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

# Structure Factor Check

## 3VRA

| | |
|---|---|
| Title: | MITOCHONDRIAL RHODOQUINOL−FUMARATE REDUCTASE FROM THE PARASI NEMATODE ASCARIS SUUM WITH THE SPECIFIC INHIBITOR ATPENIN A |
| Date: | 07−APR−12 |
| PDB code: | 3VRA |

### Crystal

Cell parameters:

a: 122.82 A  b: 132.25 A  c: 220.58 A

α: 90.00  β: 90.00  γ: 90.00

Space group: P 21 21 21

### Model

18262 atoms

| | |
|---|---|
| Number of chains: | 24 |
| Volume not occupied by model: | 56.4 % |
| <B> (for atomic model): | 96.7 A^2 |
| σ(B): | 4.70 A^2 |
| Matthews coefficient: | 3.50 |
| Corresponding solvent % : | 64.62 |

### Refinement

| | |
|---|---|
| Program: | REFMAC 5.5.0109 |
| Nominal resolution range: | 49.7 − 3.44 A |
| Reported R−factor: | 0.205 |
| Number of reflections used: | 41132 |
| Reported Rfree: | 0.28 |
| Sigma cut−off: | N.A. |

### Structure Factors

**Input**

| | | |
|---|---|---|
| Nominal resolution range: | | 49.7 − 3.44 A |
| Reflections in file: | | 43349 |
| Unique reflections | above 0: | 43349 |
| | above 1σ: | 42401 |
| | above 3σ: | 25401 |

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| | |
|---|---|
| Nominal resolution range: | 49.7 − 3.44 A |
| \05max. from input data, min. from author\05 | |
| Used reflections: | 43348 |
| Reflections out of resolution: | 1 |
| Completeness: | 89.5 % |
| R_stand(F) = <σ(F)>/<F> : | 0.097 |
| Anisotropic distribution of Structure Factors | |
| ratio of eigen values: | 0.9350 1.0000 0.9435 |
| B_overall (by Patterson): | 68.A^2 |
| Optical resolution: | 2.55 A |
| Expected opt. resol. for complete data set: | 2.55 A |
| Estimated minimal error: | 0.149 A |

### Model vs. Structure Factors

| | |
|---|---|
| R−factor for all reflections: | 0.301 |
| Correlation factor: | 0.797 |
| R−factor: | 0.307 |
| for F > 2.0 σ | |
| nom. resolution range: | 49.72 − 3.44A |
| reflections used: | 42399 |
| Rfree: | 0.358 |
| Nfree: | 2169 |
| R−factor without free−refl.: | 0.304 |
| Non free−reflections: | 40230 |
| <u> (error in coords by Luzzati plot): | 0.665 A |
| Estimated maximal error: | 0.329 A |
| DPI: | 0.651 A |

**Scaling**

| | |
|---|---|
| Scale: | 0.792 |
| Bdiff: | −3.32 |

Anisothermal Scaling (Beta):

4.4900 5.6745 4.2389 −0.0000 −0.0000 −0.0000

Solvent correction − Ks,Bs: 0.570 250.448

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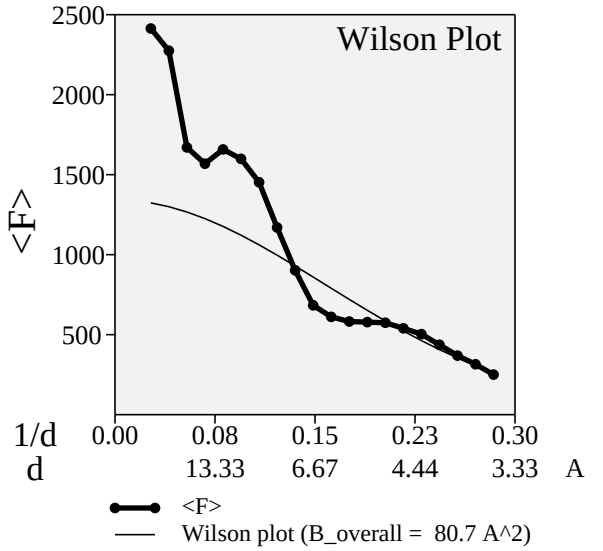
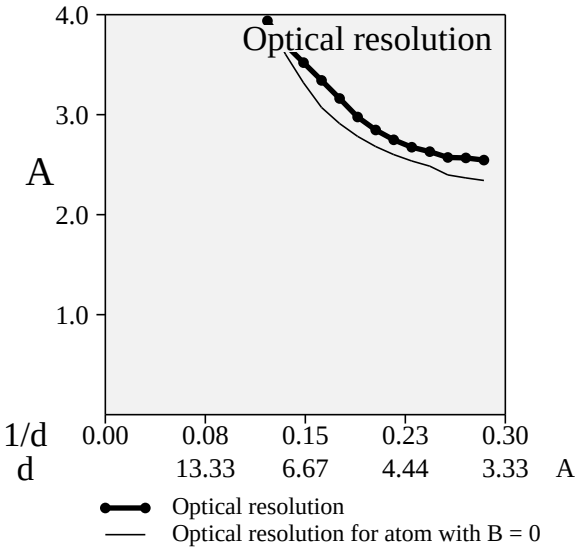
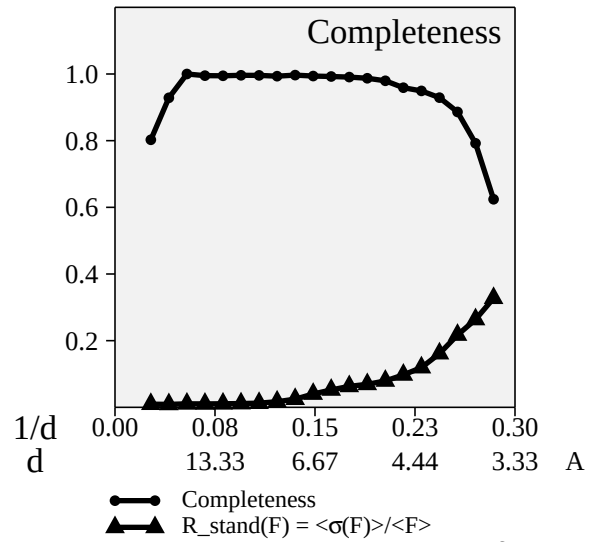
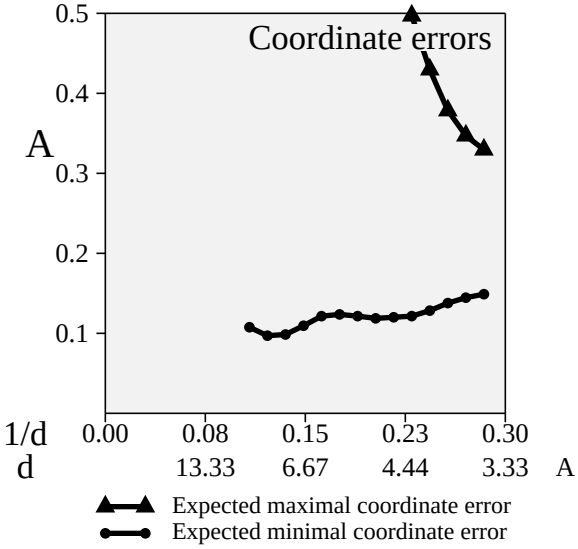
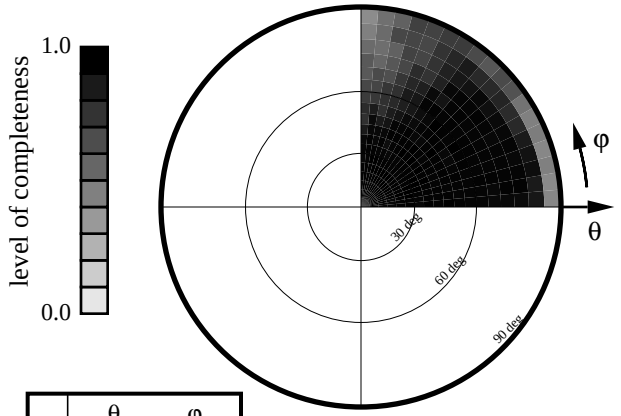


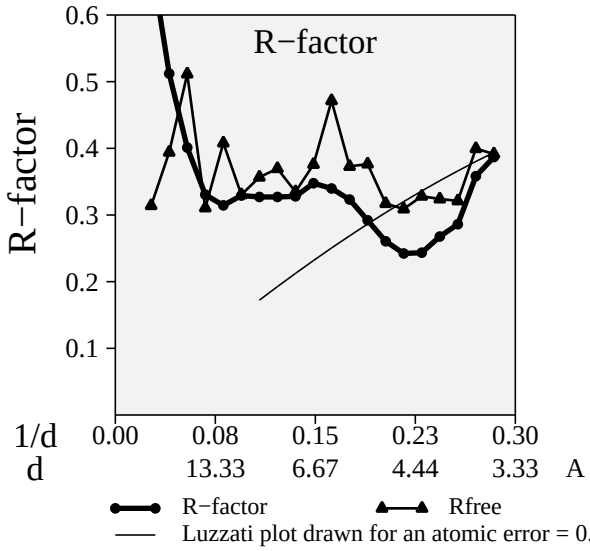




Stereographic projection of
the averaged radial completeness




| | 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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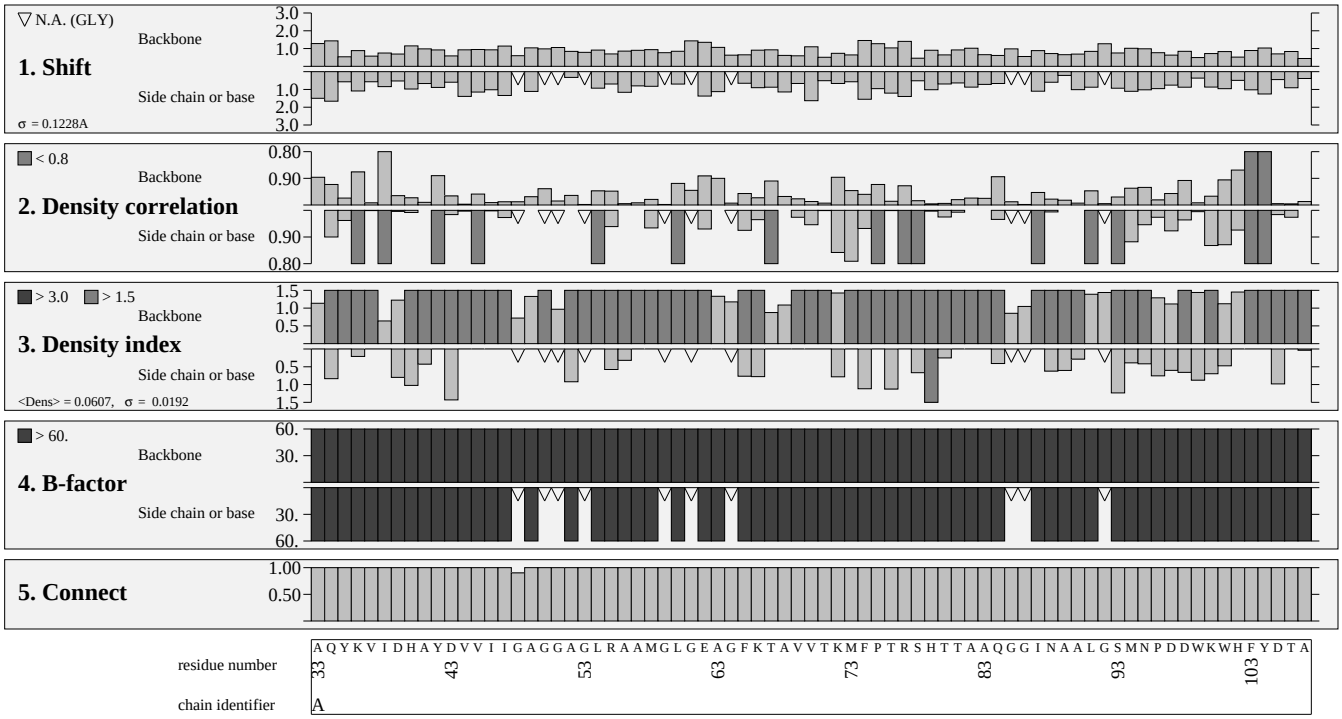
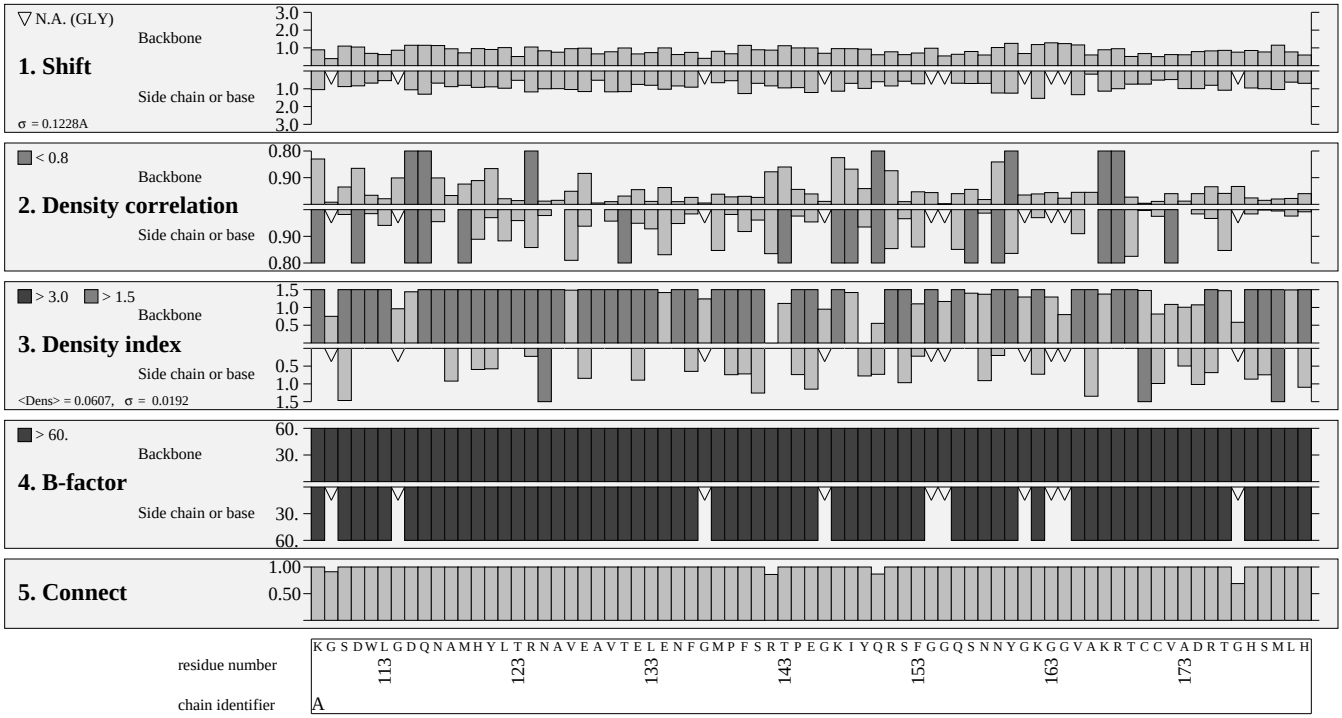
# Structure Factor Check

## 3VRA

### Local estimation

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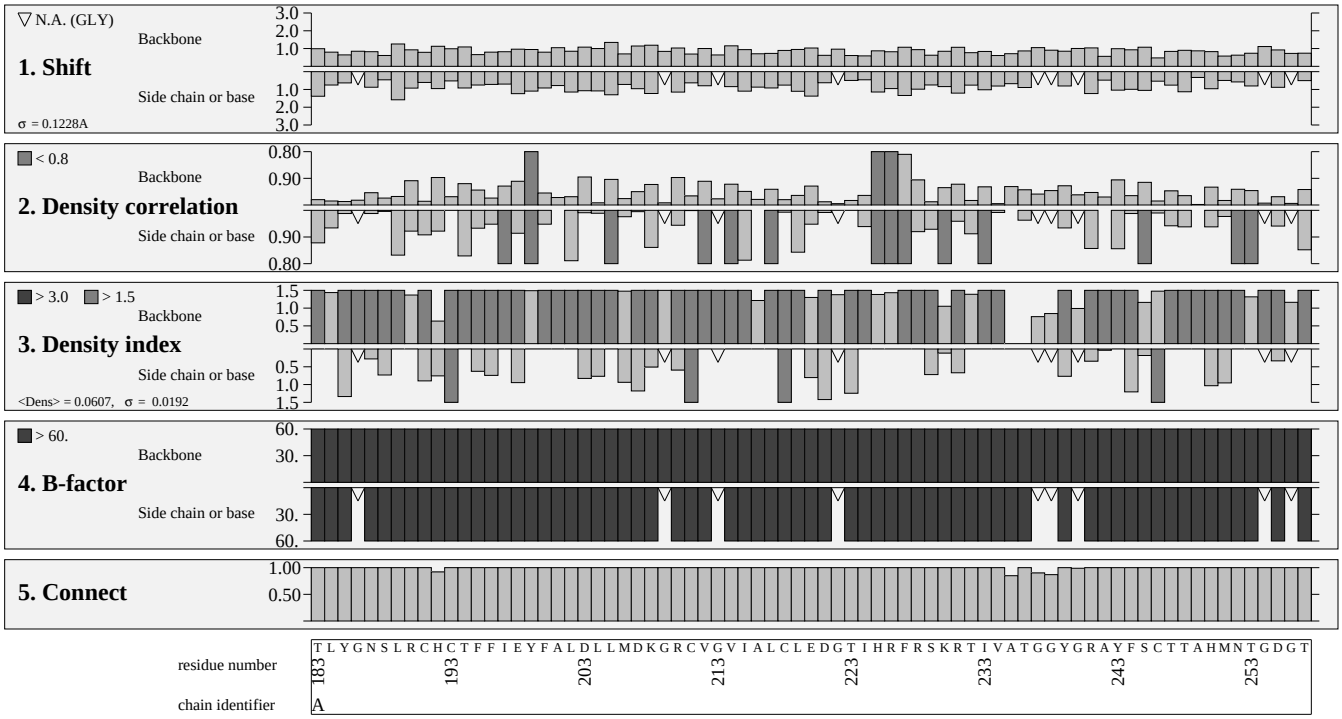
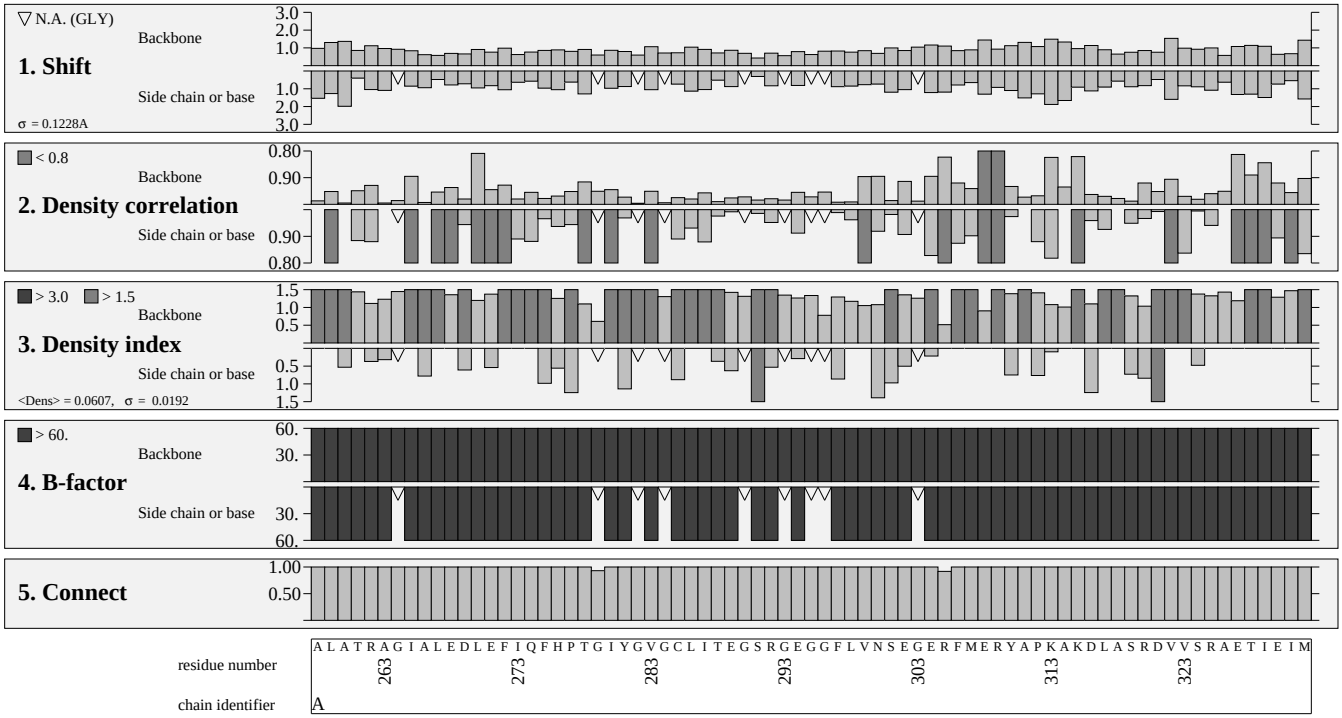
# Structure Factor Check

## 3VRA

### Local estimation (2)

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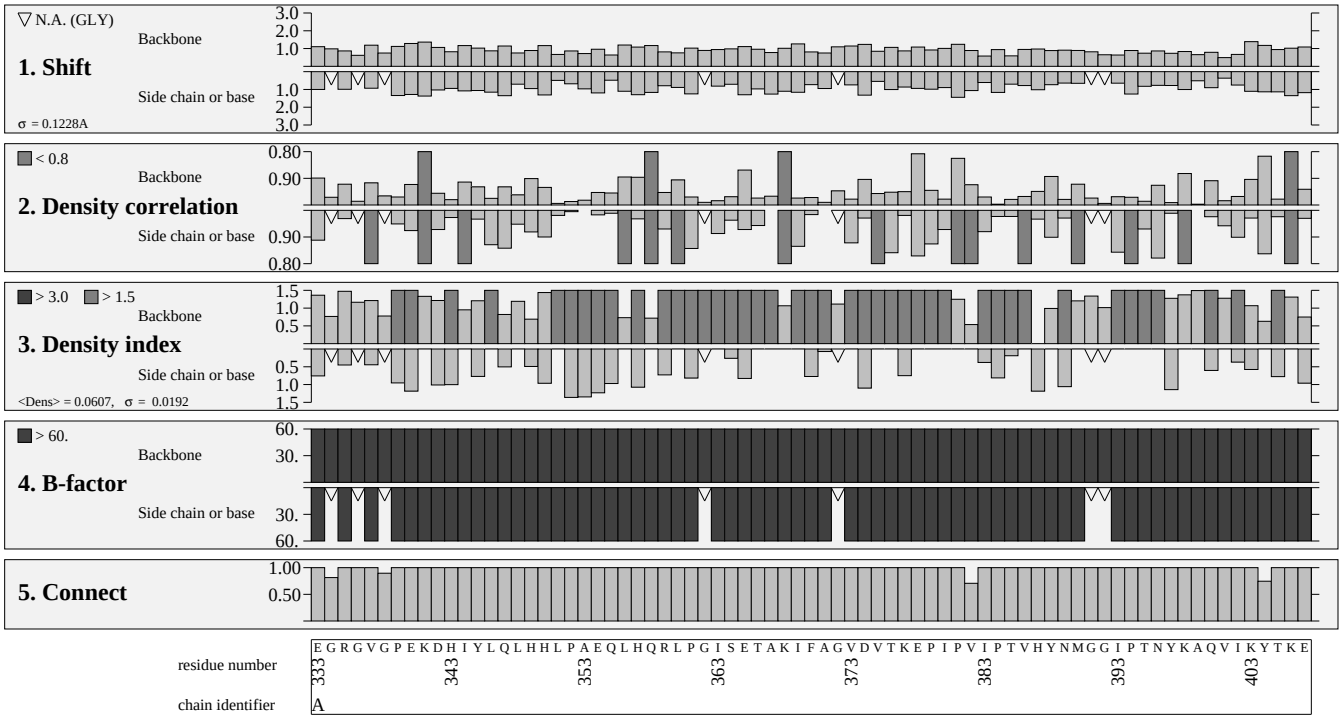
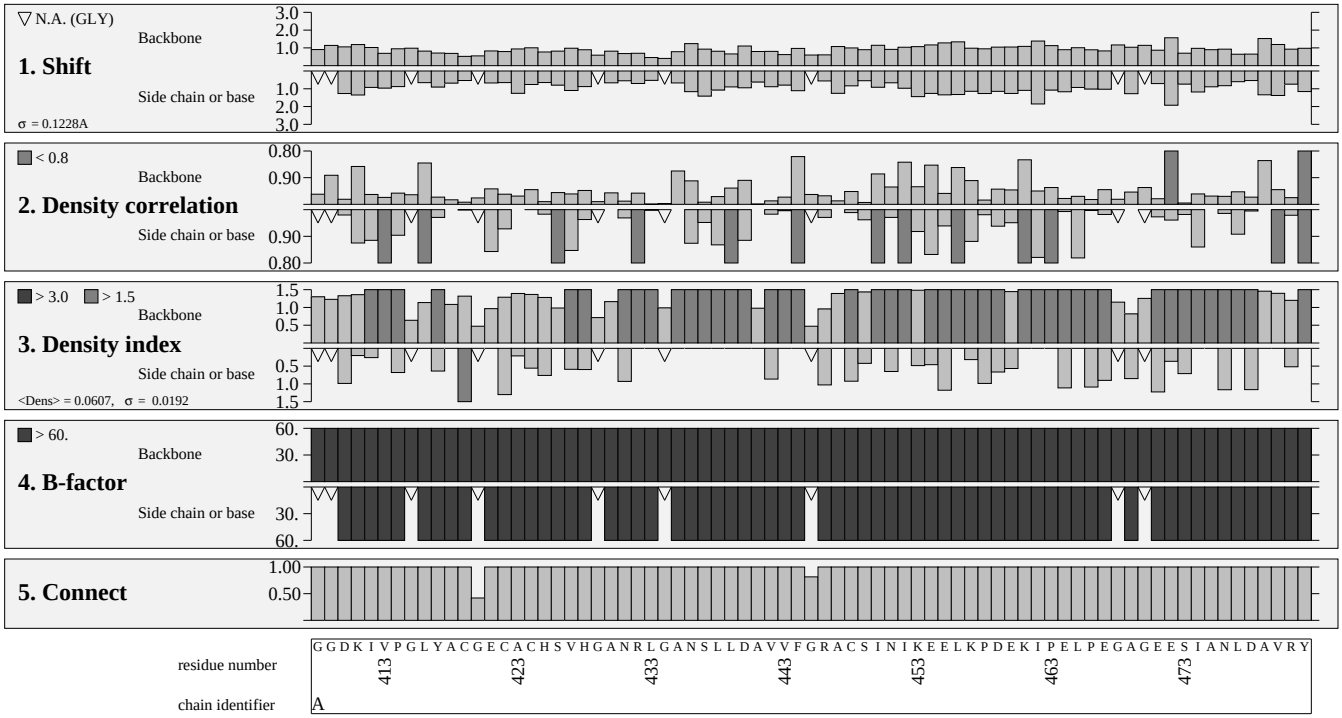
# Structure Factor Check

## 3VRA

### Local estimation (3)

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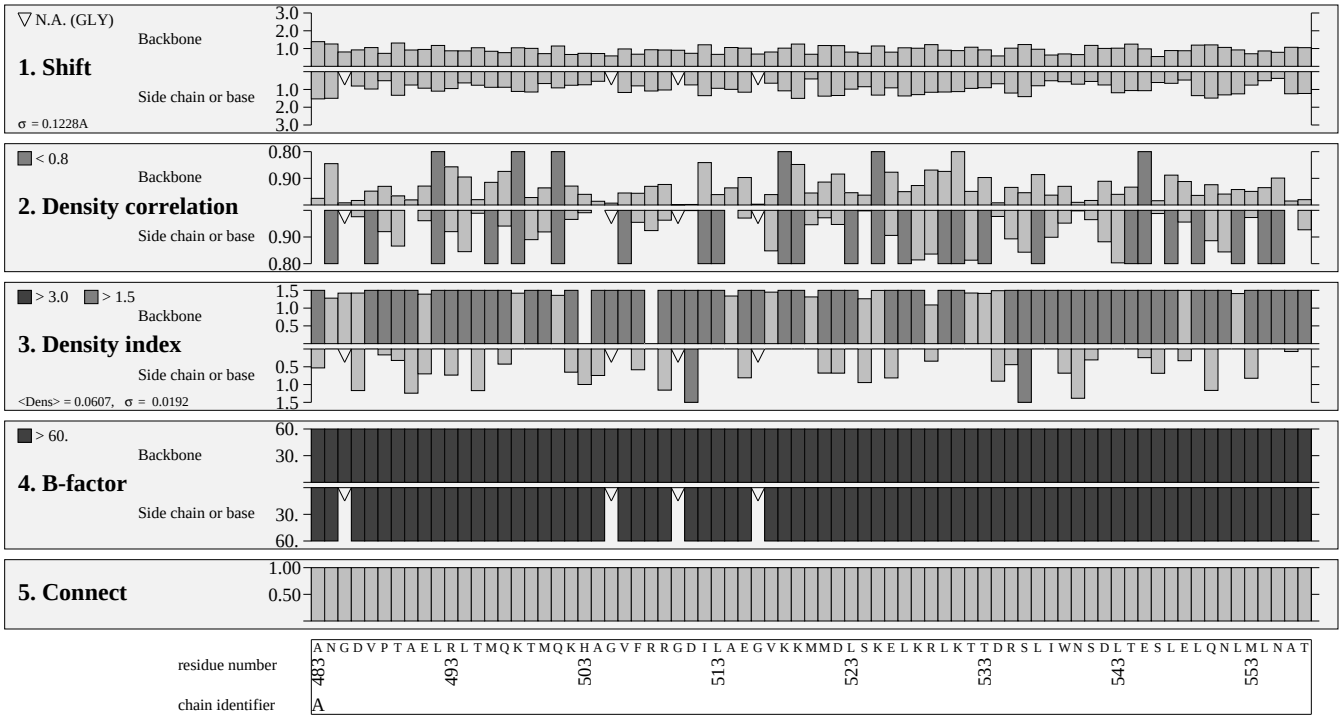
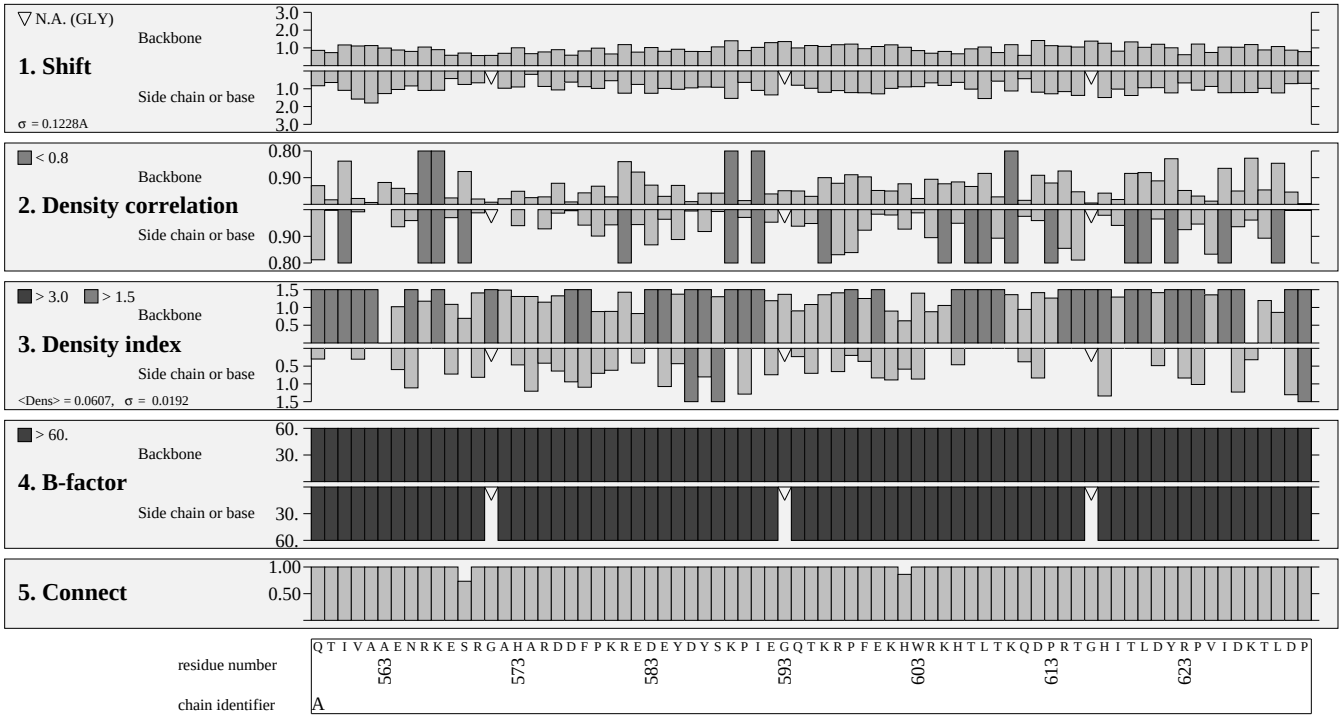
# Structure Factor Check

## 3VRA

### Local estimation (4)

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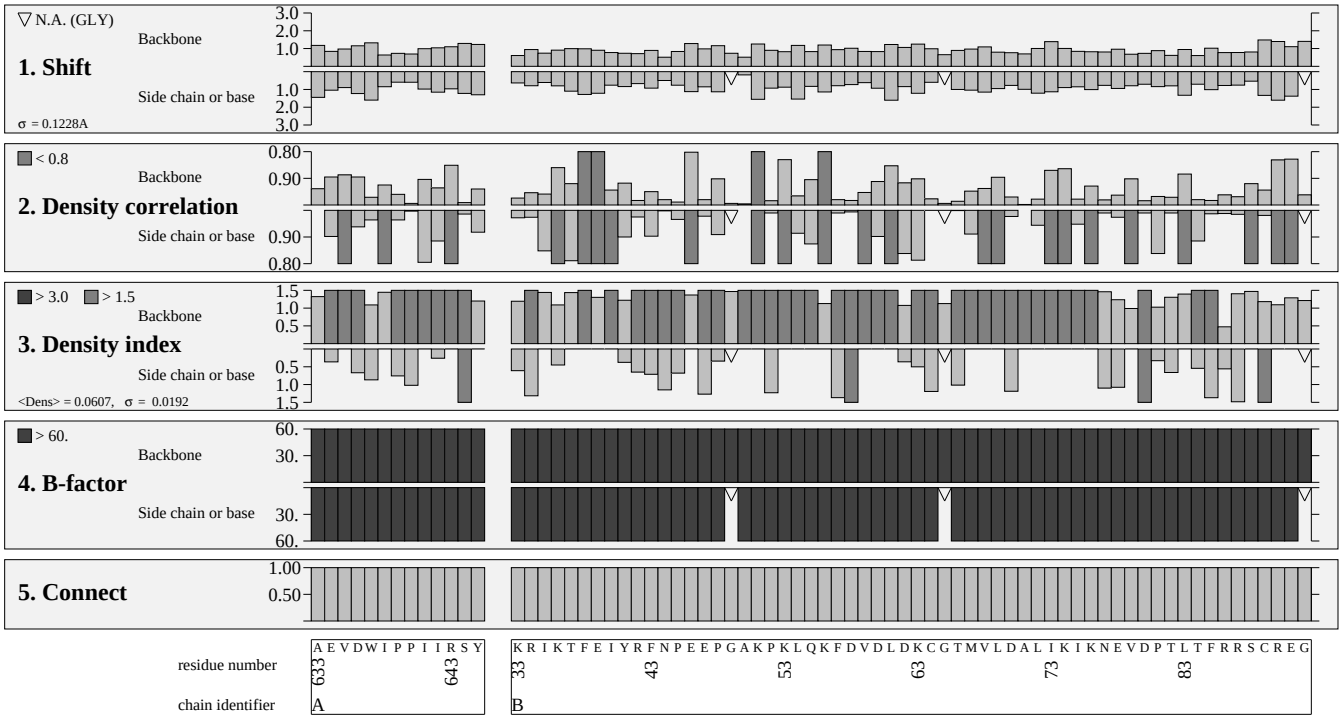
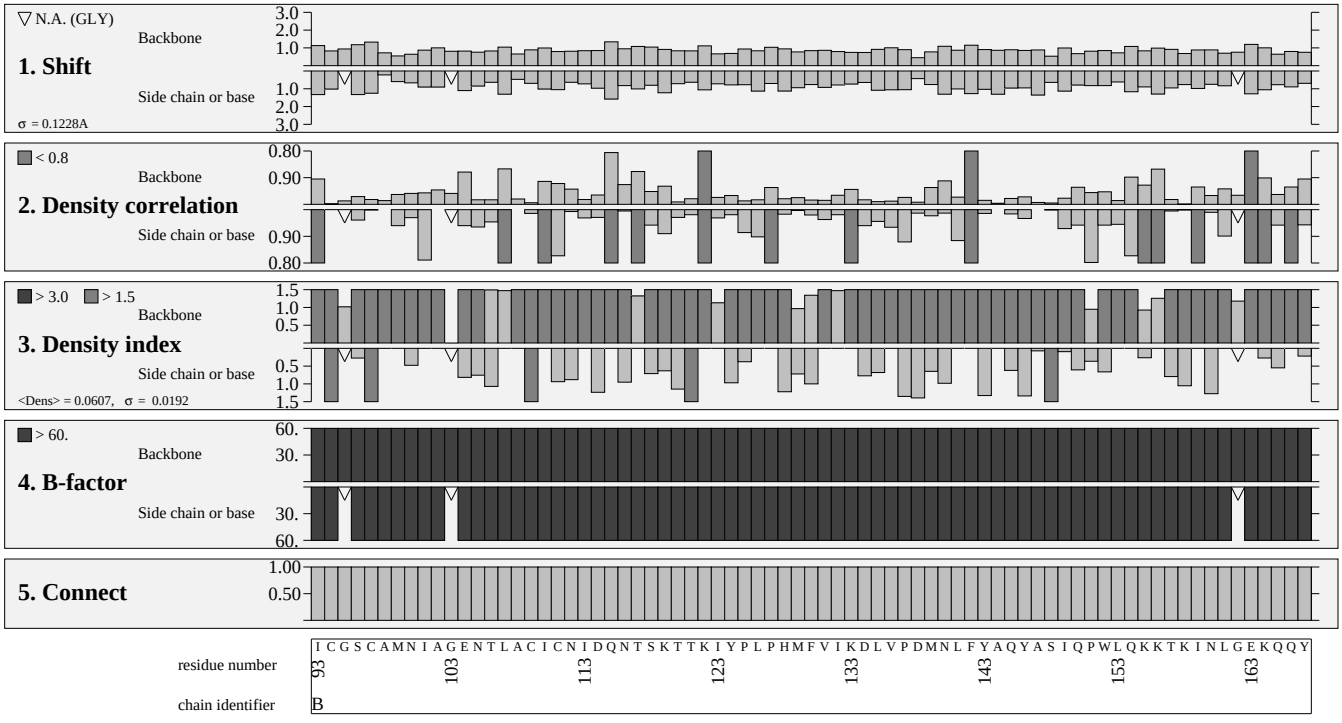
# Structure Factor Check

## 3VRA

### Local estimation (5)

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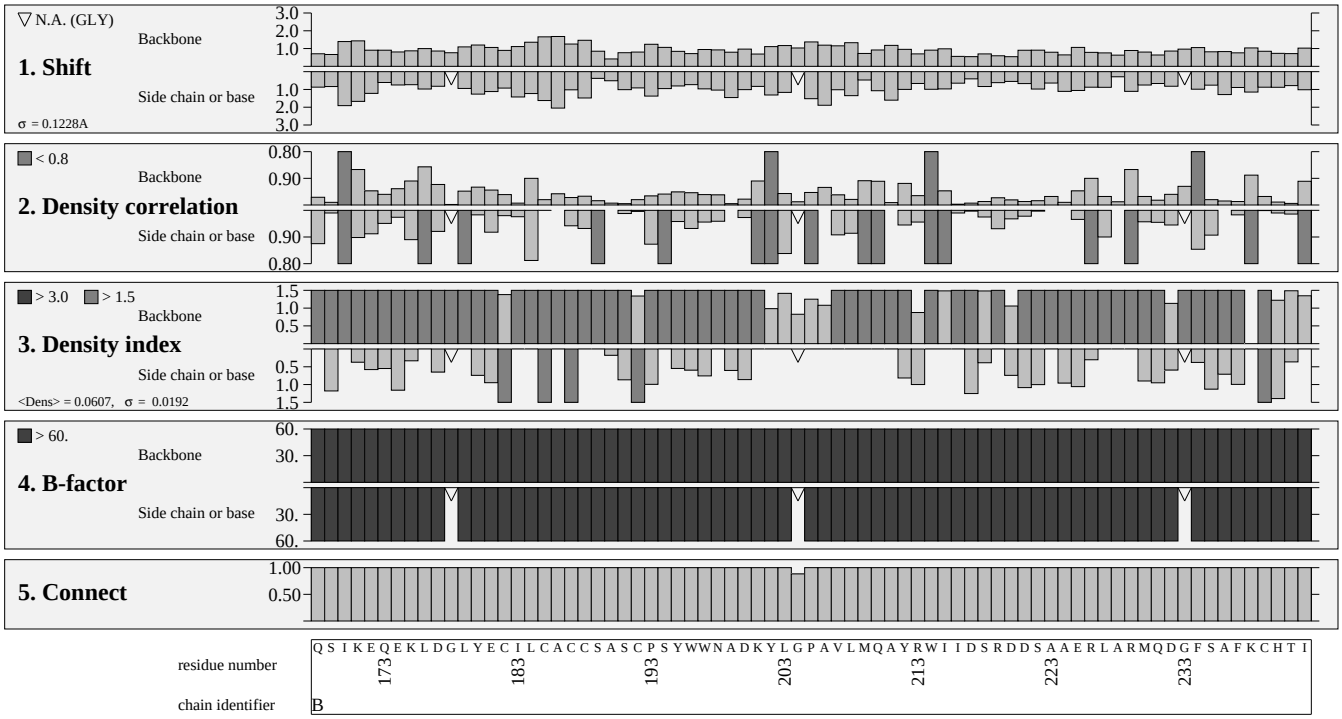
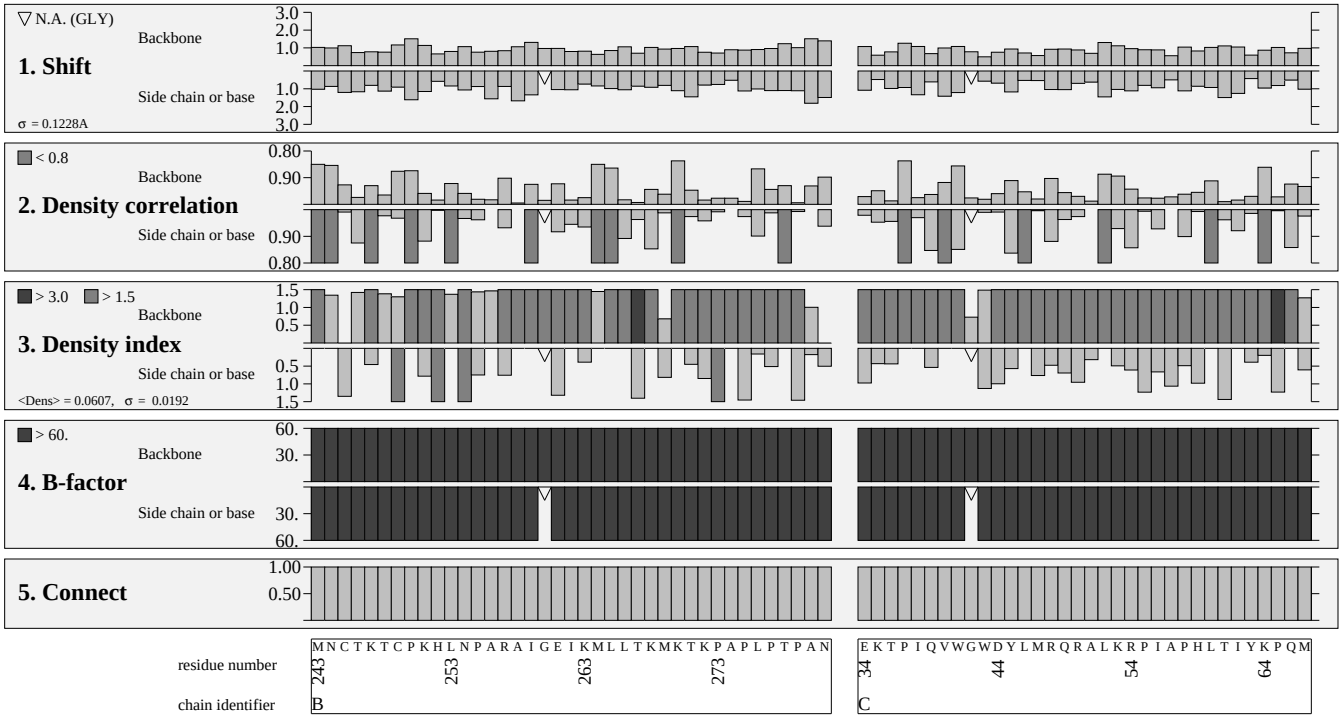
# Structure Factor Check

## 3VRA

### Local estimation (6)

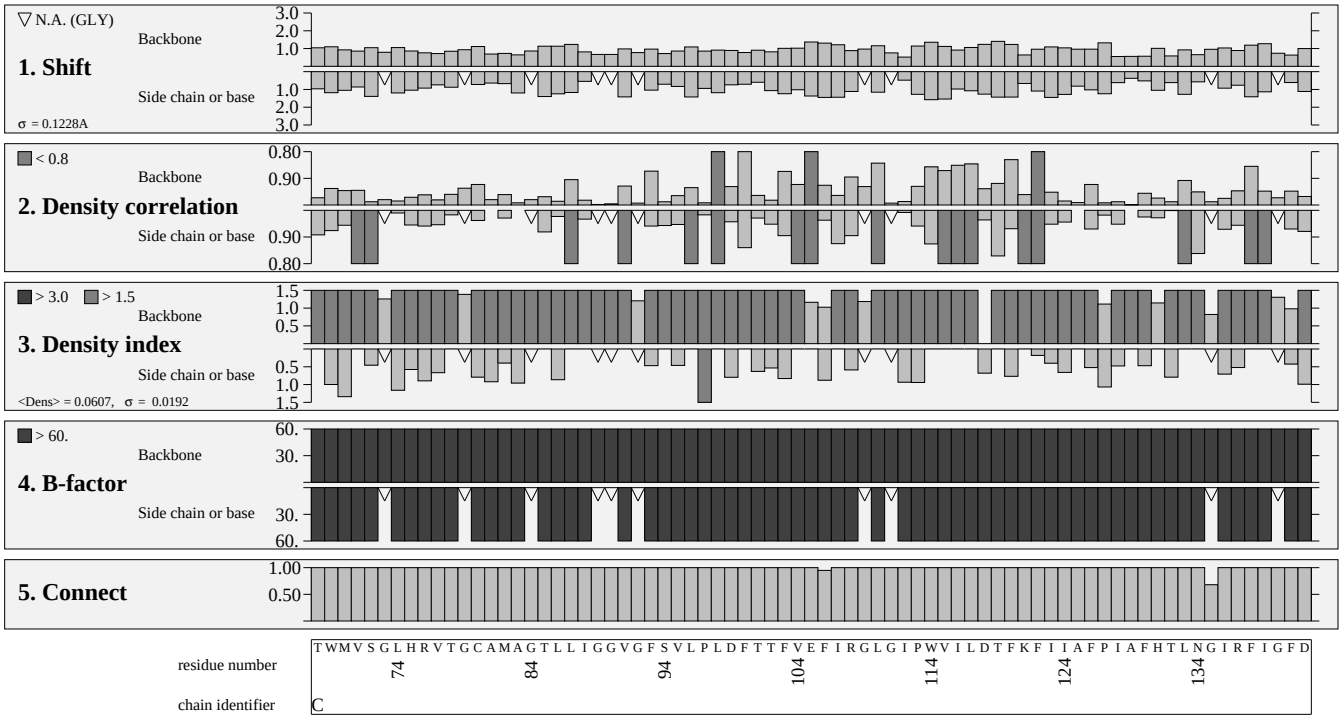


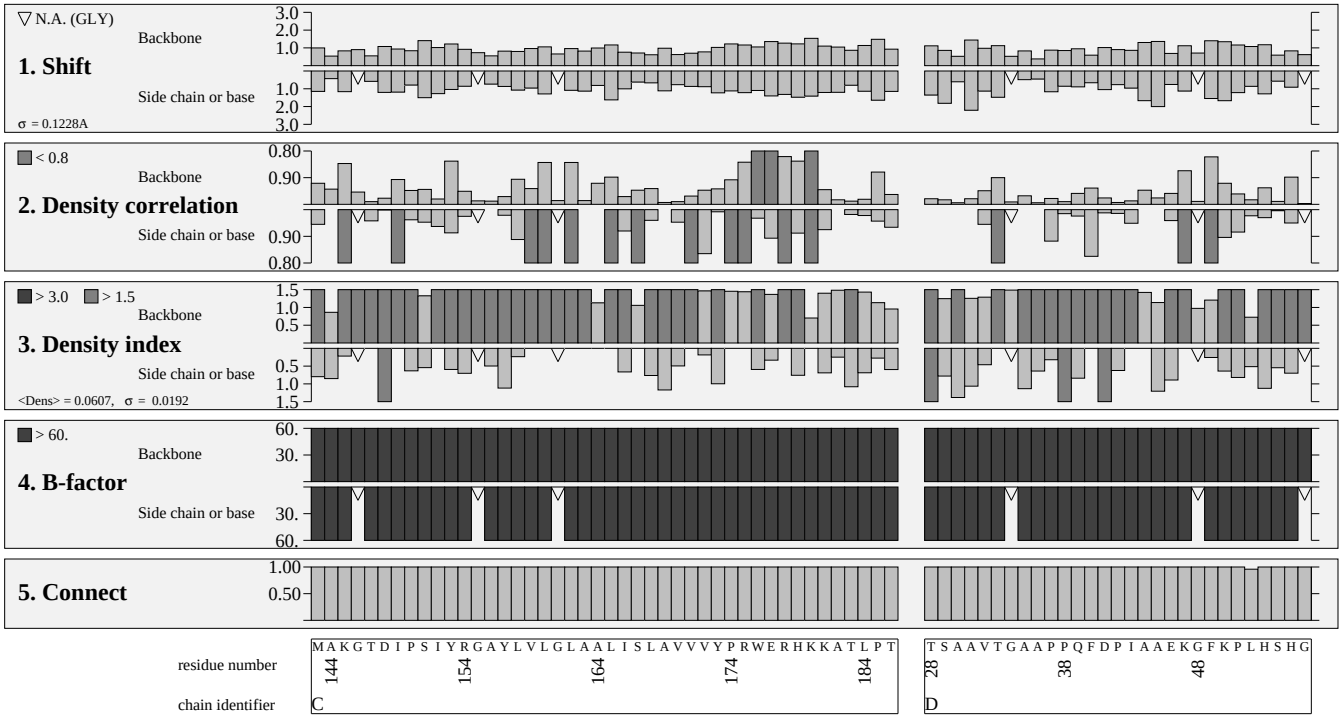



# Structure Factor Check

## 3VRA

### Local estimation (7)

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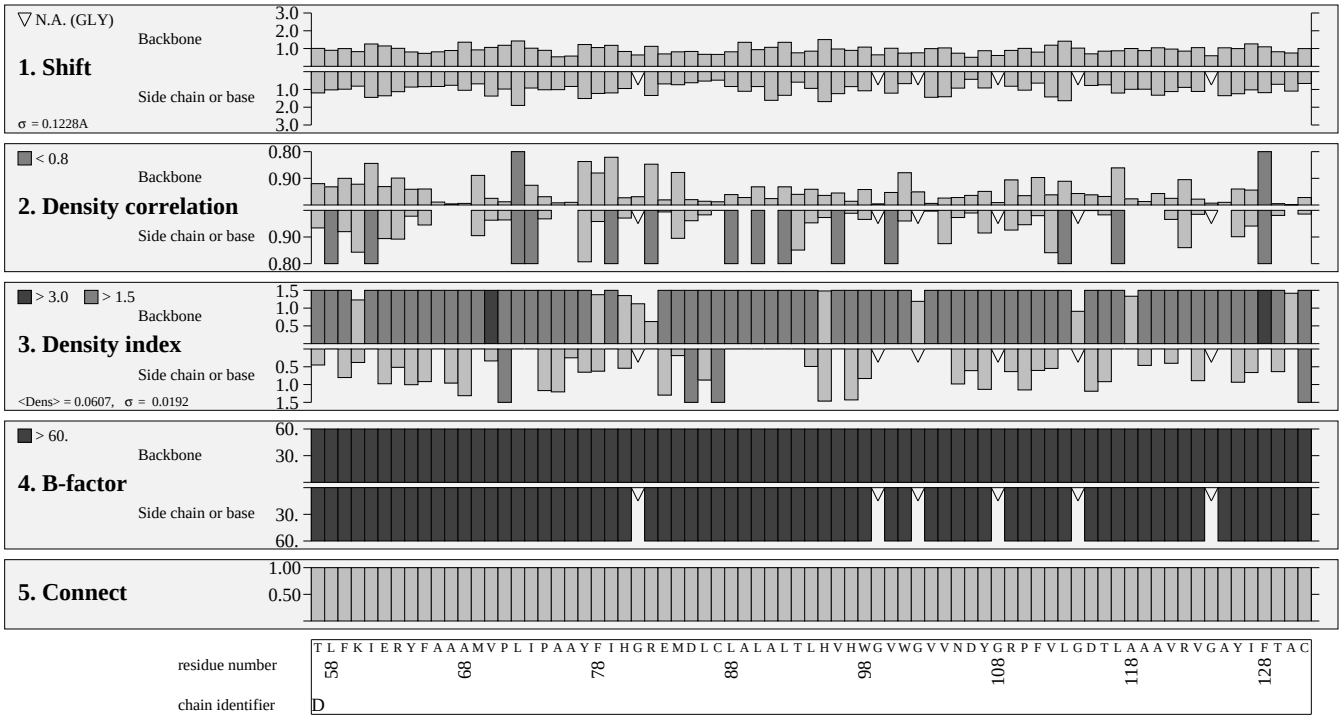
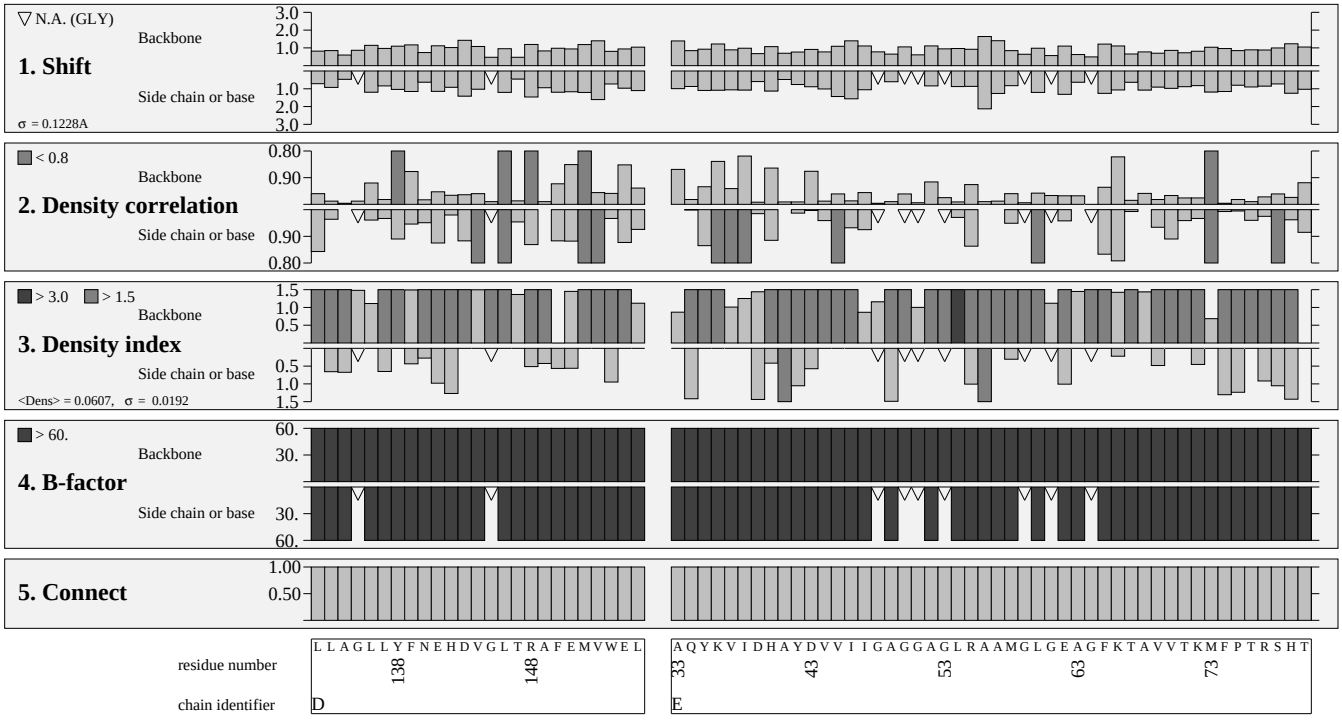
# Structure Factor Check

## 3VRA

### Local estimation (8)

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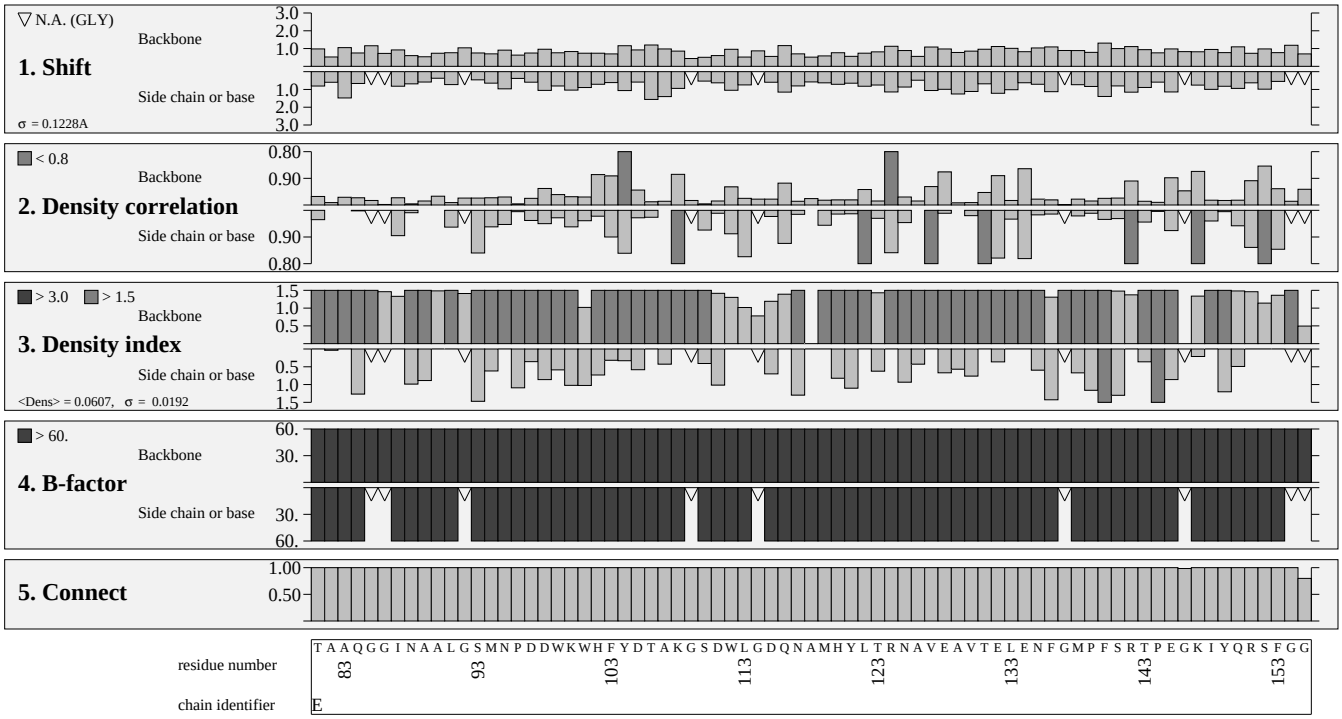
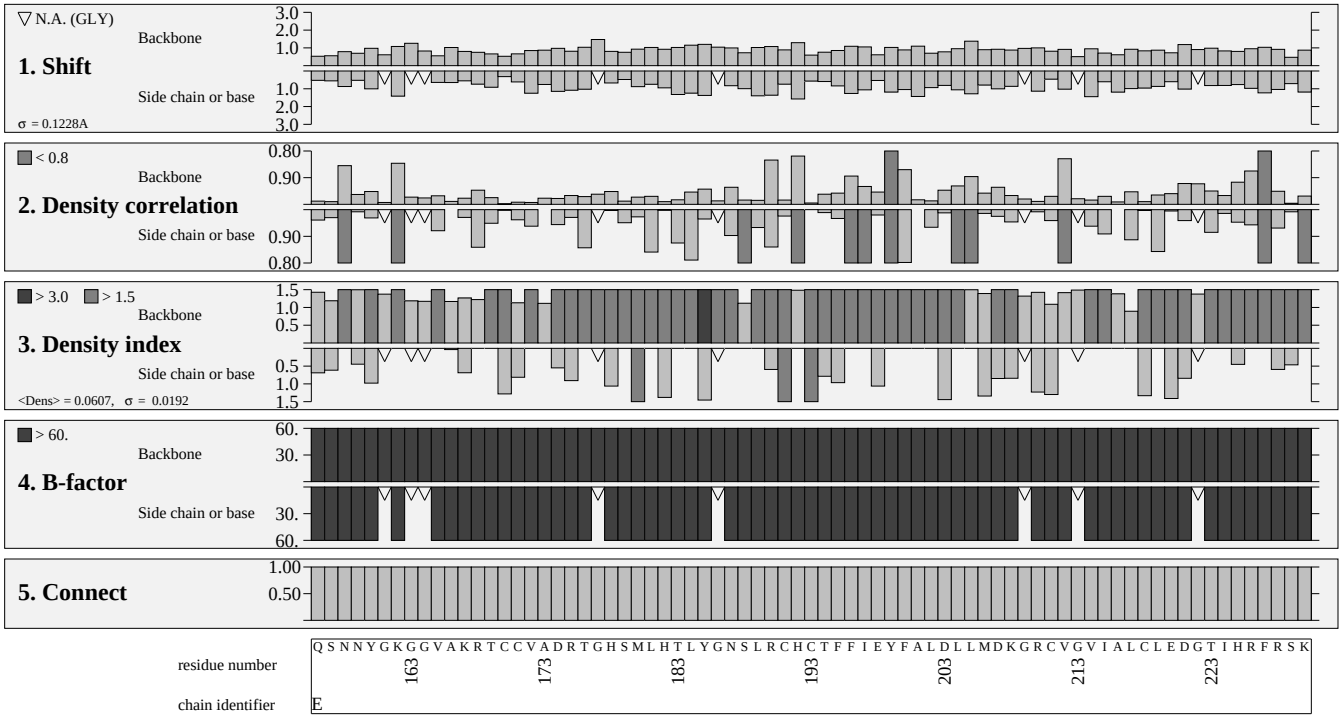
# Structure Factor Check

## 3VRA

### Local estimation (9)

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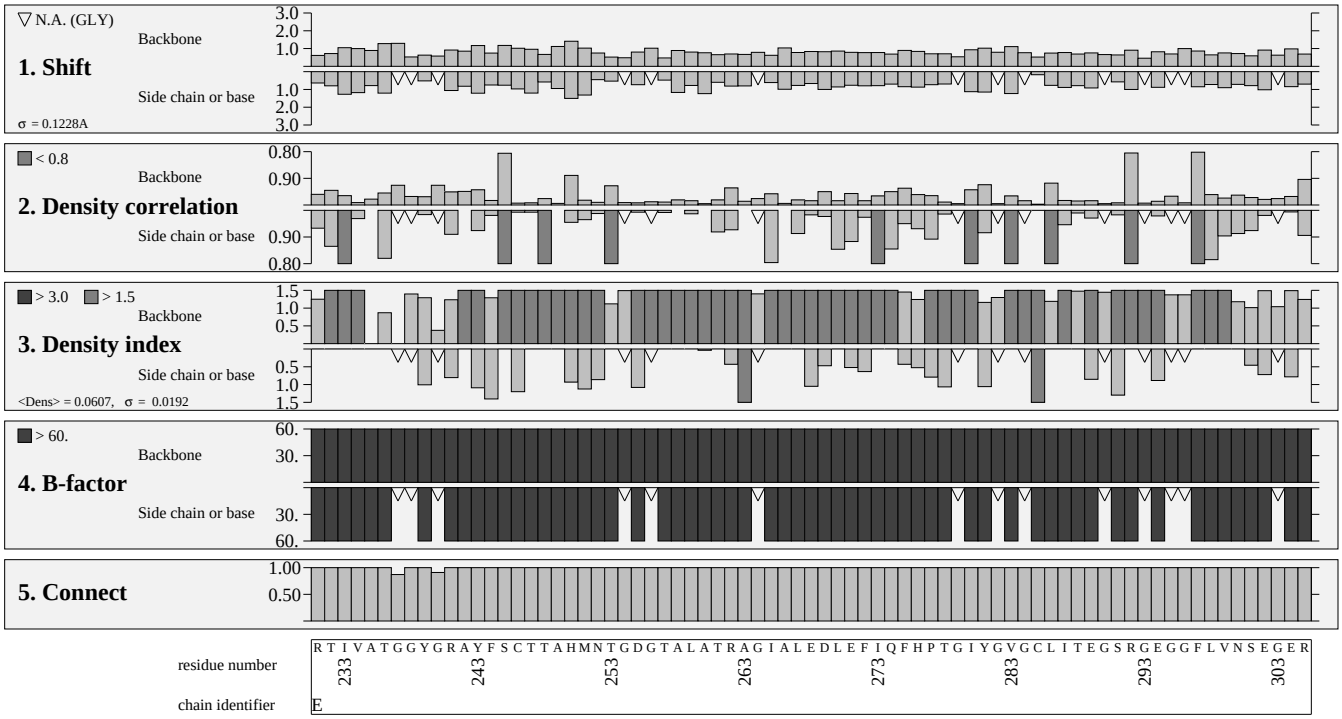
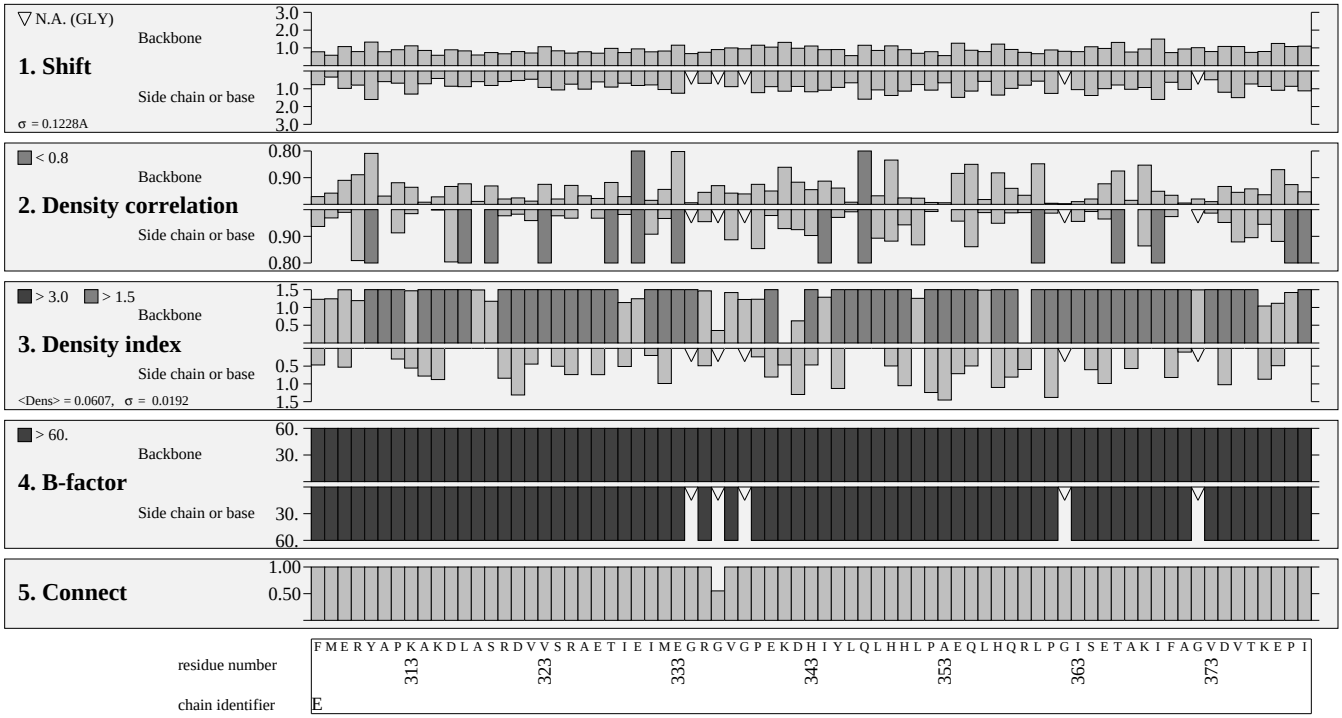
# Structure Factor Check

## 3VRA

### Local estimation (10)

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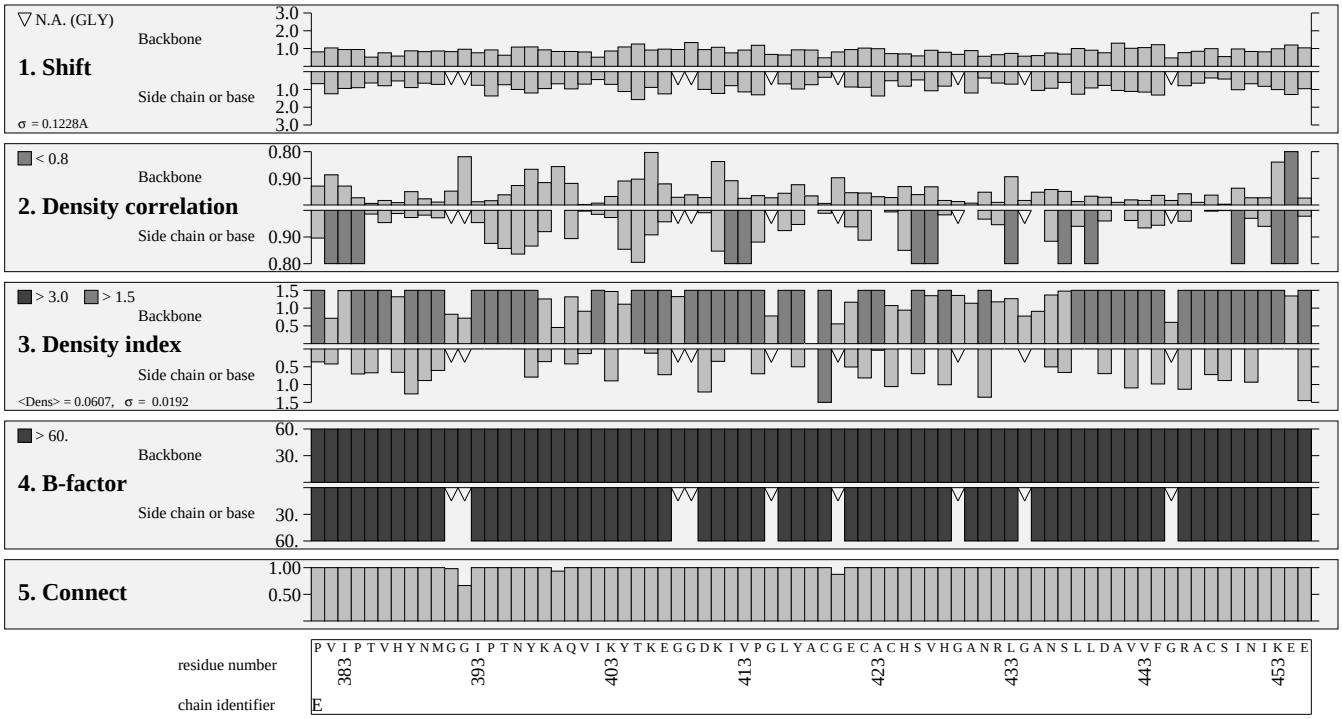
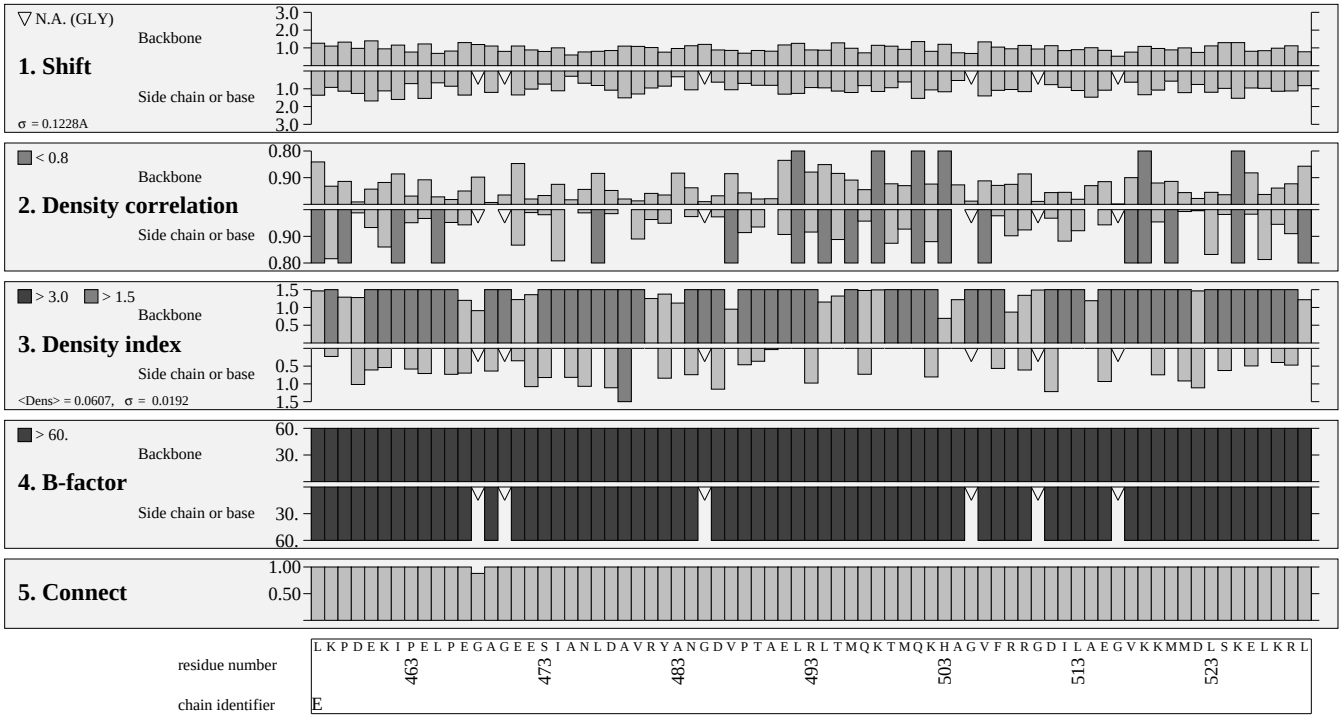
# Structure Factor Check

## 3VRA

### Local estimation (11)

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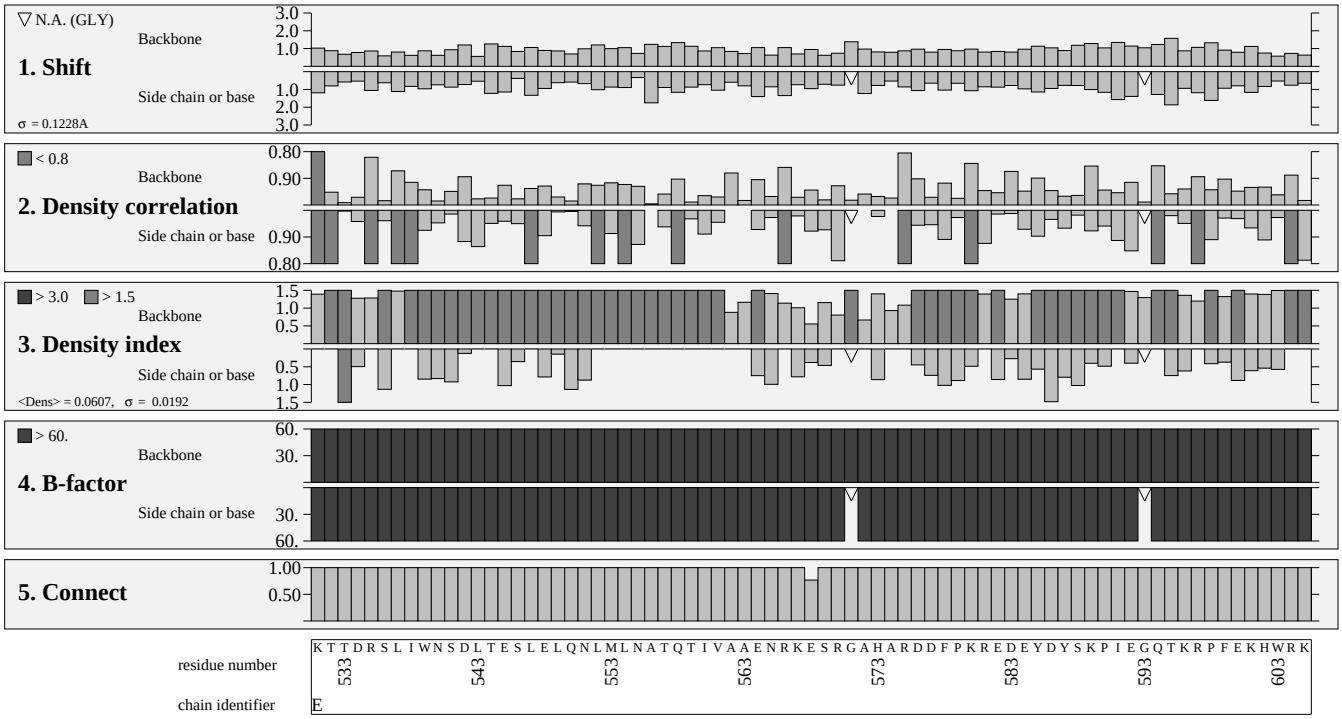
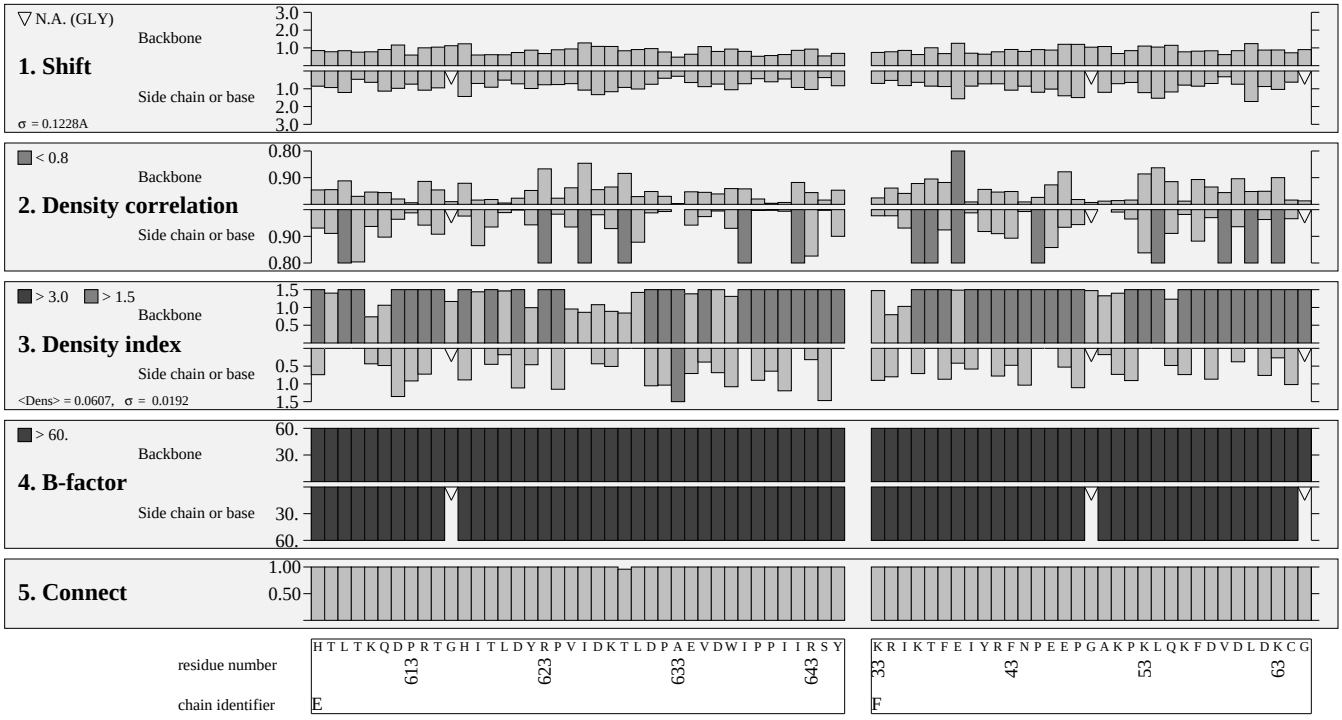
# Structure Factor Check

## 3VRA

### Local estimation (12)

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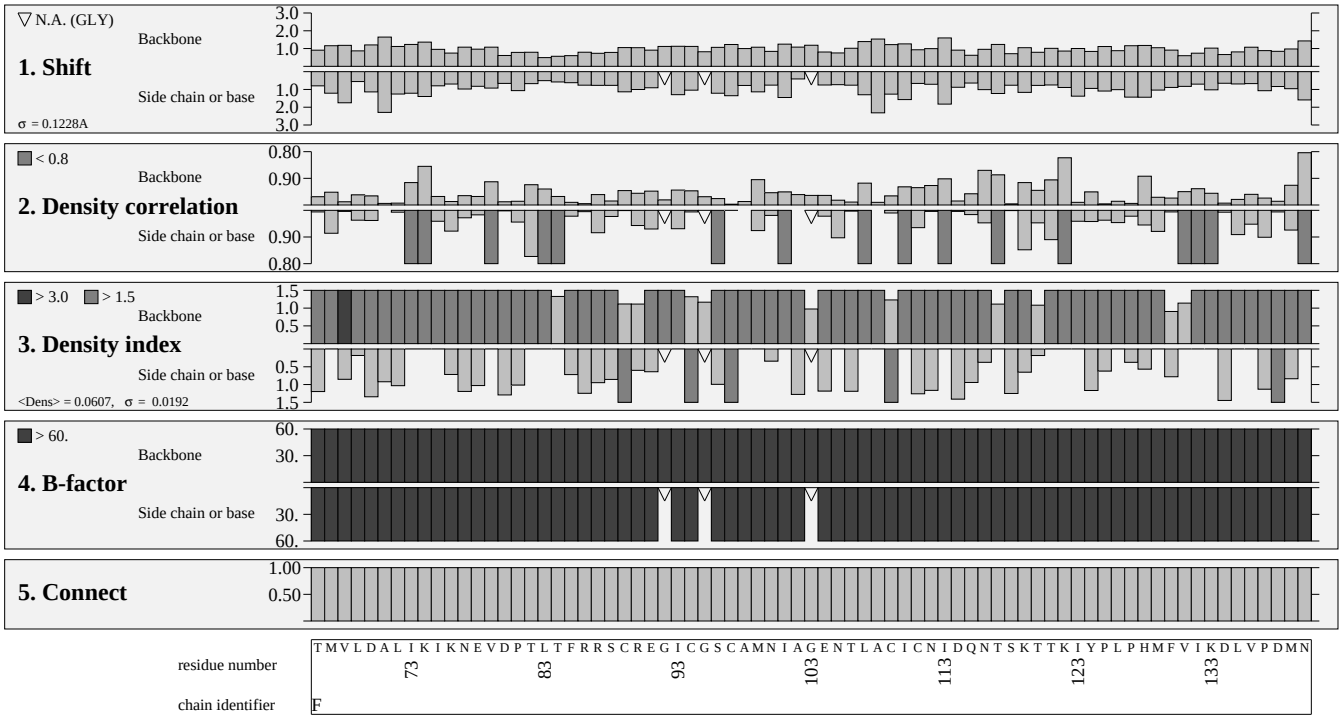
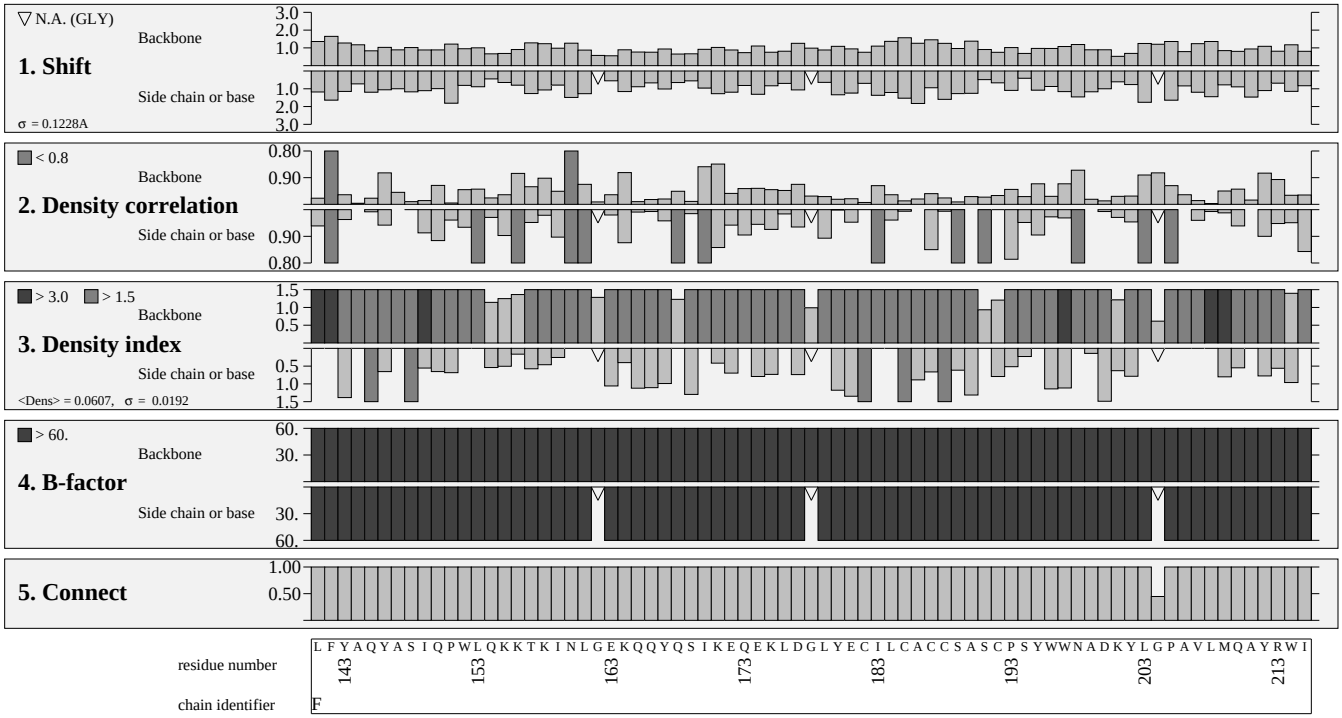
# Structure Factor Check

## 3VRA

### Local estimation (13)

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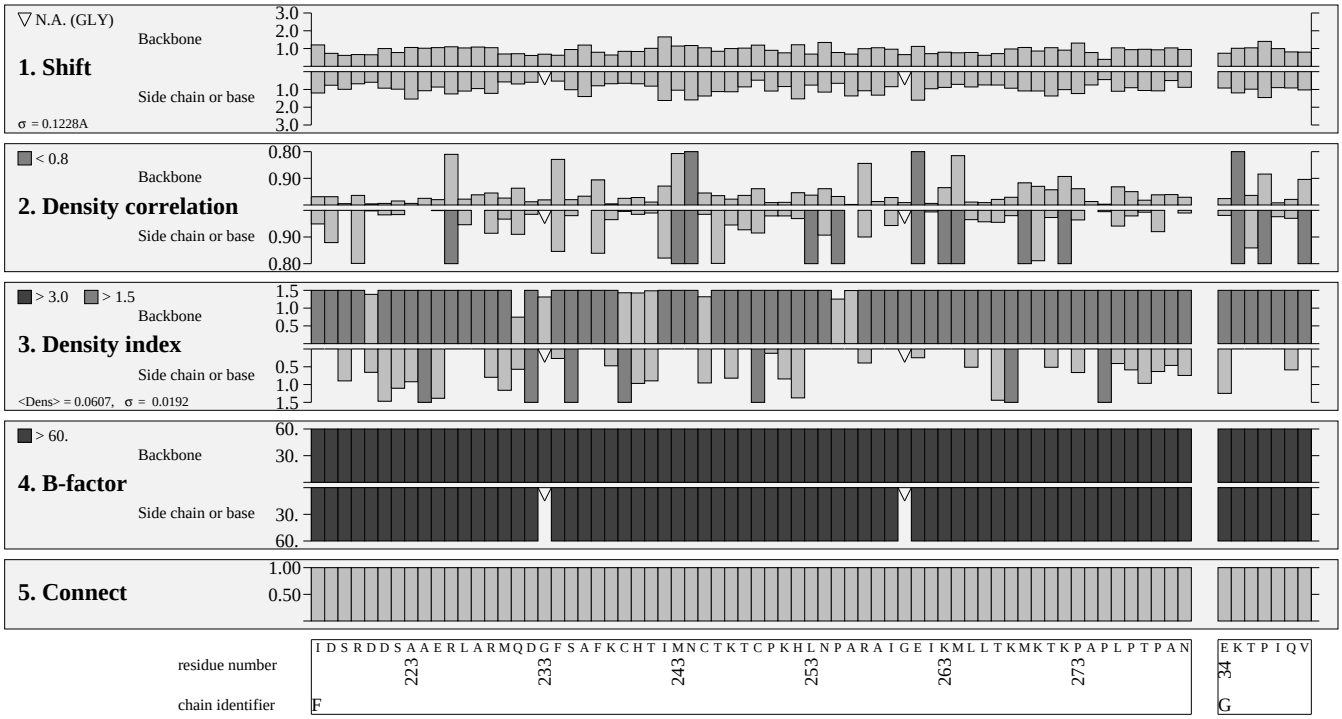
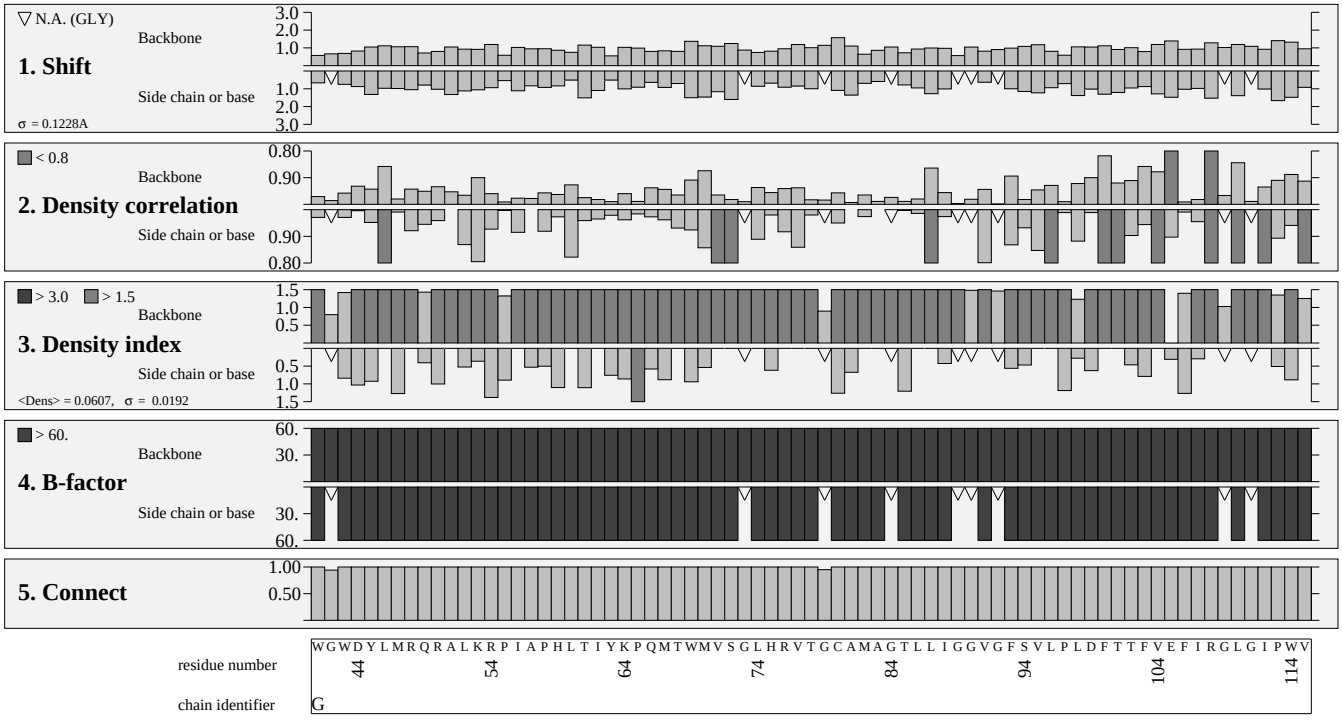
# Structure Factor Check

## 3VRA

### Local estimation (14)

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# Structure Factor Check

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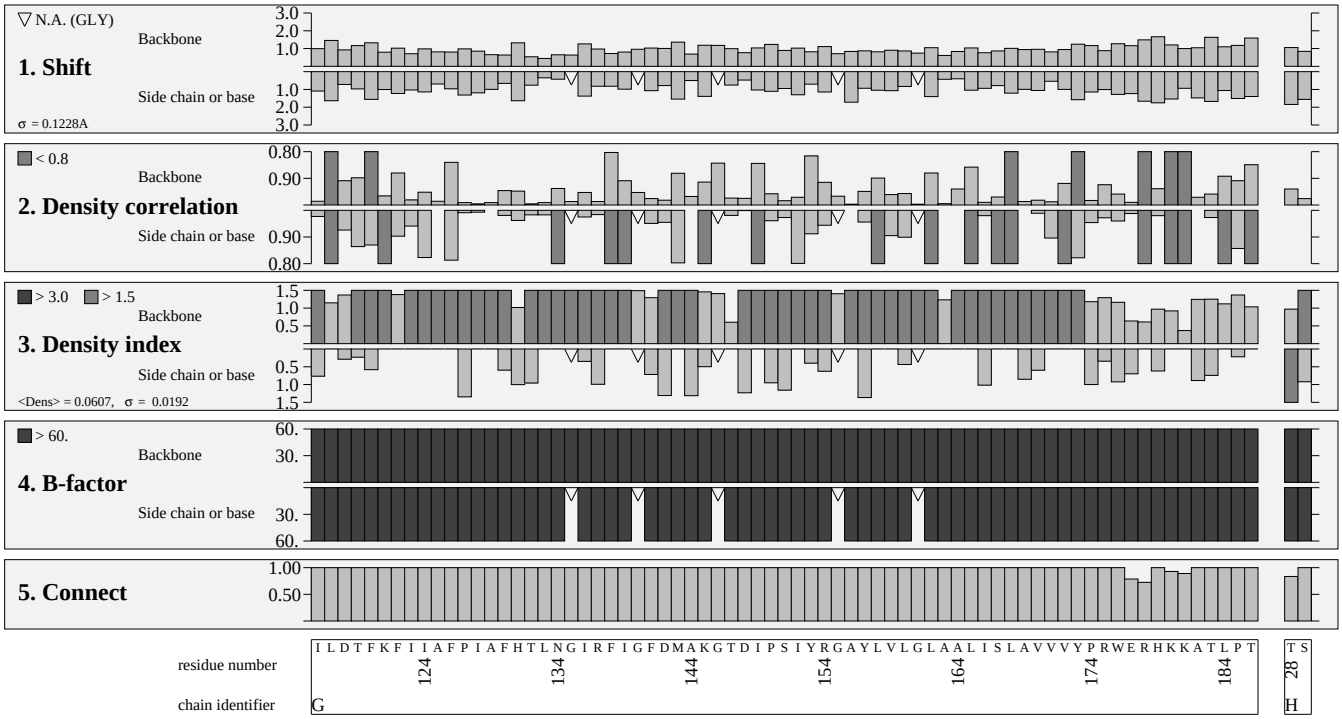
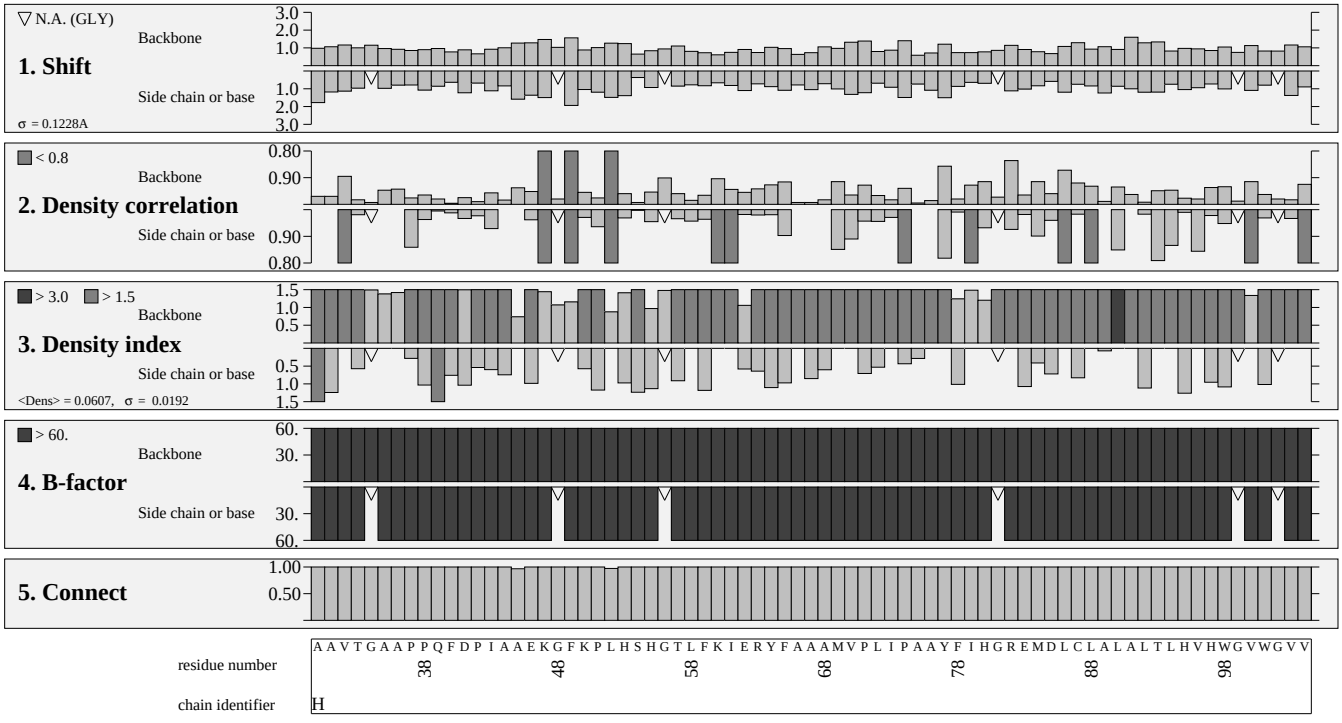
### Local estimation (15)

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# Structure Factor Check

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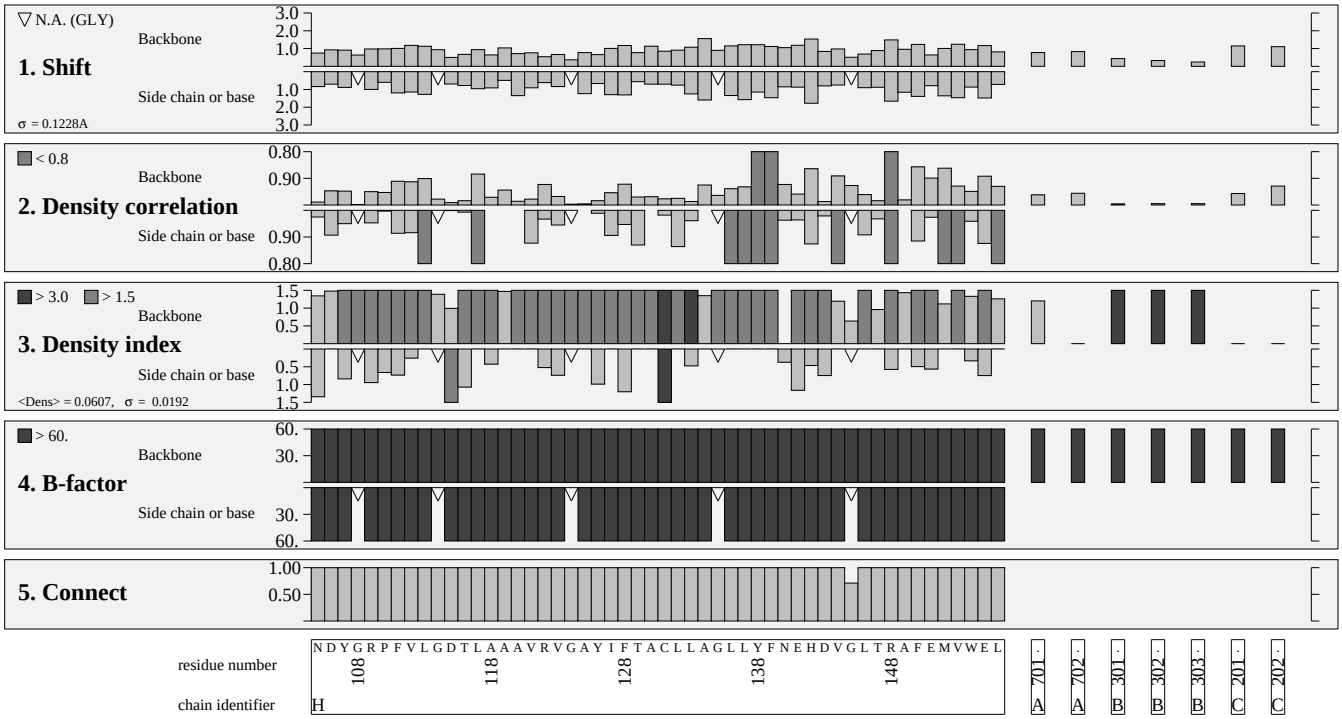
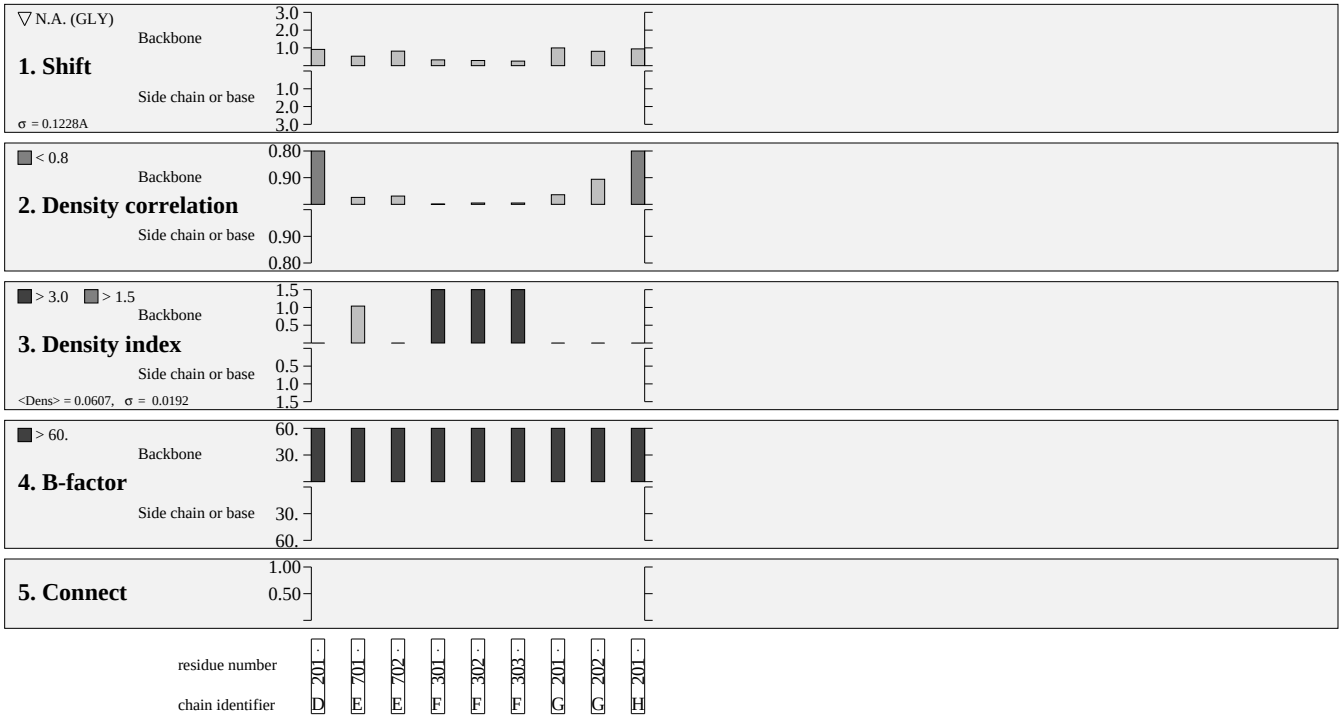
### Local estimation (16)

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