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

Structure Factor Check

3BCC

Title: STIGMATELLIN AND ANTIMYCIN BOUND CYTOCHROME BC1 COMPLEX FROM
Date: 23−MAR−98
PDB code: 3BCC

Crystal

Cell parameters:

a: 173.18 A b: 179.73 A c: 238.22 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

15645 atoms

Number of chains:	16
Volume not occupied by model:	63.6 %
<B> (for atomic model):	73.0 A^2
σ(B):	22.64 A^2
Matthews coefficient:	8.46
Corresponding solvent % :	85.35

Refinement

Program:	CNS 0.1
Nominal resolution range:	12.0 − 3.70 A
Reported R−factor:	0.289
Number of reflections used:	71026
Reported Rfree:	0.32
Sigma cut−off (F):	2.00

Structure Factors

Input

Nominal resolution range:		86.1 − 3.20 A
Reflections in file:		111780
Unique reflections	above 0:	95003
	above 1σ:	77365
	above 3σ:	48592
Reflections > 0:		16777

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Nominal resolution range: 86.1 − 3.70 A
\05max. from input data, min. from author\05

Used reflections:	67977
Reflections out of resolution:	27026
Completeness:	85.0 %
R_stand(F) = <σ(F)>/<F> :	0.114

Anisotropic distribution of Structure Factors
ratio of eigen values: 1.0000 0.5733 0.6454

B_overall (by Patterson):	70.A^2
Optical resolution:	2.65 A
Expected opt. resol. for complete data set:	2.65 A
Estimated minimal error:	0.335 A

Model vs. Structure Factors

R−factor for all reflections:	0.365
Correlation factor:	0.695
R−factor:	0.347

for F > 2.0σ
nom. resolution range: 12.00 − 3.70A
reflections used: 58453

<u> (error in coords by Luzzati plot):	0.865 A
Estimated maximal error:	0.621 A
DPI:	0.440 A

Scaling

Scale:	1.571
Bdiff:	1.22

Anisothermal Scaling (Beta):
19.6977 6.8935 8.5683 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.802 251.140

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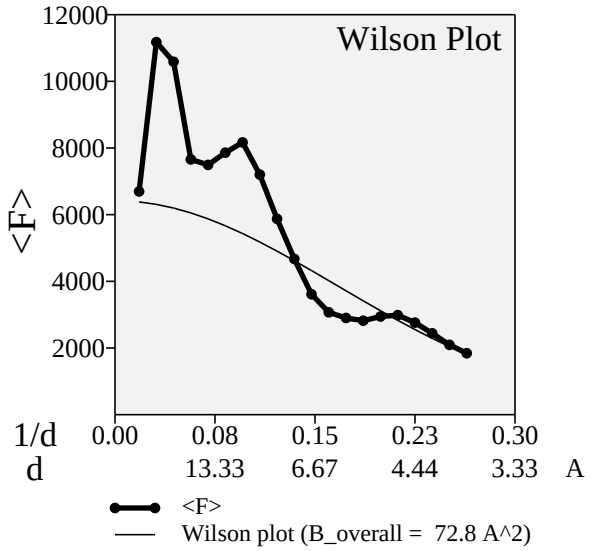
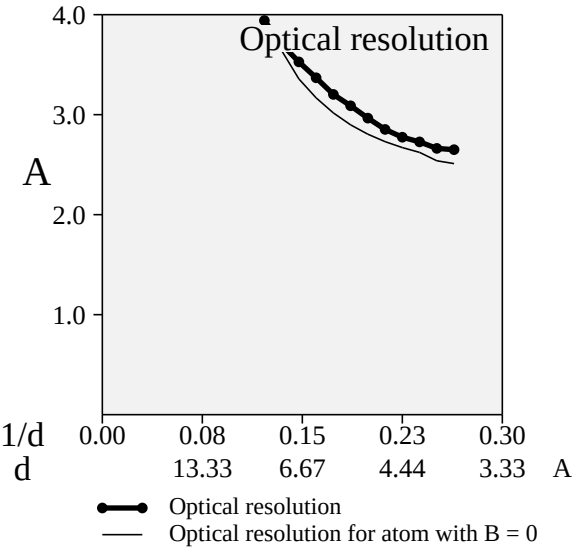
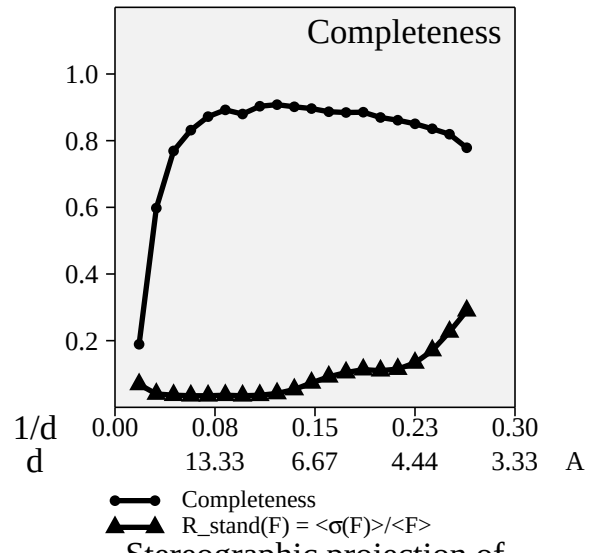


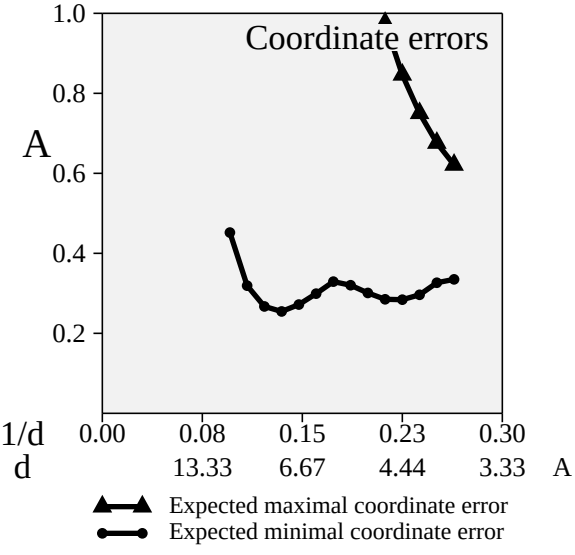
<F>
Wilson plot (B_overall = 72.8 A^2)



Optical resolution
Optical resolution for atom with B = 0

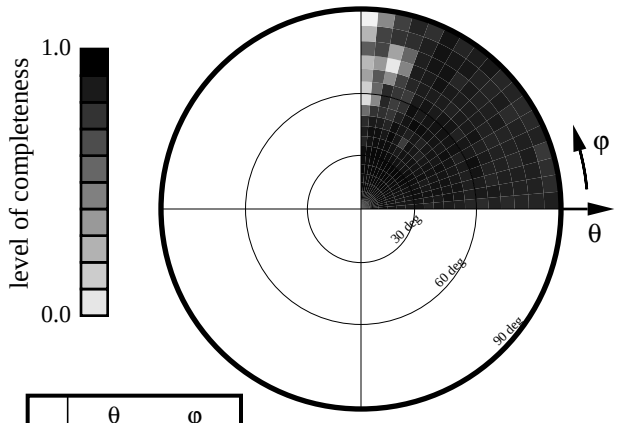


Completeness
R_stand(F) = <σ(F)>/<F>



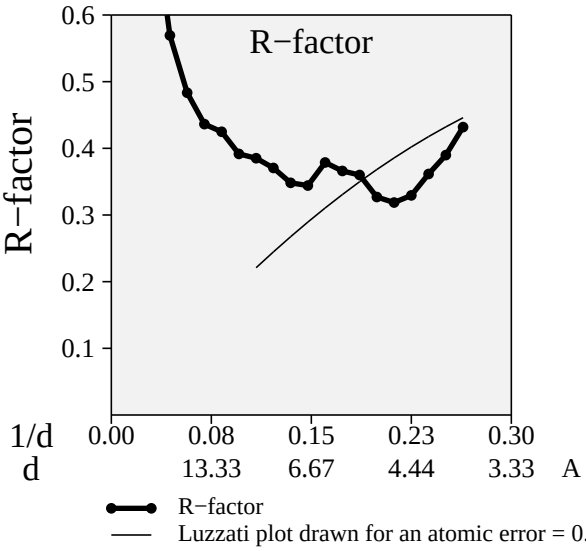
Expected maximal coordinate error
Expected minimal coordinate error

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



R−factor
Luzzati plot drawn for an atomic error = 0.865

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Structure Factor Check

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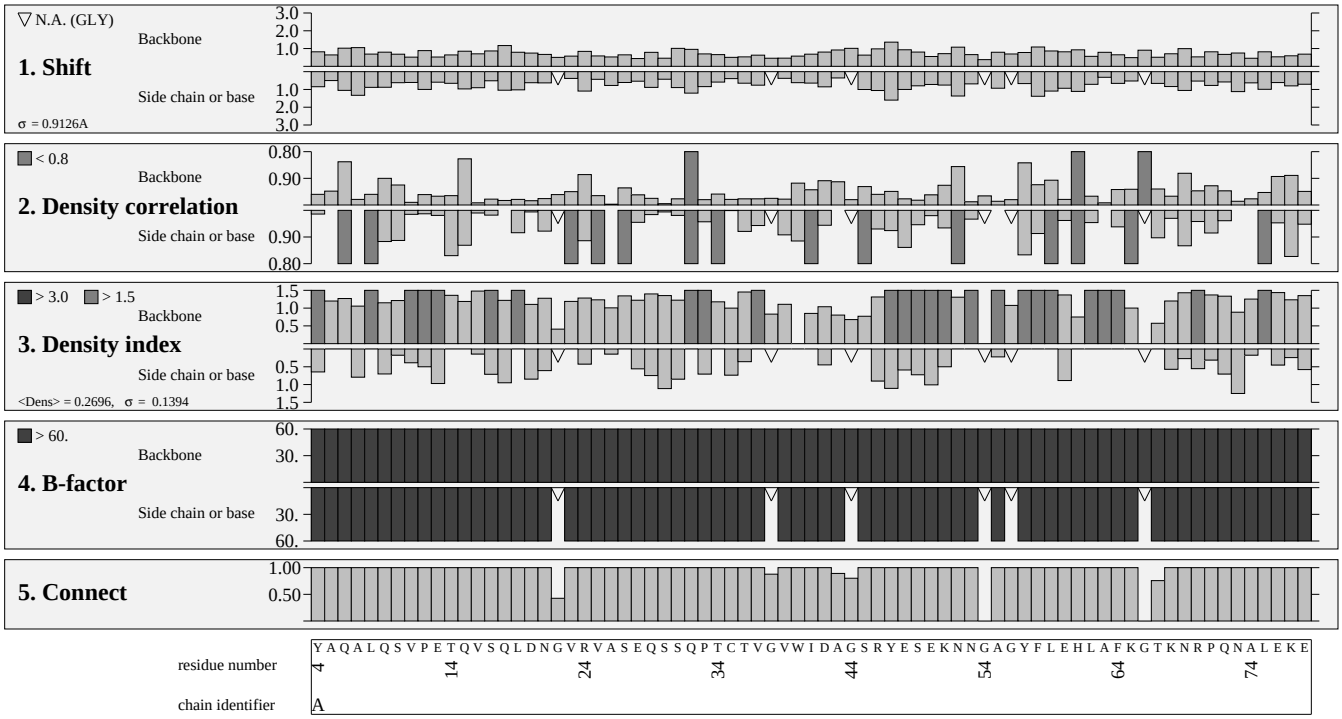
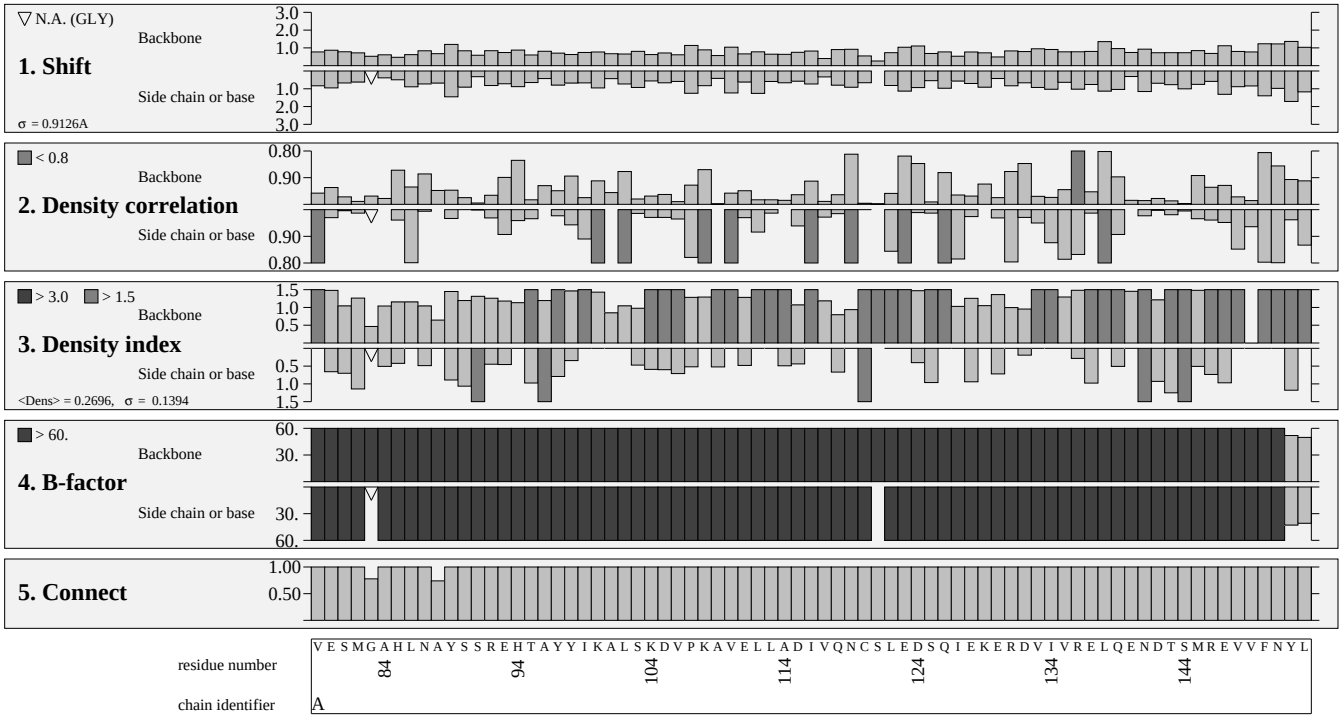
Local estimation





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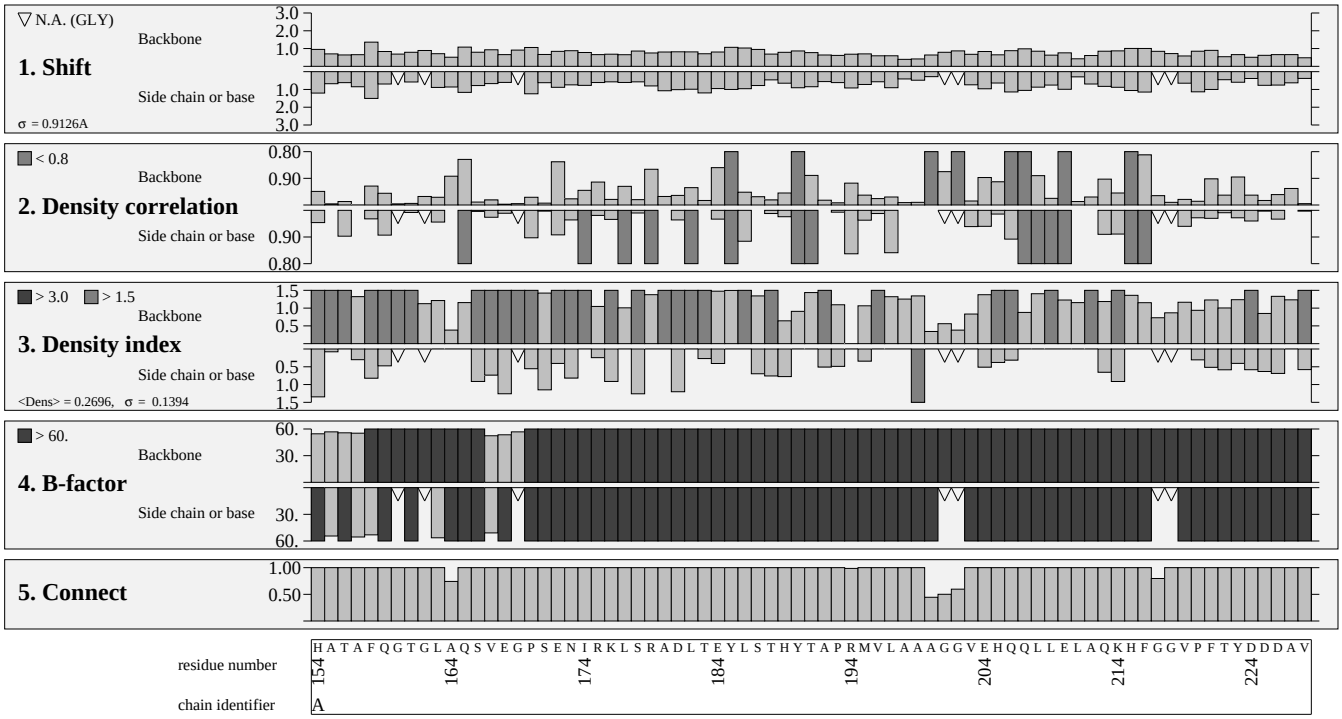
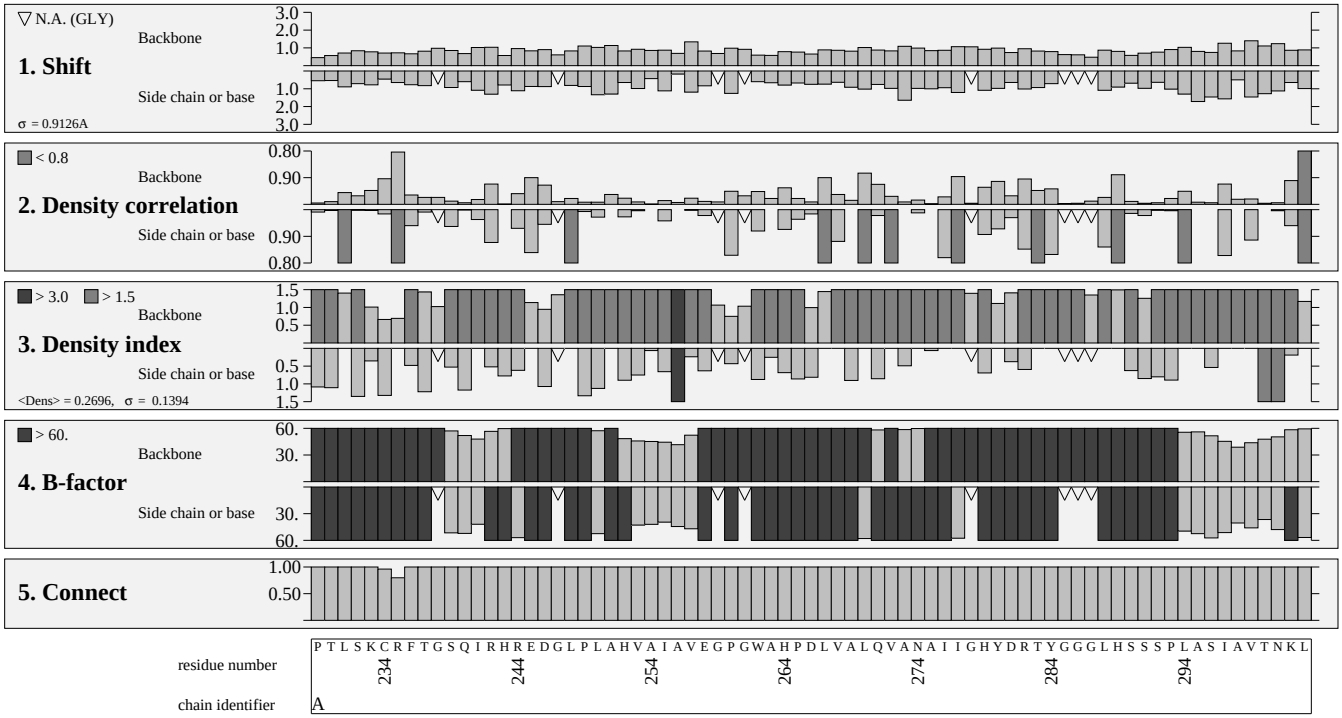
Structure Factor Check

3BCC

Local estimation (2)





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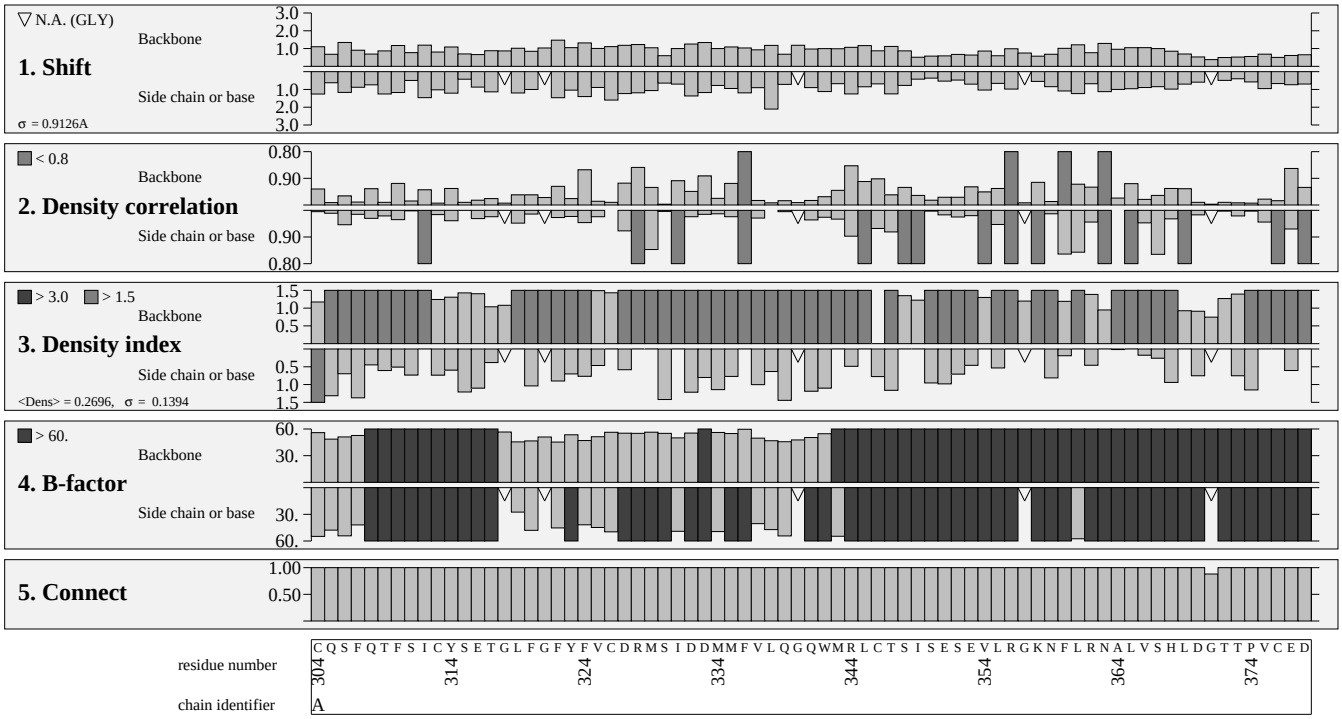
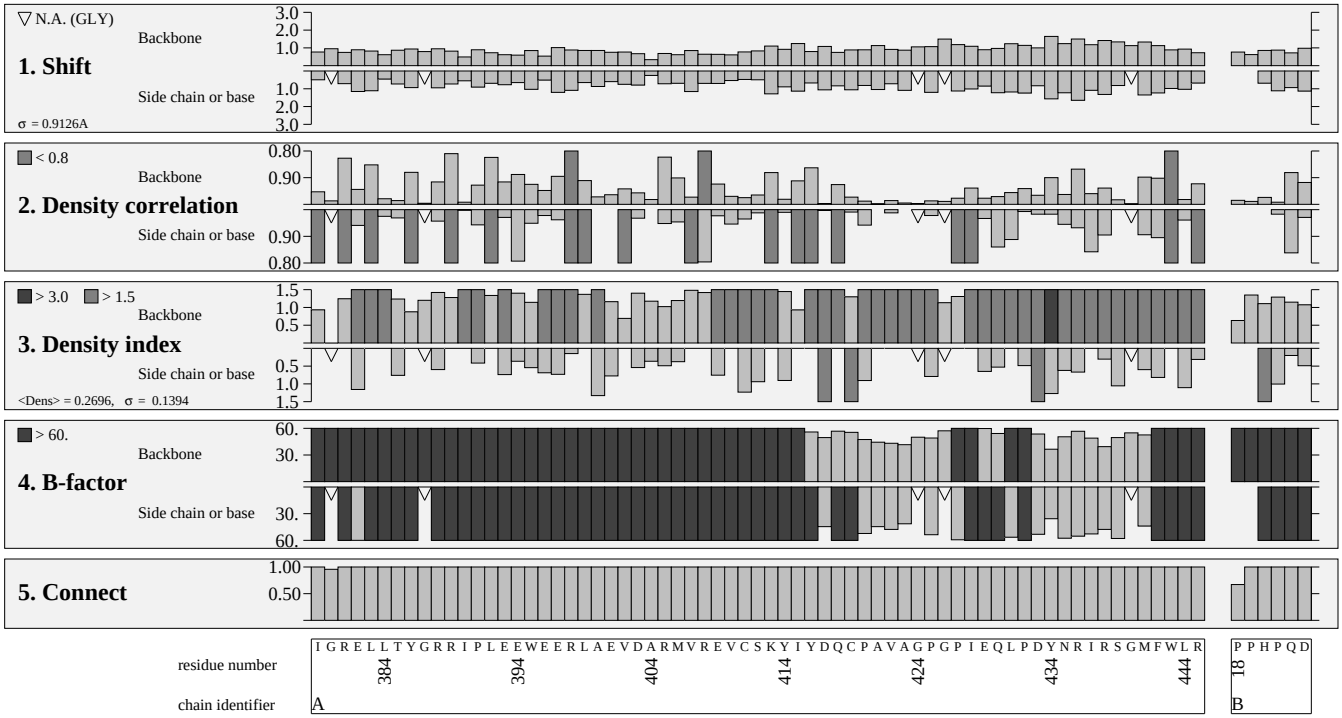
Structure Factor Check

3BCC

Local estimation (3)





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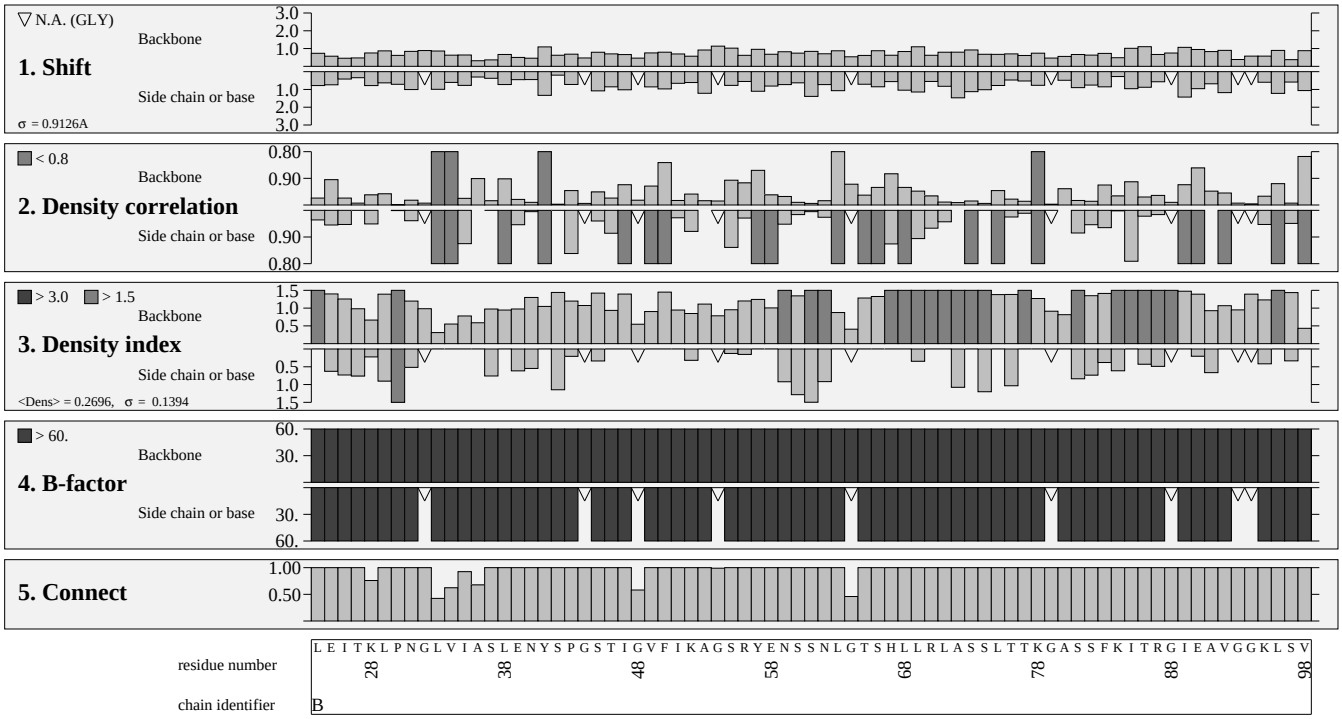
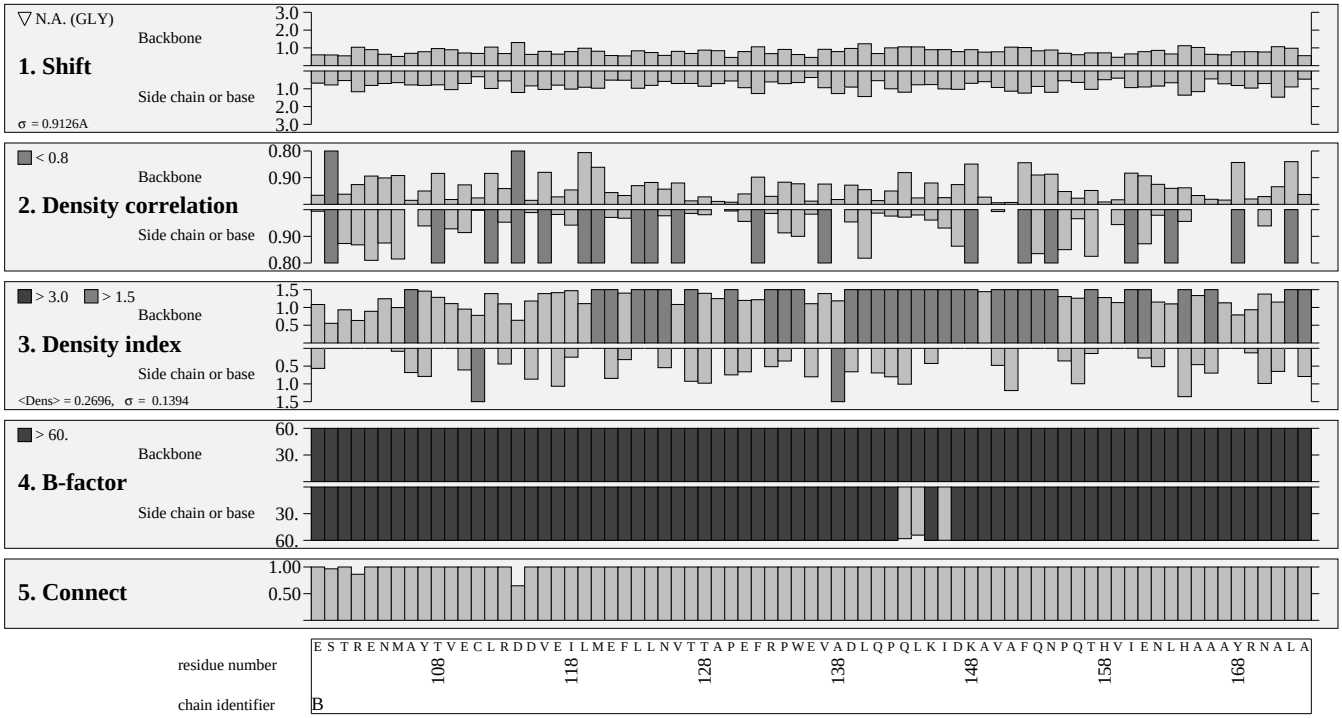
Structure Factor Check

3BCC

Local estimation (4)





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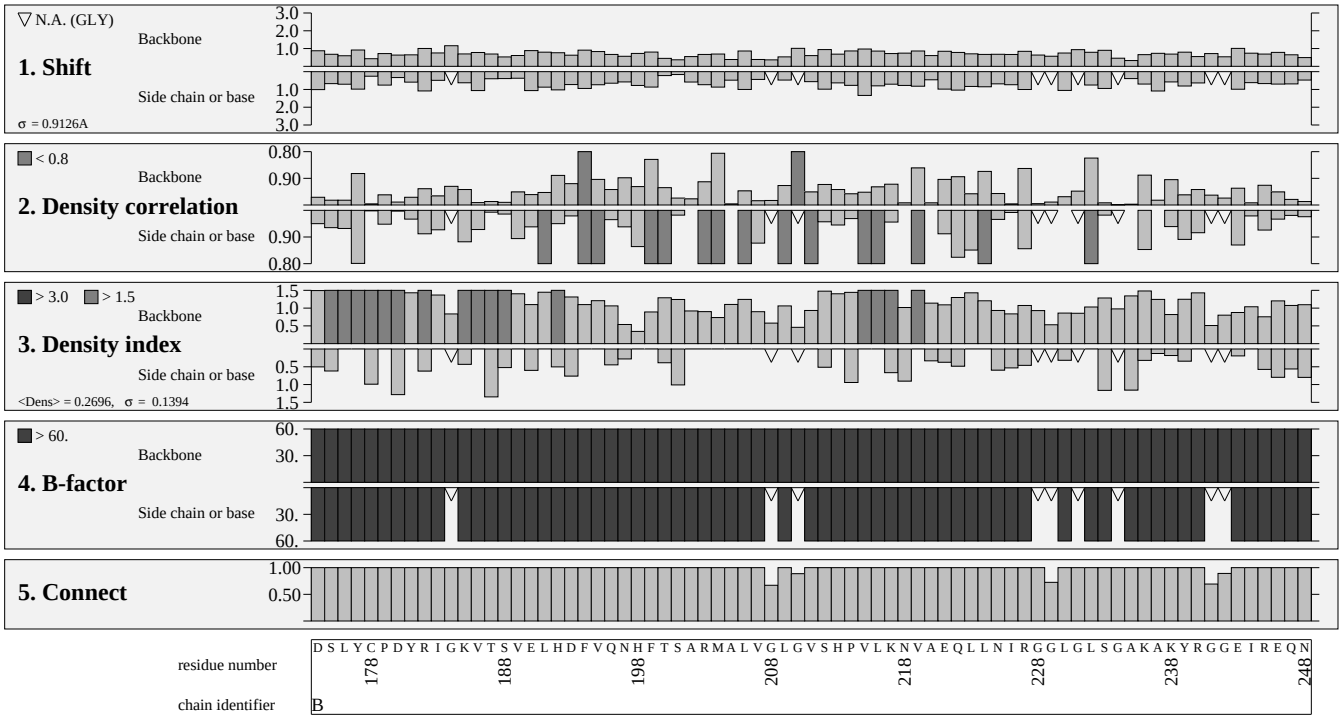
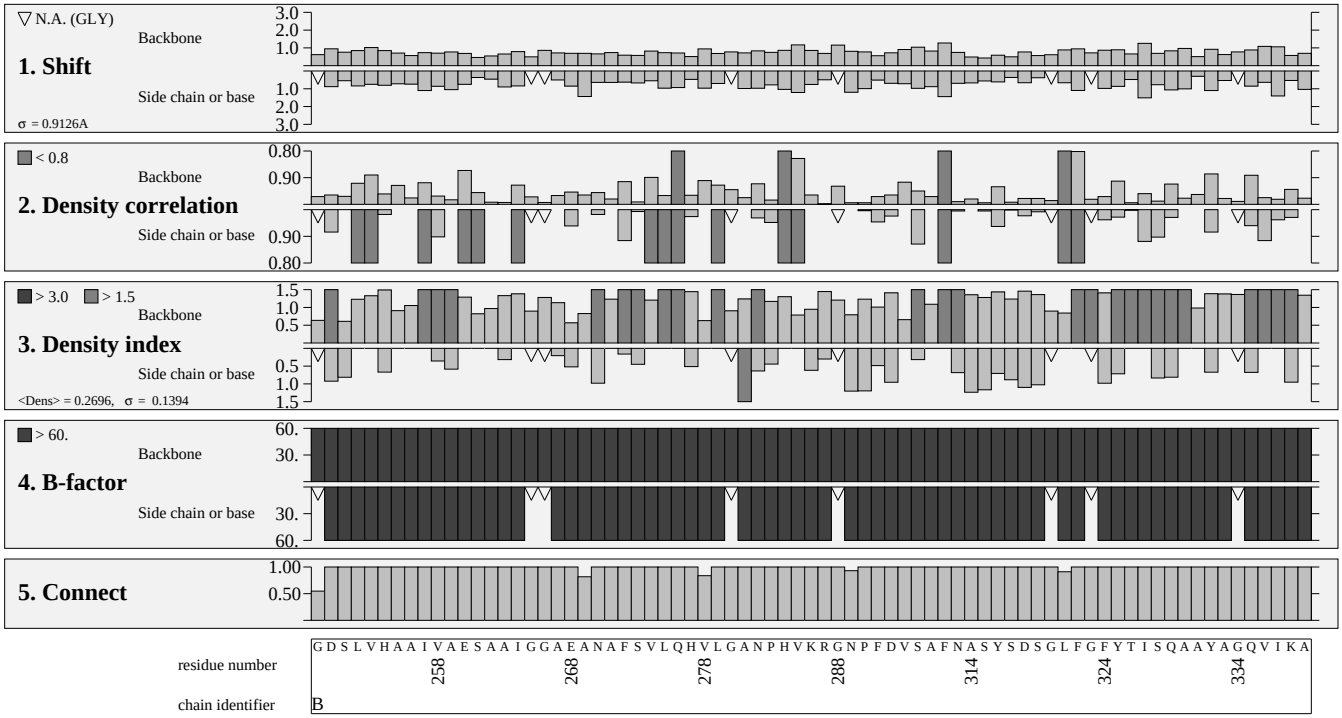
Structure Factor Check

3BCC

Local estimation (5)





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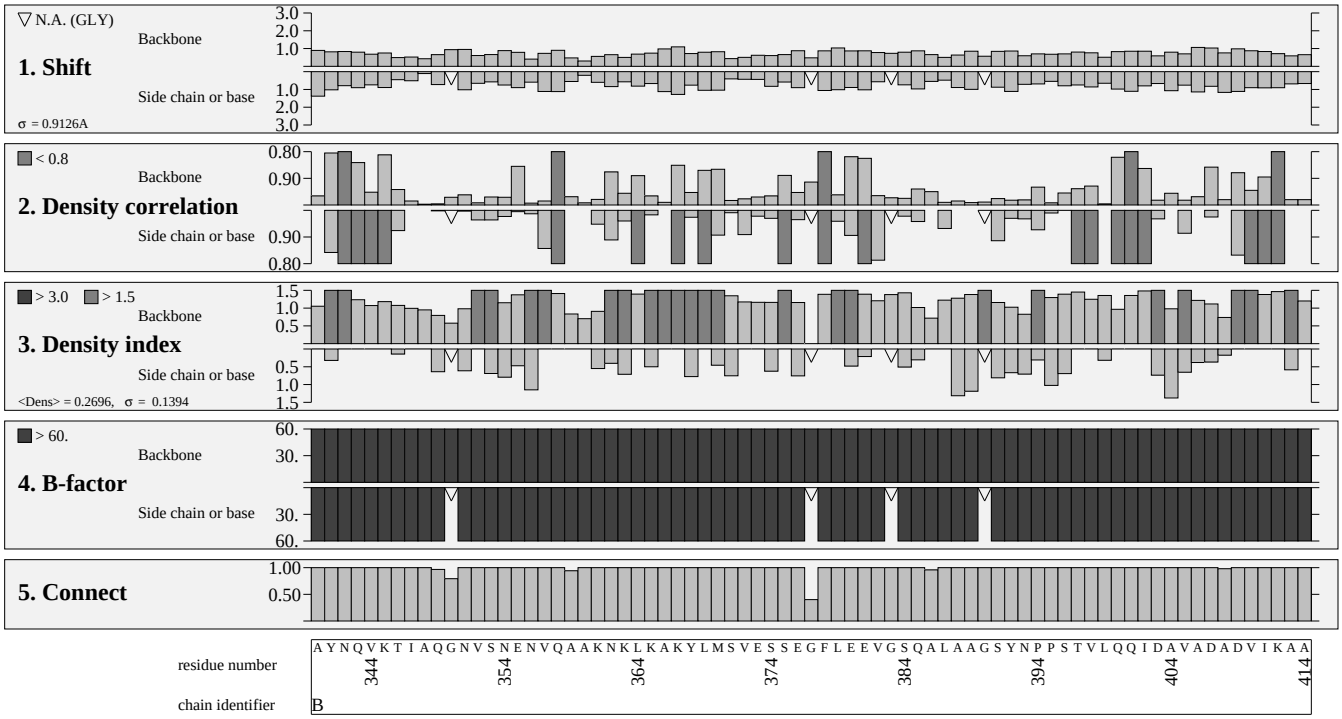
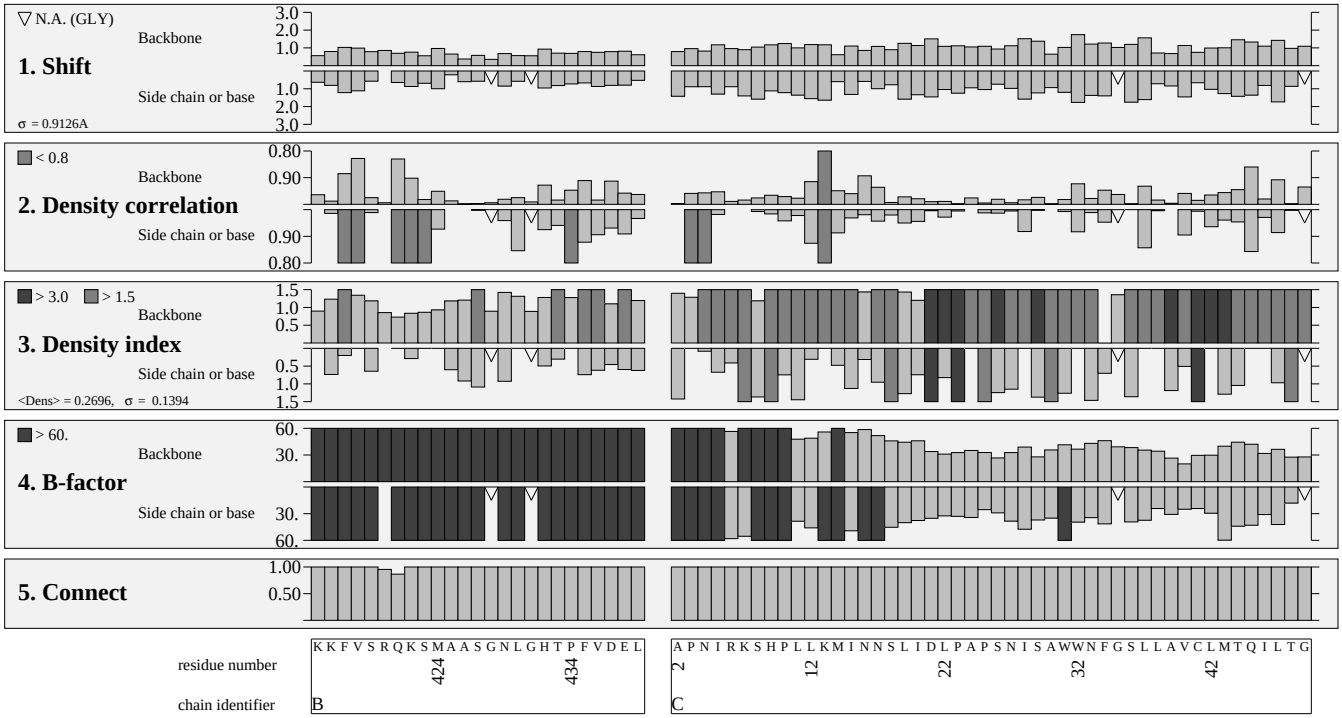
Structure Factor Check

3BCC

Local estimation (6)





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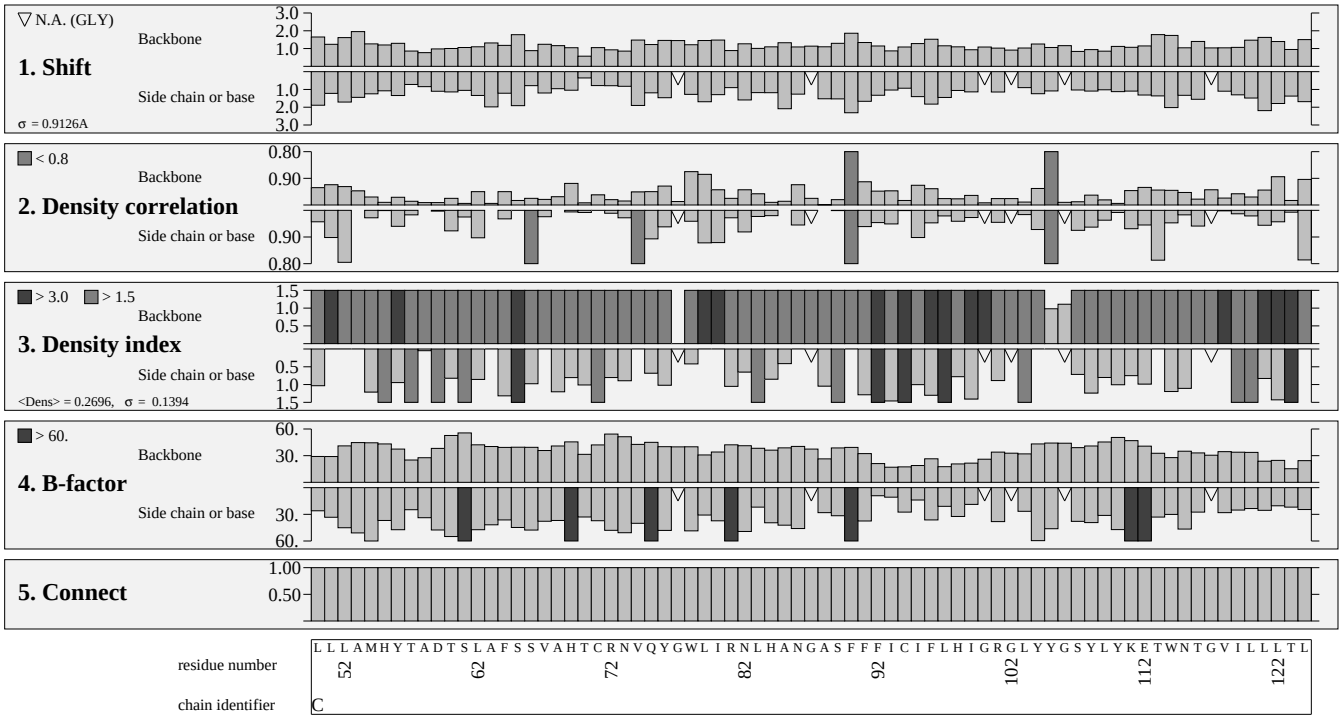
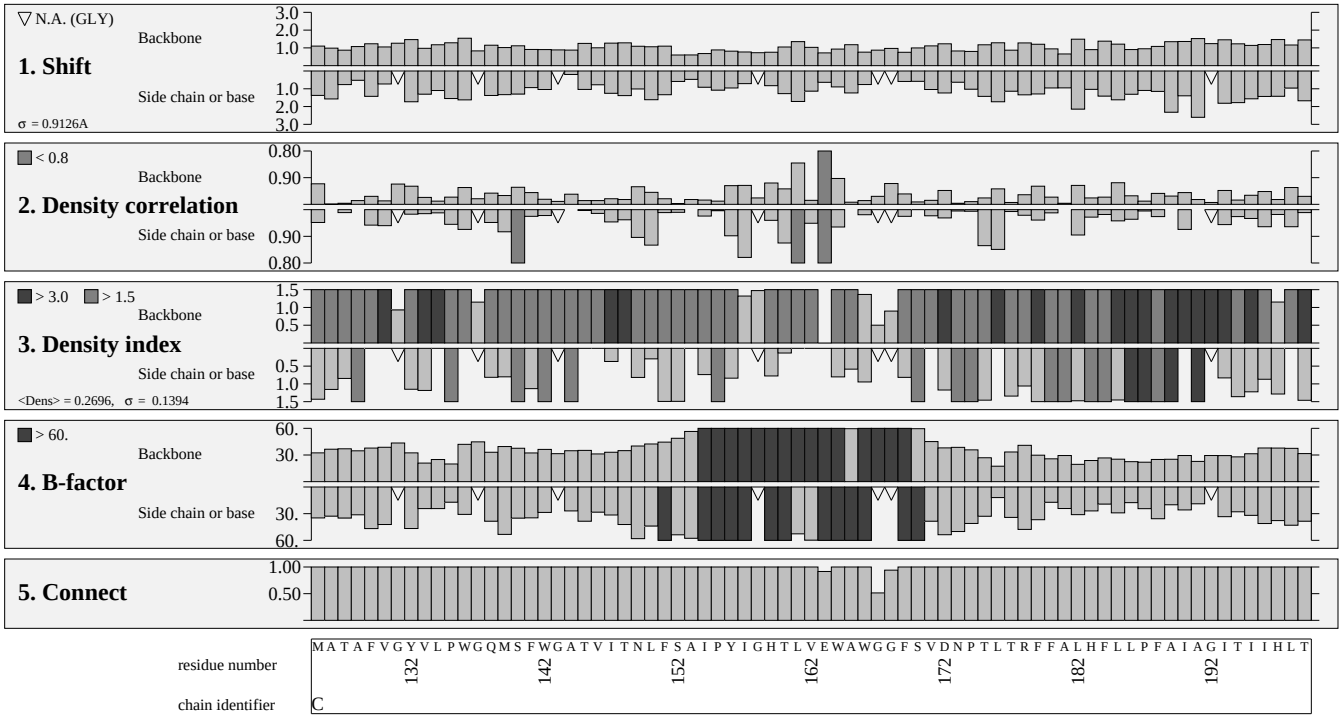
Structure Factor Check

3BCC

Local estimation (7)

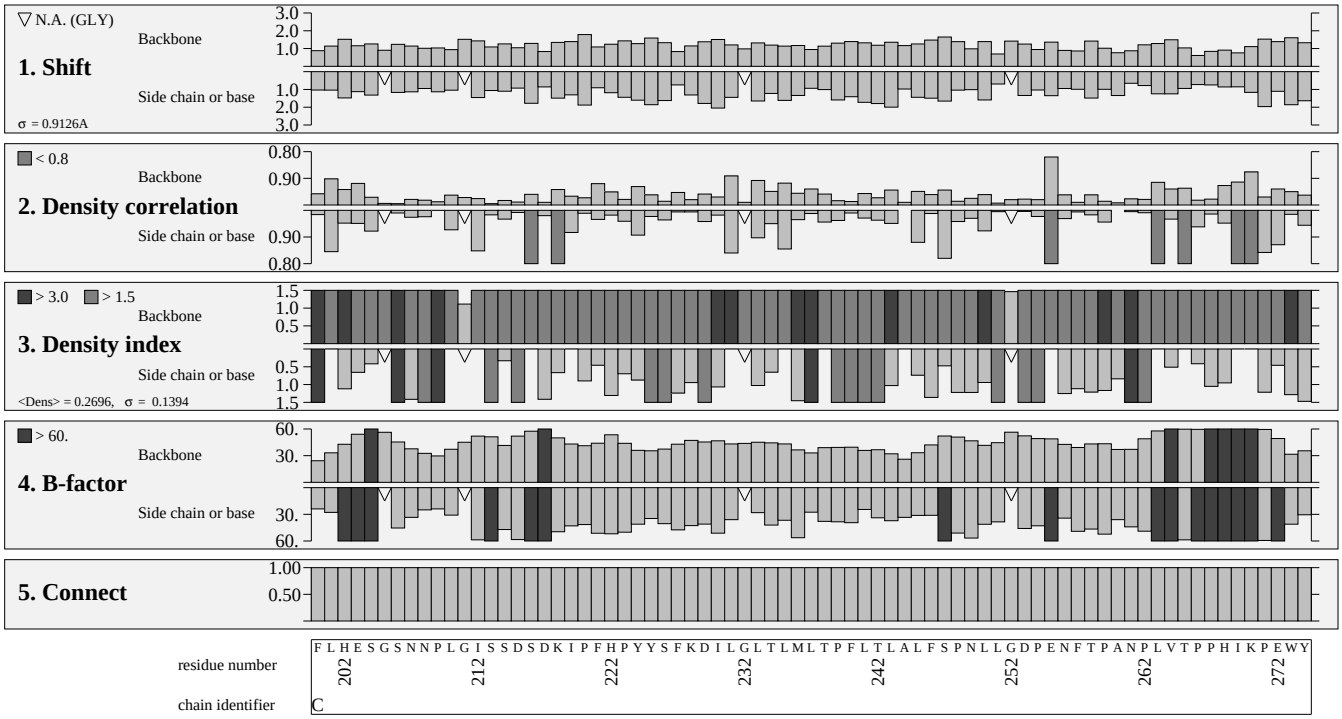


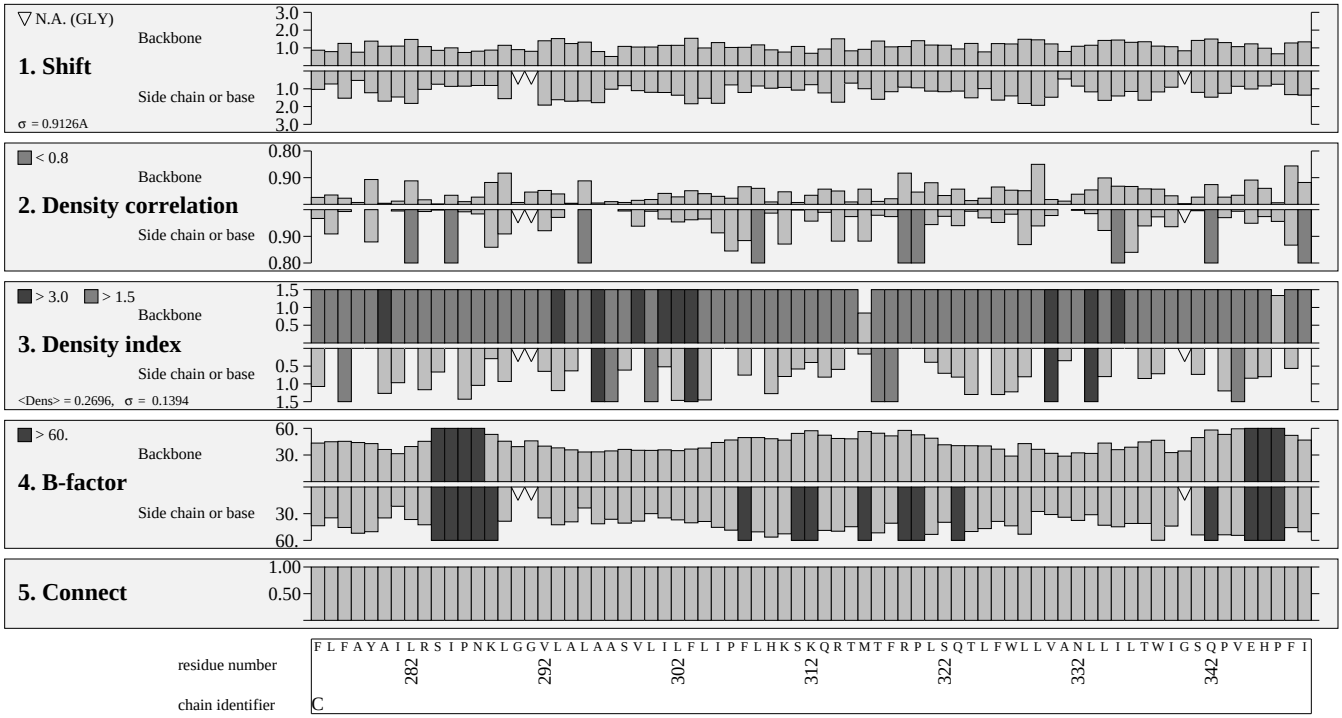


Structure Factor Check

3BCC

Local estimation (8)





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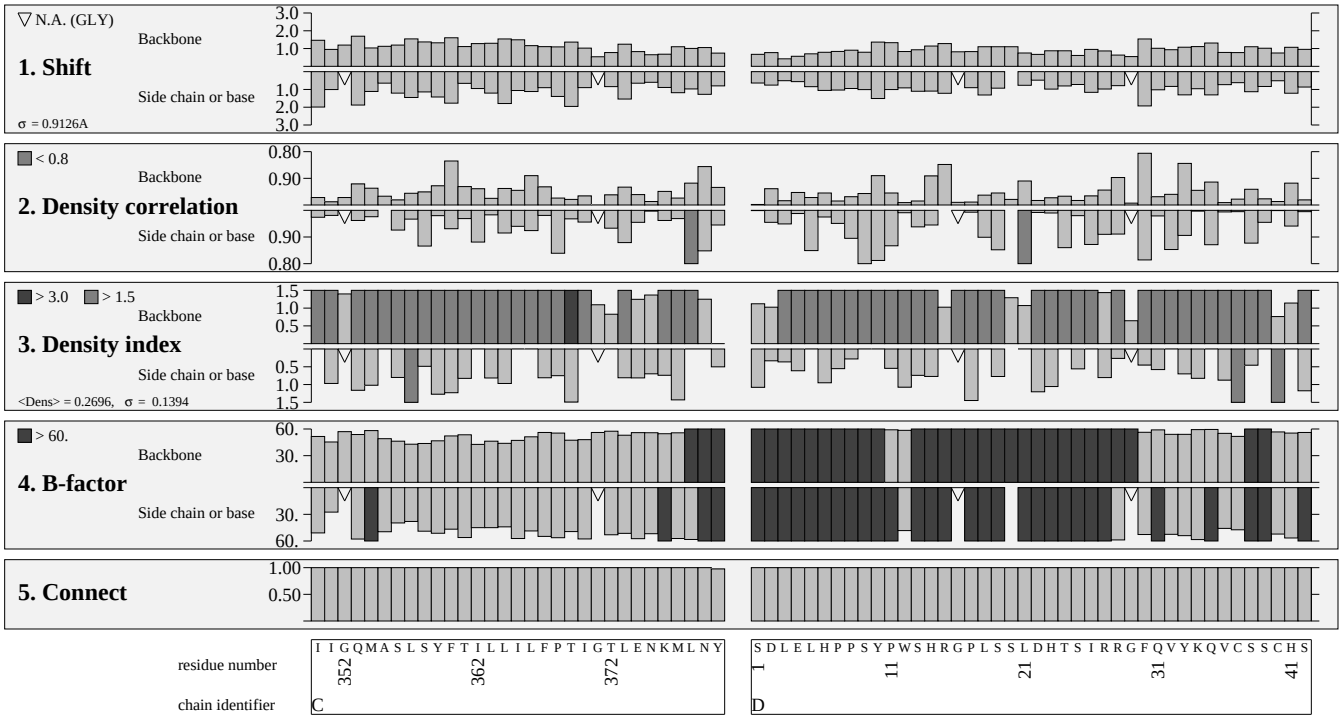
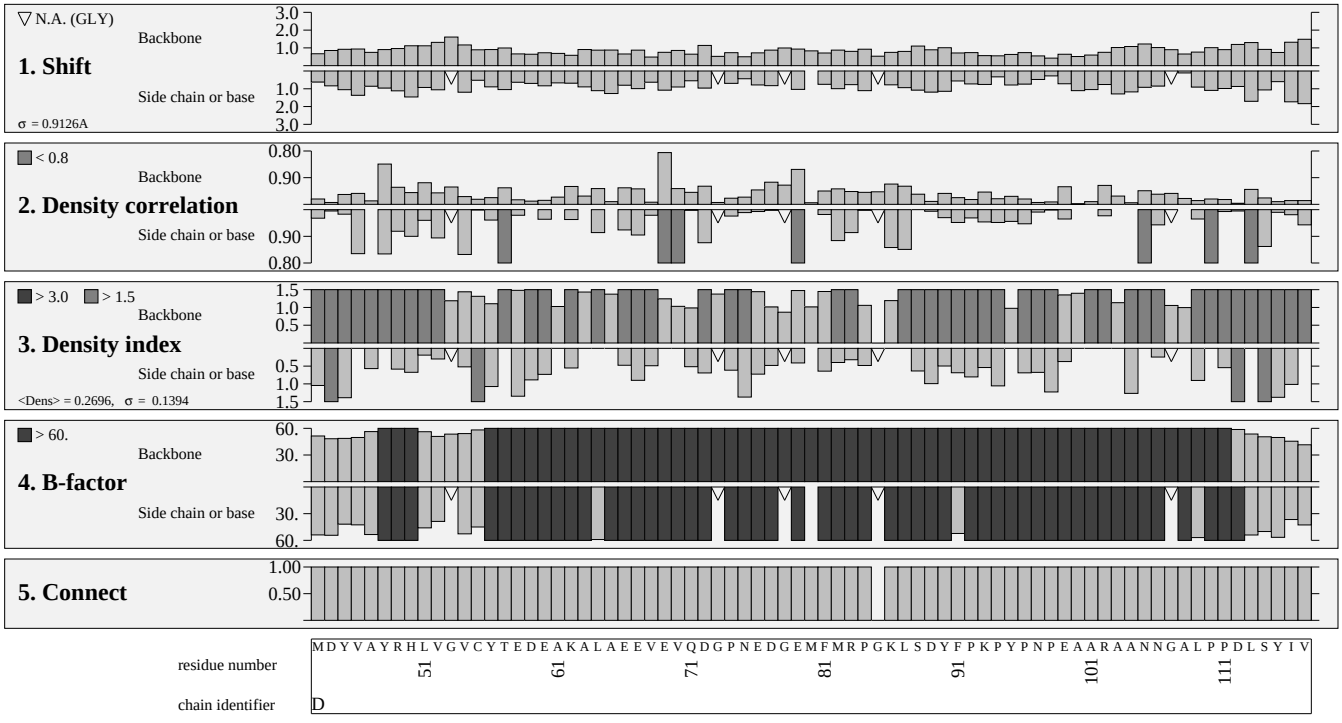
Structure Factor Check

3BCC

Local estimation (9)





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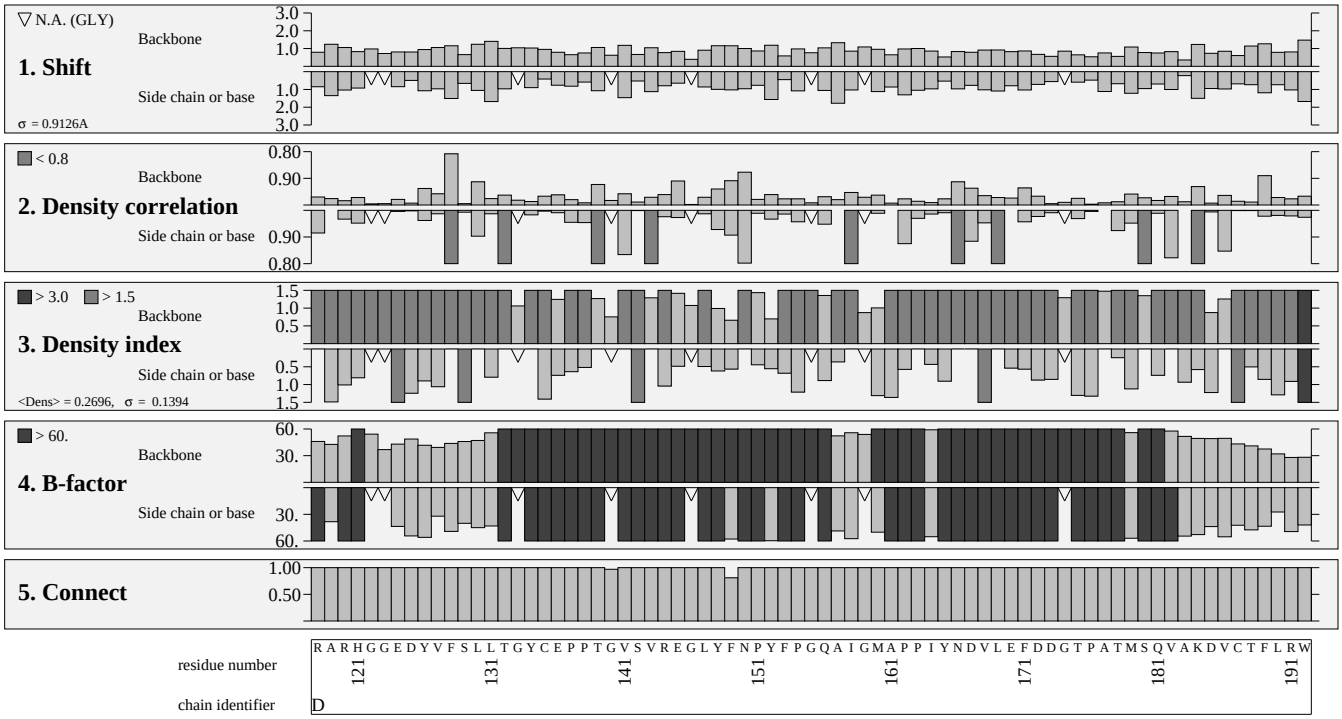
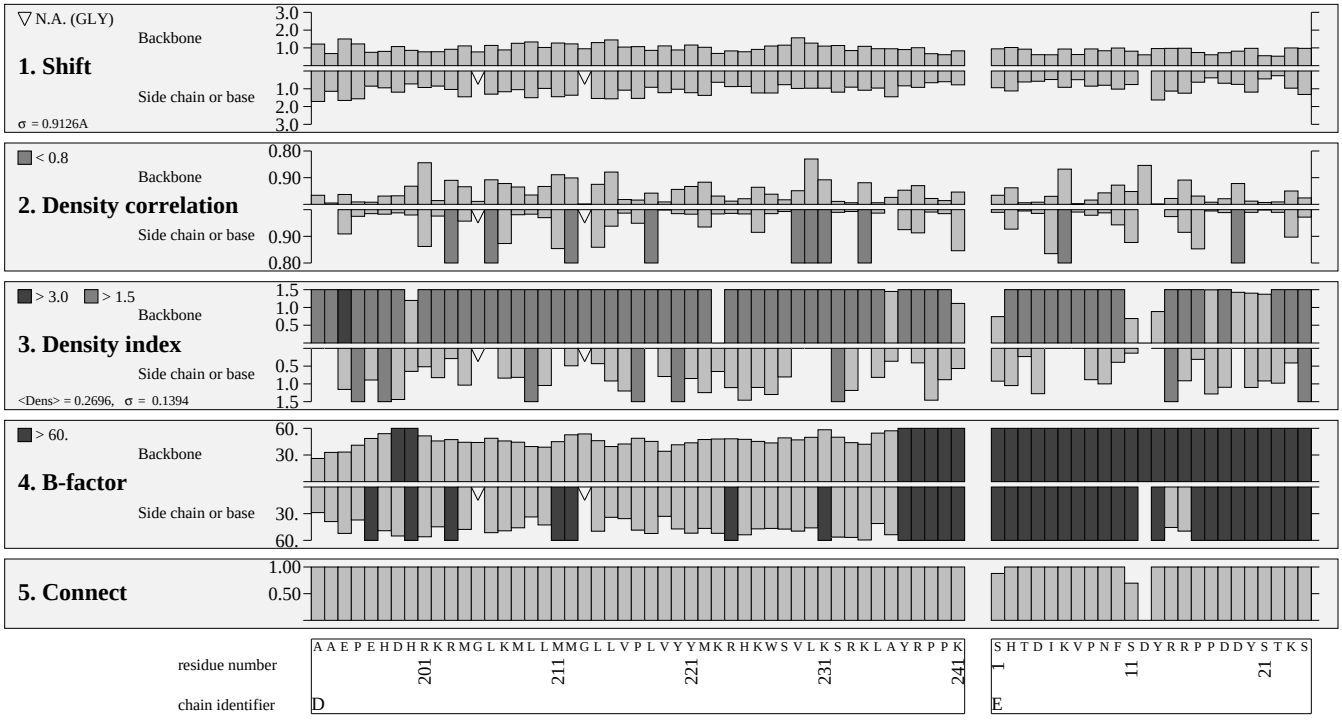
Structure Factor Check

3BCC

Local estimation (10)





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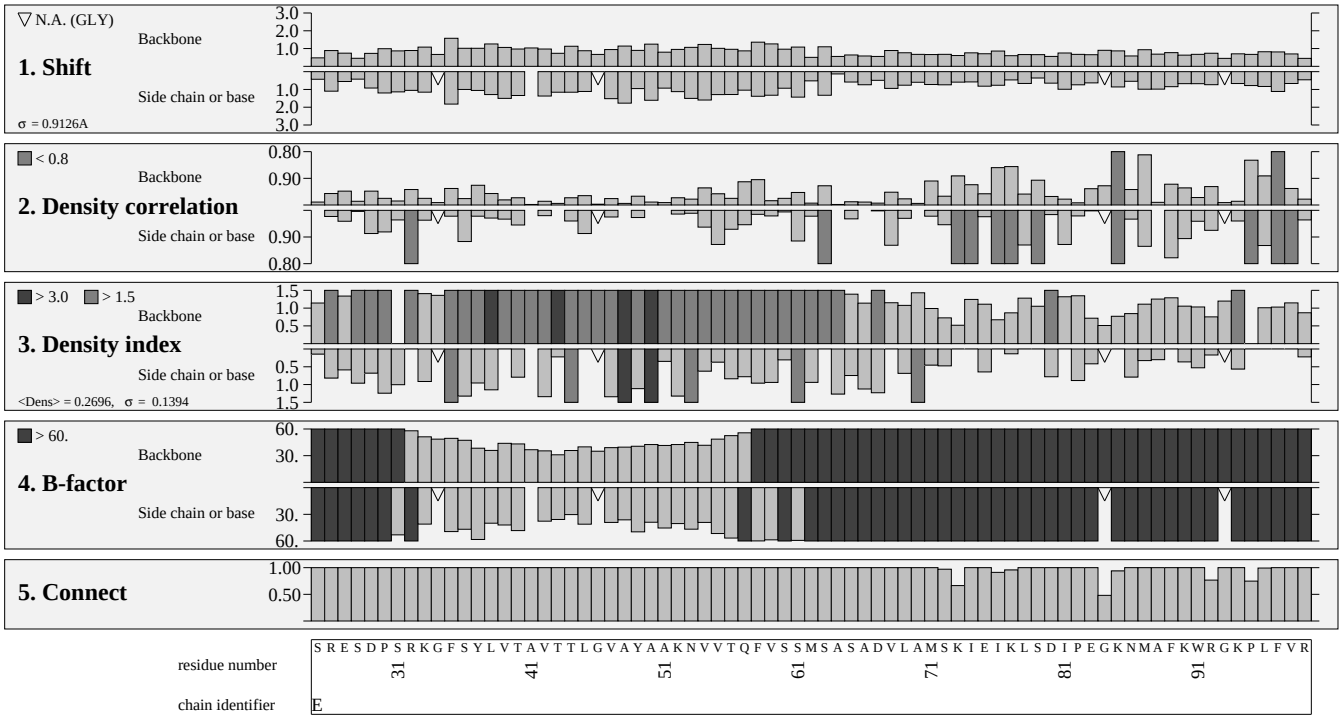
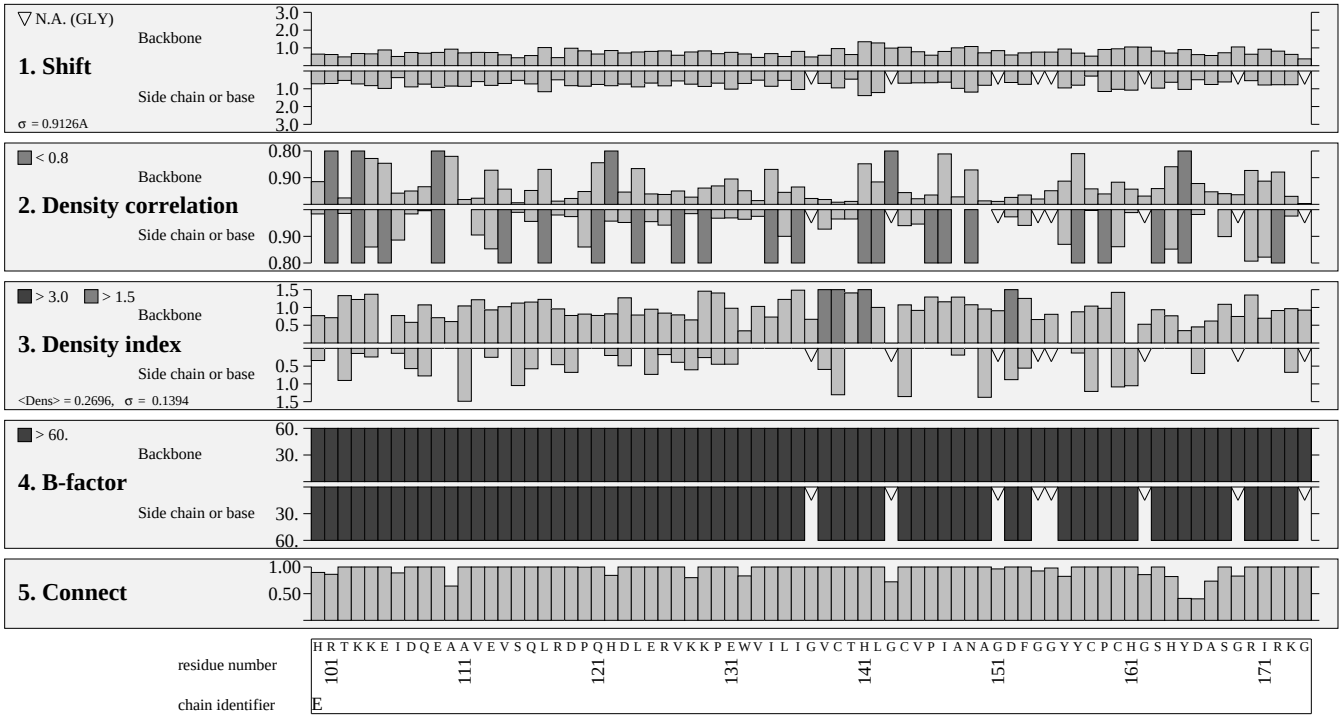
Structure Factor Check

3BCC

Local estimation (11)





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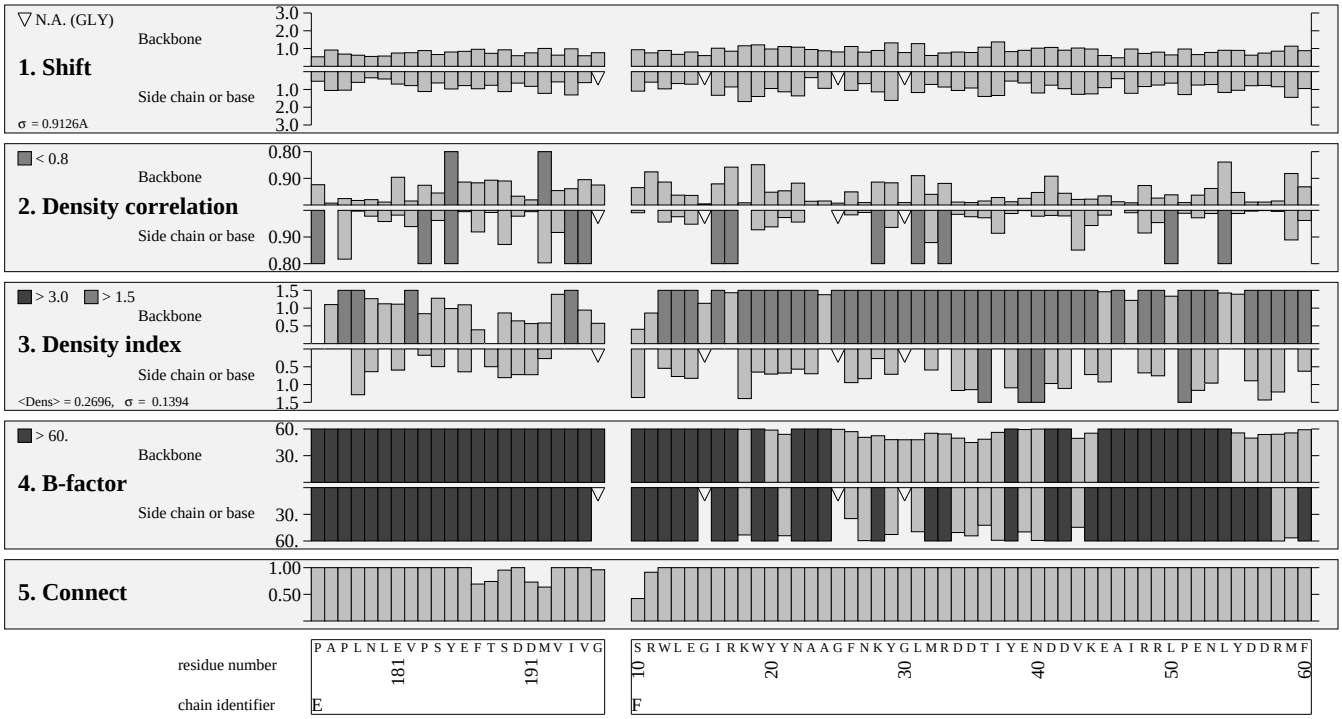
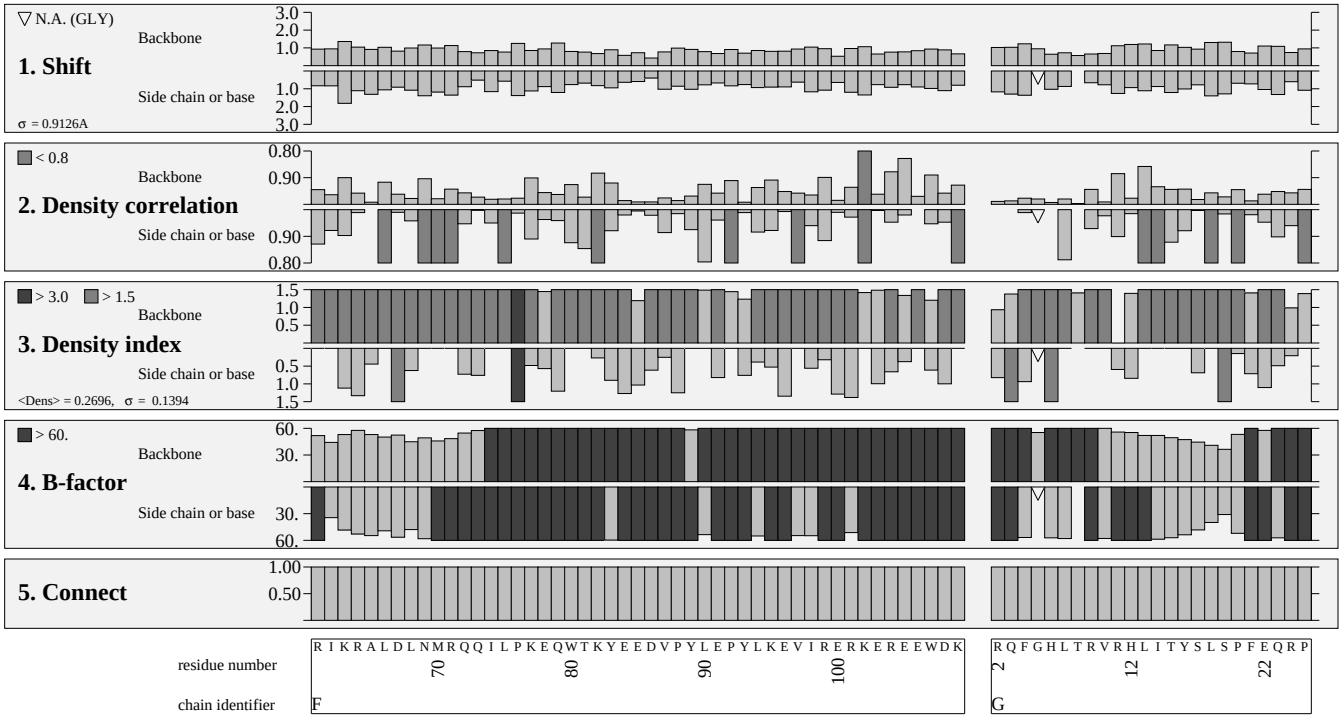
Structure Factor Check

3BCC

Local estimation (12)





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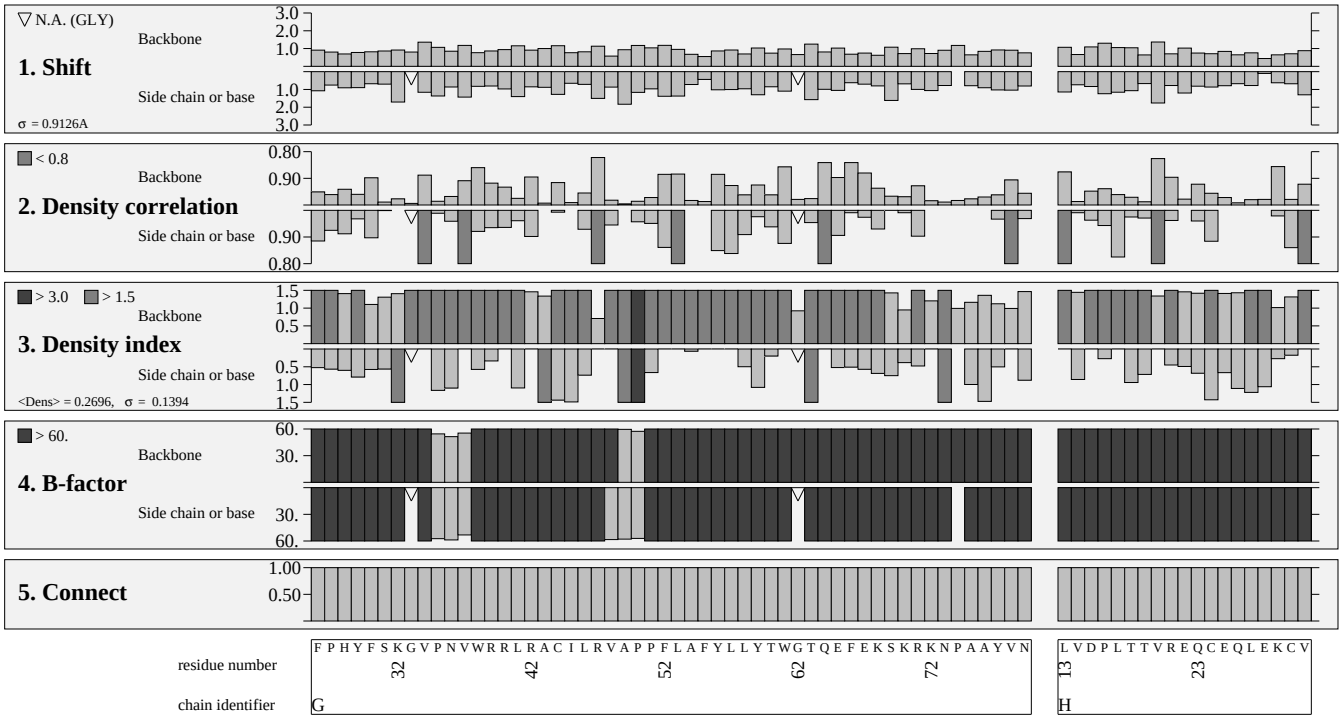
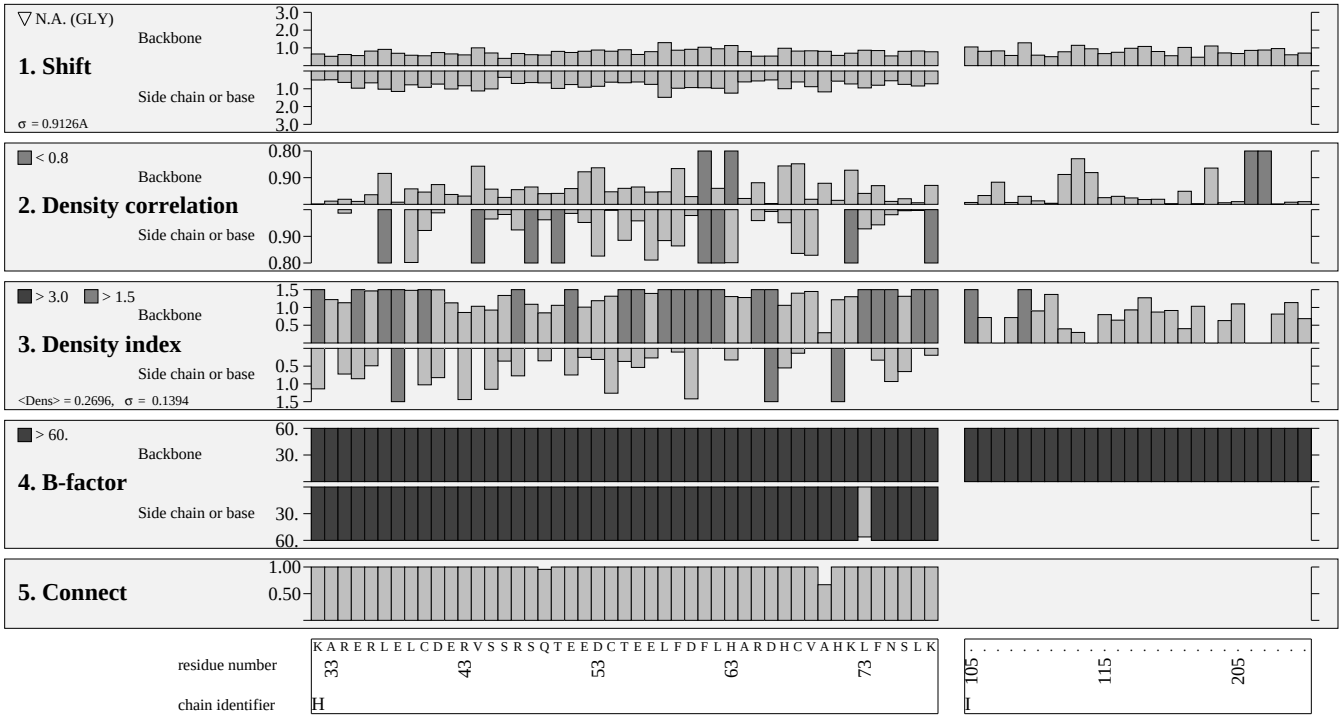
Structure Factor Check

3BCC

Local estimation (13)





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Structure Factor Check

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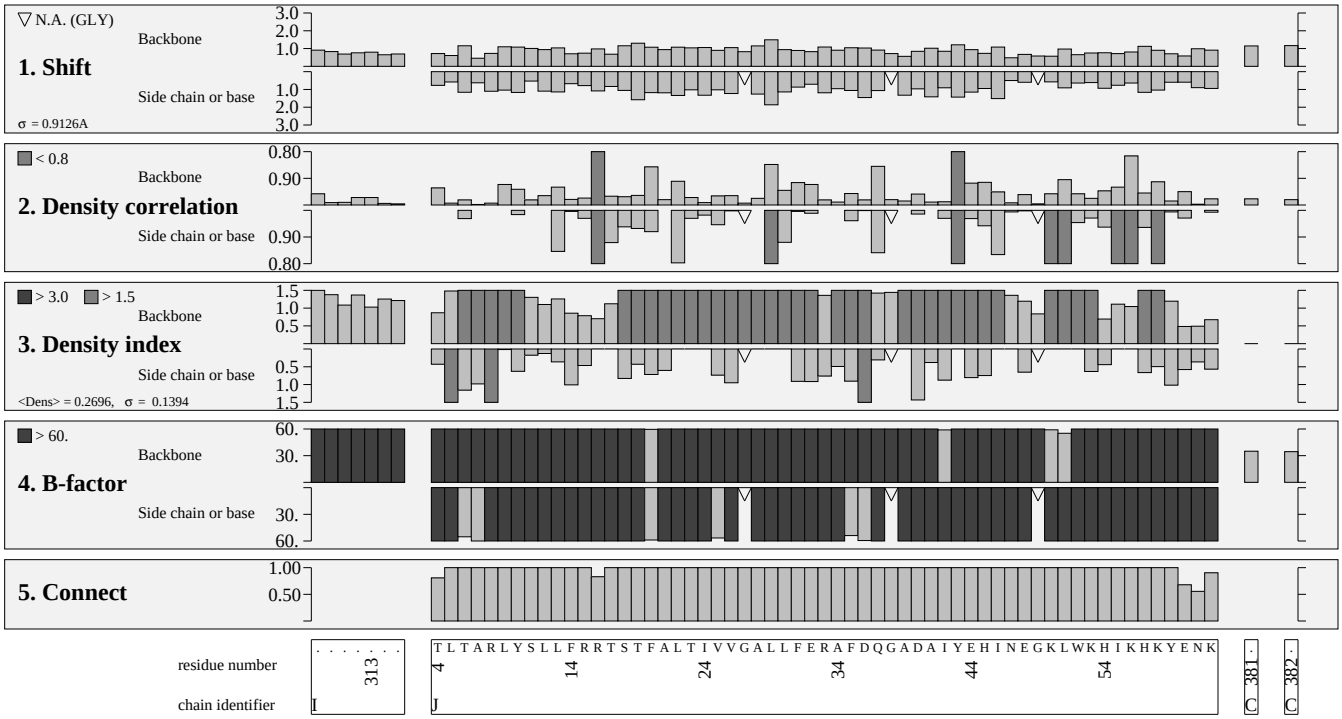
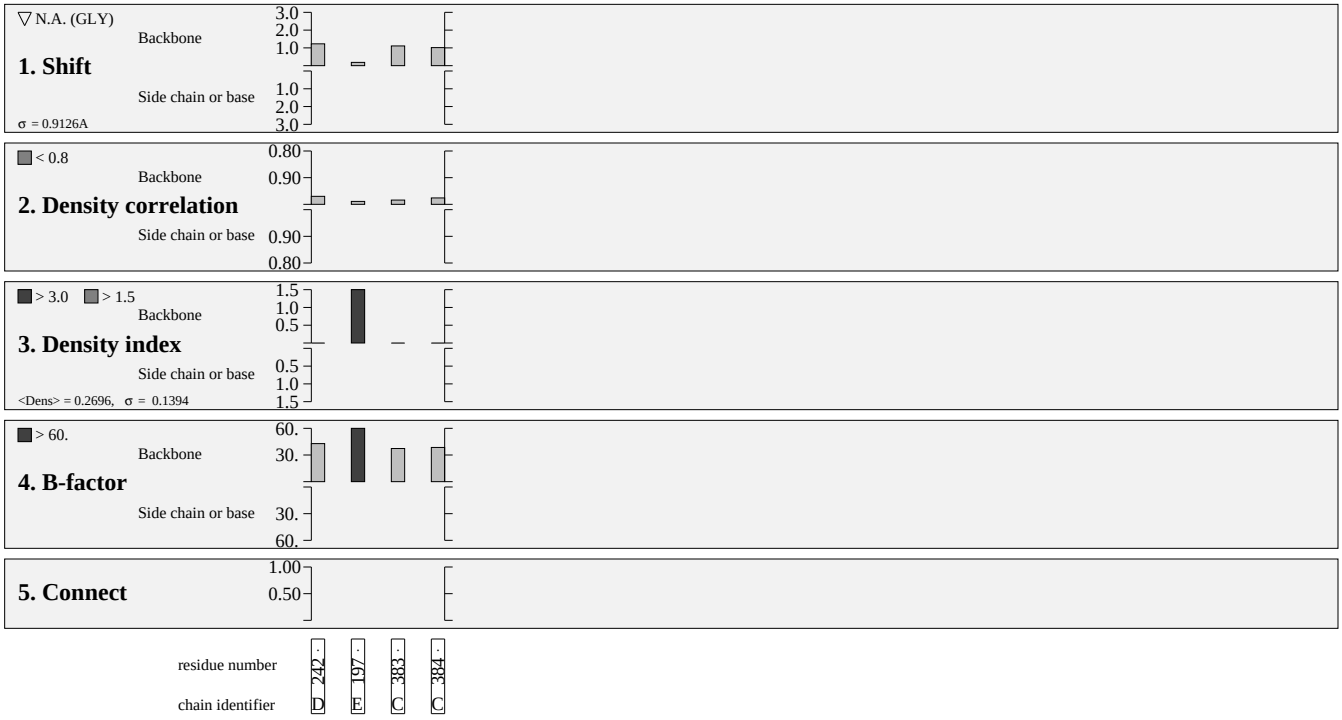
Local estimation (14)





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