"Judge not, that you be not judged" Bible, Matthew, ch.7

Structure Factor Check

4YXD

Title:	CRYSTAL STRUCTURE OF PORCINE HEART MITOCHONDRIAL COMPLEX II FLUTOLANIL
Date:	23−MAR−15
PDB code:	4YXD

Crystal

Cell parameters:

a: 70.37 A	b: 83.75 A	c: 292.63 A
α: 90.00	β: 90.00	γ: 90.00

Space group: P 21 21 21

Model

8618 atoms

Number of chains:	10
Volume not occupied by model:	57.4 %
<B> (for atomic model):	80.2 A^2
σ(B):	13.69 A^2
Matthews coefficient:	3.57
Corresponding solvent % :	65.31

Refinement

Program:	REFMAC 5.7.0029
Nominal resolution range:	20.0 − 3.00 A
Reported R−factor:	0.206
Number of reflections used:	33058
Reported Rfree:	0.26
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		20.0 − 3.00 A
Reflections in file:		35482
Unique reflections	above 0:	34645
	above 1σ:	34197
	above 3σ:	25410
Reflections > 0:		837

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Nominal resolution range: 20.0 − 3.00 A
\05max. from input data, min. from author\05

Used reflections:	34641
Reflections out of resolution:	4
Completeness:	97.6 %
R_stand(F) = <σ(F)>/<F> :	0.059

Anisotropic distribution of Structure Factors
ratio of eigen values: 0.9543 0.9389 1.0000

B_overall (by Patterson):	52.A^2
Optical resolution:	2.22 A
Expected opt. resol. for complete data set:	2.22 A
Estimated minimal error:	0.071 A

Model vs. Structure Factors

R−factor for all reflections:	0.275
Correlation factor:	0.833
R−factor:	0.284

for F > 2.0σ

nom. resolution range:	20.00 − 3.00A
reflections used:	34193

Rfree:	0.327
Nfree:	1708
R−factor without free−refl.:	0.282
Non free−reflections:	32485
<u> (error in coords by Luzzati plot):	0.400 A
Estimated maximal error:	0.195 A
DPI:	0.389 A

Scaling

Scale:	0.815
Bdiff:	−8.26

Anisothermal Scaling (Beta):
−2.5405 −2.6088 −2.3308 −0.0000 −0.0000 0.0000

Solvent correction − Ks,Bs: 0.376 249.870

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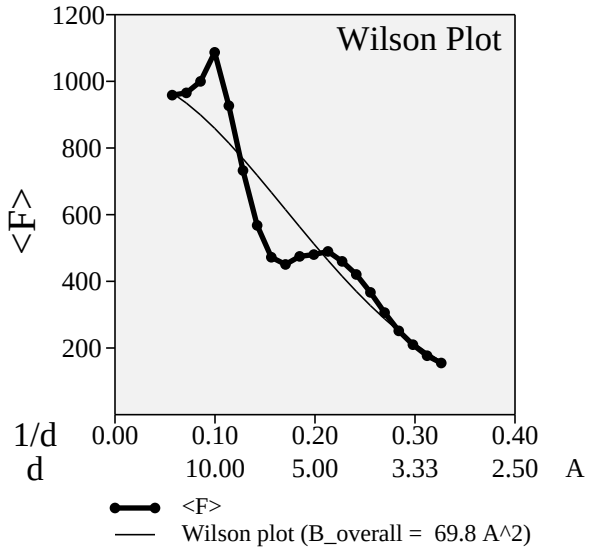
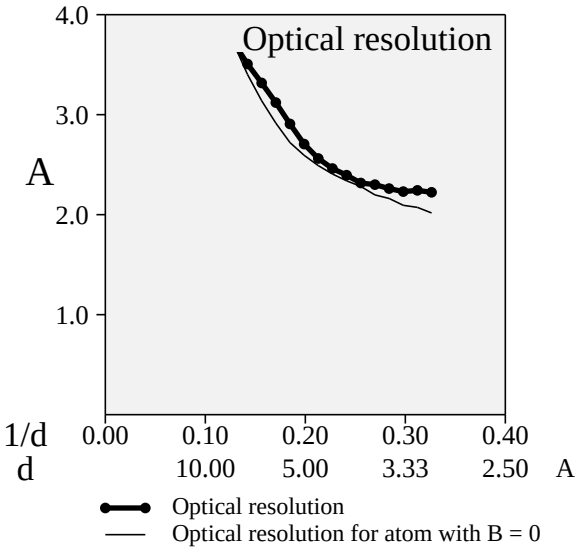
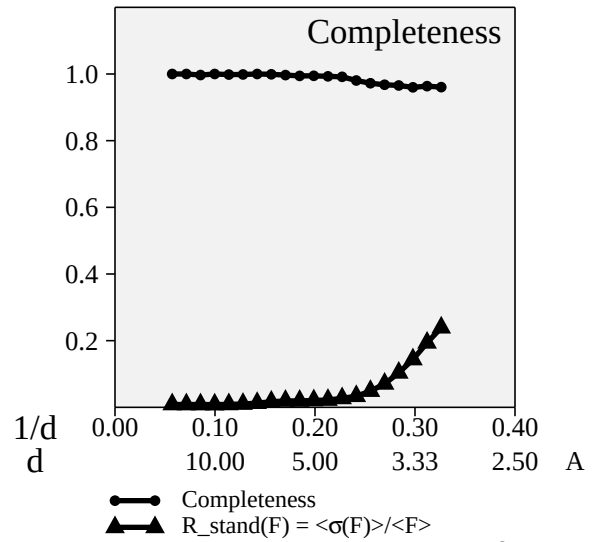
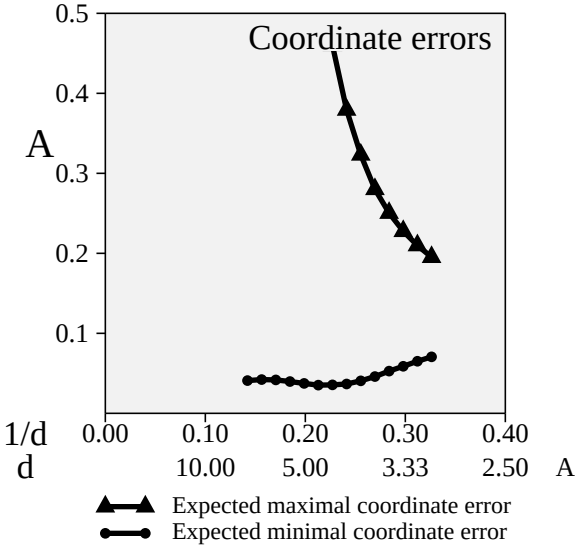
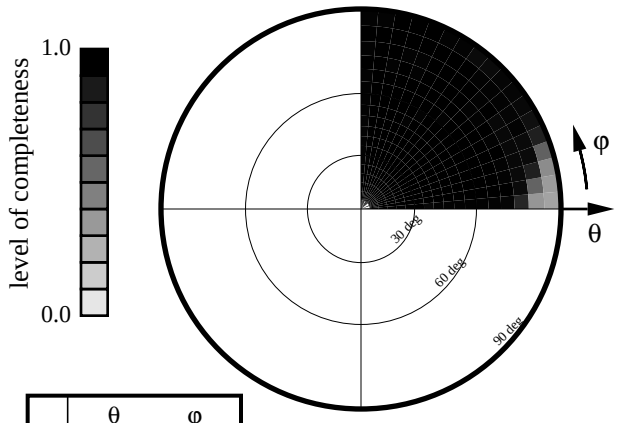






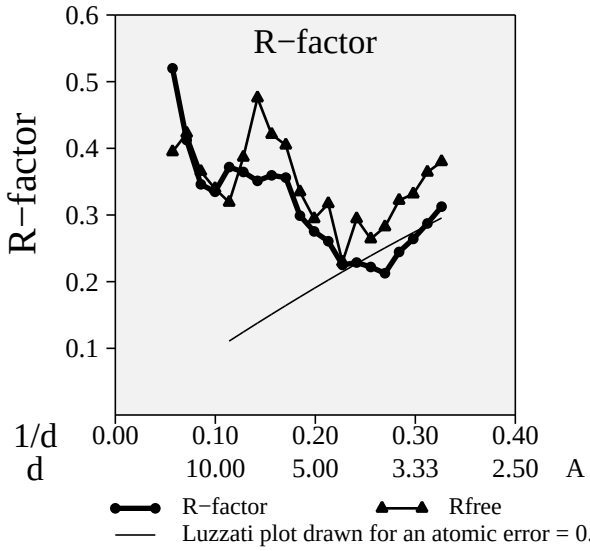


Stereographic projection of
the averaged radial completeness



	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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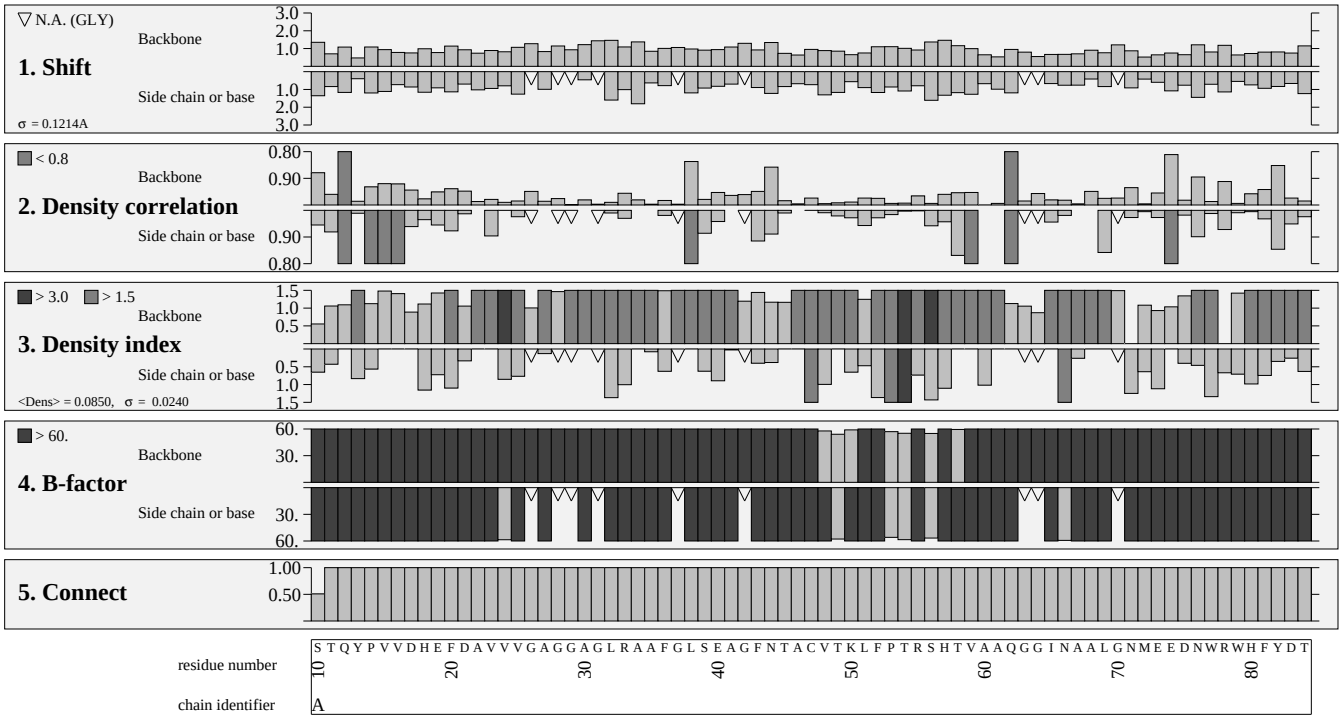
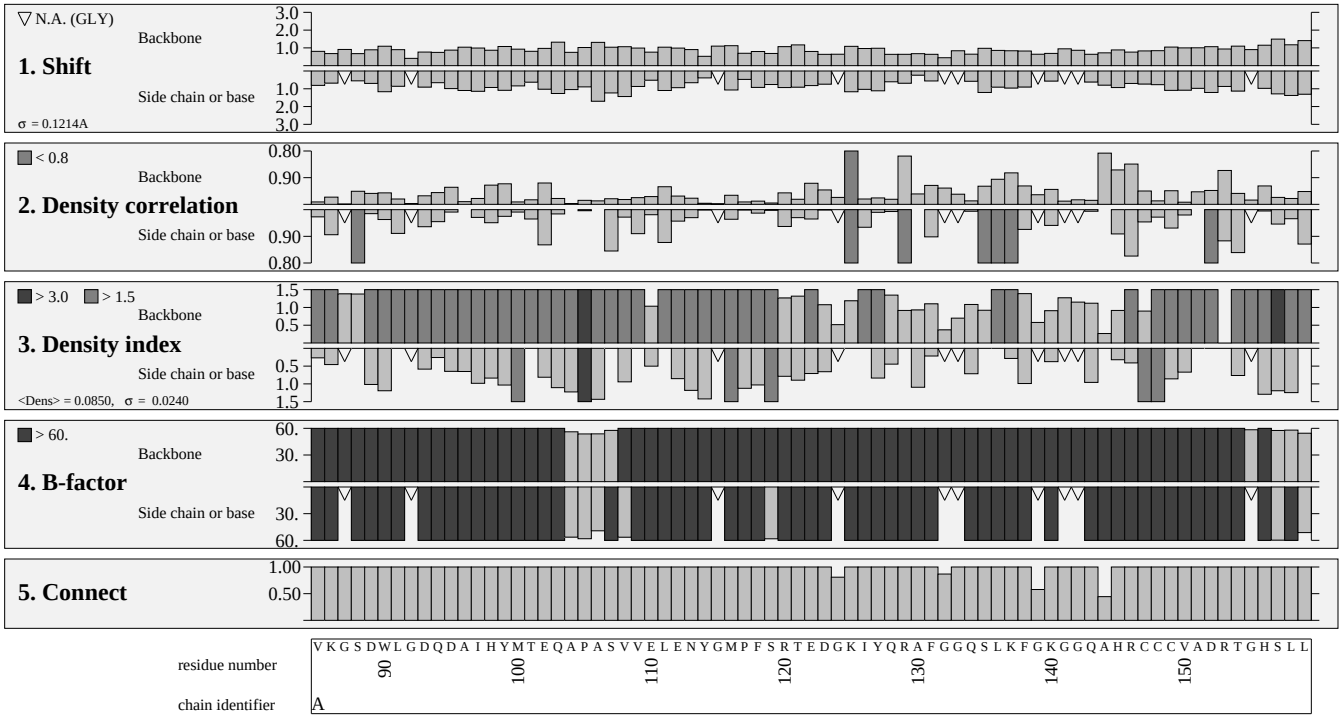
Local estimation





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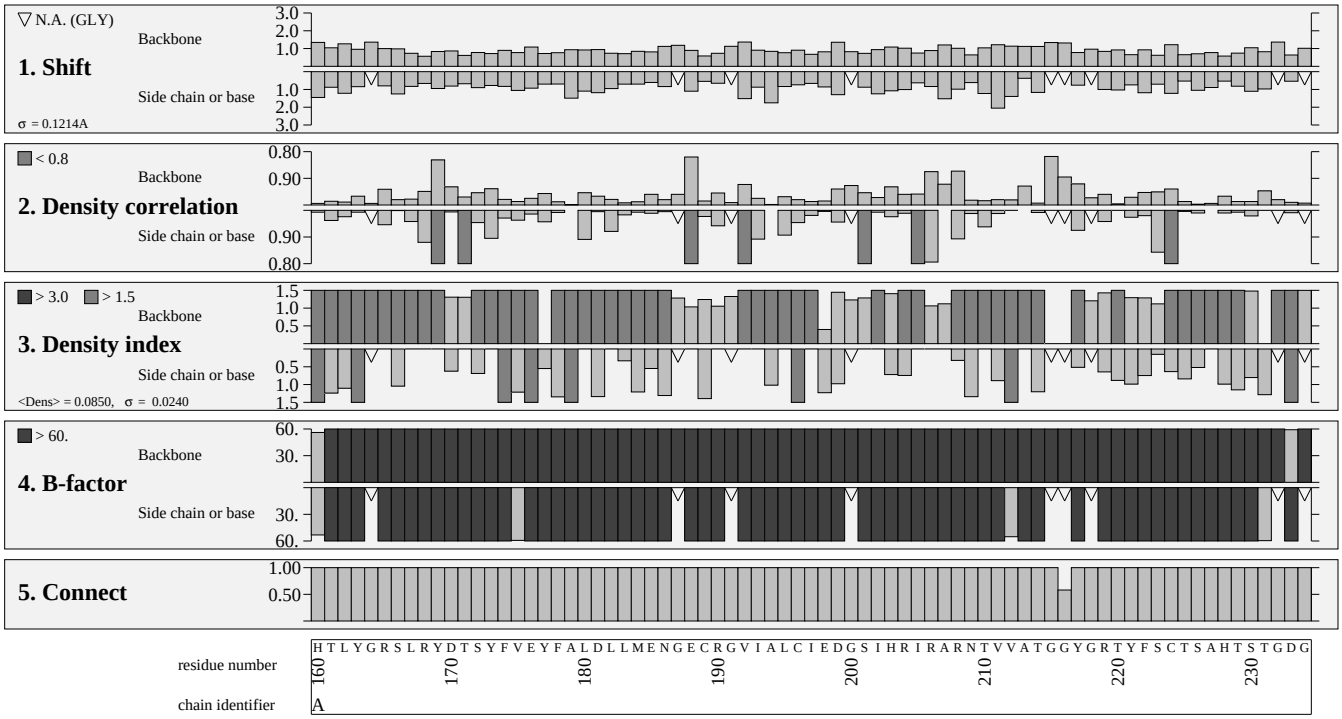
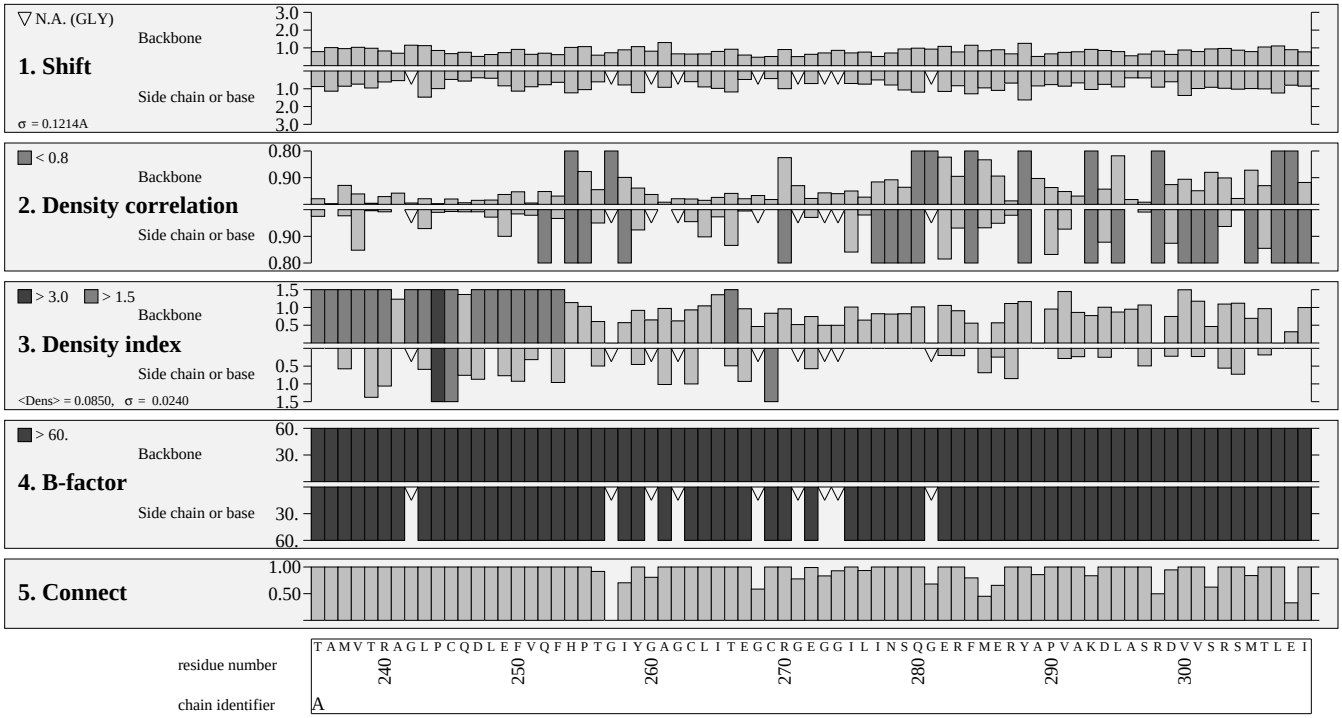
Structure Factor Check

4YXD

Local estimation (2)





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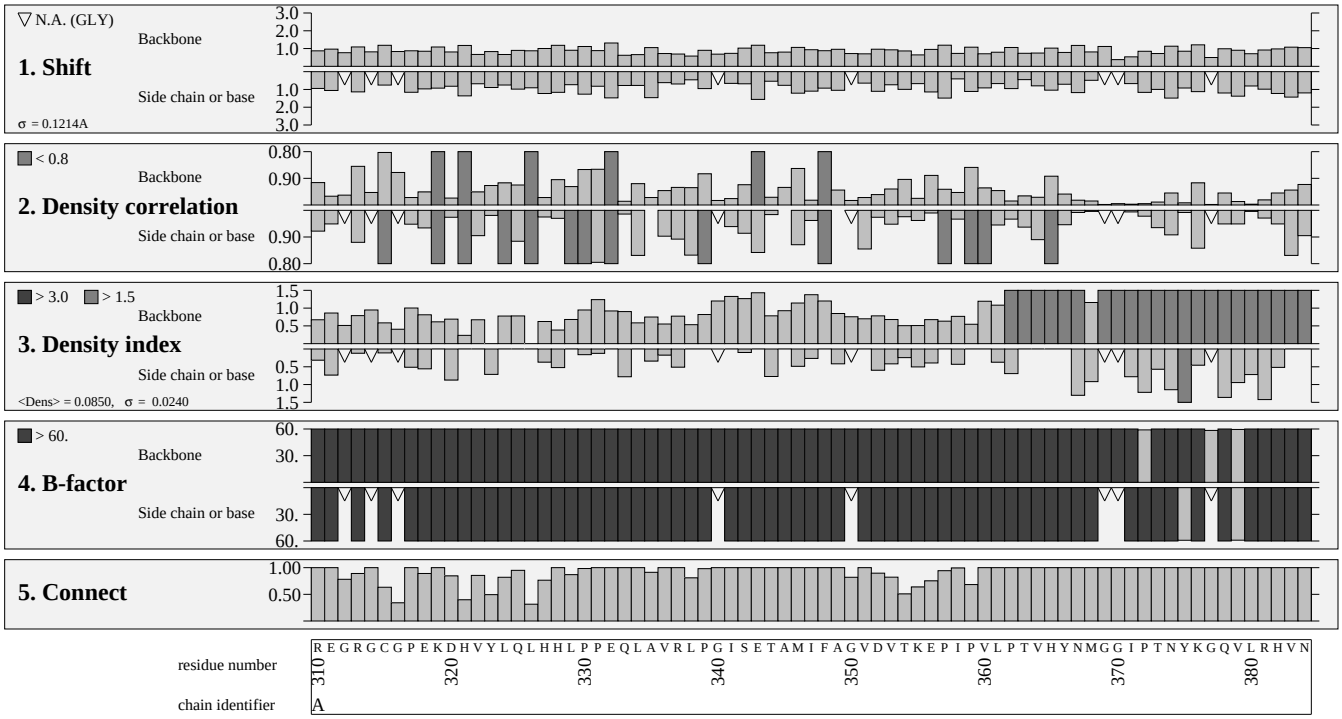
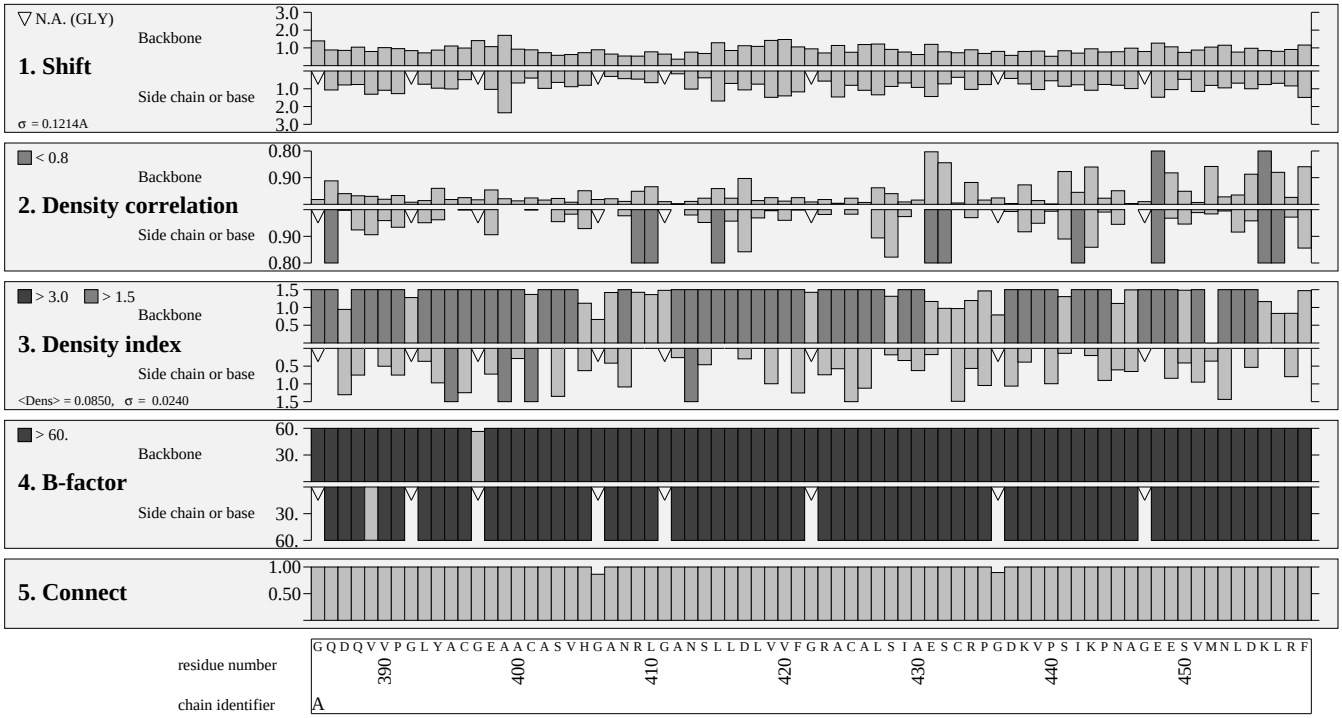
Local estimation (3)





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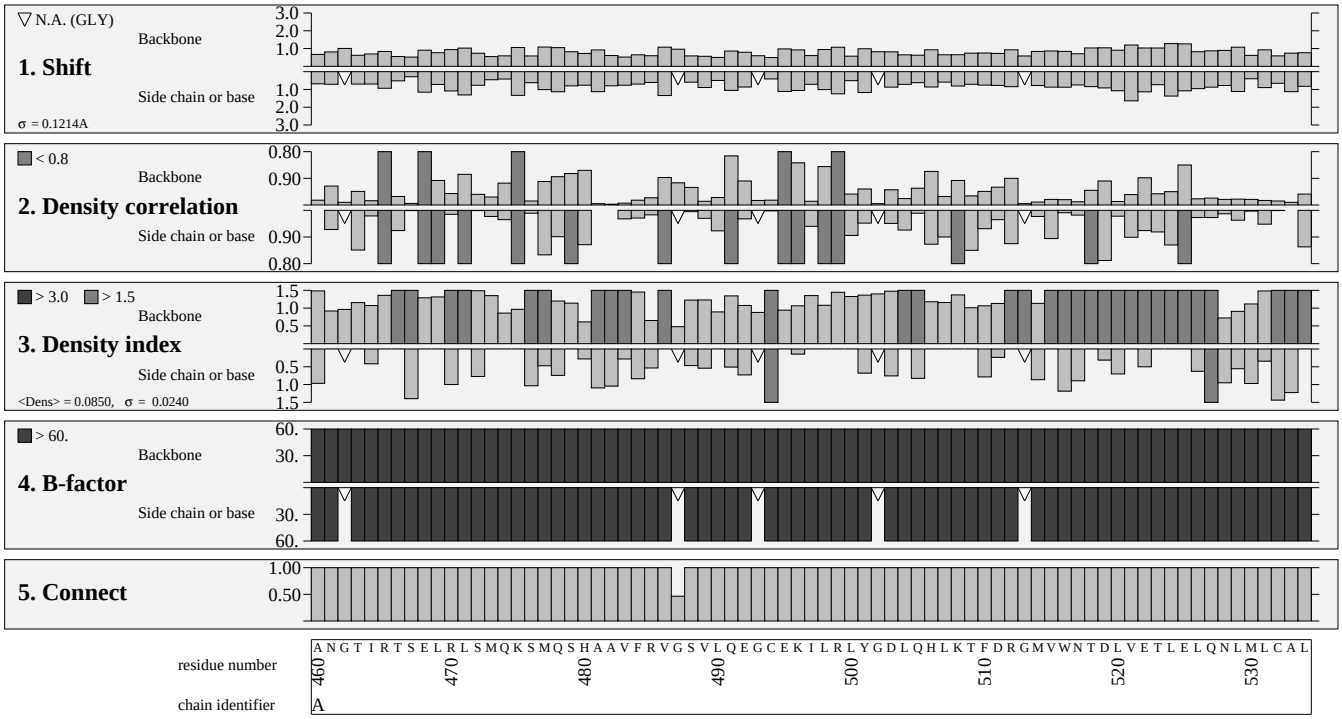
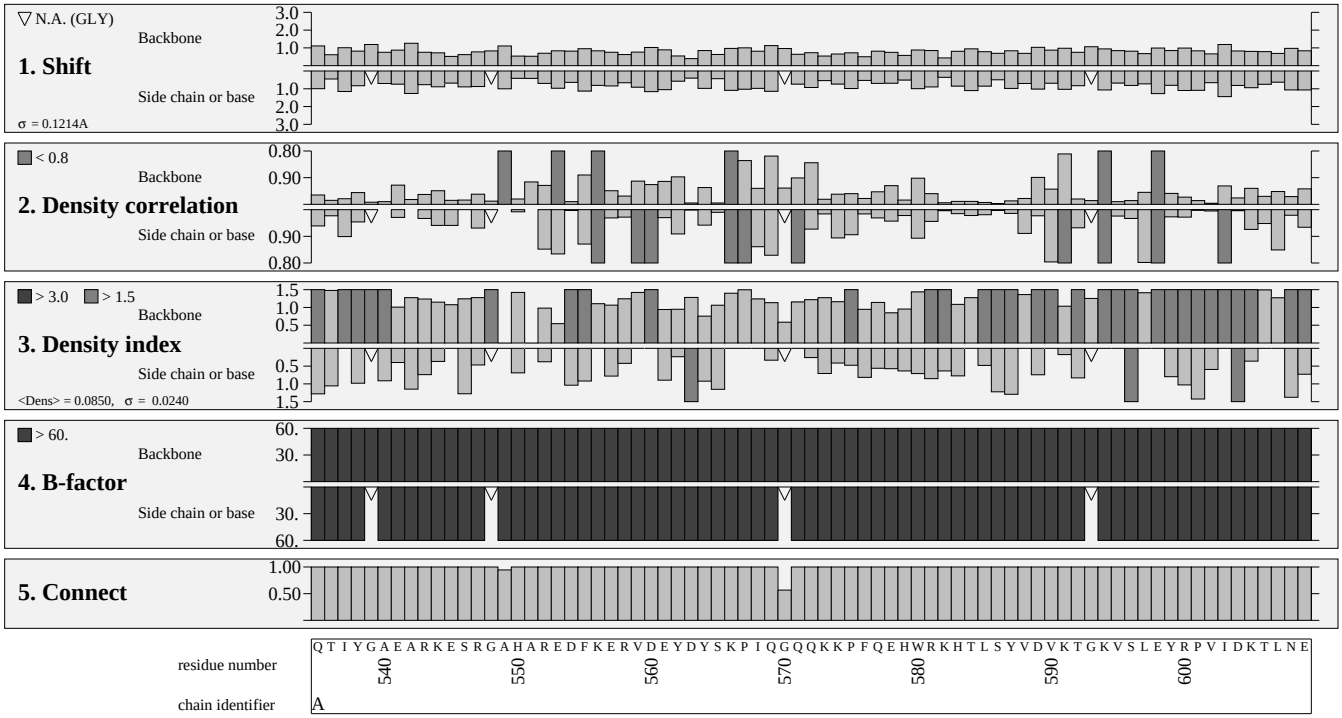
Local estimation (4)





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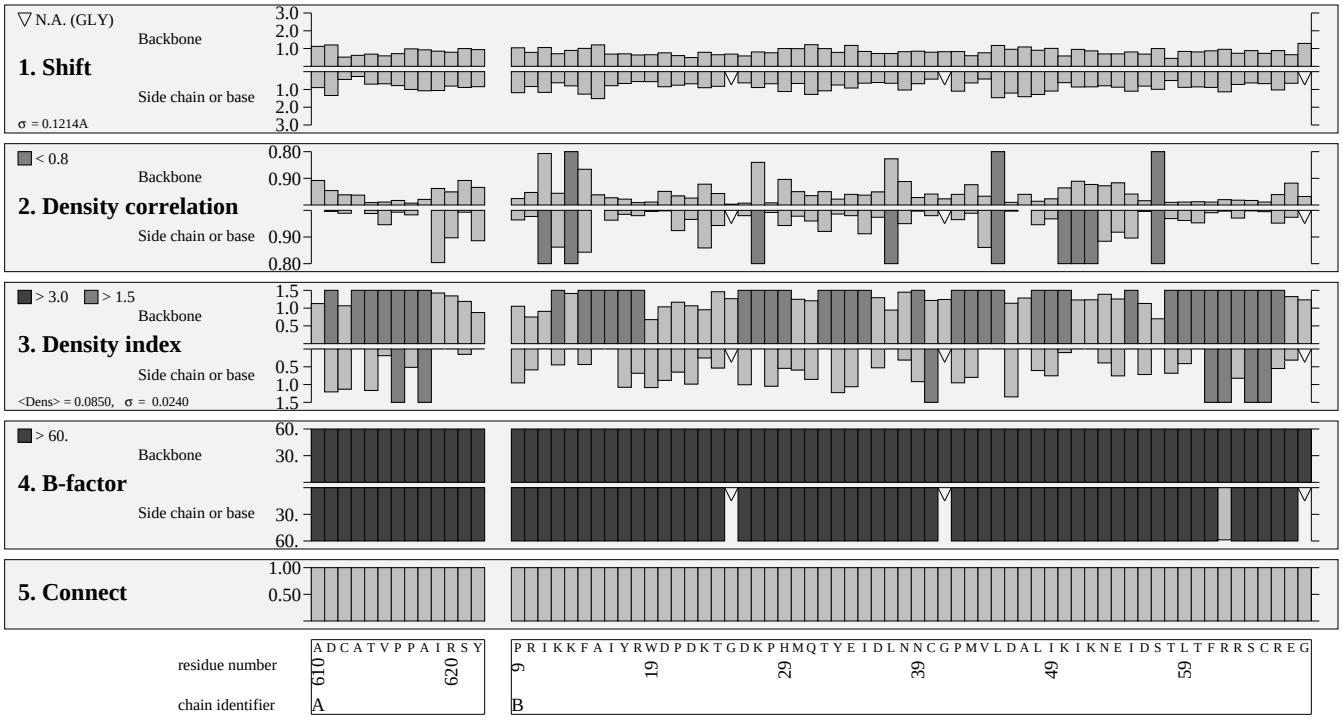
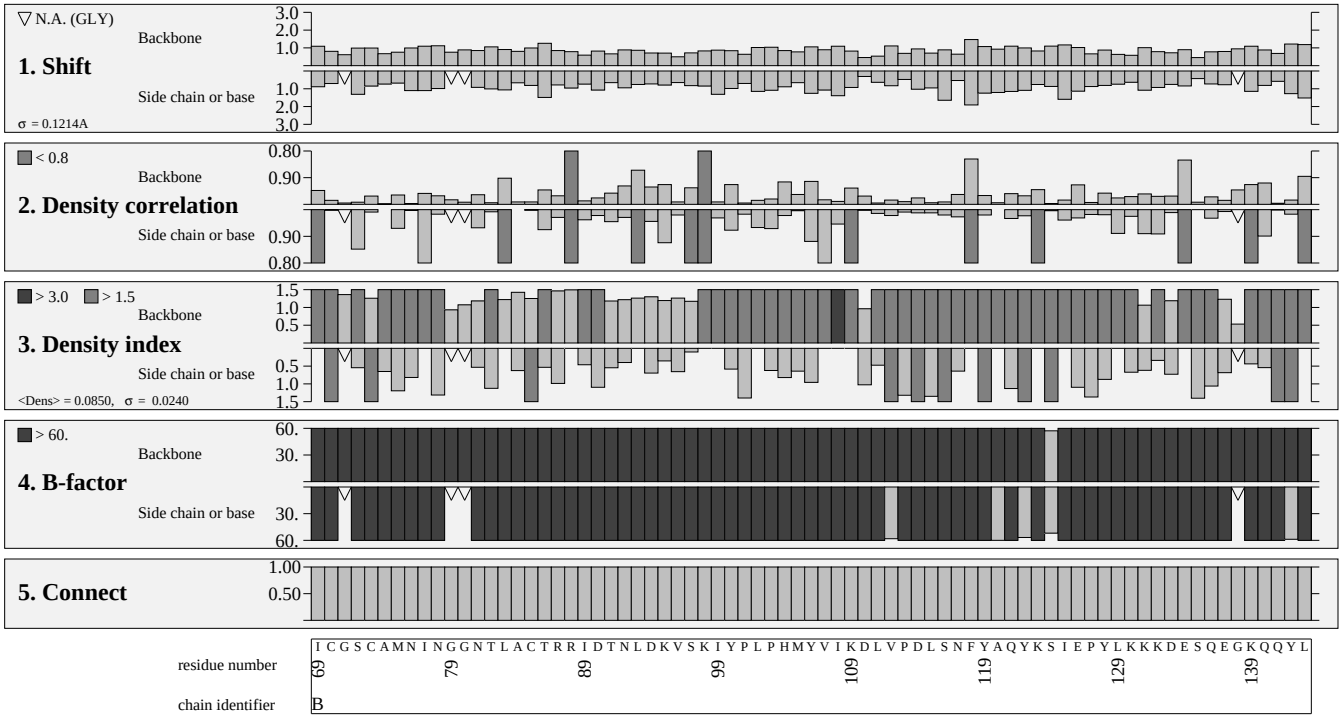
Local estimation (5)





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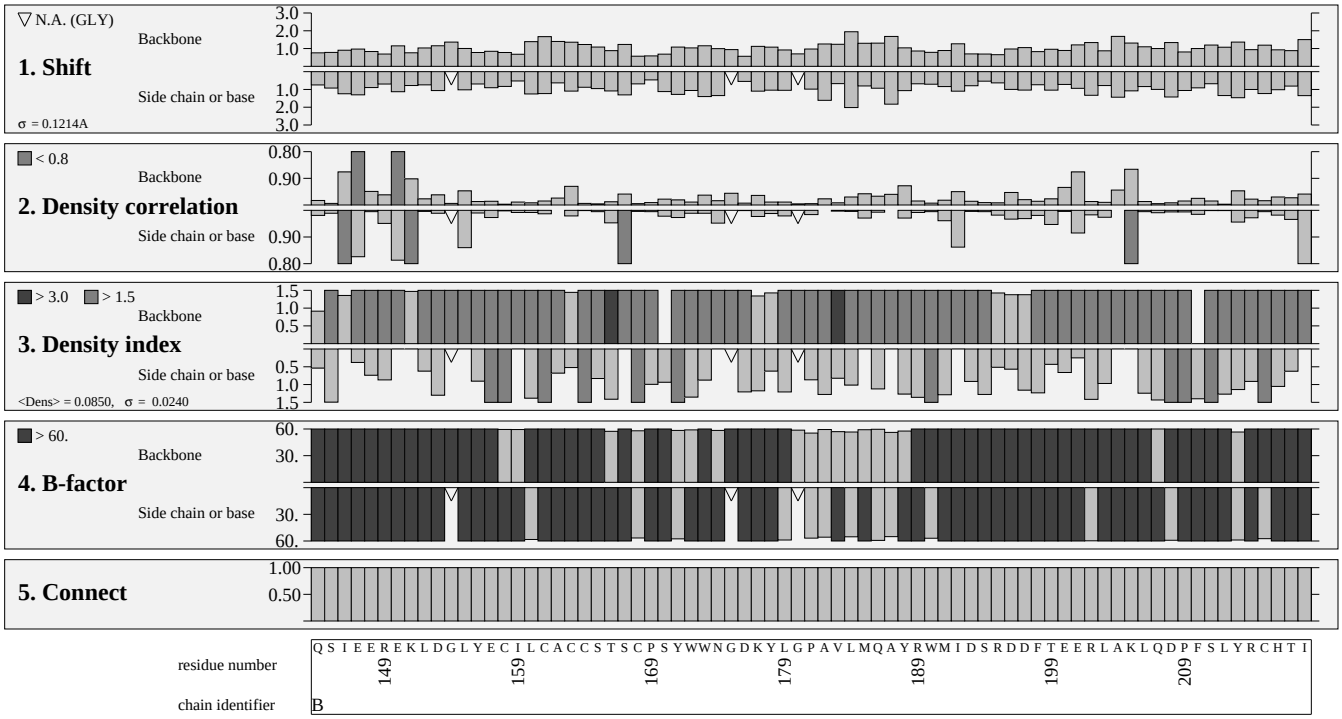
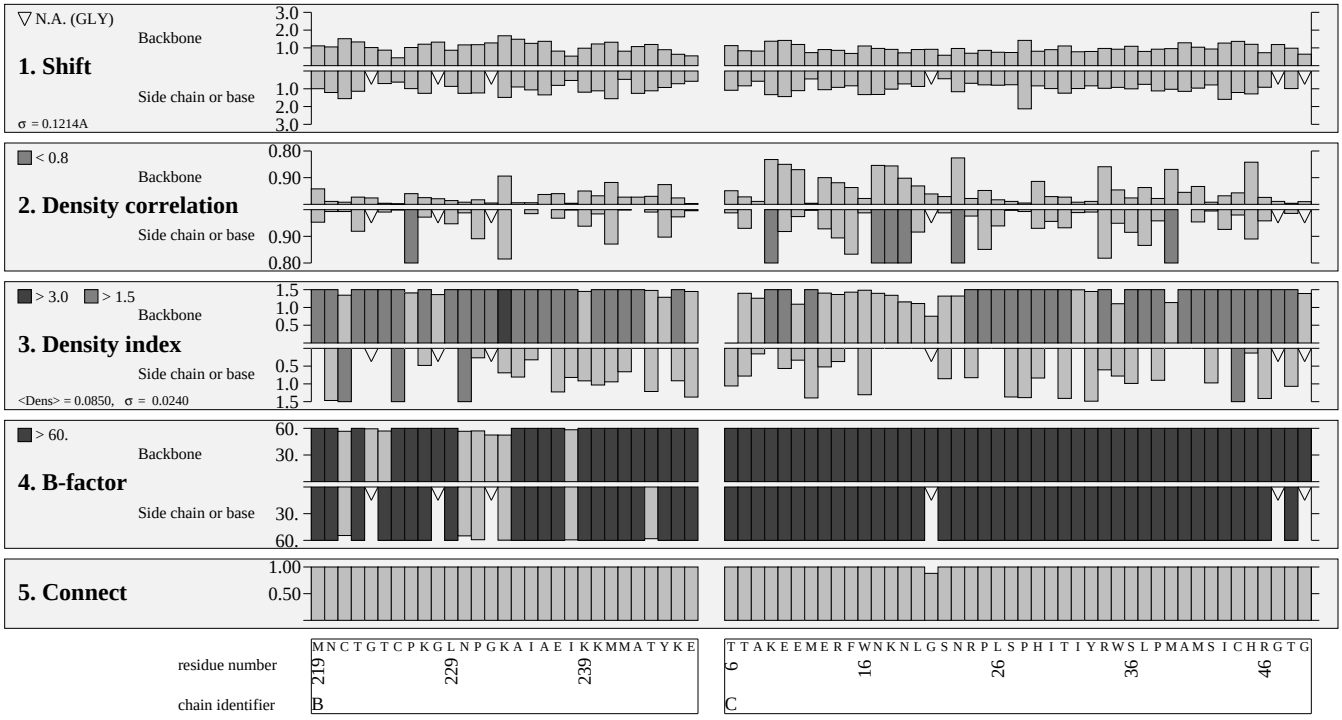
Local estimation (6)





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Structure Factor Check

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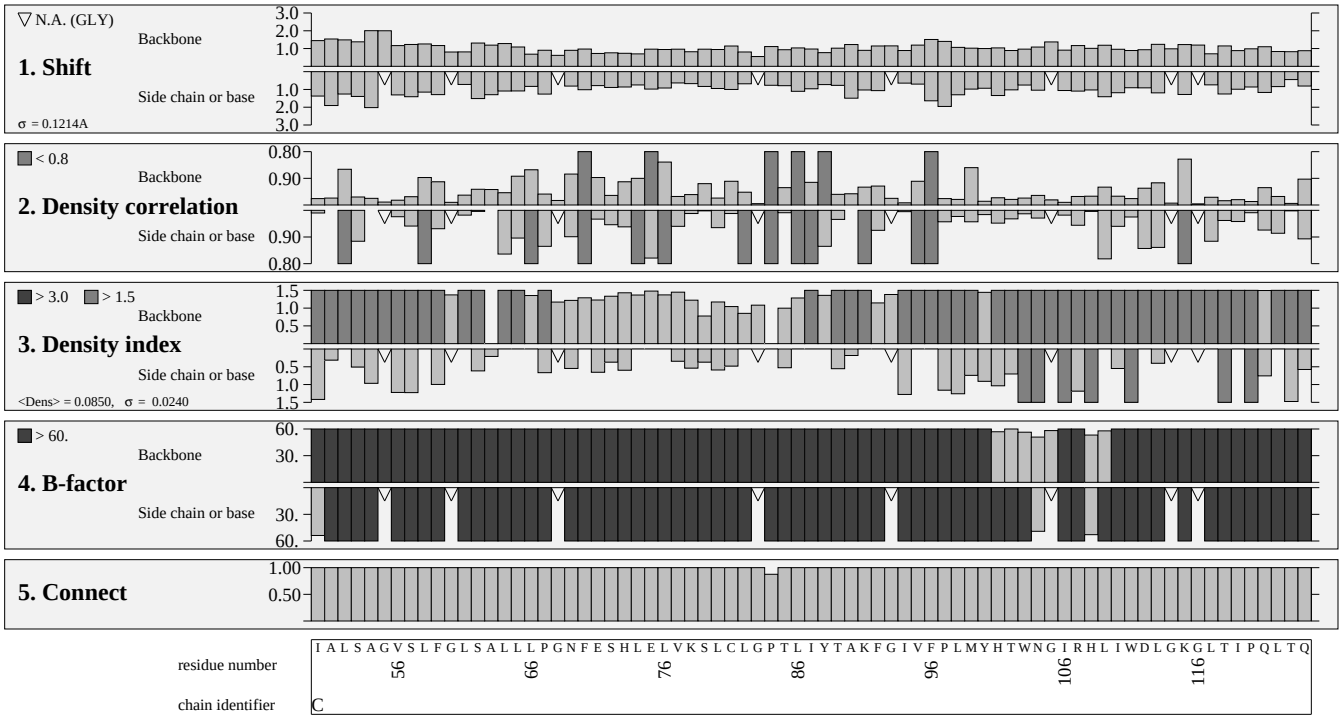
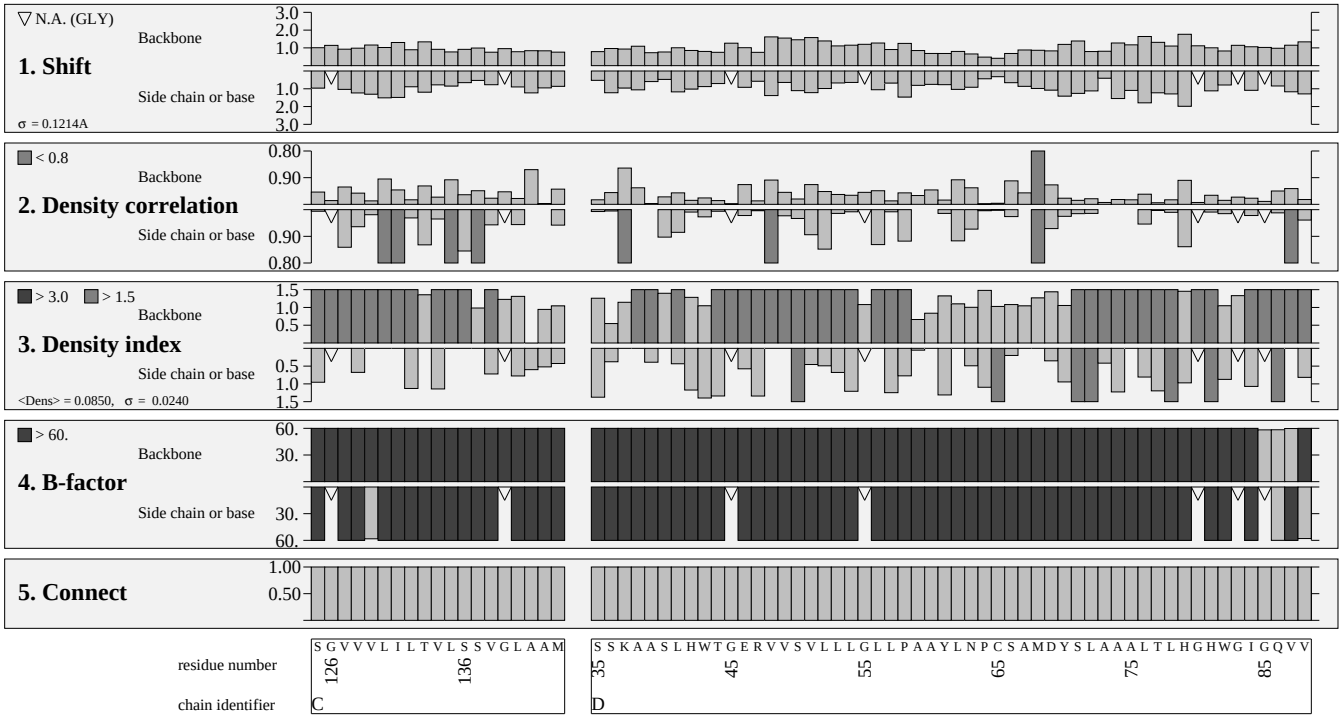
Local estimation (7)





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Local estimation (8)