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

Structure Factor Check

1PPJ

Title:	BOVINE CYTOCHROME BC1 COMPLEX WITH STIGMATELLIN AND ANTIMYCIN
Date:	16−JUN−03
PDB code:	1PPJ

Crystal

Cell parameters:

a: 128.53 Å b: 168.75 Å c: 231.53 Å

α: 90.00° β: 90.00° γ: 90.00°

Space group: P 21 21 21

Number of NCS−operators: 1

NC−symmetry only for information

Model

33549 atoms (1370 water molecules)

Number of chains:	51
Volume not occupied by model:	45.0 %
<B> (for atomic model):	49.8 Å ²
σ(B):	16.04 Å ²
Matthews coefficient:	2.79
Corresponding solvent % :	55.52

Refinement

Program:	CNS 1.1
Nominal resolution range:	93.5 − 2.10 Å
Reported R−factor:	0.224
Number of reflections used:	285060
Reported Rfree:	0.26
Sigma cut−off:	N.A.

Structure Factors

Input

Nominal resolution range:		93.5 − 2.10 Å
Reflections in file:		285058
Unique reflections	above 0:	285058
	above 1σ:	278499
	above 3σ:	213616

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Nominal resolution range:	93.5 − 2.10 Å
(max. from input data, min. from author)	
Used reflections:	285058
Completeness:	97.8 %
R_stand(F) = <σ(F)>/<F> :	0.079
Anisotropic distribution of Structure Factors	
ratio of eigen values:	1.0000 0.7563 0.6853
B_overall (by Patterson):	38.5Å ²
Optical resolution:	1.75 Å
Expected opt. resol. for complete data set:	1.75 Å
Estimated minimal error:	0.029 Å

Model vs. Structure Factors

R−factor for all reflections:	0.250
Correlation factor:	0.931
R−factor:	0.253
for F > 2.0σ	
nom. resolution range:	93.53 − 2.10Å
reflections used:	278697
Rfree:	0.274
Nfree:	13880
R−factor without free−refl.:	0.252
Non free−reflections:	264817
<u> (error in coords by Luzzati plot):	0.323 Å
Estimated maximal error:	0.104 Å
DPI:	0.189 Å

Scaling

Scale:	1.010
Bdiff:	−4.23

Anisothermal Scaling (Beta):

4.0089 0.5542 −0.7787 0.0000 0.0000 0.0000

Solvent correction − Ks,Bs: 0.841 250.032

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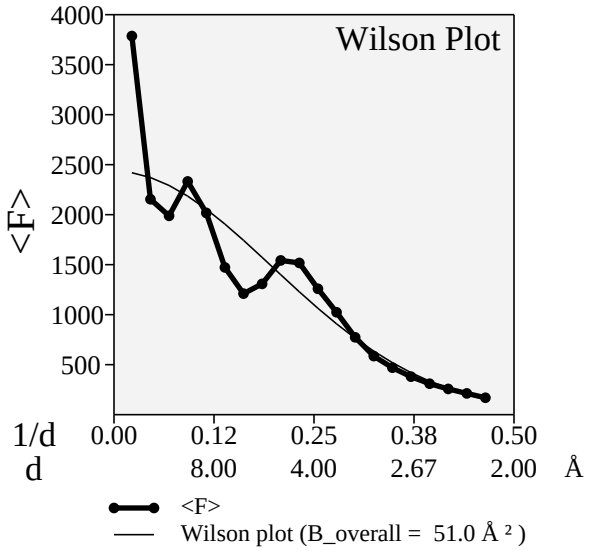
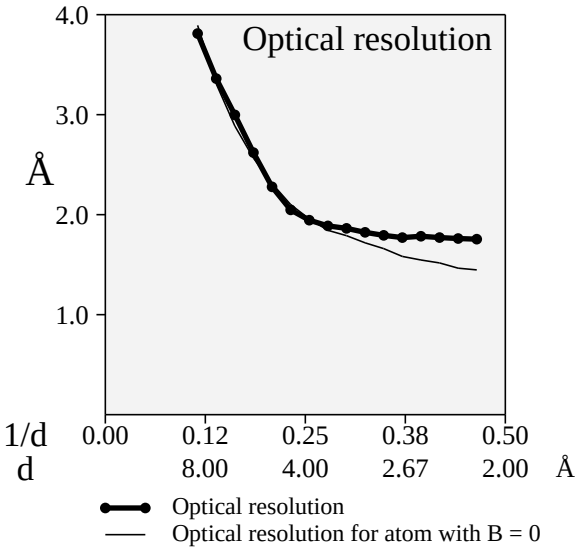
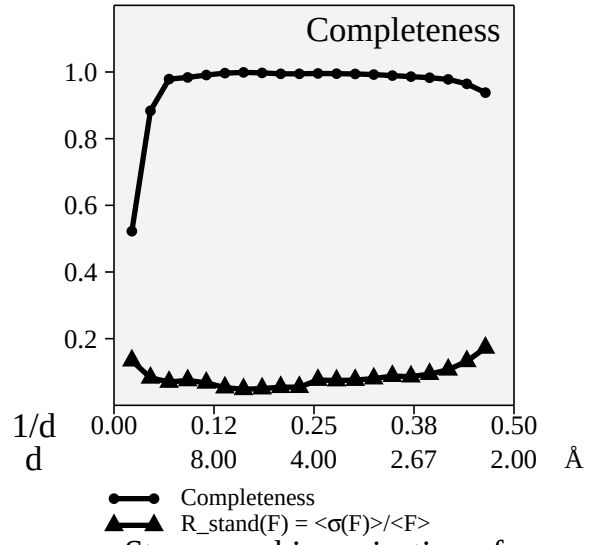
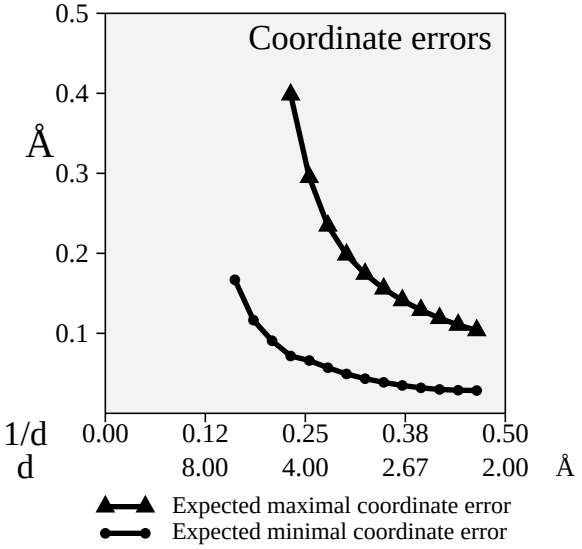
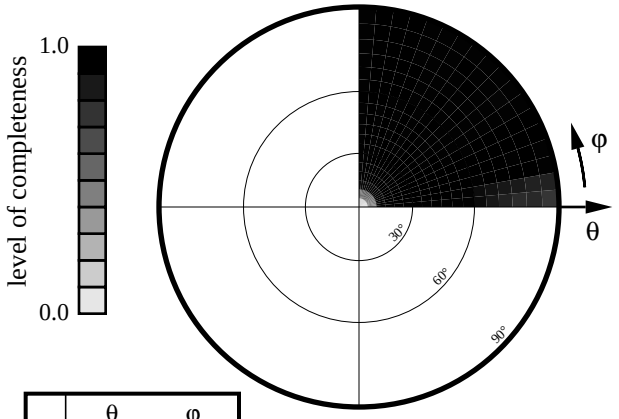






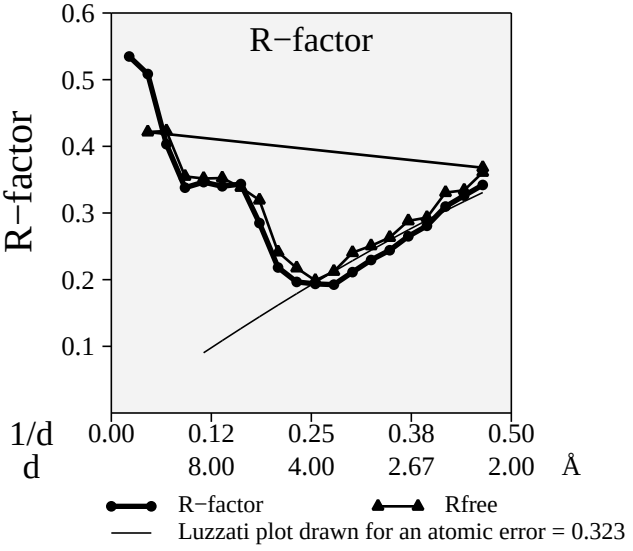


Stereographic projection of
the averaged radial completeness



	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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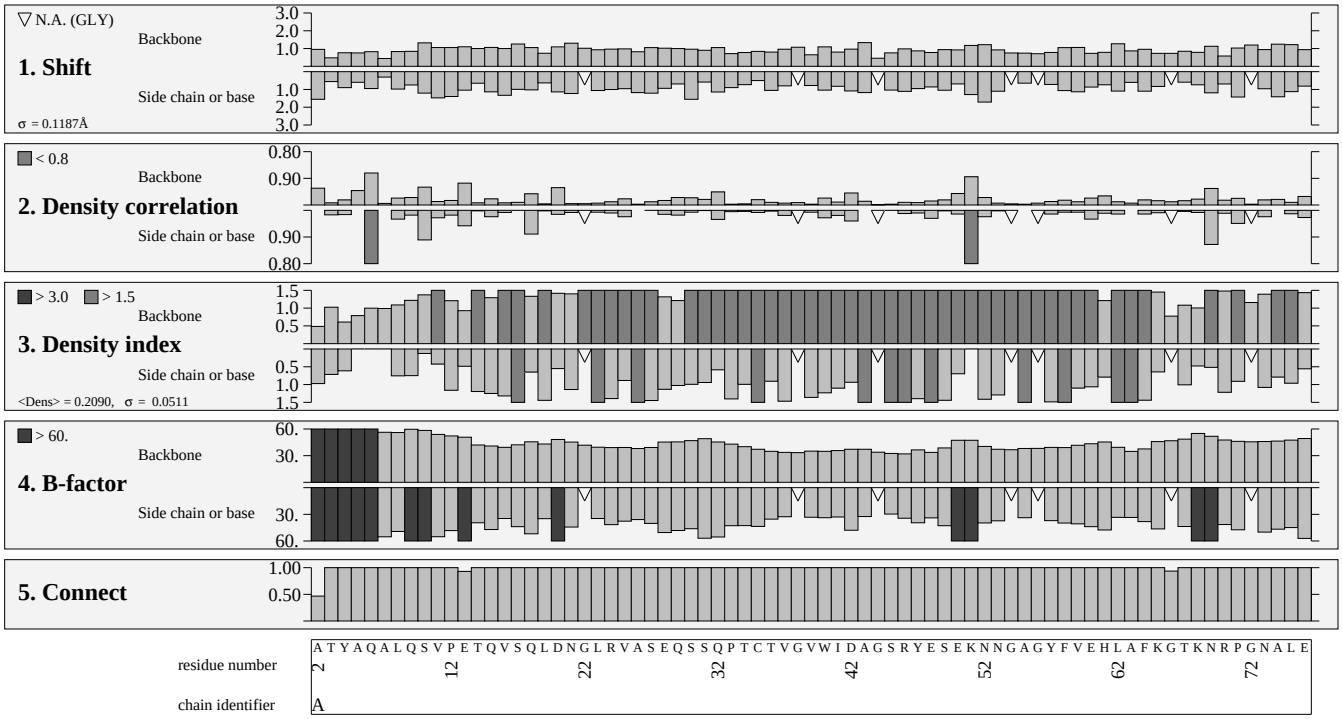
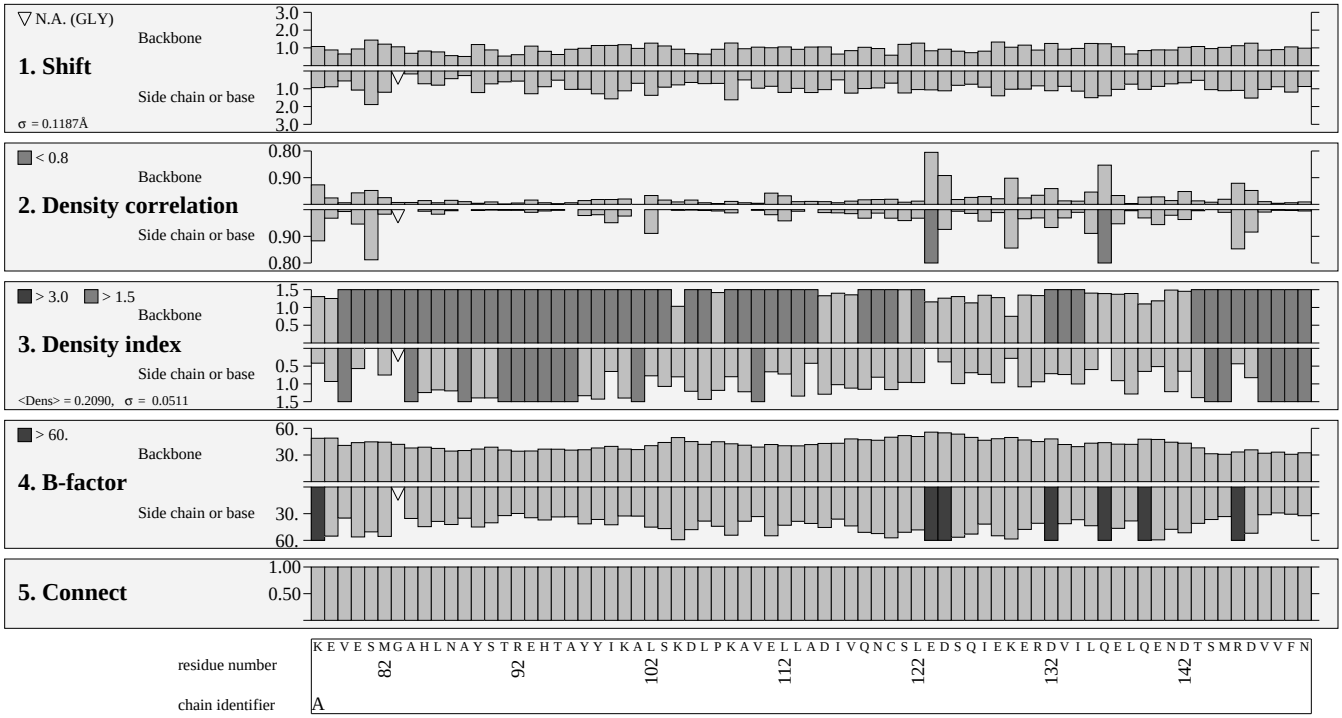
Local estimation





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Structure Factor Check

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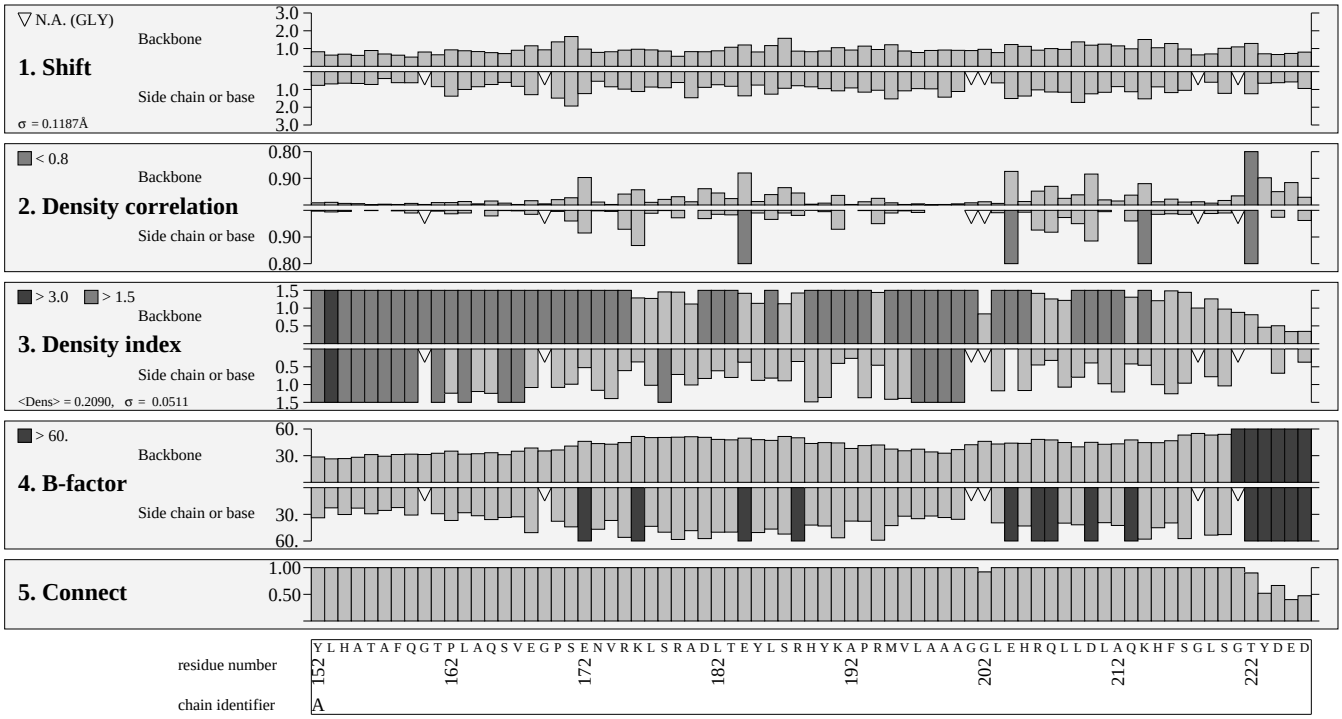
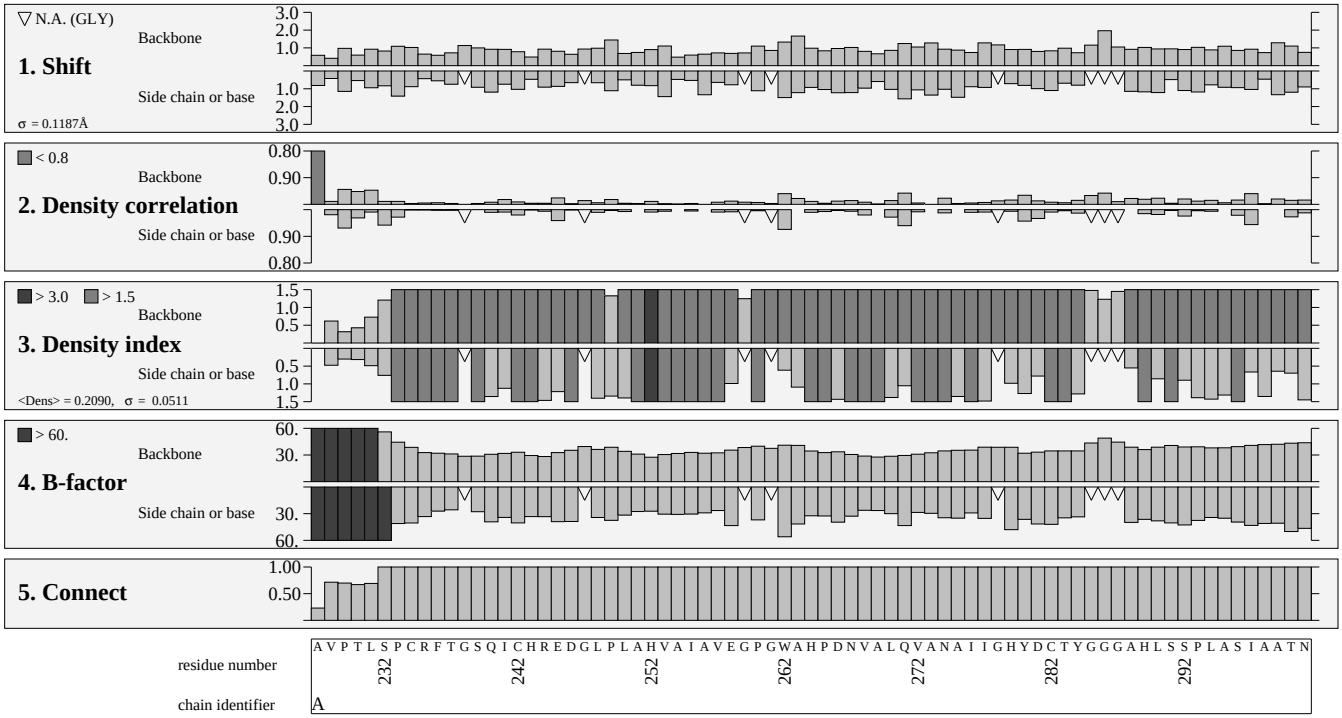
Local estimation (2)





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Structure Factor Check

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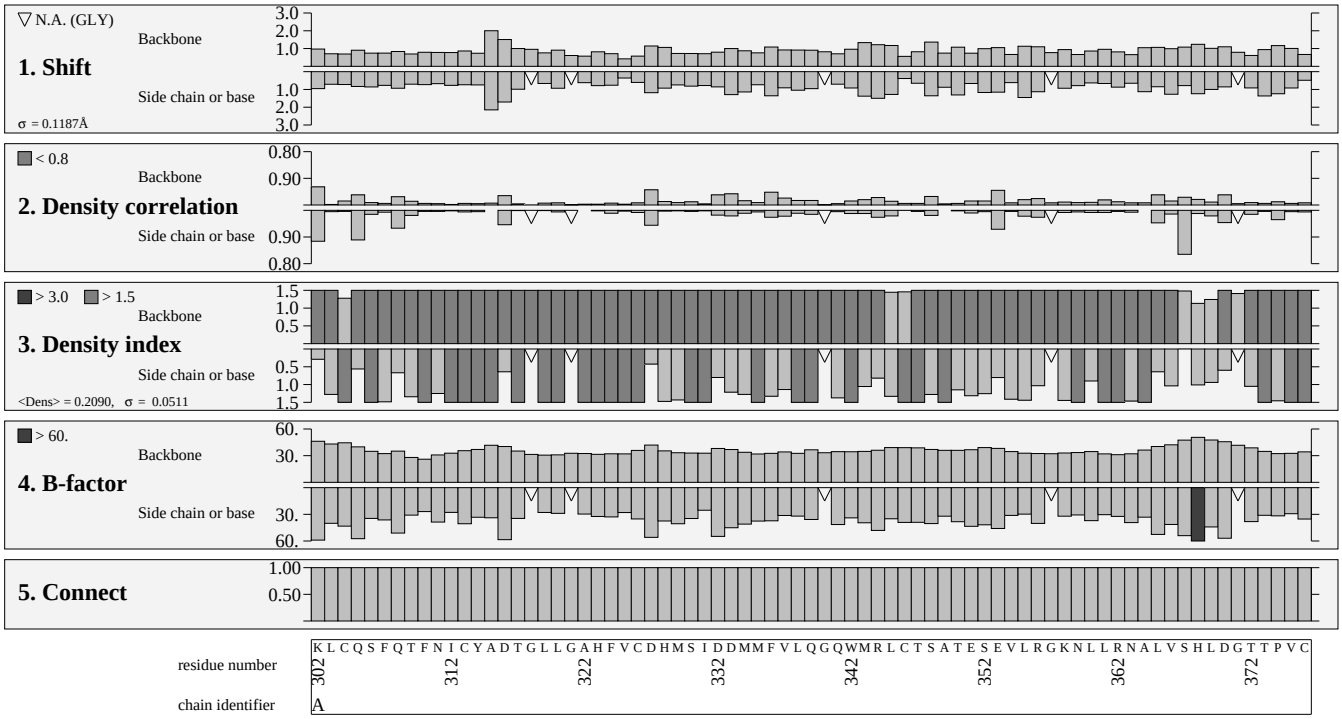
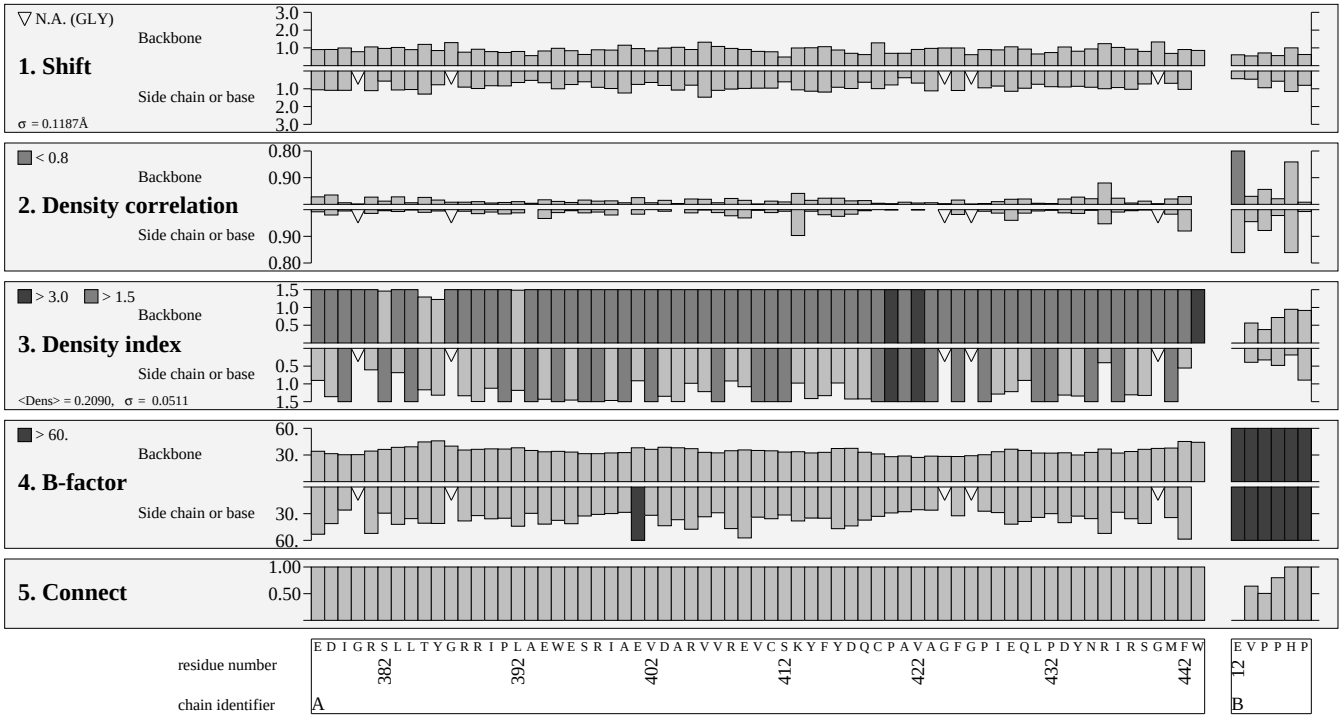
Local estimation (3)





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Structure Factor Check

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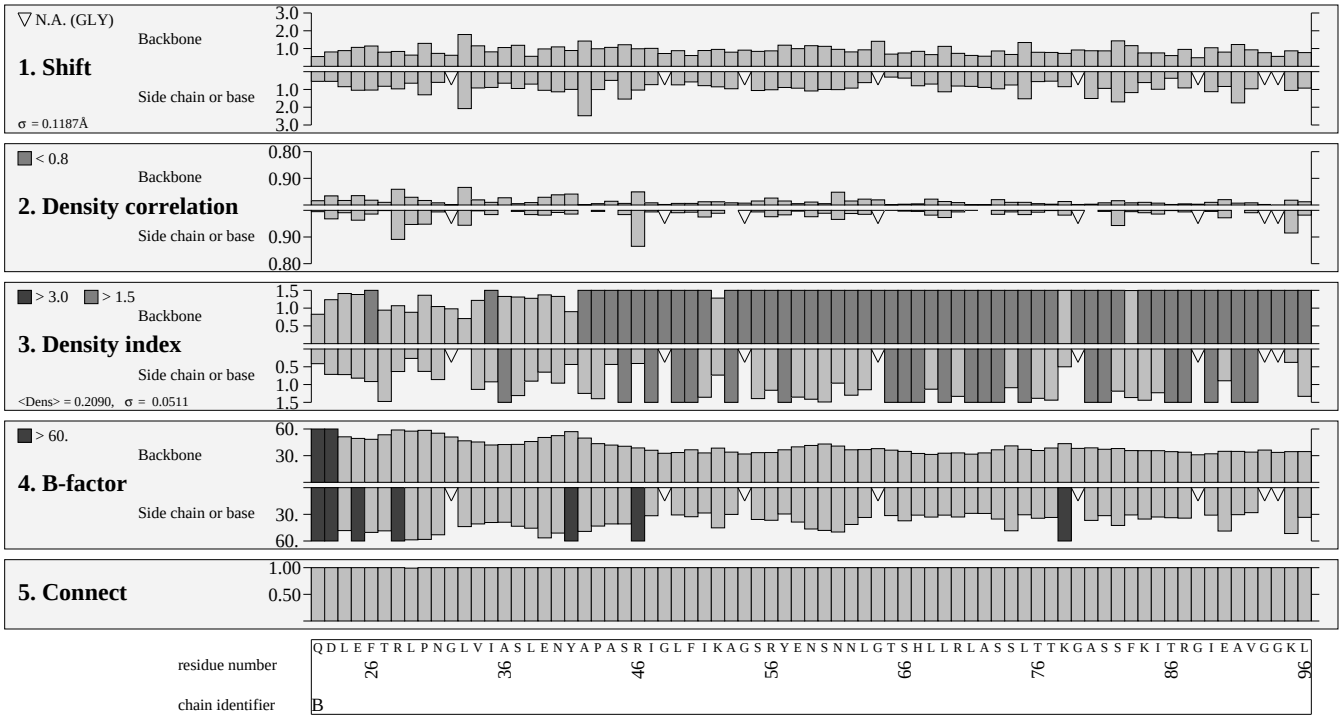
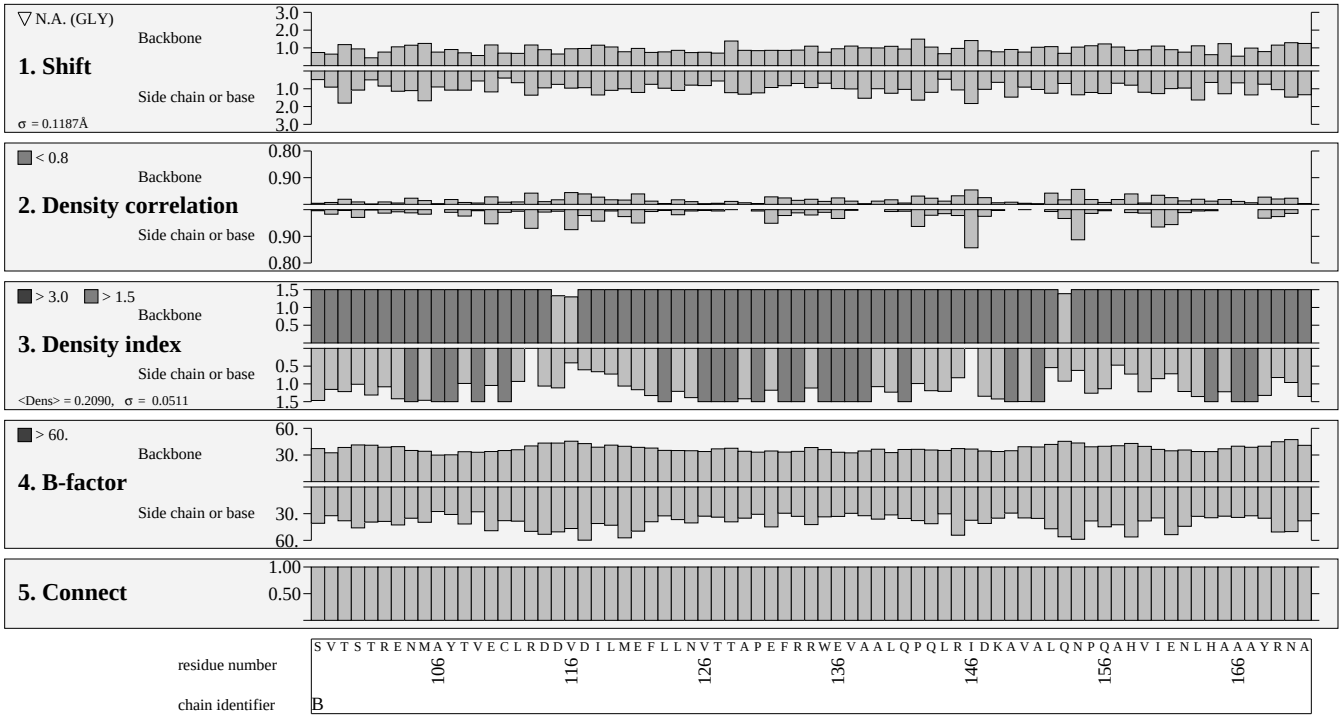
Local estimation (4)





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Structure Factor Check

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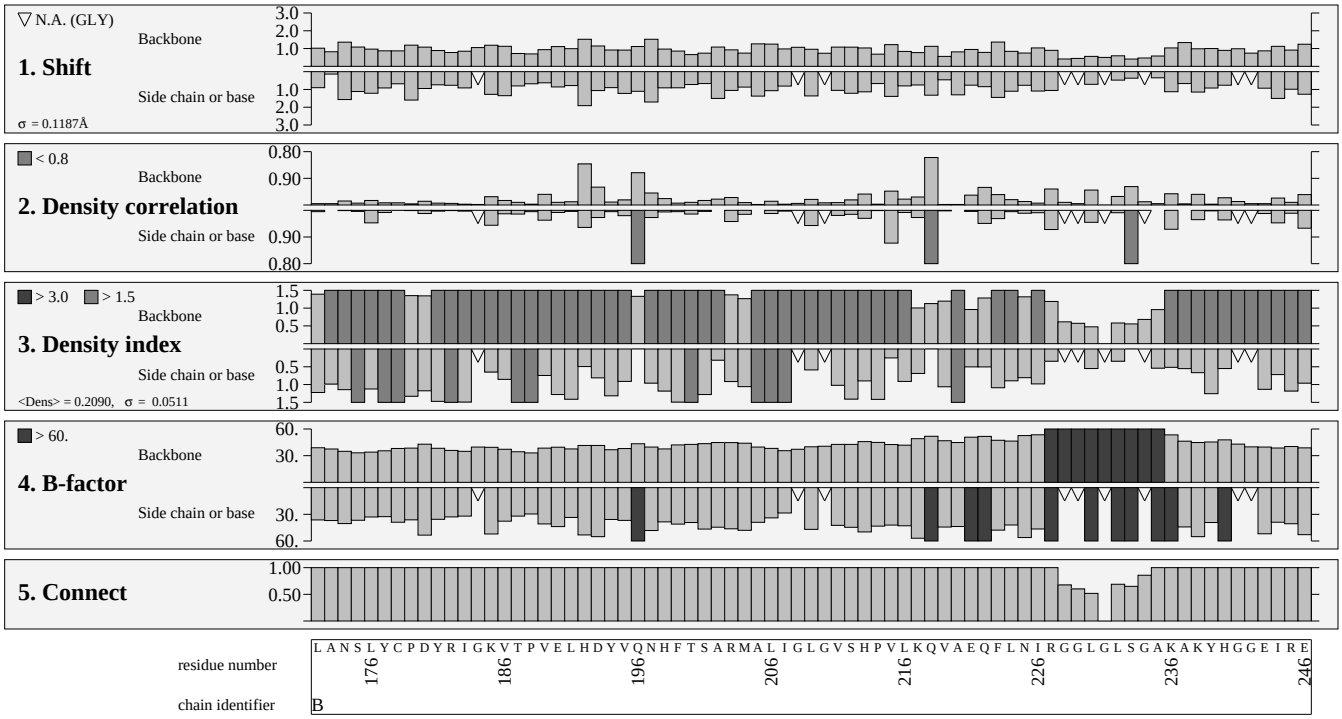
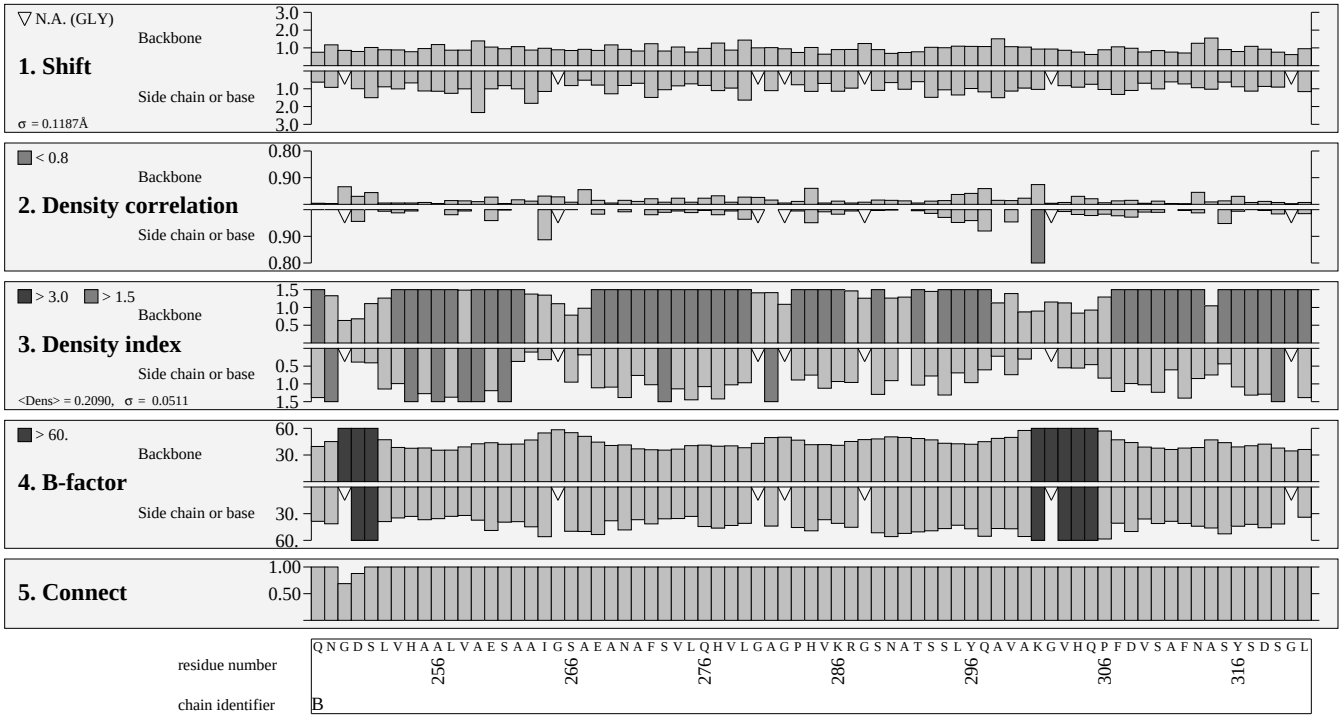
Local estimation (5)





SFCHECK 6.0.5

Structure Factor Check

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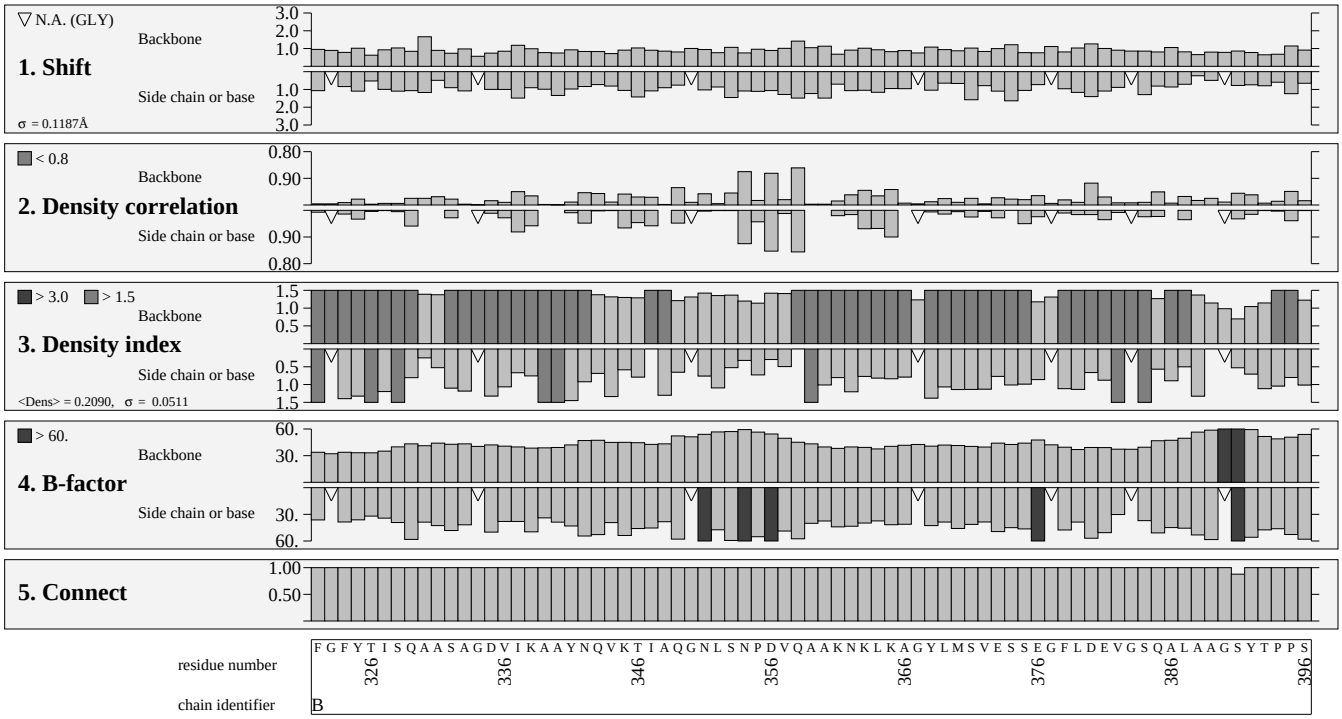
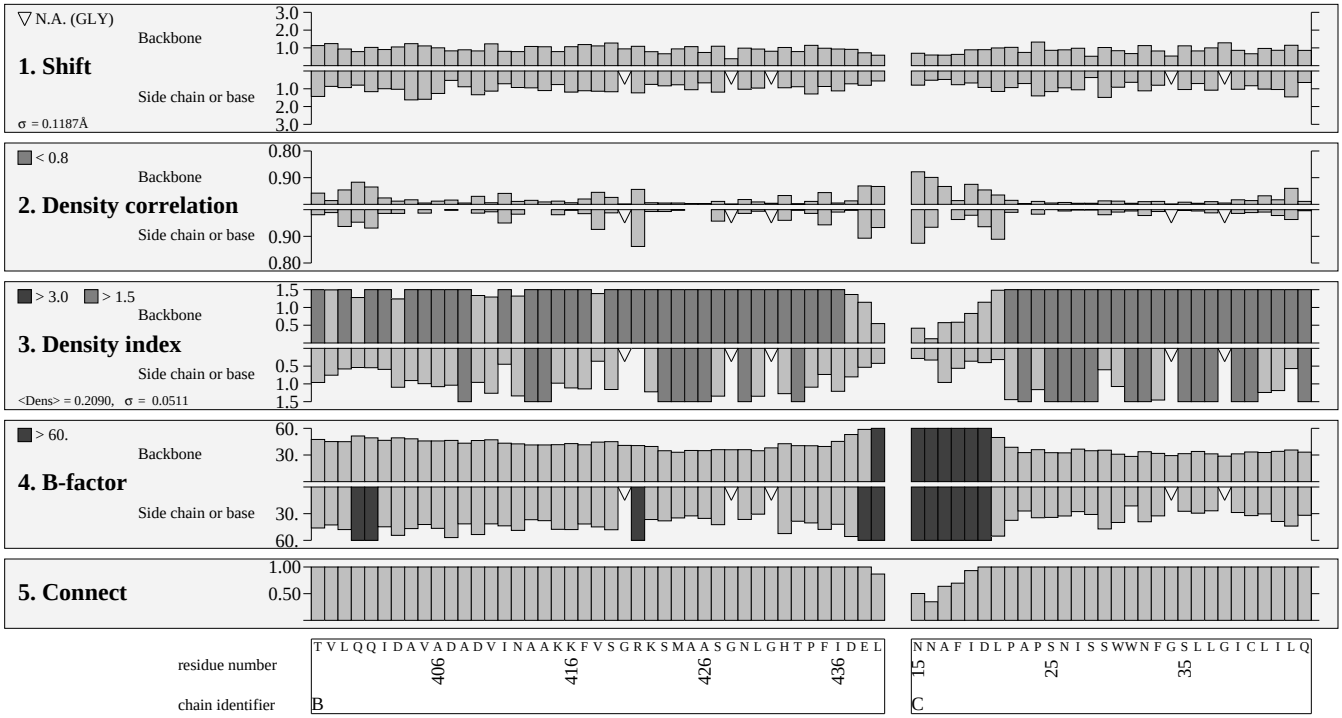
Local estimation (6)





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Structure Factor Check

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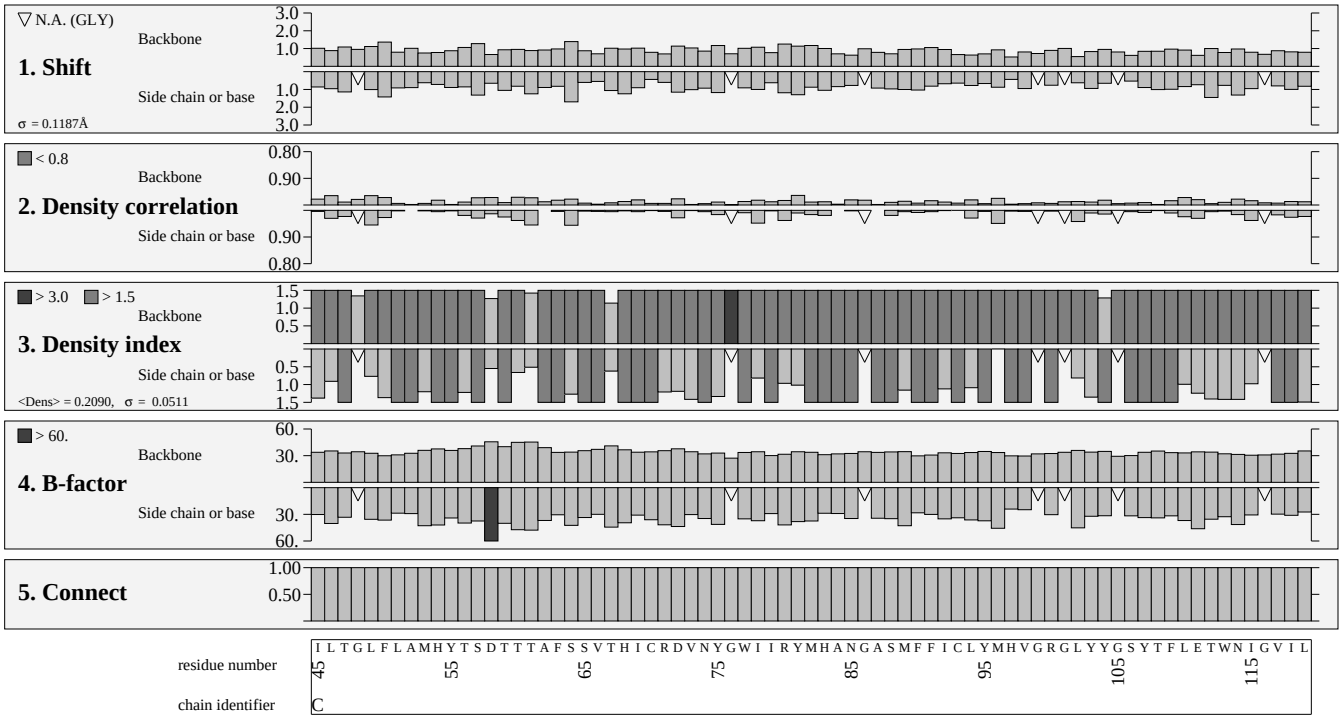
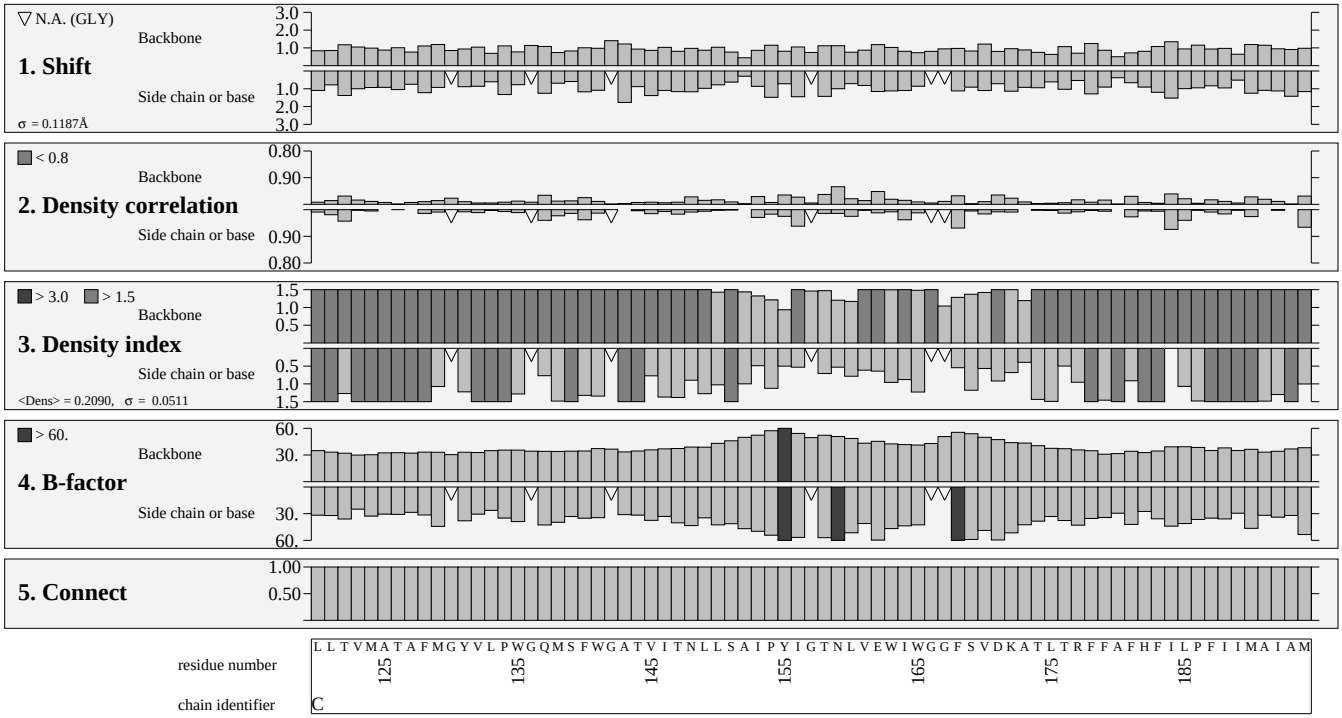
Local estimation (7)





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Structure Factor Check

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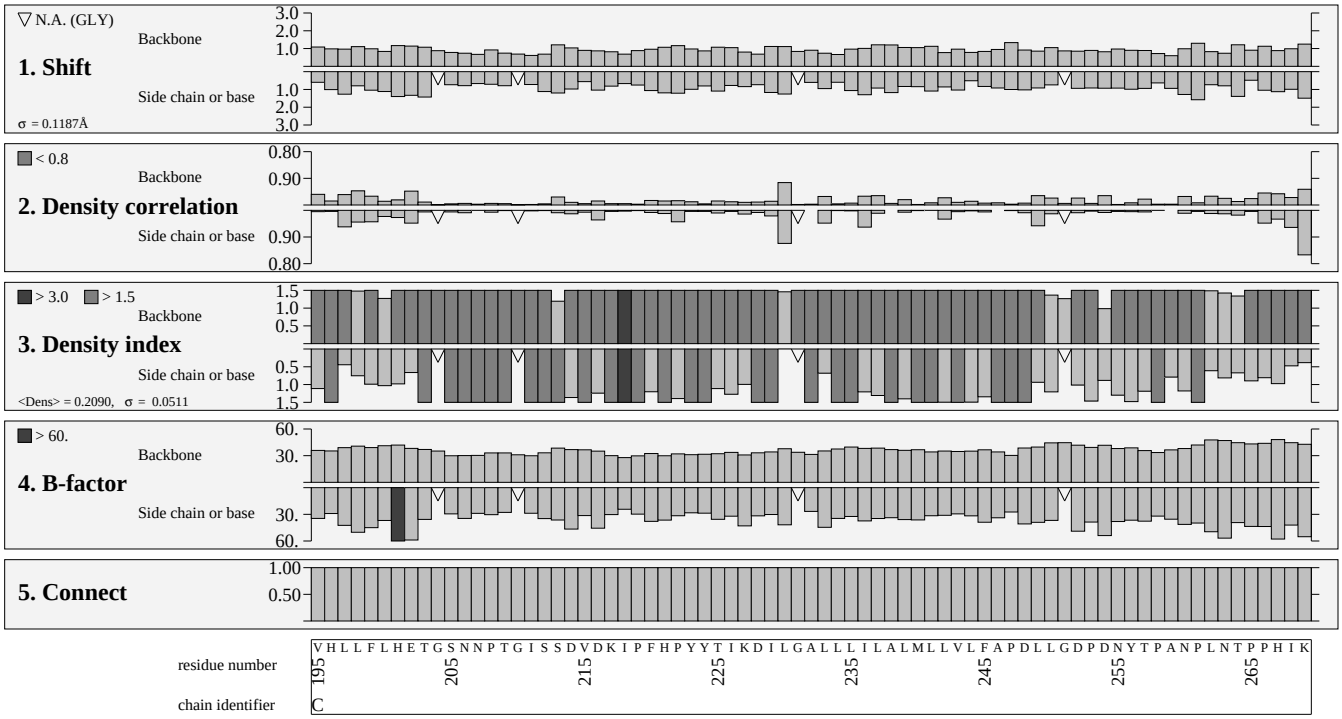
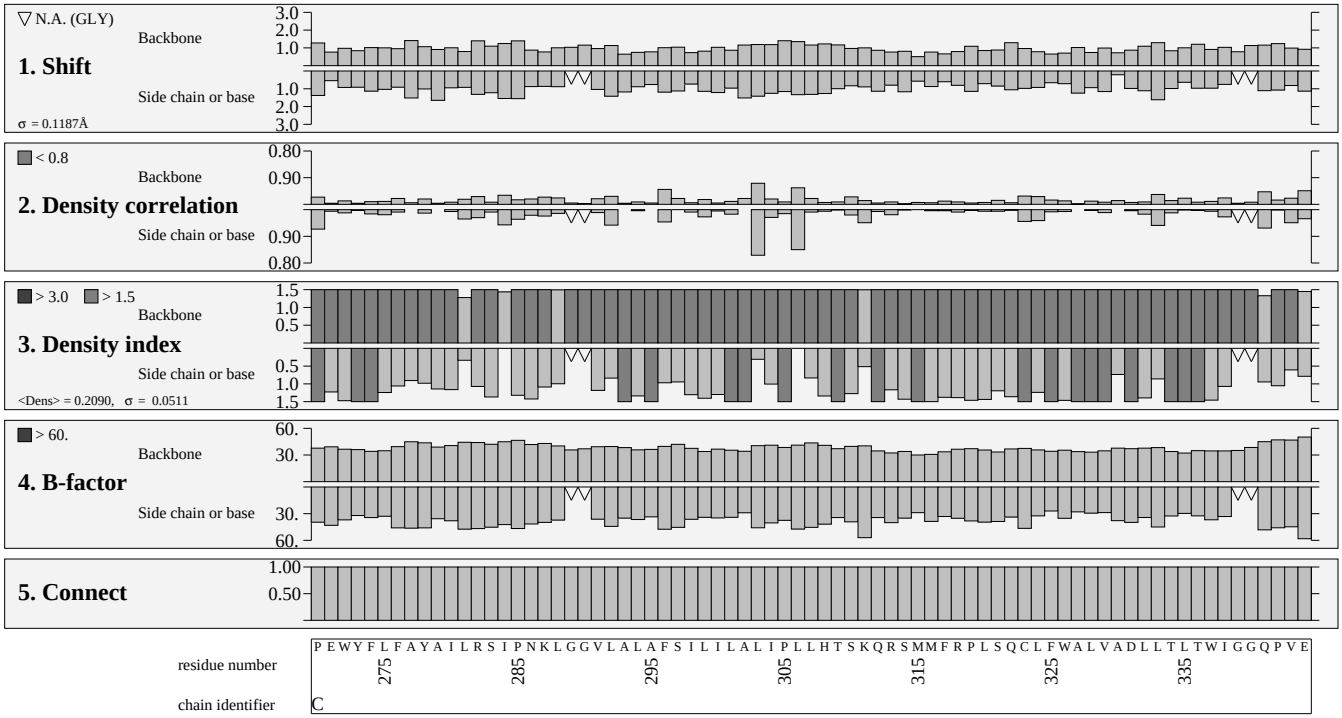
Local estimation (8)





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Structure Factor Check

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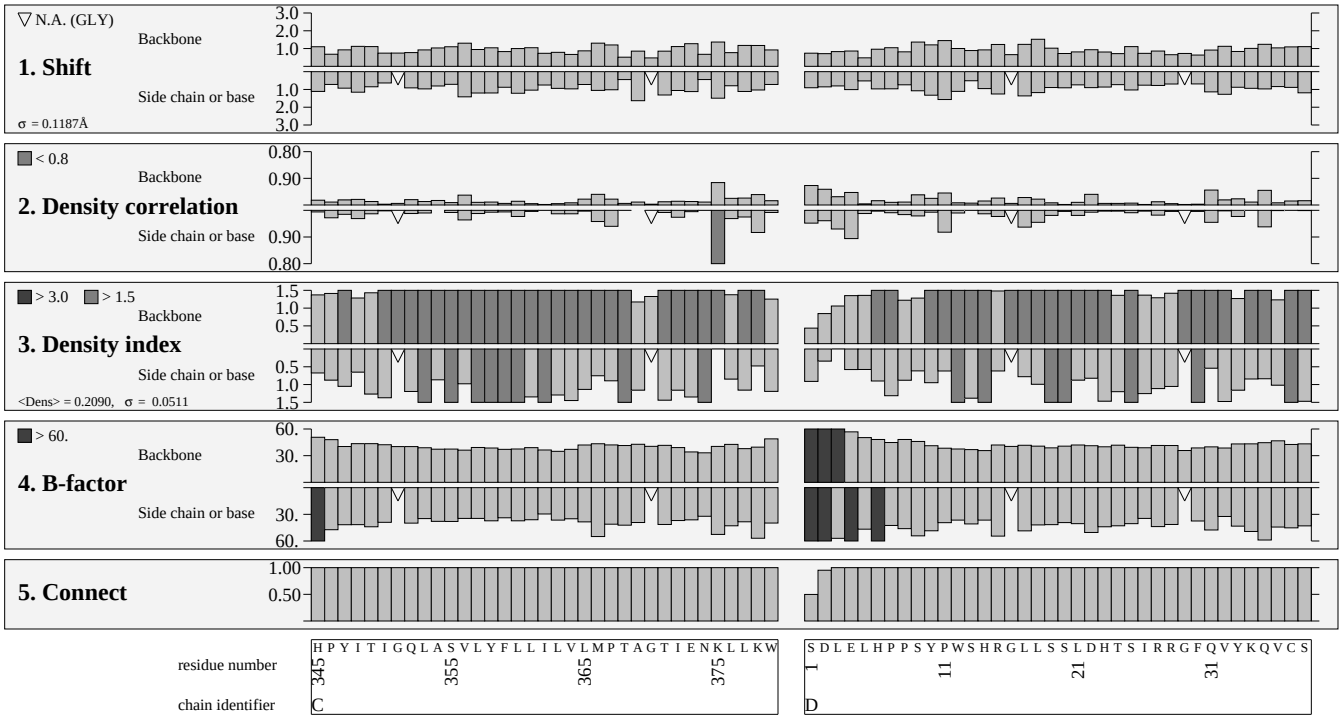
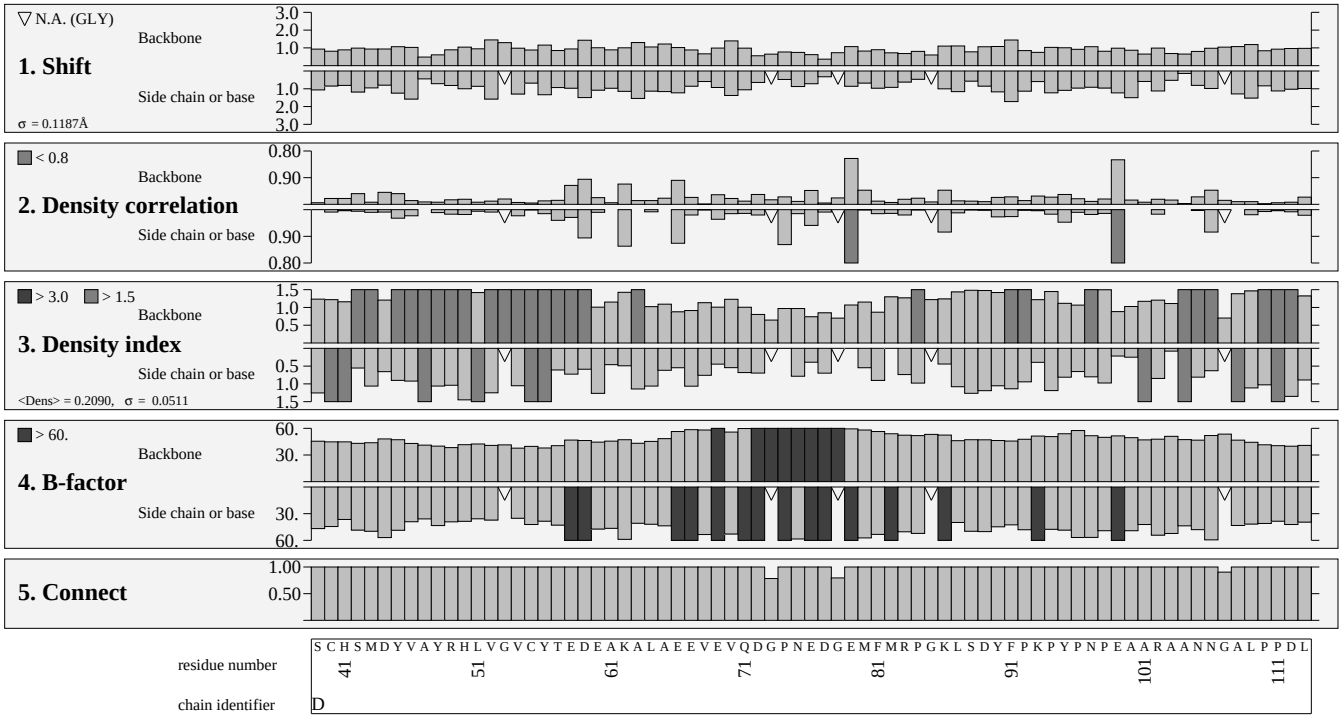
Local estimation (9)





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Structure Factor Check

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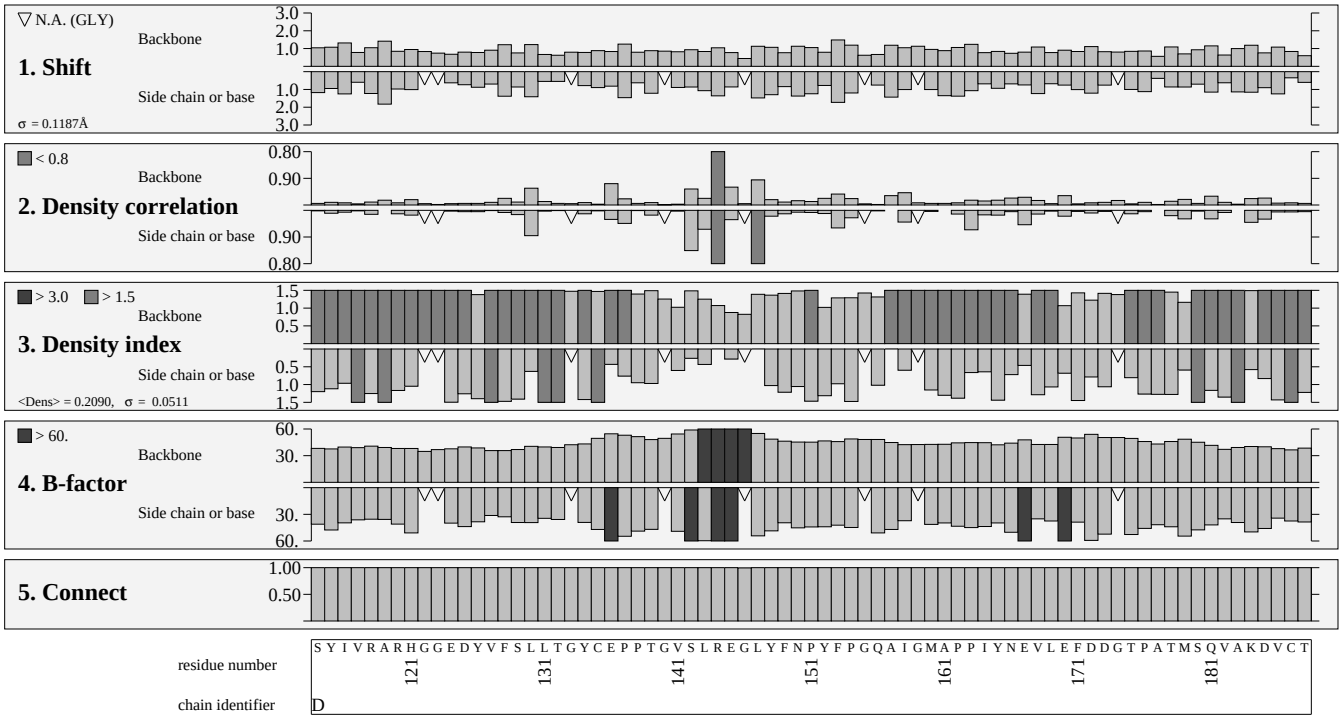
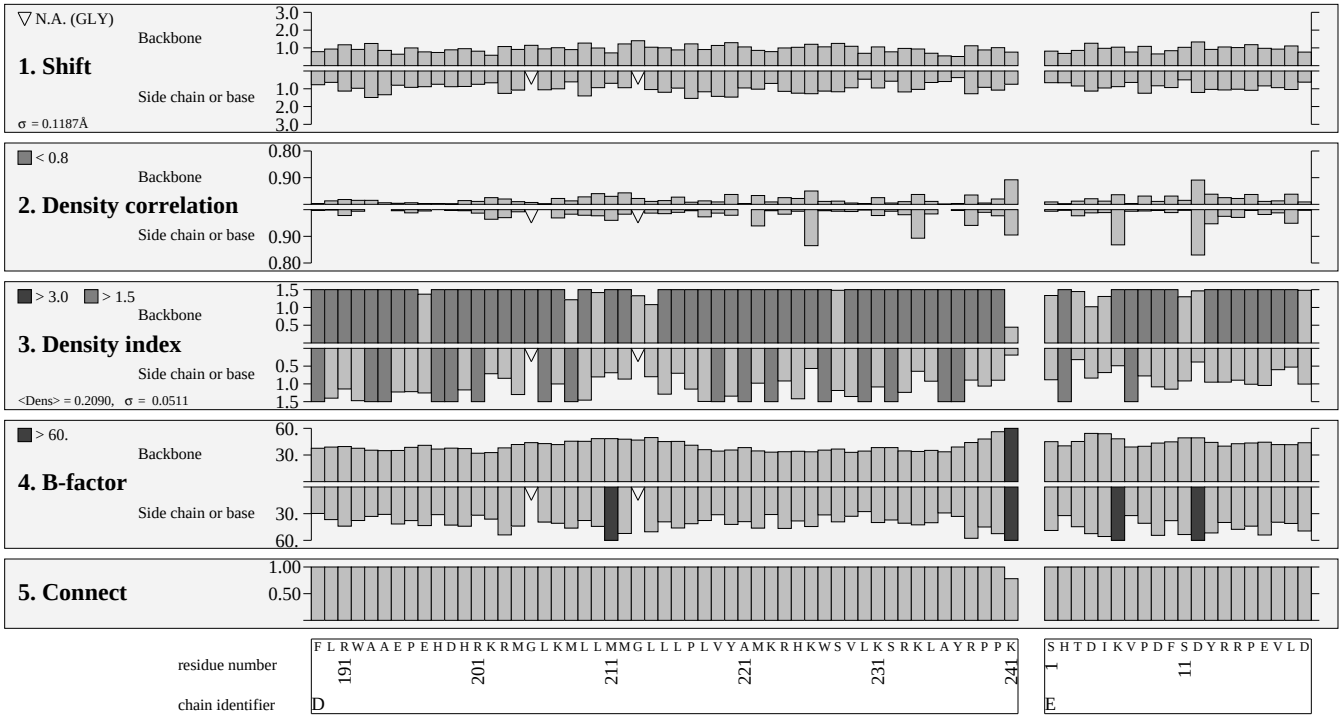
Local estimation (10)





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Structure Factor Check

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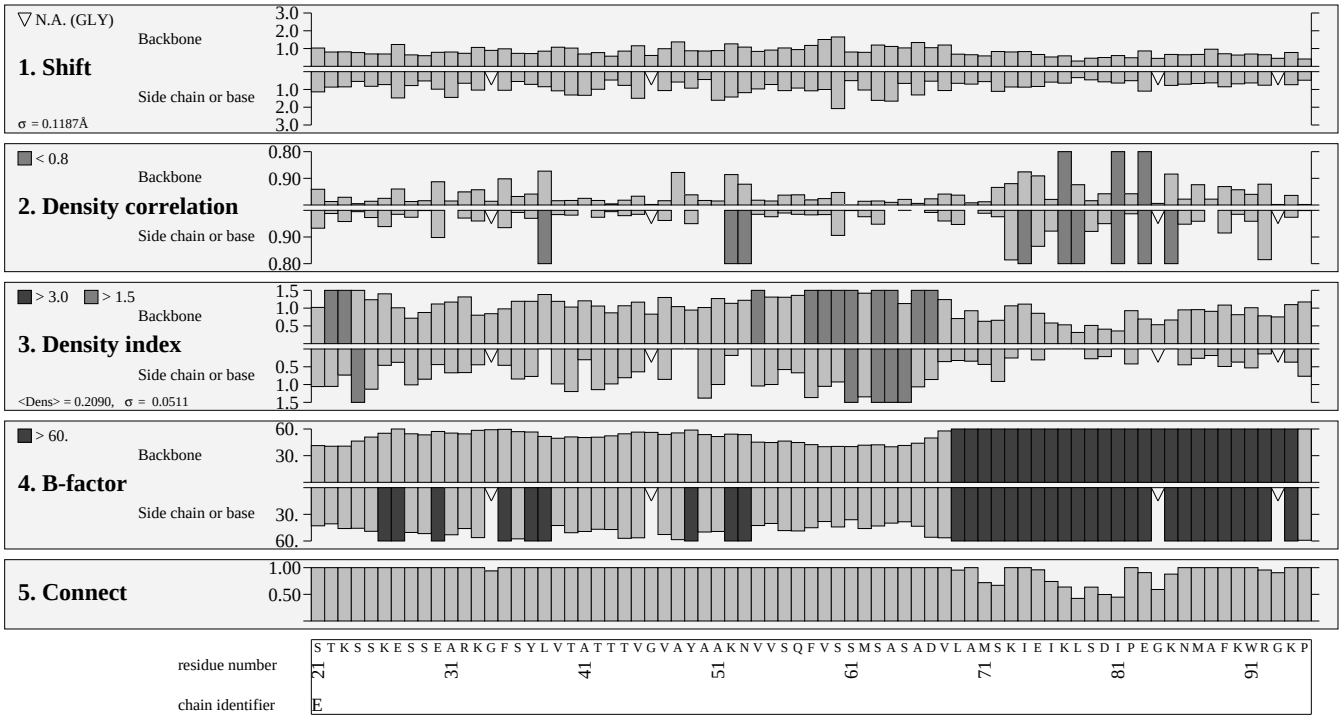
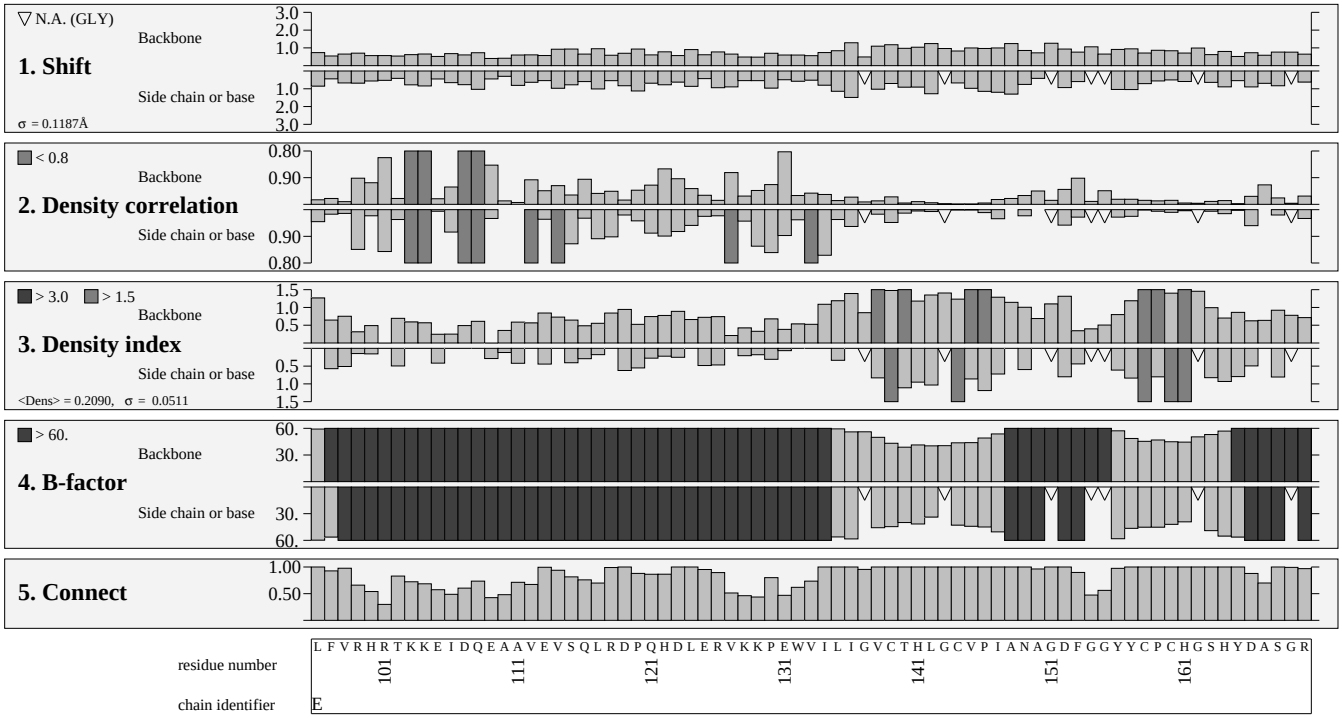
Local estimation (11)





SFCHECK 6.0.5

Structure Factor Check

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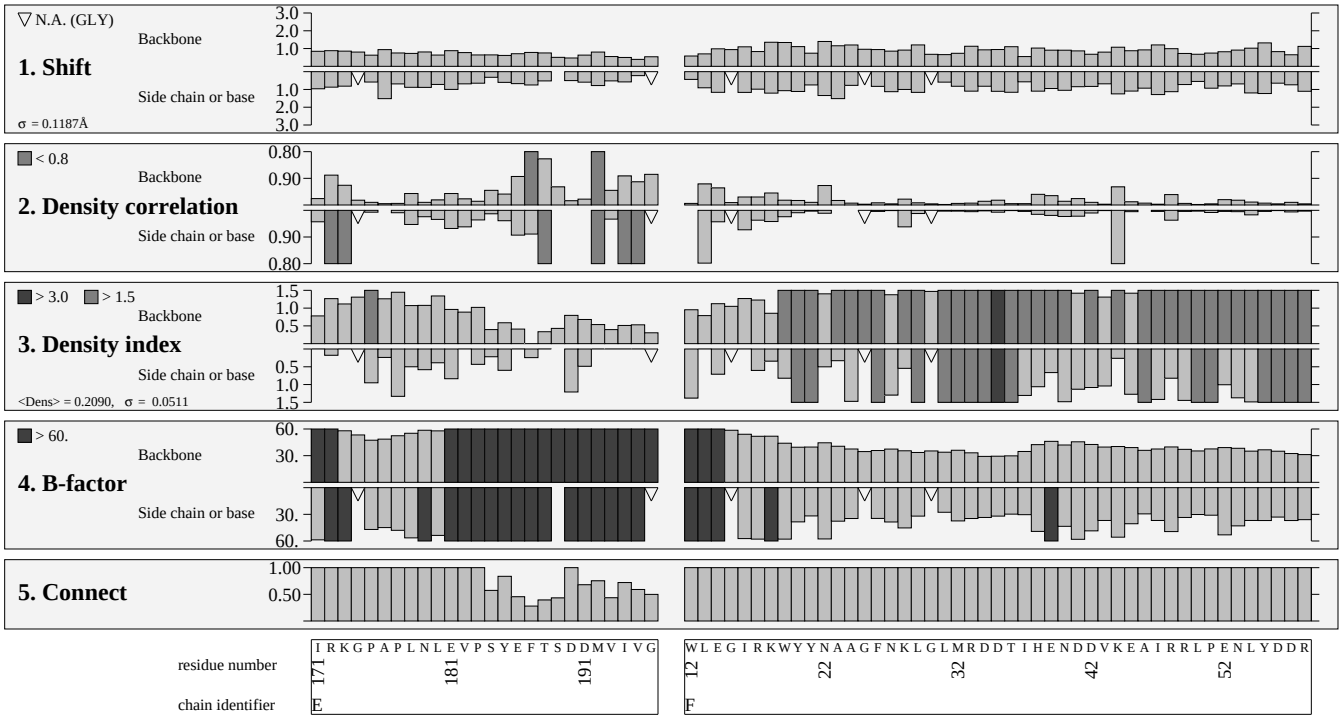
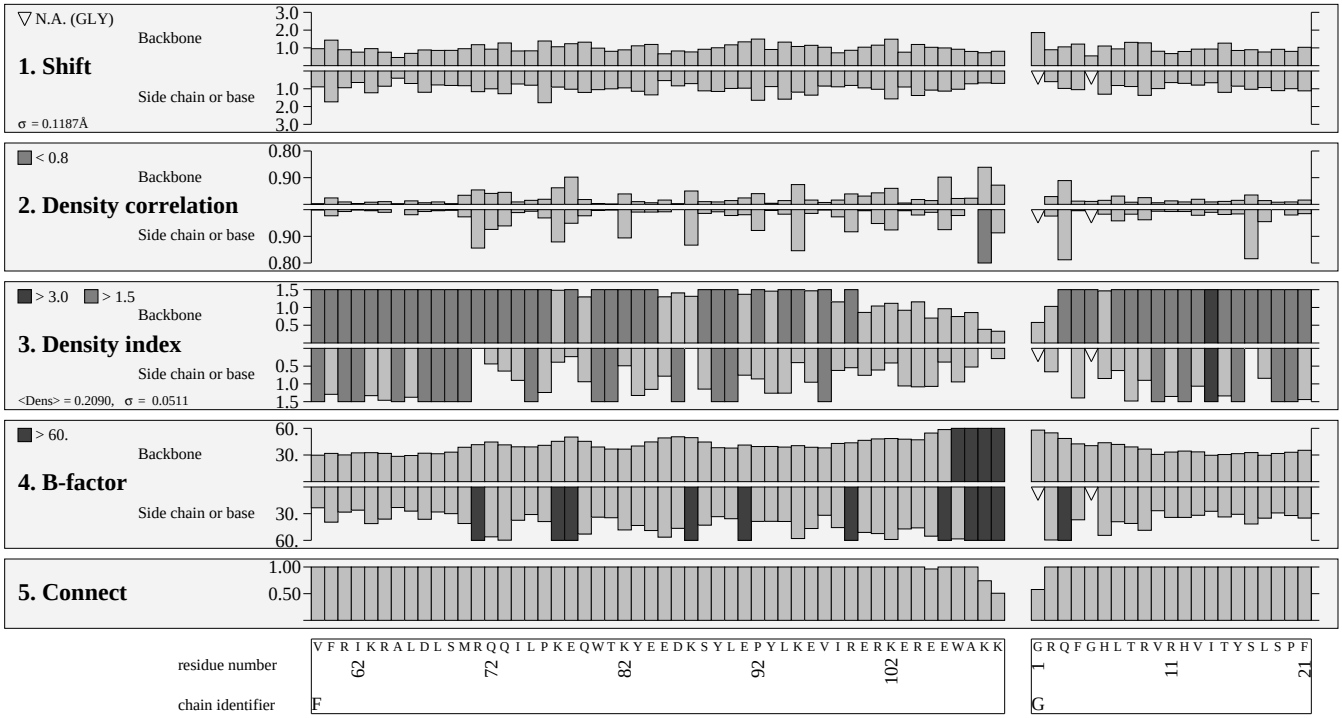
Local estimation (12)





SFCHECK 6.0.5

Structure Factor Check

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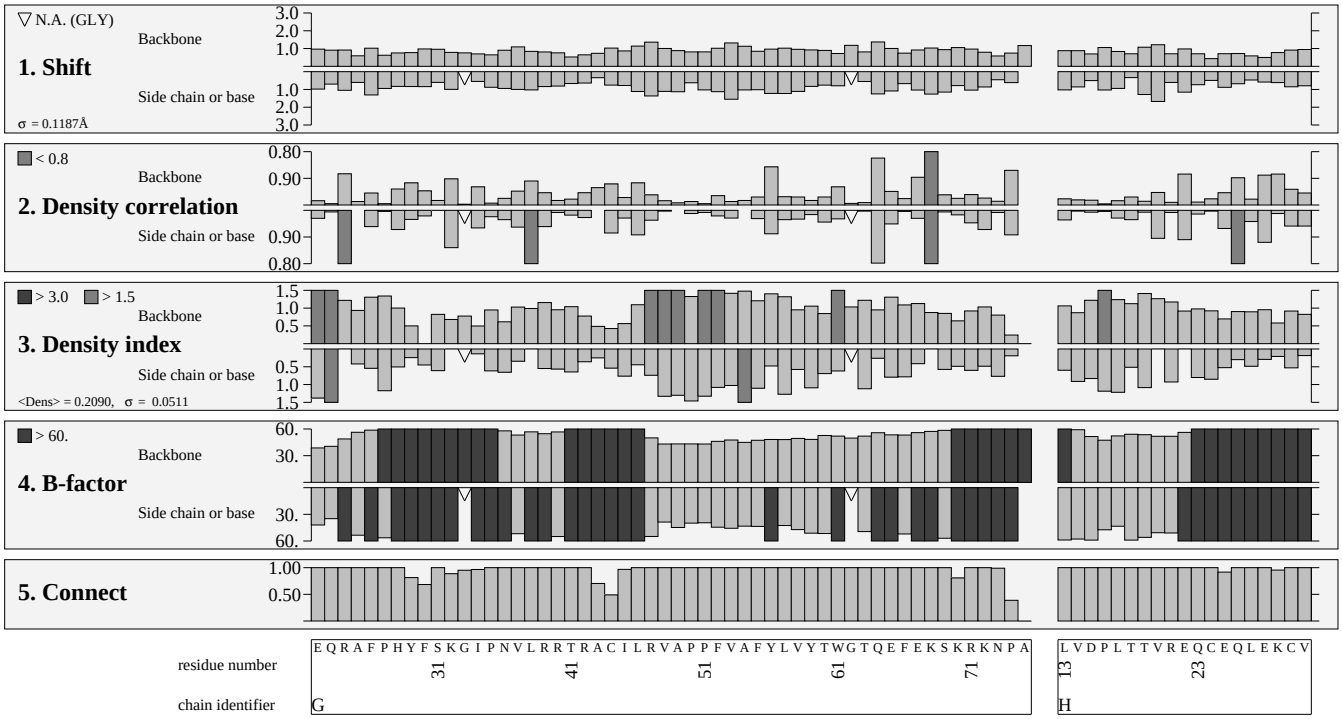
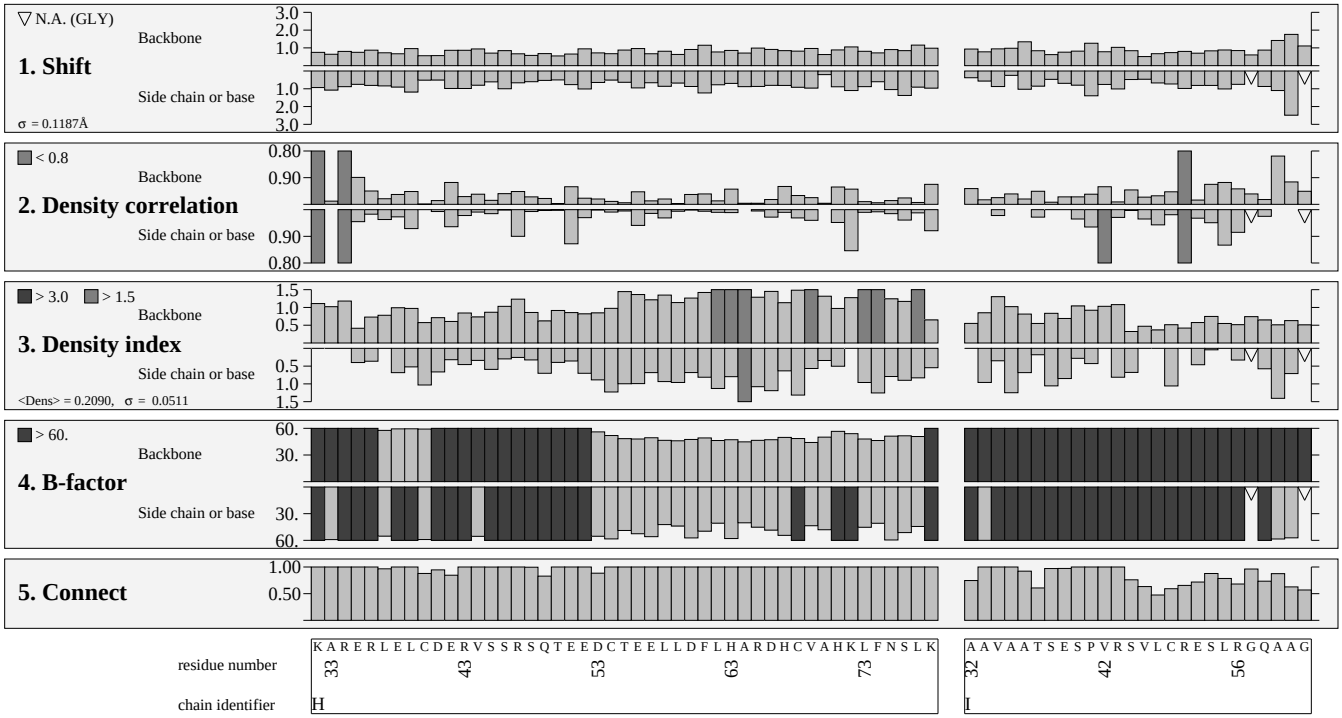
Local estimation (13)





SFCHECK 6.0.5

Structure Factor Check

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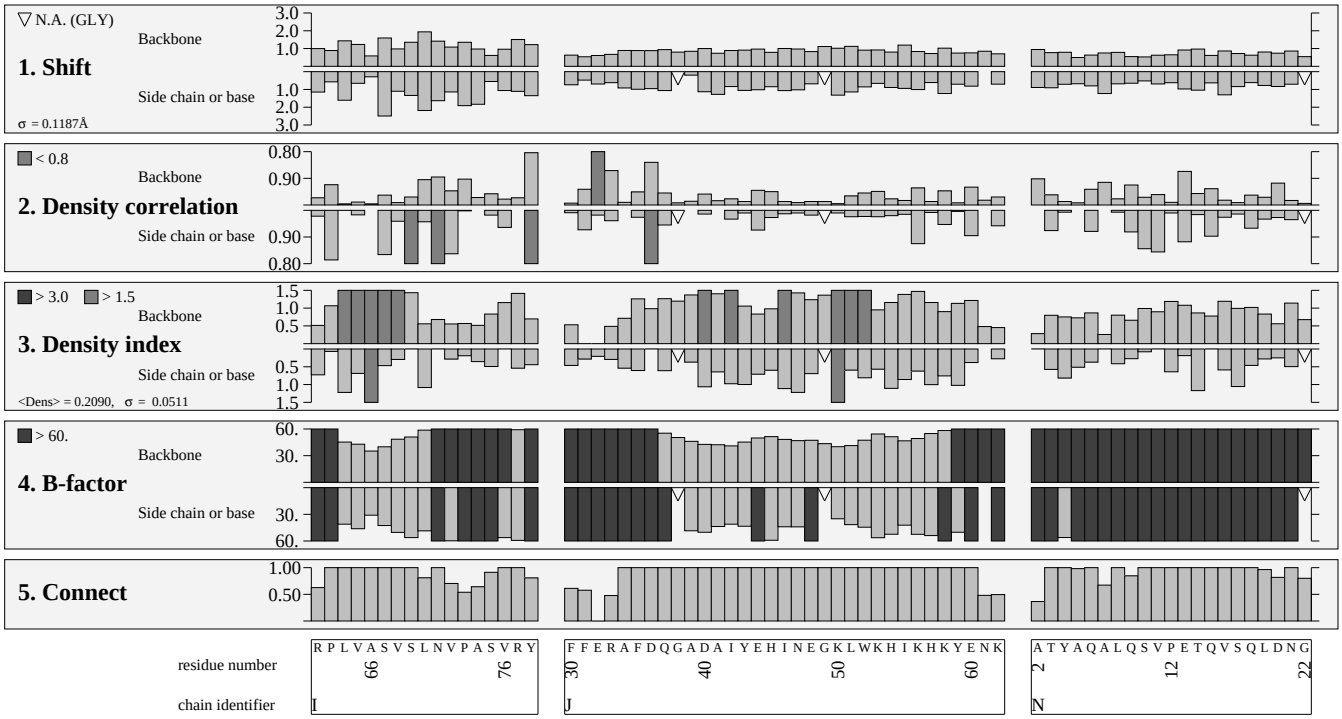
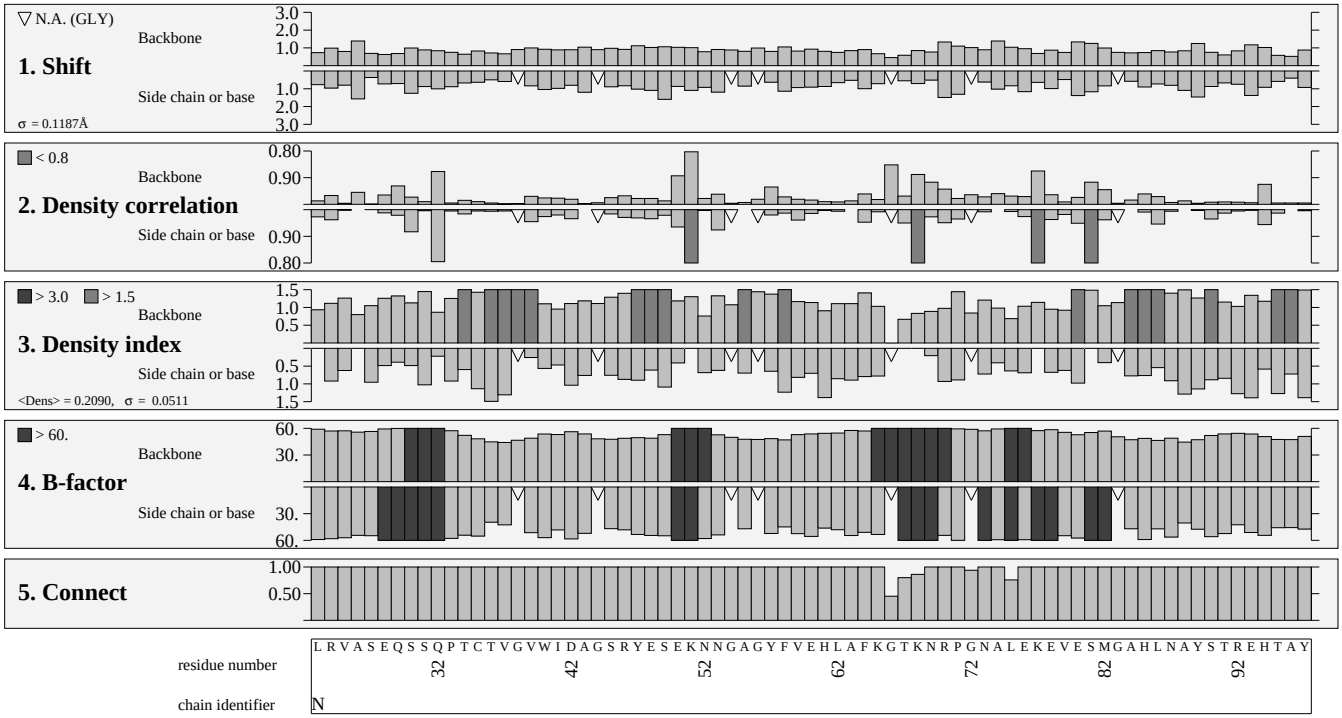
Local estimation (14)





SFCHECK 6.0.5

Structure Factor Check

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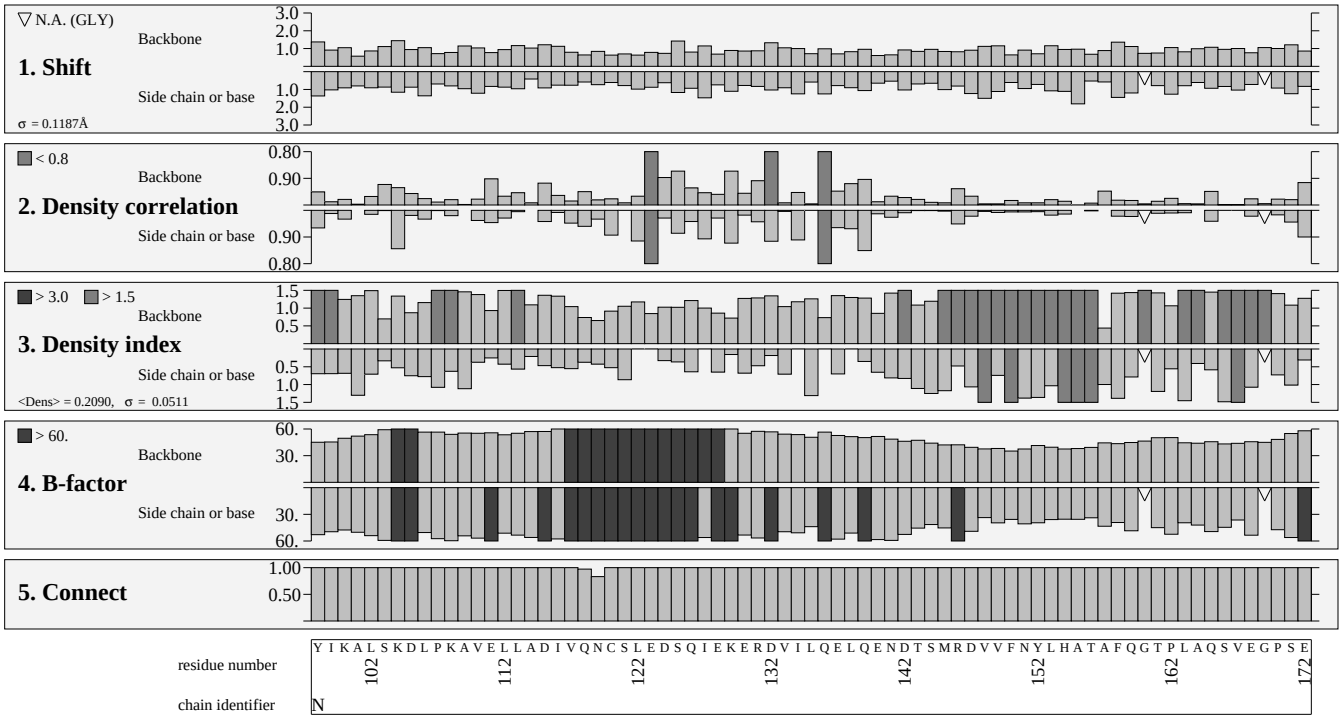
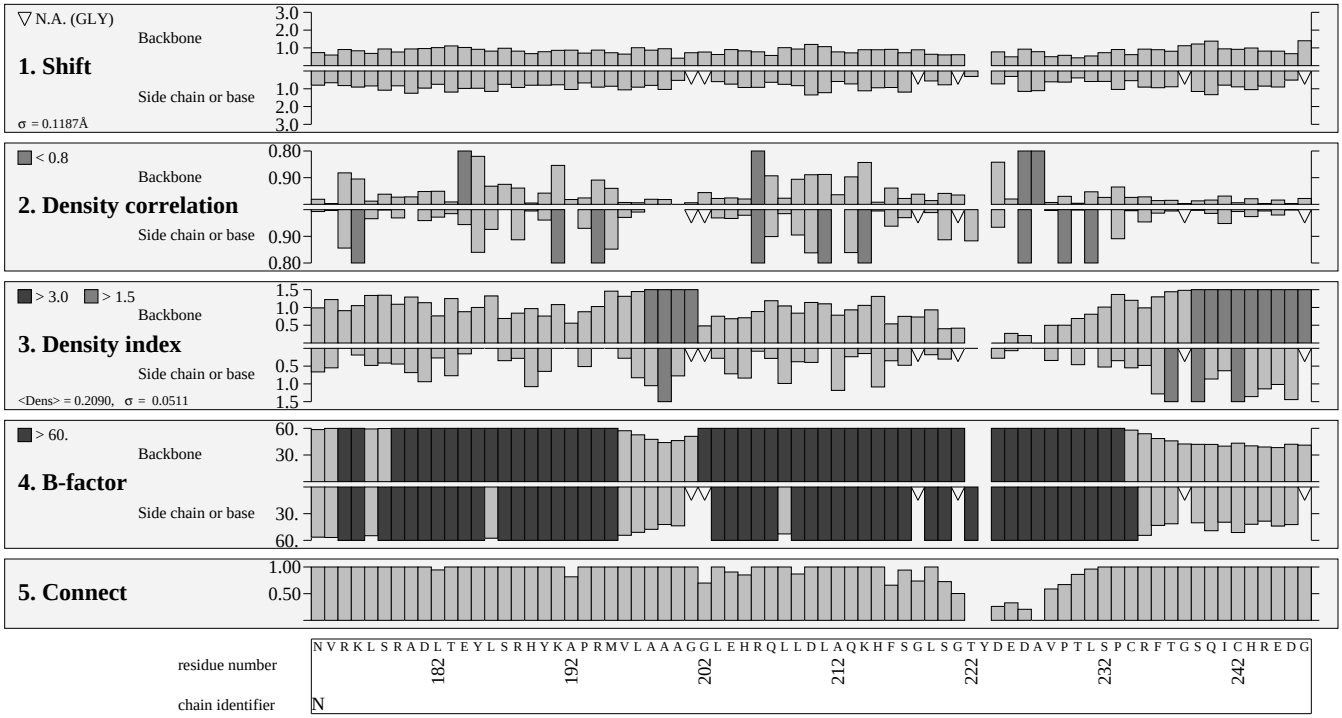
Local estimation (15)





SFCHECK 6.0.5

Structure Factor Check

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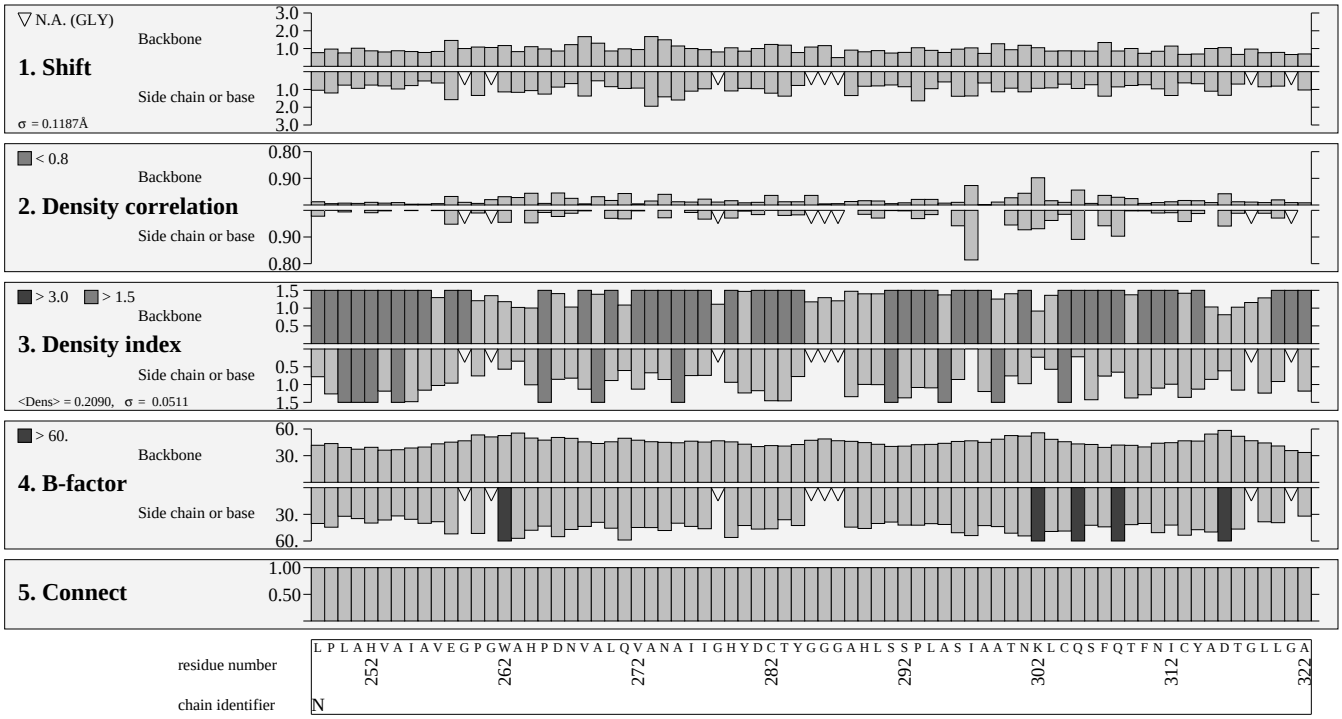
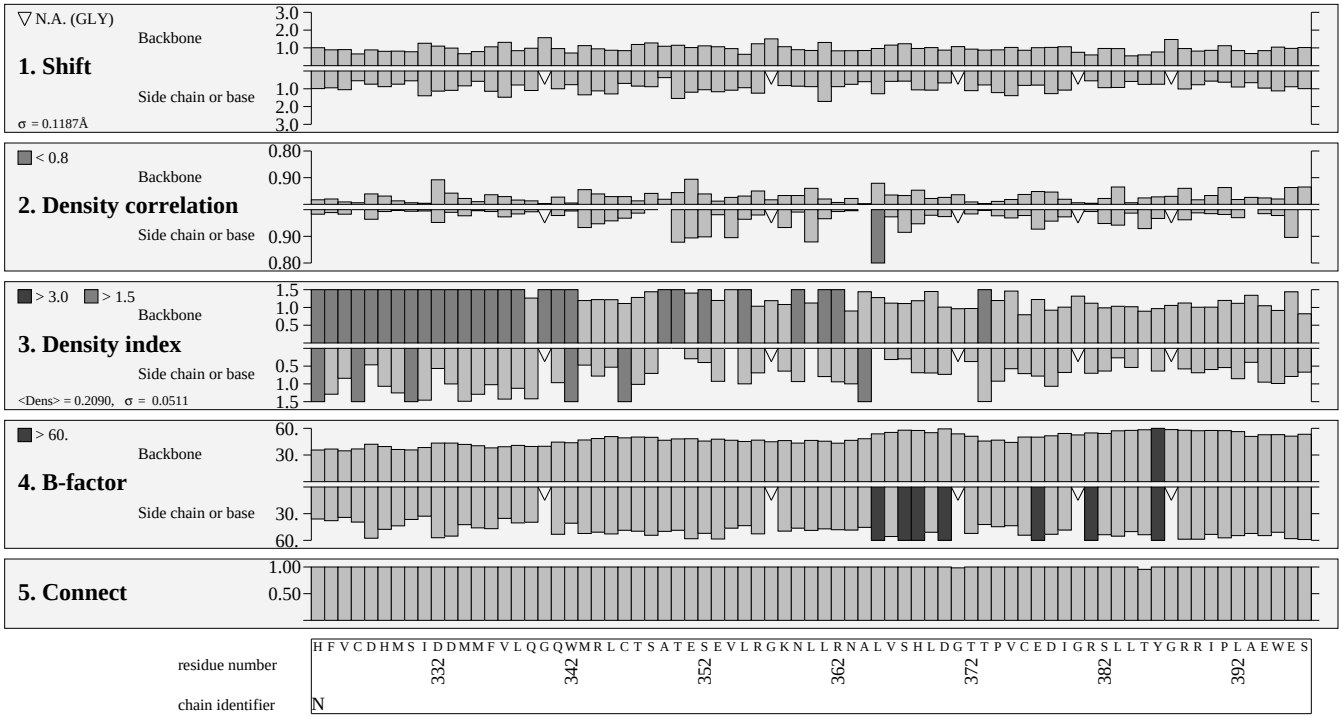
Local estimation (16)





SFCHECK 6.0.5

Structure Factor Check

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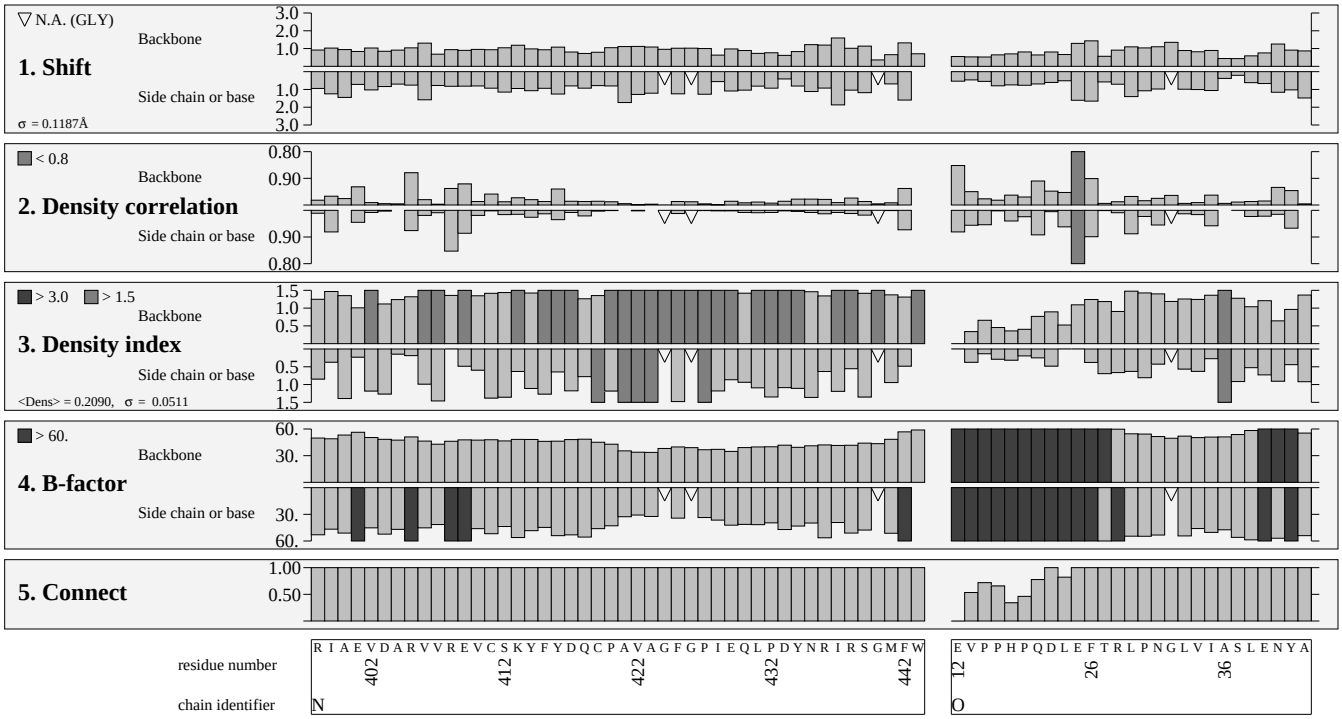
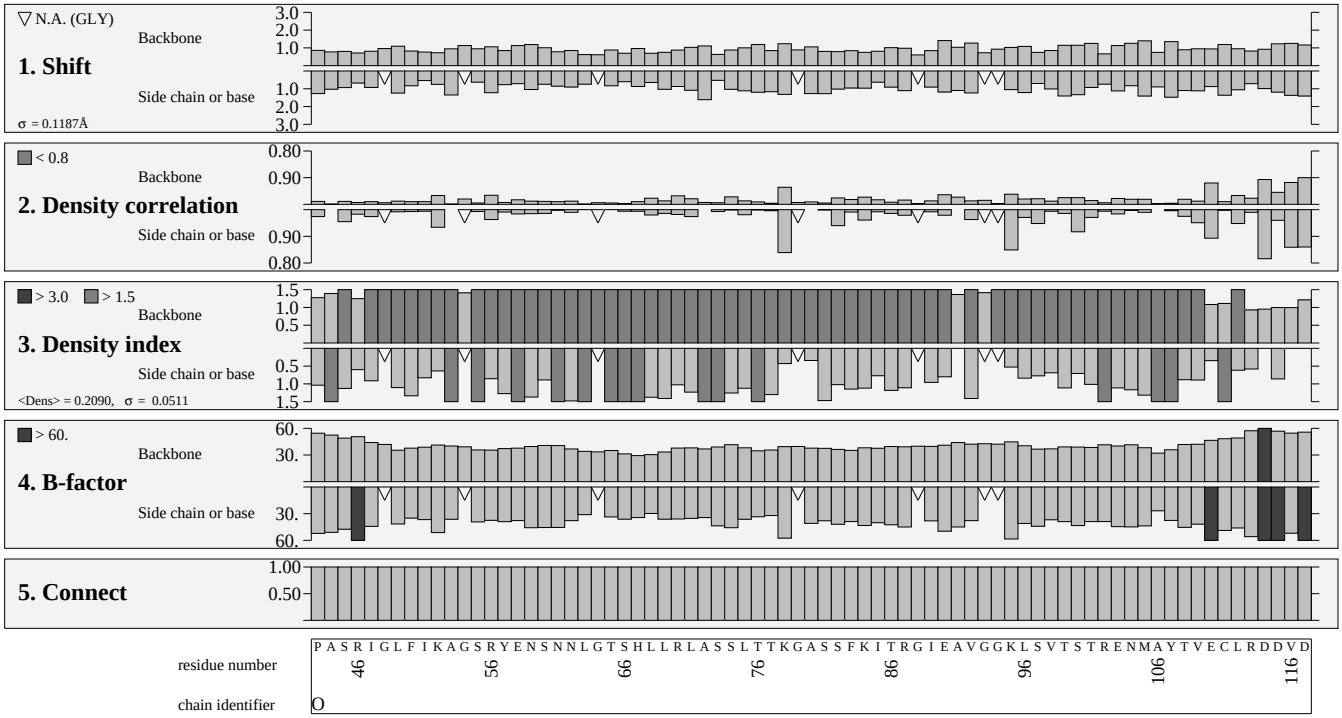
Local estimation (17)





SFCHECK 6.0.5

Structure Factor Check

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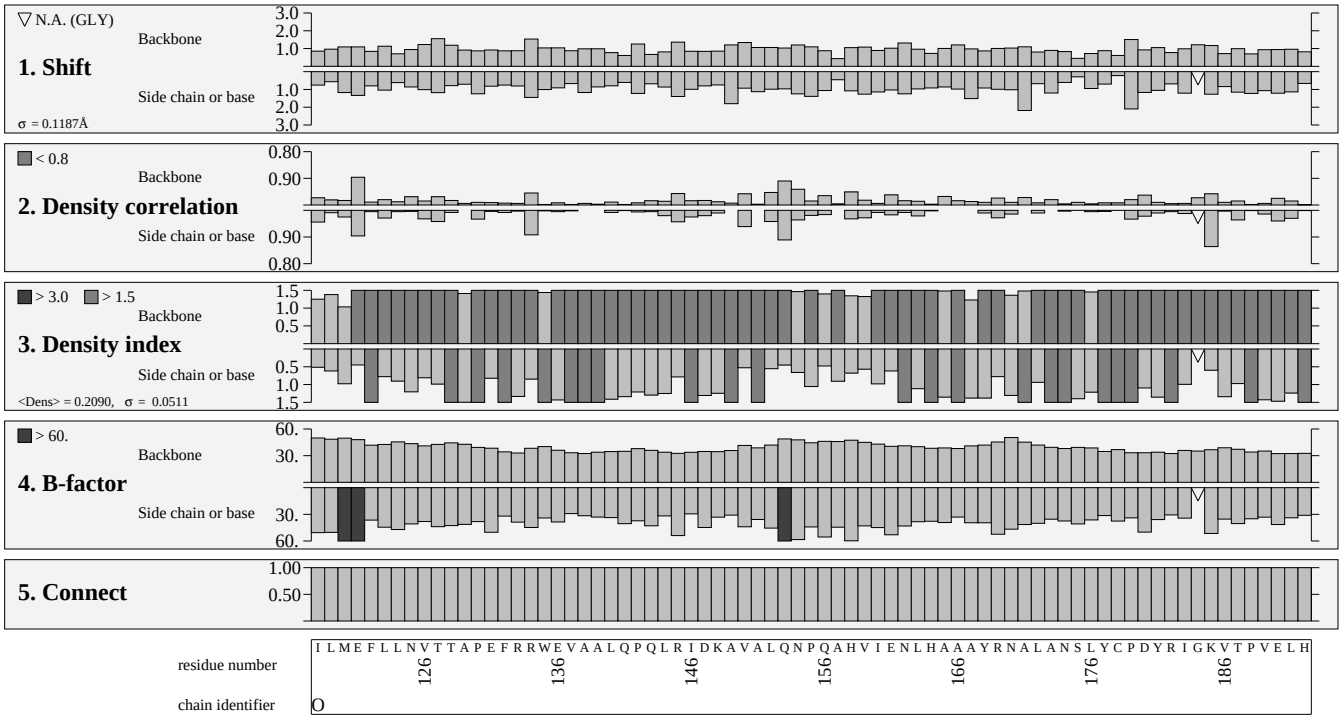
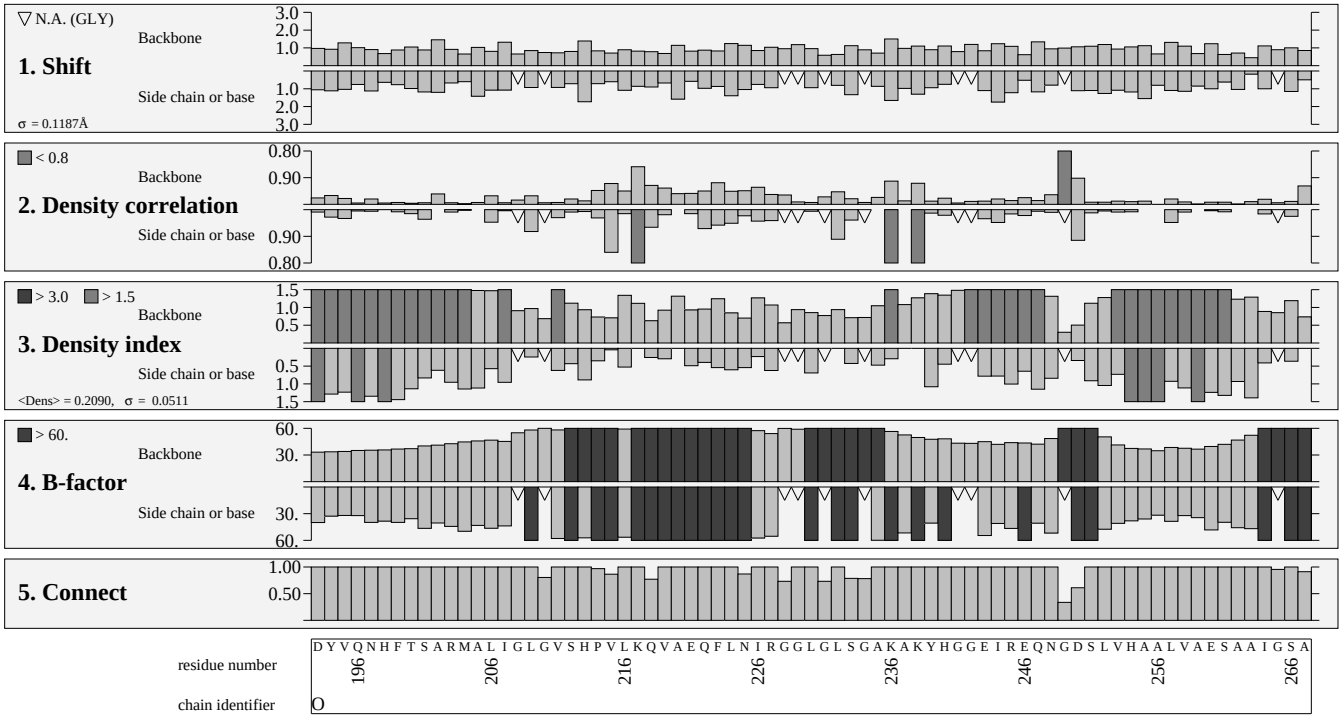
Local estimation (18)





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Structure Factor Check

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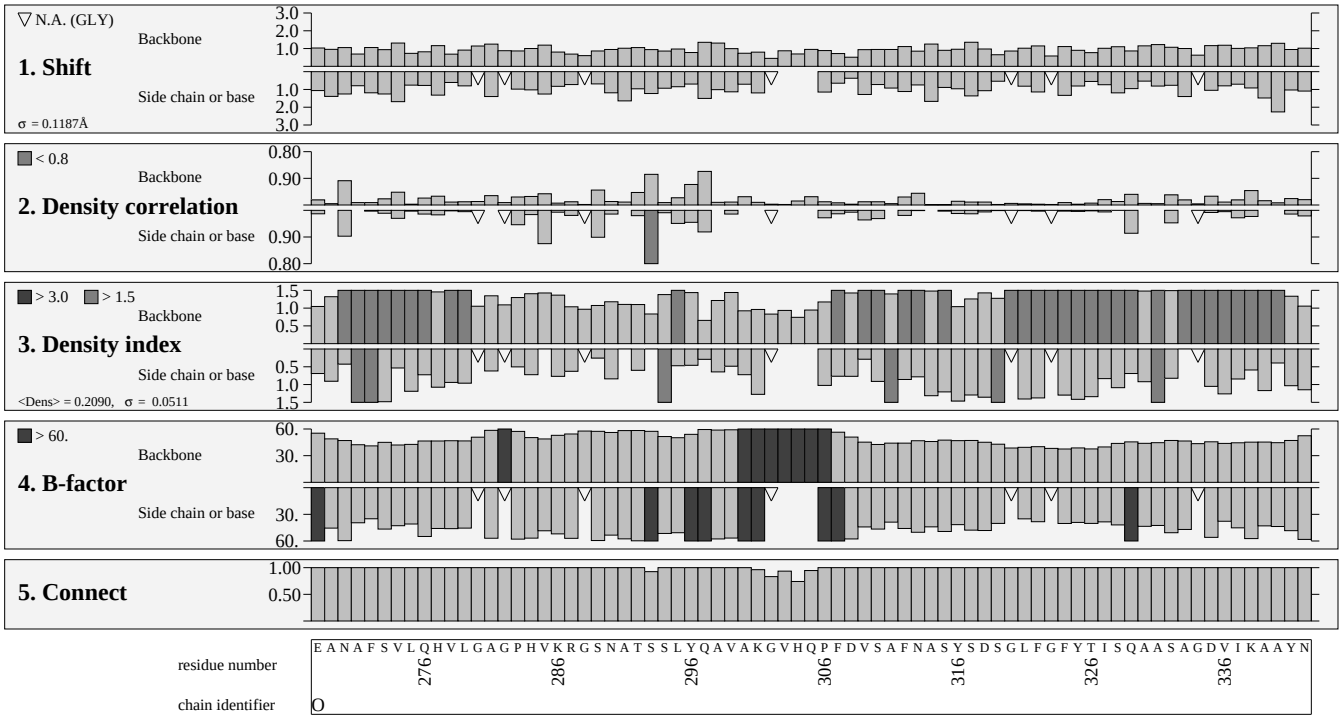
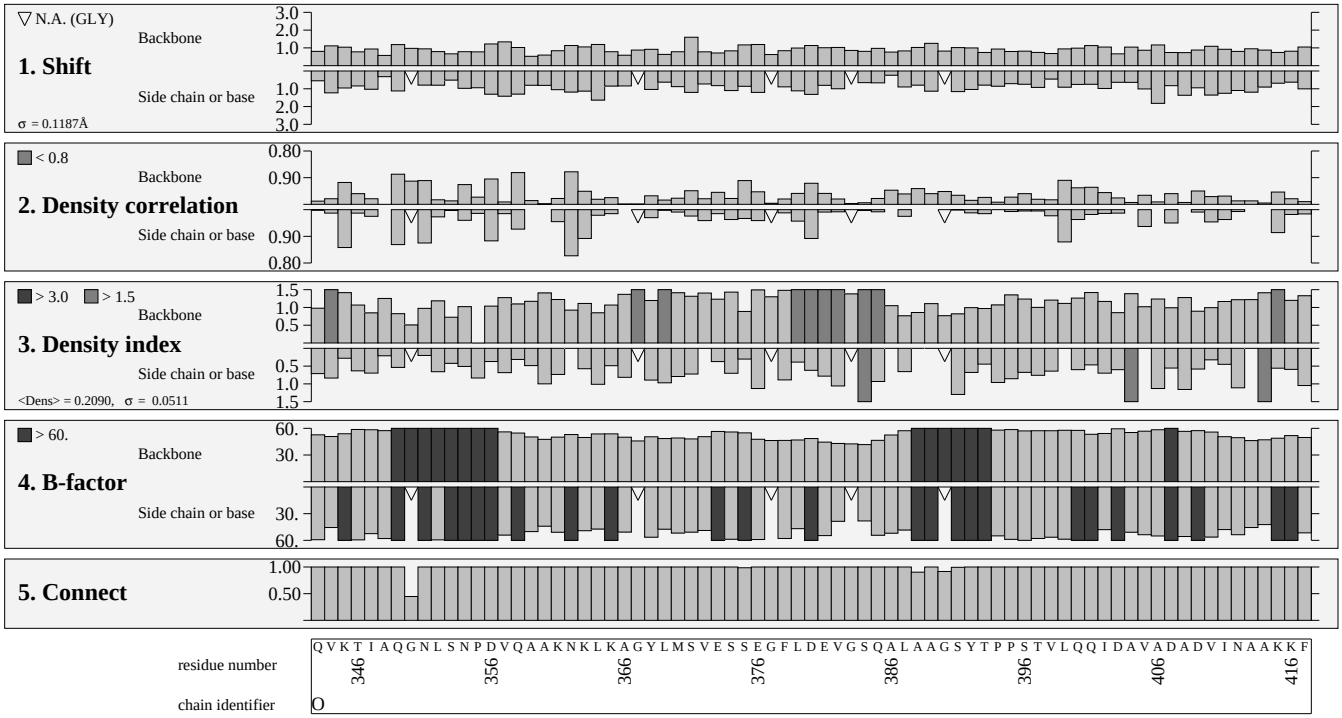
Local estimation (19)





SFCHECK 6.0.5

Structure Factor Check

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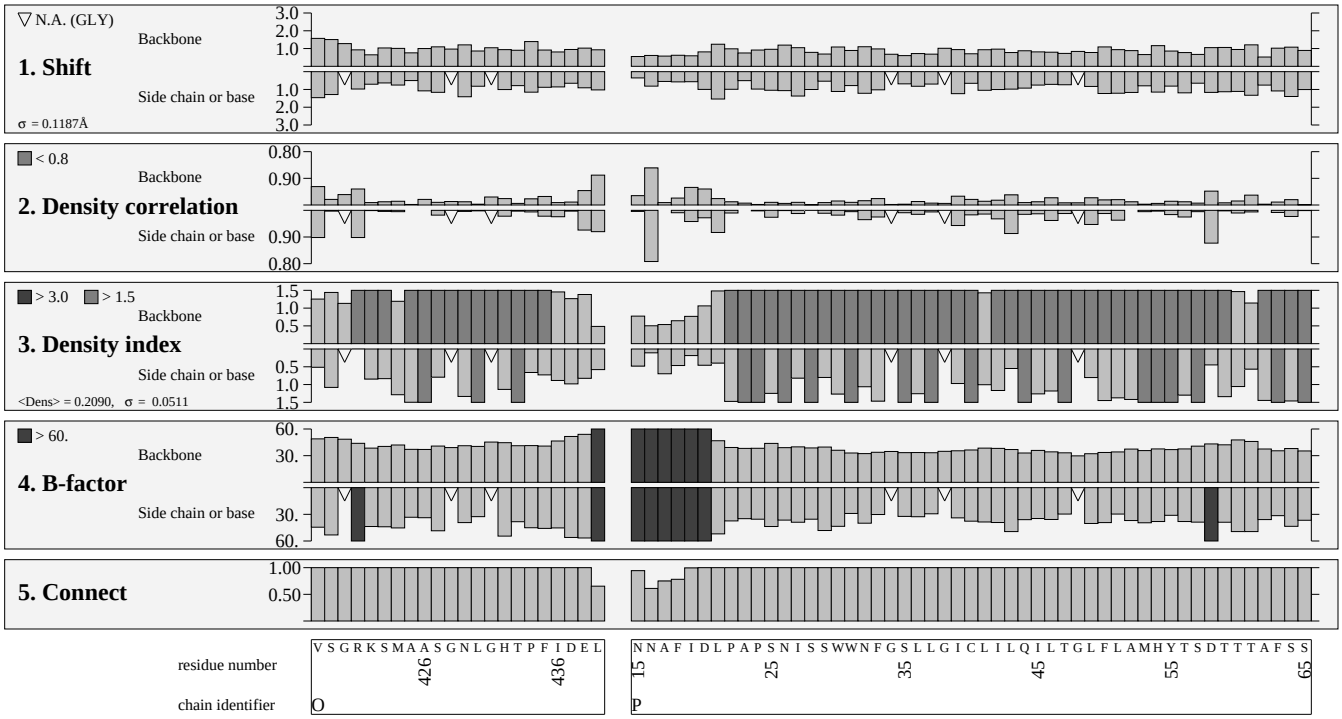
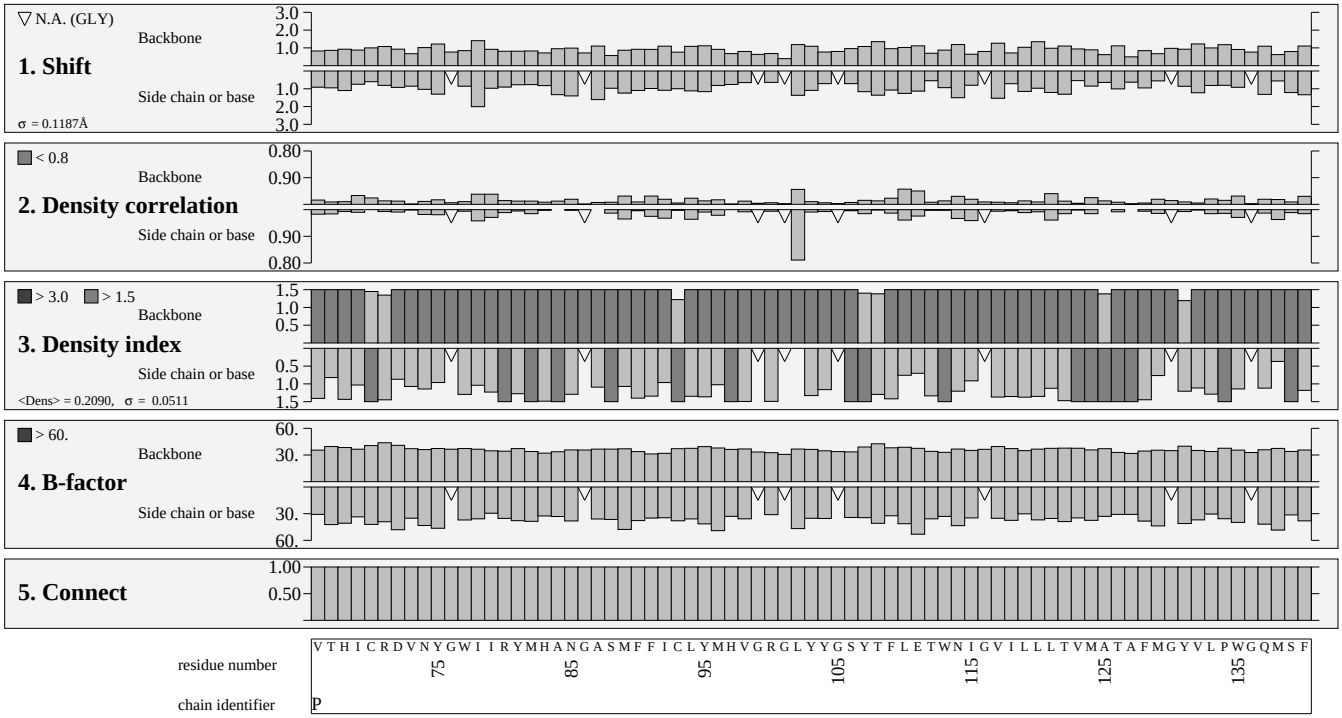
Local estimation (20)





SFCHECK 6.0.5

Structure Factor Check

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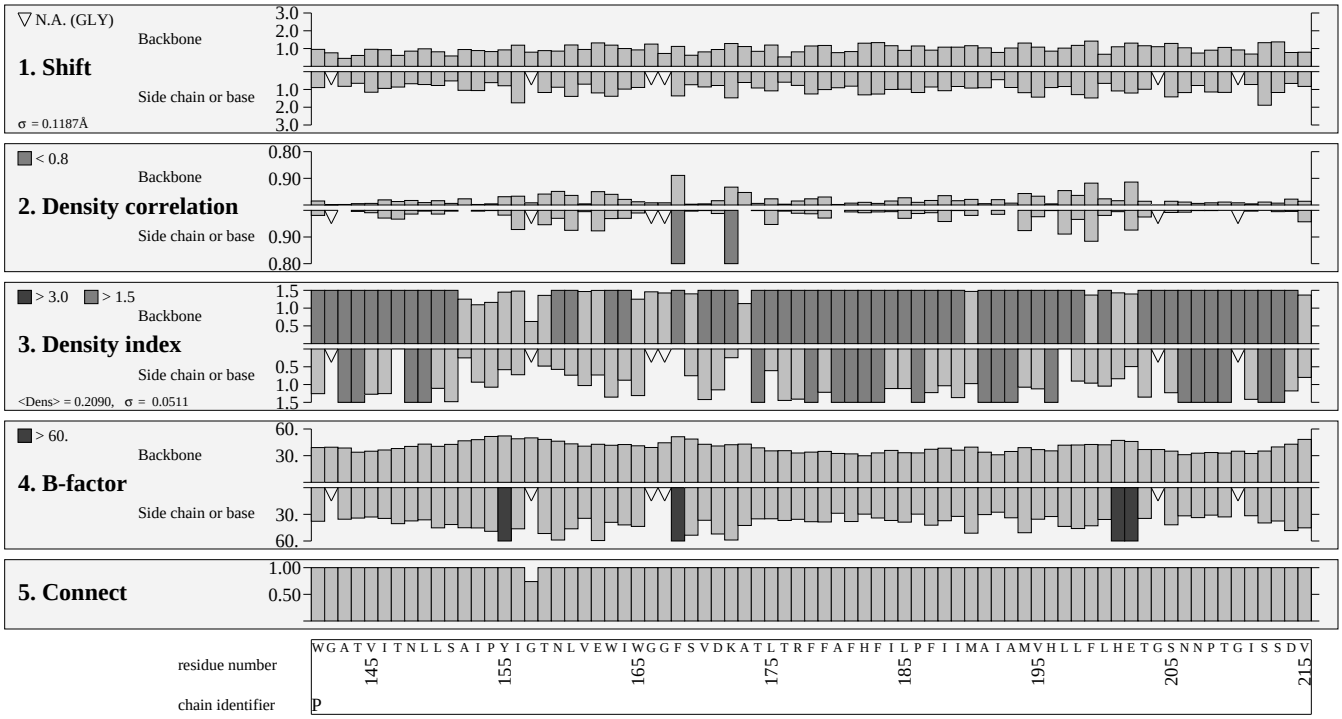
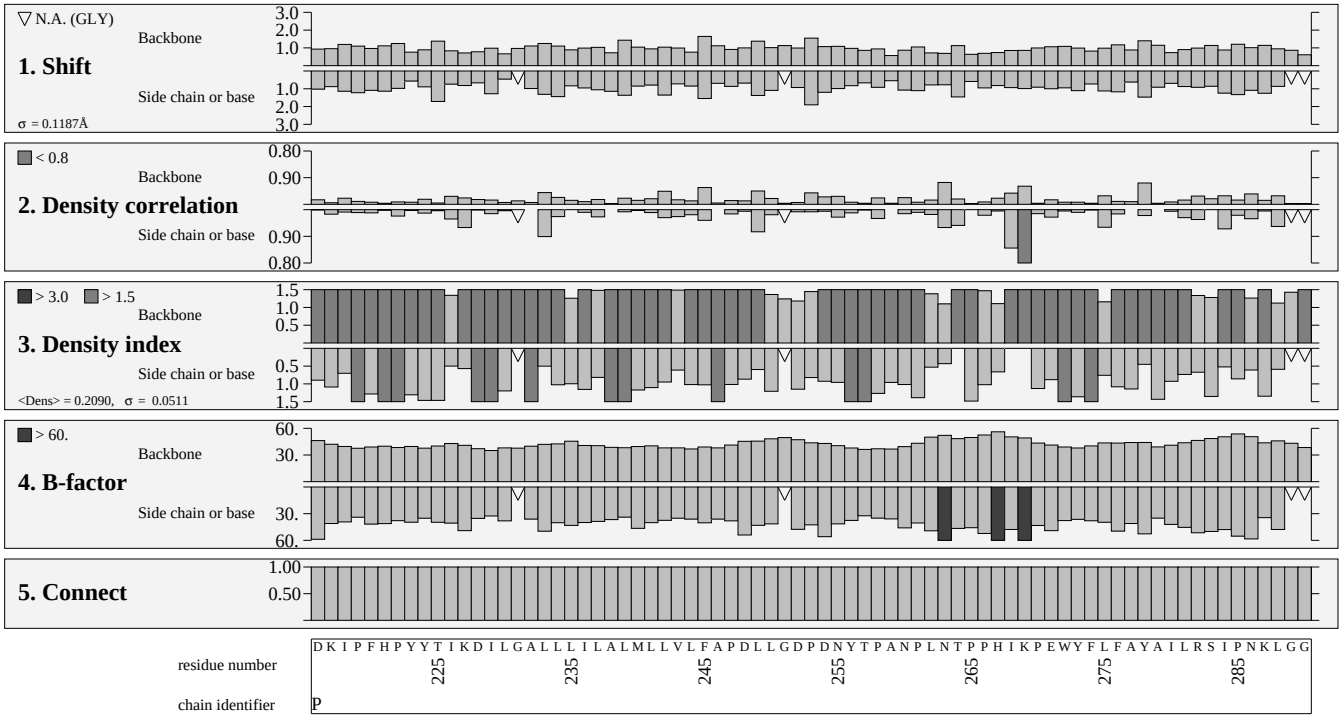
Local estimation (21)





SFCHECK 6.0.5

Structure Factor Check

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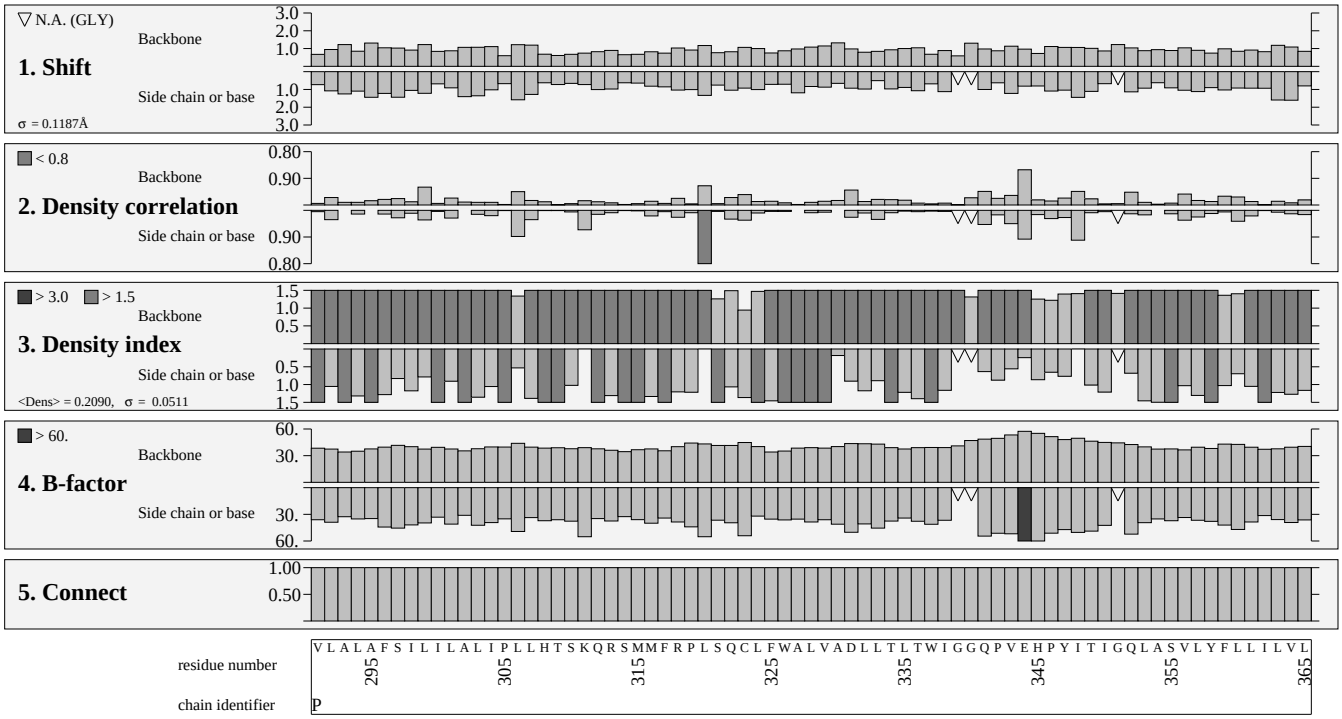
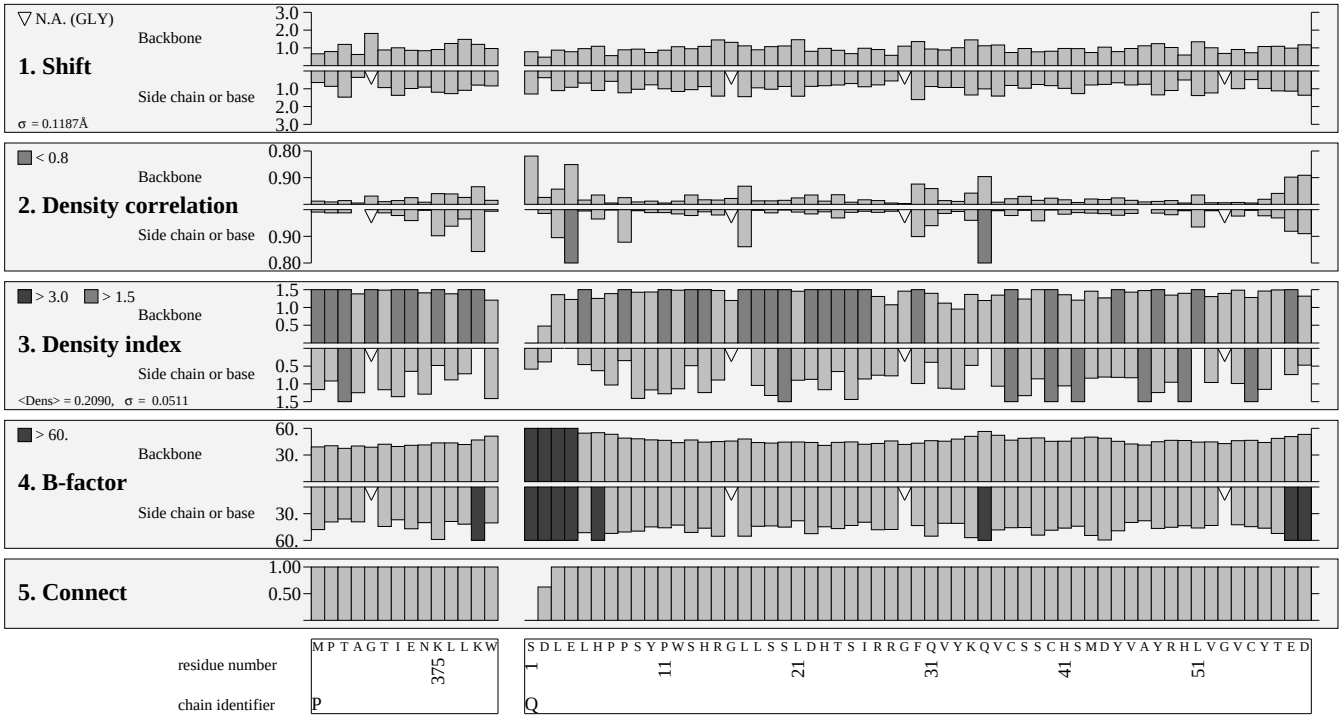
Local estimation (22)





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Structure Factor Check

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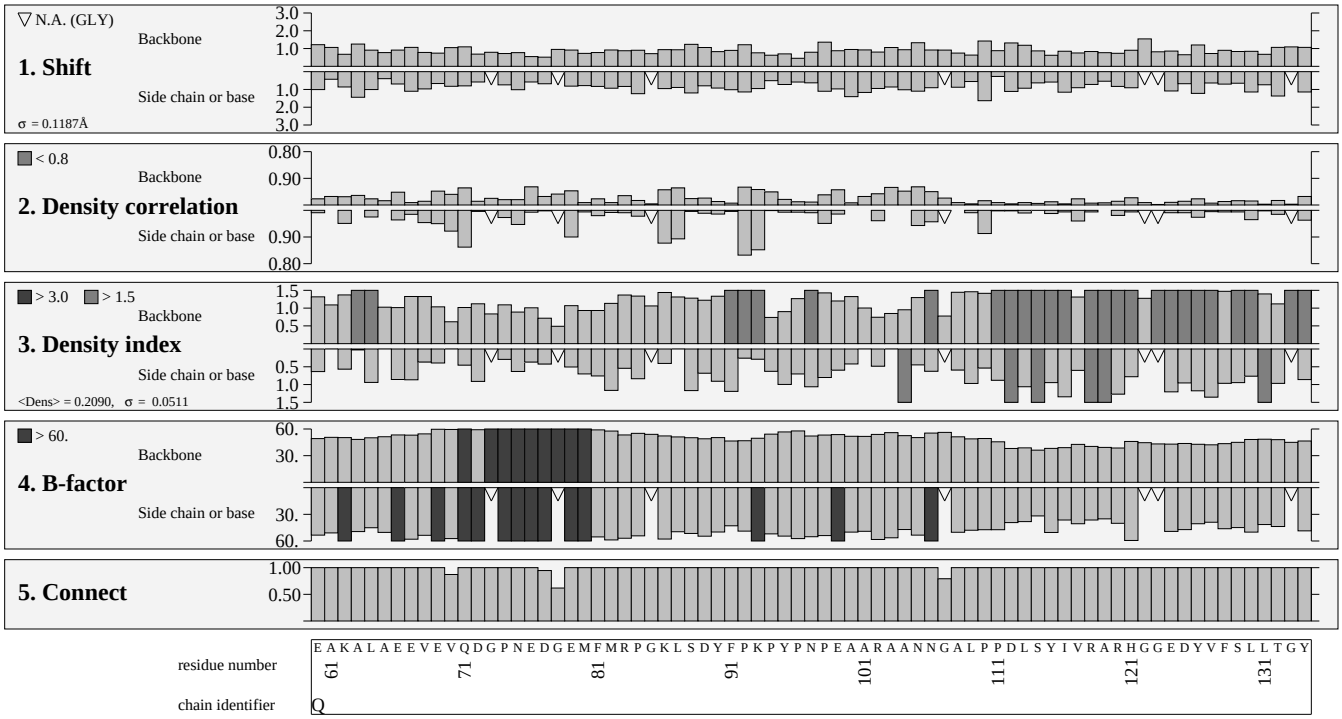
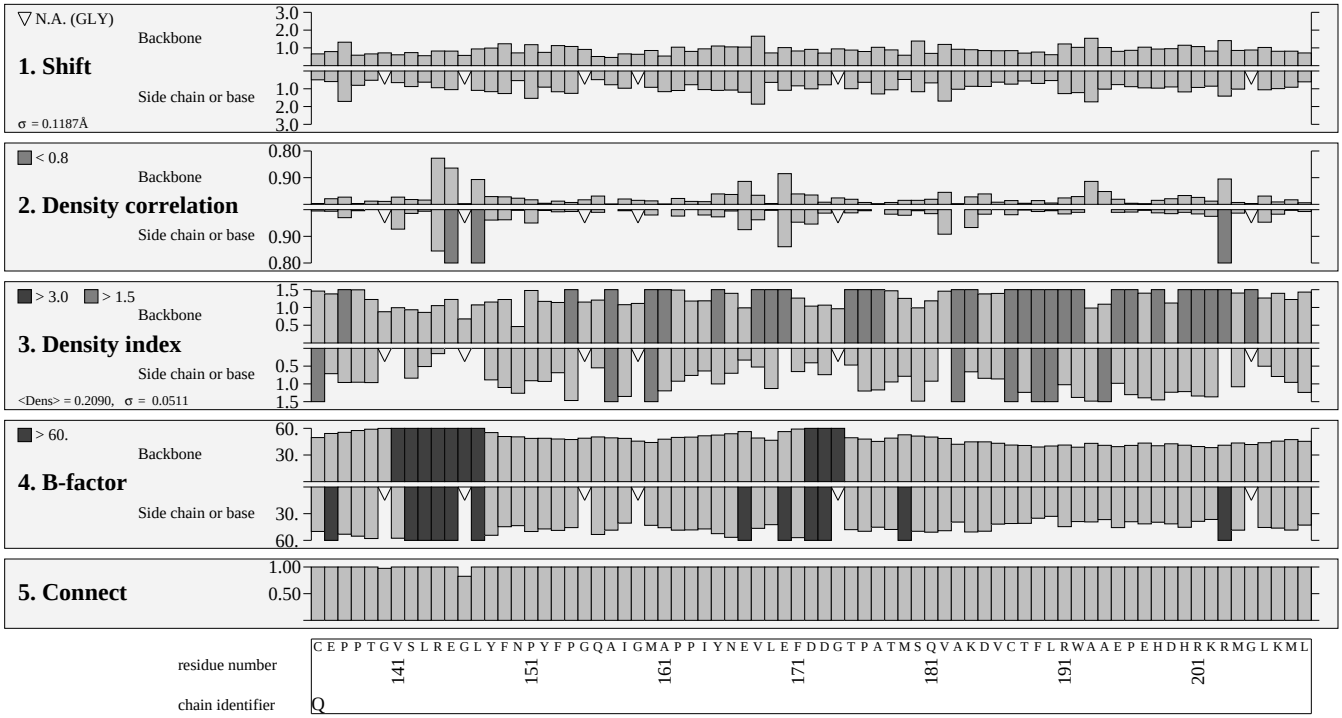
Local estimation (23)



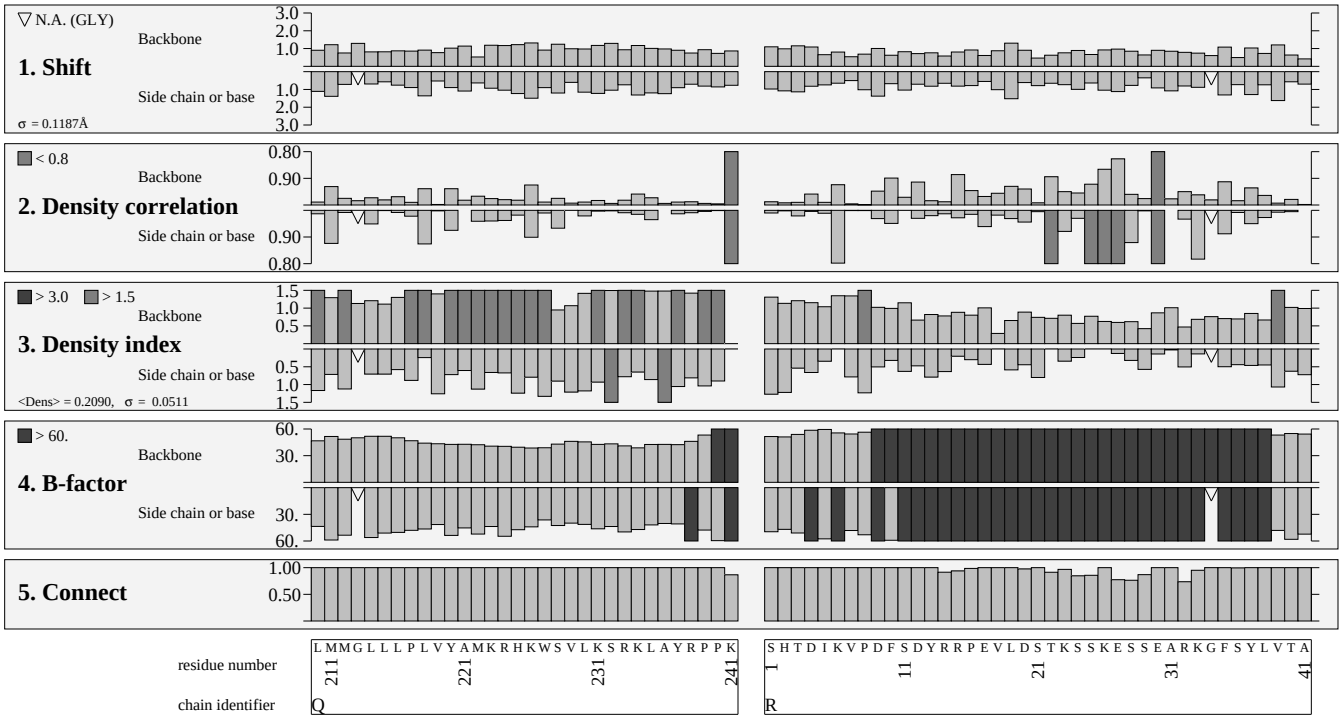


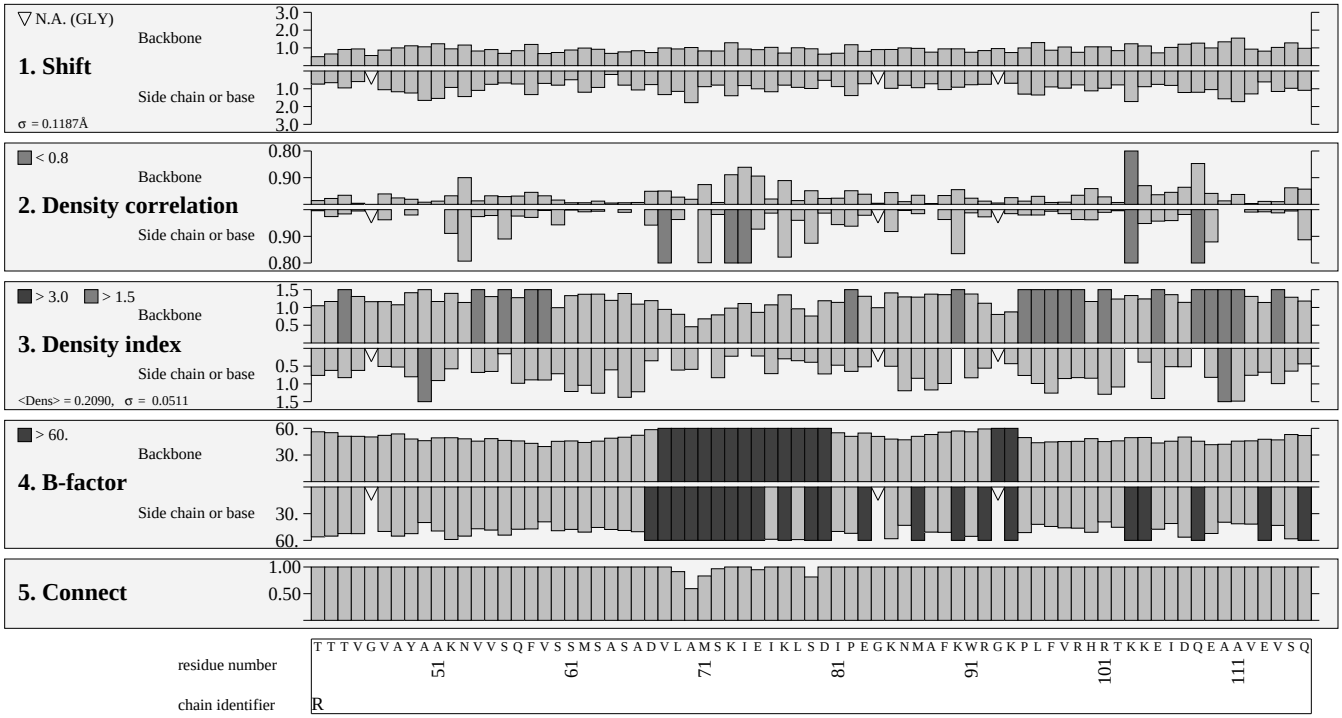
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (24)



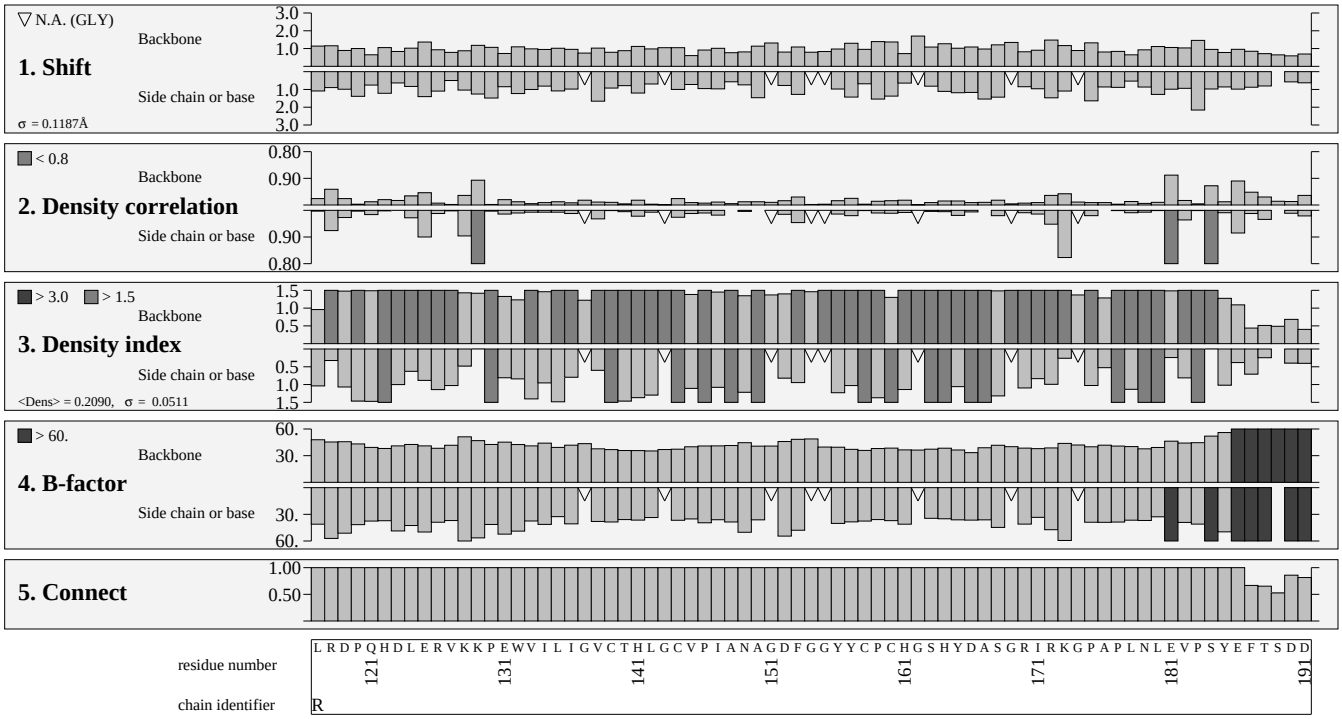


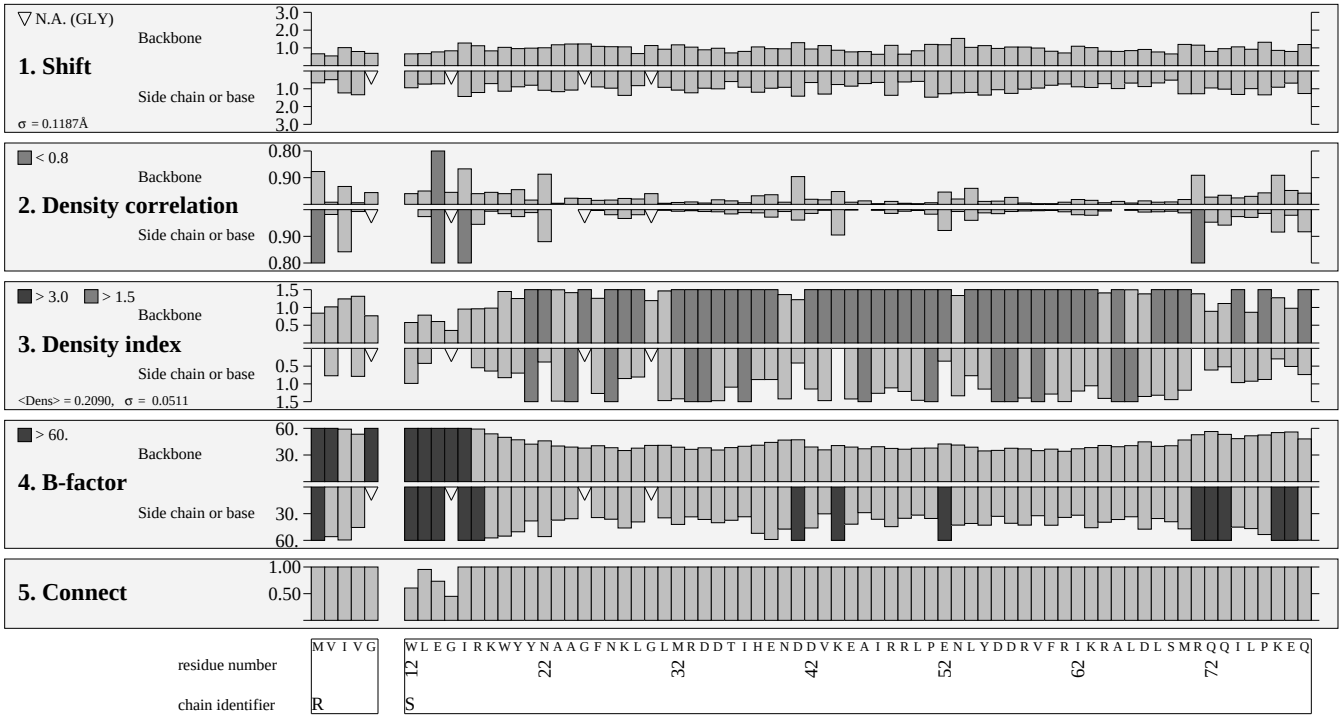
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (25)



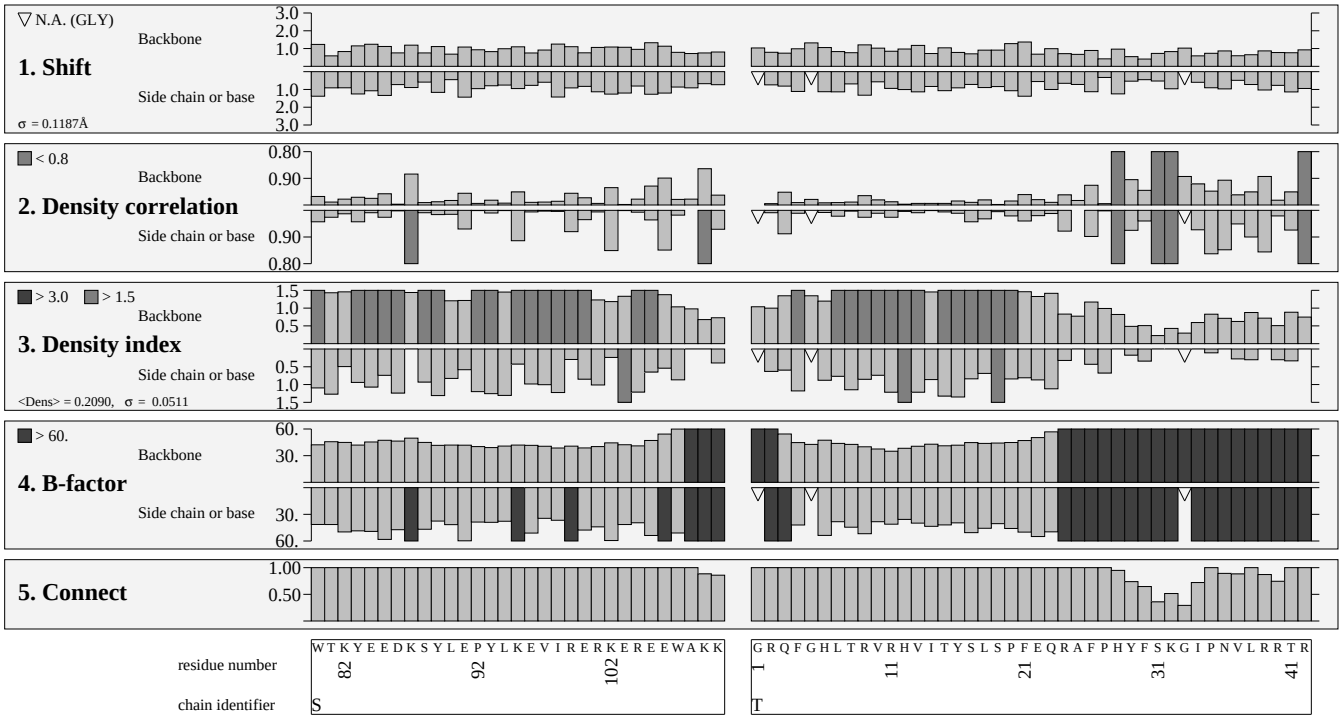


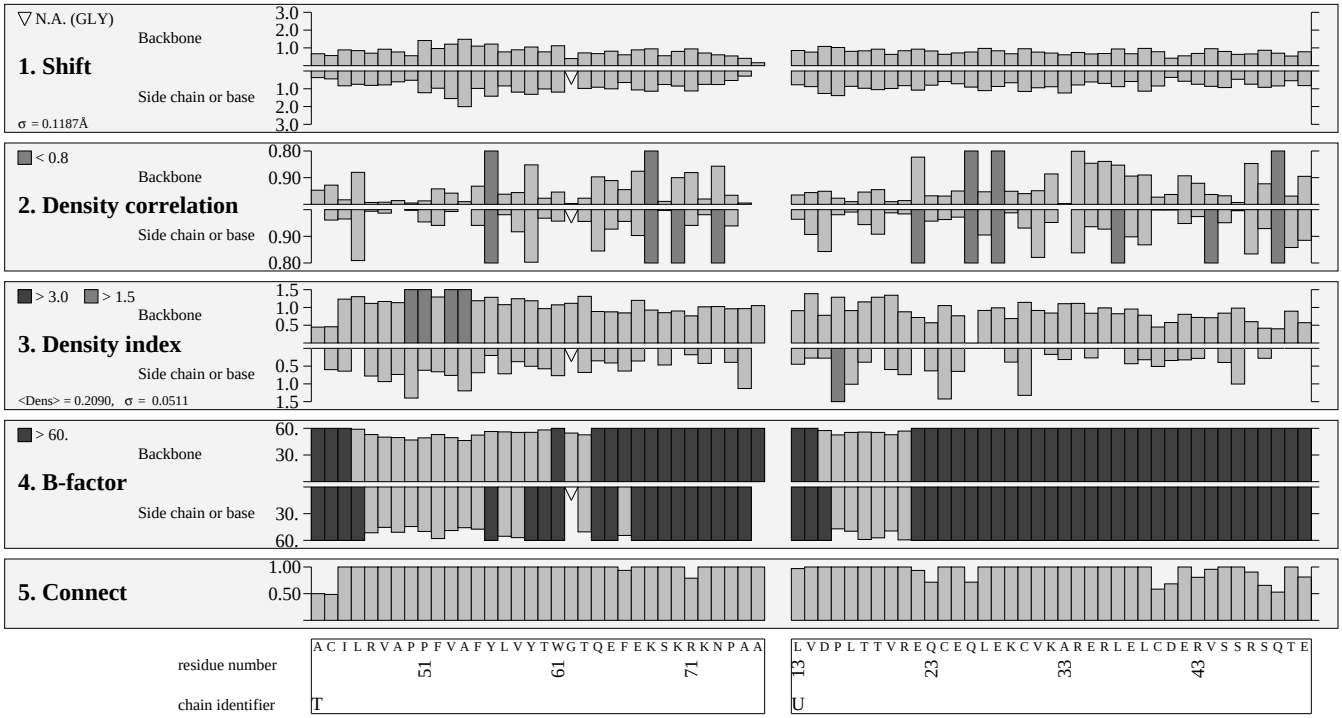
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (26)



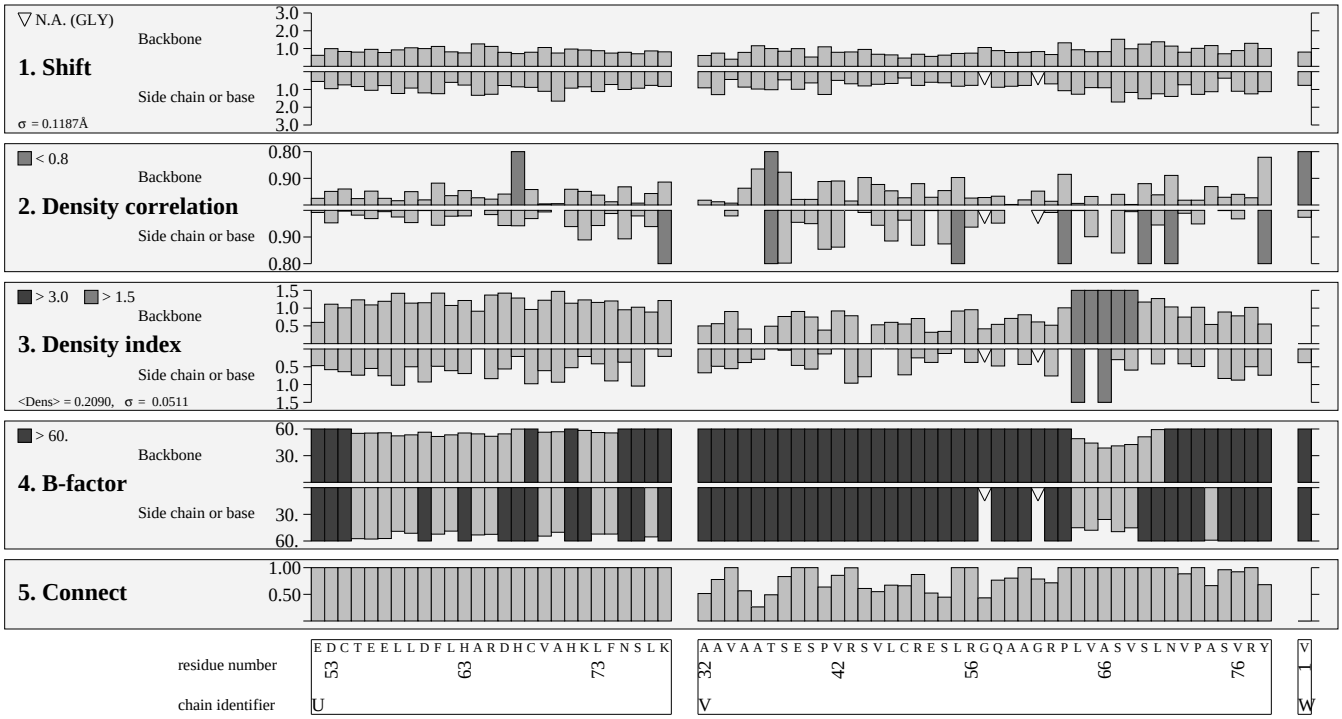


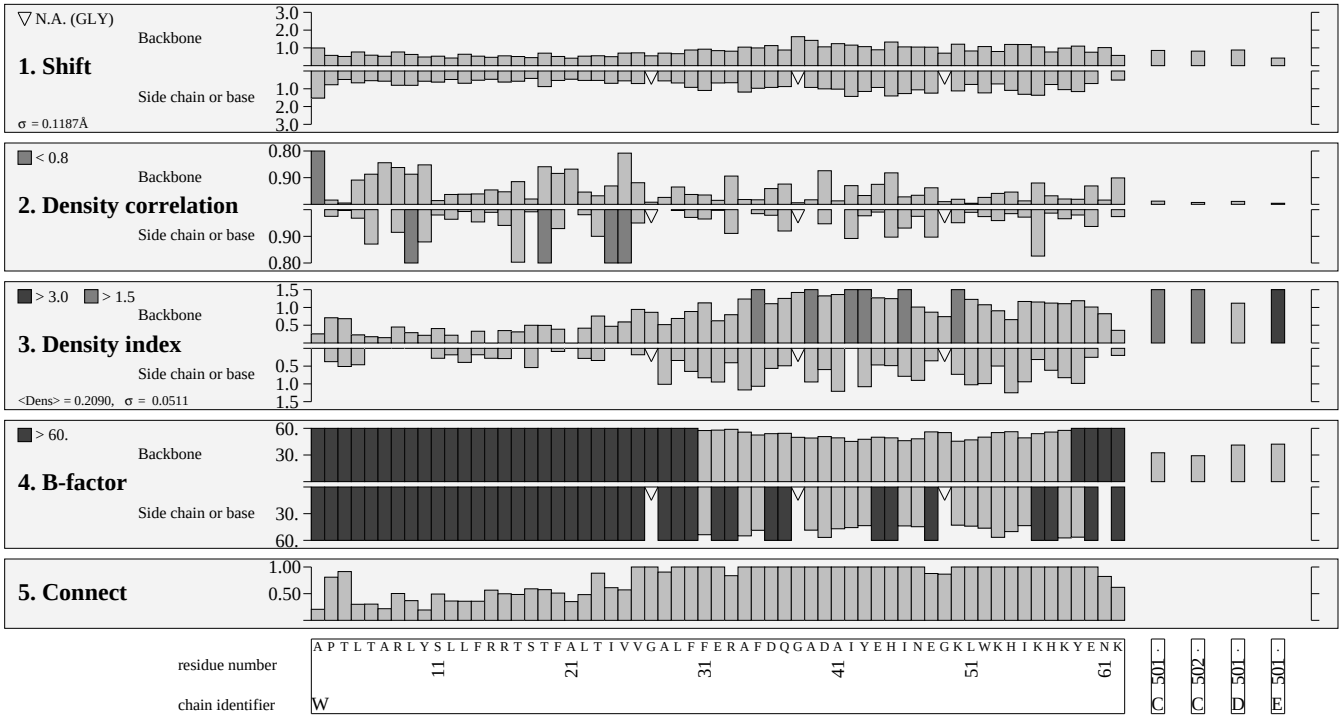
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (27)



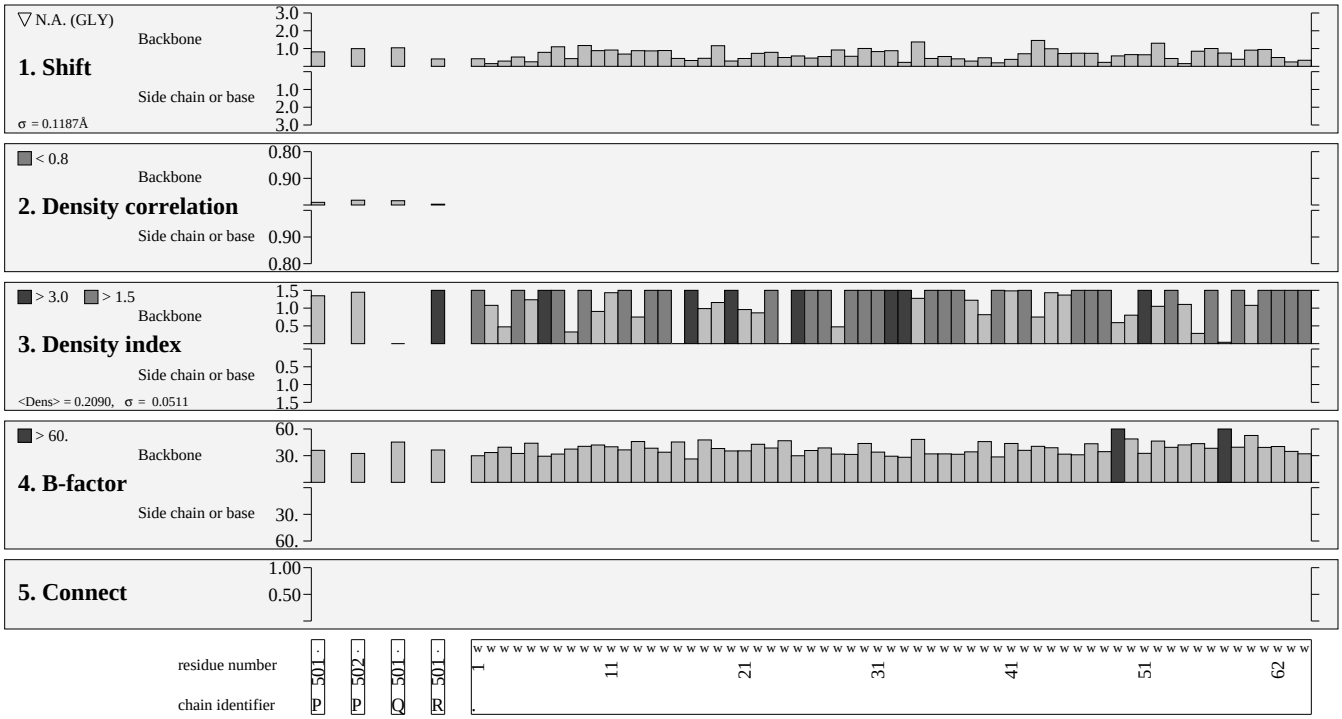


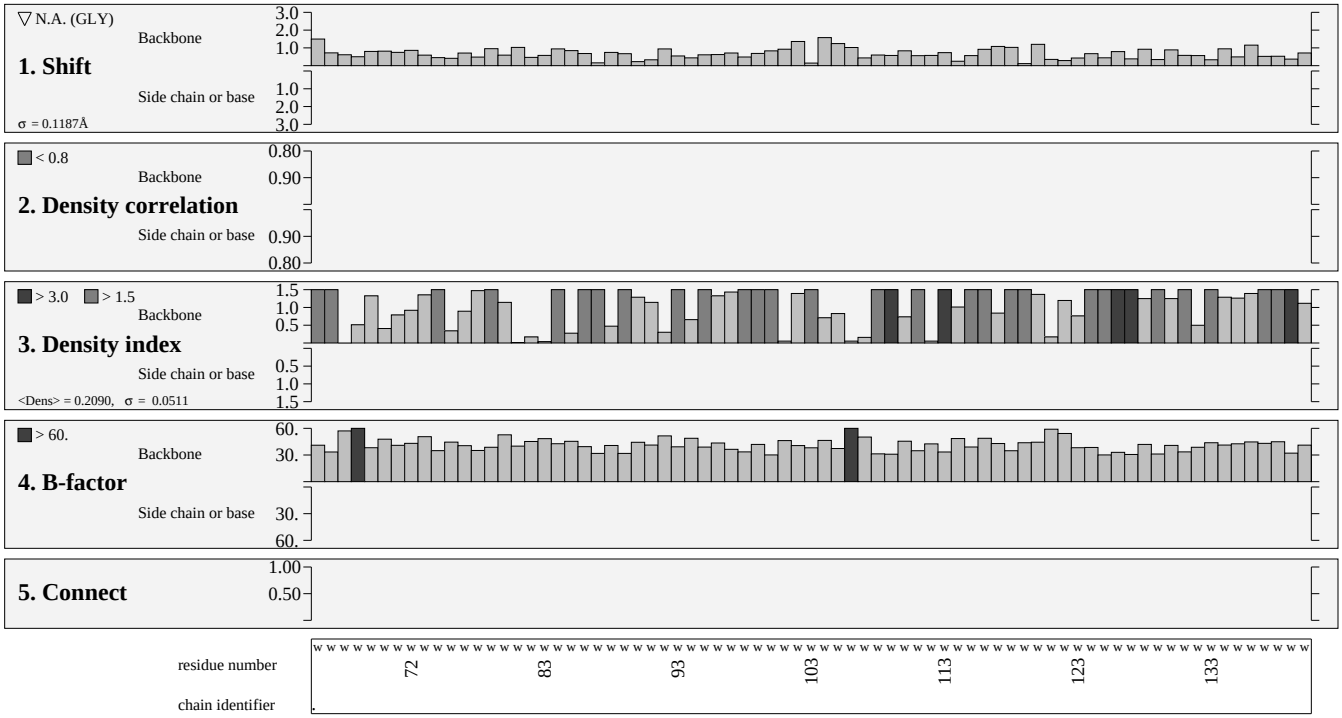
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (28)



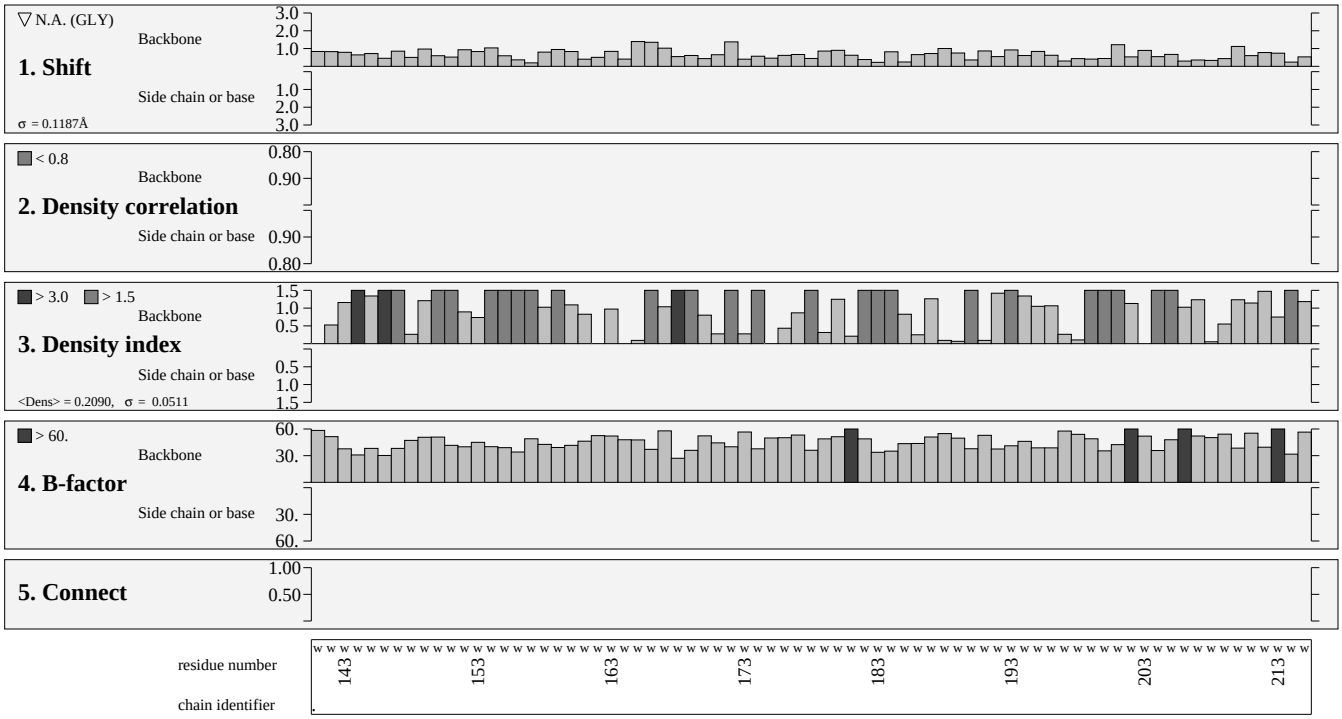


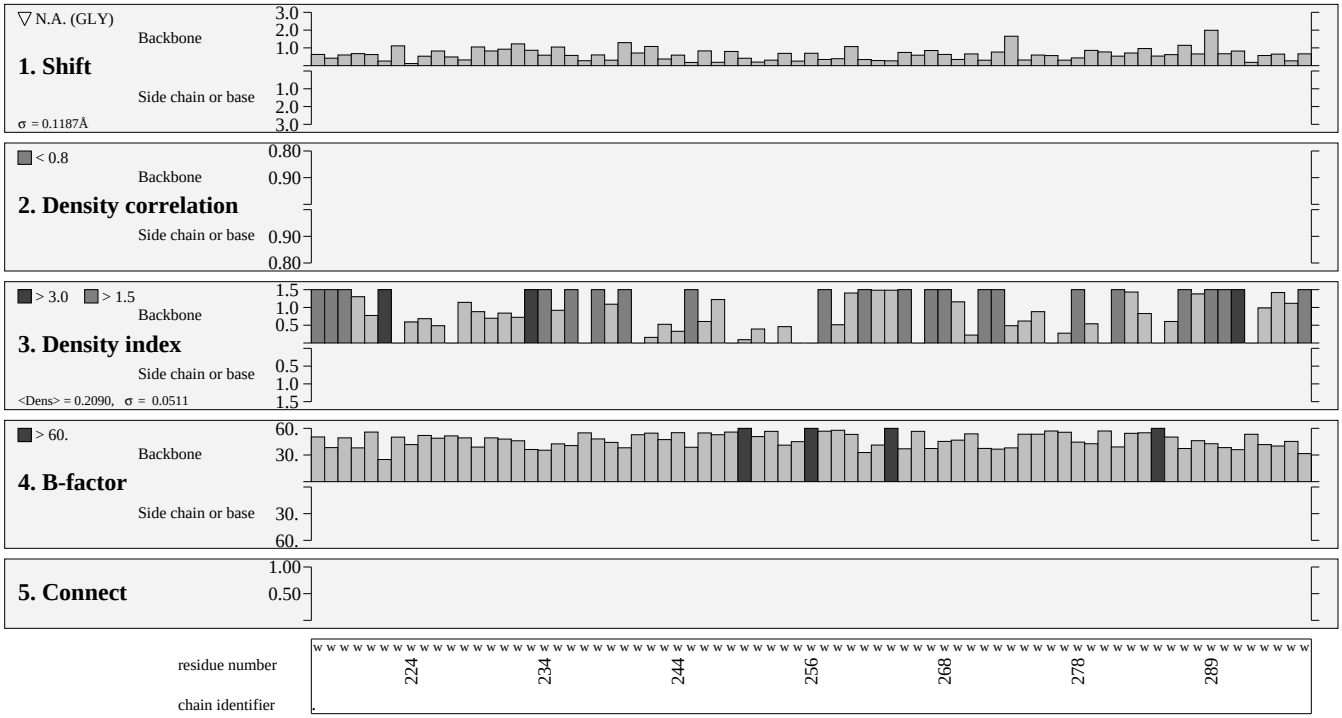
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (29)



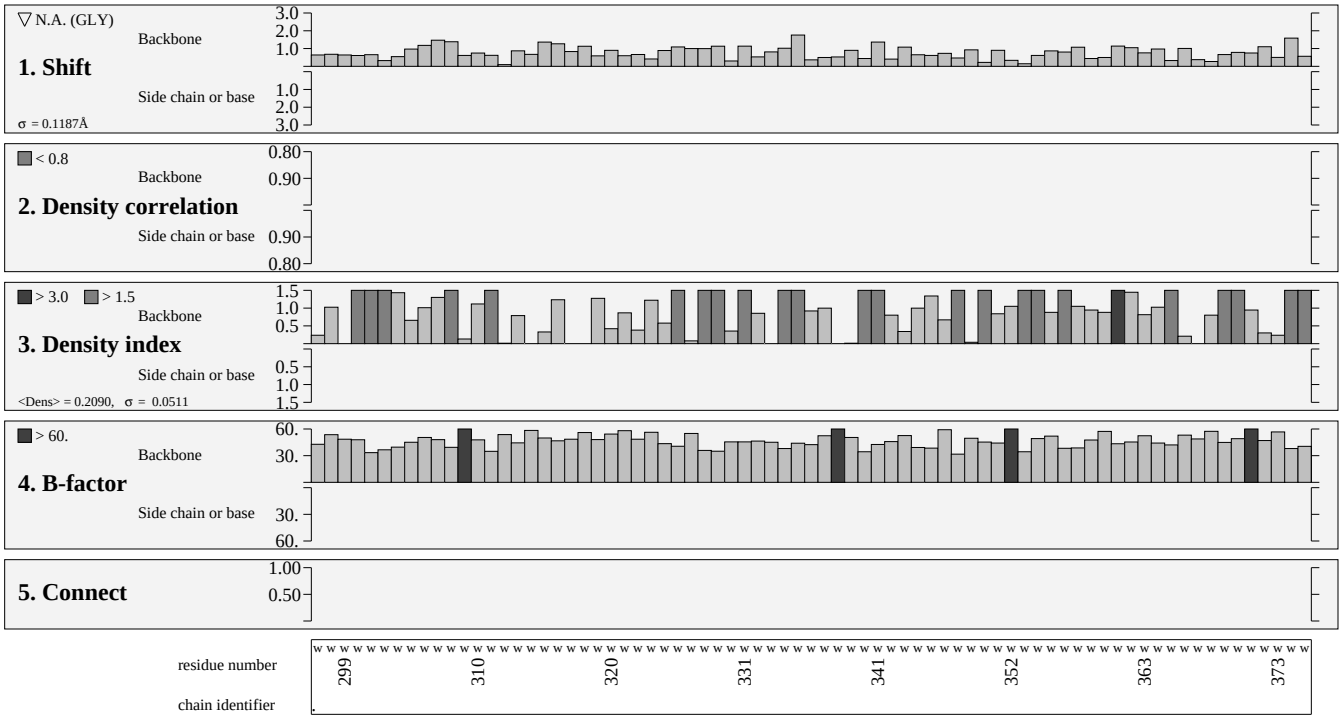


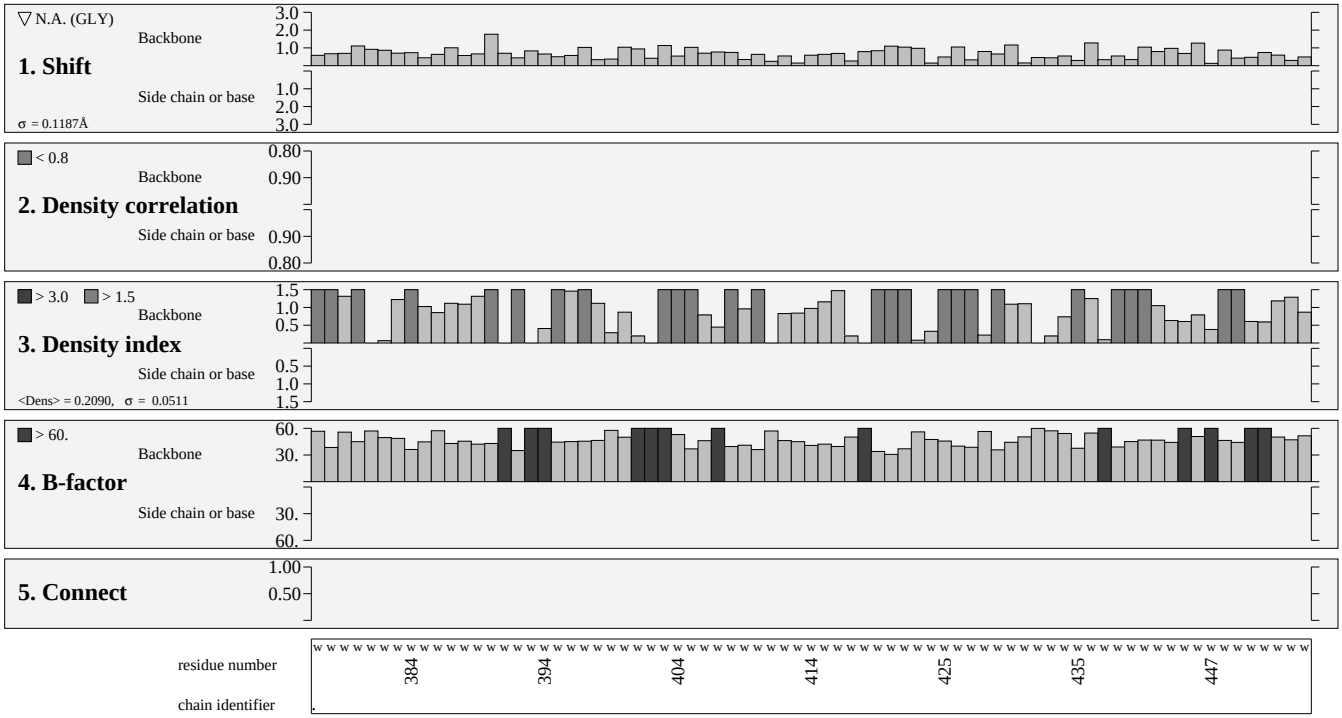
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (30)



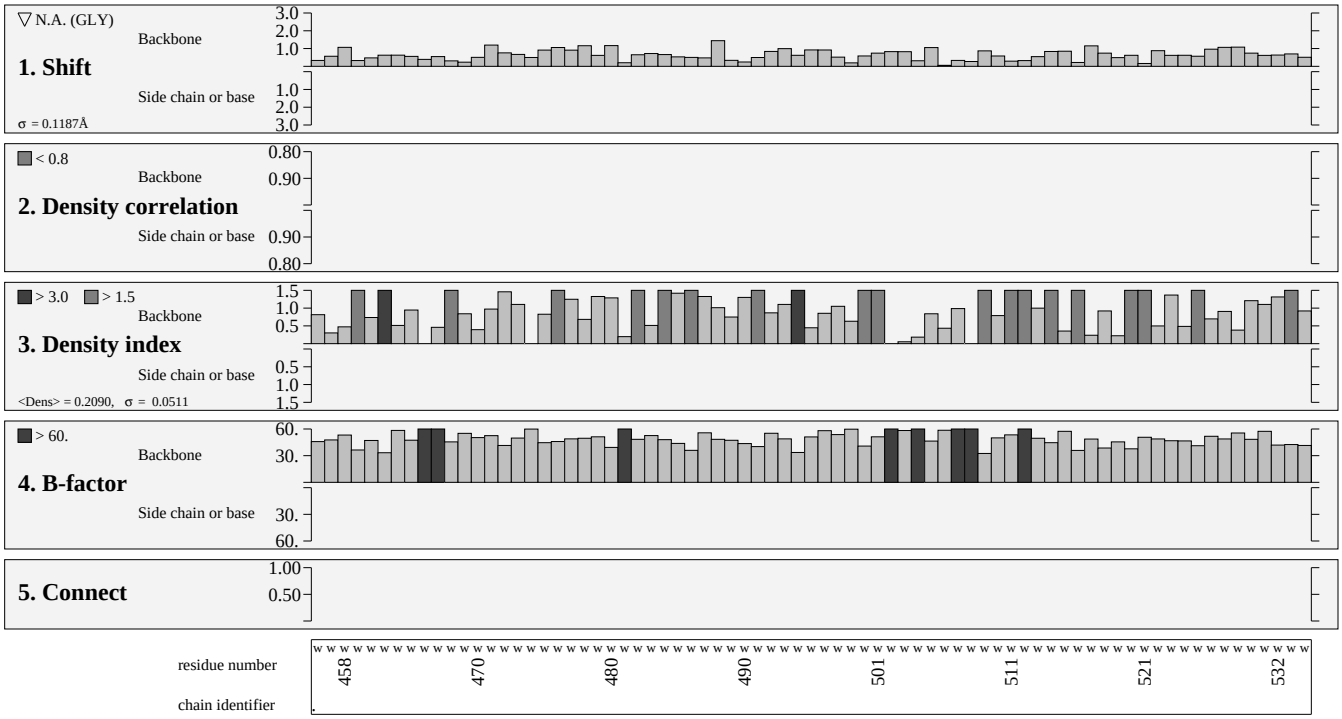


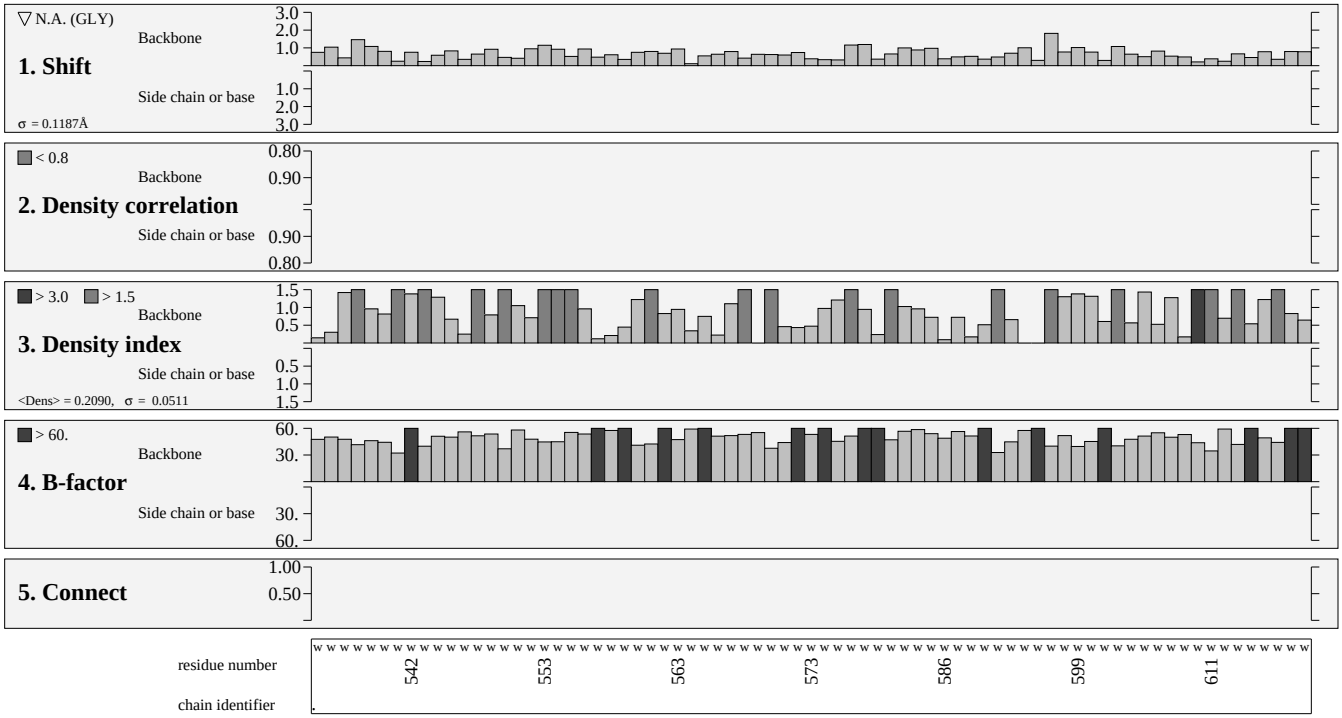
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (31)



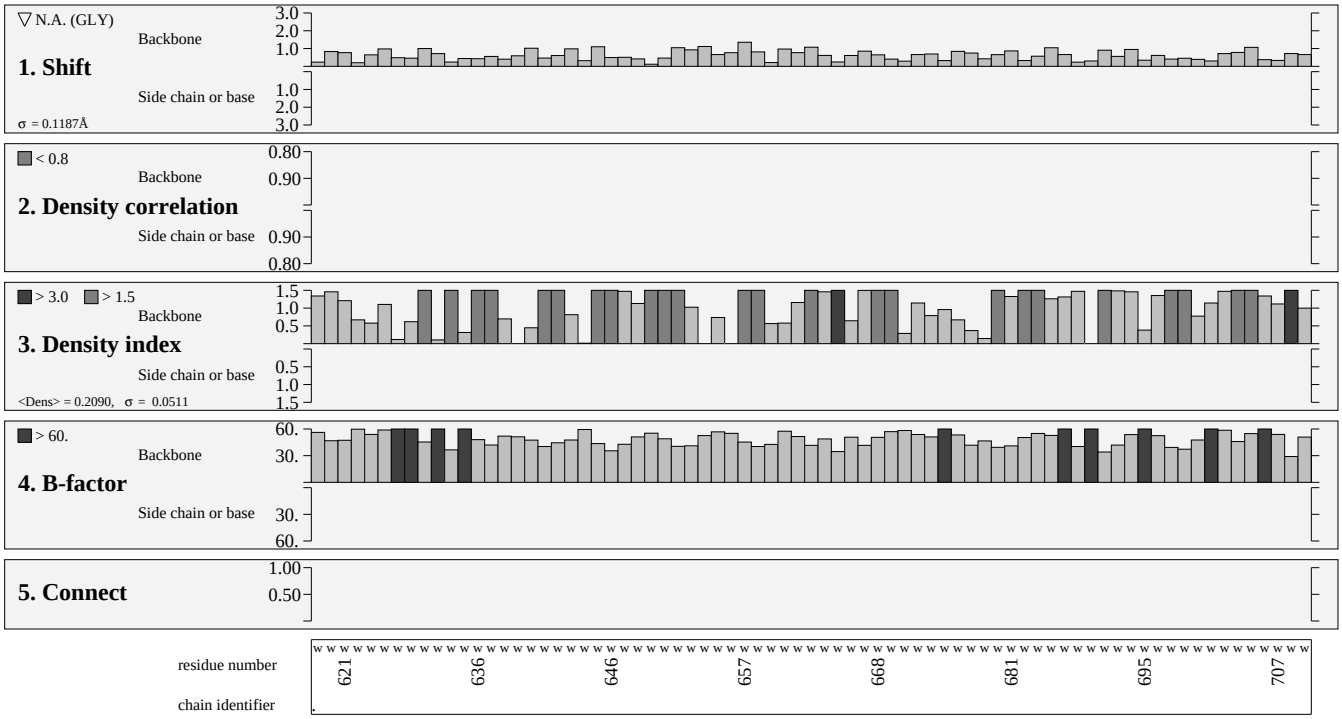


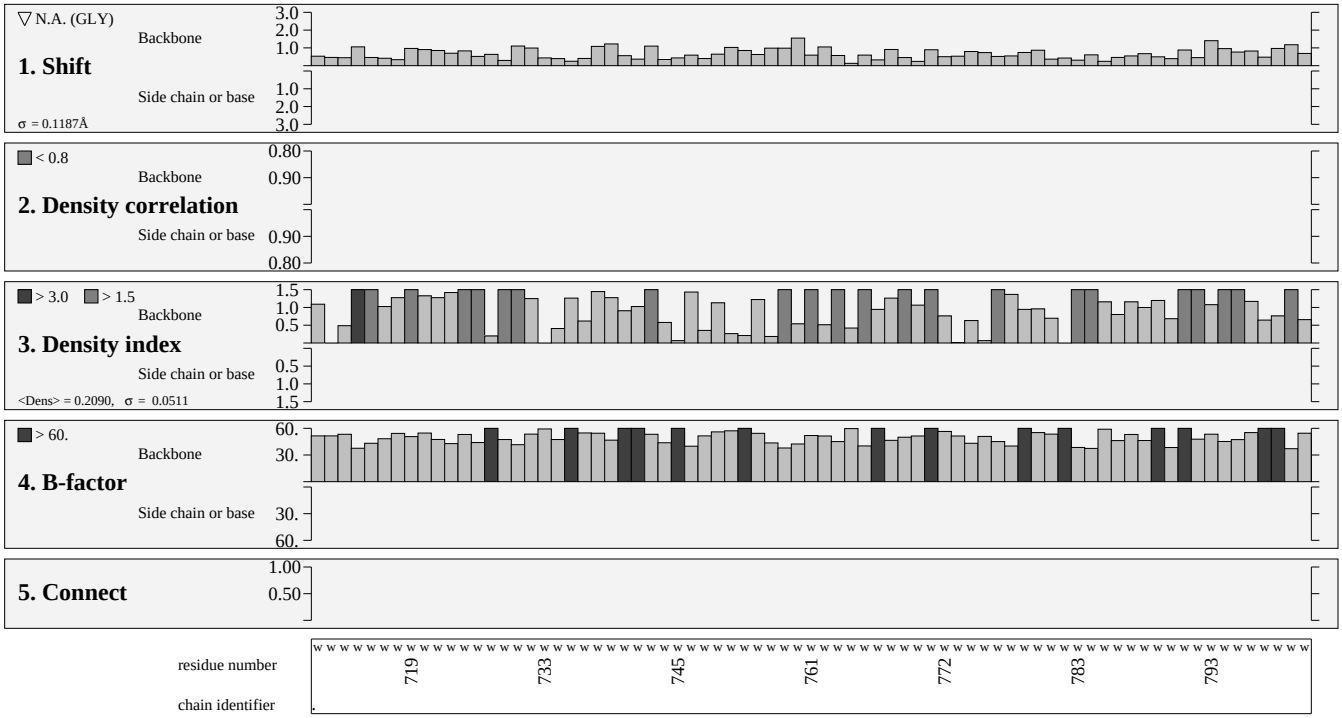
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (32)



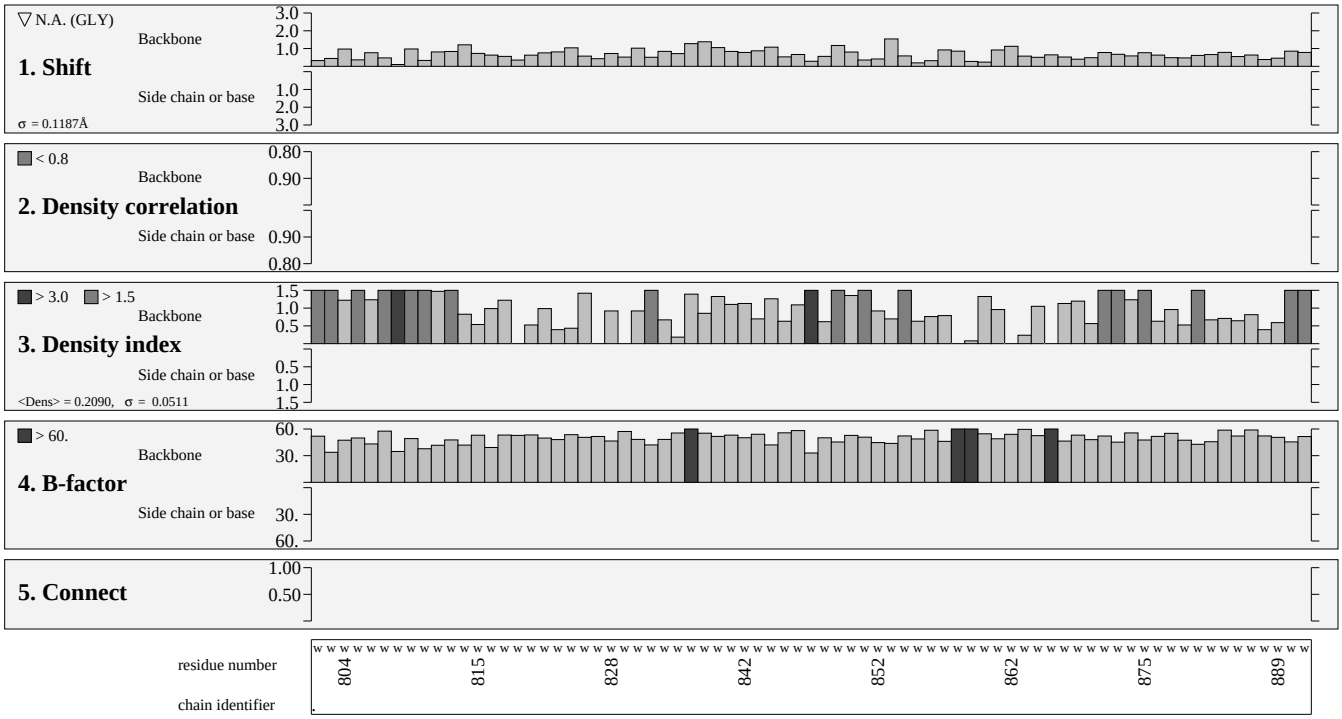


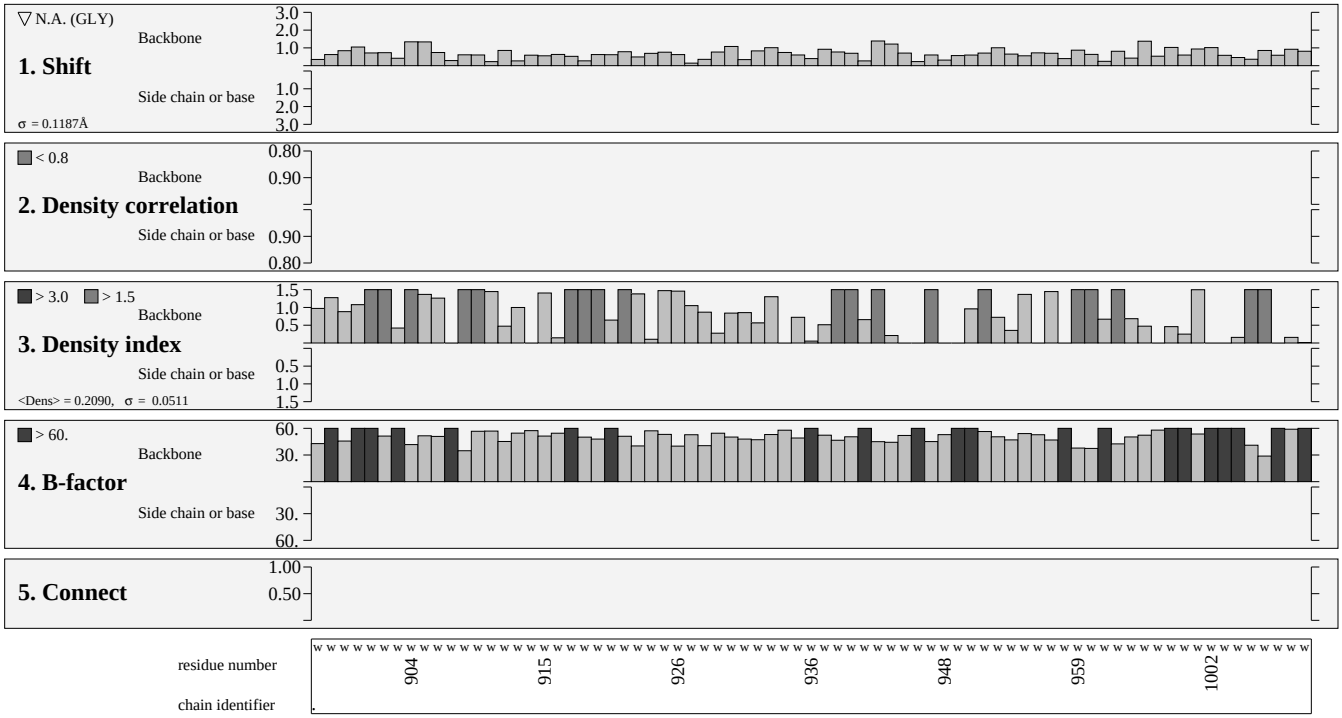
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (33)



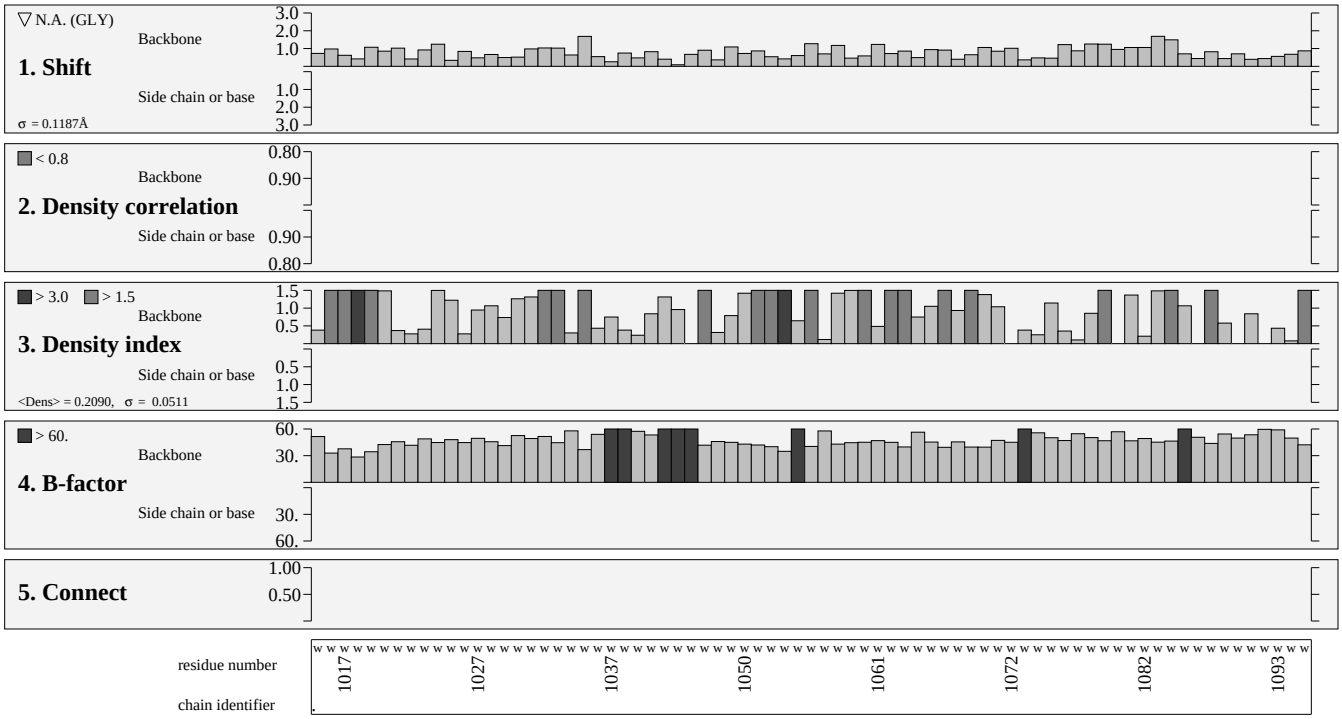


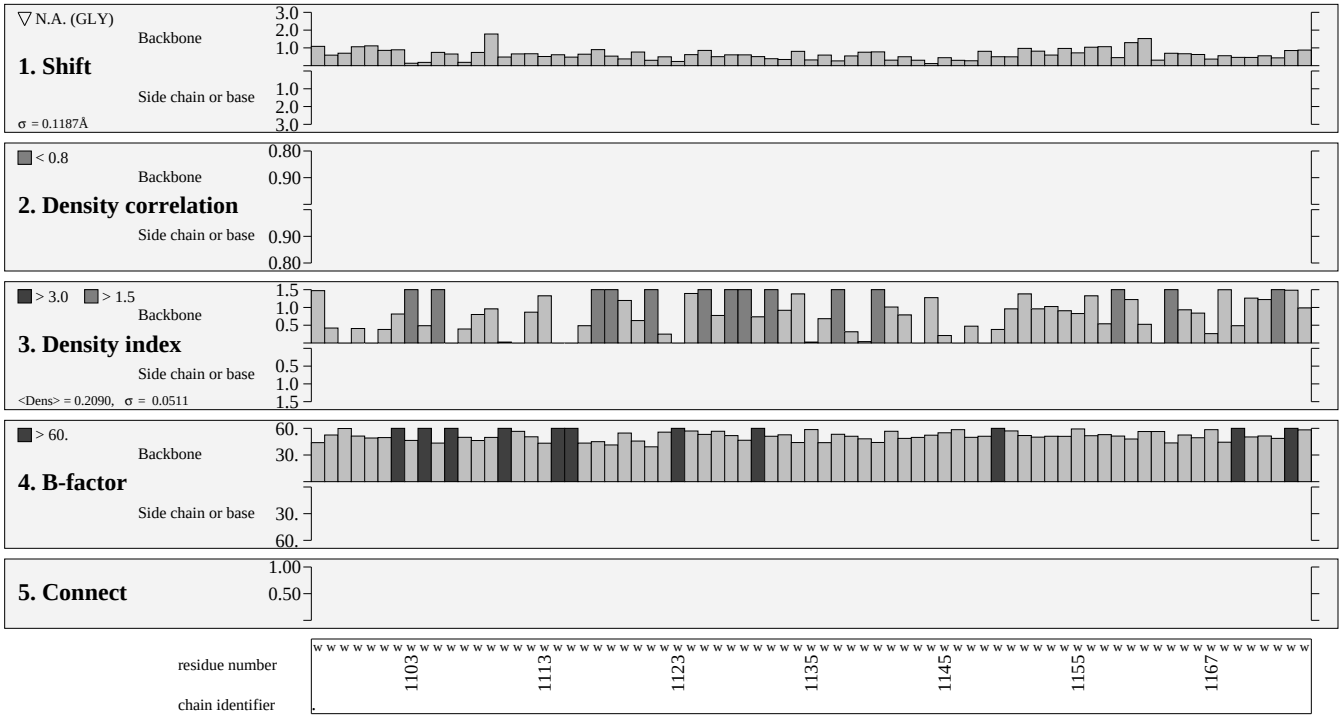
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (34)



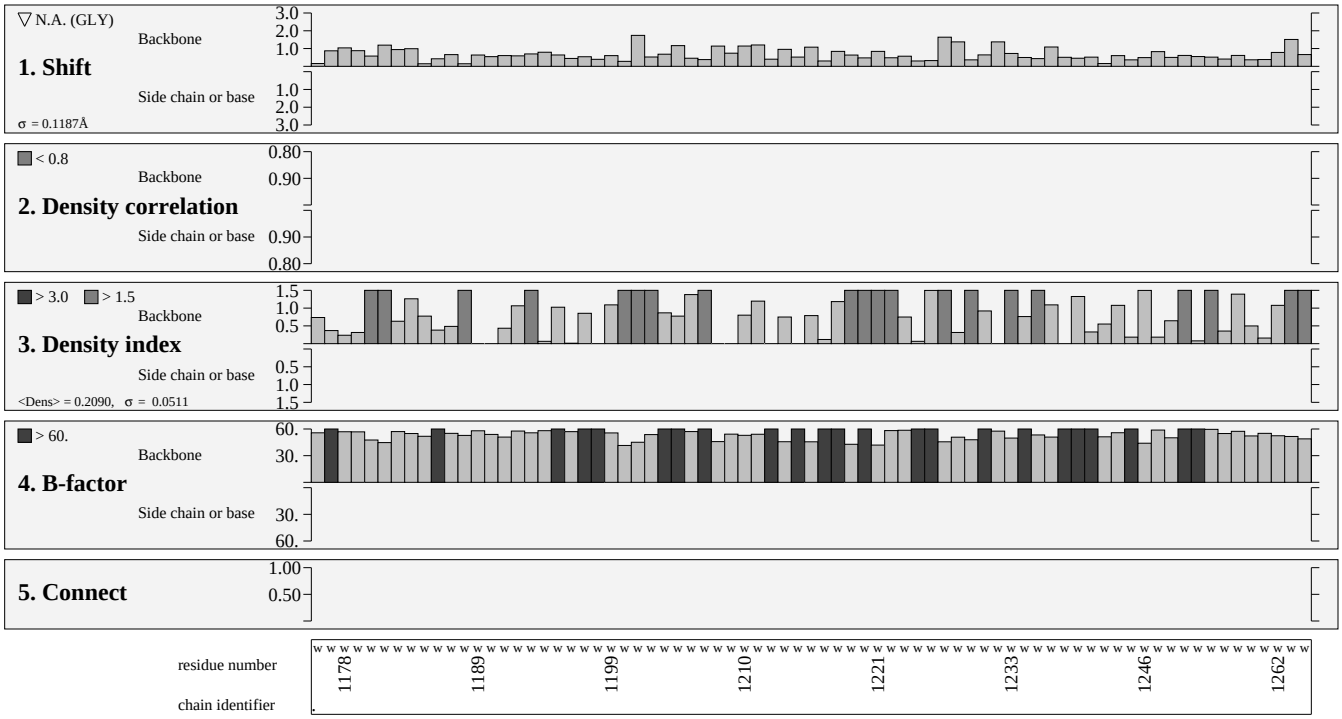


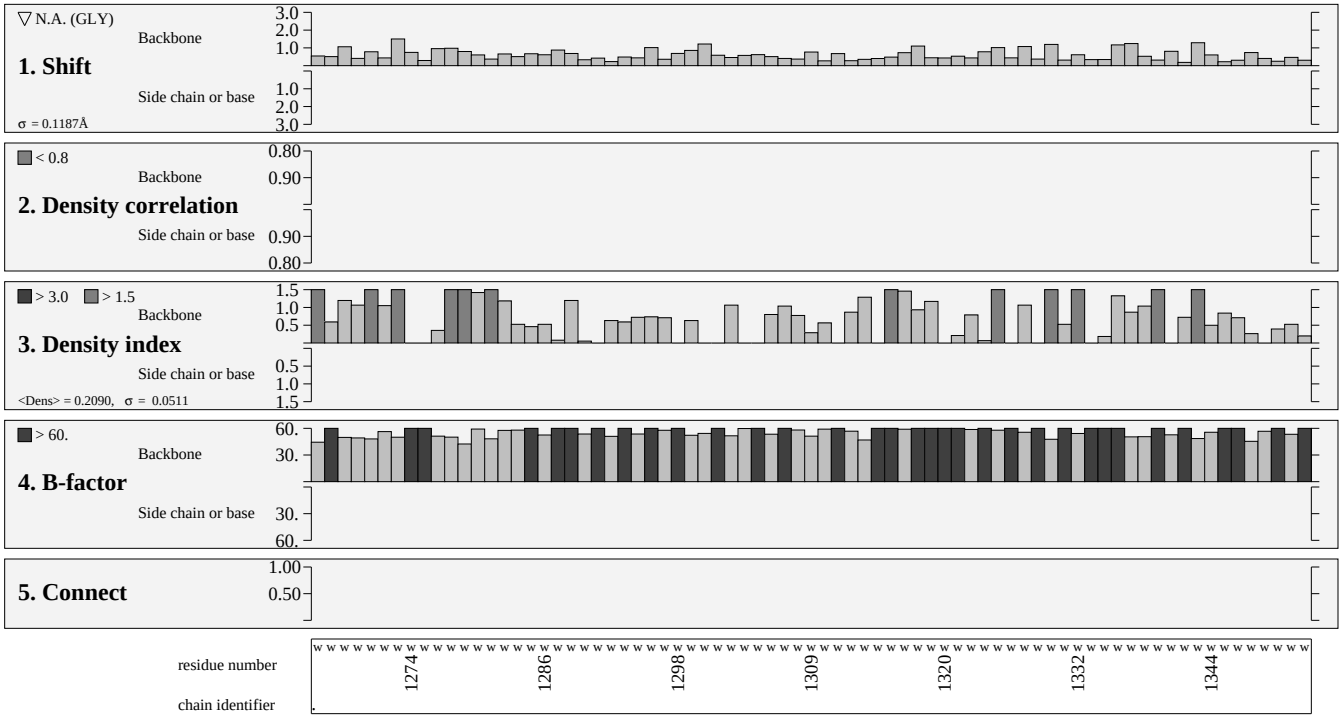
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (35)



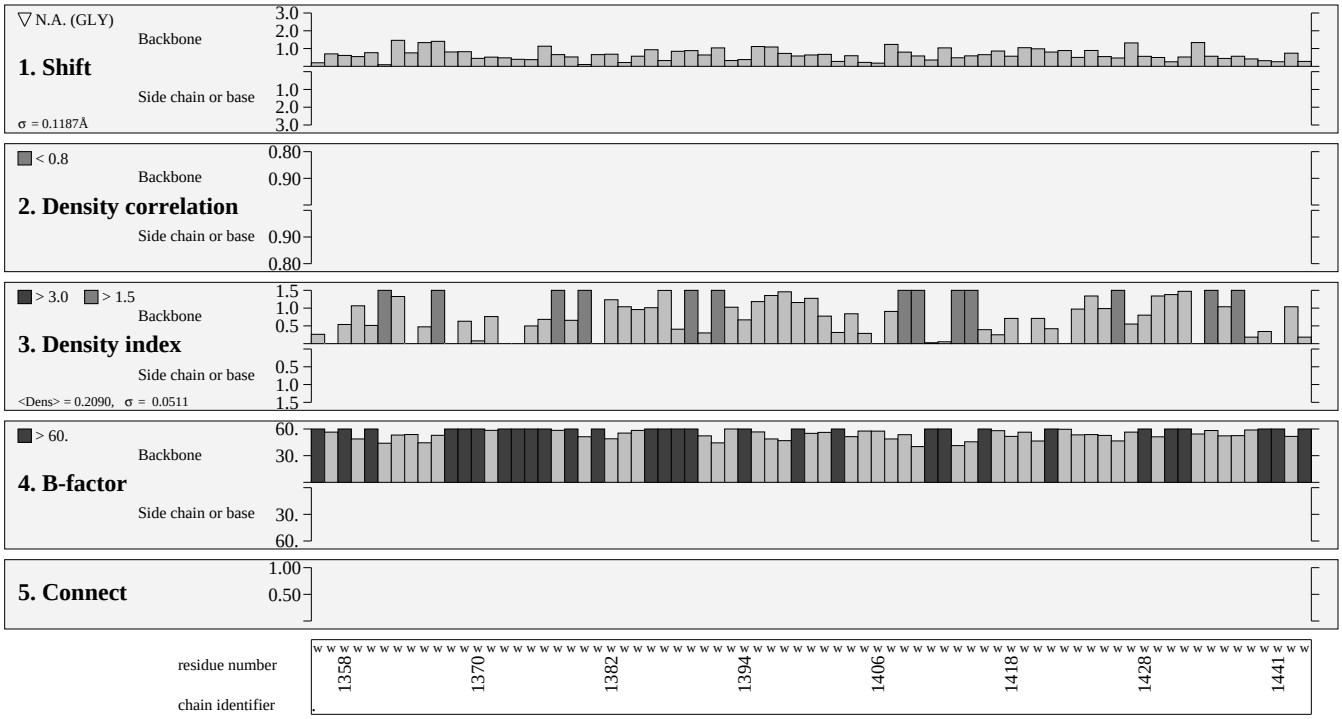


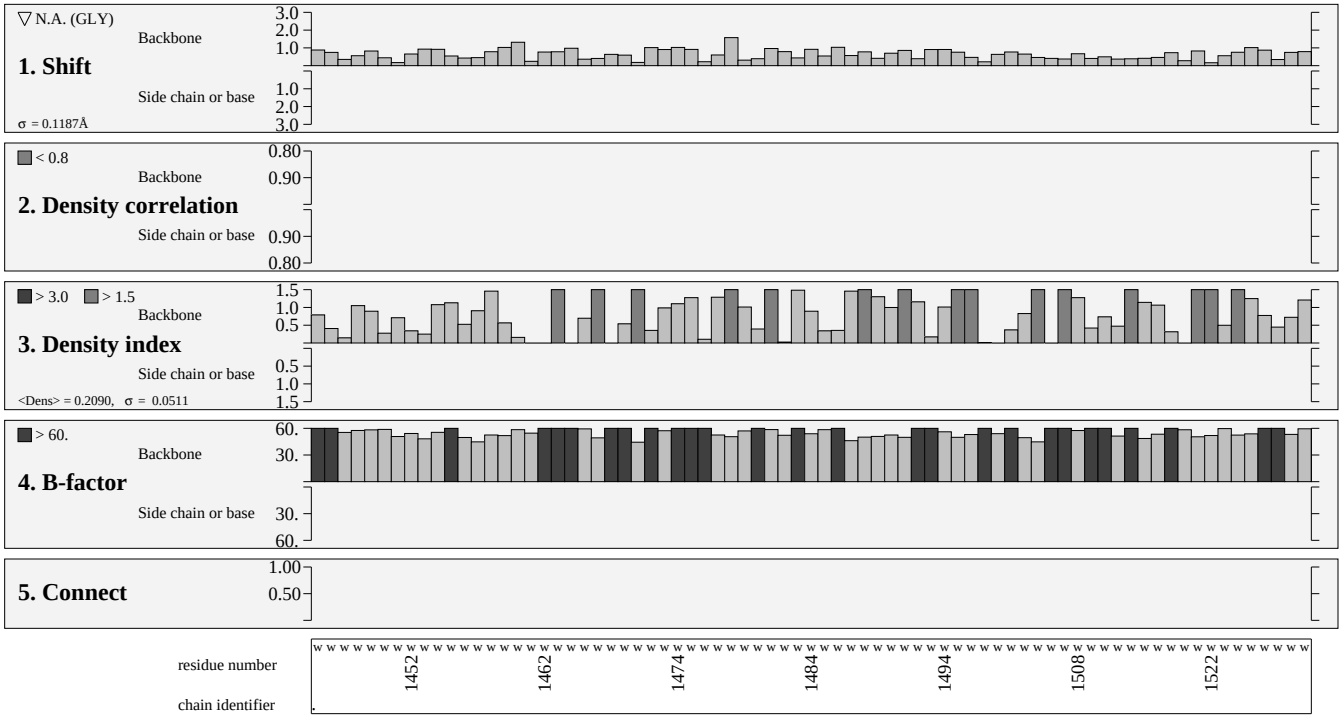
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (36)



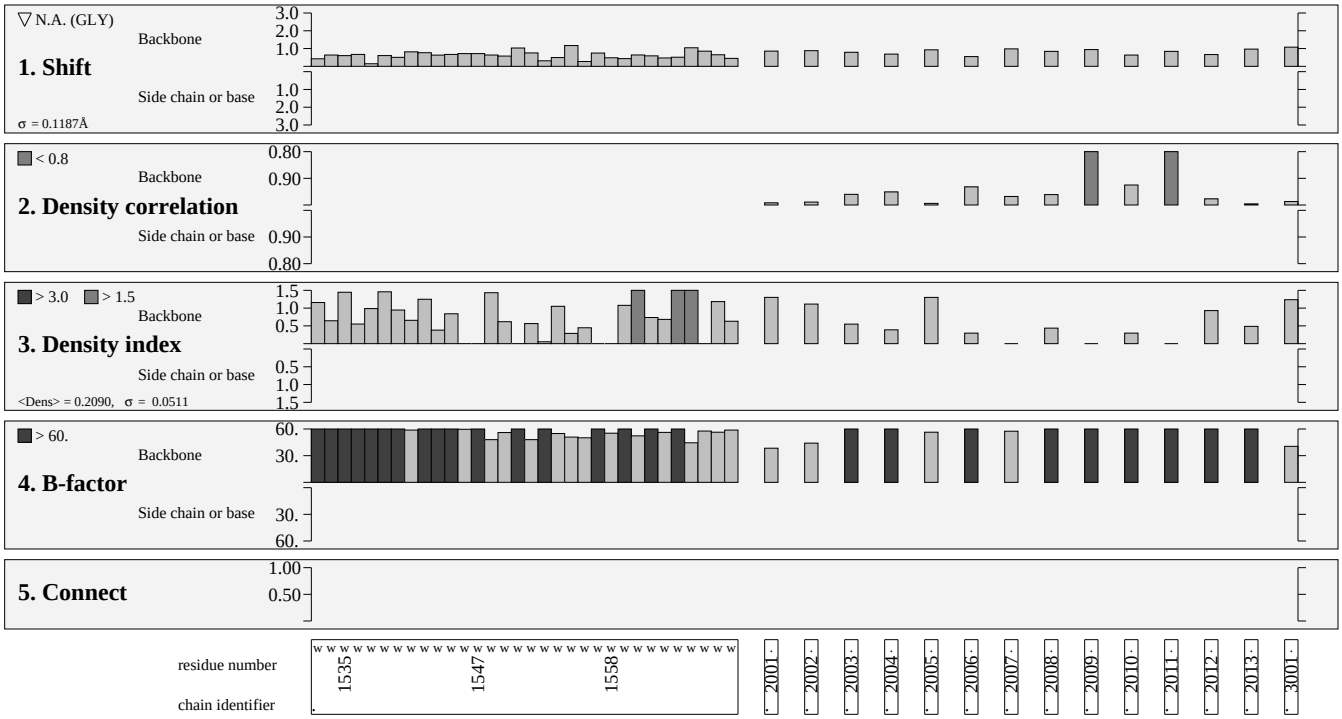


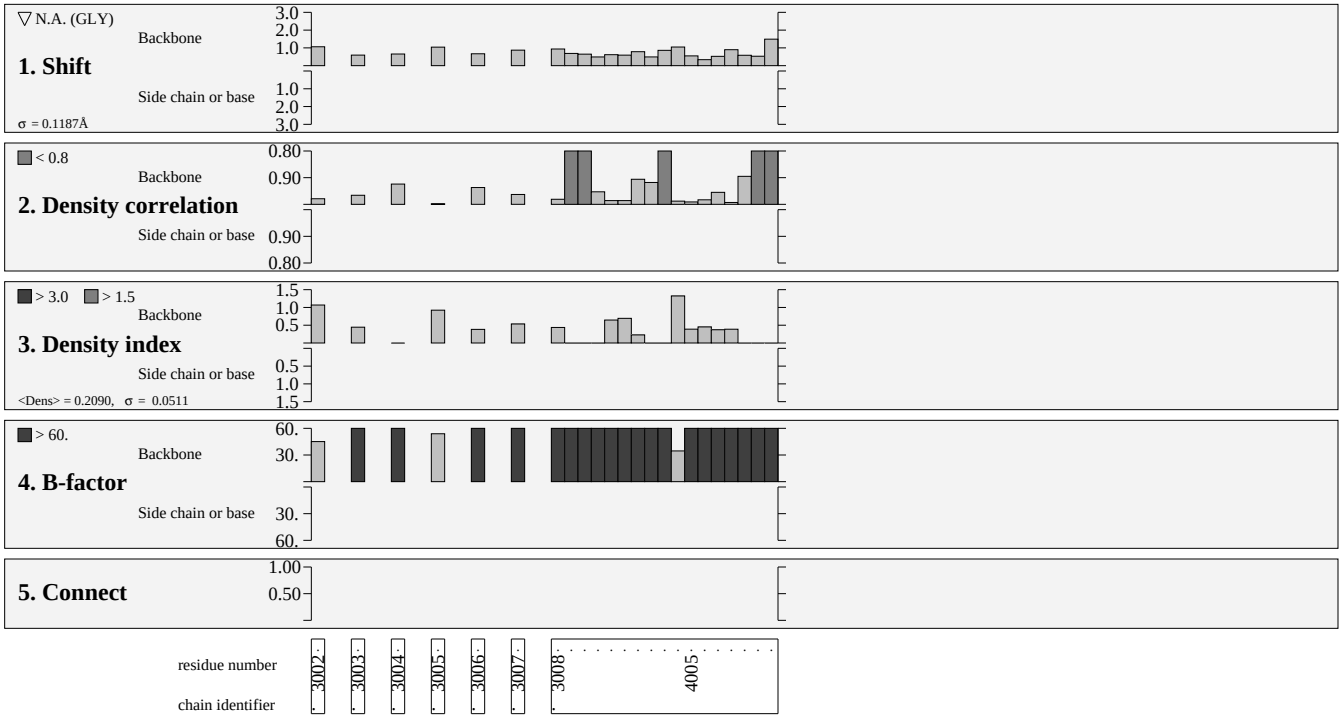
SFCHECK 6.0.5

Structure Factor Check

1PPJ

Local estimation (37)





SFCHECK 6.0.5