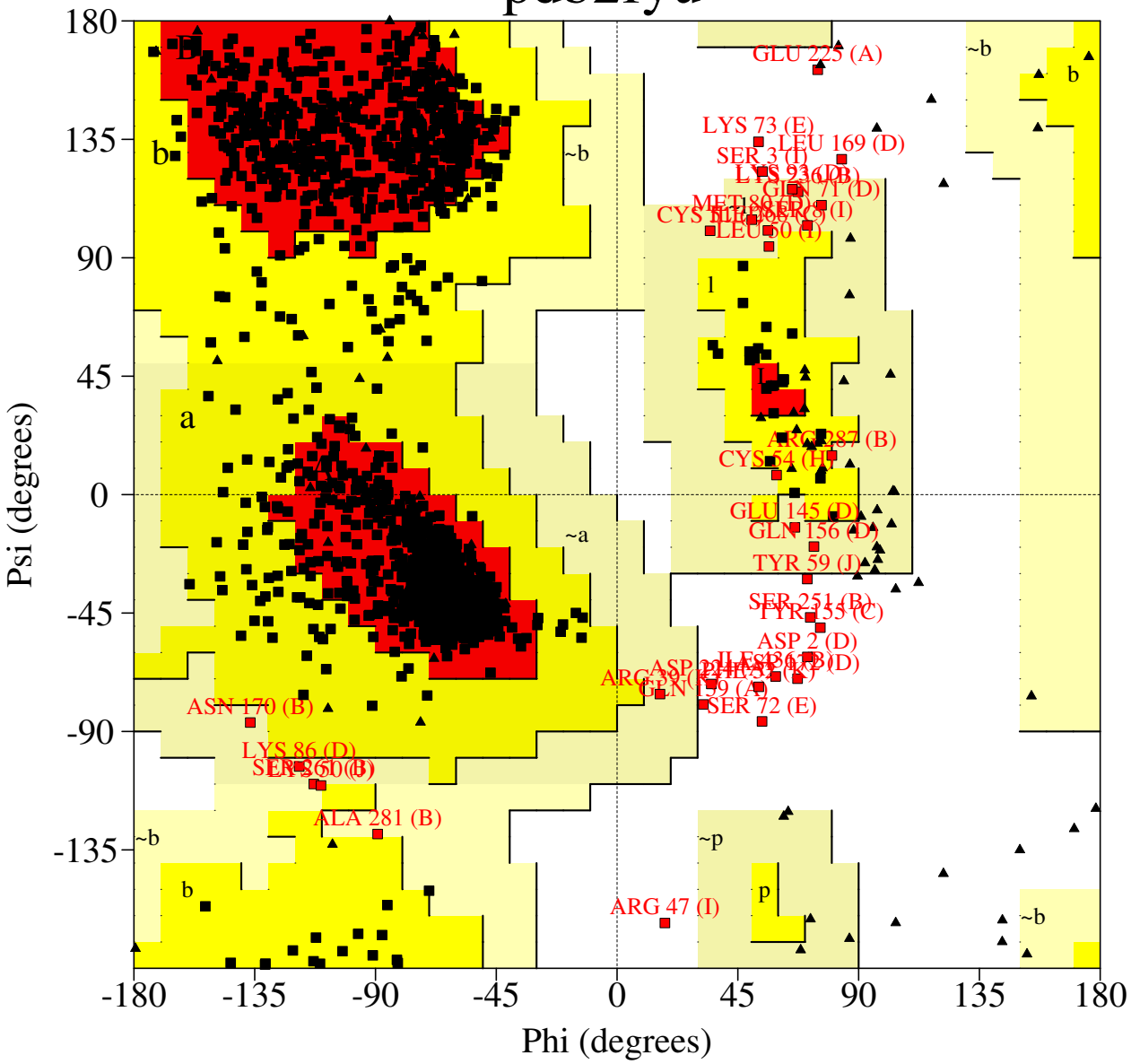
# Ramachandran Plot

## pdb2fyu



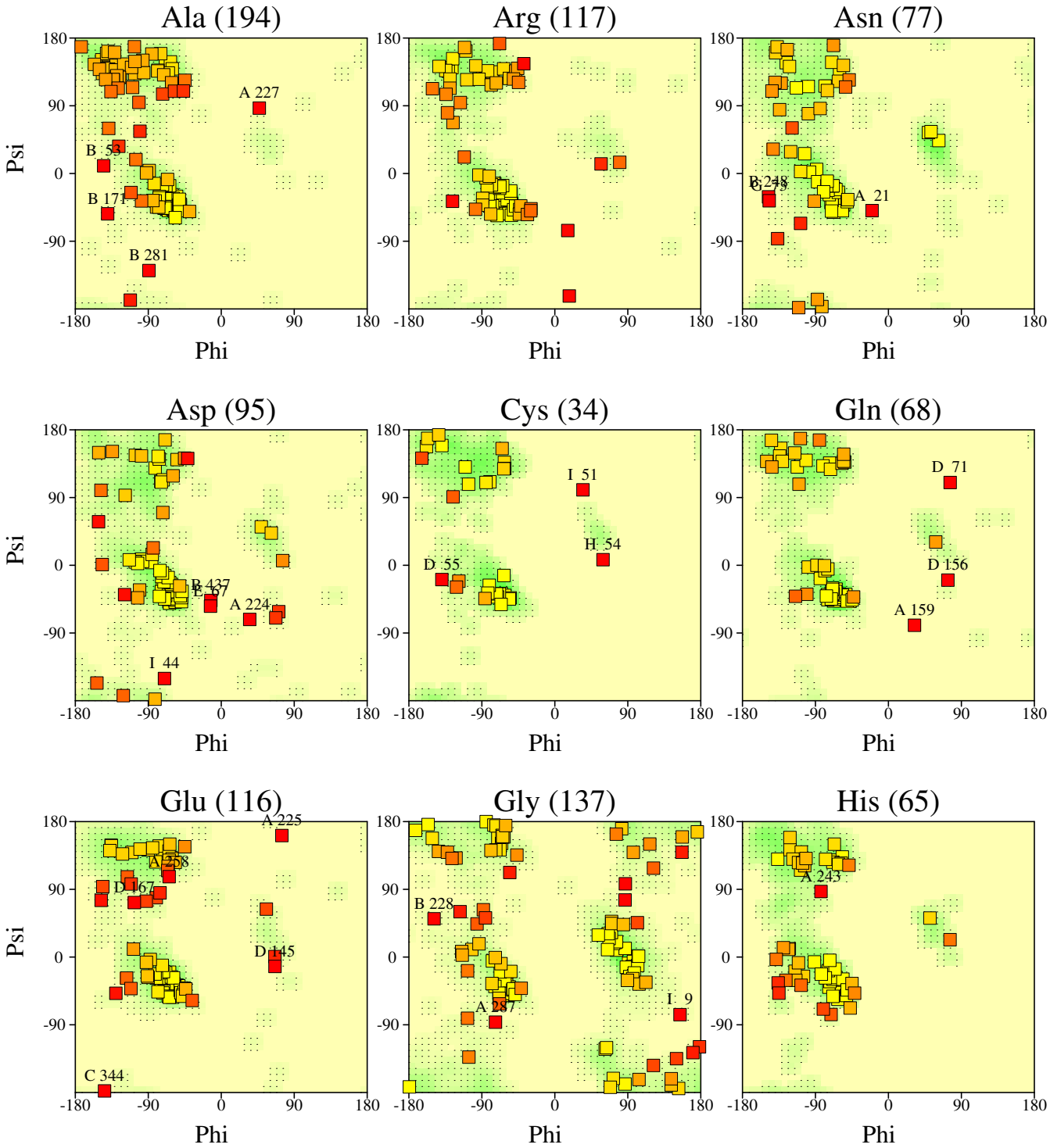

### Plot statistics

| | | |
|---|---|---|
| Residues in most favoured regions [A,B,L] | 1624 | 88.7% |
| Residues in additional allowed regions [a,b,l,p] | 174 | 9.5% |
| Residues in generously allowed regions [~a,~b,~l,~p] | 18 | 1.0% |
| Residues in disallowed regions | 15 | 0.8% |
| | ---- | ------ |
| Number of non-glycine and non-proline residues | 1831 | 100.0% |
| Number of end-residues (excl. Gly and Pro) | 19 | |
| Number of glycine residues (shown as triangles) | 140 | |
| Number of proline residues | 109 | |
| | ---- | |
| Total number of residues | 2099 | |

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

# Ramachandran plots for all residue types

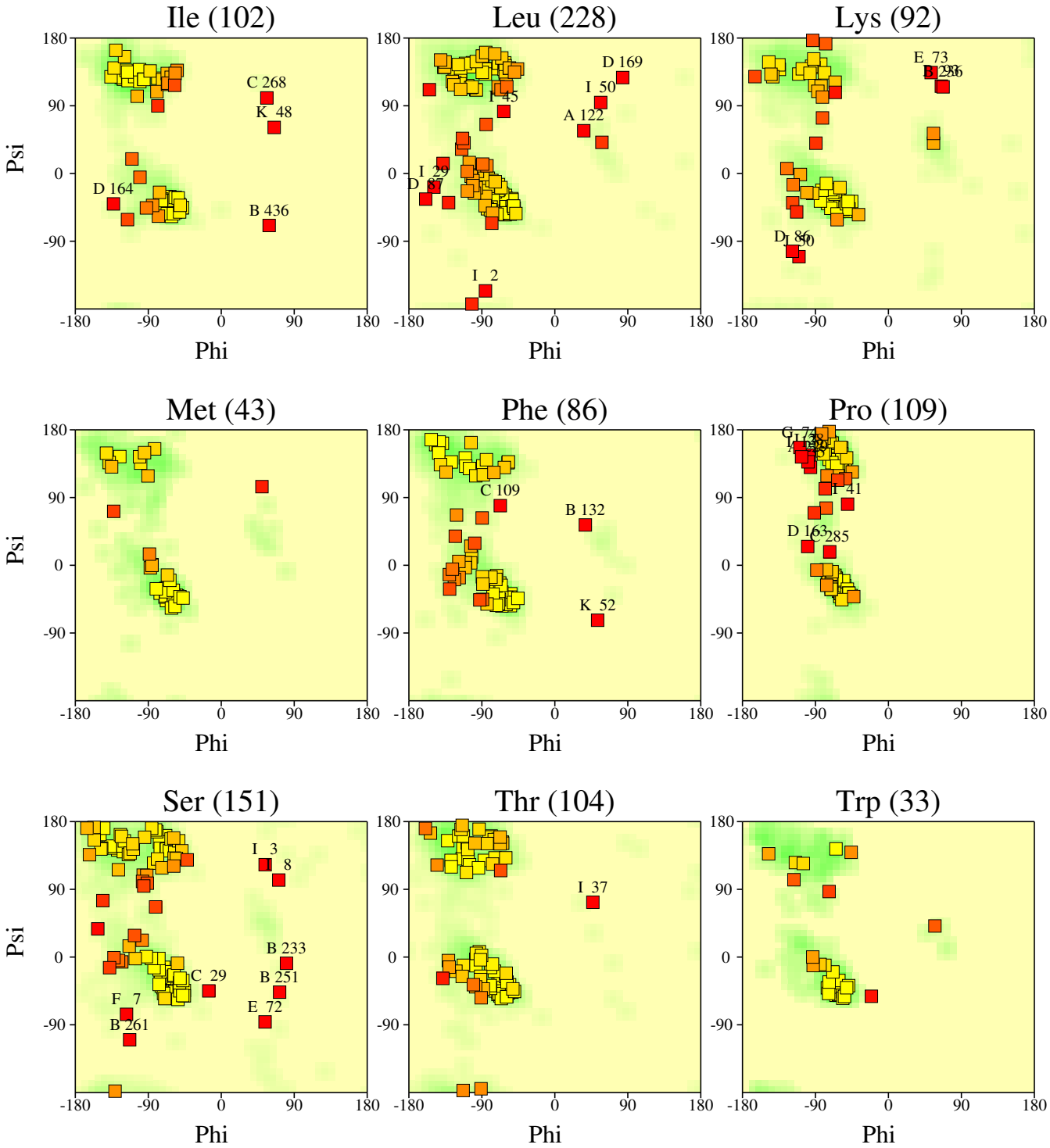
## pdb2fyu




Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Ramachandran plots for all residue types

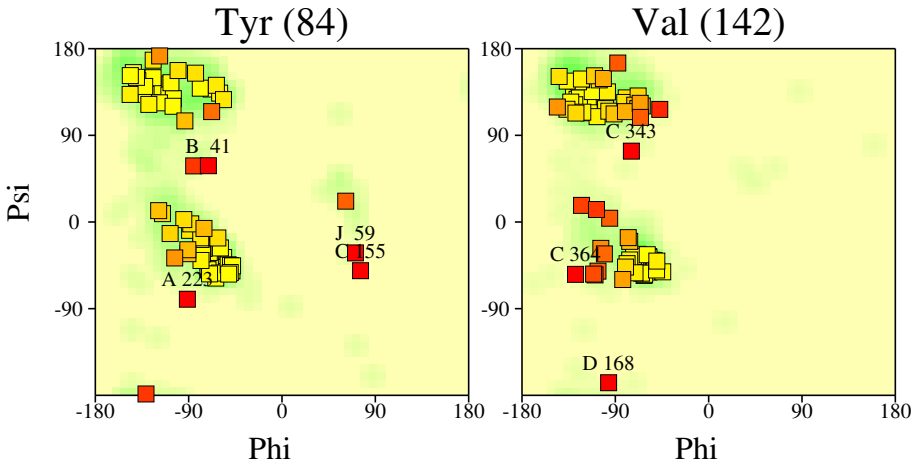
## pdb2fyu




Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Ramachandran plots for all residue types

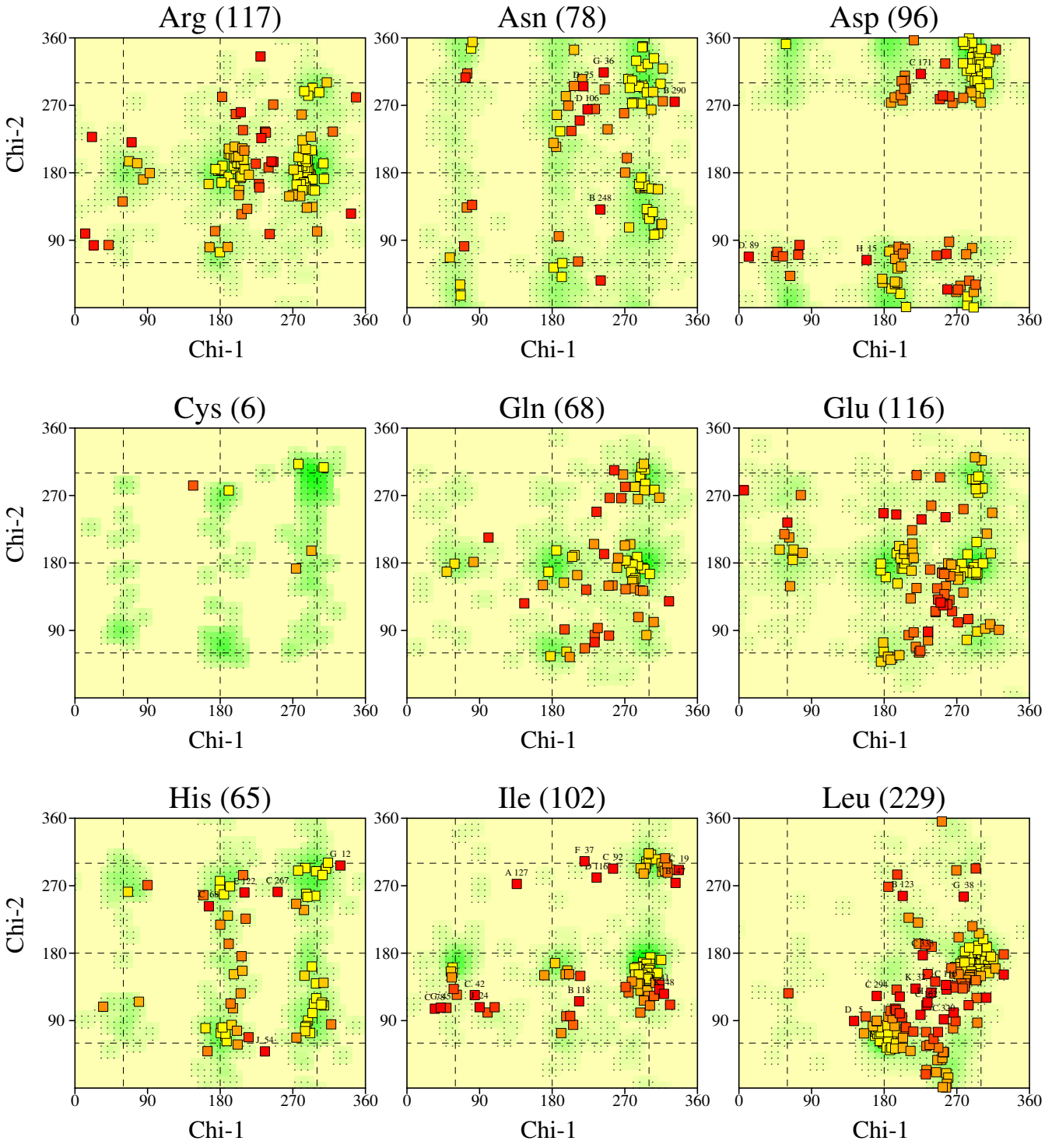
## pdb2fyu




Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Chi1-Chi2 plots

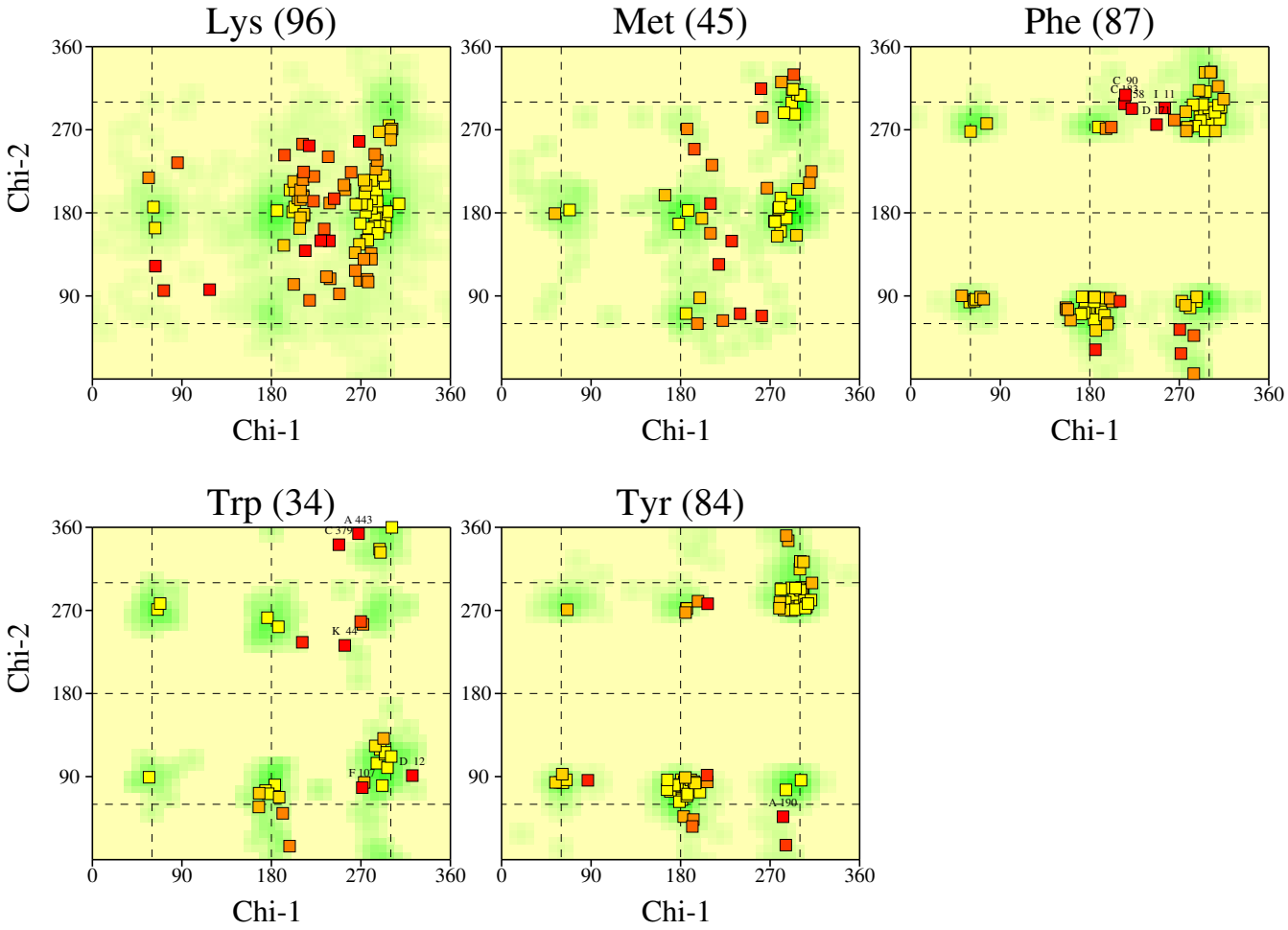
## pdb2fyu




Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

# Chi1-Chi2 plots

## pdb2fyu



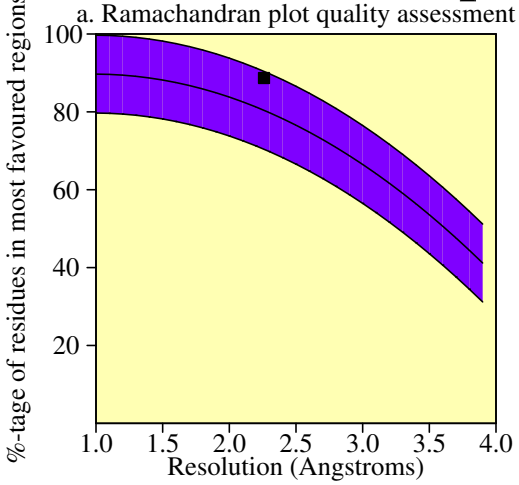

Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

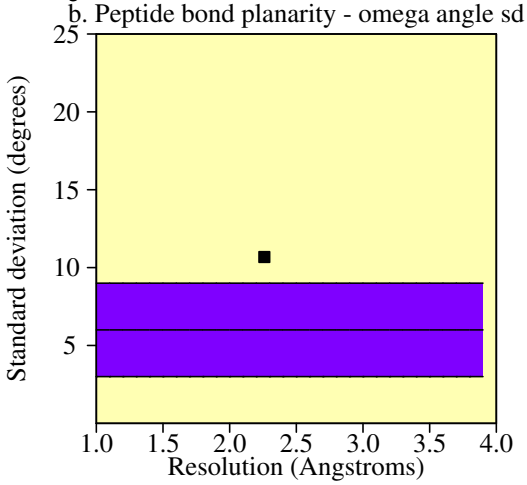
# Main-chain parameters

## pdb2fyu

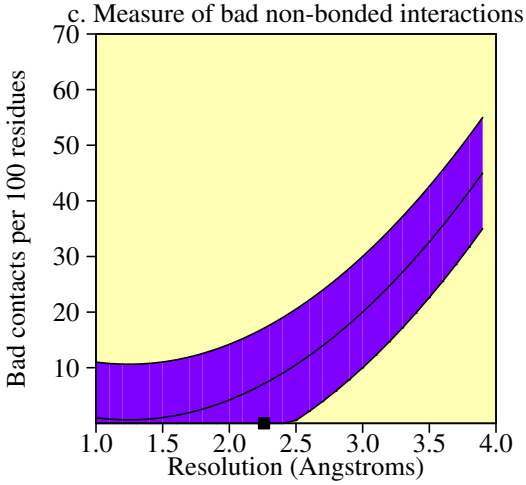
a. Ramachandran plot quality assessment



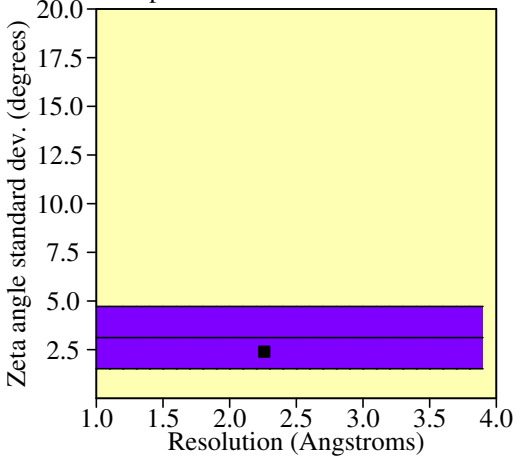

b. Peptide bond planarity - omega angle sd



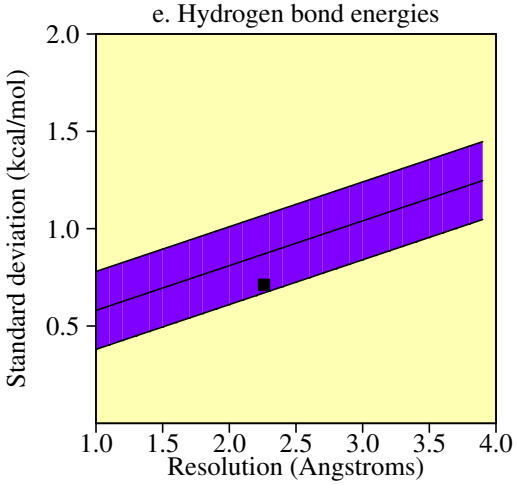

c. Measure of bad non-bonded interactions



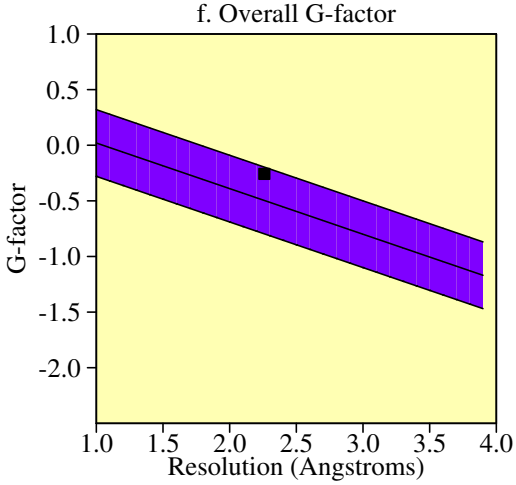

d. Alpha carbon tetrahedral distortion




e. Hydrogen bond energies




f. Overall G-factor



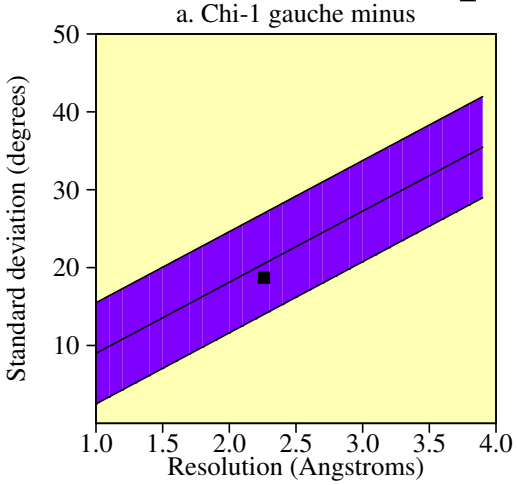

### Plot statistics

| Stereochemical parameter | No. of data pts | Parameter value | Comparison values Typical value | Band width | No. of band widths from mean | |
|---|---|---|---|---|---|---|
| a. %-tage residues in A, B, L | 1831 | 88.7 | 80.4 | 10.0 | 0.8 | Inside |
| b. Omega angle st dev | 2087 | 10.7 | 6.0 | 3.0 | 1.6 | WORSE |
| c. Bad contacts / 100 residues | 0 | 0.0 | 7.1 | 10.0 | -0.7 | Inside |
| d. Zeta angle st dev | 1959 | 2.4 | 3.1 | 1.6 | -0.5 | Inside |
| e. H-bond energy st dev | 1354 | 0.7 | 0.9 | 0.2 | -0.8 | Inside |
| f. Overall G-factor | 2099 | -0.3 | -0.5 | 0.3 | 0.8 | Inside |

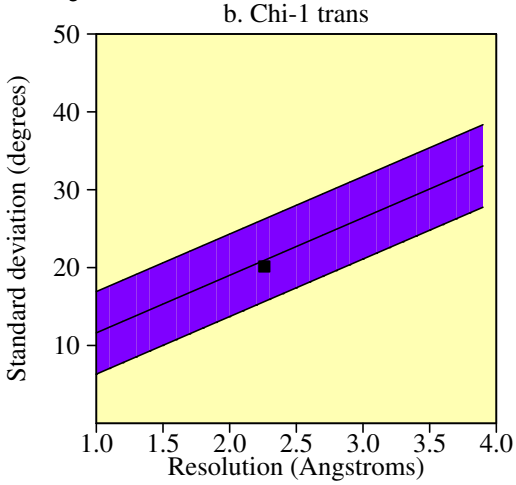
# Side-chain parameters

## pdb2fyu

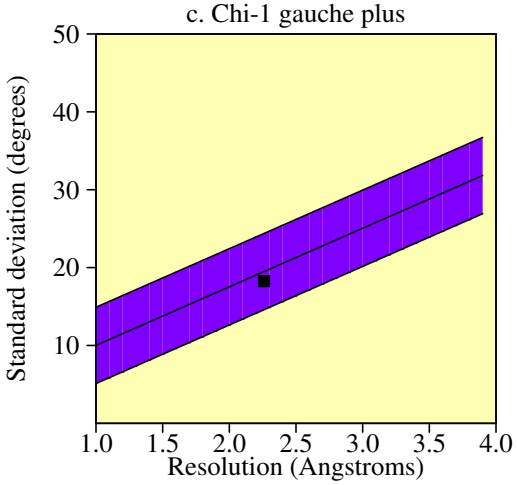
a. Chi-1 gauche minus



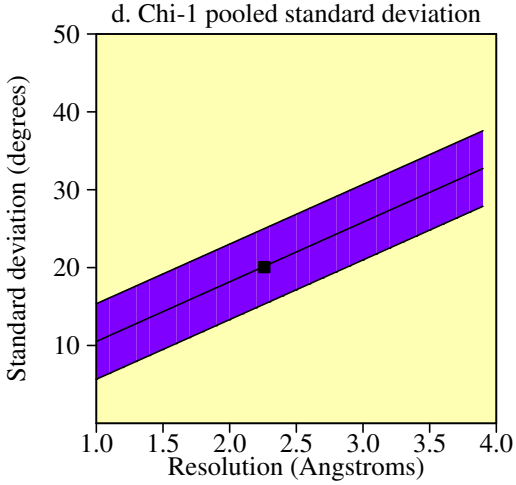

b. Chi-1 trans



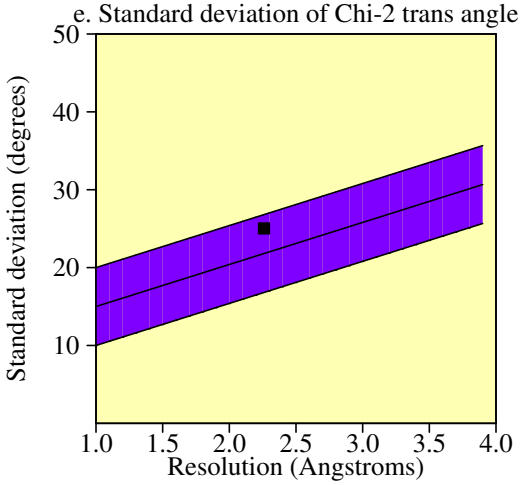

c. Chi-1 gauche plus




d. Chi-1 pooled standard deviation




e. Standard deviation of Chi-2 trans angle




pdb2fyu

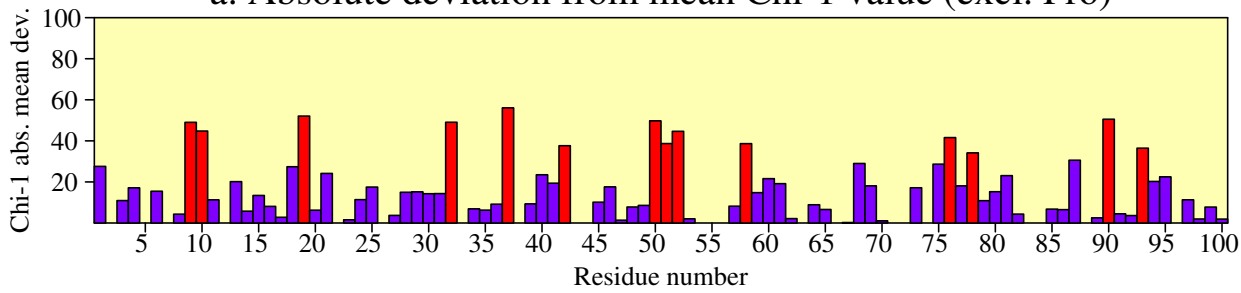
### Plot statistics

| Stereochemical parameter | No. of data pts | Parameter value | Comparison values Typical value | Band width | No. of band widths from mean | |
|---|---|---|---|---|---|---|
| a. Chi-1 gauche minus st dev | 226 | 18.7 | 20.5 | 6.5 | -0.3 | Inside |
| b. Chi-1 trans st dev | 590 | 20.1 | 20.9 | 5.3 | -0.1 | Inside |
| c. Chi-1 gauche plus st dev | 837 | 18.3 | 19.5 | 4.9 | -0.3 | Inside |
| d. Chi-1 pooled st dev | 1653 | 20.1 | 20.2 | 4.8 | 0.0 | Inside |
| e. Chi-2 trans st dev | 506 | 25.0 | 21.8 | 5.0 | 0.6 | Inside |

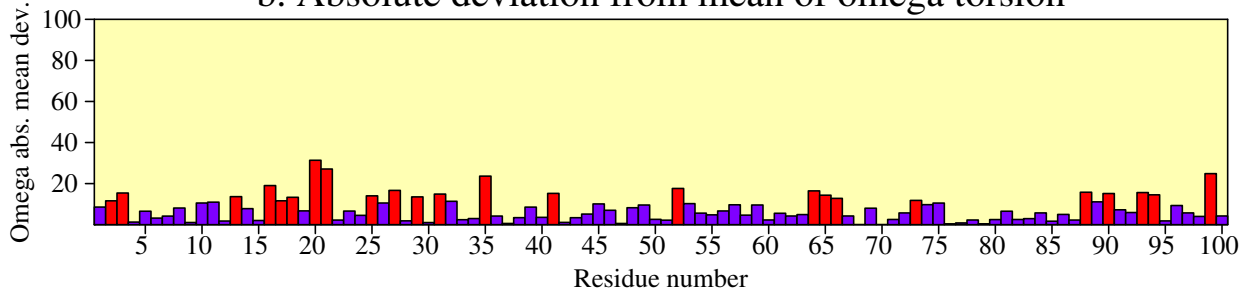
# Residue properties

## pdb2fyu

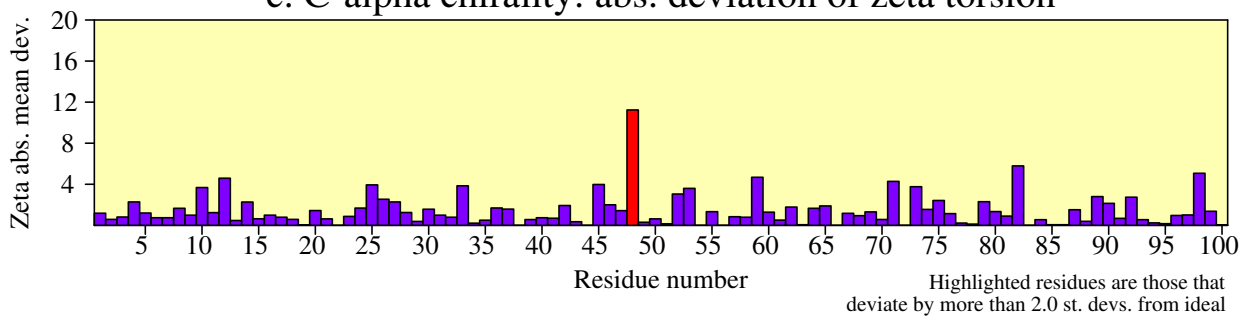
### a. Absolute deviation from mean Chi-1 value (excl. Pro)




### b. Absolute deviation from mean of omega torsion

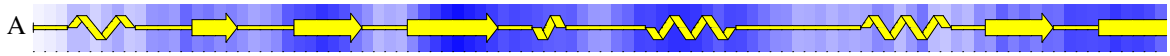



### c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



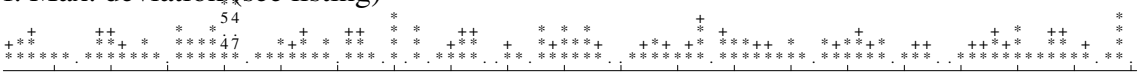

Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

### e. Sequence & Ramachandran regions

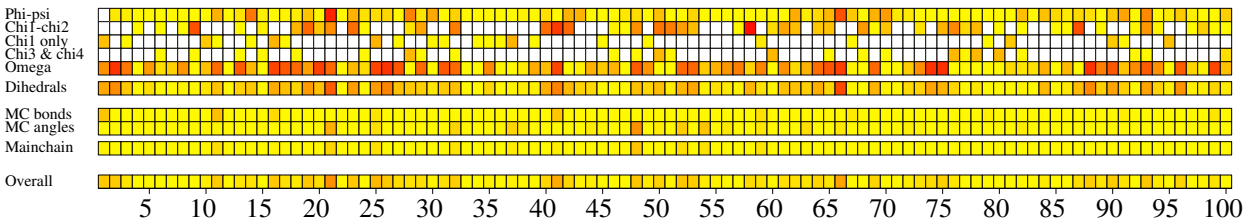
Most favoured Allowed Generous Disallowed

TATYAQALQSVPETQVSQLDNGLRVASEQSSQPTCTVGVWIDAGSRYESEKNNGAGYFVEHLAFKGTKNRPGNALEKEVESMGAHLNAYSTREHTAYYIK

### f. Max. deviation (see listing)



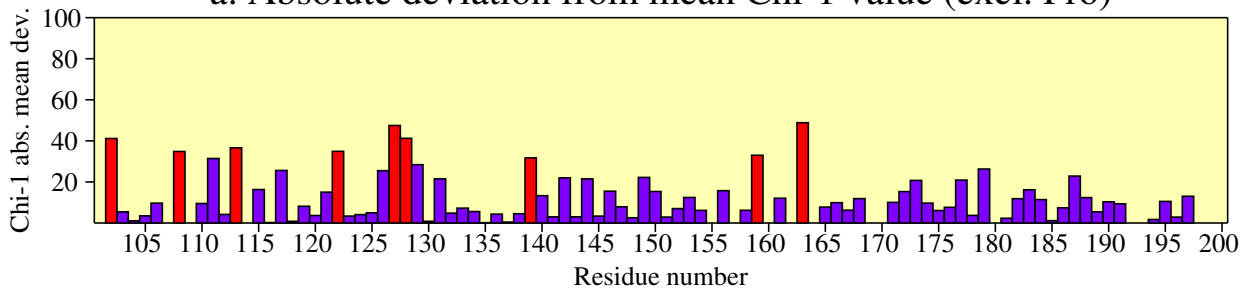

### g. G-factors



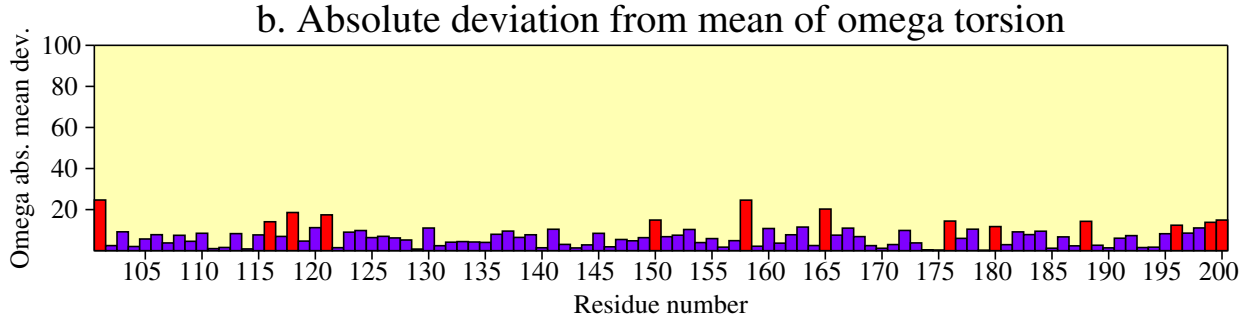
# Residue properties

## pdb2fyu

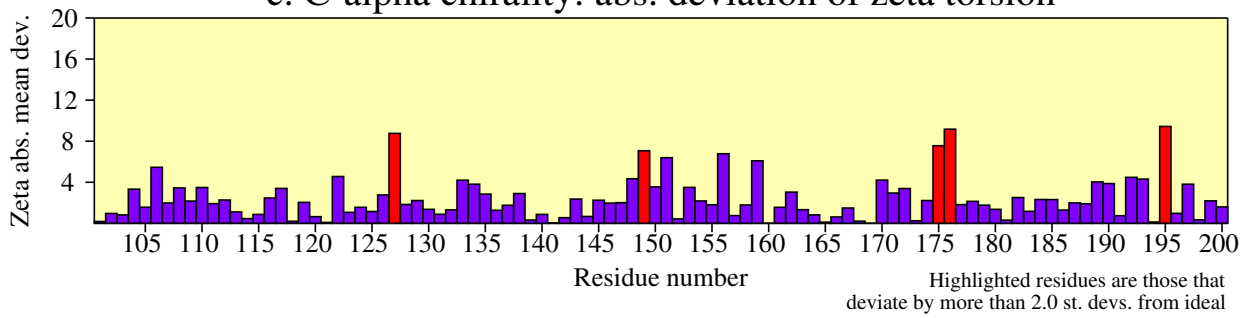
### a. Absolute deviation from mean Chi-1 value (excl. Pro)




### b. Absolute deviation from mean of omega torsion




### c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility

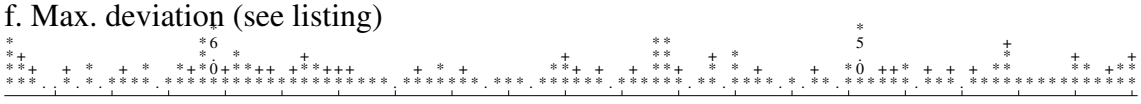
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

### e. Sequence & Ramachandran regions

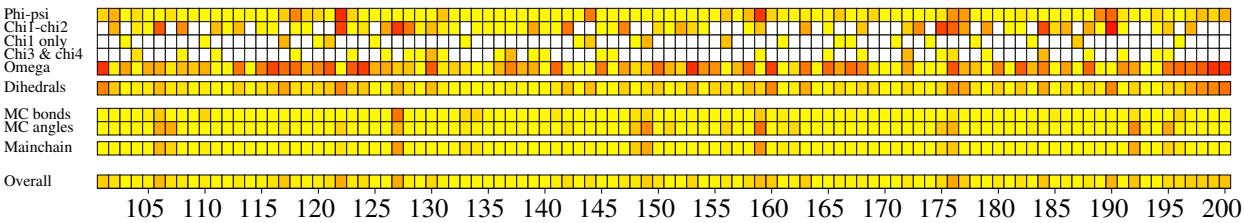
Most favoured Allowed Generous Disallowed

ALSKDLPKAVELLADIVQNCSLEDSQIEKERDVILQELQENDTSMRDVVFNYLHATAFQGTPLAQSVEGPSENVRKLSRADLTEYLSRHYKAPRMVLAAA

### f. Max. deviation (see listing)

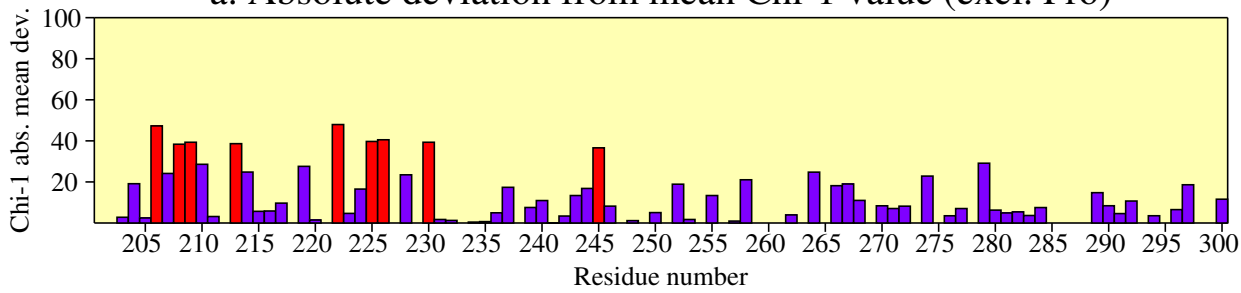


### g. G-factors

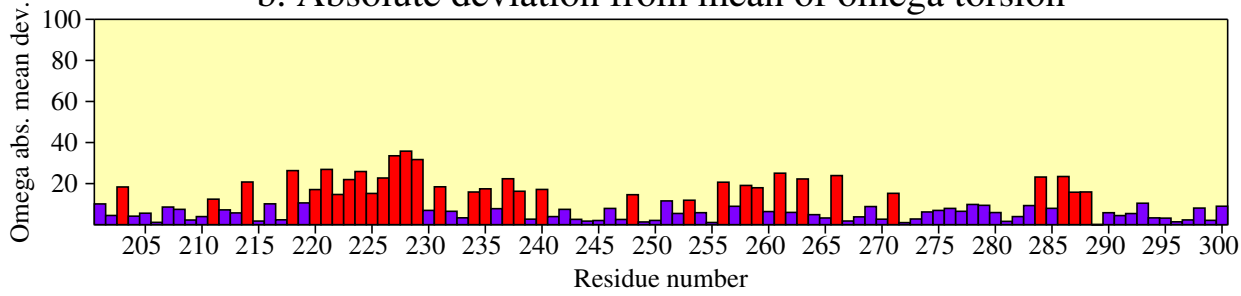


# Residue properties
## pdb2fyu

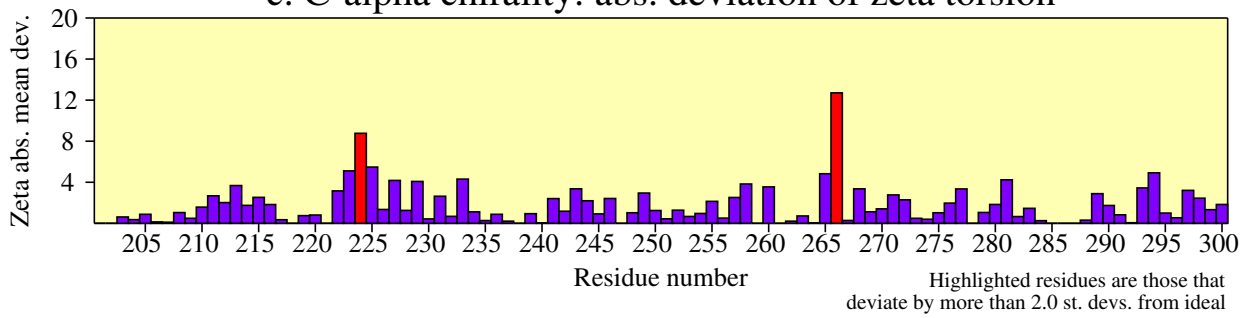
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion




c. C-alpha chirality: abs. deviation of zeta torsion

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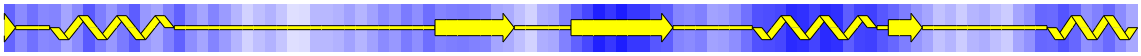
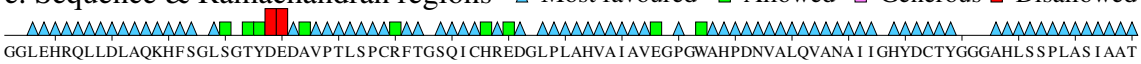
d. Secondary structure & estimated accessibility



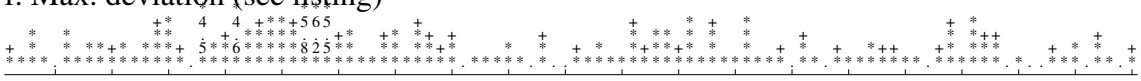
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

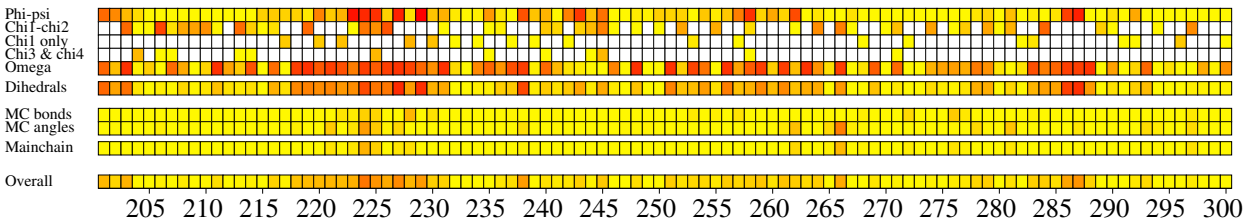


GGLEHRQLLDLAQKHFSGLSGTYDEDAVPTLSPCRFTGSQICHREDGLPLAHVAIAVEGPGWAHPDNVALQVANAIIGHYDCTYGGGAHLSSPLASIAAT

f. Max. deviation (see listing)



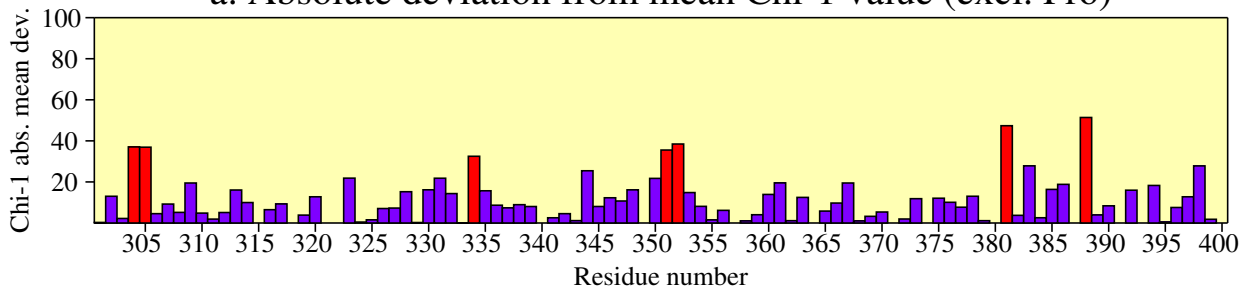
g. G-factors



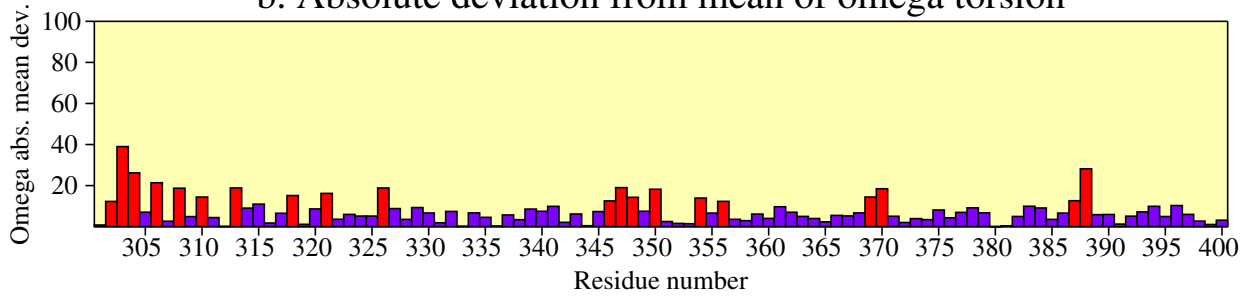
# Residue properties

## pdb2fyu

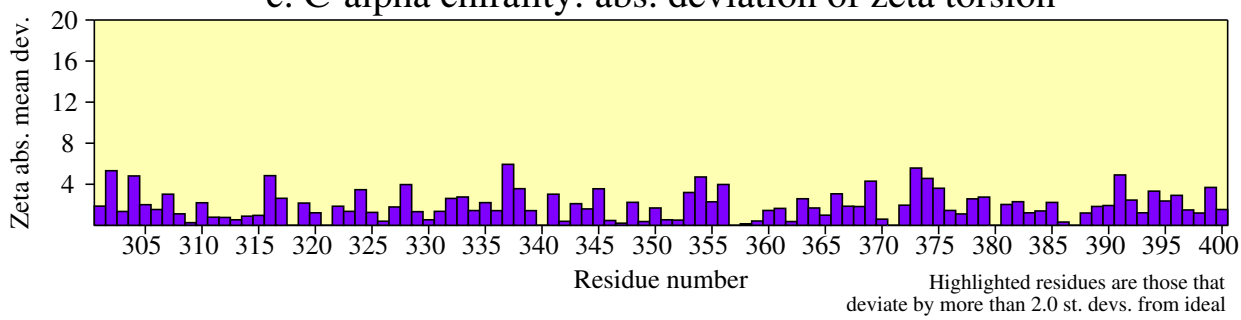
### a. Absolute deviation from mean Chi-1 value (excl. Pro)




### b. Absolute deviation from mean of omega torsion




### c. C-alpha chirality: abs. deviation of zeta torsion



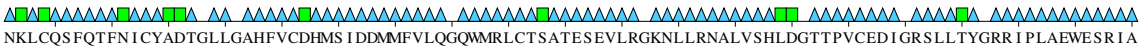

Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility

Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

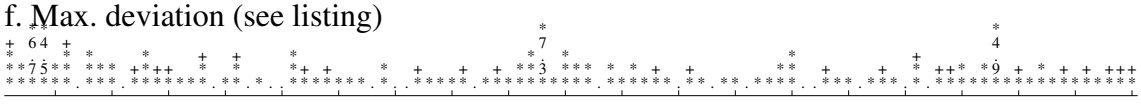
### e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

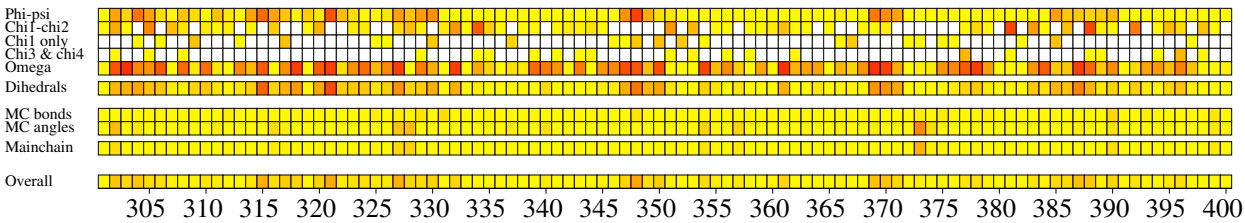


NKLCQSFQTFNICYADTGLLGAHFVCDHMSIDDMMFVLQGQWMRLCTSATESEVLRGKNLLRNALVSHLDGTTPVCEDIGRSLLTYGRRIPLAEWESRIA

### f. Max. deviation (see listing)

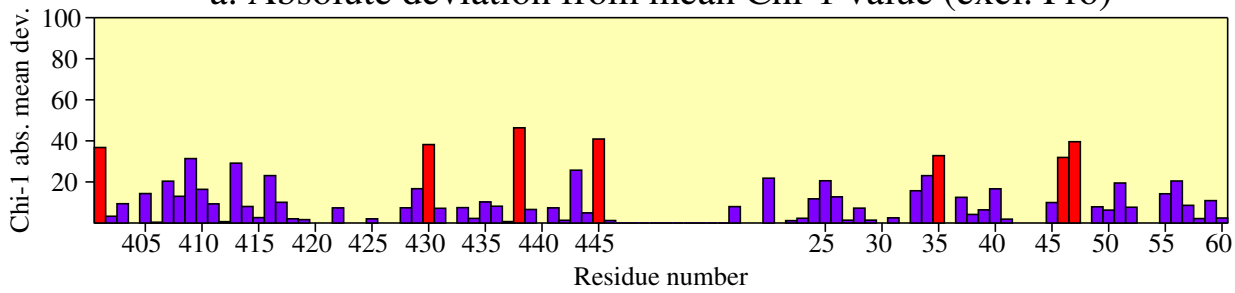


### g. G-factors

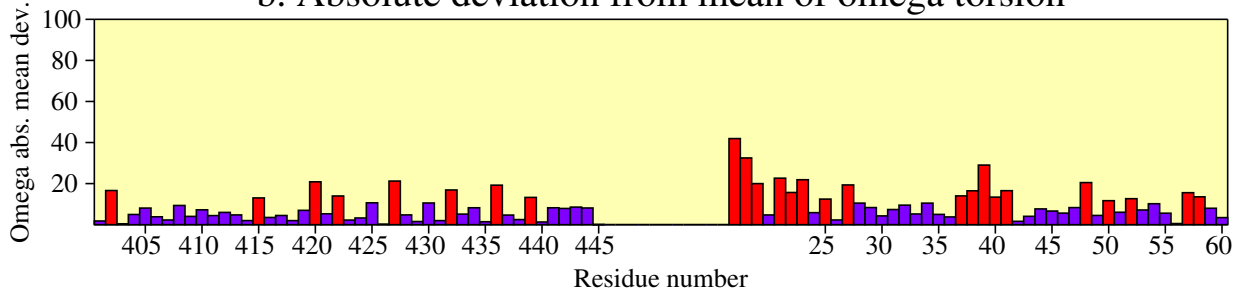


# Residue properties
## pdb2fyu

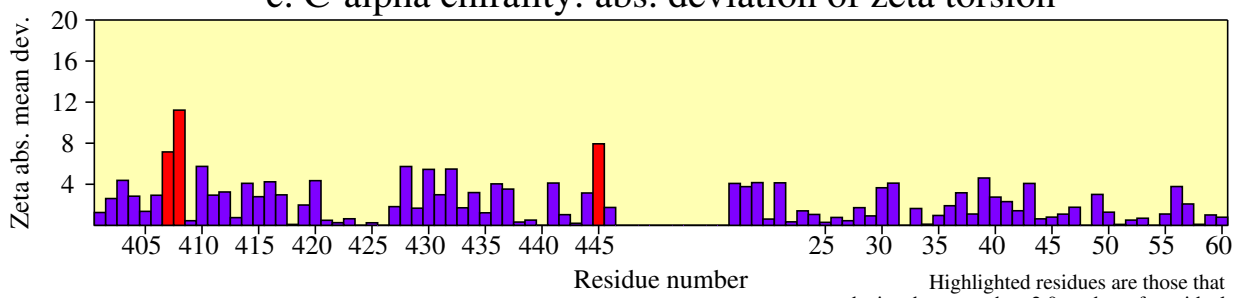
### a. Absolute deviation from mean Chi-1 value (excl. Pro)




### b. Absolute deviation from mean of omega torsion

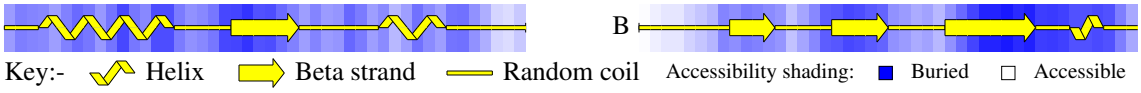



### c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility

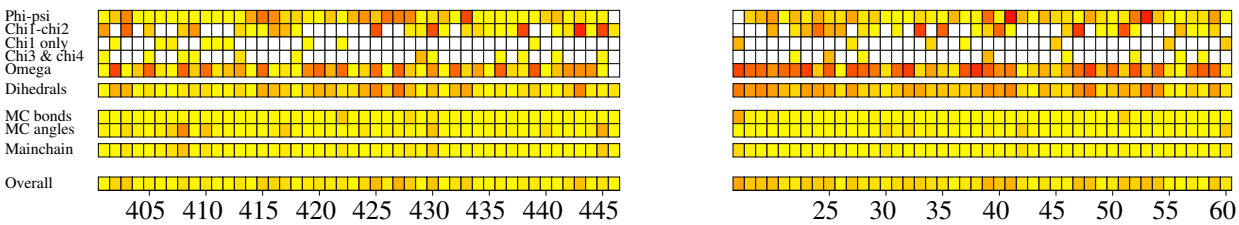



### e. Sequence & Ramachandran regions

Most favoured  Allowed  Generous  Disallowed

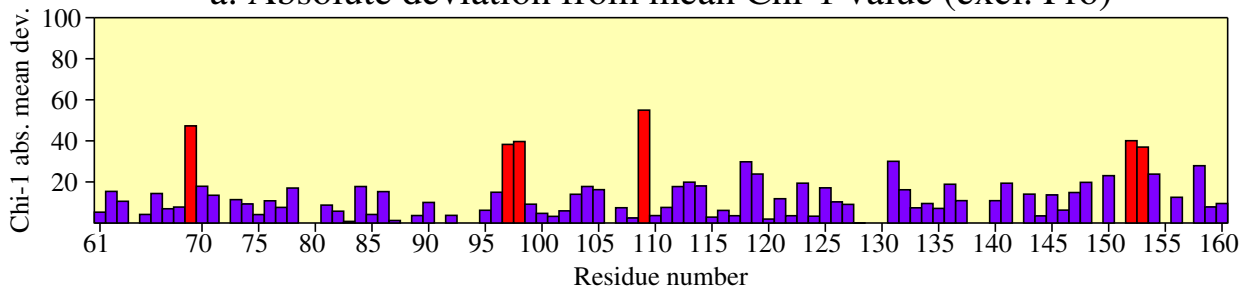

### f. Max. deviation (see listing)

### g. G-factors

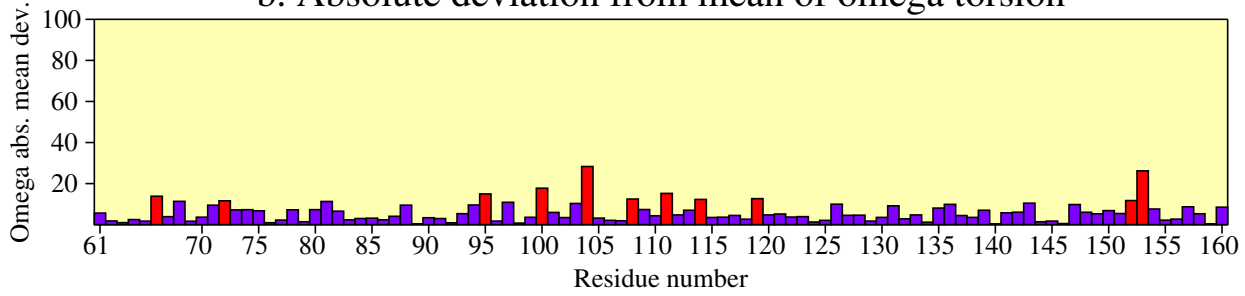


# Residue properties
## pdb2fyu

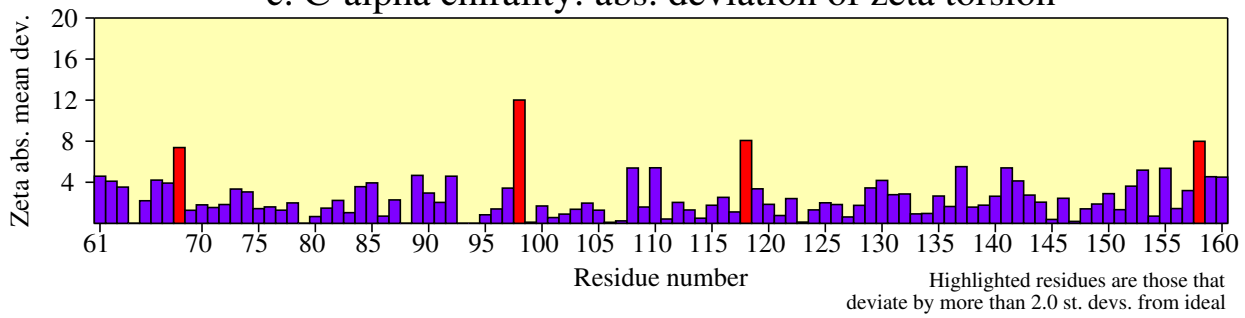
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion

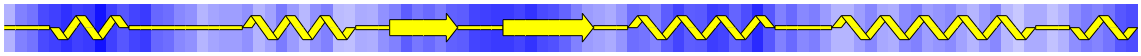



c. C-alpha chirality: abs. deviation of zeta torsion



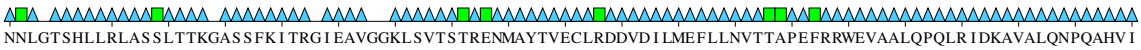

Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



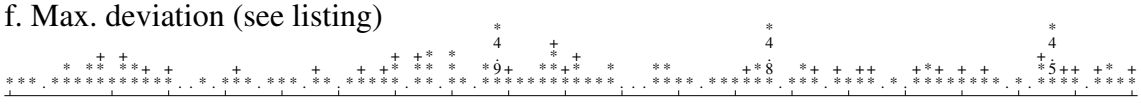
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

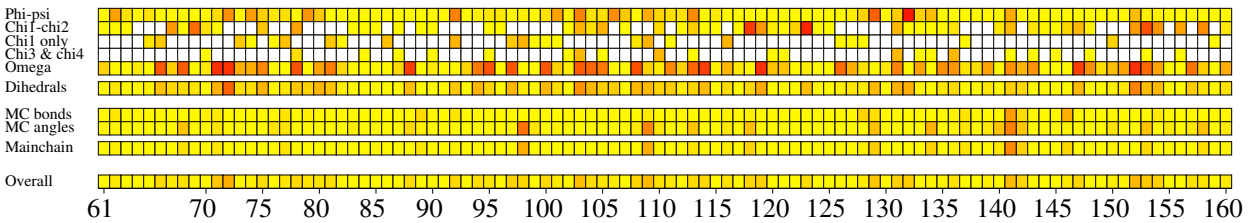


NNLGTSHLLRLASSLTTKGASSFKITRGIEAVGGKLSVTSTRENMAYTVECLRDDVDILMEFLLNVTTAPEFRRWEVAALQPQLRIDKAVALQNPQAHVI

f. Max. deviation (see listing)

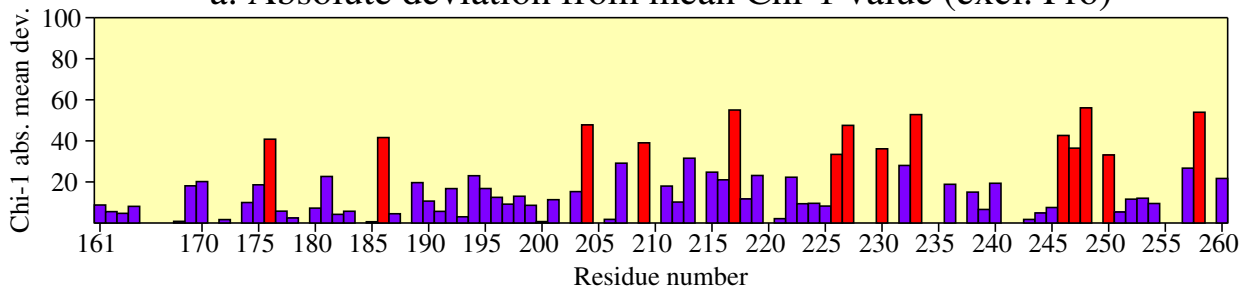


g. G-factors

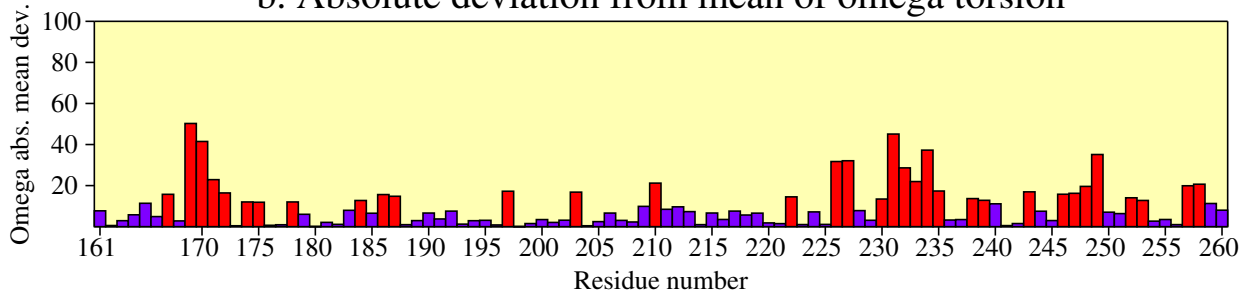


# Residue properties
## pdb2fyu

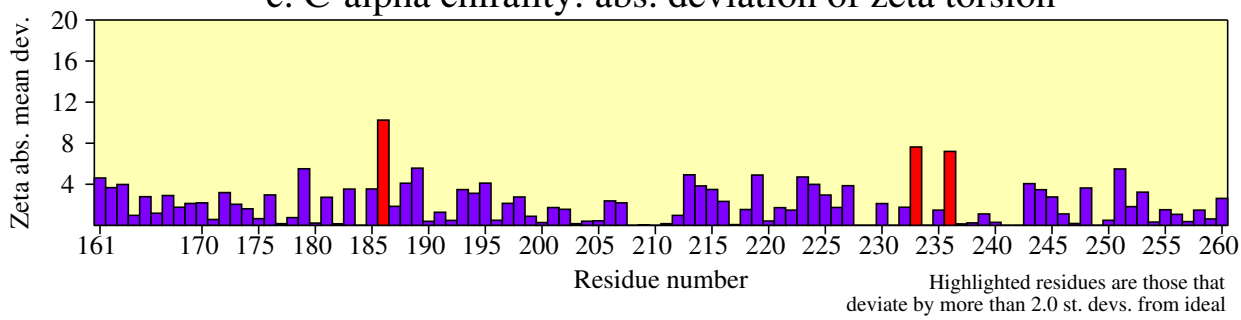
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion

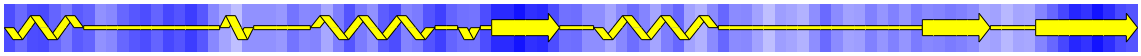



c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

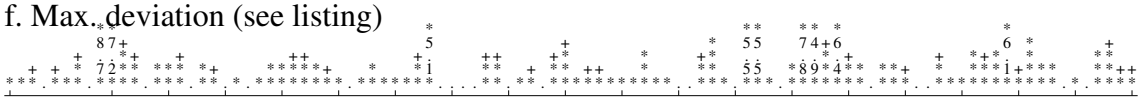


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

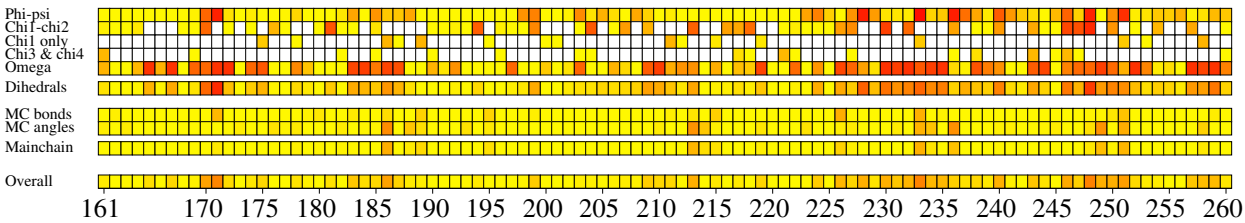
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

ENLHAAAYRNALANSLYCPDYRIGKVTPVELHDYVQNHFTSARMALIGLGVSHPVLKQVAEQFLNIRGGLGLSGAKAKYHGGEIREQNGDSLVHAALVAE

f. Max. deviation (see listing)

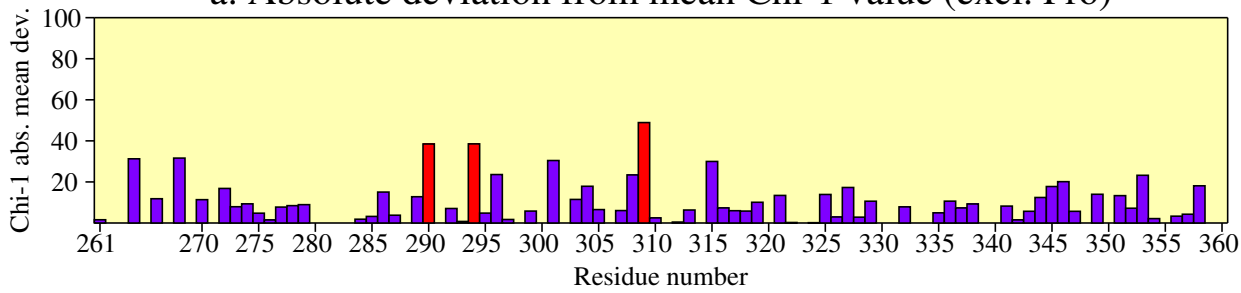


g. G-factors

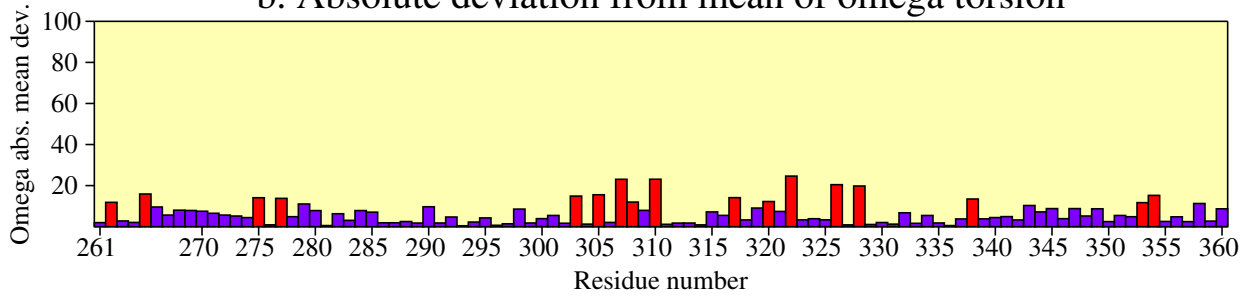


# Residue properties
## pdb2fyu

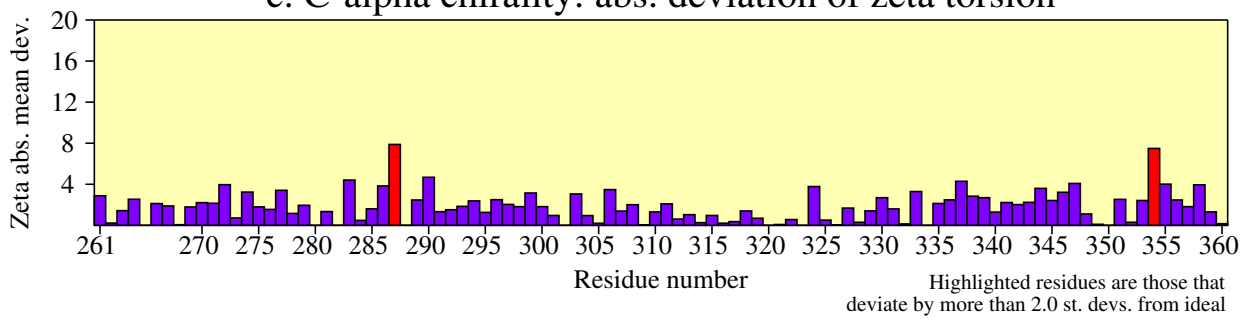
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion




c. C-alpha chirality: abs. deviation of zeta torsion

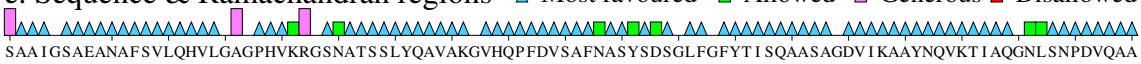



Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

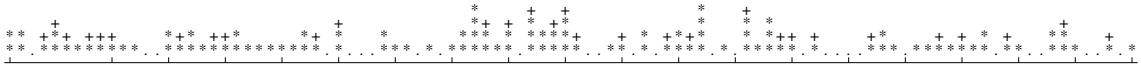
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

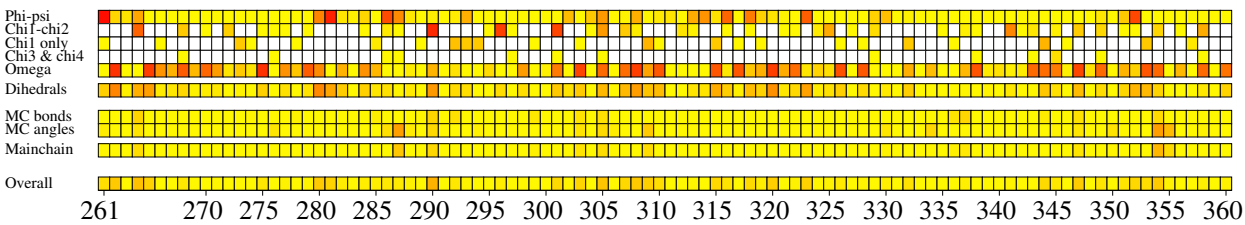


SAAIGSAEANAFSVLQHVLGAGPHVKRGSNATSSLYQAVAKGVHQPFDVSAFNASYSDSGLFGFYTISQAASAGDVIKAAYNQVKTIAQGNLSNPDVQAA

f. Max. deviation (see listing)

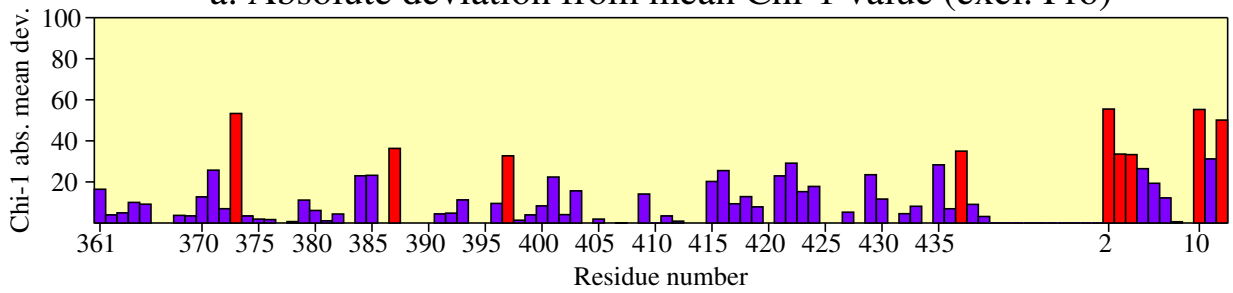


g. G-factors

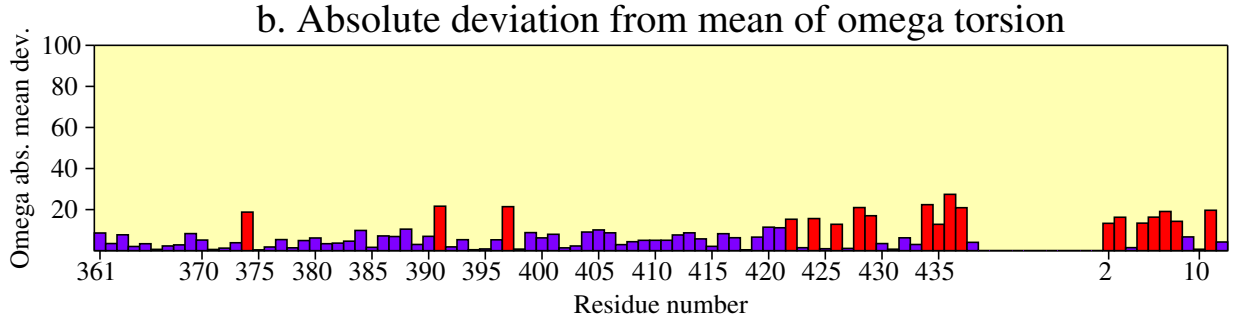


# Residue properties
## pdb2fyu

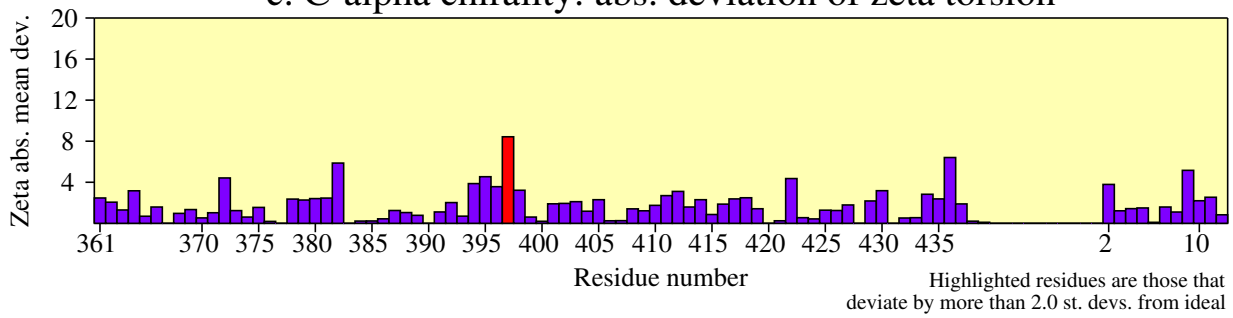
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion




c. C-alpha chirality: abs. deviation of zeta torsion



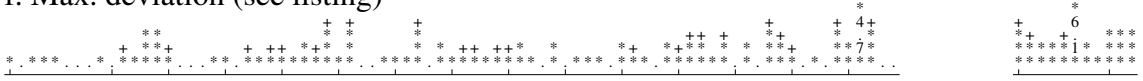

Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

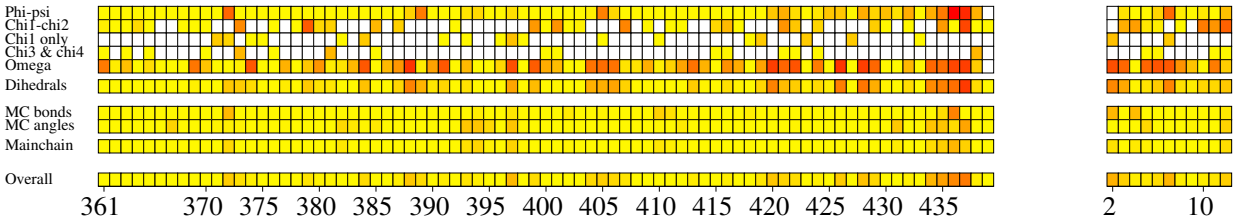

Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed


f. Max. deviation (see listing)



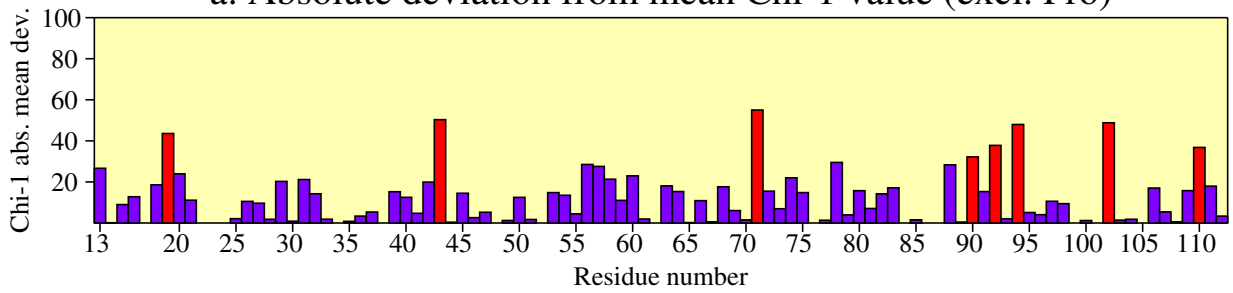
g. G-factors



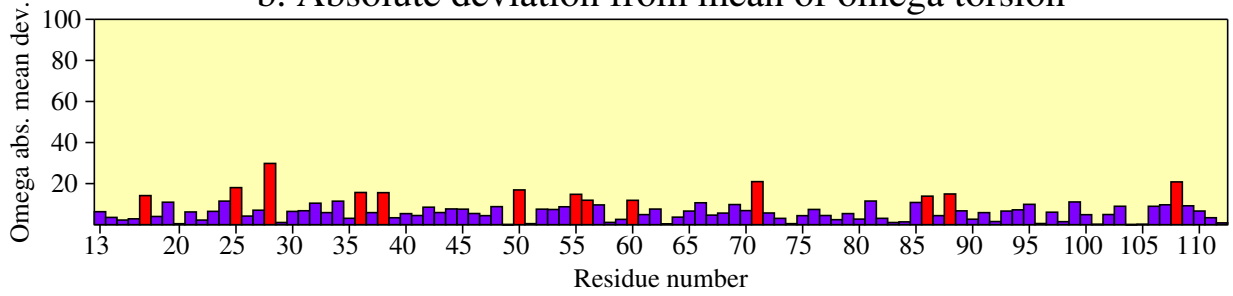
# Residue properties

## pdb2fyu

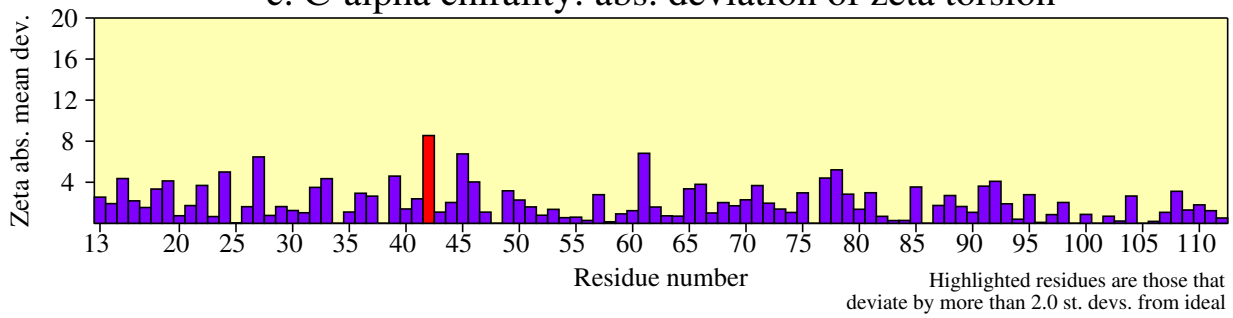
### a. Absolute deviation from mean Chi-1 value (excl. Pro)




### b. Absolute deviation from mean of omega torsion




### c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility

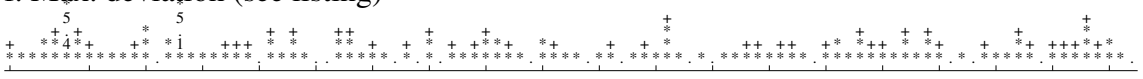
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

### e. Sequence & Ramachandran regions

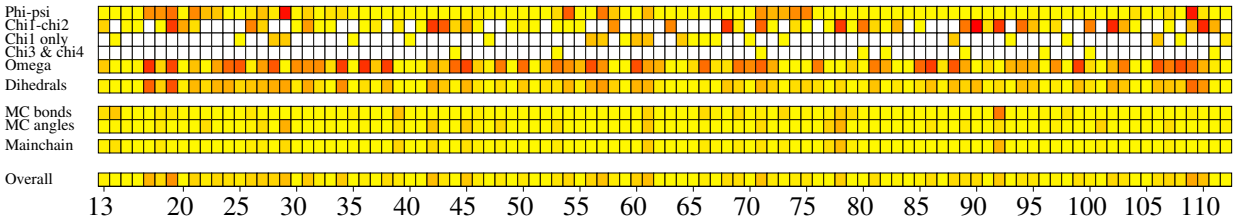
Most favoured Allowed Generous Disallowed

I V N N A F I D L P A P S N I S S W W N F G S L L G I C L I L Q I L T G L F L A M H Y T S D T T T A F S S V T H I C R D V N Y G W I I R Y M H A N G A S M F F I C L Y M H V G R G L Y Y G S Y T F L E T

### f. Max. deviation (see listing)

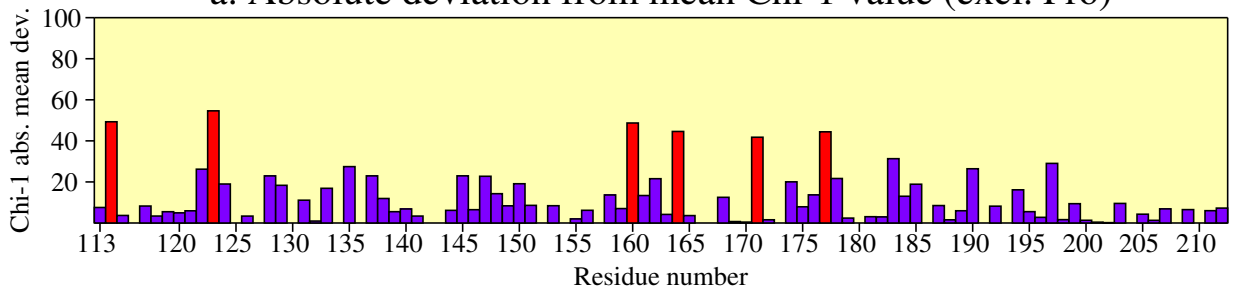


### g. G-factors

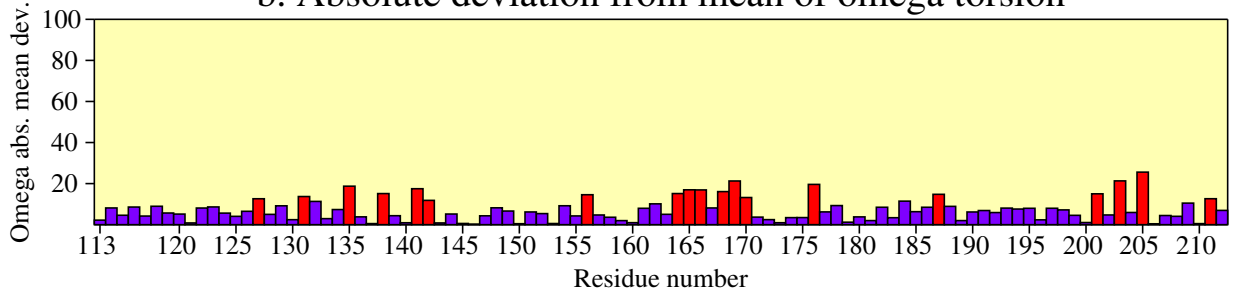


# Residue properties
## pdb2fyu

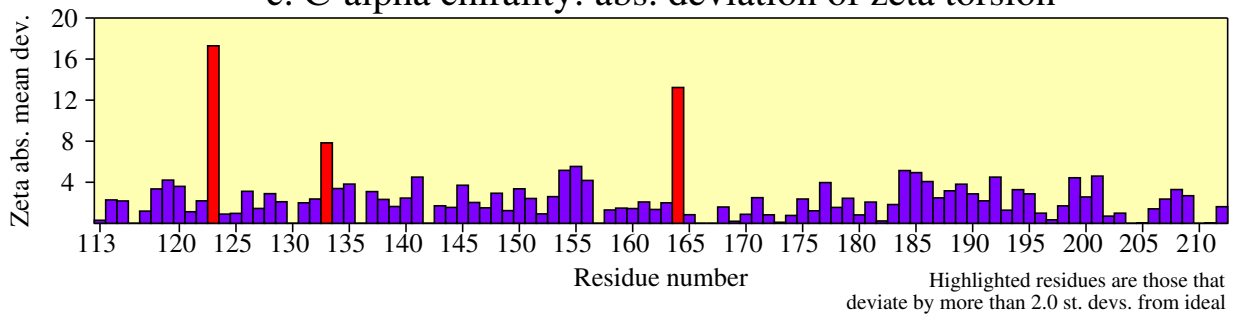
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion




c. C-alpha chirality: abs. deviation of zeta torsion



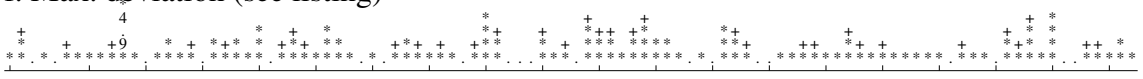

Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

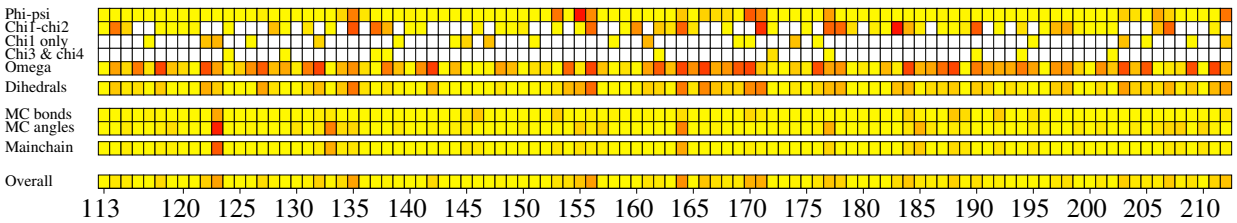
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed


f. Max. deviation (see listing)

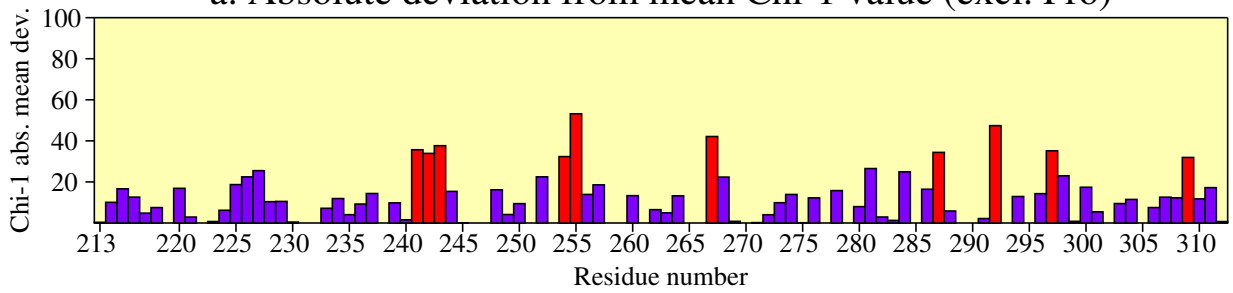


g. G-factors

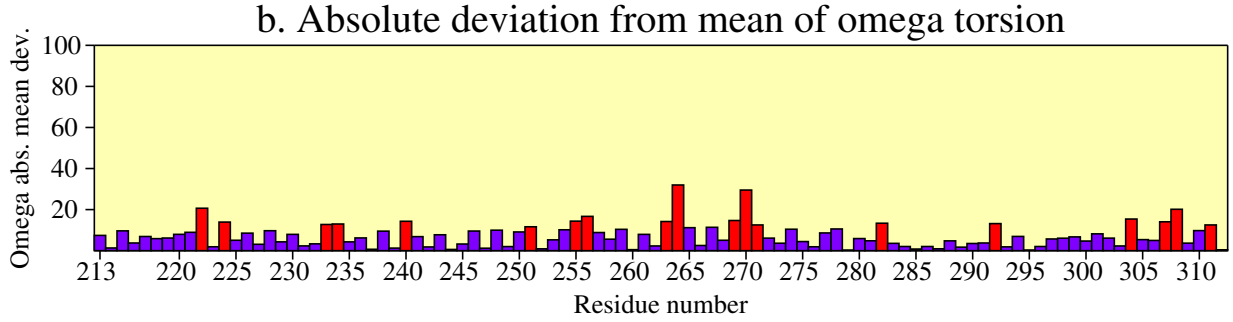


# Residue properties
## pdb2fyu

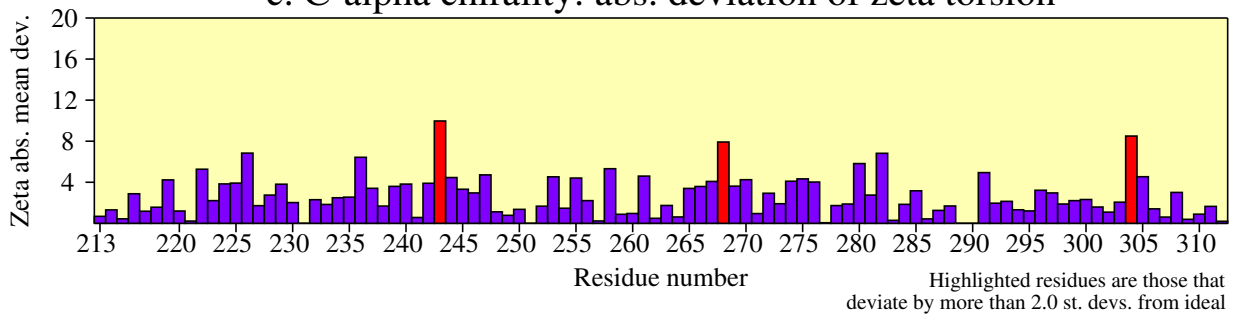
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion

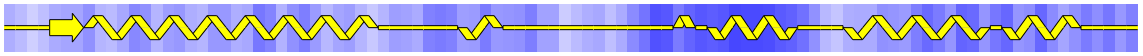



c. C-alpha chirality: abs. deviation of zeta torsion



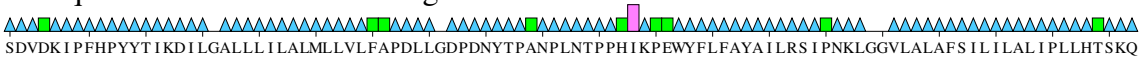

Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



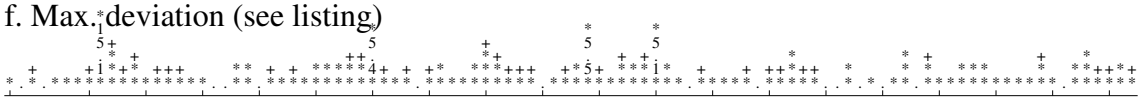
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

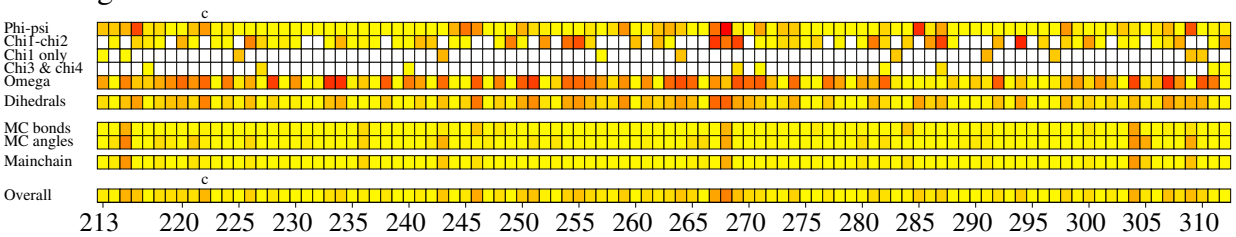


SDVDK I PFHPYYT I KD I LGALLL I LALMLLVLFAPDLLGDPDNYTPANPLNTPPH I KPEWYFLFAYA I LRS I PNKLGGVLALAFS I L I LAL I PLLHTSKQ

f. Max. deviation (see listing)



g. G-factors

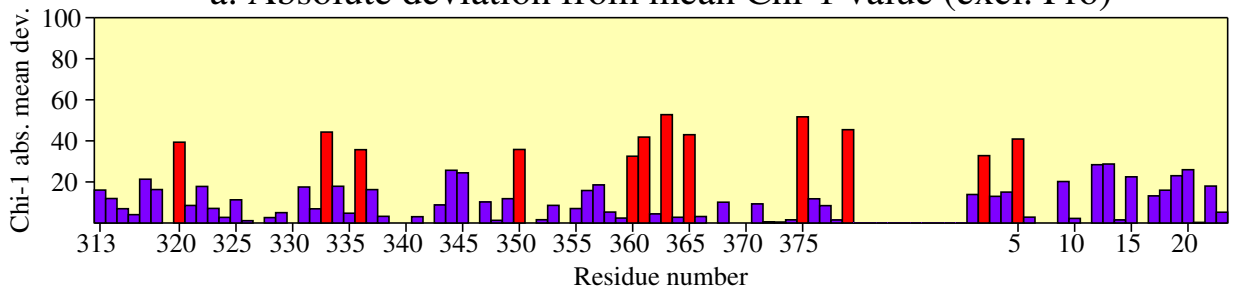



c = cis-peptide

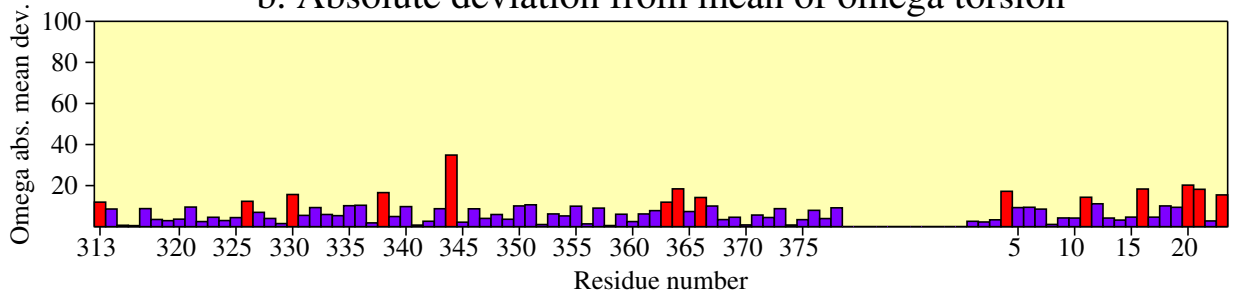
# Residue properties

## pdb2fyu

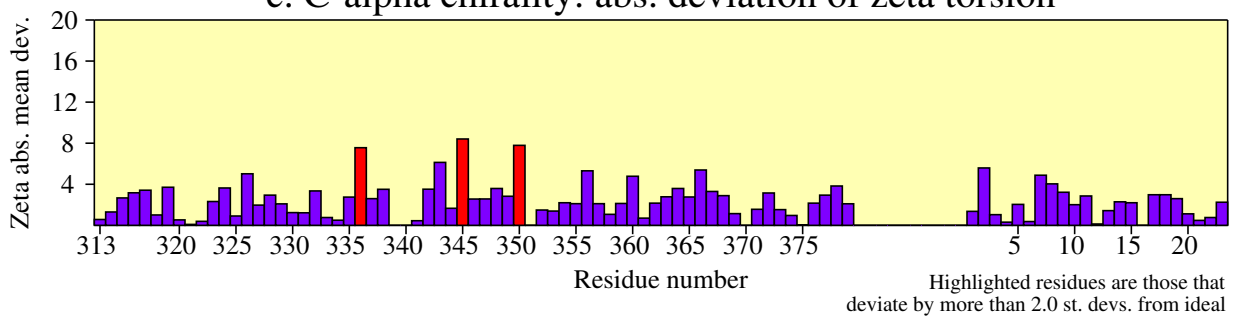
### a. Absolute deviation from mean Chi-1 value (excl. Pro)




### b. Absolute deviation from mean of omega torsion




### c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

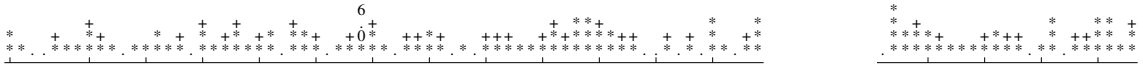
### d. Secondary structure & estimated accessibility


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

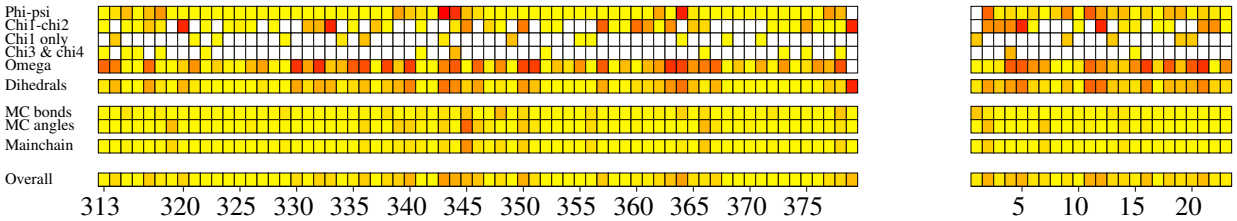
### e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed


### f. Max. deviation (see listing)

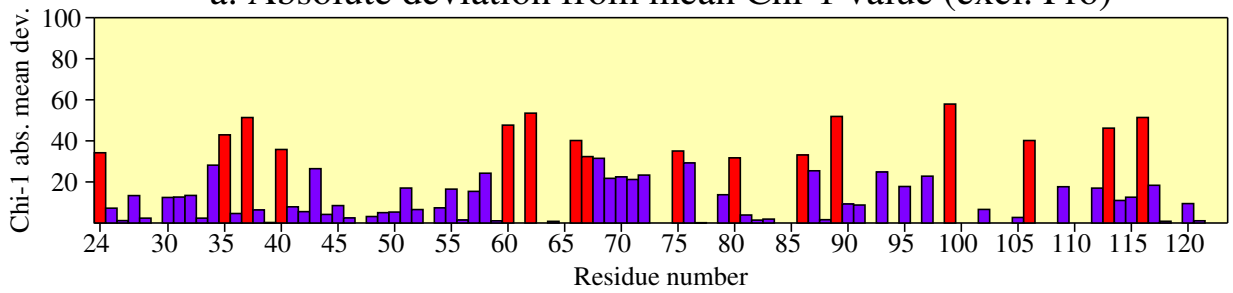


### g. G-factors

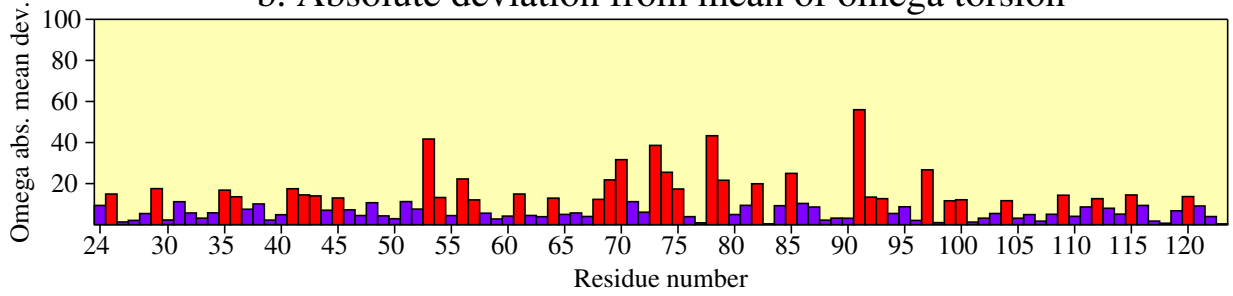


# Residue properties
## pdb2fyu

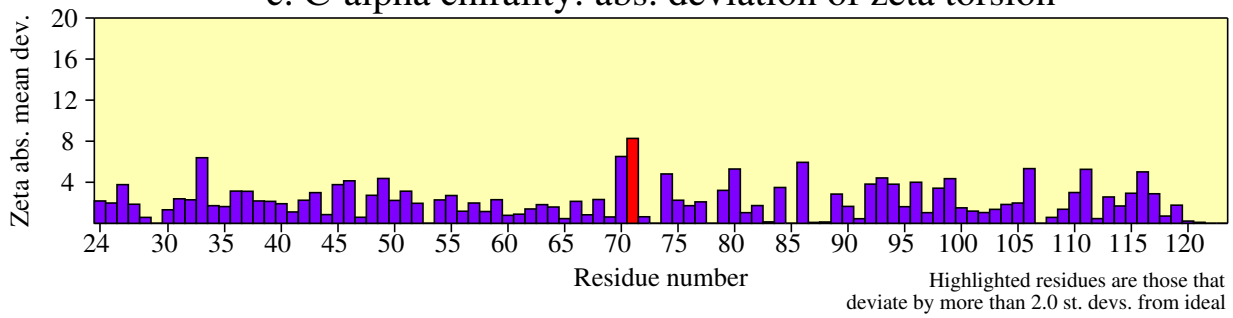
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion

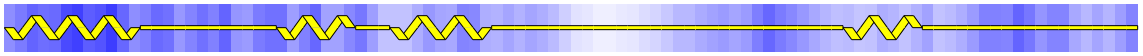



c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

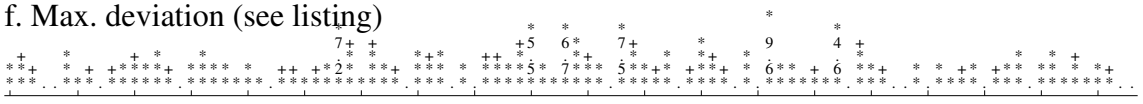


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

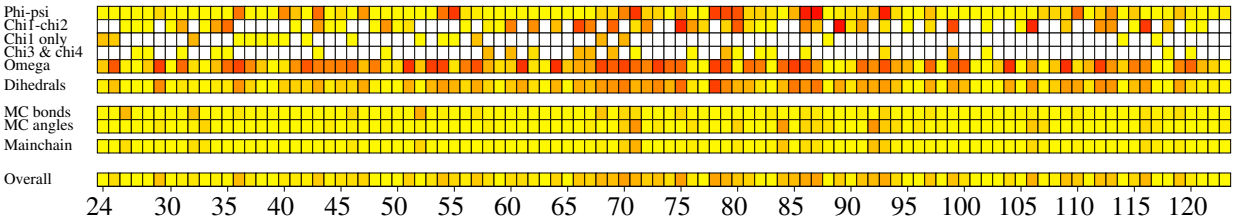
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

T S I R R G F Q V Y K Q V C S S C H S M D Y V A Y R H L V G V C Y T E D E A K A L A E E V E V Q D G P N E D G E M F M R P G K L S D Y F P K P Y P N P E A A R A A N N G A L P P D L S Y I V R A R H G G

f. Max. deviation (see listing)

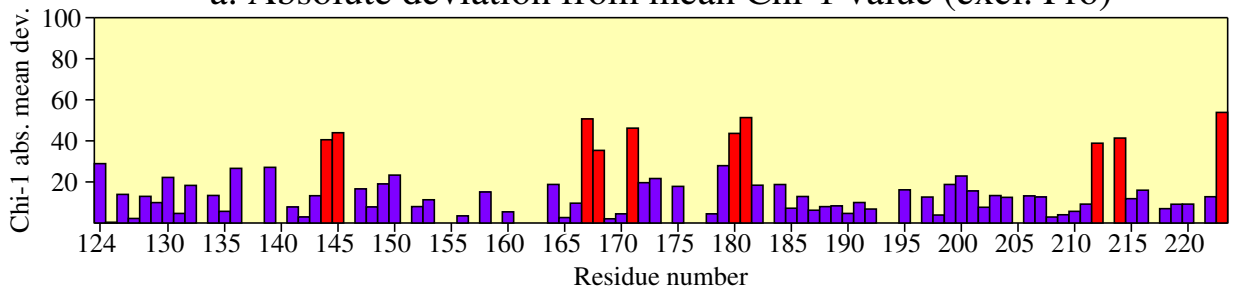


g. G-factors

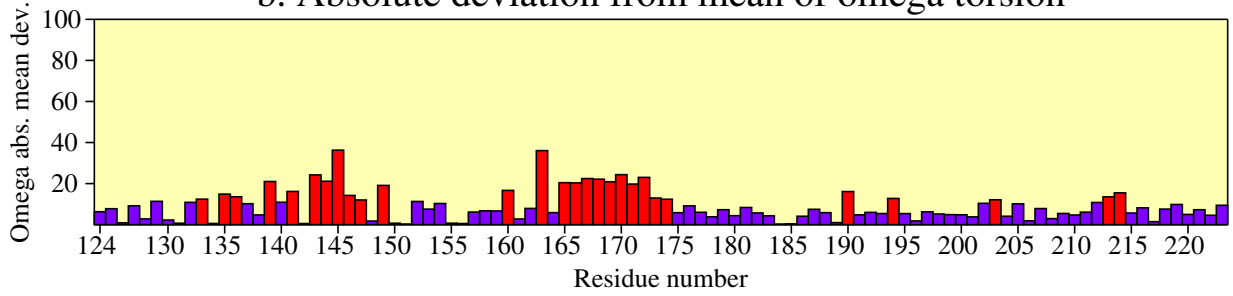


# Residue properties
## pdb2fyu

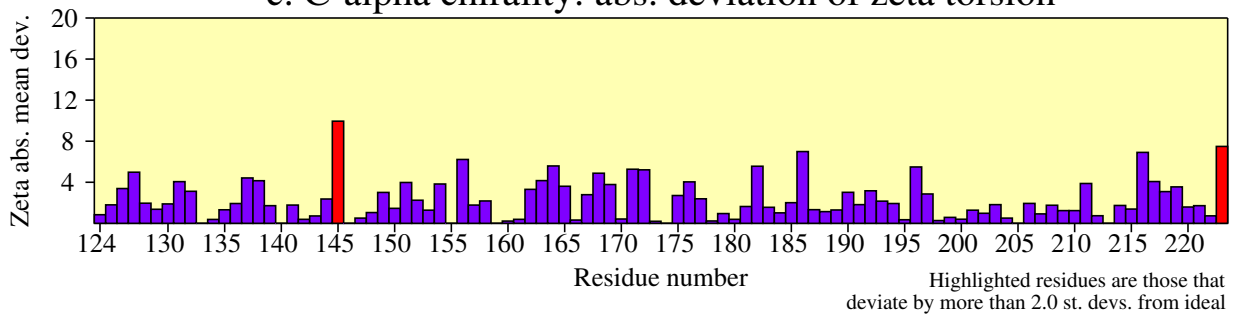
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion

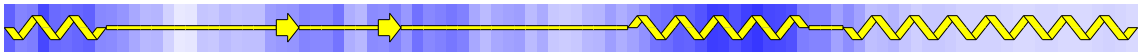



c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

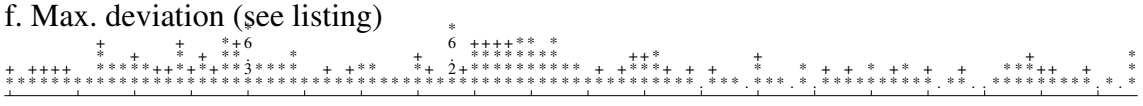


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

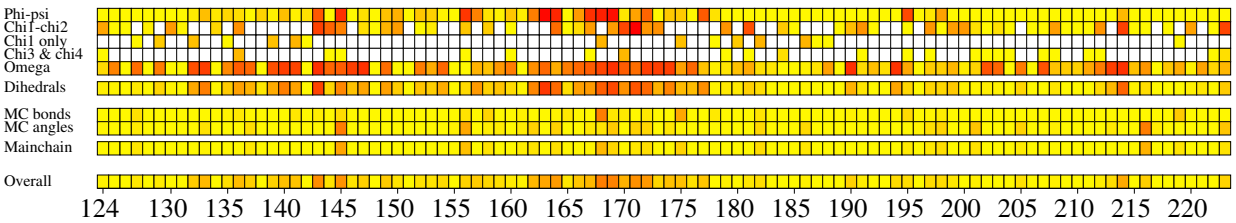
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

EDYVFSLLTGYCEPPTGVSLREGLYFNPYFPGQAIGMAPPIYNEVLEFDDGTPATMSQVAKDVCTFLRWAAEPEHDHRKRMGLKMLLMMGLLLPLVYAMK

f. Max. deviation (see listing)



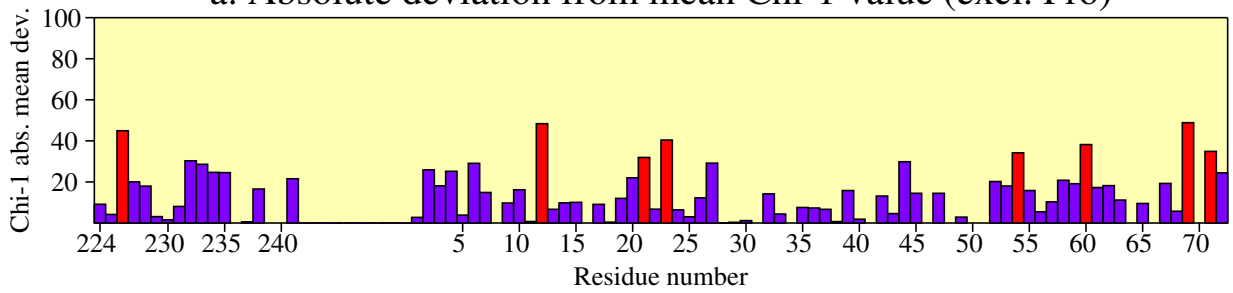
g. G-factors



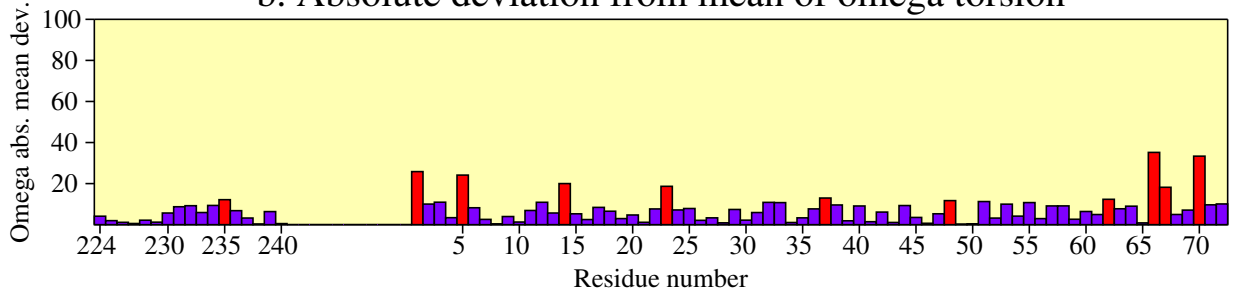
# Residue properties

## pdb2fyu

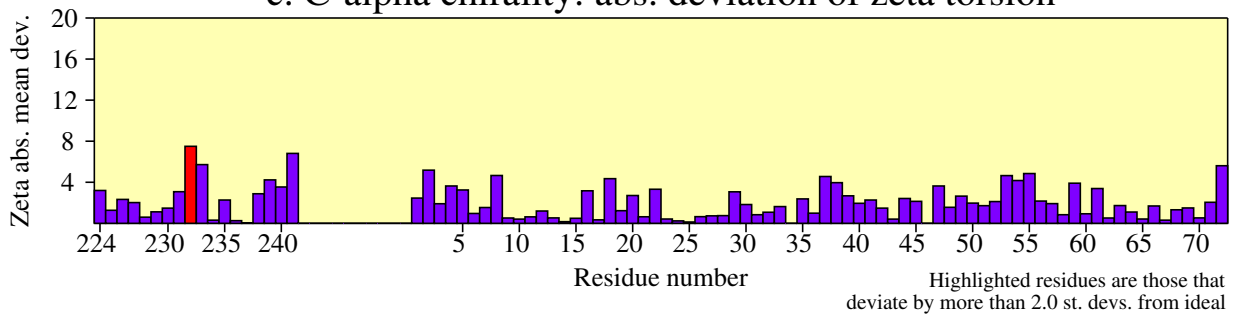
### a. Absolute deviation from mean Chi-1 value (excl. Pro)




### b. Absolute deviation from mean of omega torsion

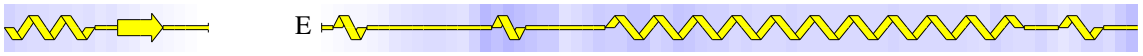



### c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility

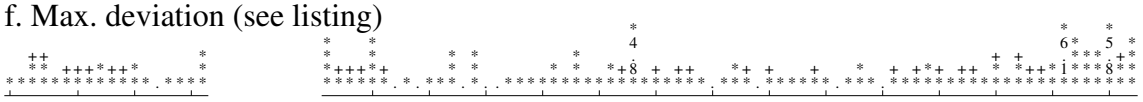



Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

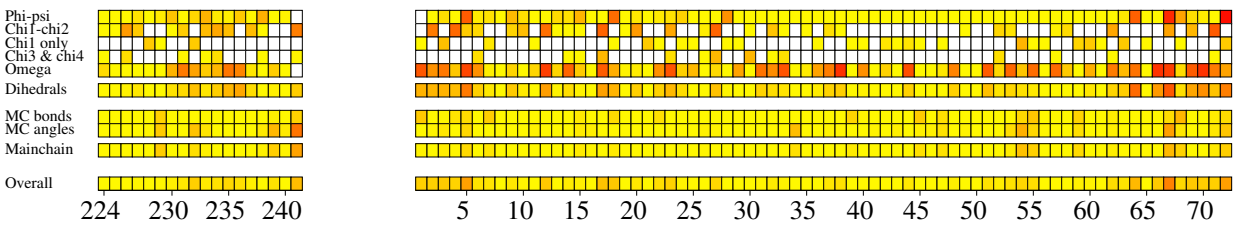
### e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed


### f. Max. deviation (see listing)

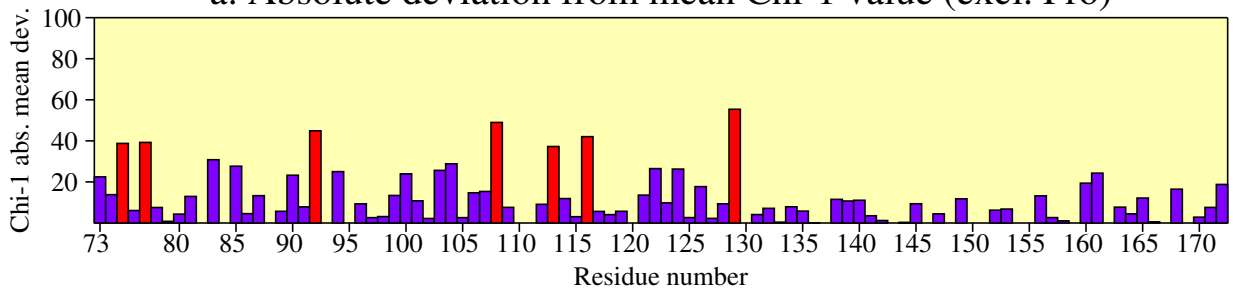


### g. G-factors

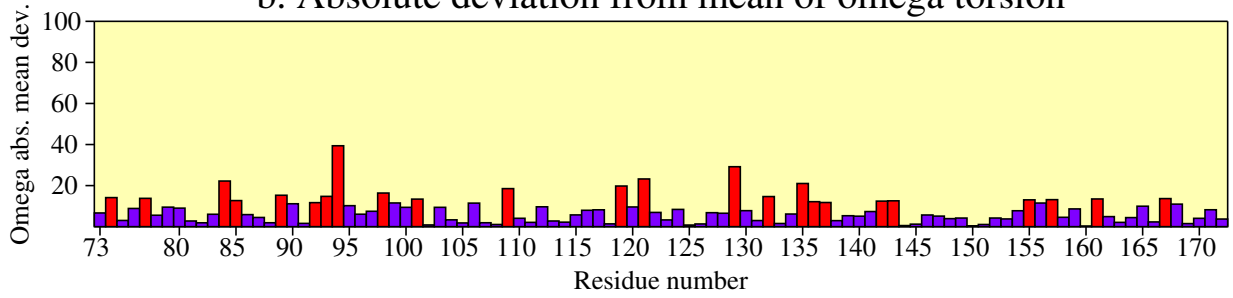


# Residue properties
## pdb2fyu

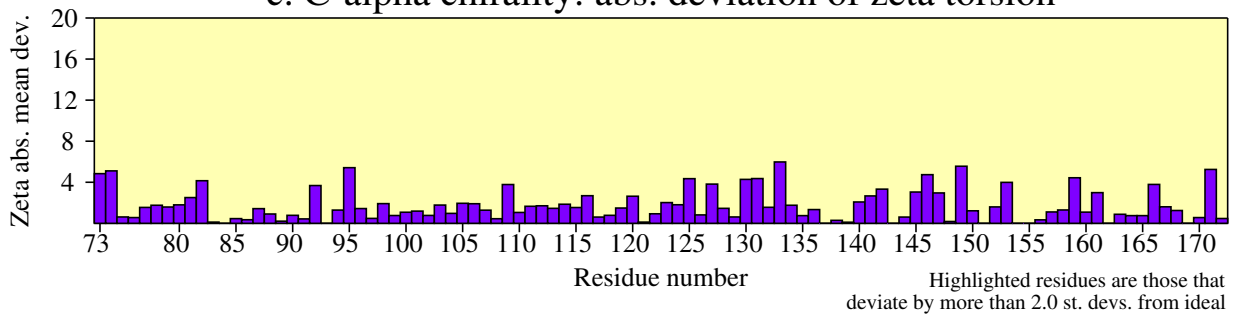
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion

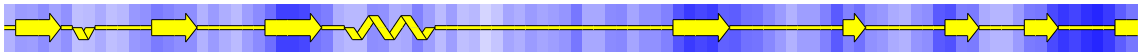



c. C-alpha chirality: abs. deviation of zeta torsion



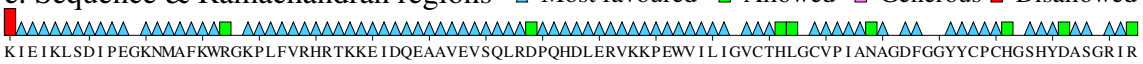

Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



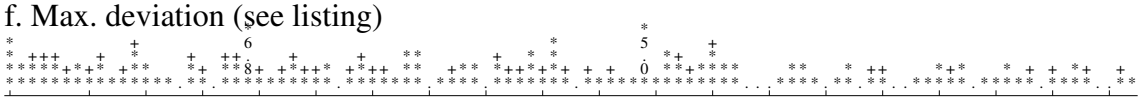
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

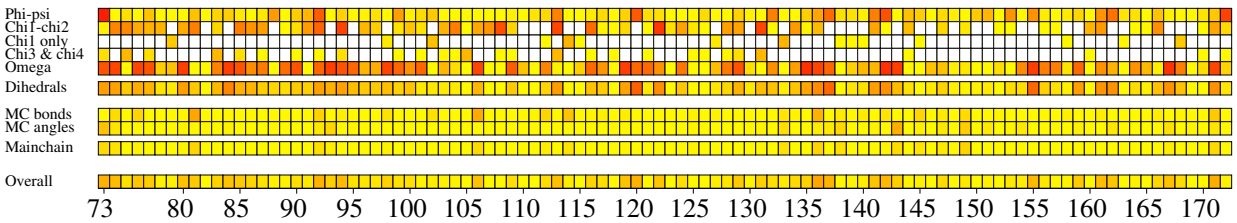


K I E I K L S D I P E G K N M A F K W R G K P L F V R H R T K K E I D Q E A A V E V S Q L R D P Q H D L E R V K K P E W V I L I G V C T H L G C V P I A N A G D F G G Y Y C P C H G S H Y D A S G R I R

f. Max. deviation (see listing)

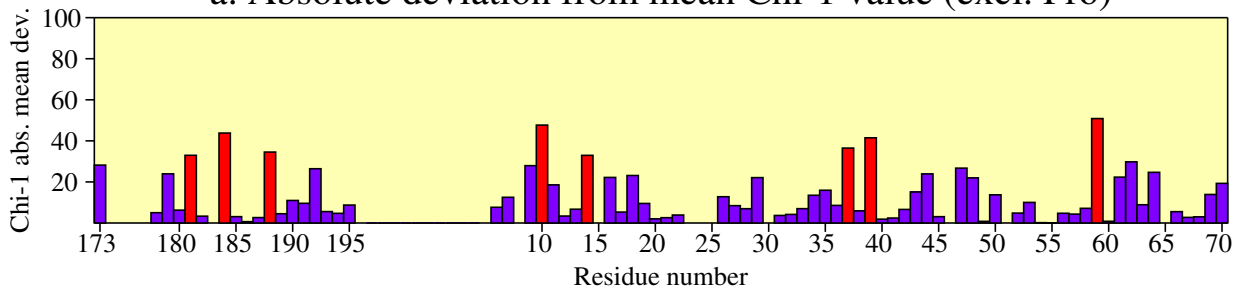


g. G-factors

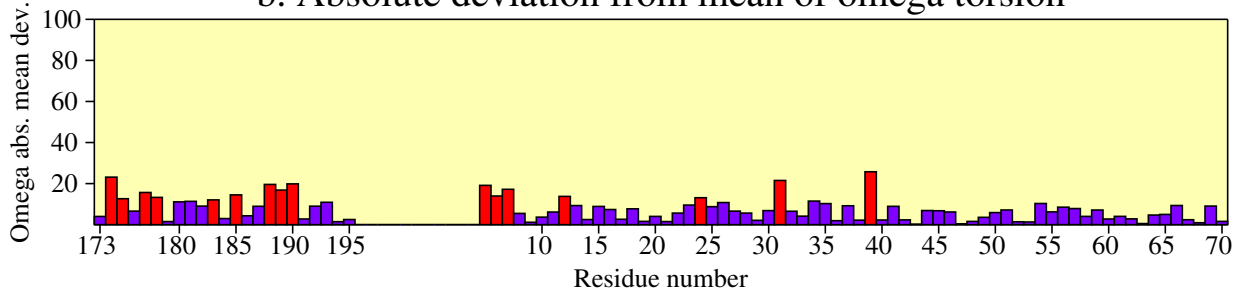


# Residue properties
## pdb2fyu

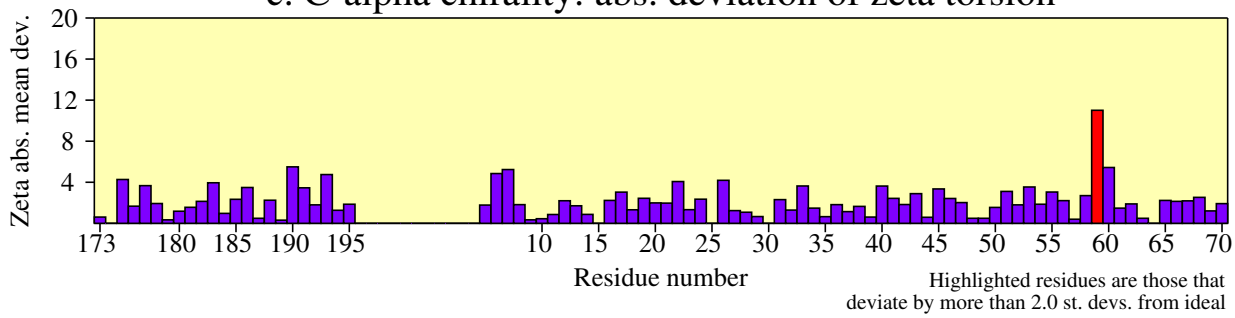
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion




c. C-alpha chirality: abs. deviation of zeta torsion



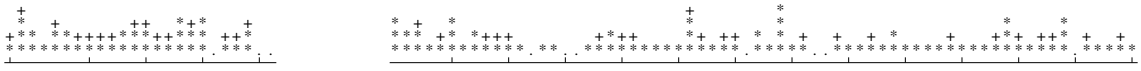

Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

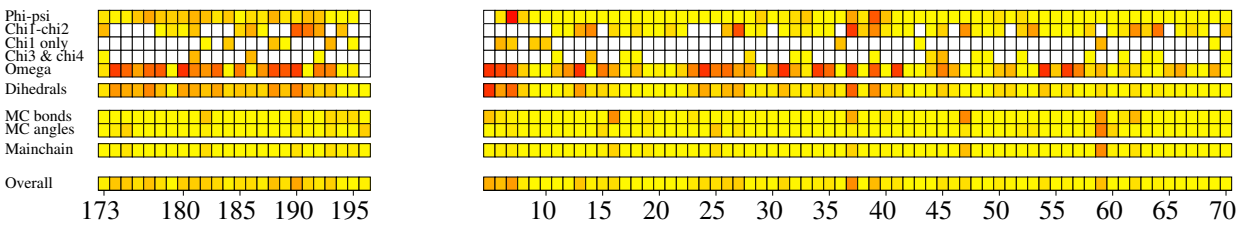

Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed


f. Max. deviation (see listing)

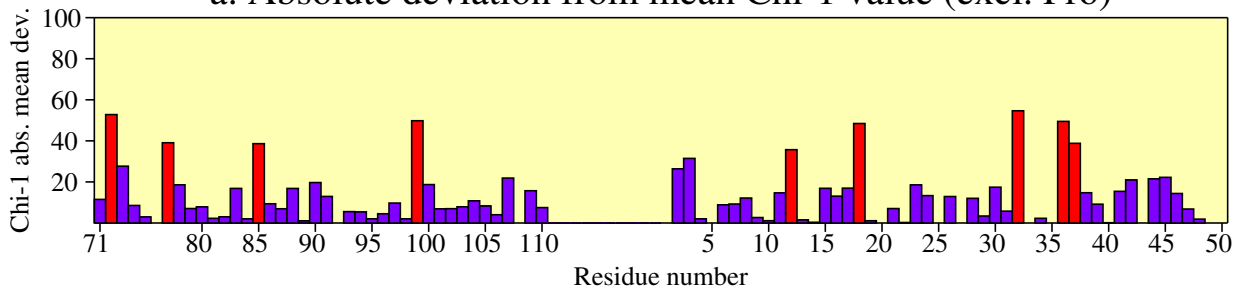


g. G-factors

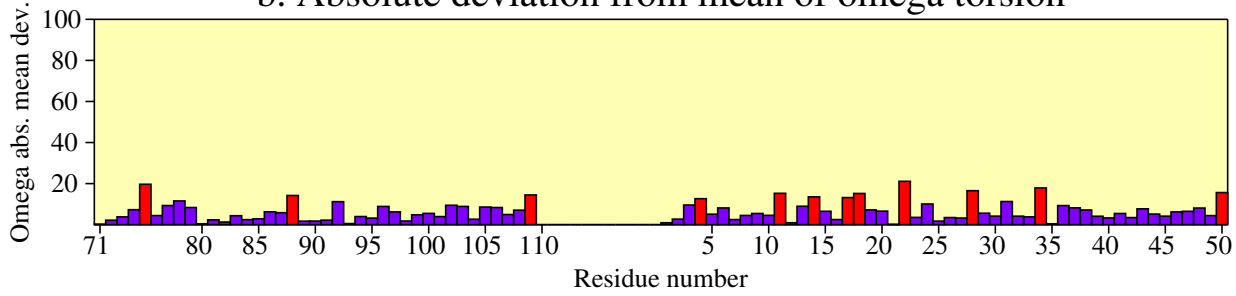


# Residue properties
## pdb2fyu

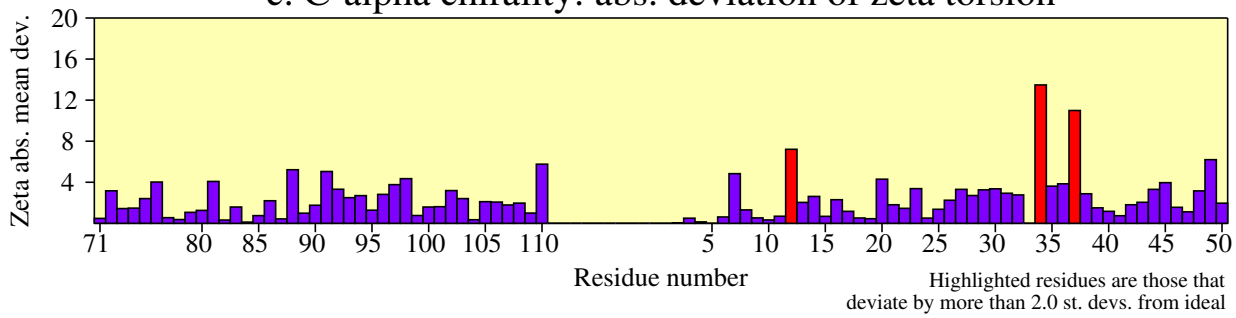
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion

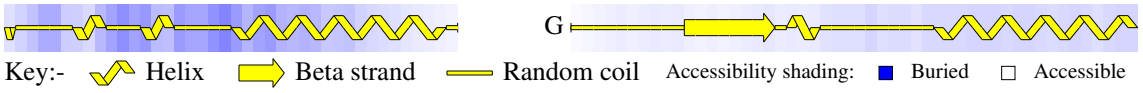



c. C-alpha chirality: abs. deviation of zeta torsion




Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

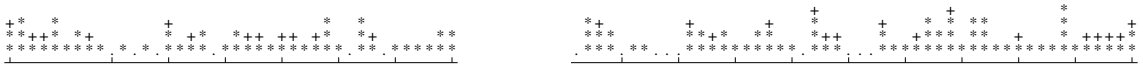
d. Secondary structure & estimated accessibility



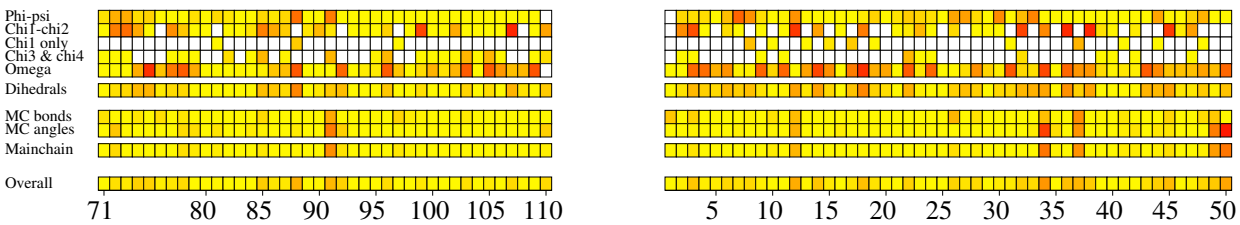

e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed


f. Max. deviation (see listing)

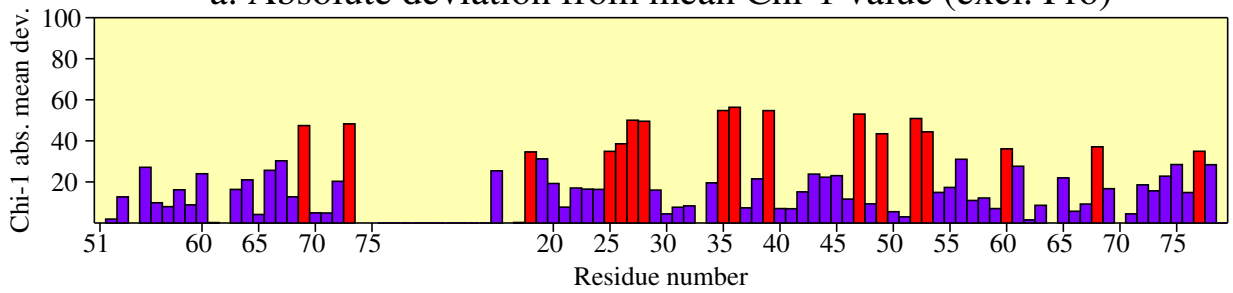


g. G-factors

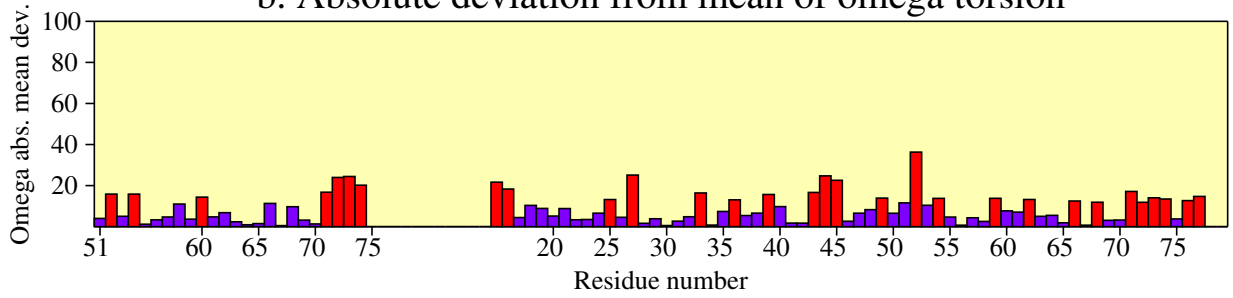


# Residue properties
## pdb2fyu

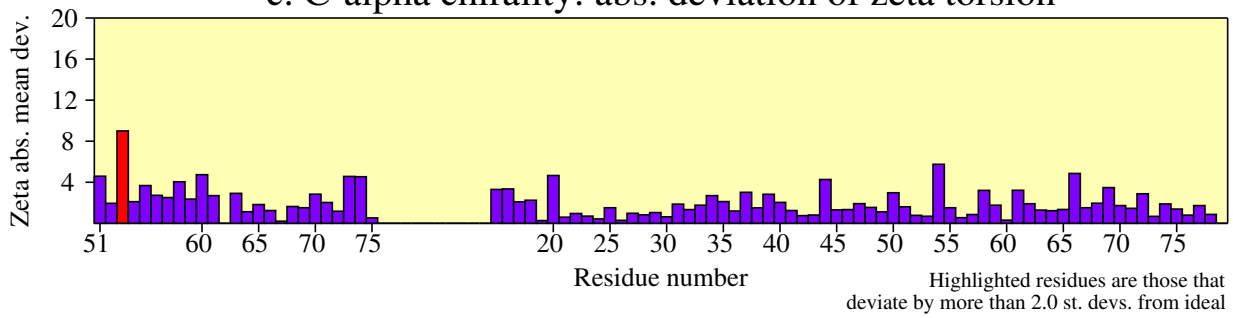
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion




c. C-alpha chirality: abs. deviation of zeta torsion



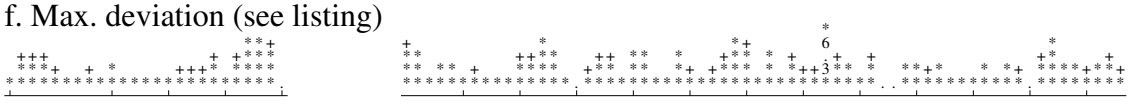

Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

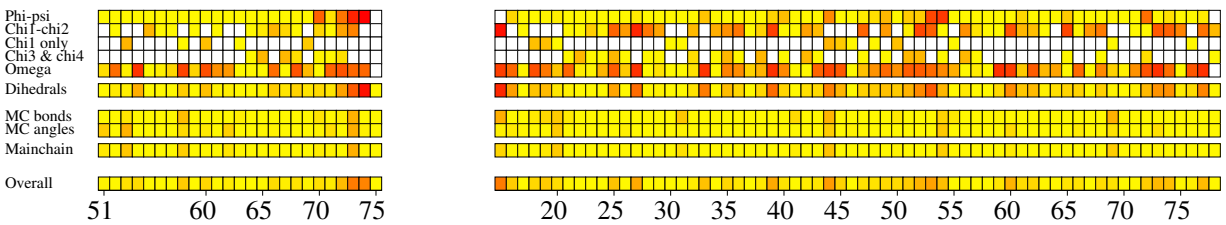

Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed


f. Max. deviation (see listing)

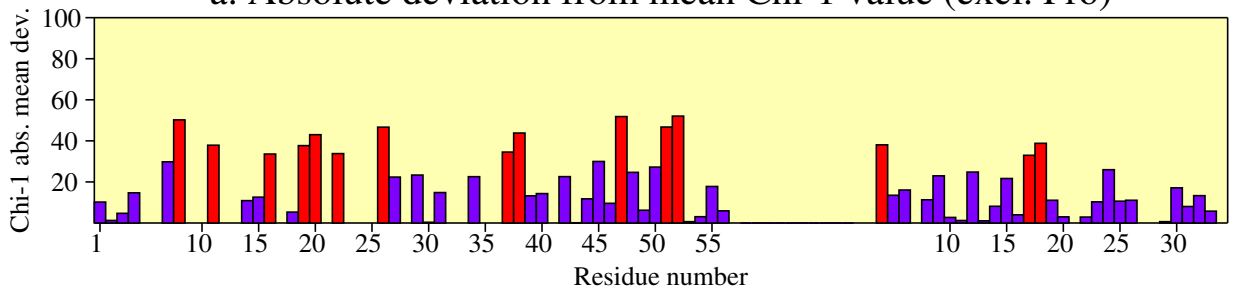


g. G-factors

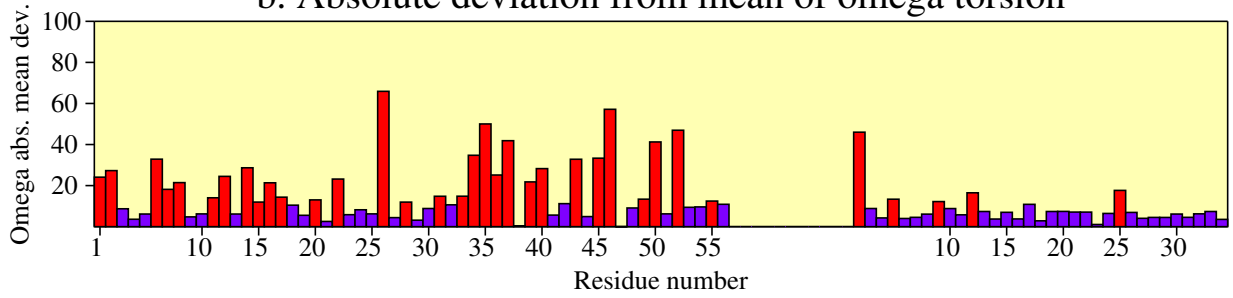


# Residue properties
## pdb2fyu

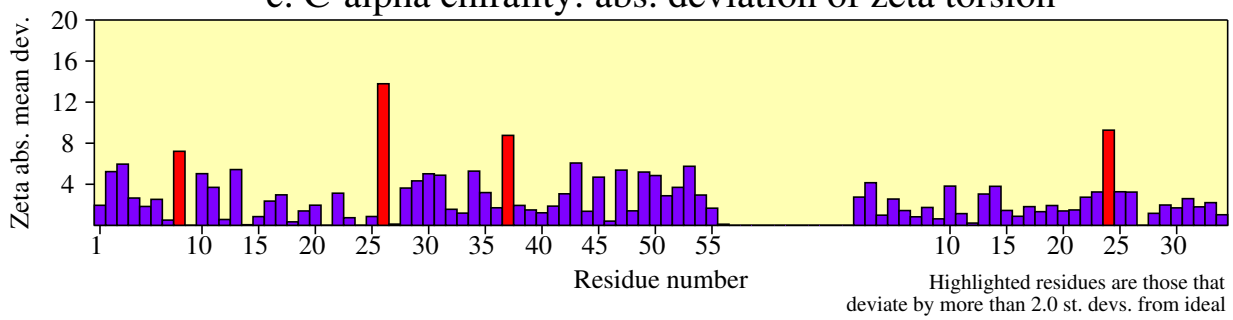
a. Absolute deviation from mean Chi-1 value (excl. Pro)



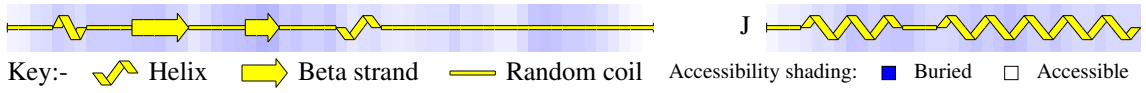

b. Absolute deviation from mean of omega torsion




c. C-alpha chirality: abs. deviation of zeta torsion

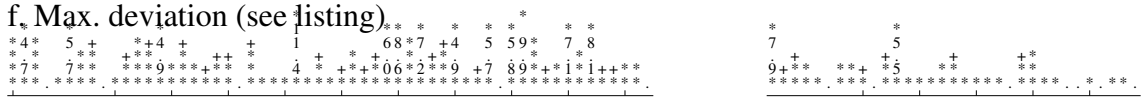



d. Secondary structure & estimated accessibility

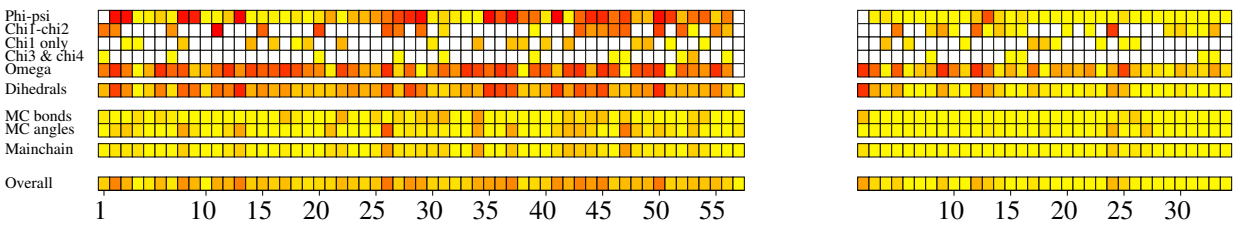



e. Sequence & Ramachandran regions


f. Max. deviation (see listing)

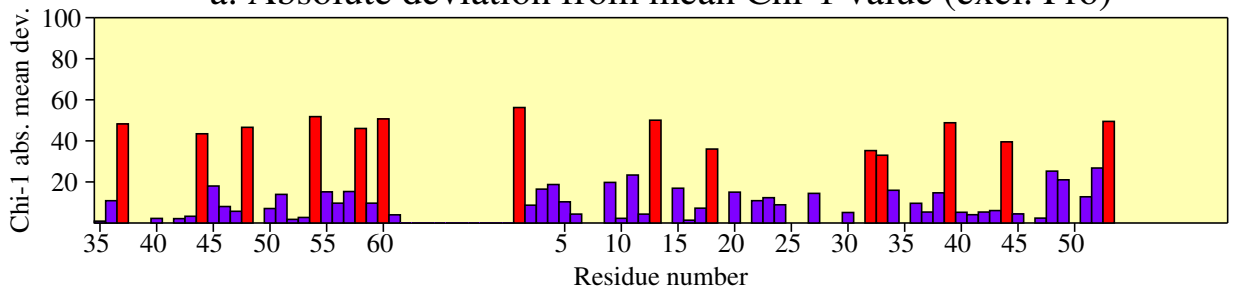


g. G-factors

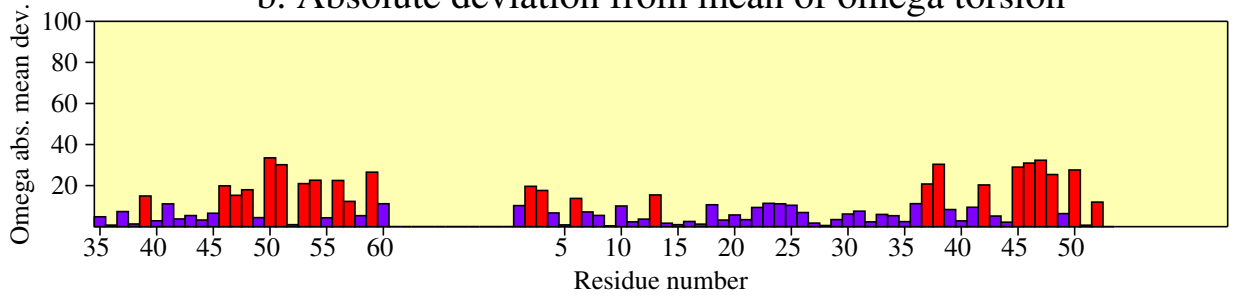


# Residue properties
## pdb2fyu

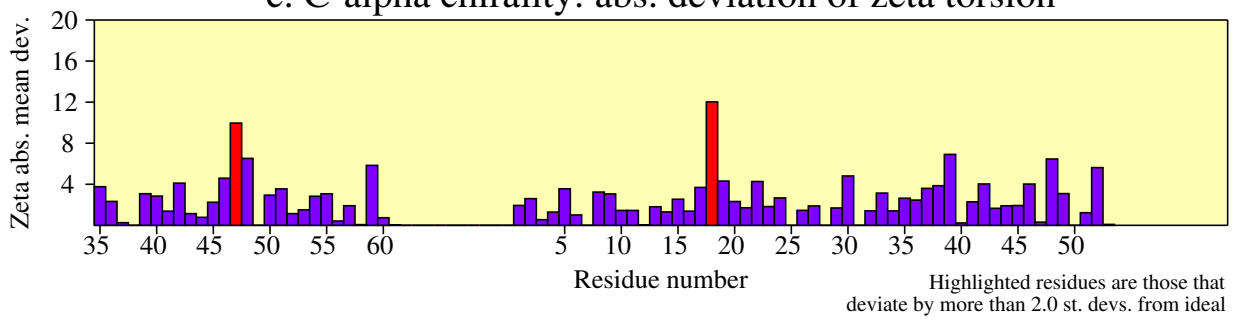
a. Absolute deviation from mean Chi-1 value (excl. Pro)




b. Absolute deviation from mean of omega torsion




c. C-alpha chirality: abs. deviation of zeta torsion



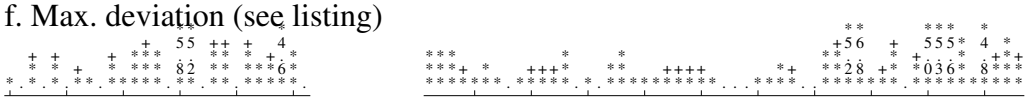

Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

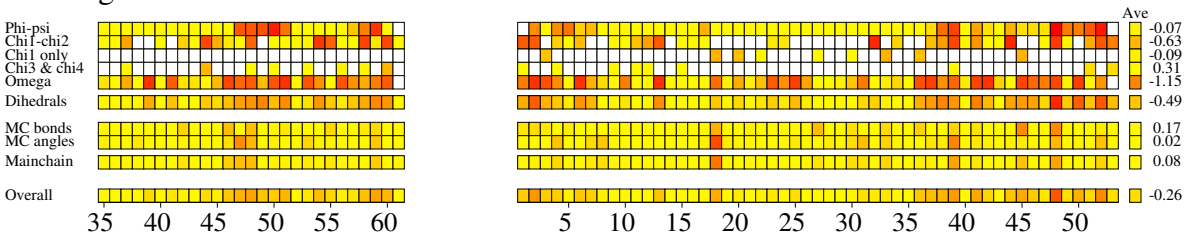

Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed


f. Max. deviation (see listing)

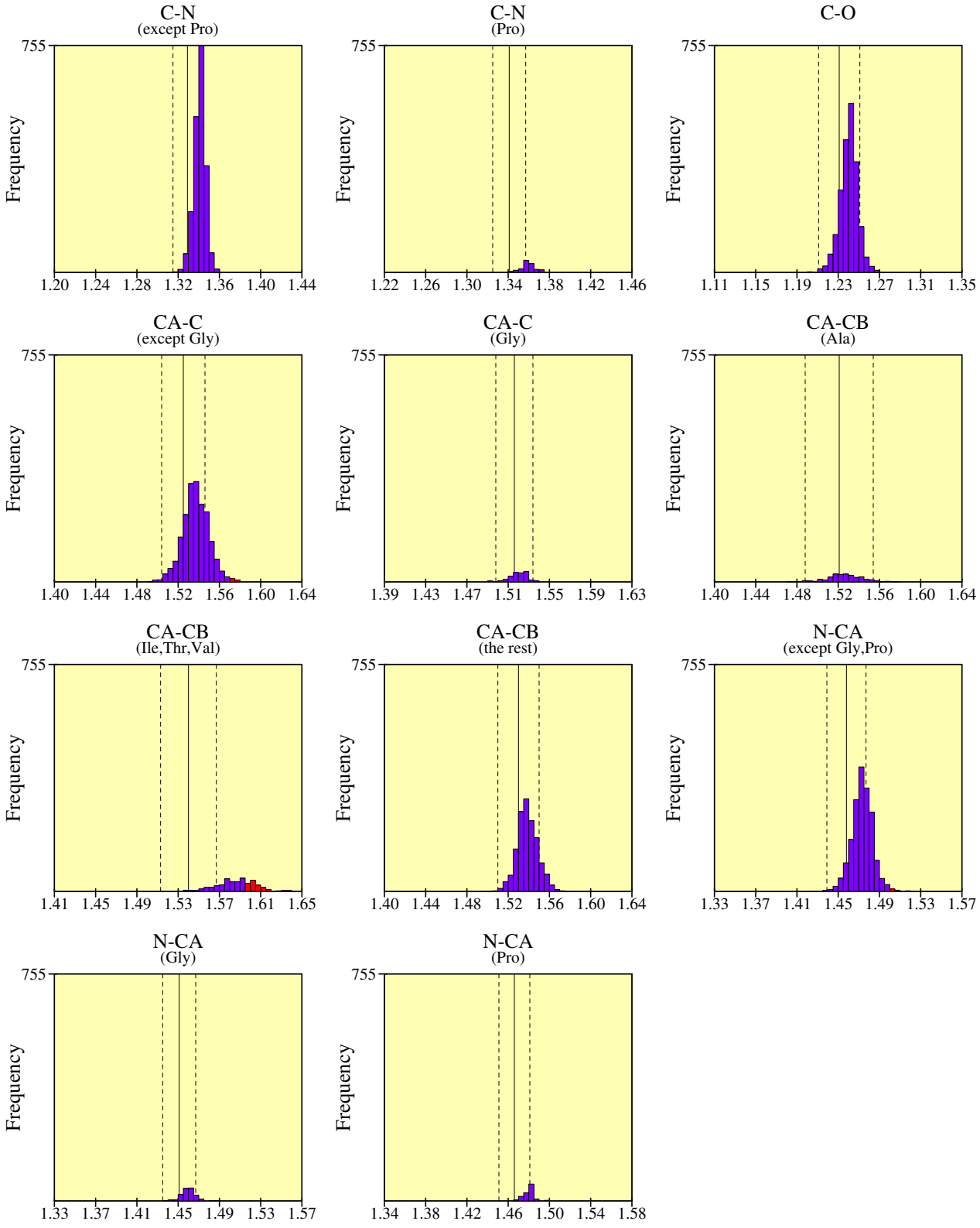


g. G-factors



# Main-chain bond lengths

## pdb2fyu

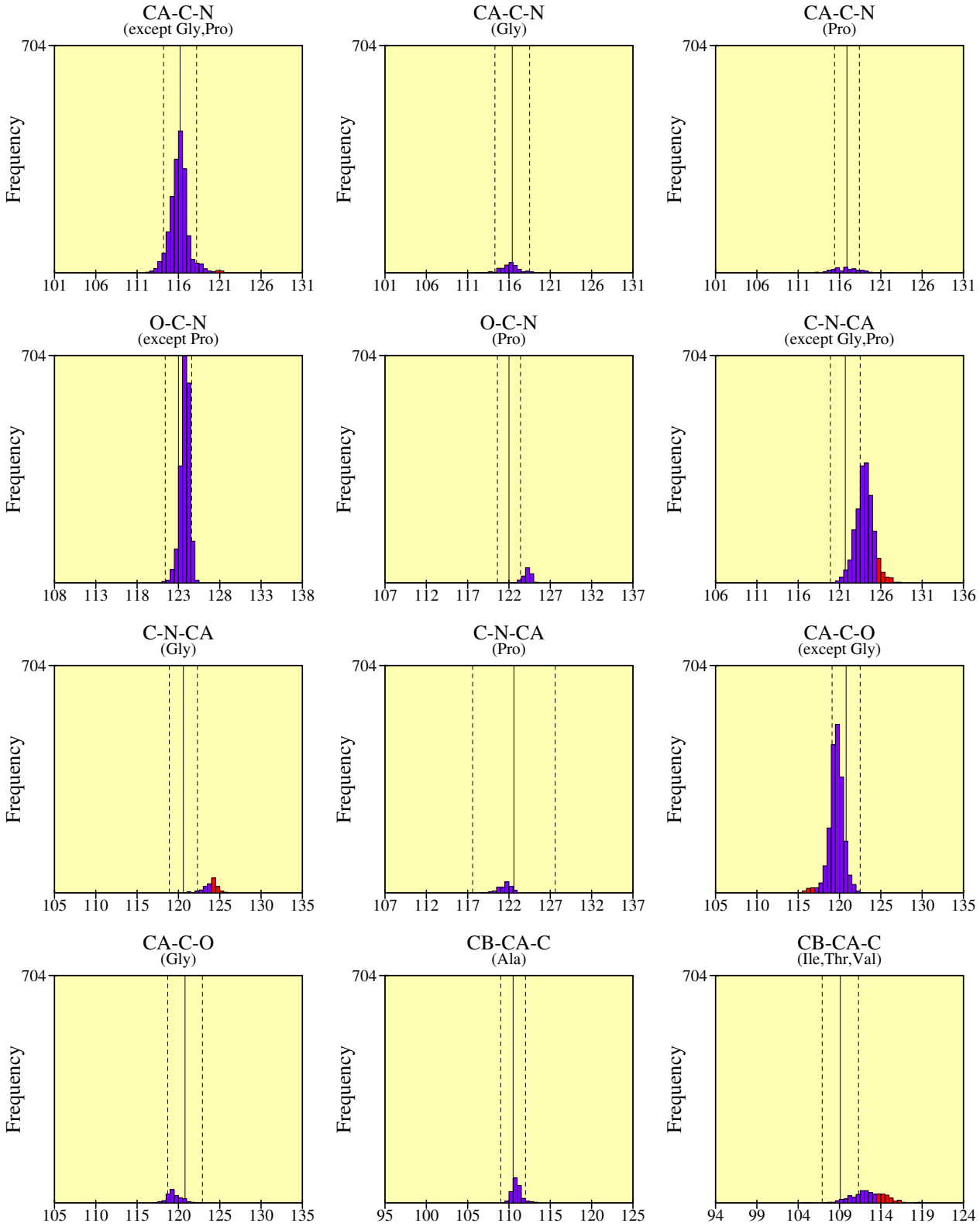



Black bars > 2.0 st. devs. from mean.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# Main-chain bond angles

## pdb2fyu

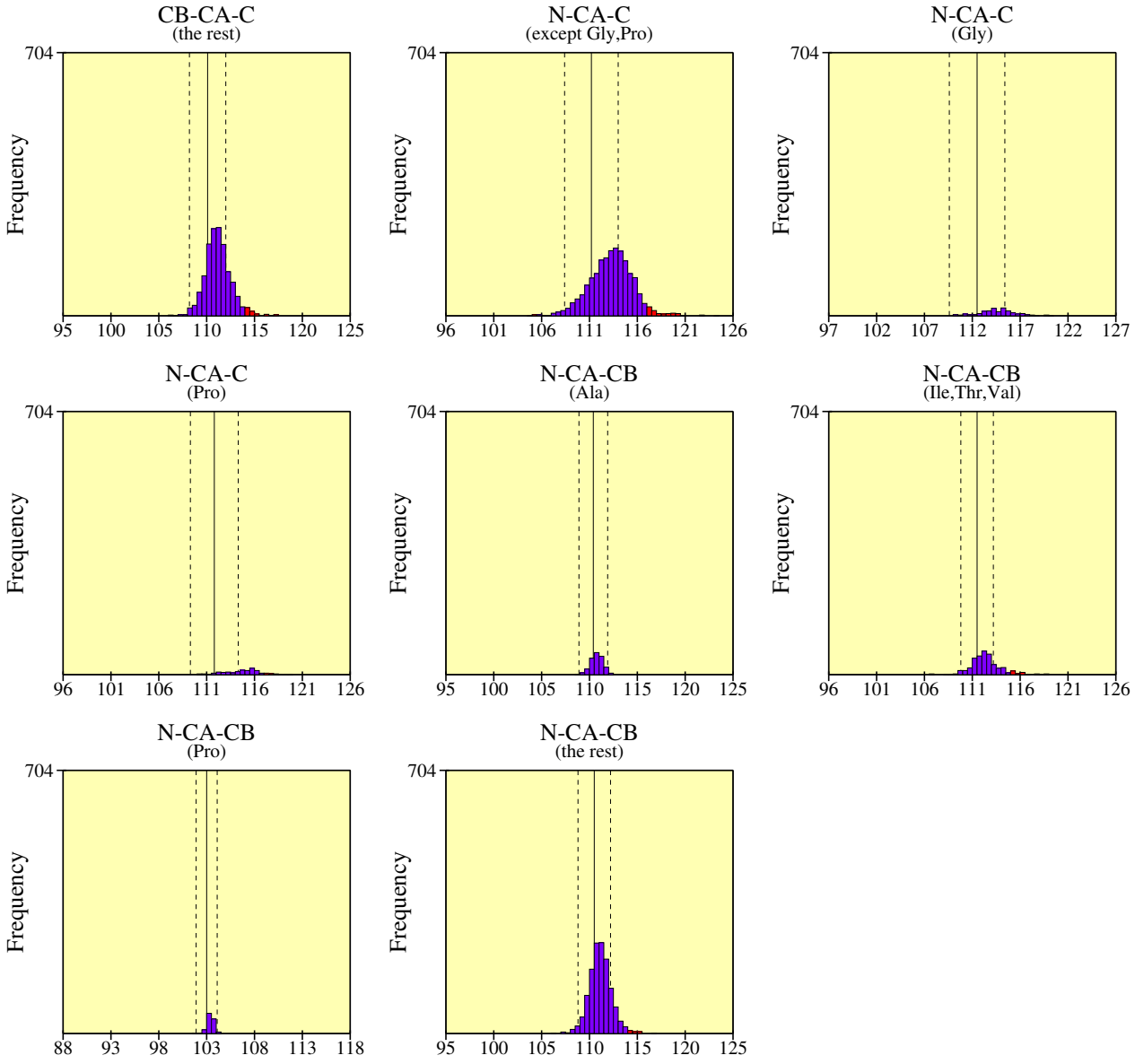



Black bars > 2.0 st. devs. from mean.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# Main-chain bond angles

## pdb2fyu

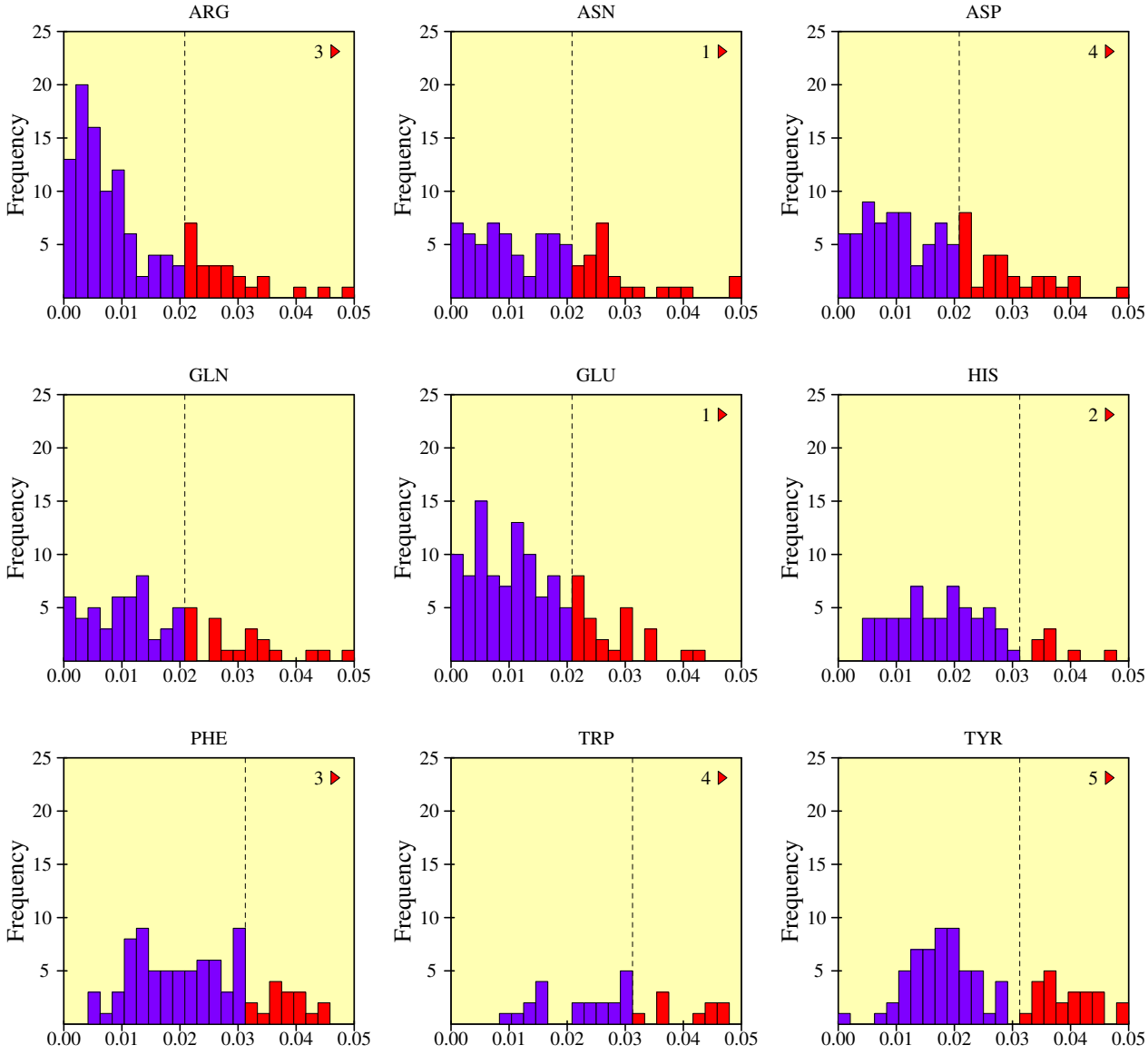



Black bars > 2.0 st. devs. from mean.

Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

# RMS distances from planarity

## pdb2fyu

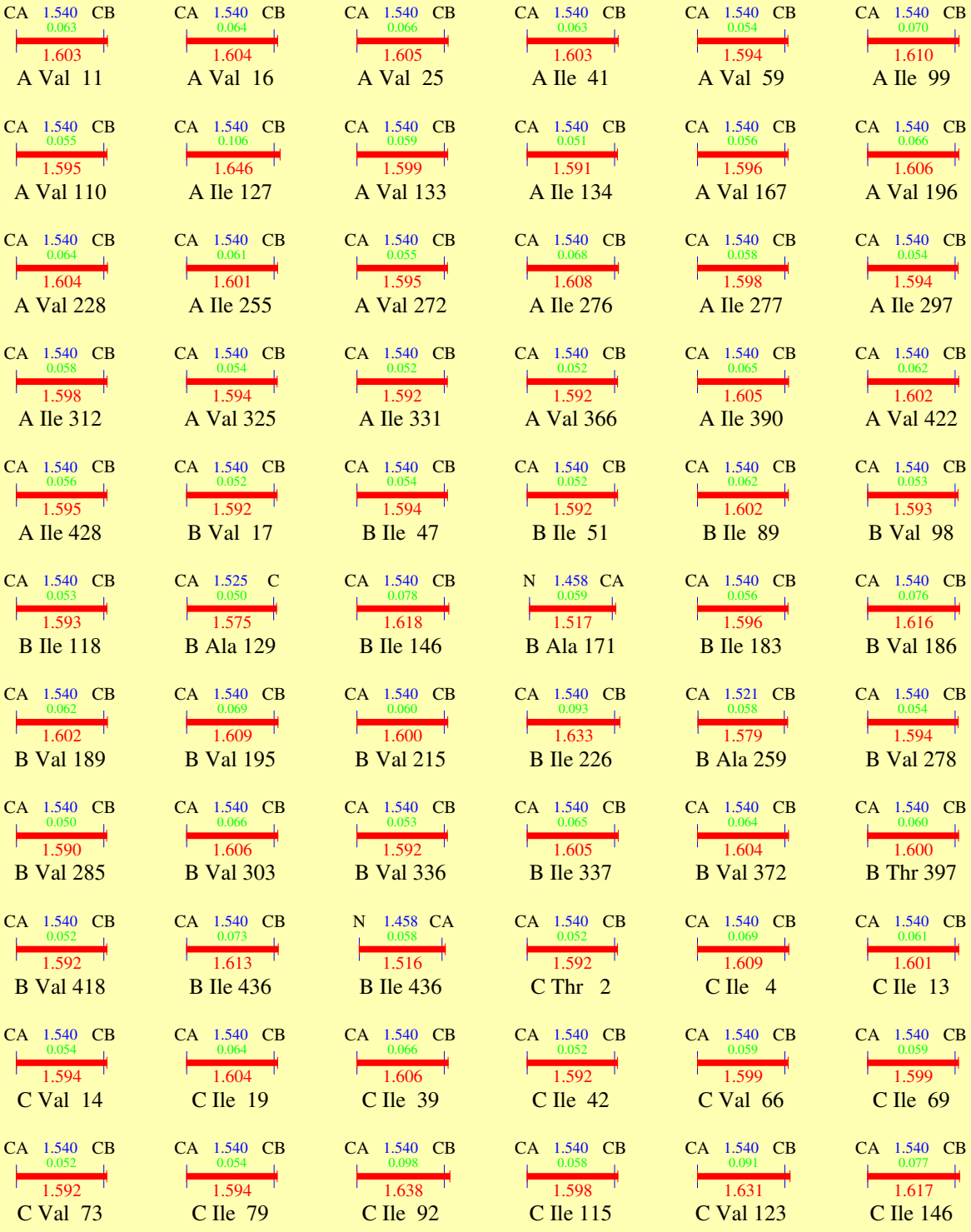



Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

▸ signifies data points off the graph in the direction shown.

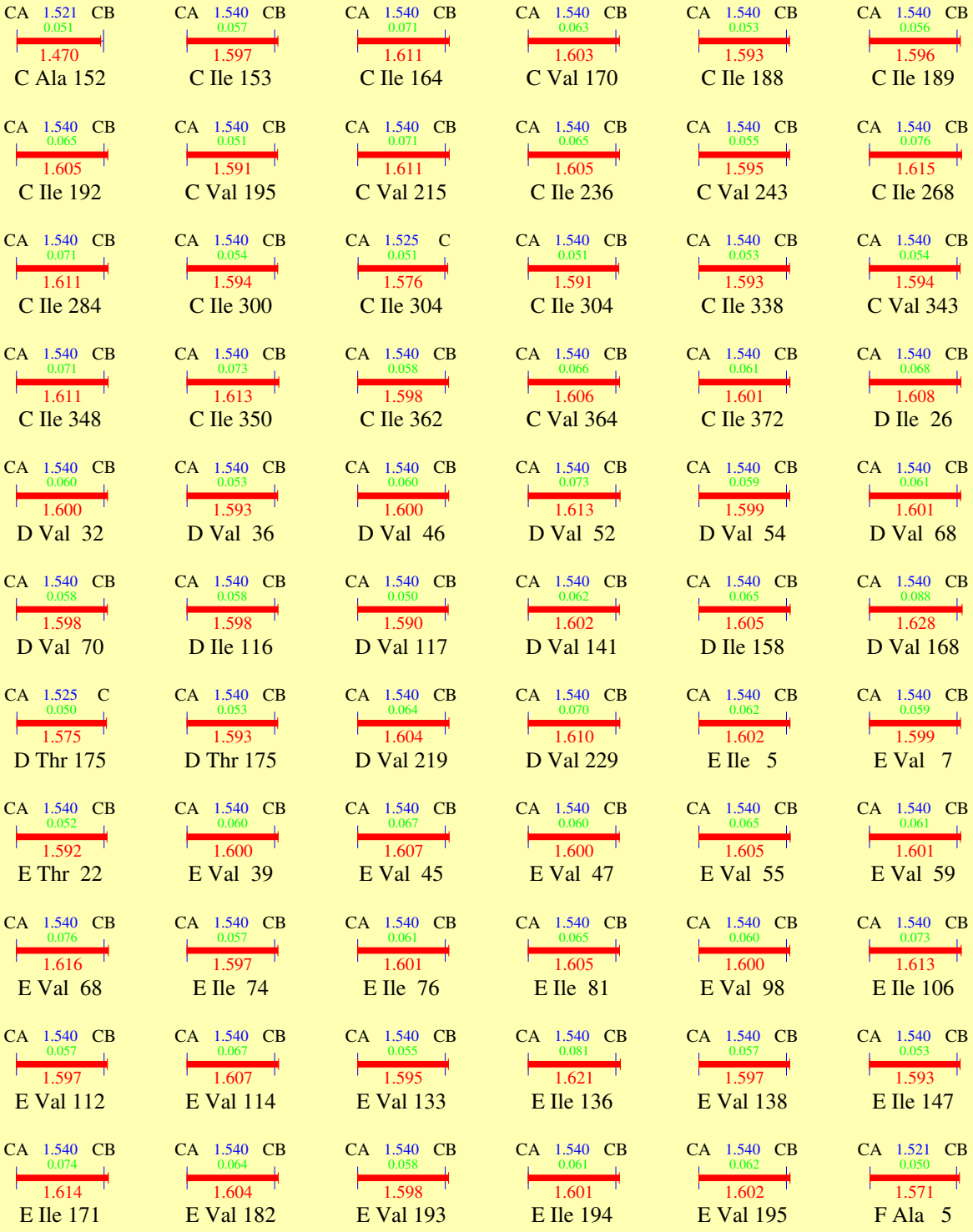
# Distorted geometry
## pdb2fyu

### Main-chain bond lengths



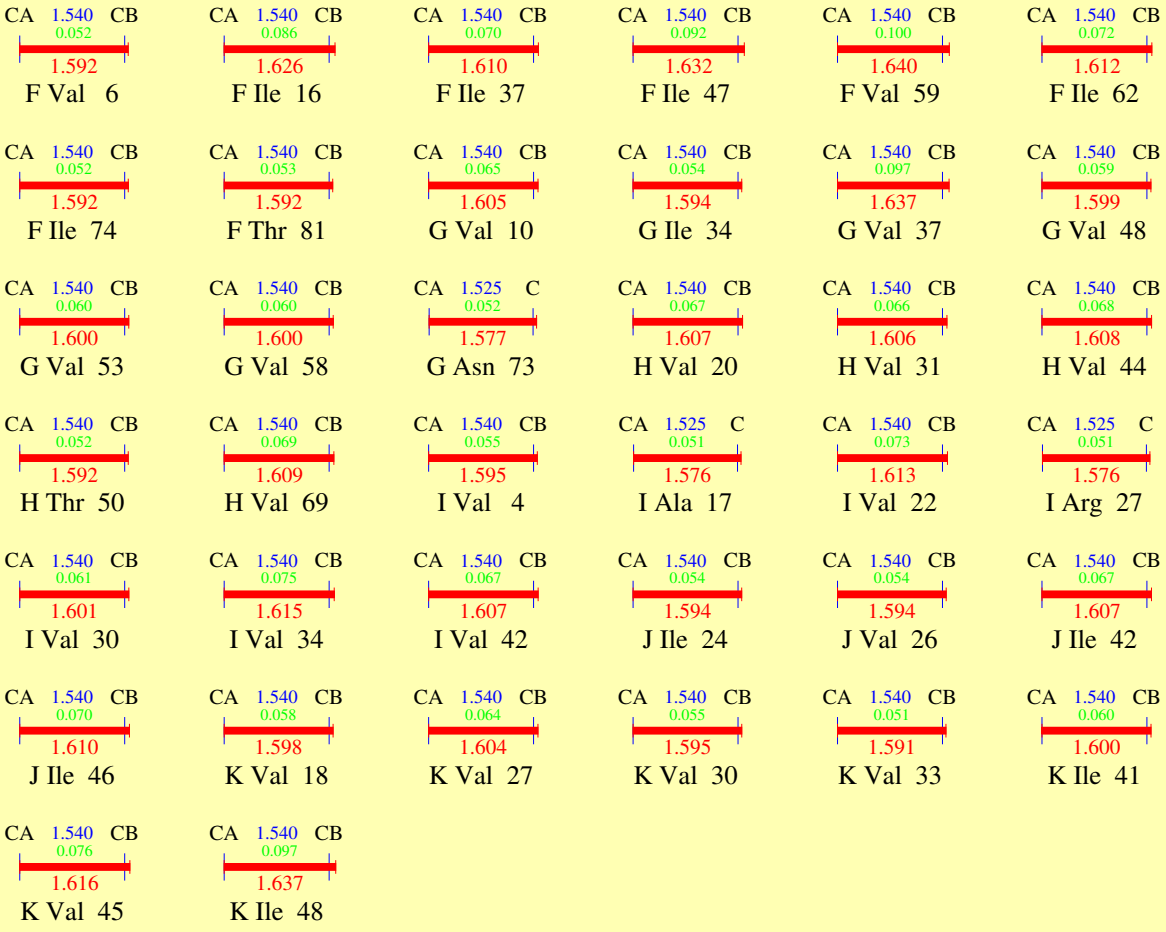
# Distorted geometry
## pdb2fyu

### Main-chain bond lengths (contd)



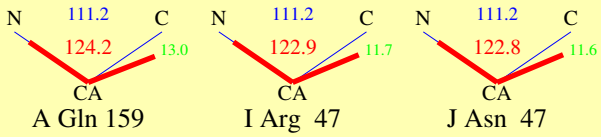
# Distorted geometry
## pdb2fyu

### Main-chain bond lengths (contd)




Bonds differing by > 0.05A from small-molecule values. Values shown: "ideal", difference, actual

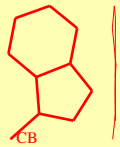
### Main-chain bond angles



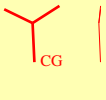

Bond angles differing by > 10.0 degrees from small-molec values. Values shown: "ideal", actual, diff.

# Distorted geometry
## pdb2fyu

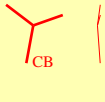
### Planar groups



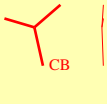

0.045
A Trp 40



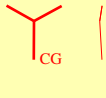

0.029
A Glu 48



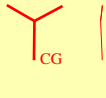

0.048
A Asn 52



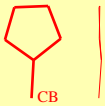

0.025
A Asn 53




0.039
A Glu 60

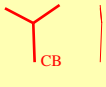



0.029
A Glu 80

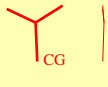



0.033
A His 85

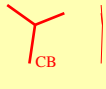

0.027
A Glu 93




0.026
A Asp 105

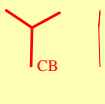



0.022
A Glu 111

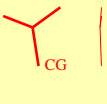



0.022
A Asn 119

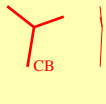

0.020
A Gln 126



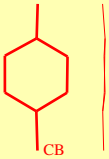

0.022
A Asp 132



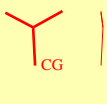

0.025
A Gln 139



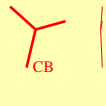

0.036
A Asn 141



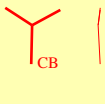

0.035
A Tyr 152



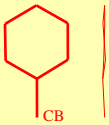

0.033
A Gln 159




0.028
A Asn 173

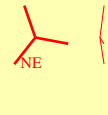



0.035
A Asp 181

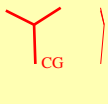



0.037
A Phe 236

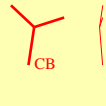

0.031
A Gln 240



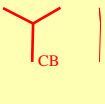

0.069
A Arg 244




0.061
A Glu 245

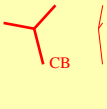



0.053
A Asp 266

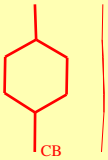



0.020
A Asn 267

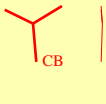

0.043
A Gln 271



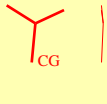

0.071
A Asp 281



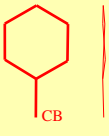

0.035
A Tyr 284



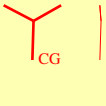

0.021
A Asn 301



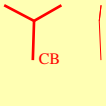

0.030
A Gln 305



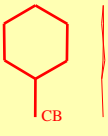

0.036
A Phe 307



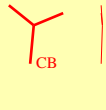

0.021
A Gln 308



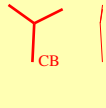

0.030
A Asn 311




0.039
A Phe 324




0.021
A Asp 327

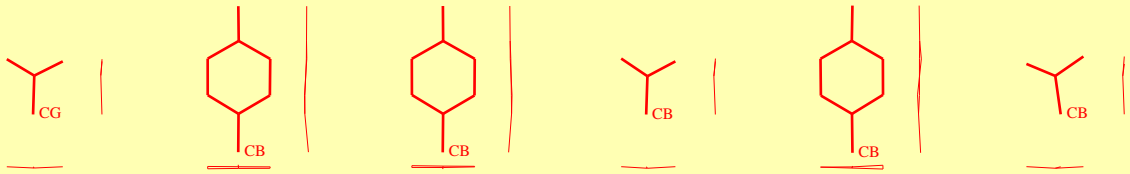



0.039
A Asp 332

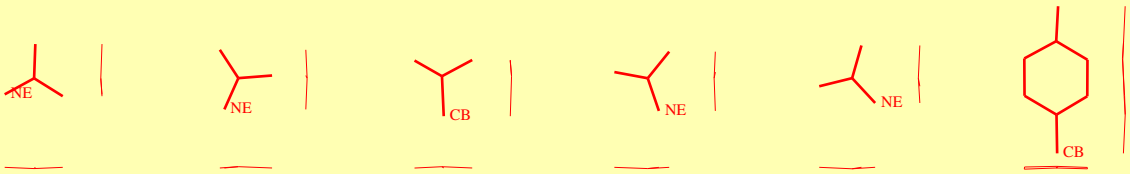
# Distorted geometry
## pdb2fyu

### Planar groups (contd)

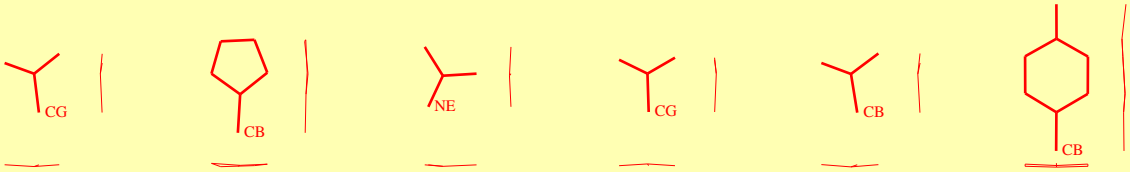

0.020 A Glu 353 | 0.082 A Arg 389 | 0.028 A Glu 394 | 0.021 A Arg 398 | 0.048 A Asp 403 | 0.047 A Arg 408




0.020 A Glu 409 | 0.048 A Tyr 414 | 0.040 A Tyr 416 | 0.026 A Asp 417 | 0.043 A Tyr 434 | 0.026 A Asn 435

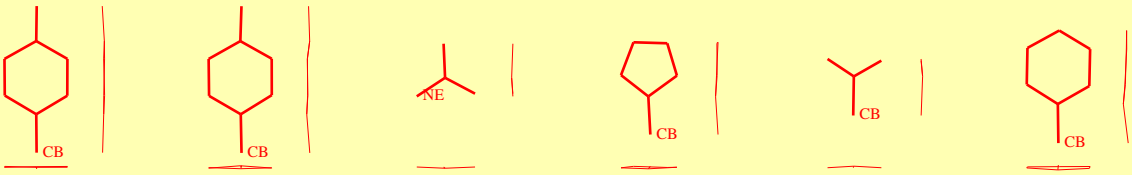



0.020 A Arg 436 | 0.023 A Arg 445 | 0.022 B Asn 31 | 0.020 B Arg 46 | 0.025 B Arg 56 | 0.038 B Tyr 57




0.030 B Glu 58 | 0.045 B His 67 | 0.025 B Arg 102 | 0.029 B Glu 103 | 0.038 B Asn 104 | 0.049 B Tyr 107

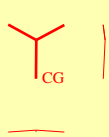

0.042 B Glu 110 | 0.021 B Glu 131 | 0.021 B Arg 133 | 0.021 B Gln 143 | 0.035 B Asp 147 | 0.046 B Asn 162



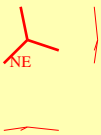

0.032 B Tyr 168 | 0.041 B Tyr 177 | 0.021 B Arg 182 | 0.034 B His 192 | 0.026 B Asp 193 | 0.057 B Phe 199

# Distorted geometry
## pdb2fyu

### Planar groups (contd)



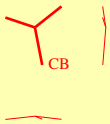

0.032
B Glu 243



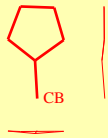

0.057
B Arg 245


0.020
B Glu 246

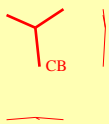

0.034
B Gln 247



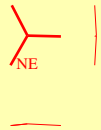

0.054
B Asn 248



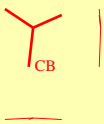

0.036
B His 254



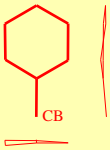

0.038
B Asn 270



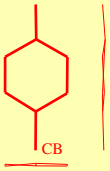

0.029
B Arg 287



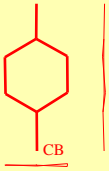

0.025
B Asn 313



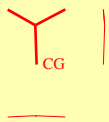

0.073
B Phe 322



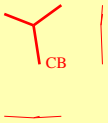

0.038
B Tyr 325



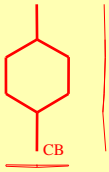

0.032
B Tyr 341



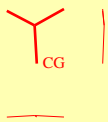

0.022
B Gln 349



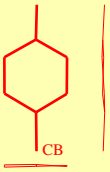

0.026
B Asn 354



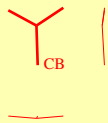

0.035
B Tyr 368



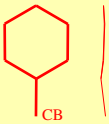

0.026
B Gln 385



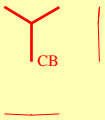

0.035
B Tyr 392




0.038
B Asp 409



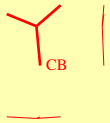

0.053
B Phe 435



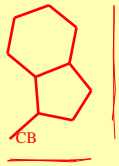

0.021
B Asp 437


0.033
B Glu 438

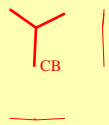

0.029
C Arg 5



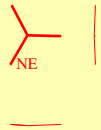

0.027
C Asp 20



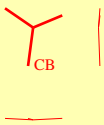

0.031
C Trp 31



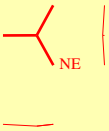

0.025
C Asp 58



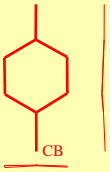

0.020
C Arg 71



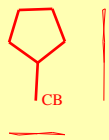

0.024
C Asn 74



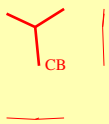

0.031
C Arg 80



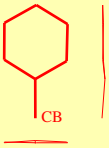

0.041
C Tyr 81



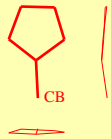

0.035
C His 83



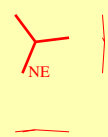

0.024
C Asn 85



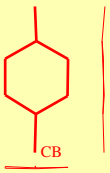

0.034
C Phe 90



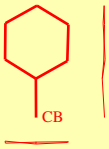

0.078
C His 97




0.034
C Arg 100



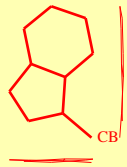

0.034
C Tyr 103



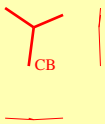

0.035
C Phe 109

# Distorted geometry
## pdb2fyu

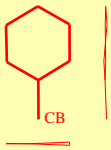
### Planar groups (contd)



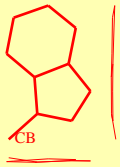

0.045
C Trp 113



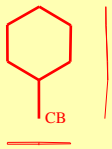

0.026
C Asn 114



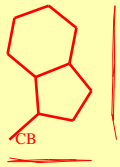

0.038
C Phe 128



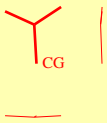

0.054
C Trp 135



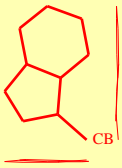

0.040
C Phe 140



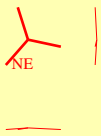

0.049
C Trp 141



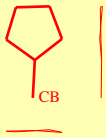

0.024
C Glu 162



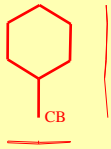

0.036
C Trp 165



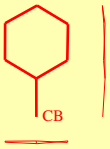

0.027
C Arg 177



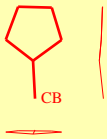

0.035
C His 182



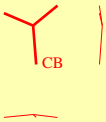

0.040
C Phe 183



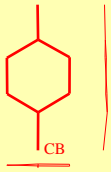

0.040
C Phe 187



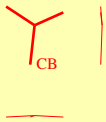

0.051
C His 196



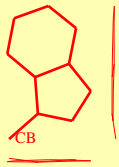

0.049
C Asp 214




0.048
C Tyr 224




0.025
C Asn 263

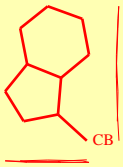



0.044
C Trp 272

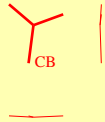

0.028
C Gln 312


0.025
C Arg 318


0.024
C Gln 322

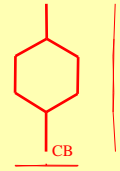



0.034
C Trp 326



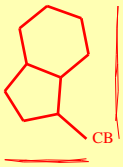

0.022
C Asp 331


0.030
C Gln 341

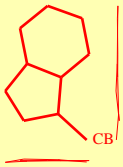



0.035
C Tyr 347

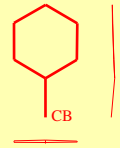

0.028
C Gln 352



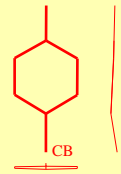

0.043
C Trp 379



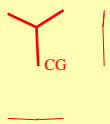

0.036
D Trp 12



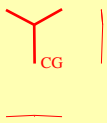

0.042
D Phe 30



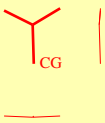

0.073
D Tyr 33



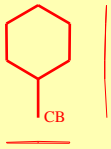

0.022
D Glu 66



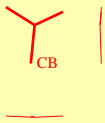

0.023
D Glu 79



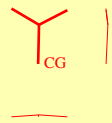

0.021
D Glu 136



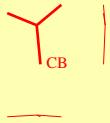

0.032
D Phe 149




0.023
D Asn 166



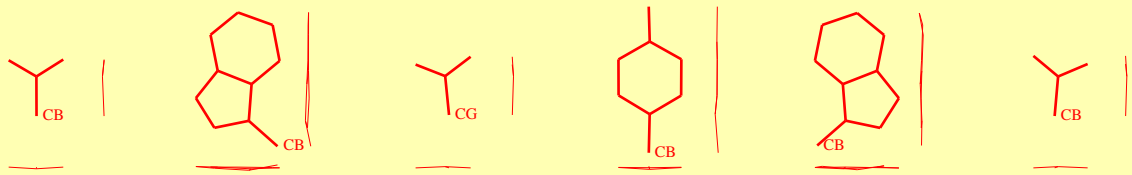

0.032
D Glu 167



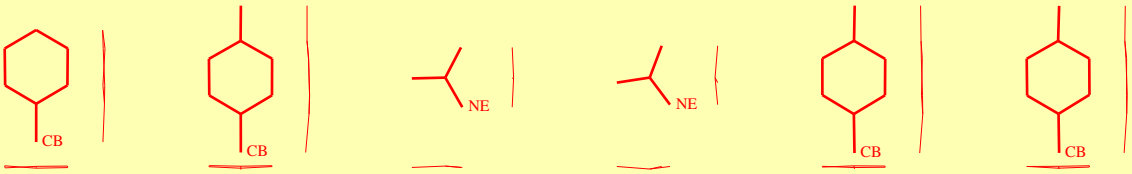

0.028
D Asp 173

# Distorted geometry
## pdb2fyu

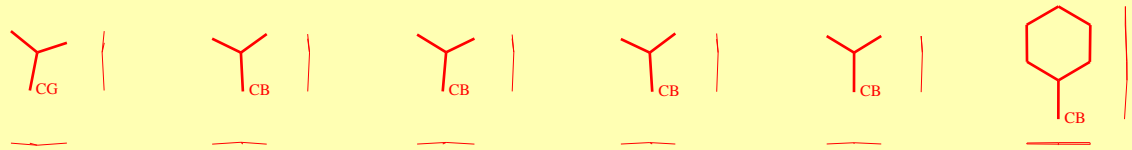
### Planar groups (contd)




0.028 D Asp 185 | 0.052 D Trp 192 | 0.021 D Glu 197 | 0.031 D Tyr 220 | 0.042 D Trp 227 | 0.021 E Asp 4

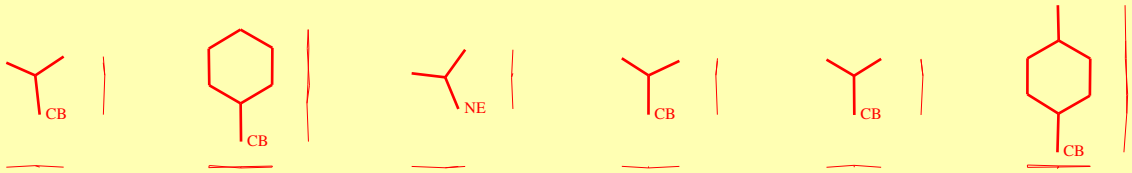



0.036 E Phe 10 | 0.052 E Tyr 13 | 0.023 E Arg 14 | 0.044 E Arg 32 | 0.038 E Tyr 37 | 0.040 E Tyr 49




0.035 E Gln 57 | 0.031 E Asp 67 | 0.028 E Asn 86 | 0.025 E Asp 107 | 0.021 E Asp 119 | 0.034 E Phe 153


0.037 E Tyr 157 | 0.040 E His 161 | 0.050 E Asp 166 | 0.021 E Asp 190 | 0.048 F Trp 19 | 0.070 F Tyr 20

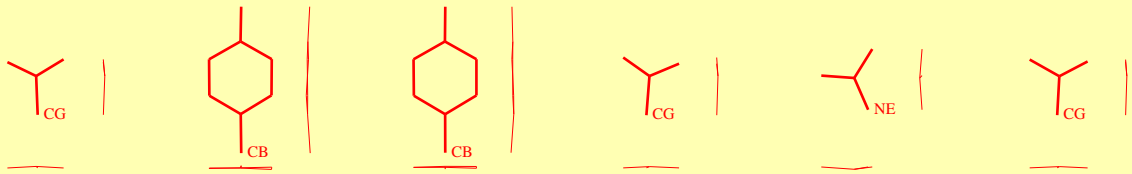



0.025 F Asn 22 | 0.031 F Phe 26 | 0.022 F Arg 33 | 0.026 F Asn 40 | 0.033 F Asp 42 | 0.043 F Tyr 55

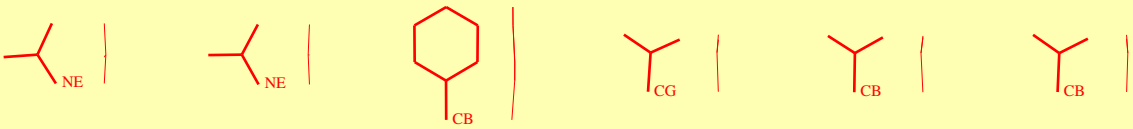

0.026 F Asp 57 | 0.027 F Arg 58 | 0.032 F Arg 61 | 0.036 F Asp 67 | 0.048 F Gln 72 | 0.026 F Gln 73

# Distorted geometry
## pdb2fyu

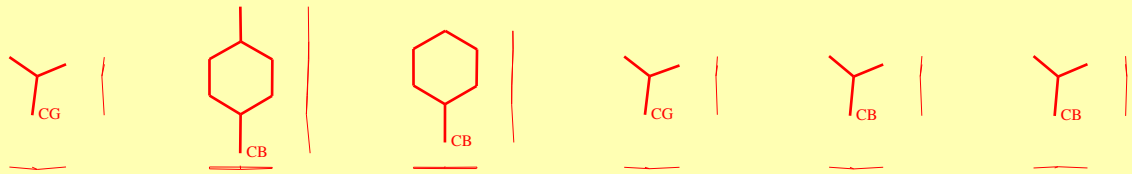
### Planar groups (contd)




0.026 F Glu 85 | 0.048 F Tyr 89 | 0.034 F Tyr 93 | 0.021 F Glu 96 | 0.039 G Arg 2 | 0.021 G Gln 3




0.027 G Arg 9 | 0.022 G Arg 47 | 0.043 G Phe 55 | 0.023 H Glu 38 | 0.033 H Asp 41 | 0.021 H Asp 60




0.041 I Gln 31 | 0.044 J Tyr 10 | 0.030 J Phe 31 | 0.024 J Glu 32 | 0.028 J Asp 36 | 0.021 K Asp 43

Sidechains with RMS dist. from planarity > 0.03A for rings, or > 0.02A otherwise. Value shown is RMS dist.