

Structure Factor Check

4YTN

Title: CRYSTAL STRUCTURE OF MITOCHONDRIAL RHODOQUINOL-FUMARATE REDU
 ASCARIS SUUM WITH N-[3-(5-PENTAFLUOROPHENOXY)PHENYL]-2-
 (5-TRIFLUOROMETHYL)BENZAMIDE
 Date: 18-MAR-15
 PDB code: 4YTN

Crystal

Cell parameters:

a: 123.61 Å b: 125.48 Å c: 219.67 Å
 α : 90.00 β : 90.00 γ : 90.00

Space group: P 21 21 21

Number of NCS-operators: 5
 NC-symmetry only for information

Structure Factors

Input

Nominal resolution range: 20.0 – 3.00 Å
 Reflections in file: 68829
 Unique reflections above 0: 64636
 above 1 σ : 63900
 above 3 σ : 51203
 Reflections > 0: 4193

SFCHECK

Nominal resolution range: 20.0 – 3.00 Å
\05max. from input data, min. from author\05
 Used reflections: 64629
 Reflections out of resolution: 7
 Completeness: 93.9 %
 $R_{\text{stand}}(F) = \langle \sigma(F) \rangle / \langle F \rangle$: 0.048
 Anisotropic distribution of Structure Factors
 ratio of eigen values: 1.0000 0.9304 0.9069
 B_{overall} (by Patterson): 48.Å²
 Optical resolution: 2.17 Å
 Expected opt. resol. for complete data set: 2.17 Å
 Estimated minimal error: 0.042 Å

Model

18320 atoms (40 water molecules)
 Number of chains: 28
 Volume not occupied by model: 54.2 %
 $\langle B \rangle$ (for atomic model): 62.9 Å²
 $\sigma(B)$: 15.25 Å²
 Matthews coefficient: 3.32
 Corresponding solvent % : 62.68

Model vs. Structure Factors

R-factor for all reflections: 0.245
 Correlation factor: 0.856
 R-factor: 0.250
 for $F > 2.0\sigma$
 nom. resolution range: 20.00 – 3.00Å
 reflections used: 63891
 Rfree: 0.293
 Nfree: 3231
 R-factor without free-refl.: 0.248
 Non free-reflections: 60660
 $\langle u \rangle$ (error in coords by Luzzati plot): 0.357 Å
 Estimated maximal error: 0.218 Å
 DPI: 0.385 Å

Refinement

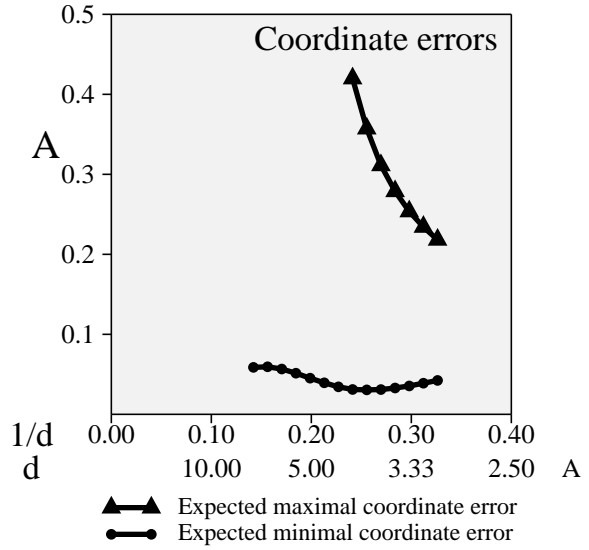
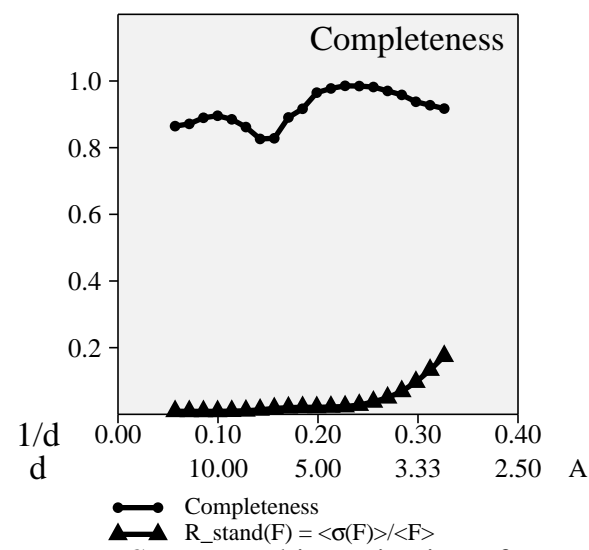
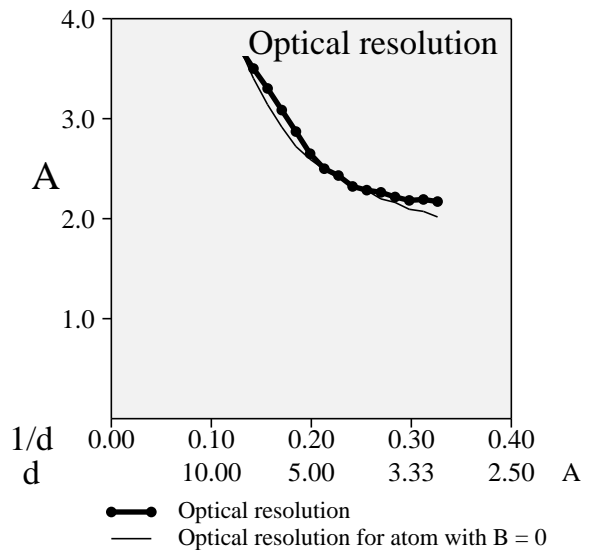
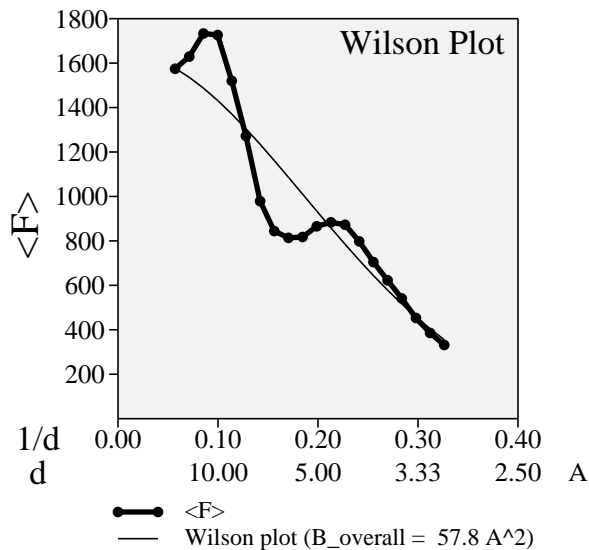
Program: REFMAC 5.7.0029
 Nominal resolution range: 20.0 – 3.00 Å
 Reported R-factor: 0.190
 Number of reflections used: 61648
 Reported Rfree: 0.24
 Sigma cut-off: N.A.

Scaling

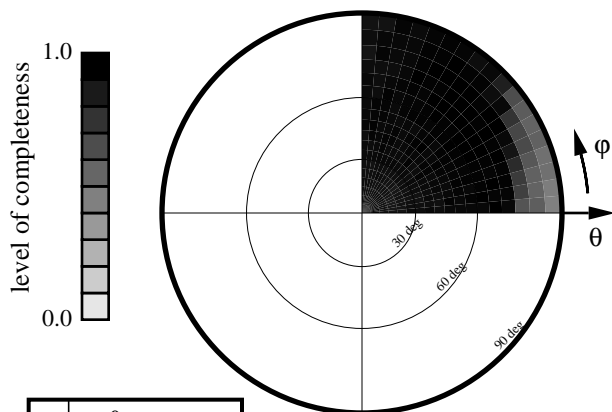
Scale: 0.888
 Bdiff: -5.58
 Anisothermal Scaling (Beta):
 -2.8059 -2.8872 -3.0322 0.0000 0.0000 0.0000
 Solvent correction – Ks,Bs: 0.365 249.860

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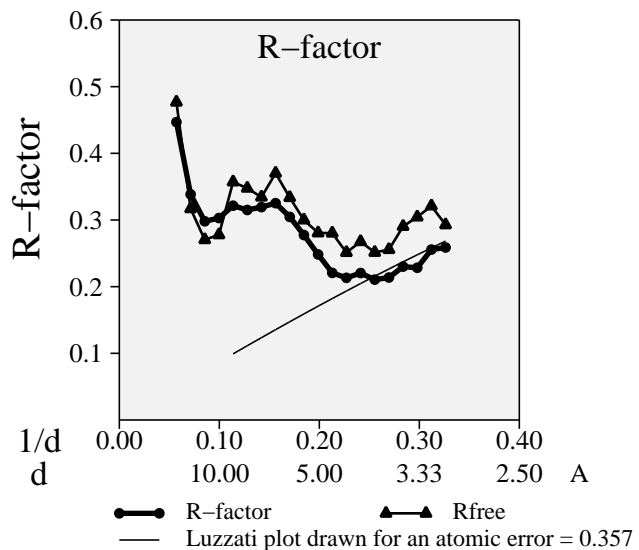


Stereographic projection of the averaged radial completeness



	θ	ϕ
h	90.00	0.00
k	90.00	90.00
l	0.00	0.00

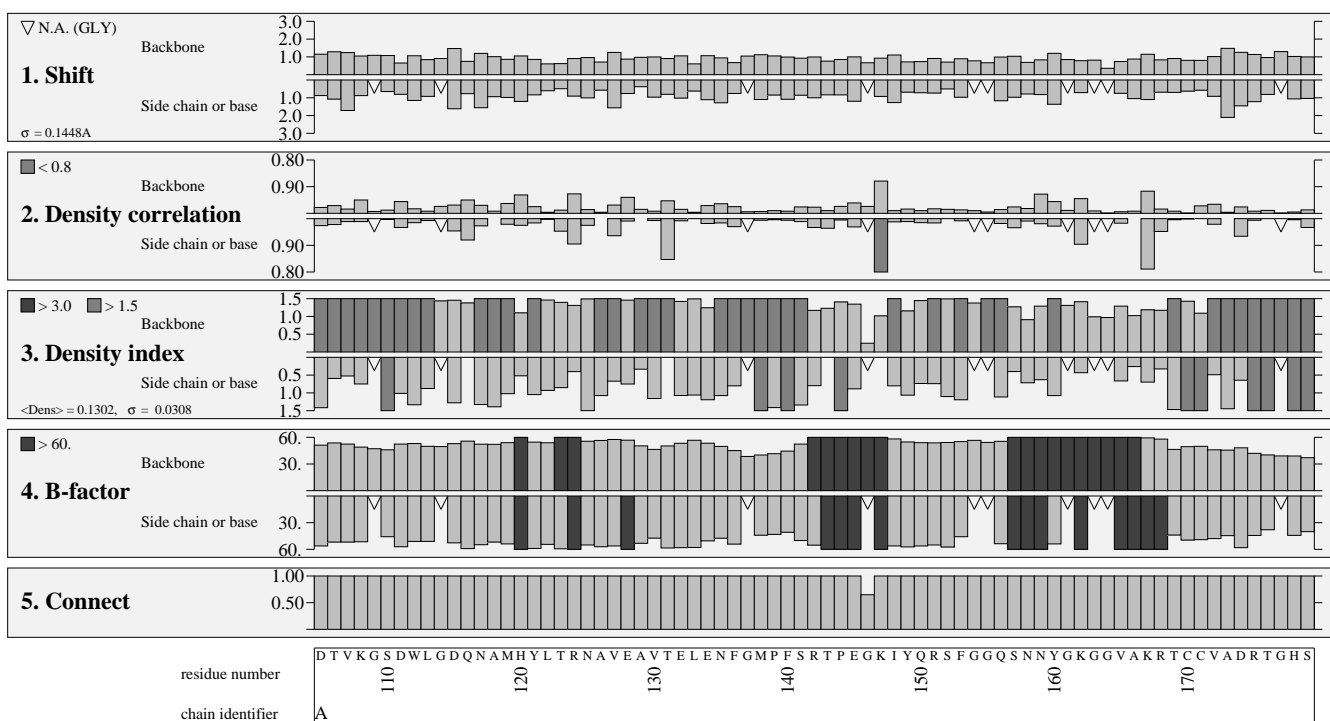
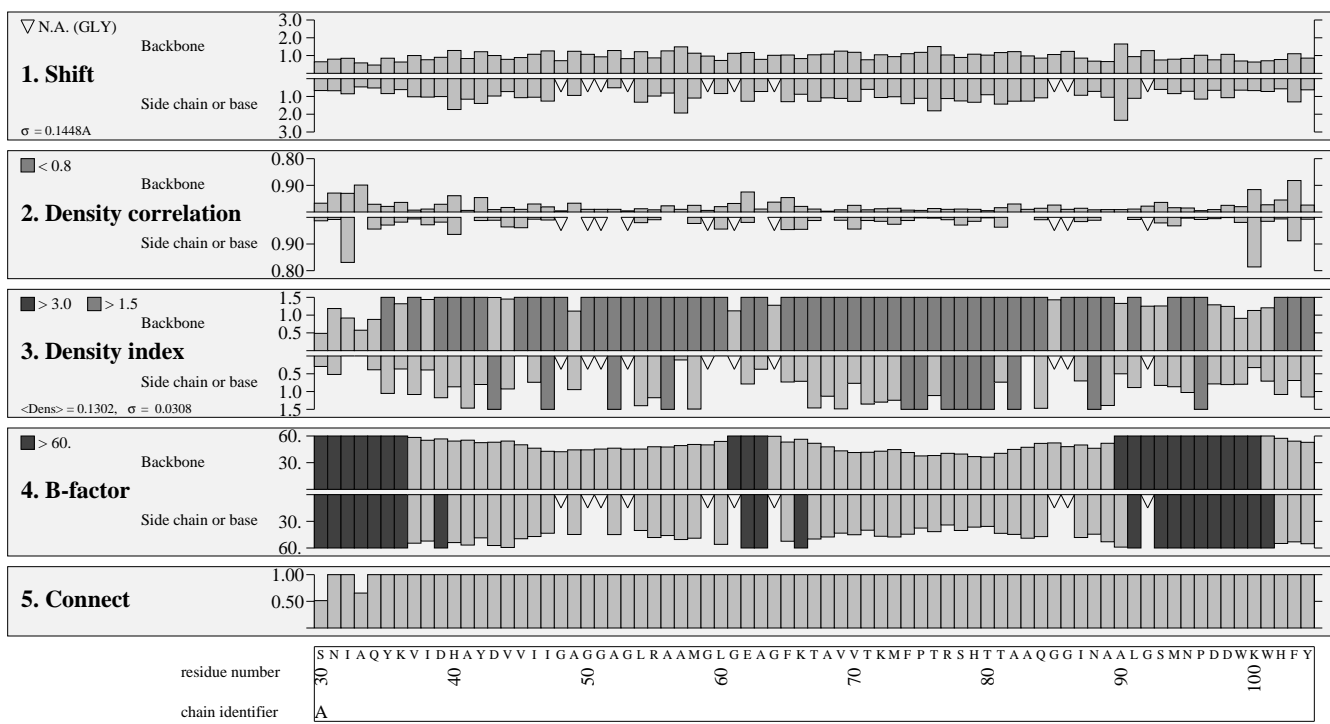
polar coordinates of the crystallographical axes



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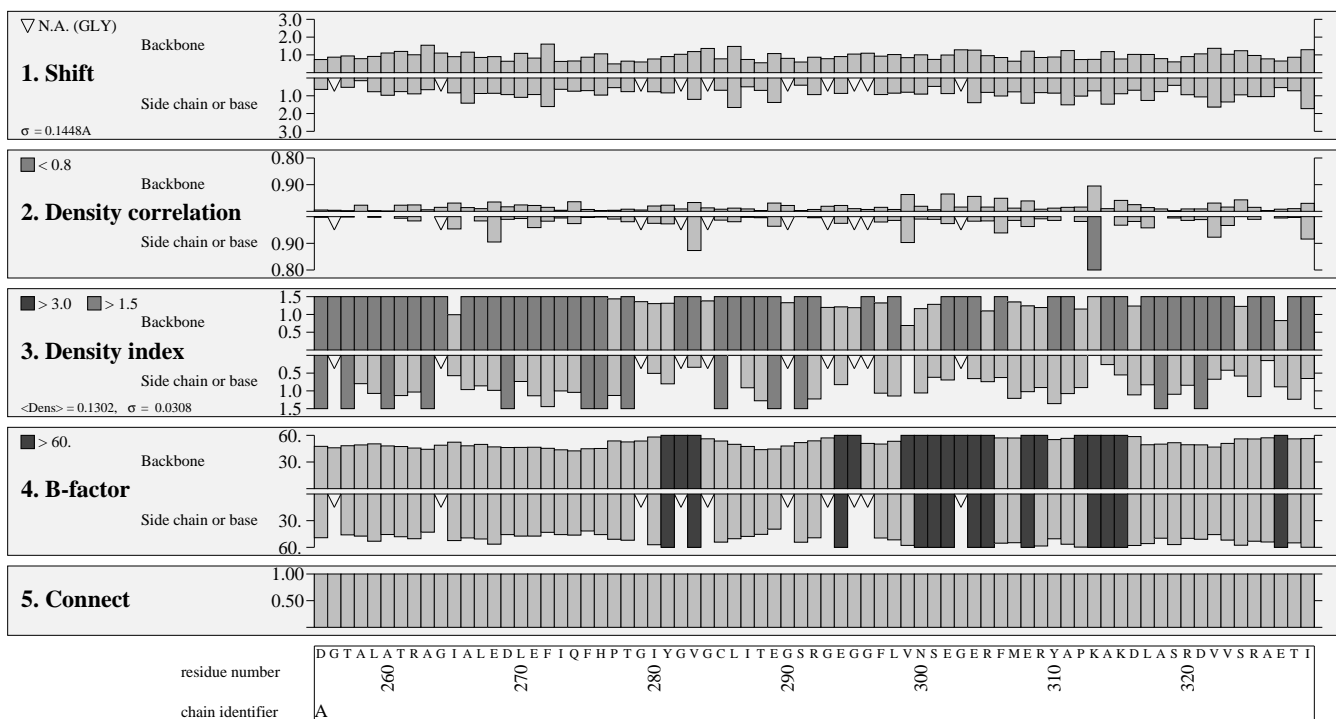
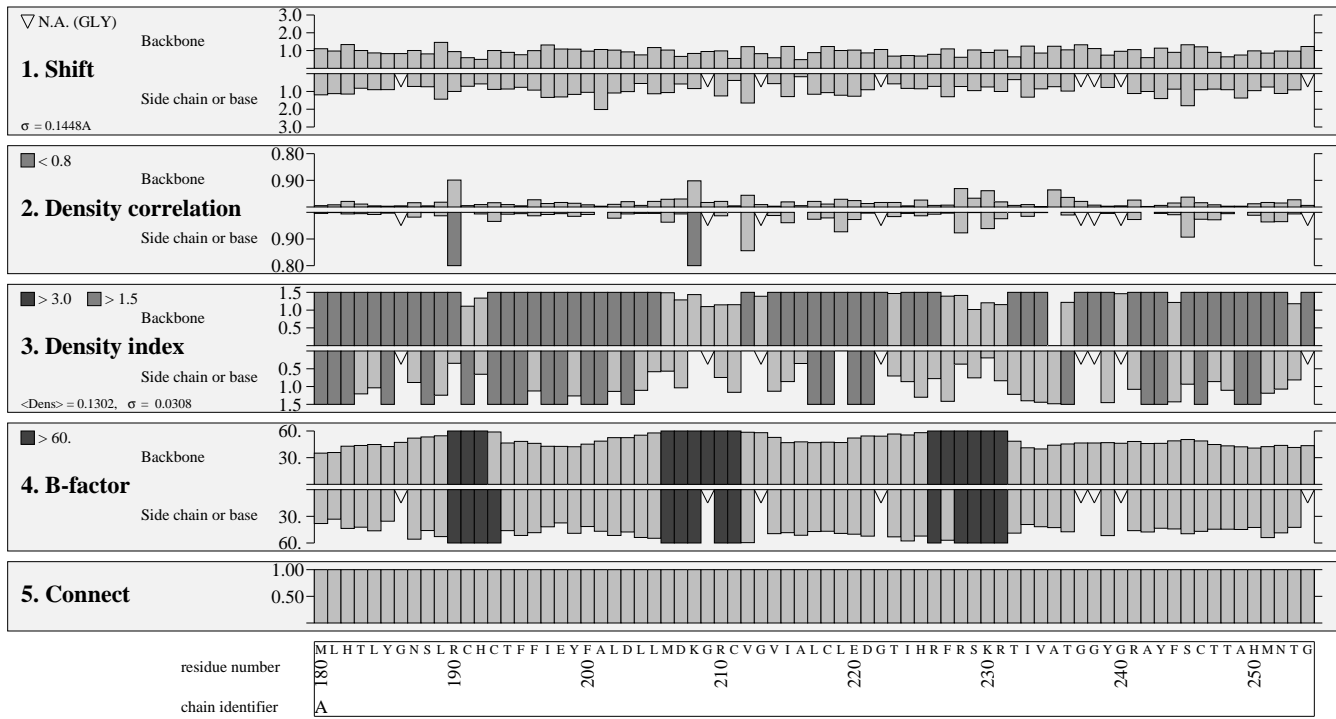
Local estimation



Structure Factor Check

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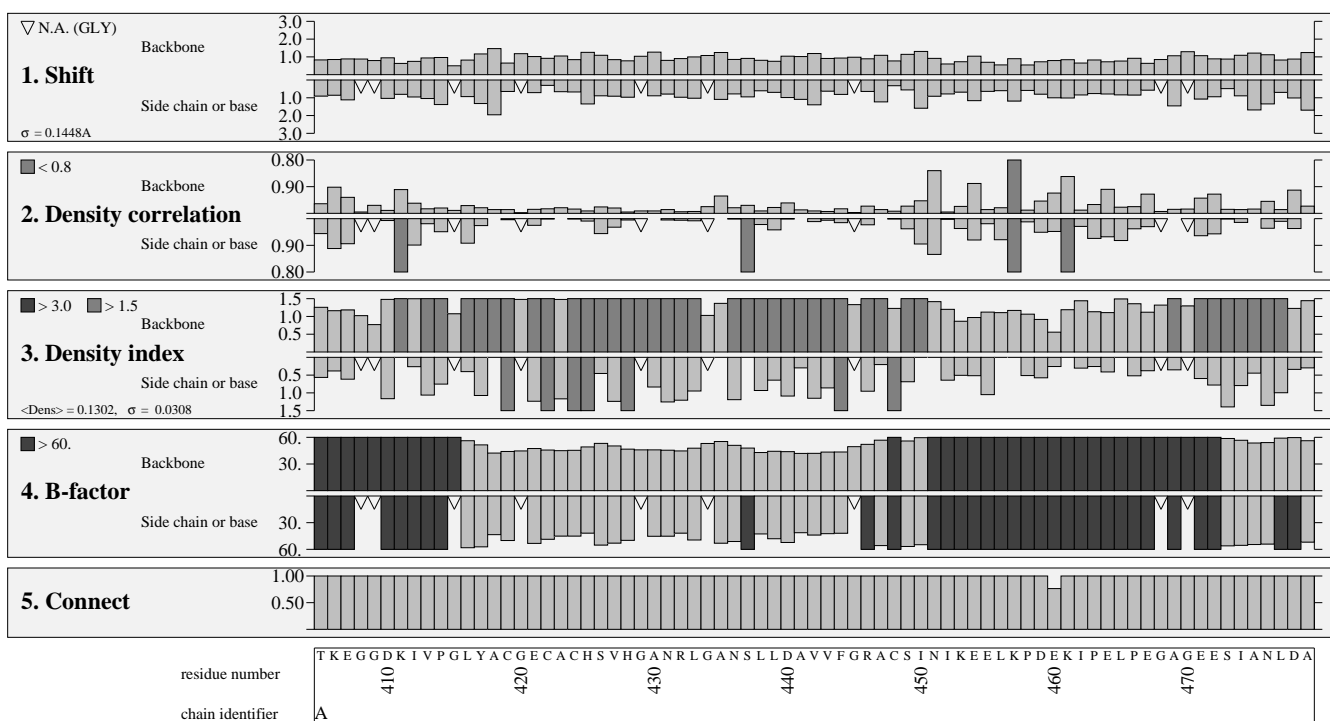
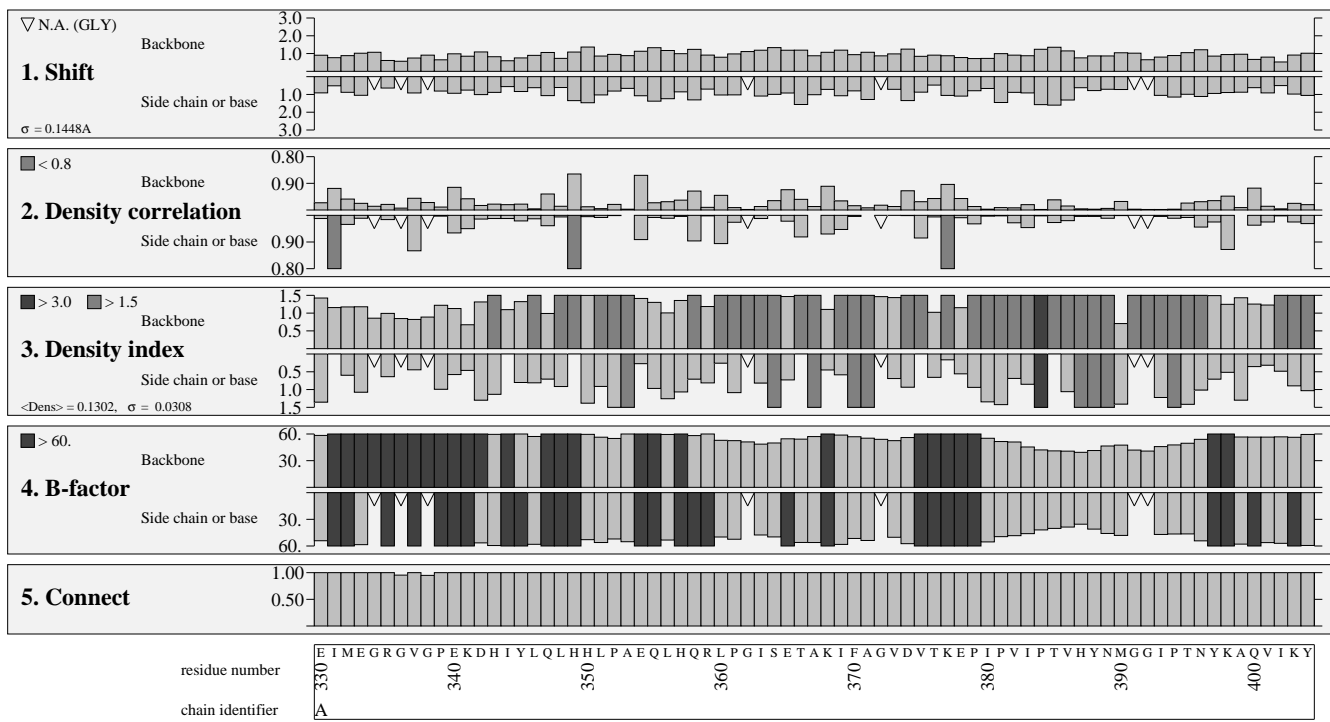
Local estimation (2)



Structure Factor Check

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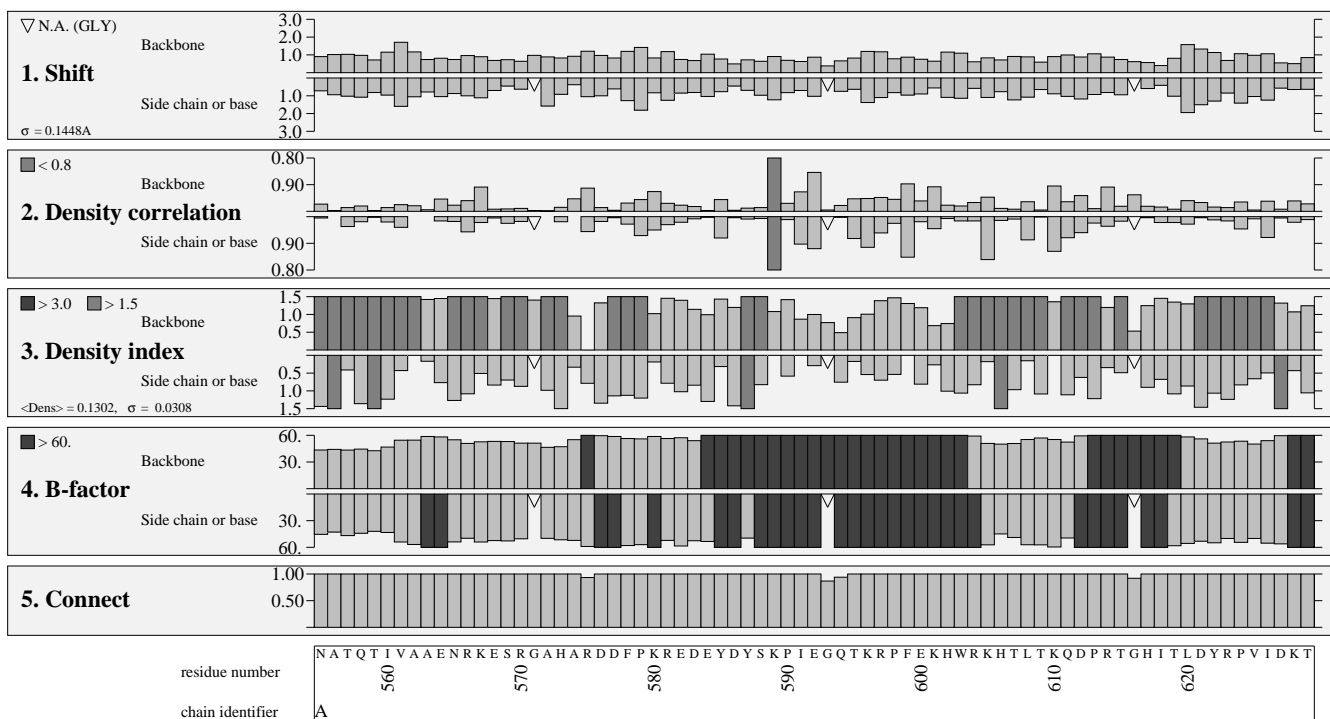
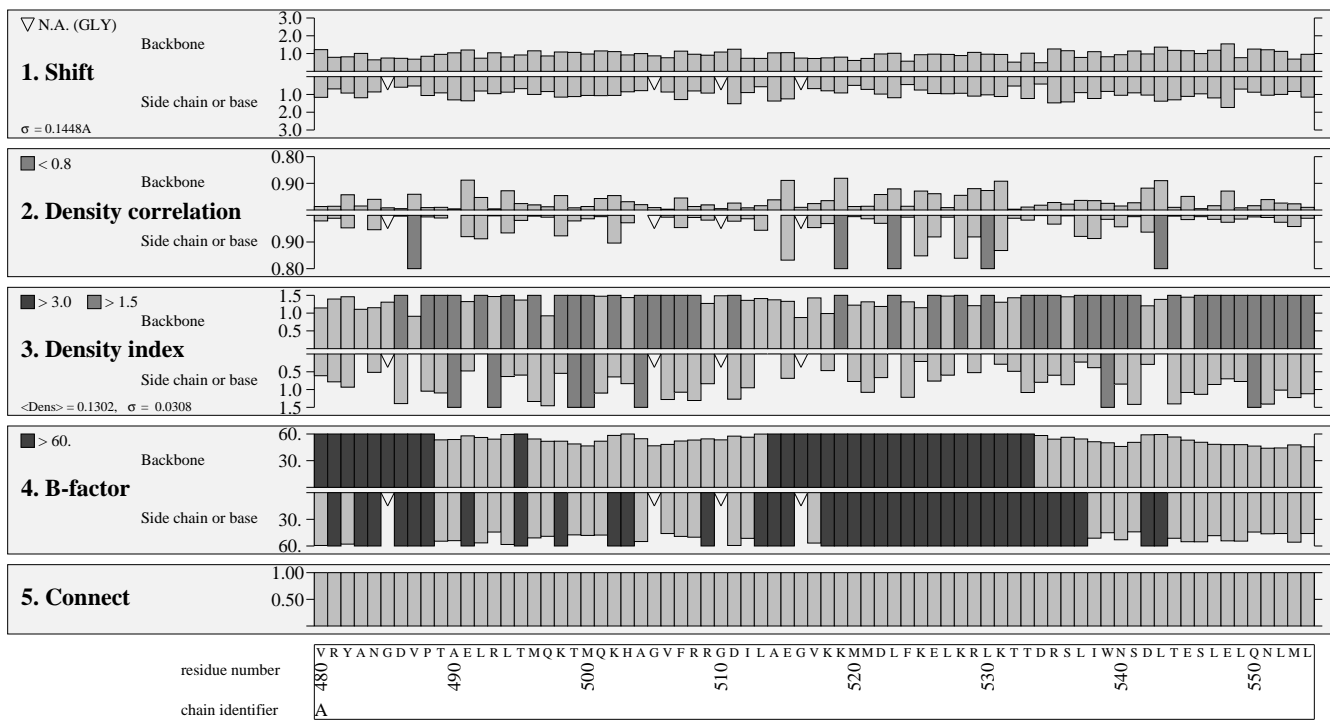
Local estimation (3)



Structure Factor Check

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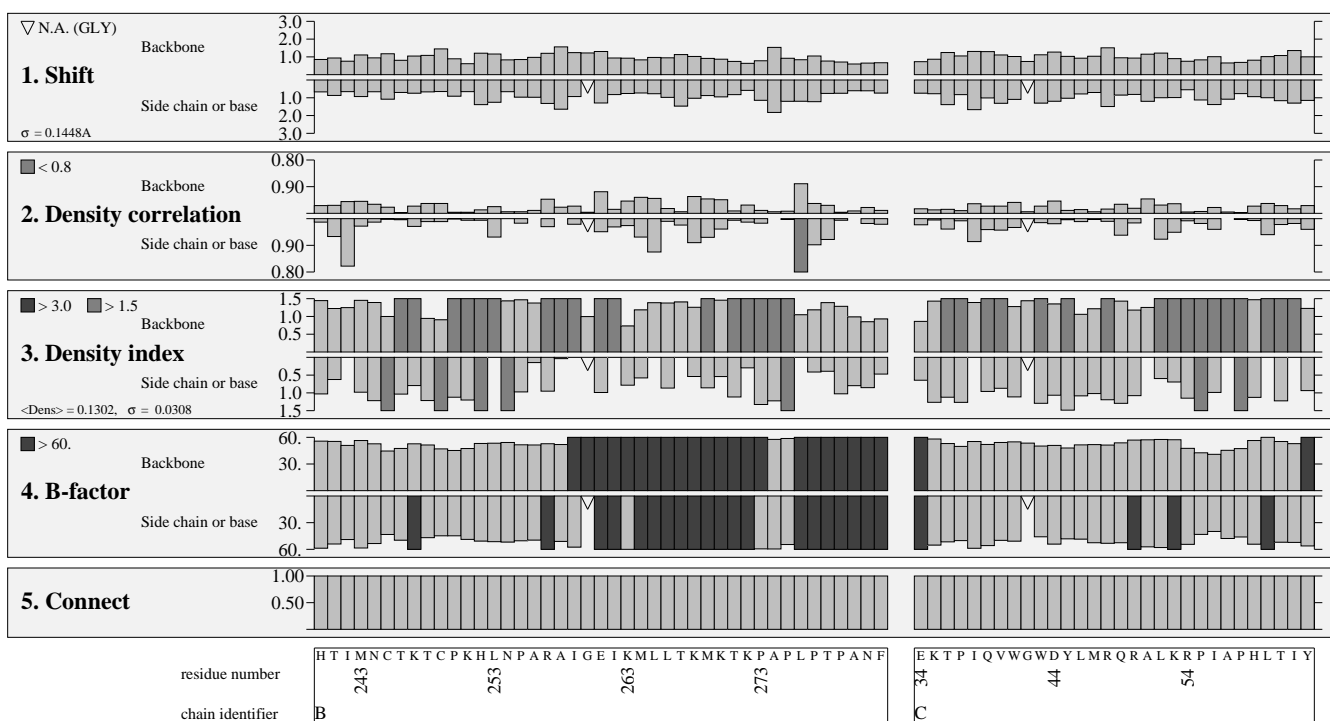
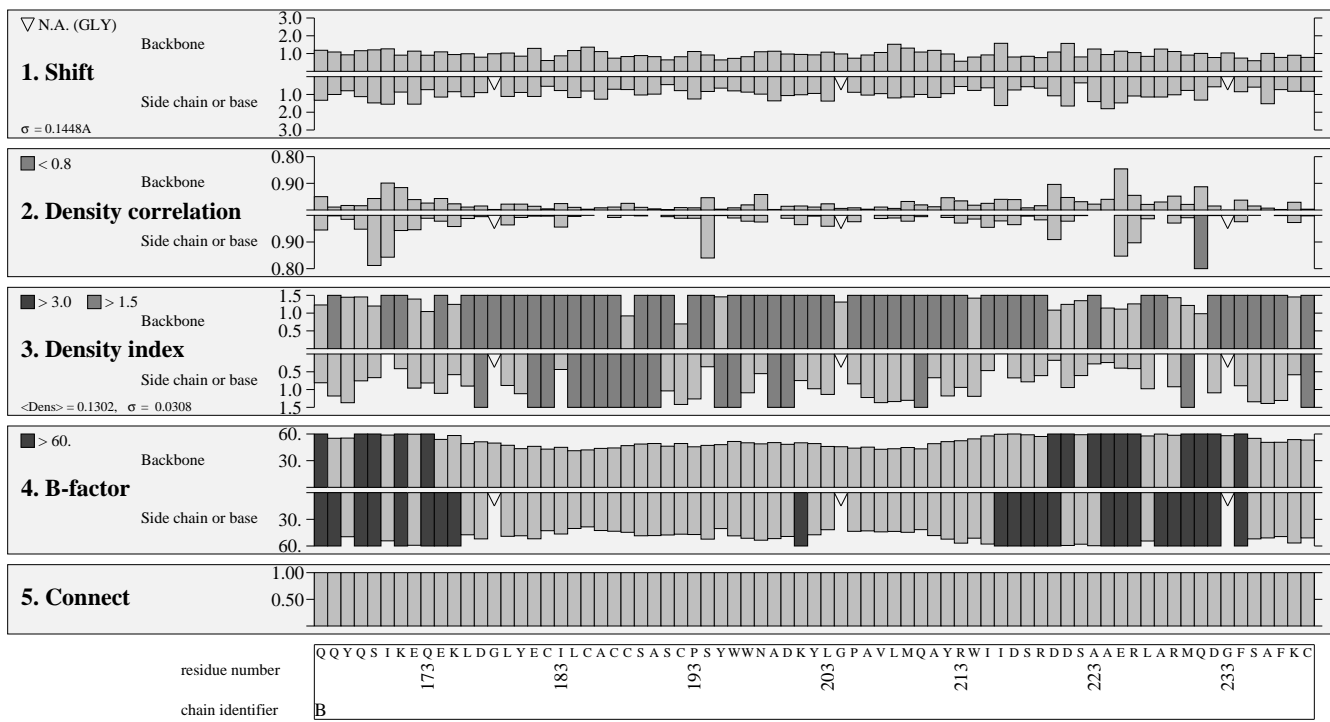
Local estimation (4)



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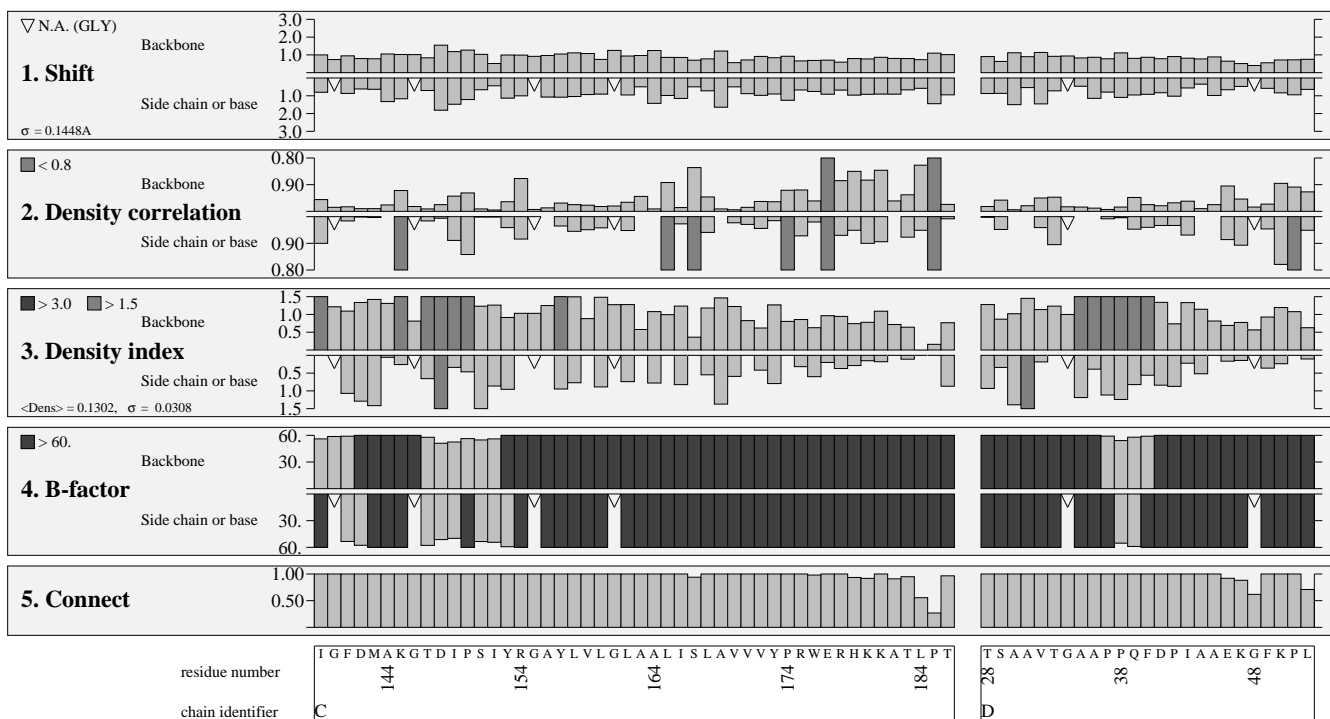
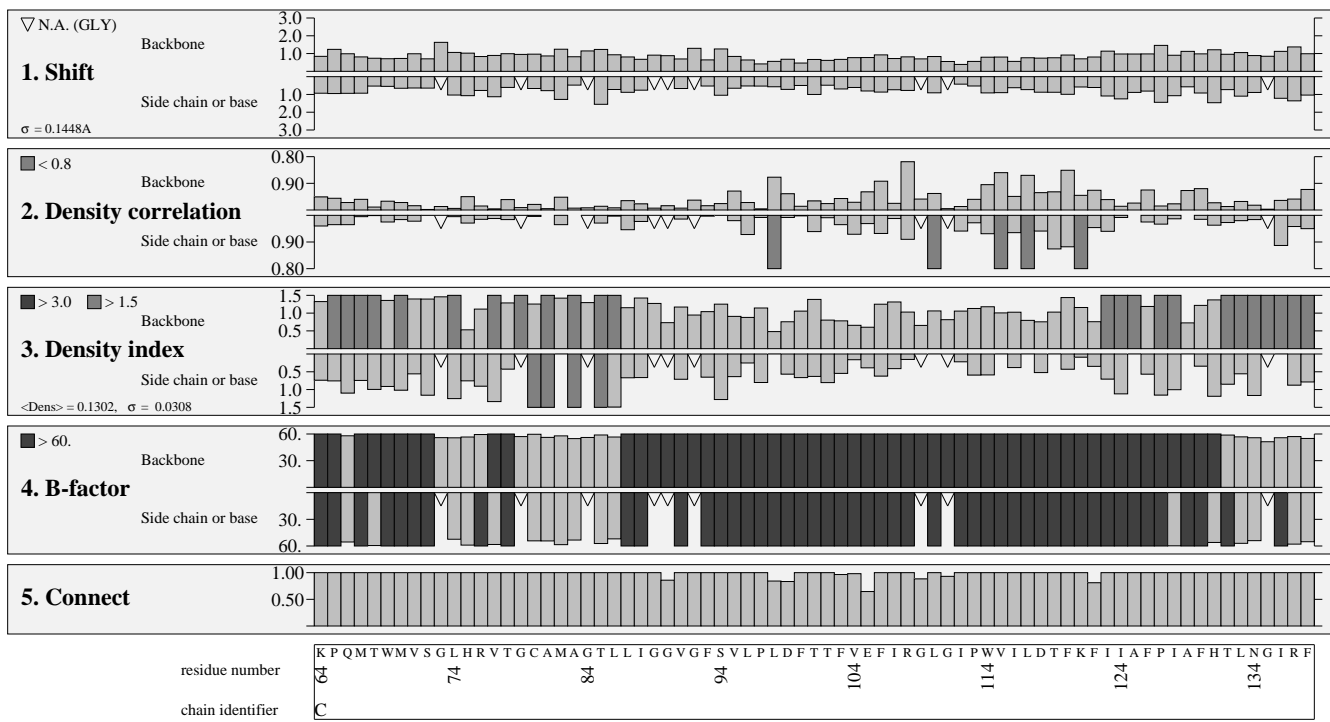
Local estimation (6)



Structure Factor Check

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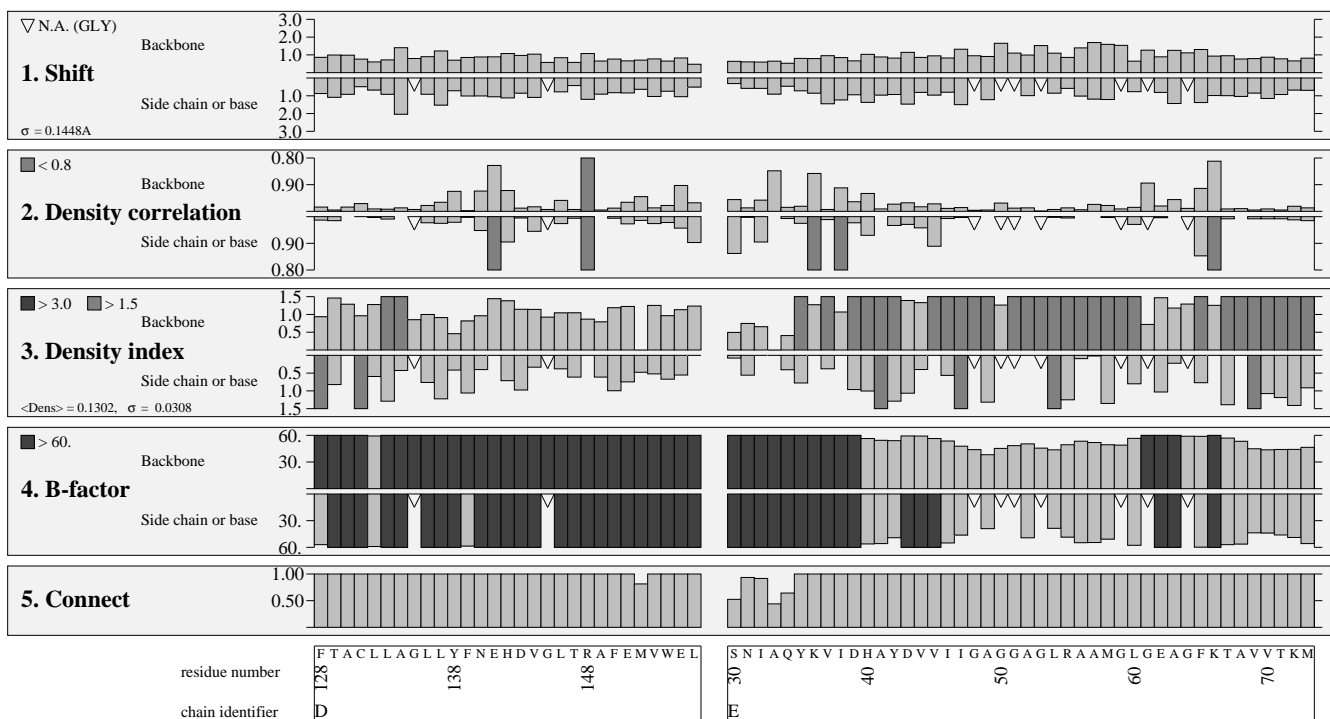
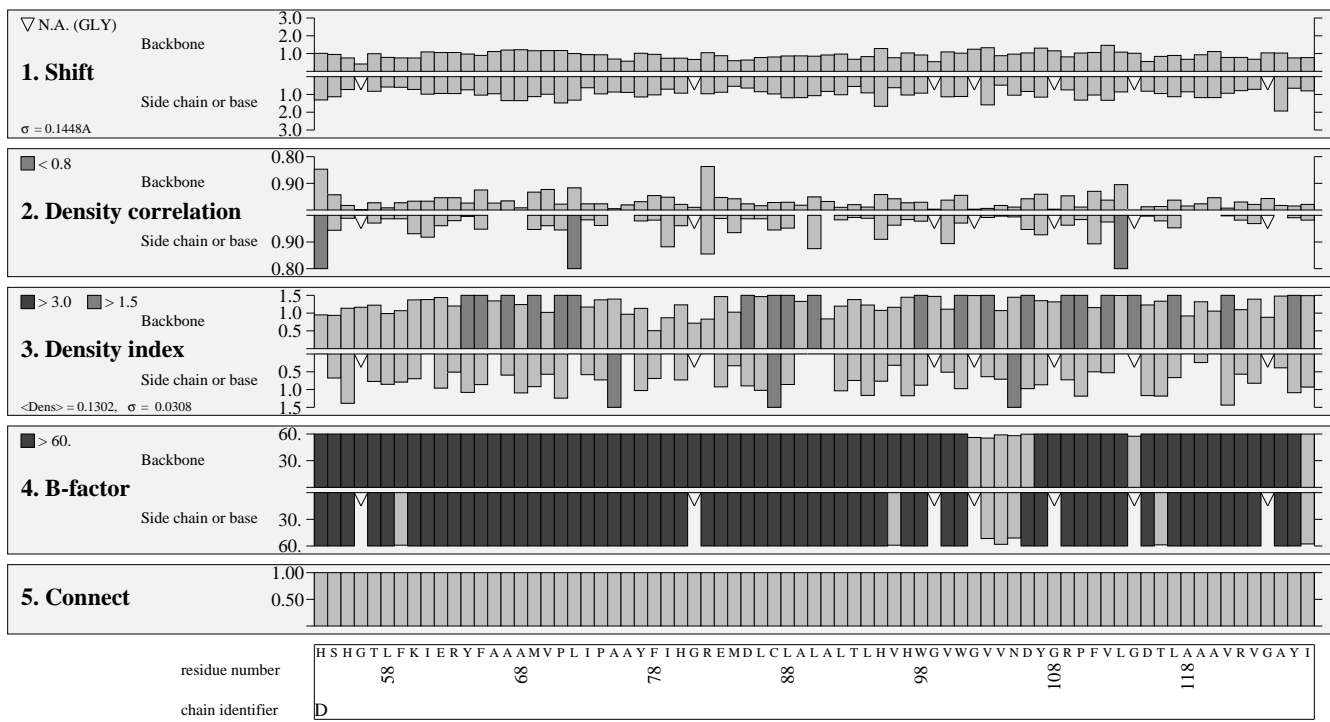
Local estimation (7)



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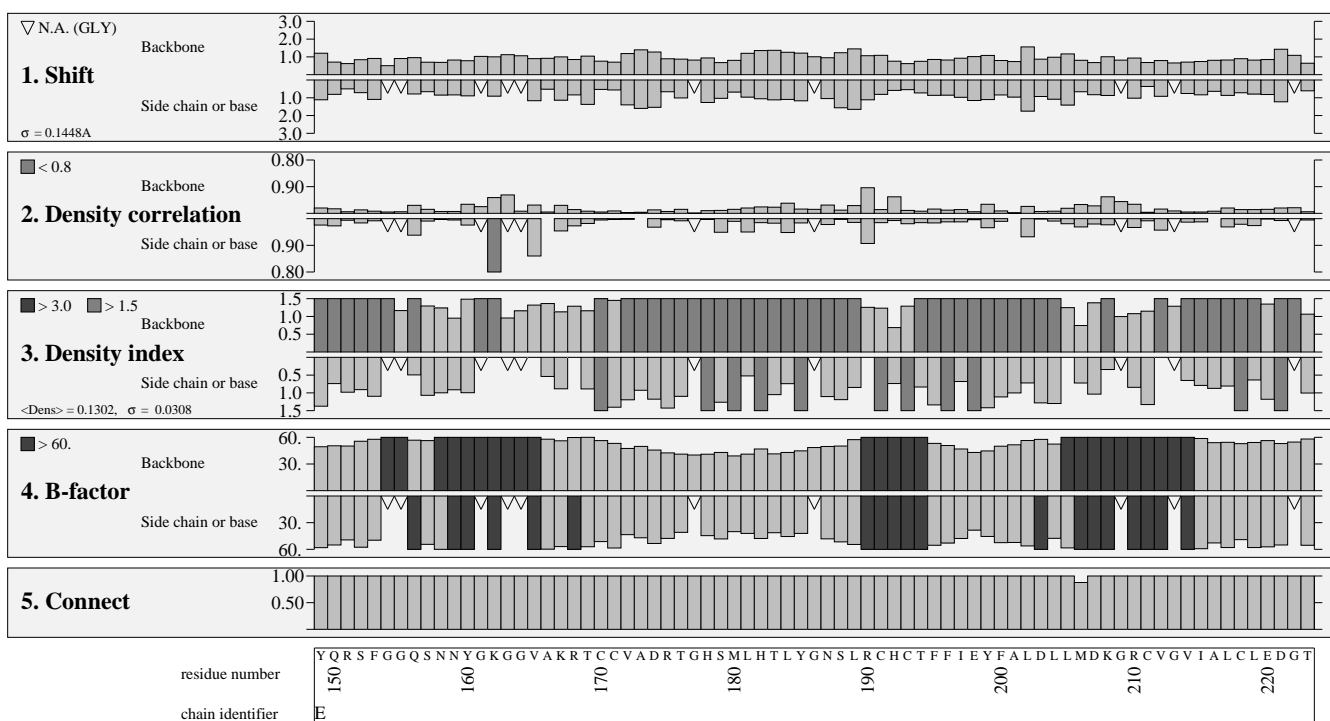
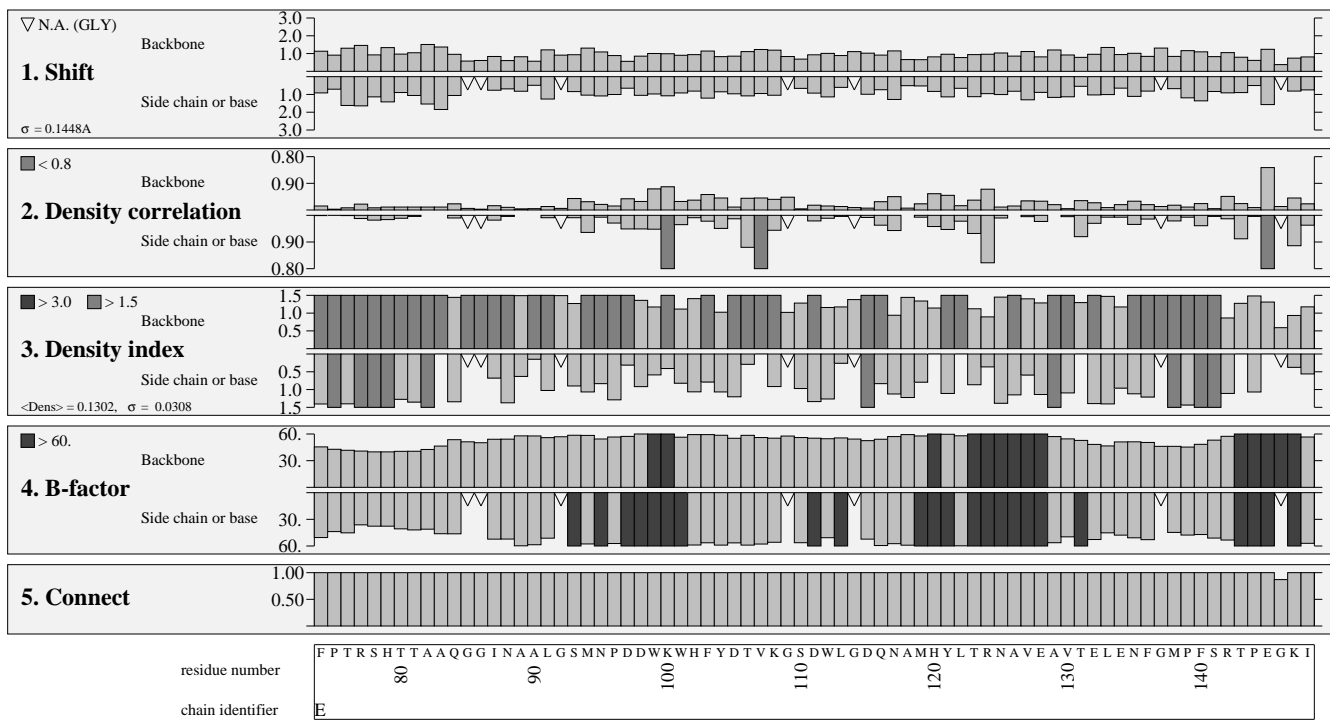
Local estimation (8)



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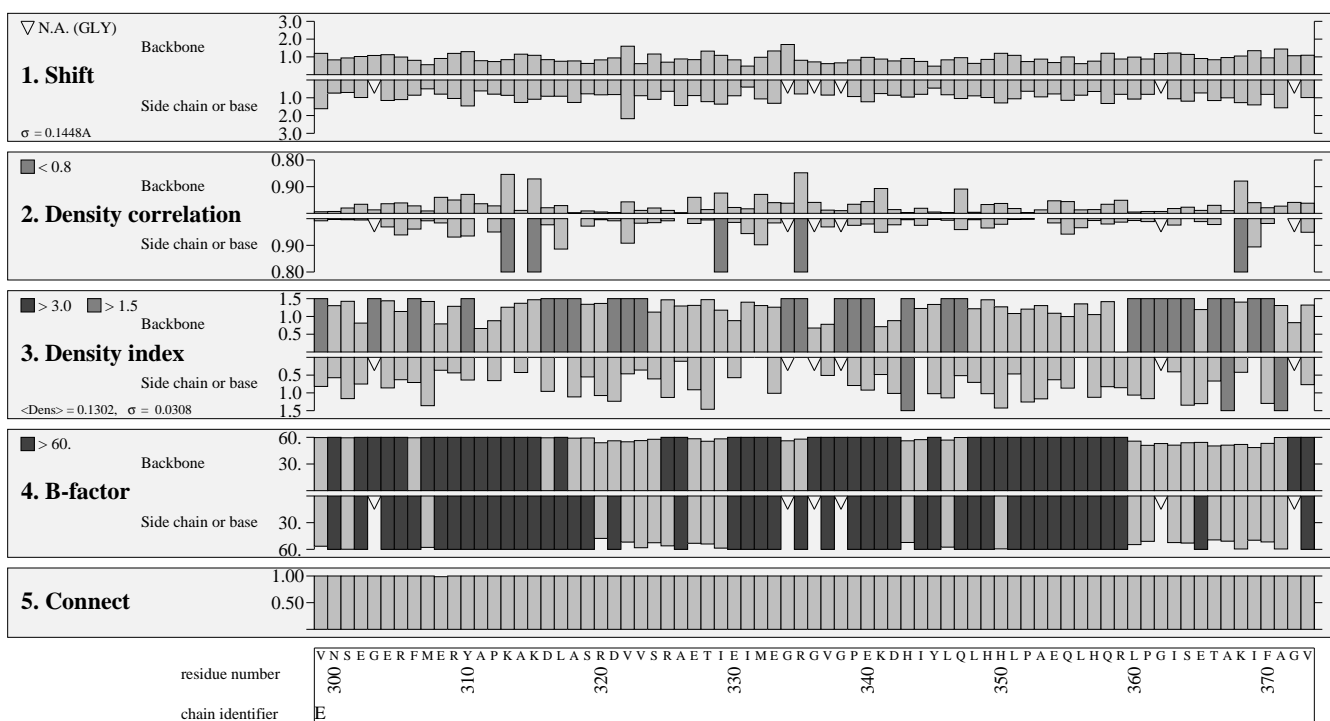
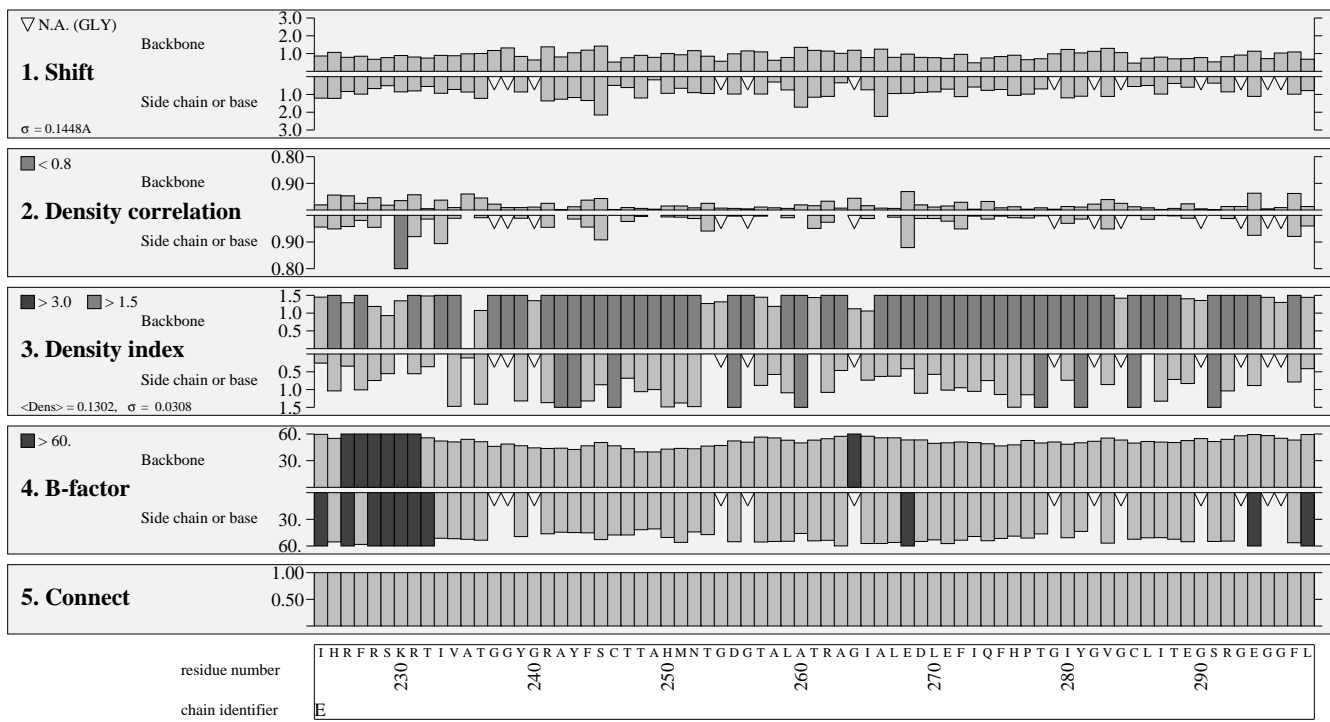
Local estimation (9)



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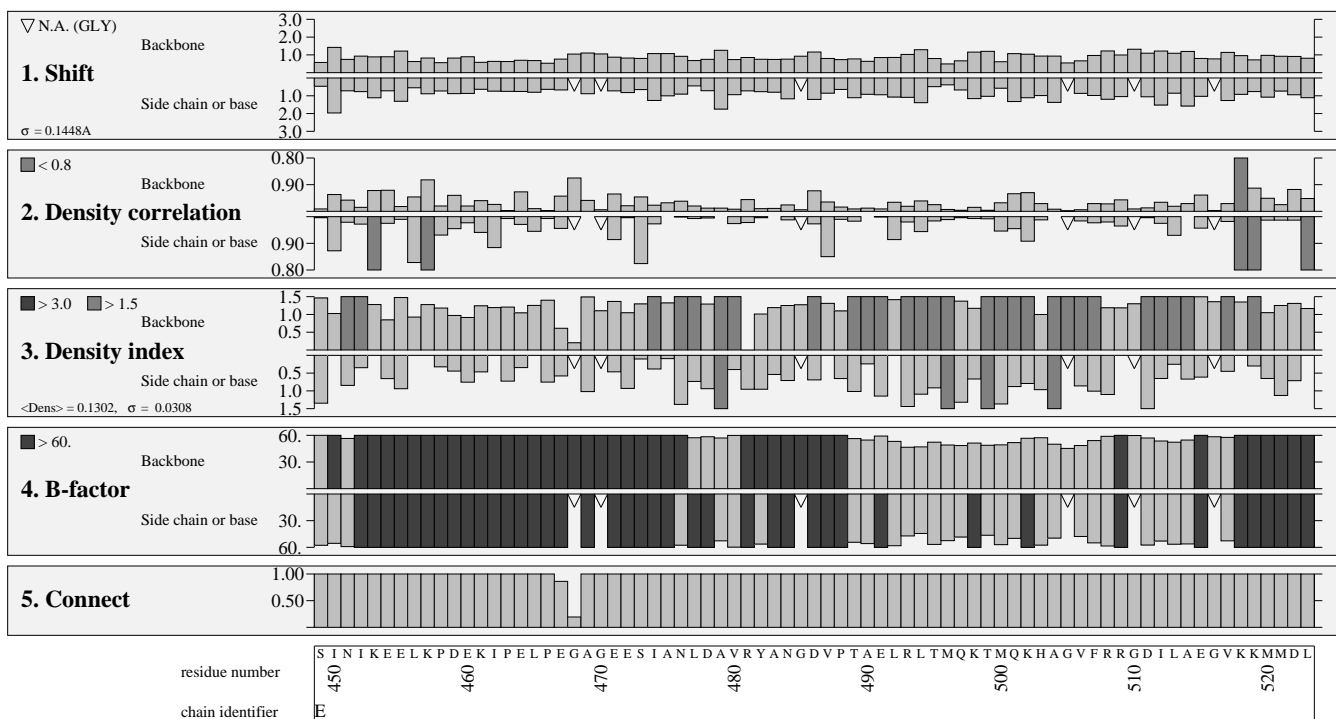
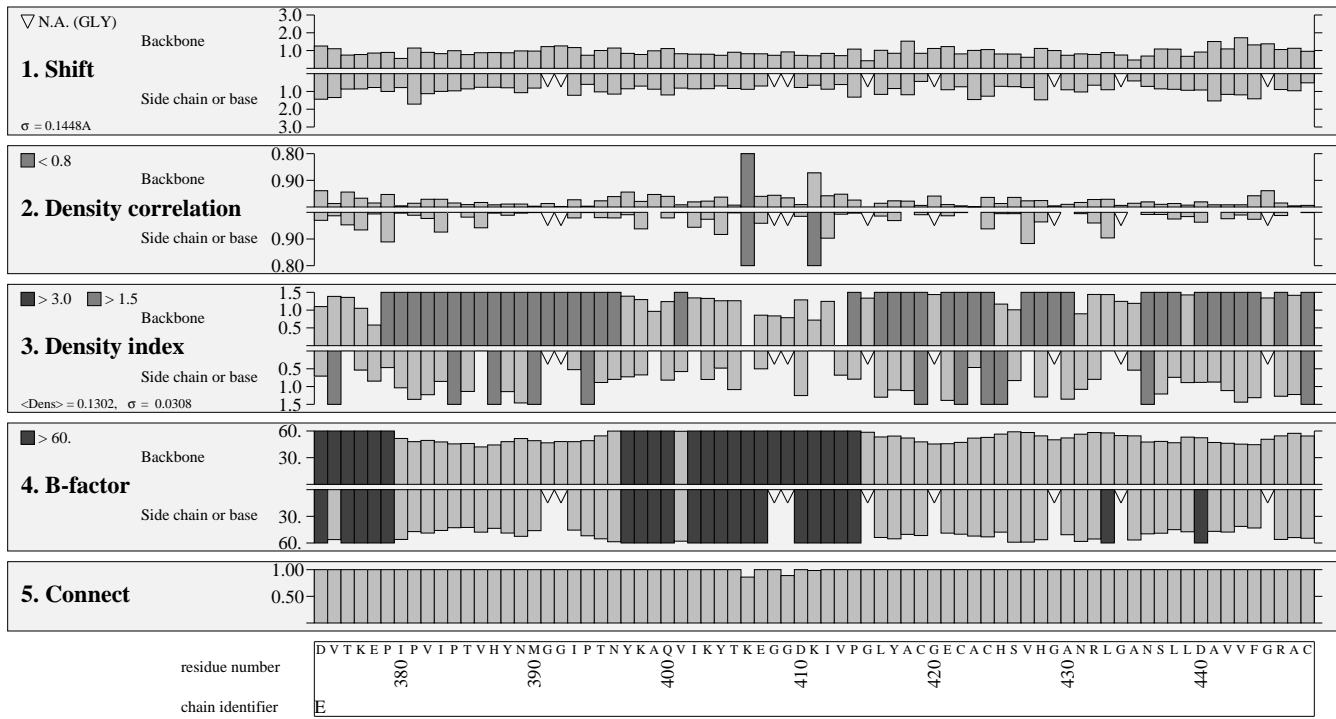
Local estimation (10)



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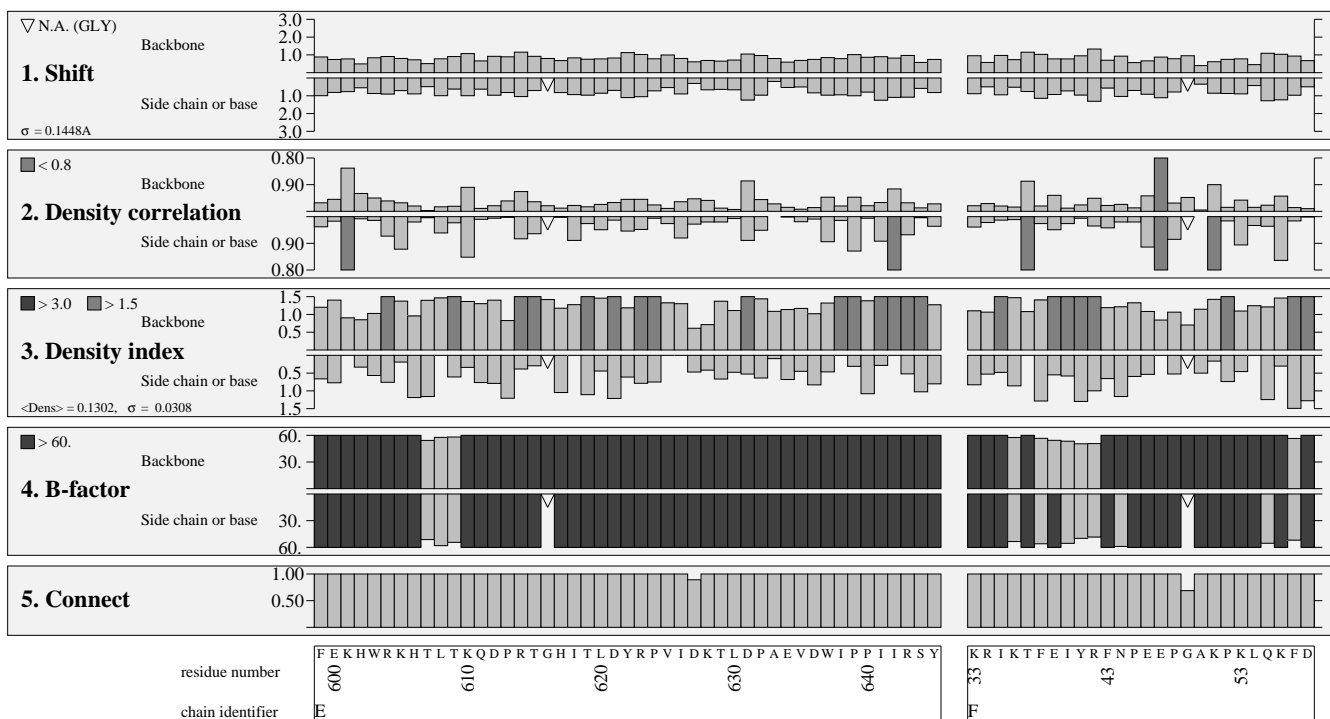
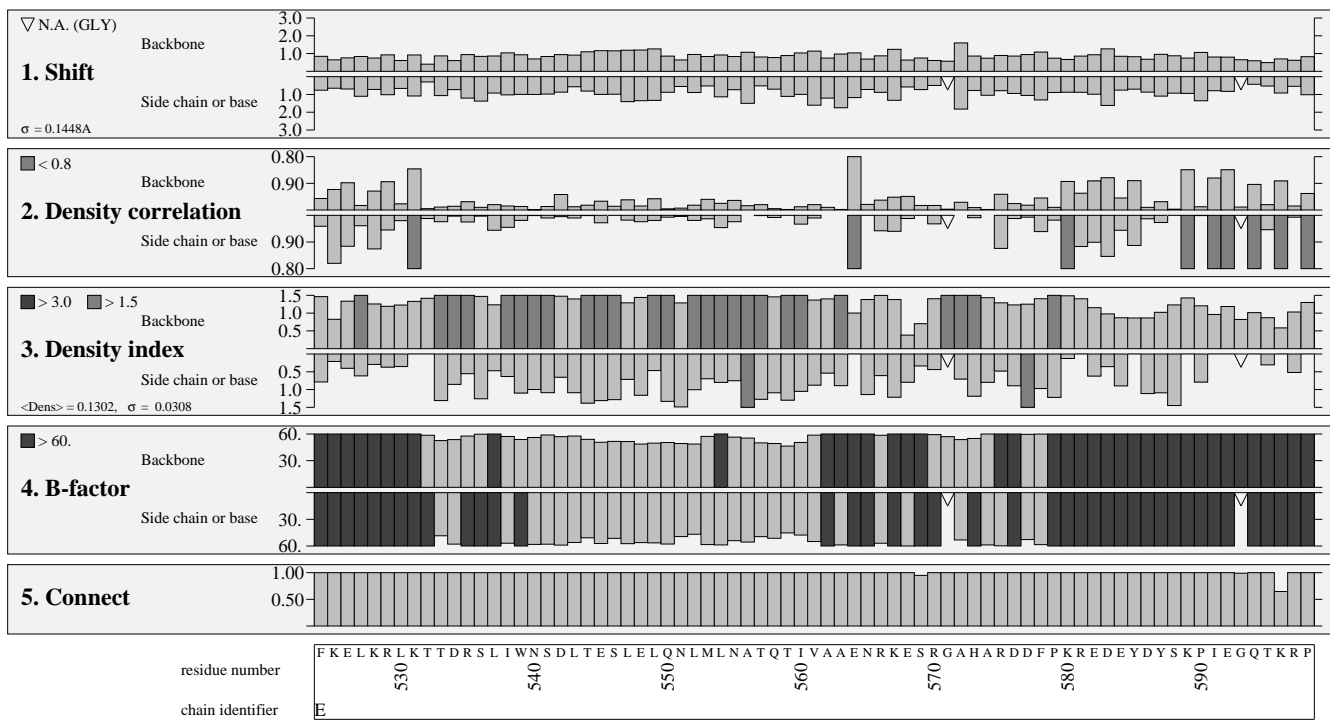
Local estimation (11)



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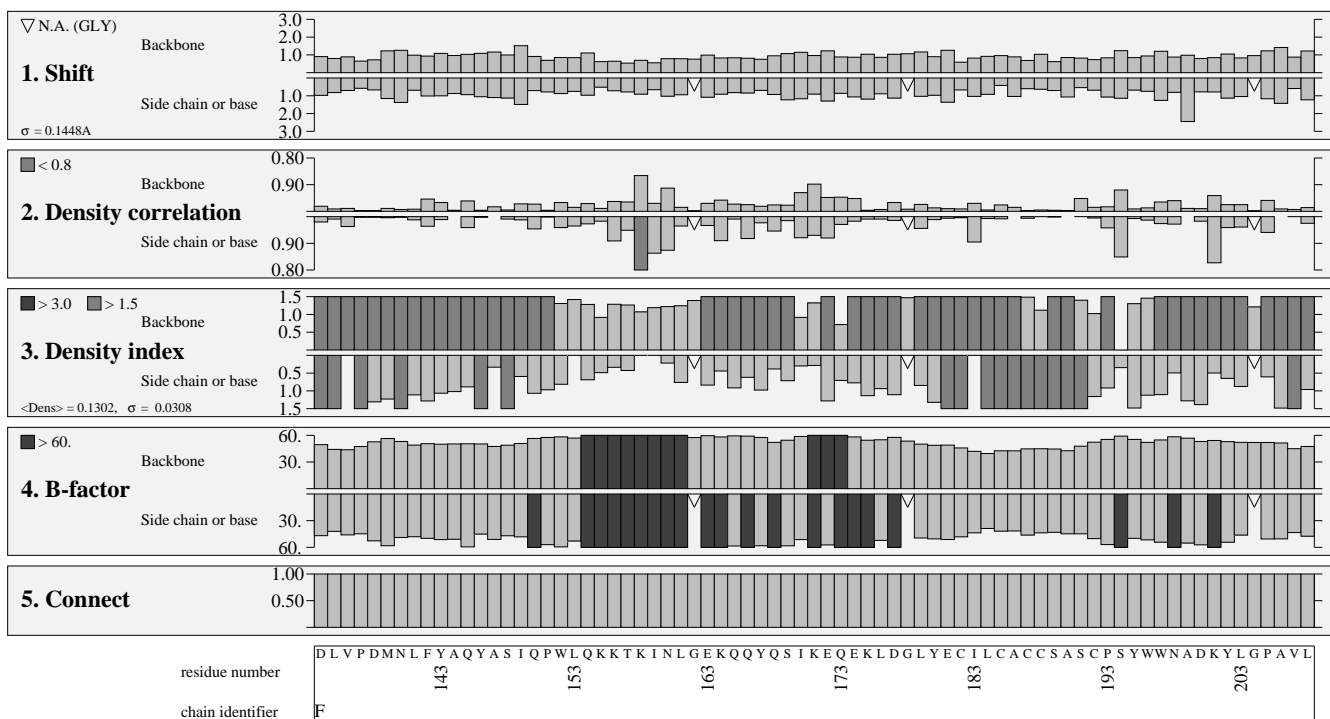
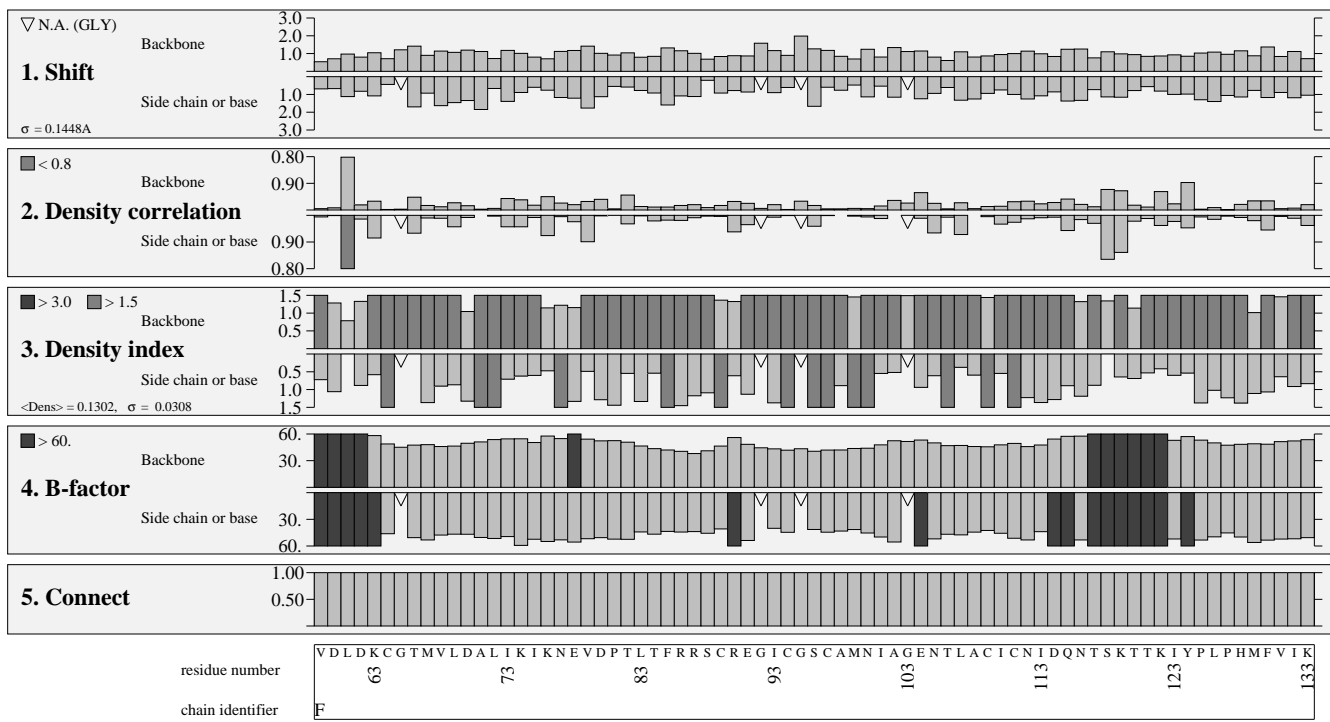
Local estimation (12)



Structure Factor Check

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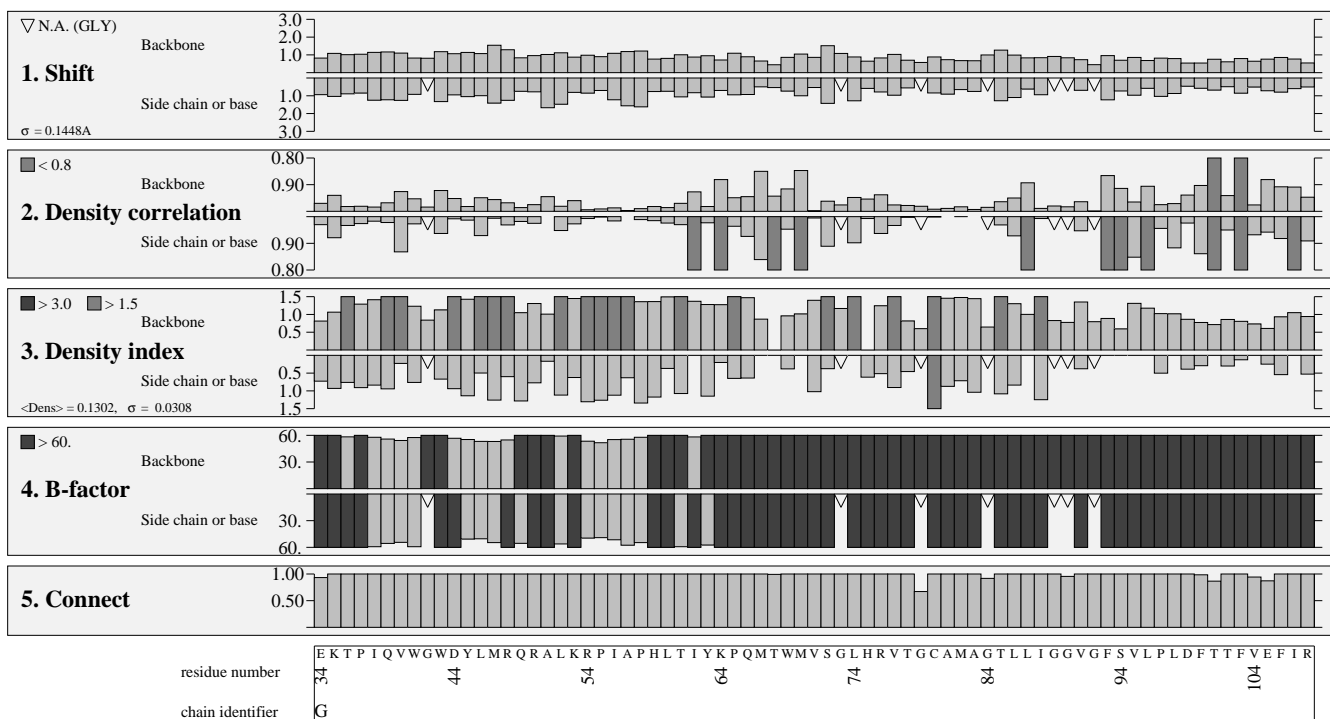
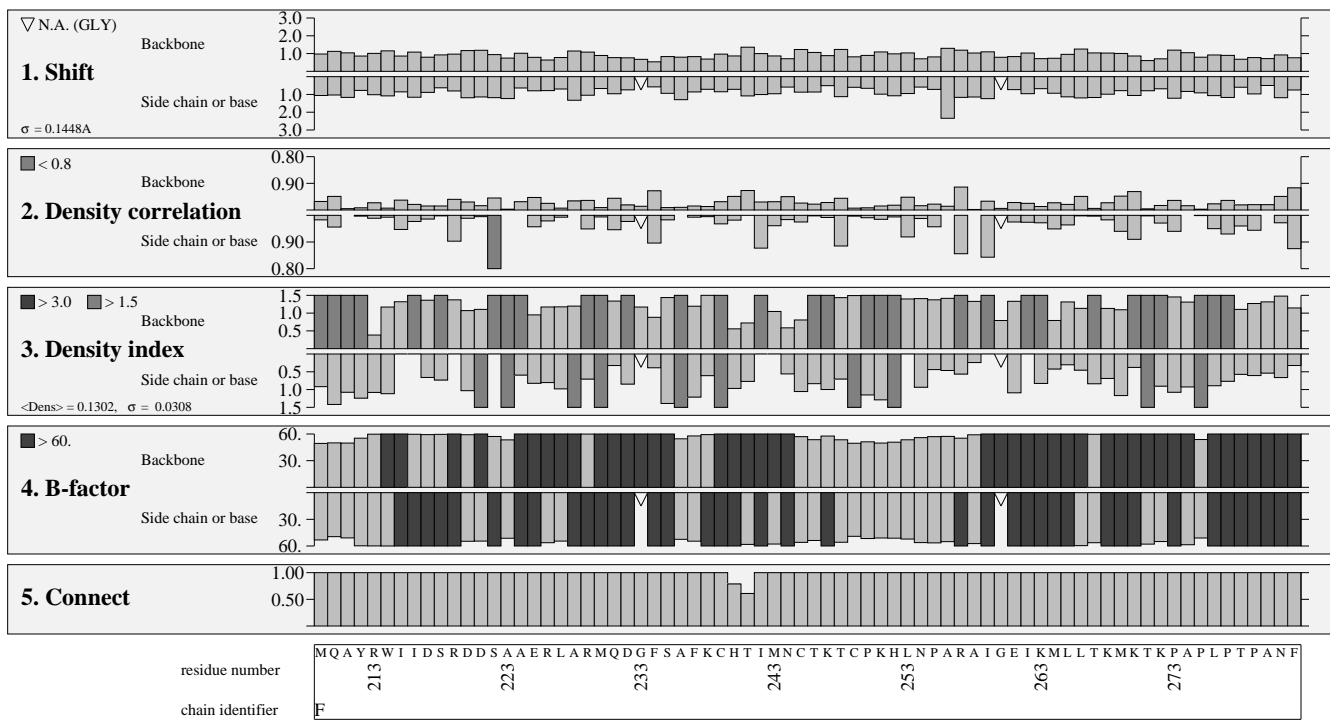
Local estimation (13)



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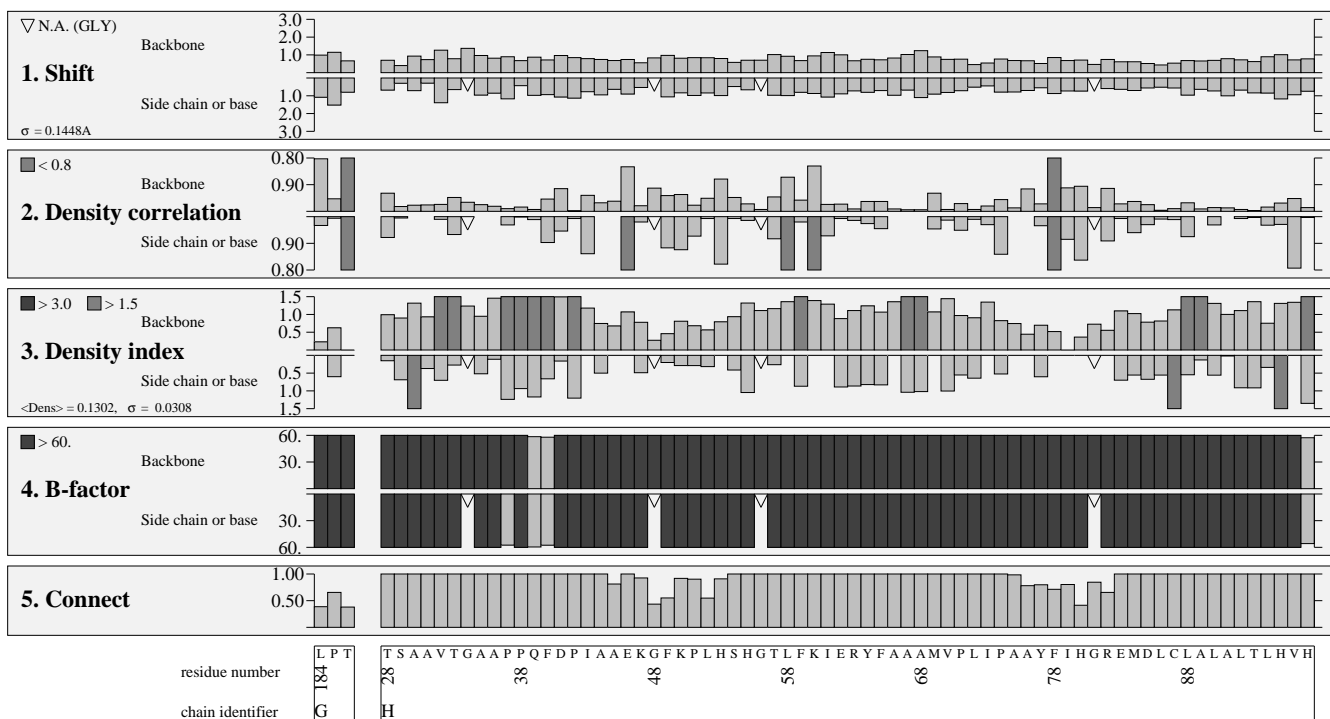
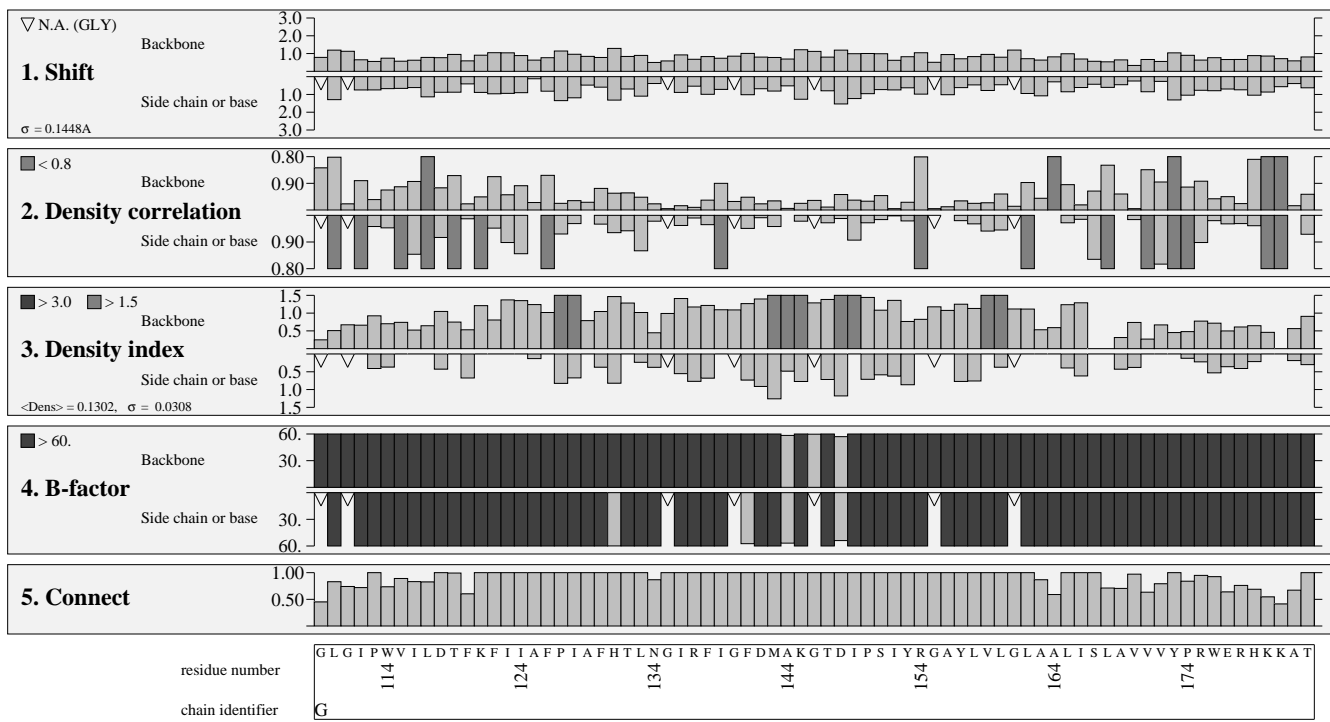
Local estimation (14)



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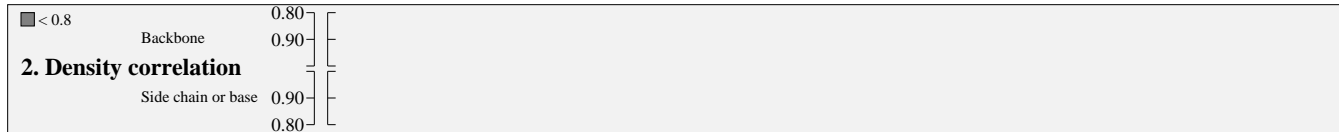
Local estimation (15)



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Local estimation (17)



residue number

chain identifier