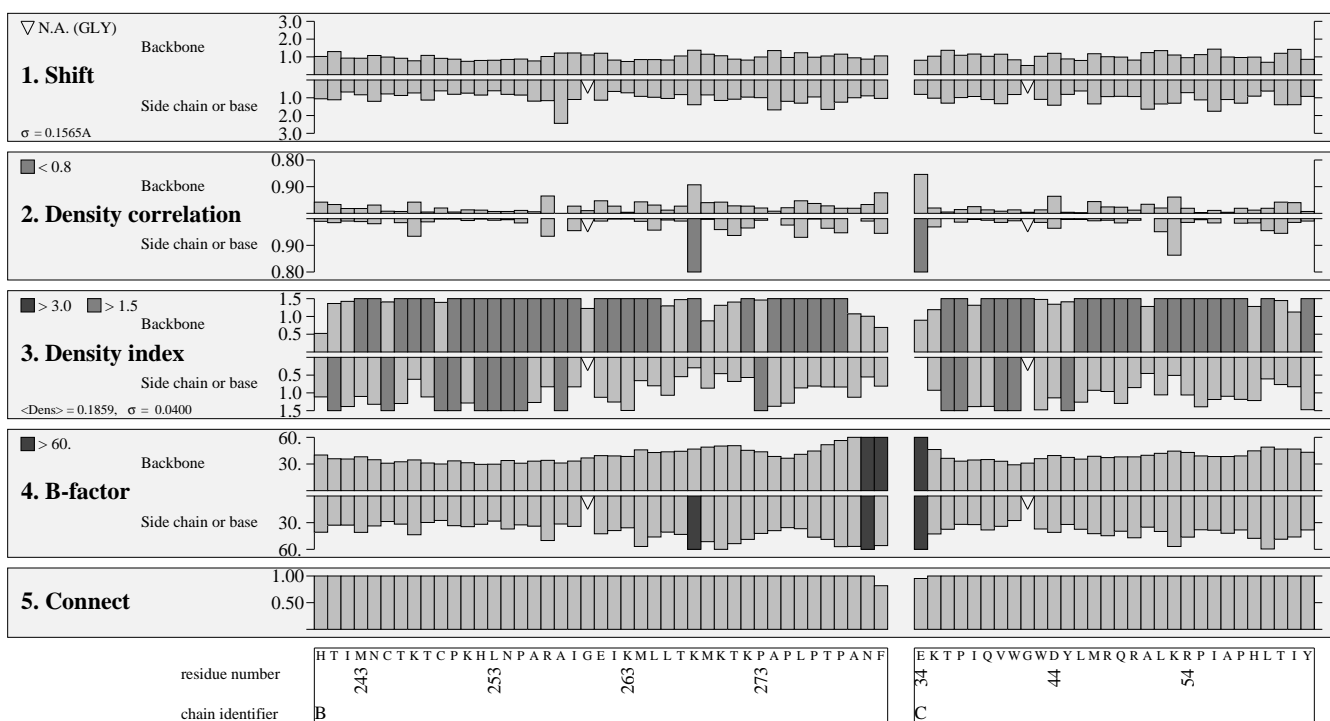
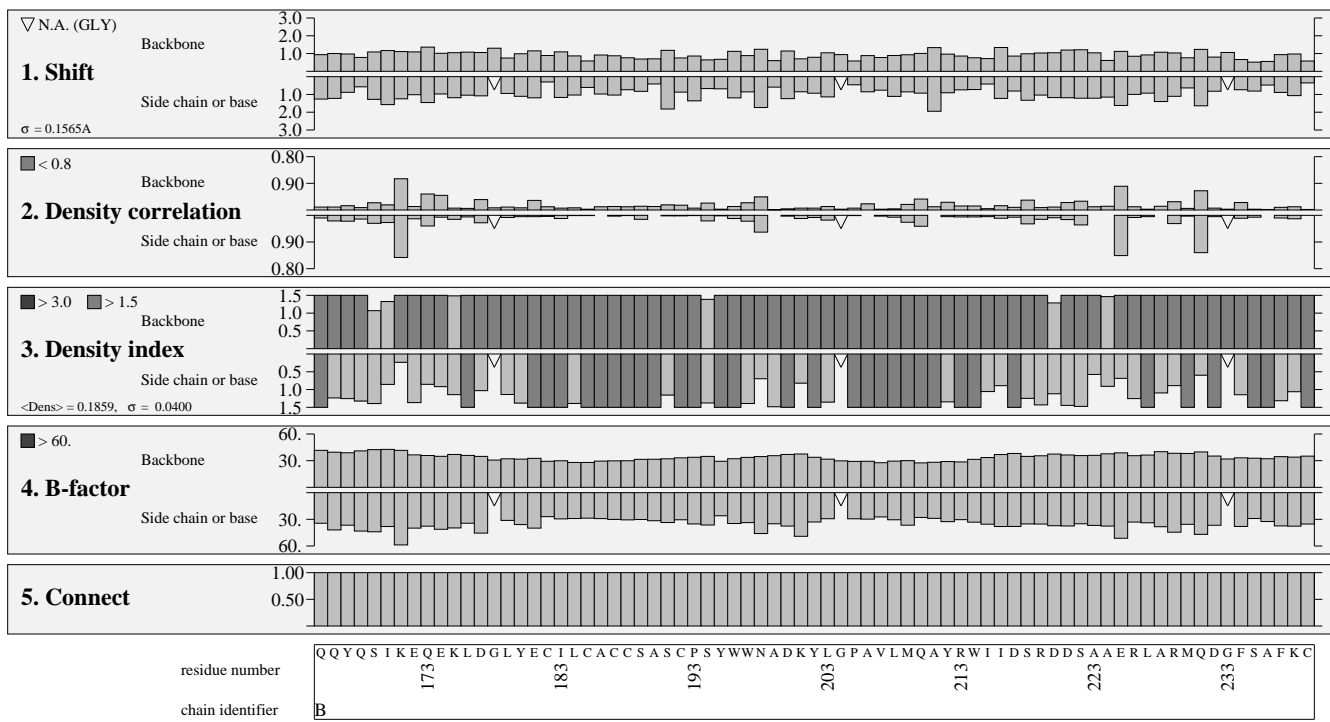
Local estimation (5)



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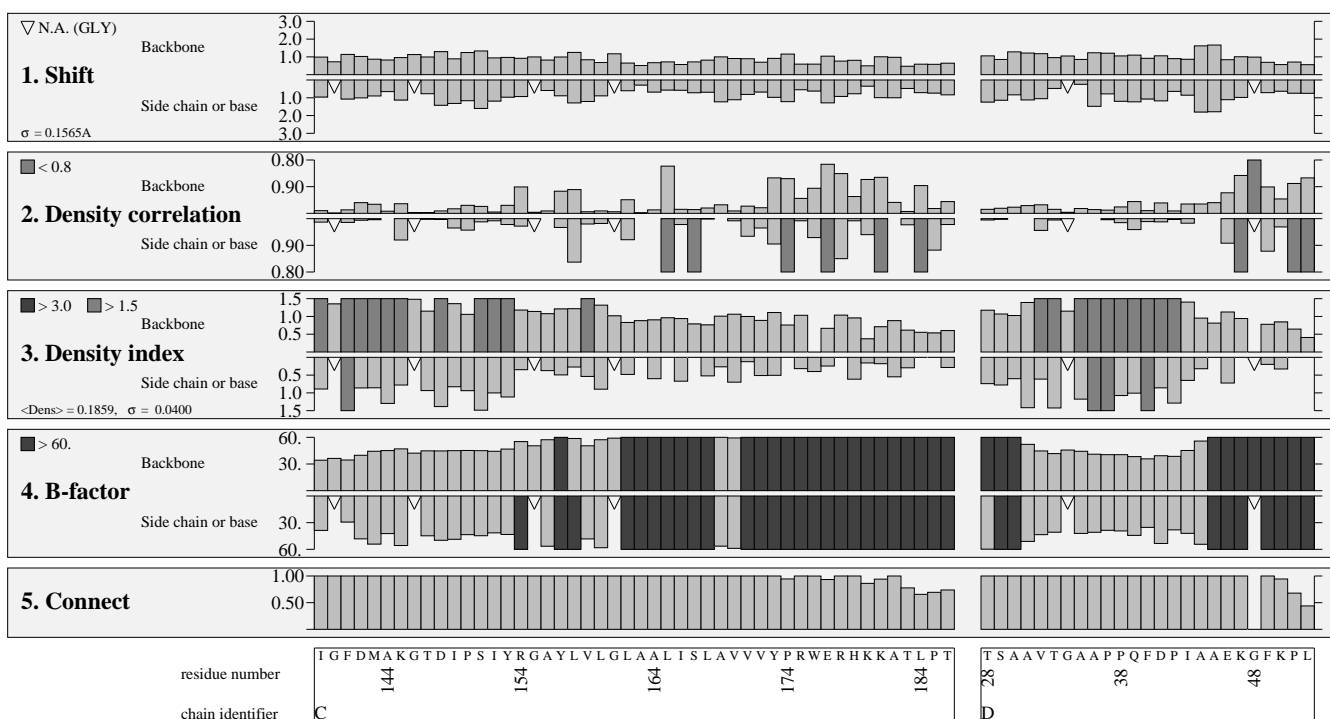
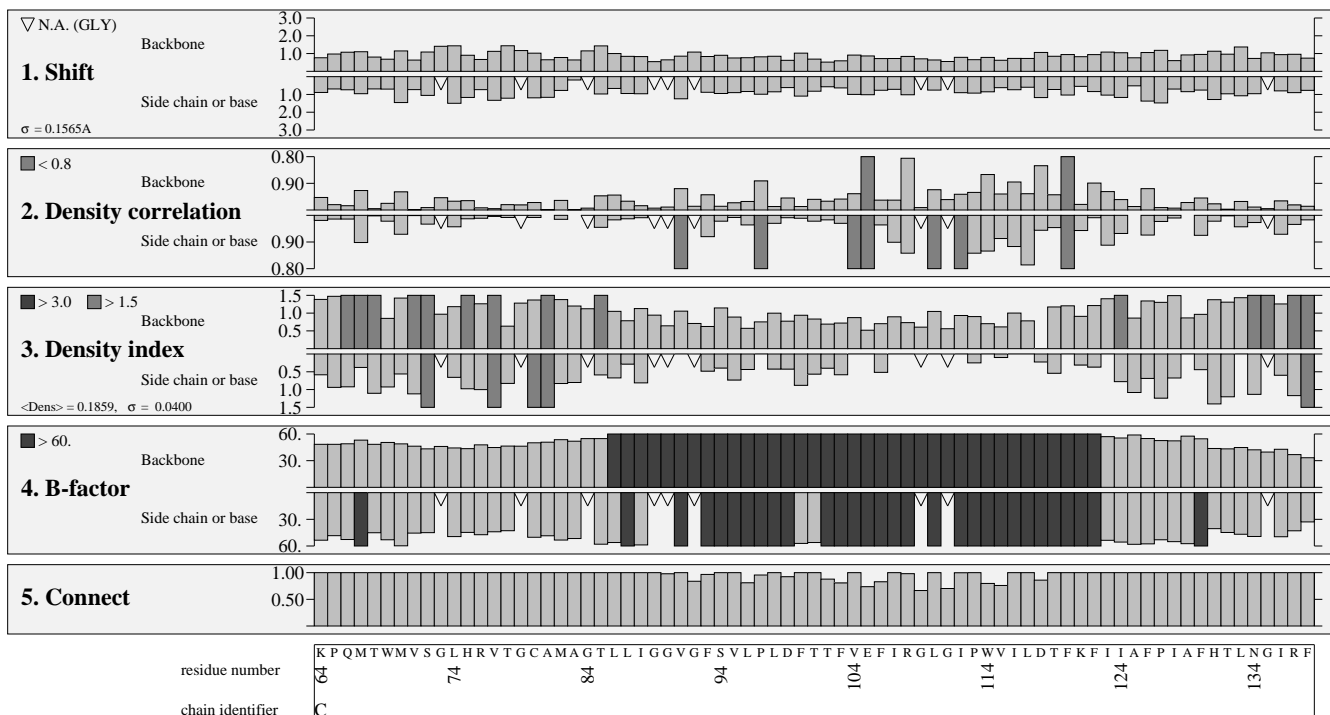
Local estimation (6)



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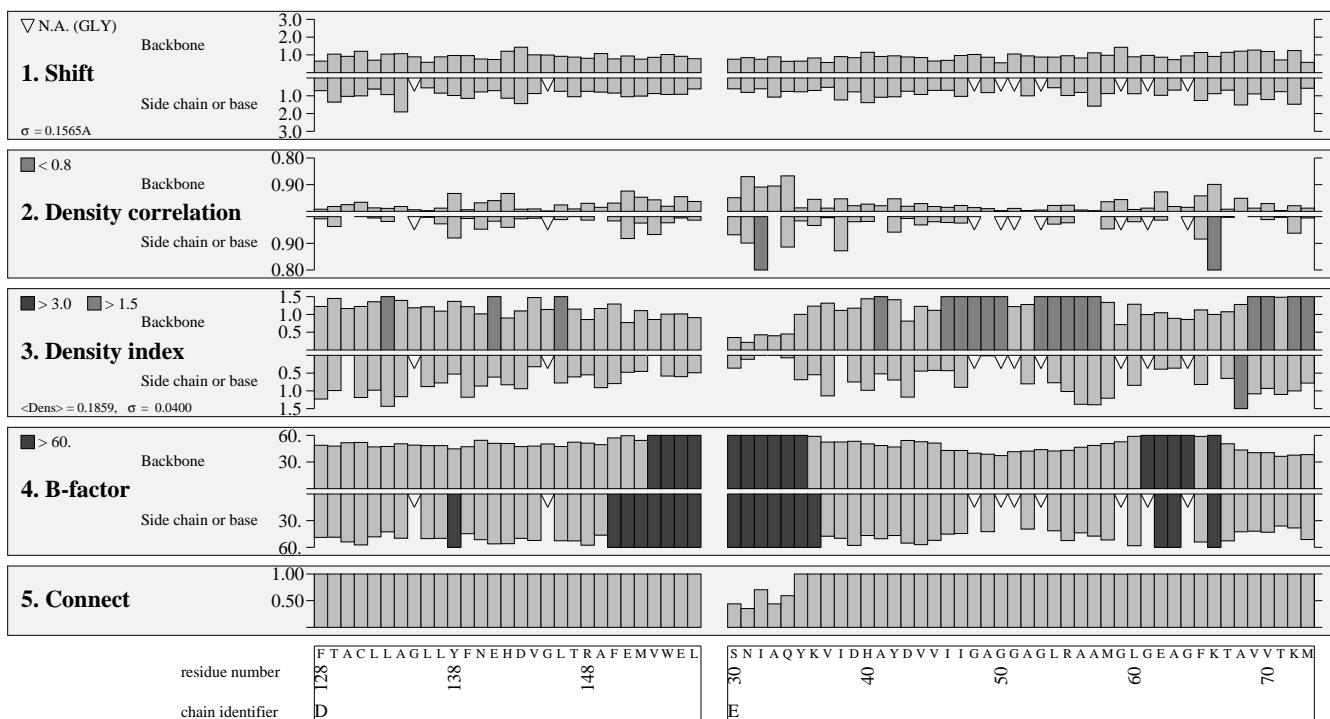
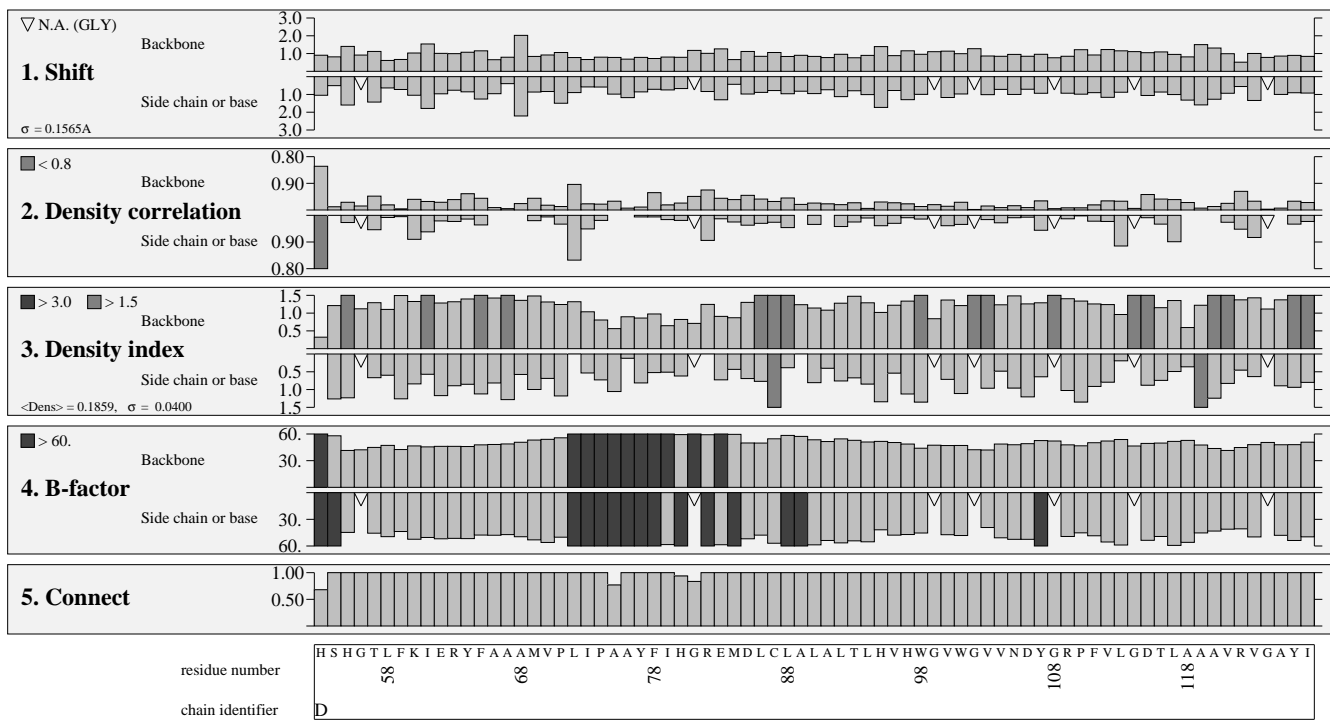
Local estimation (7)



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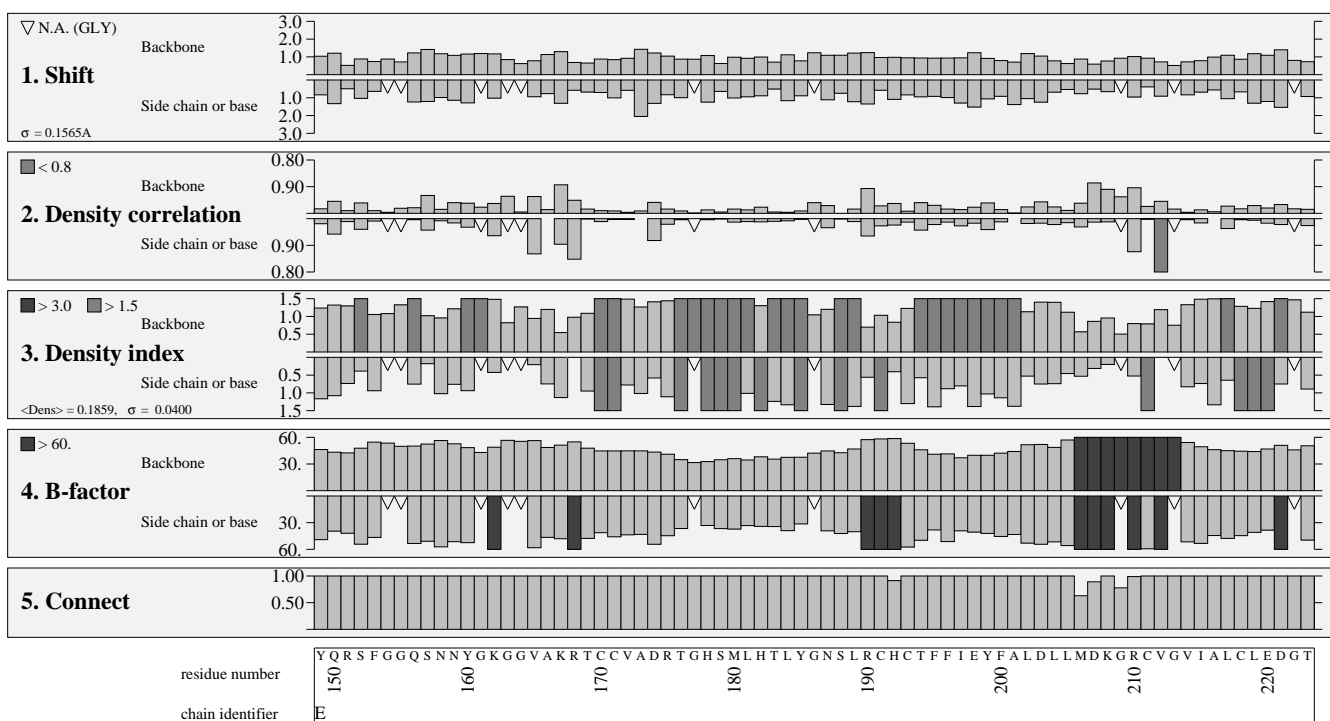
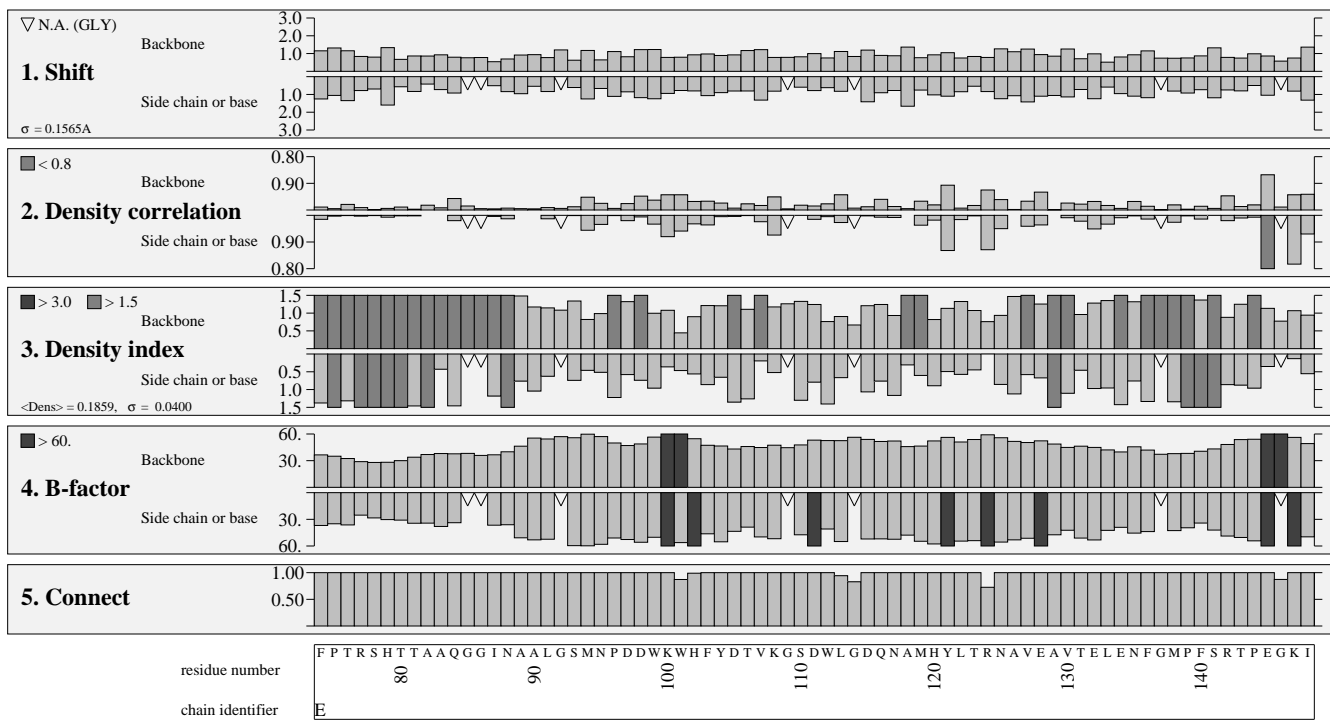
Local estimation (8)



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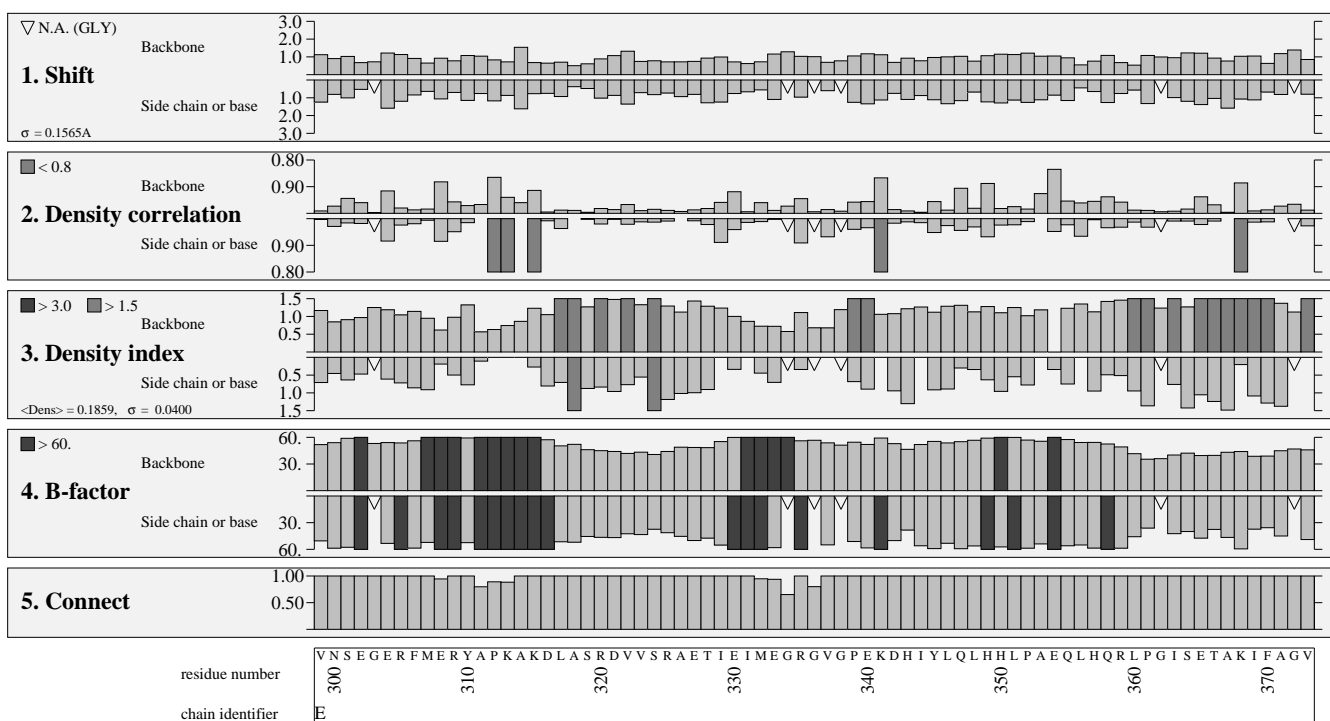
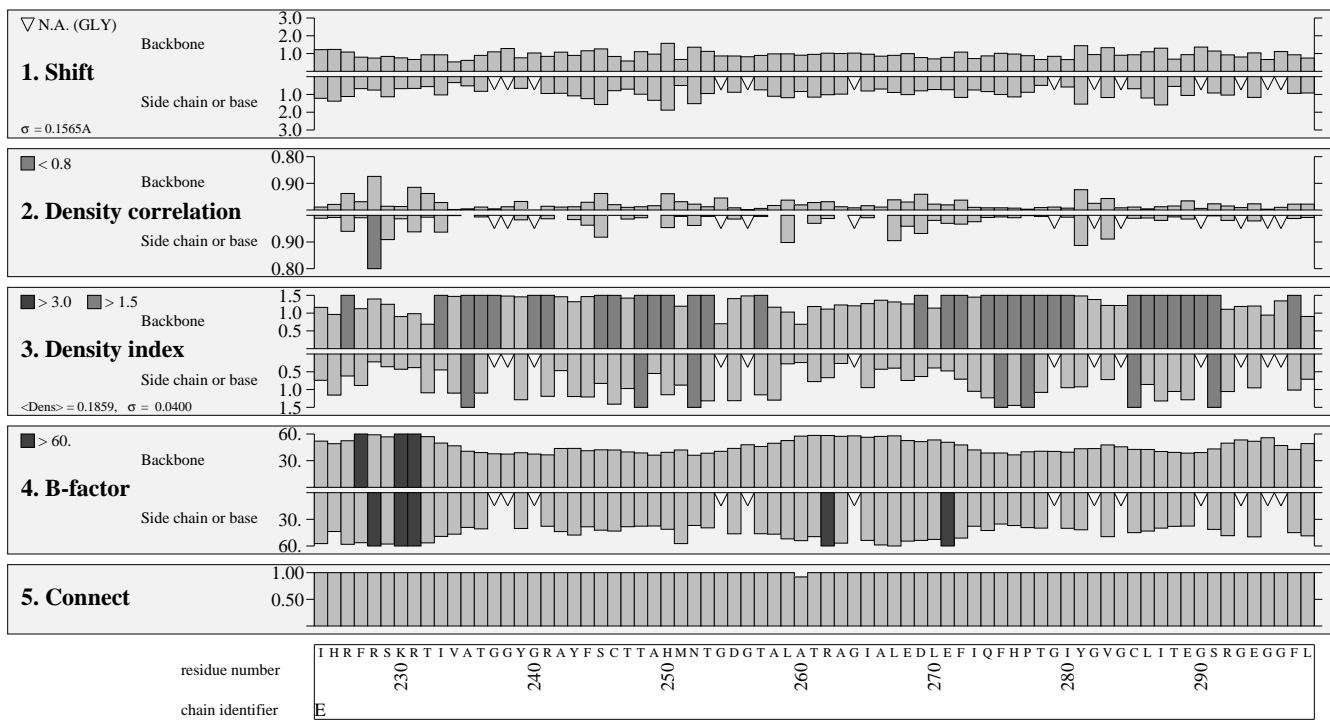
Local estimation (9)



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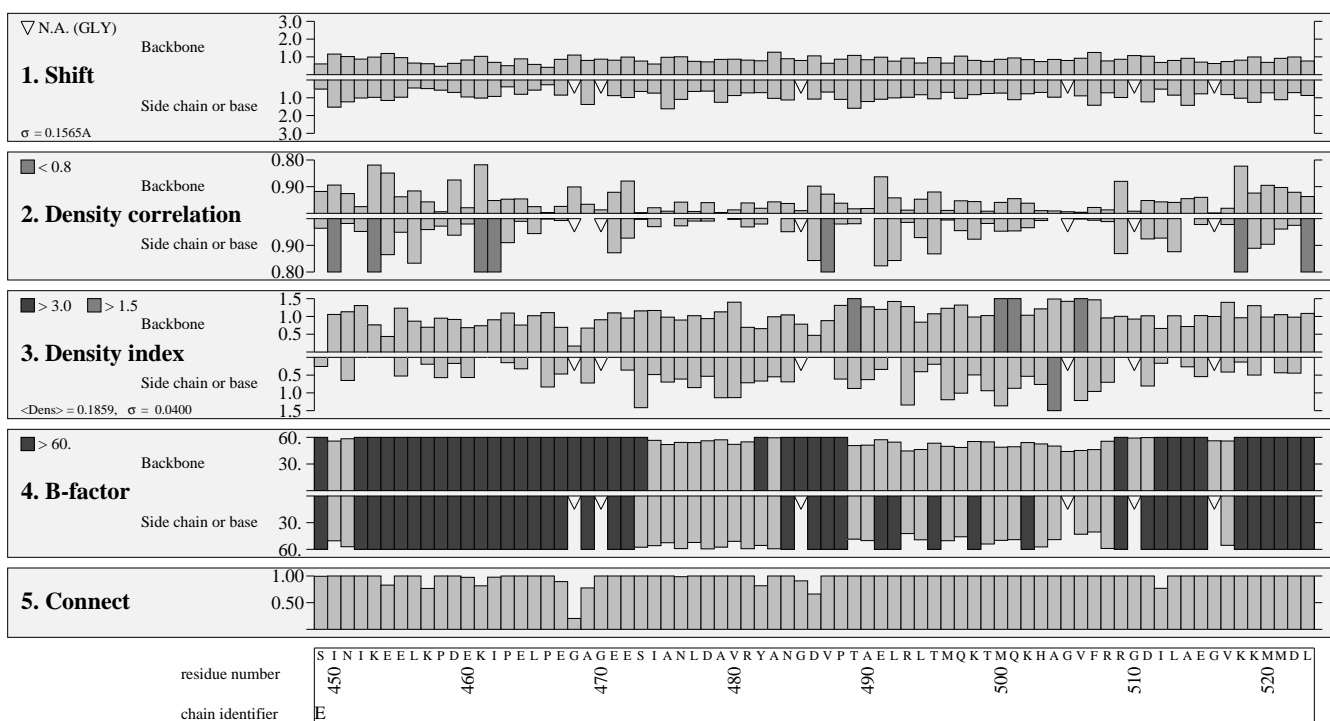
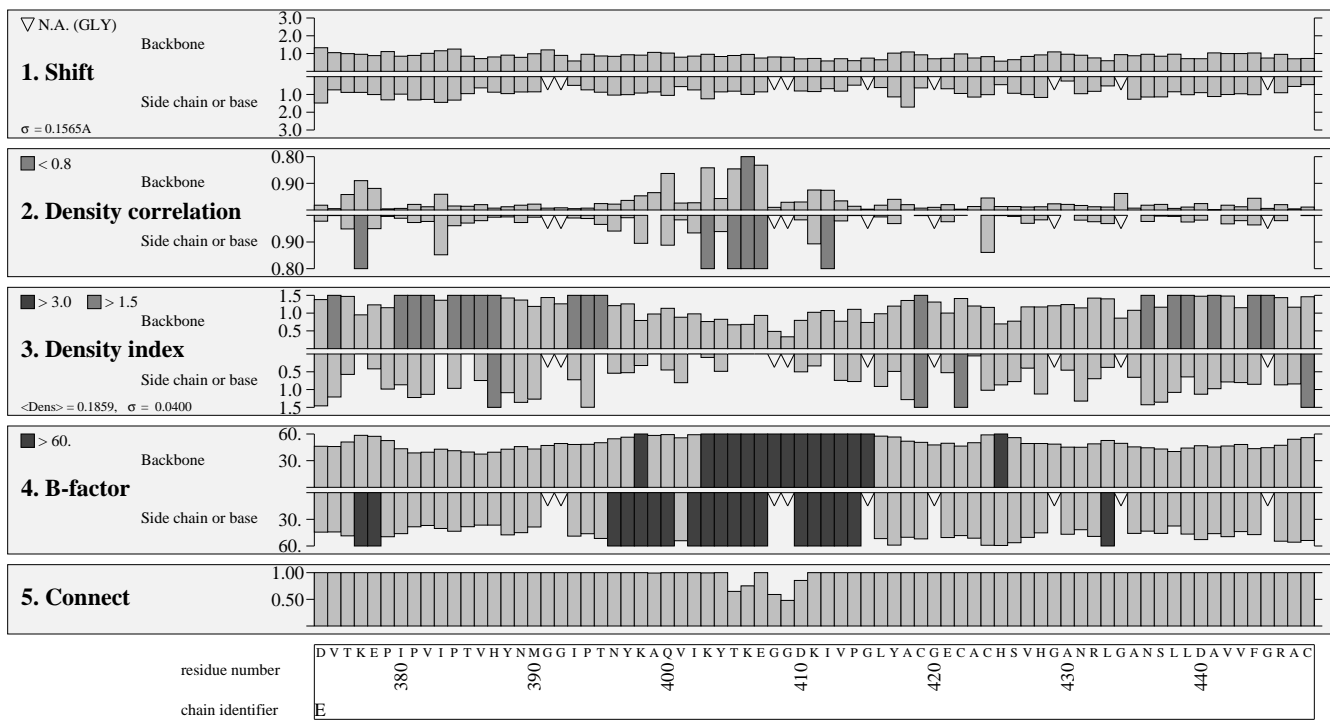
Local estimation (10)



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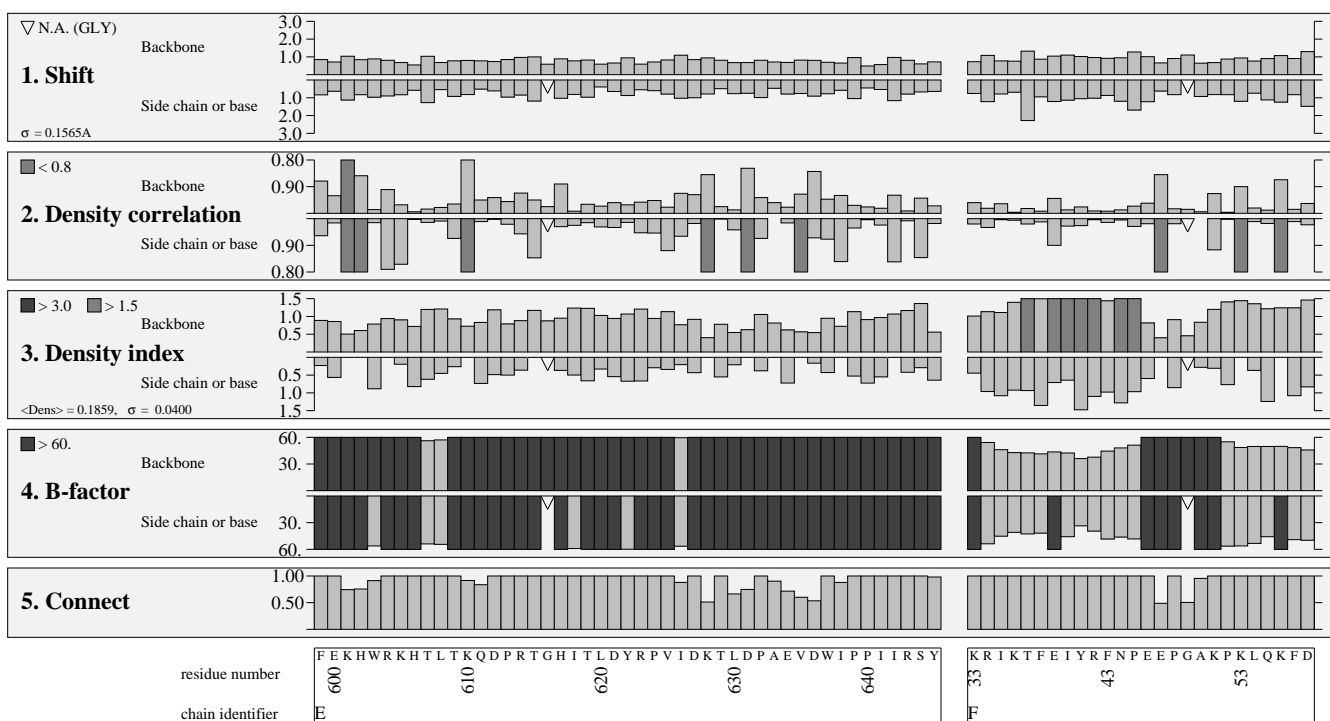
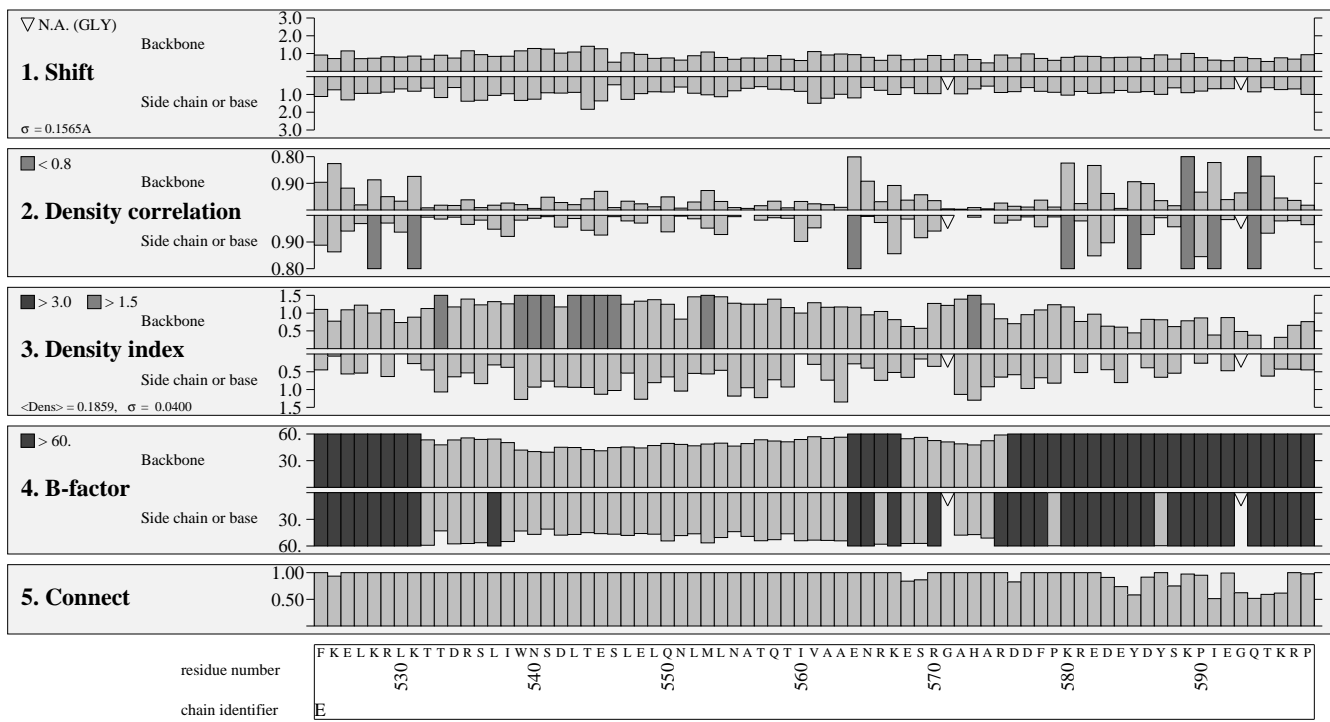
Local estimation (11)



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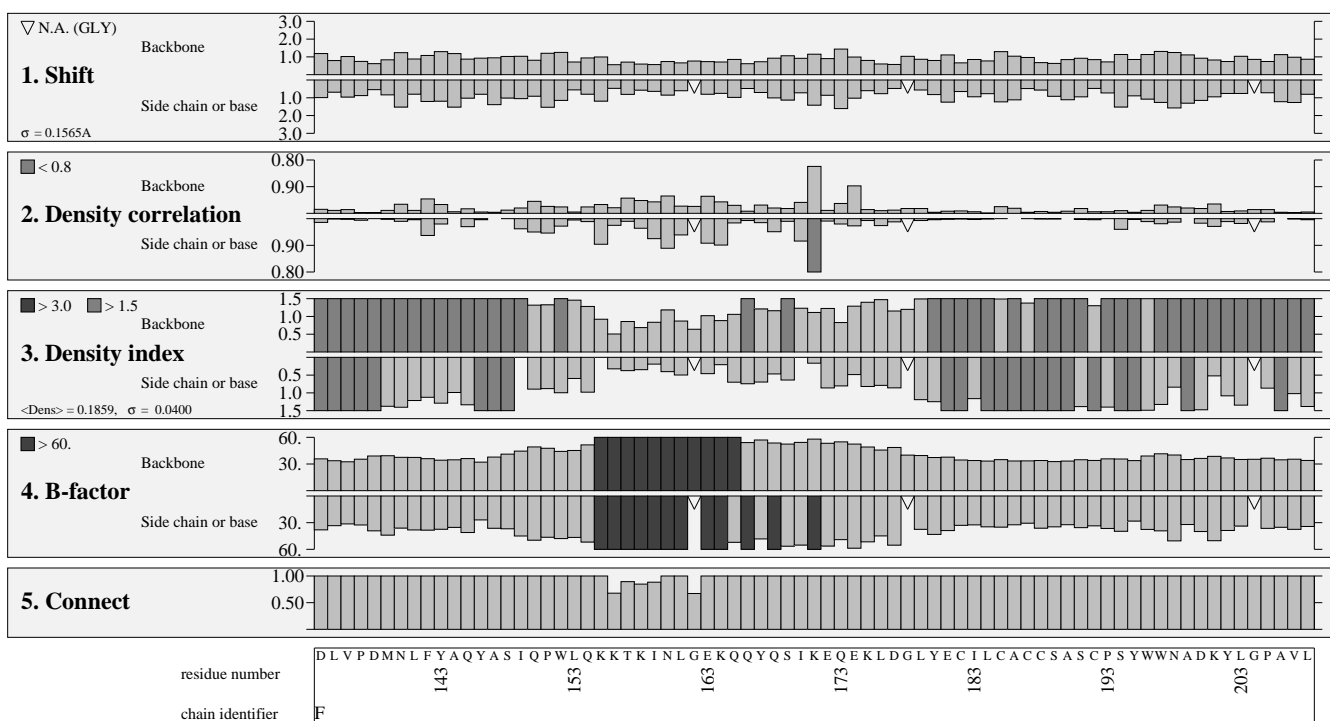
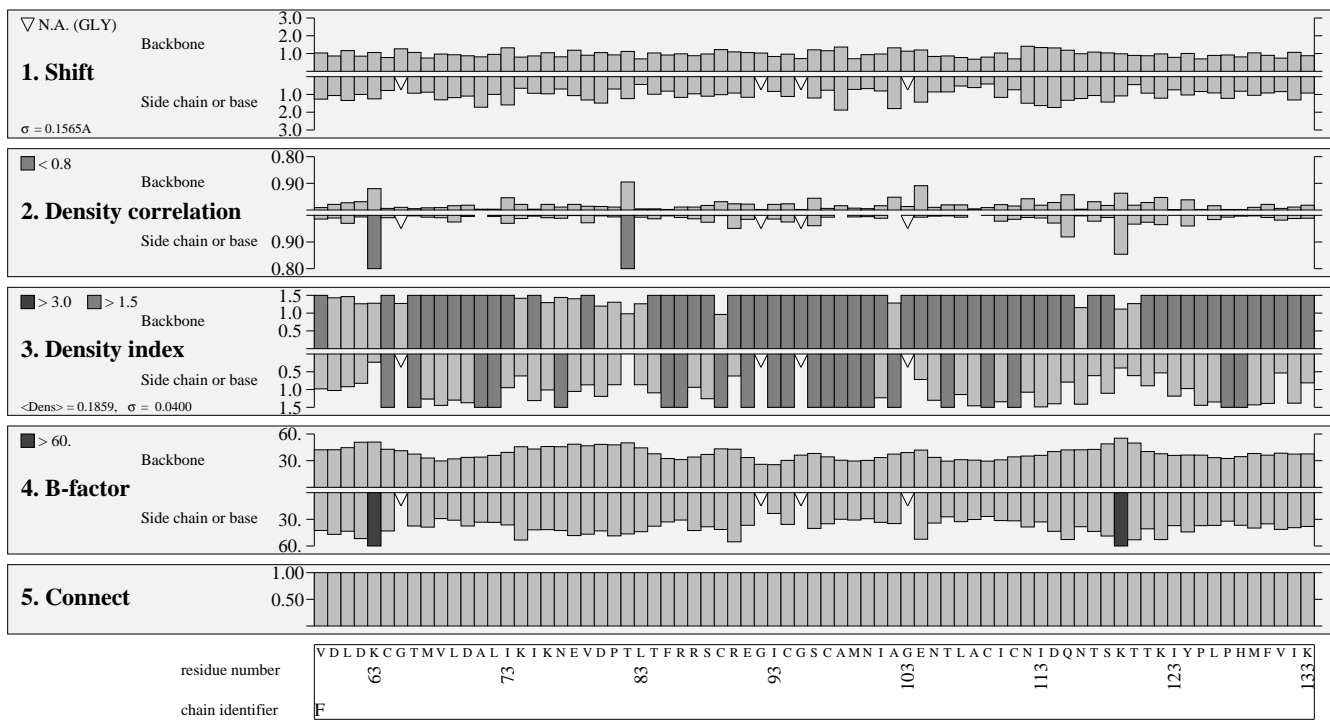
Local estimation (12)



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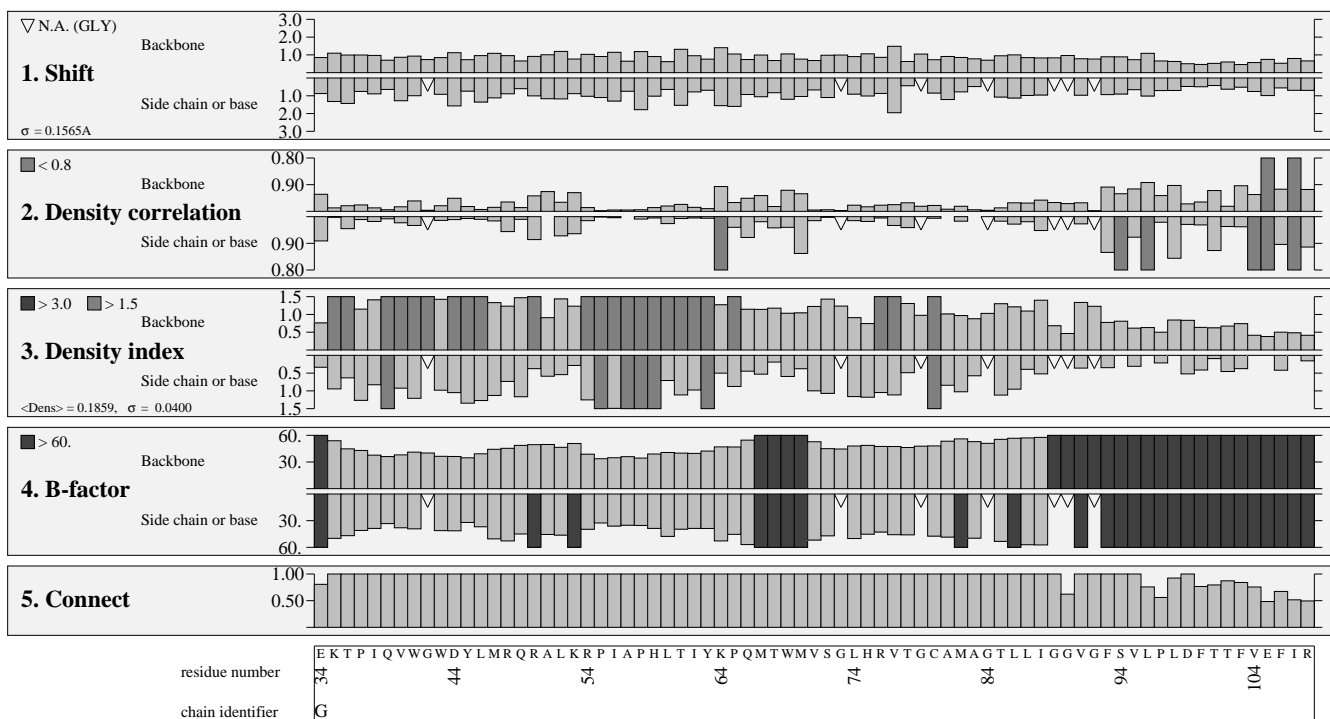
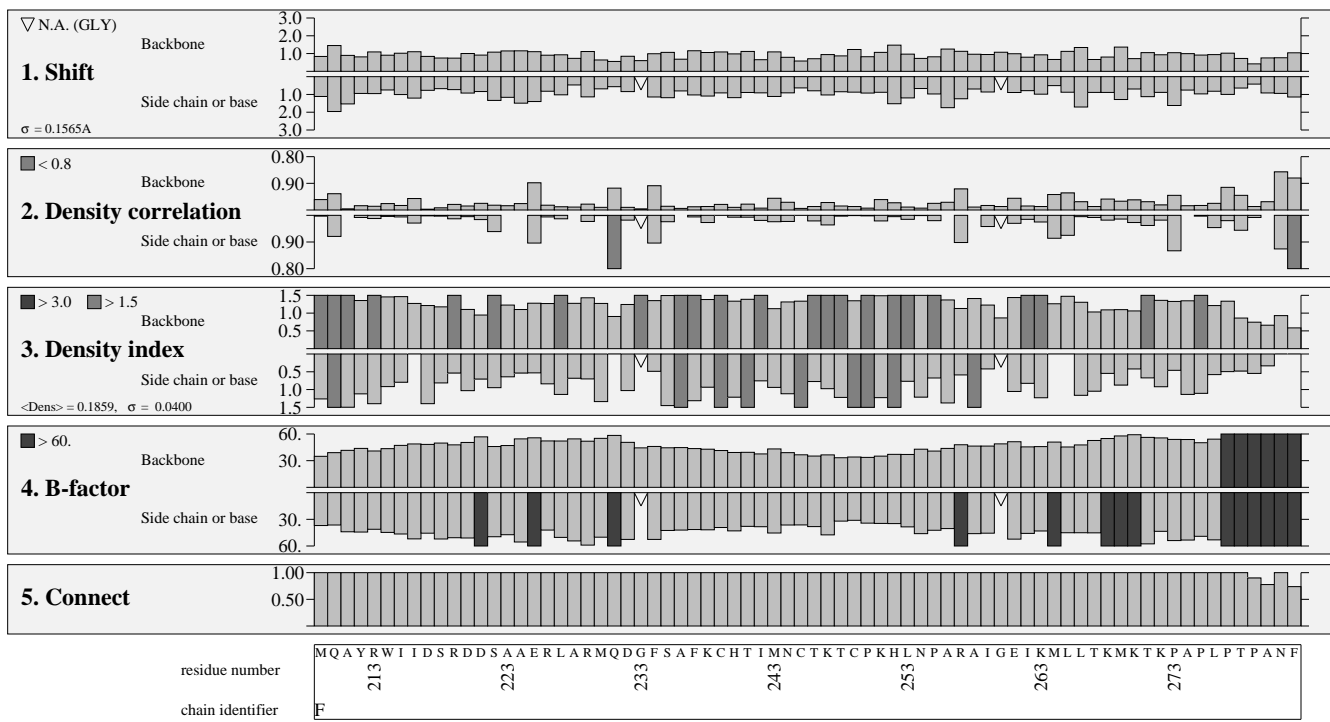
Local estimation (13)



Structure Factor Check

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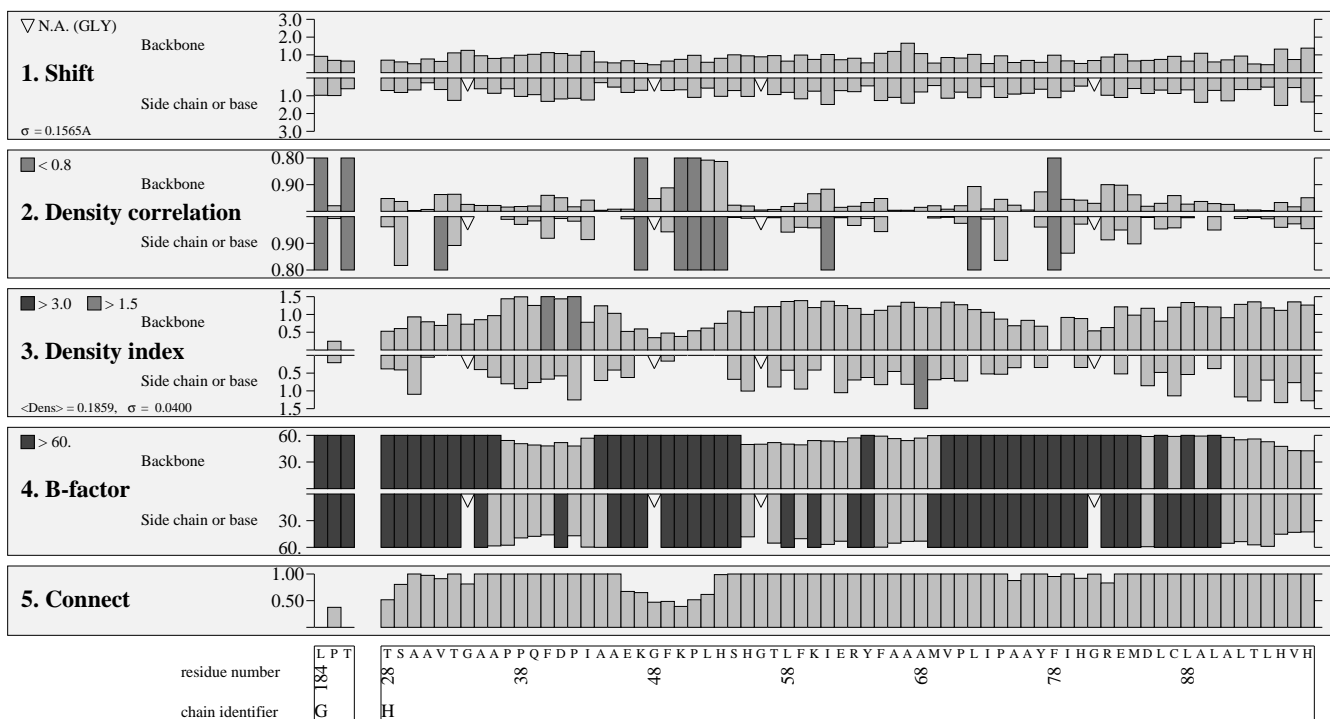
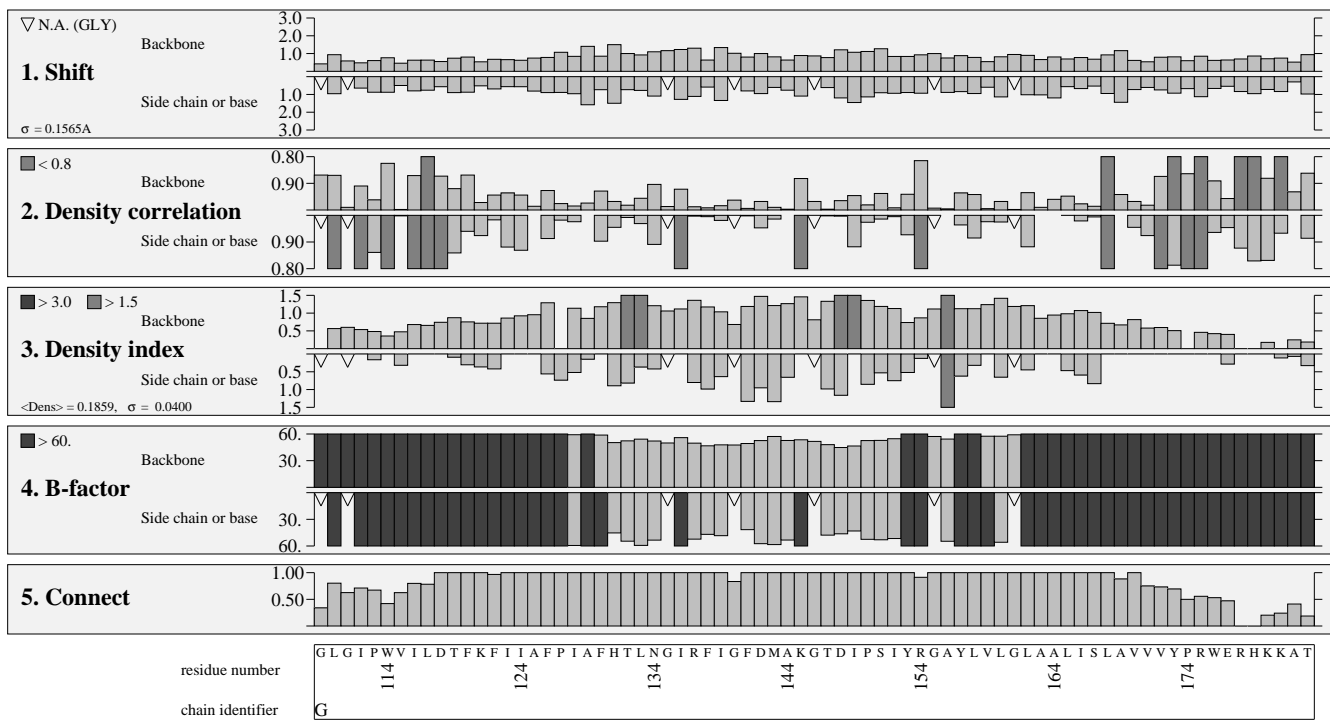
Local estimation (14)



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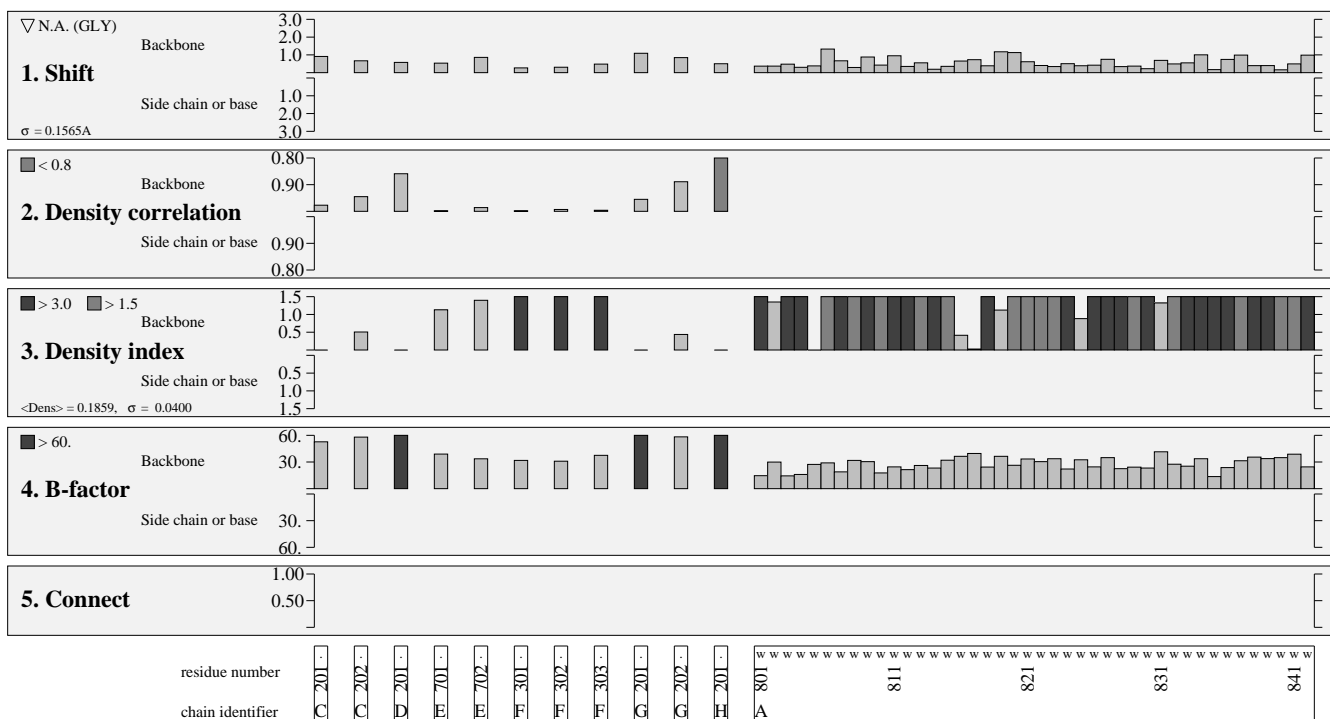
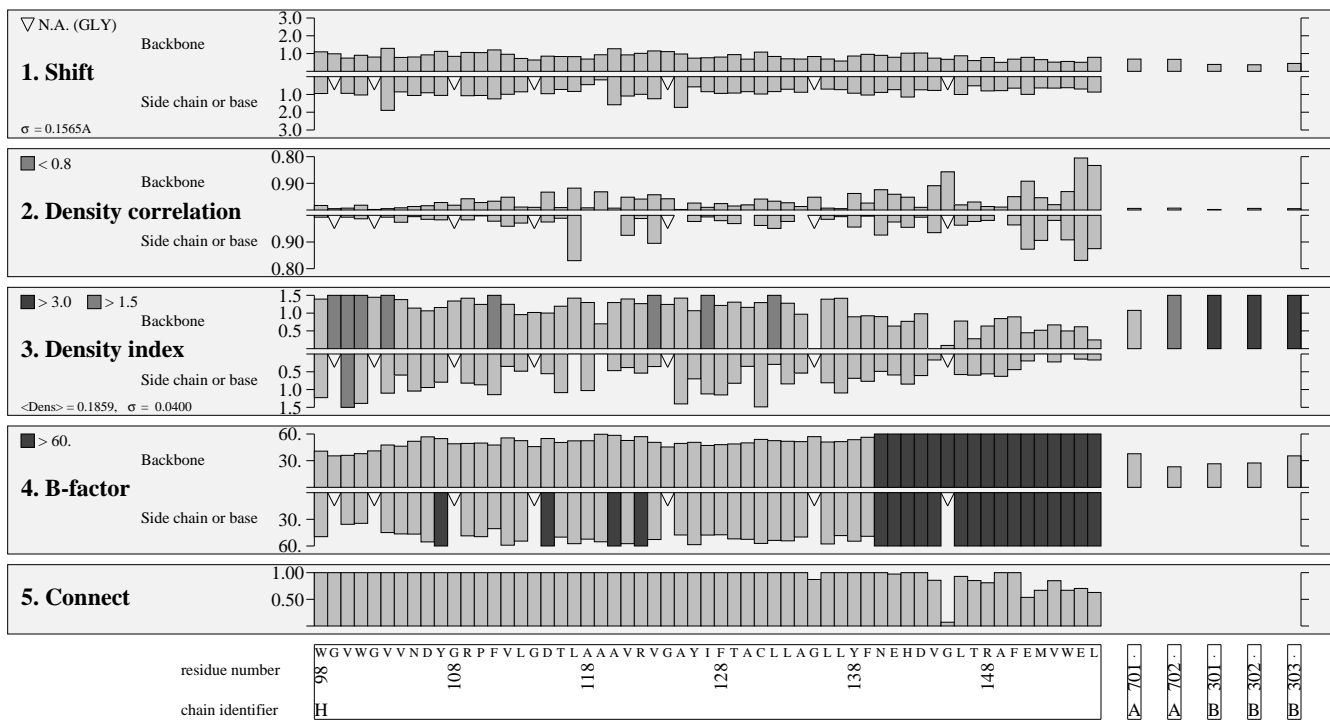
Local estimation (15)



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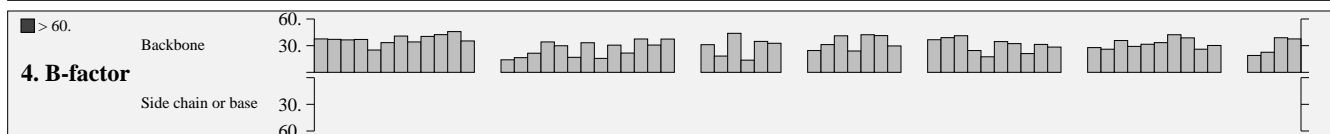
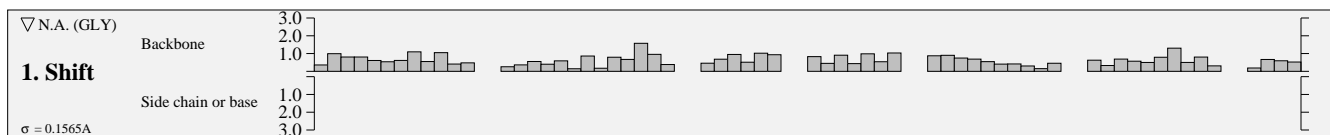
Local estimation (16)



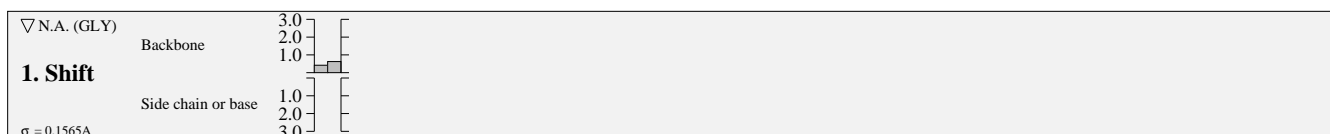
Structure Factor Check

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Local estimation (17)



residue number	w w w w w w w w w w	w w w w w w w w w w w w	w w w w w w	w w w w w w w	w w w w w w w w w w w	w w w w w w w w w w w	w w w w
	851	401 411	301	301	801	401	301
chain identifier	A	B	C	D	E	F	G



residue number	w w
	301
chain identifier	H