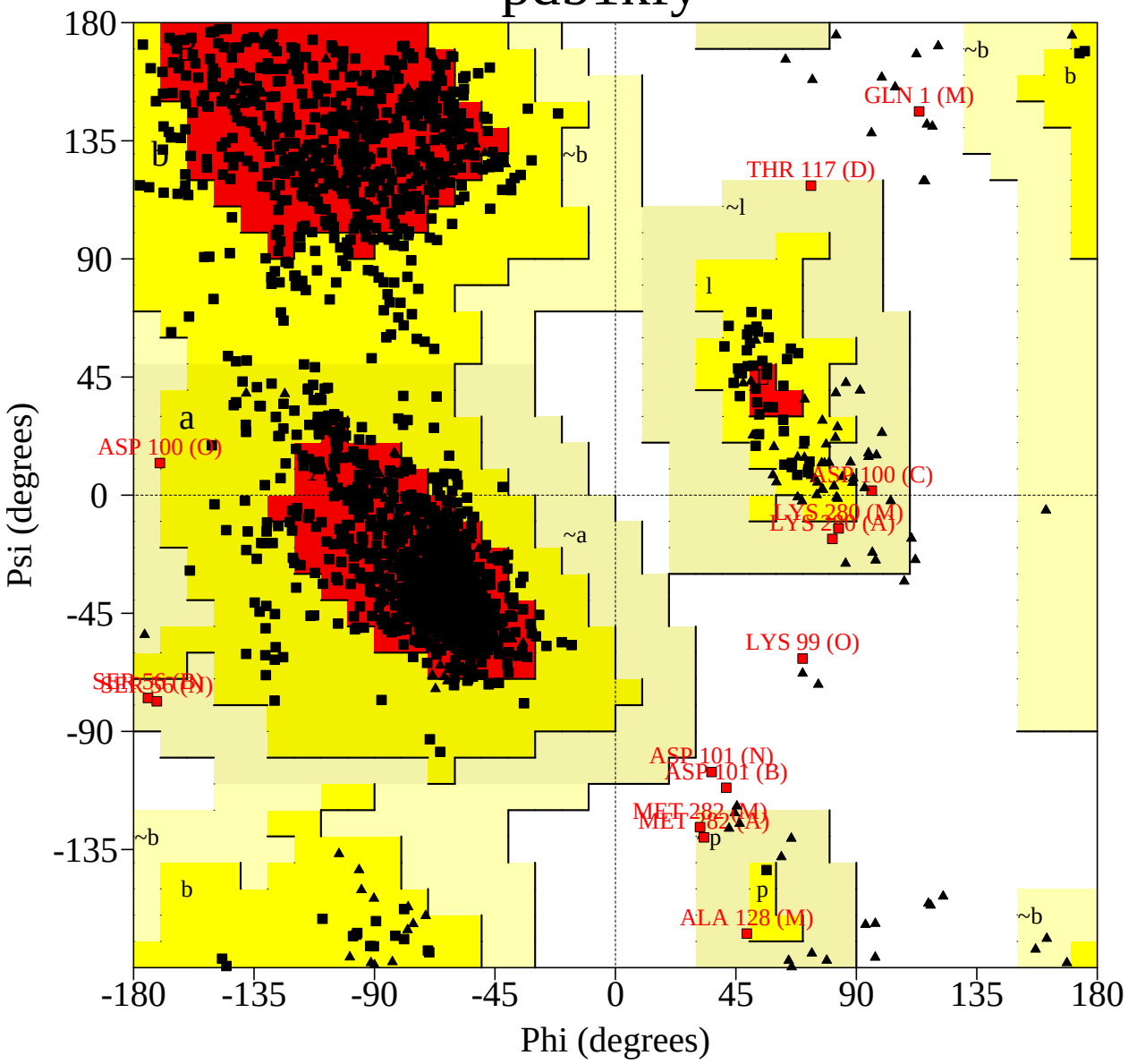
Ramachandran Plot

pdb1kfy



Plot statistics

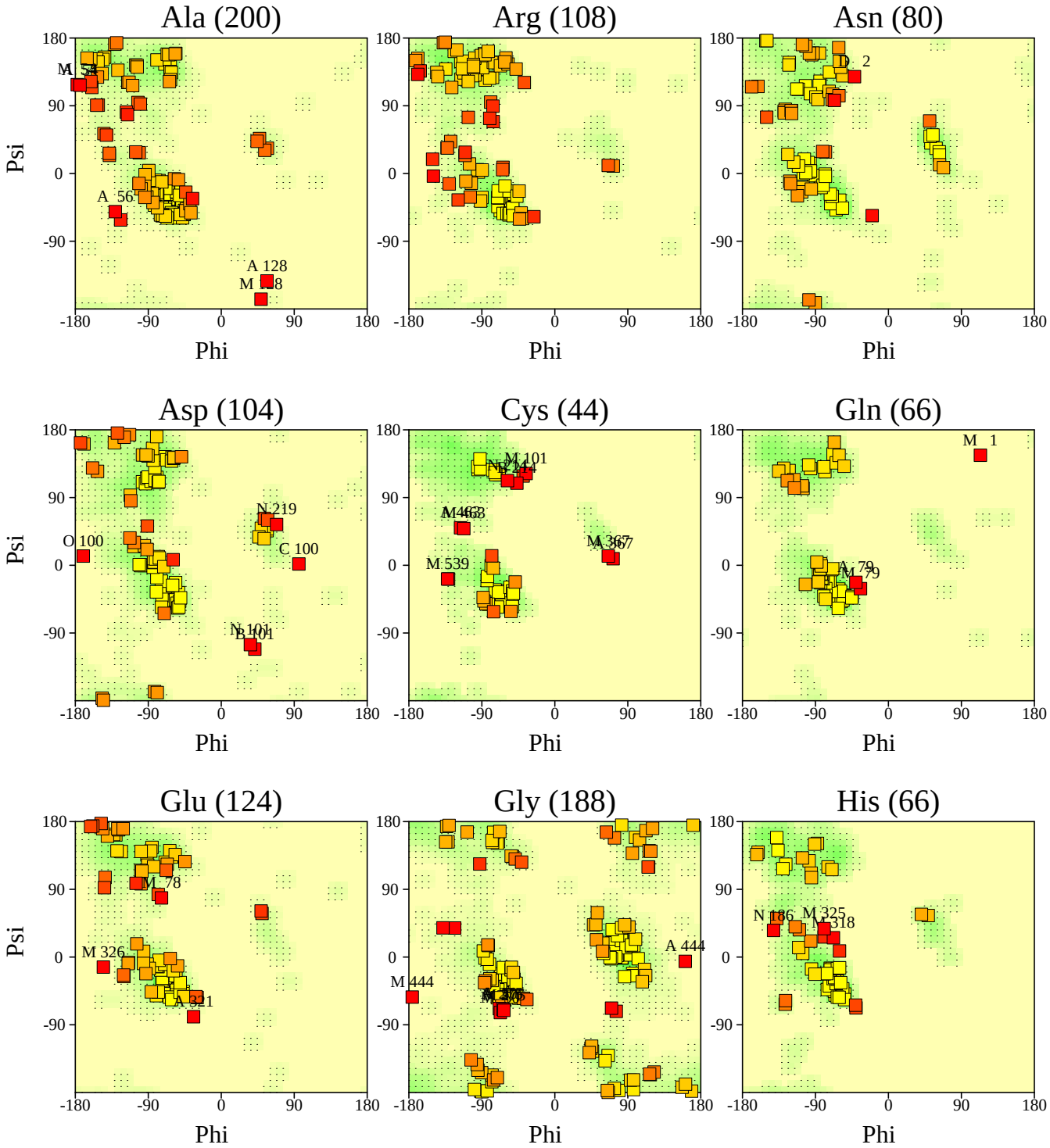
Residues in most favoured regions [A,B,L]	1545	84.5%
Residues in additional allowed regions [a,b,l,p]	269	14.7%
Residues in generously allowed regions [~a,~b,~l,~p]	10	0.5%
Residues in disallowed regions	4	0.2%
	----	------
Number of non-glycine and non-proline residues	1828	100.0%
Number of end-residues (excl. Gly and Pro)	16	
Number of glycine residues (shown as triangles)	188	
Number of proline residues	106	

Total number of residues	2138	

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

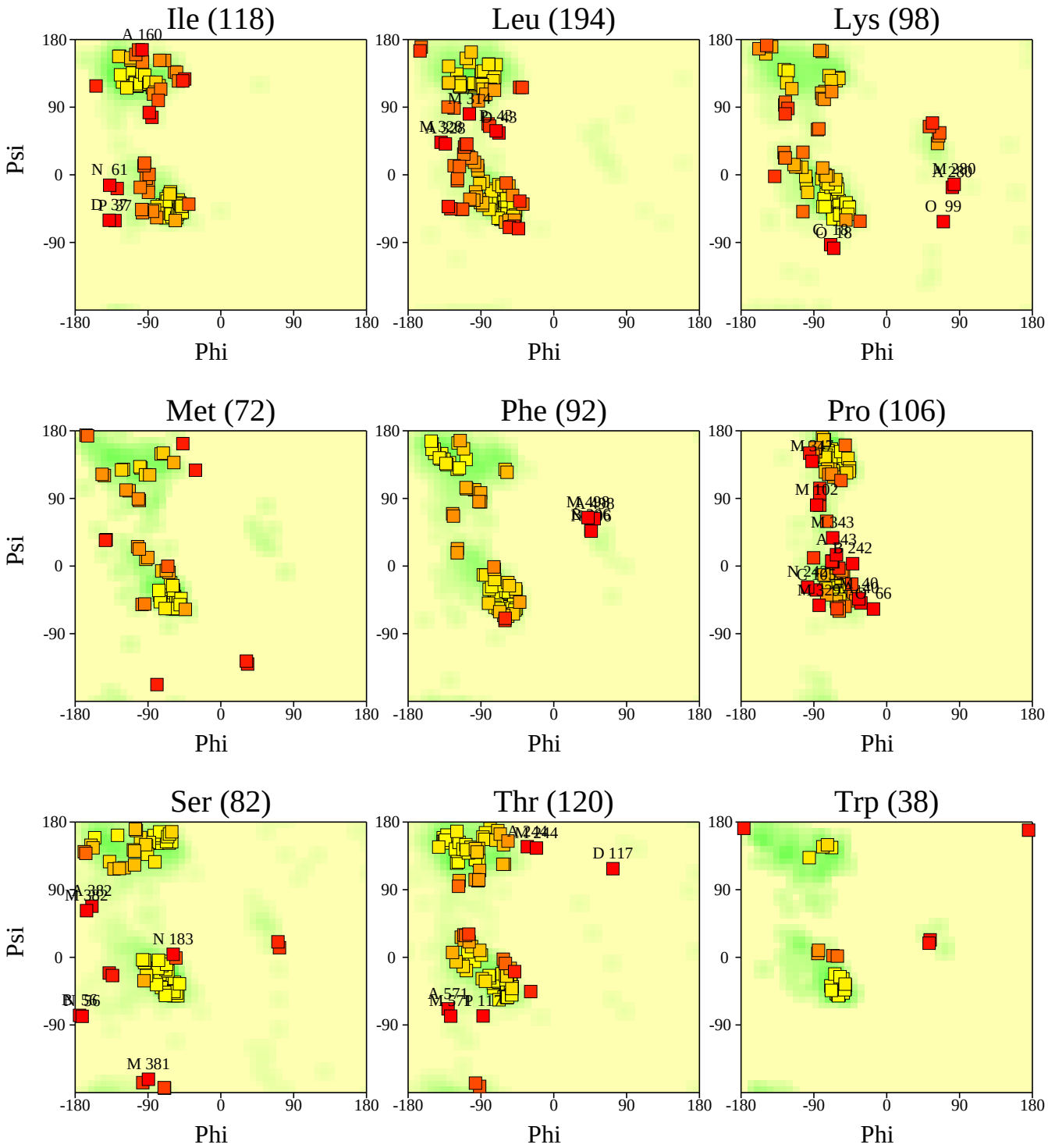
pdb1kfy



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

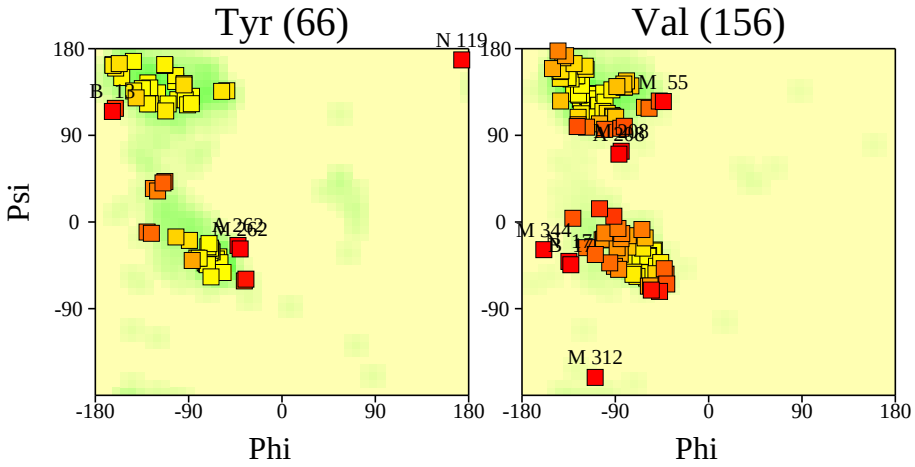
pdb1kfy



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

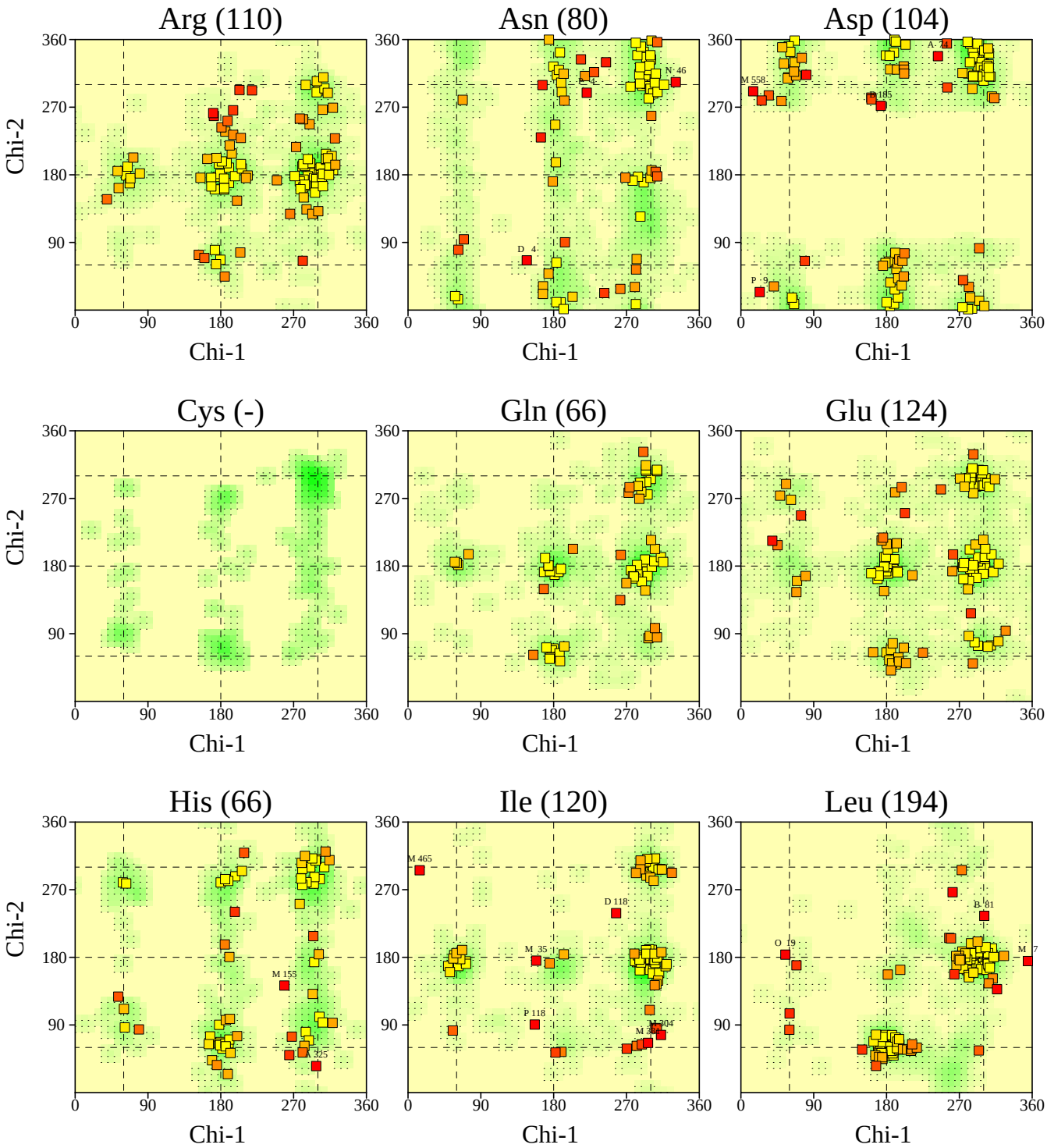
pdb1kfy



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

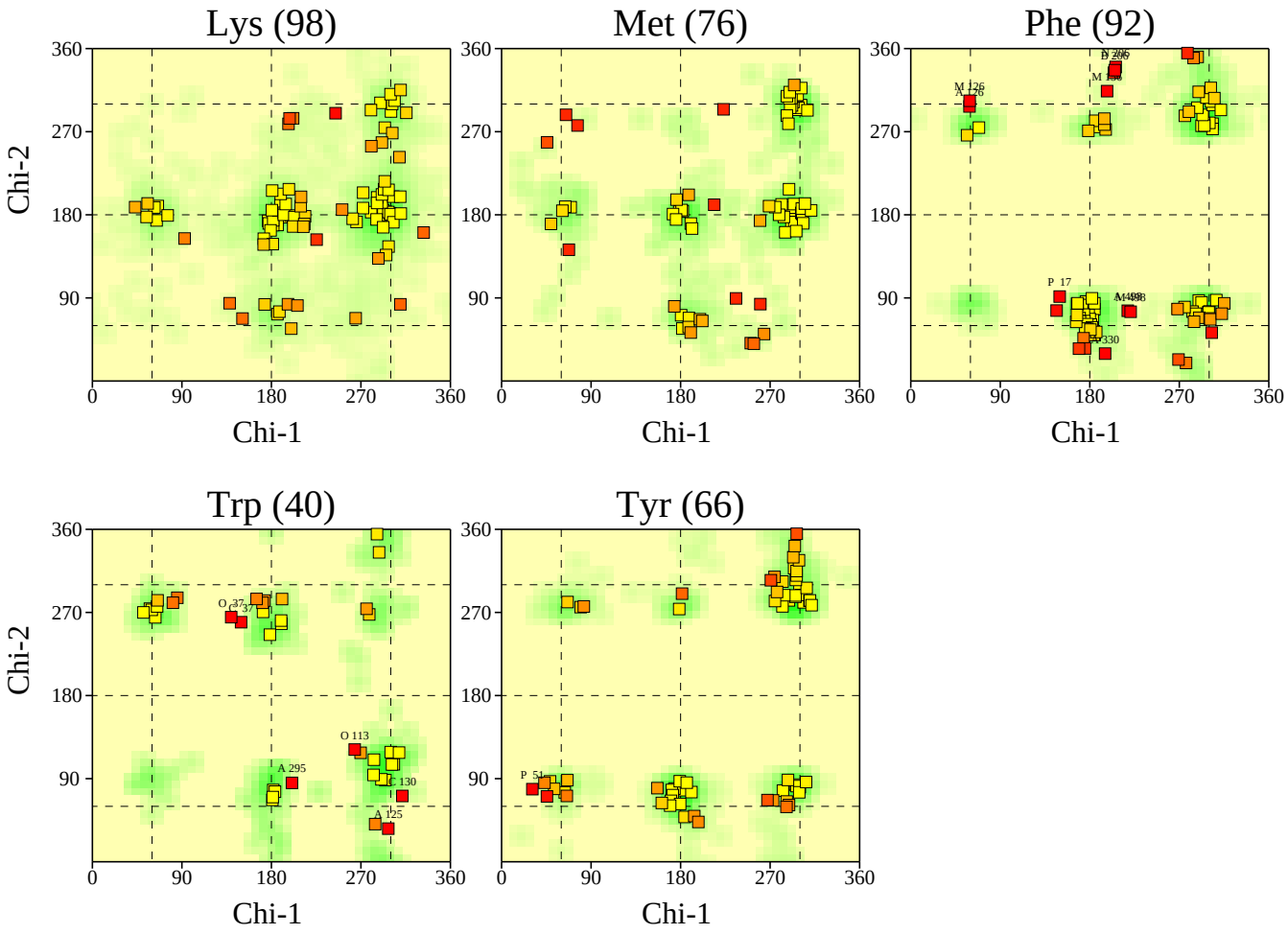
pdb1kfy



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

pdb1kfy

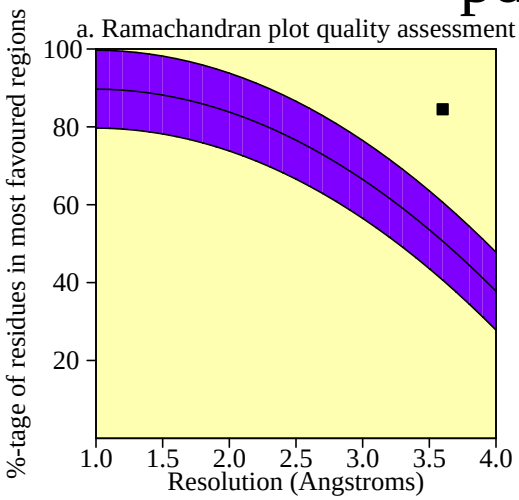


Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

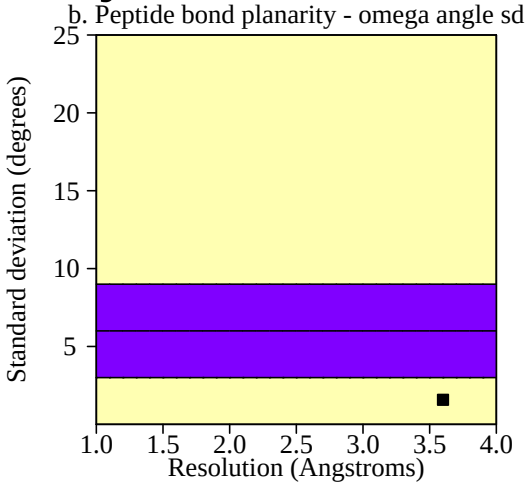
Main-chain parameters

pdb1kfy

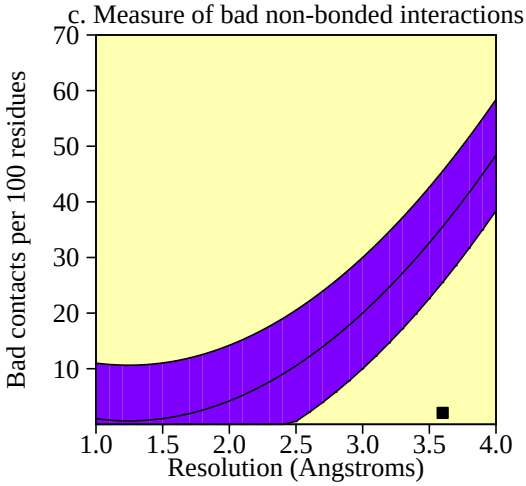
a. Ramachandran plot quality assessment



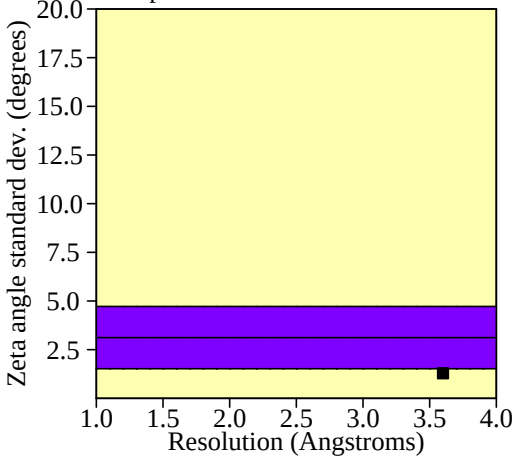
b. Peptide bond planarity - omega angle sd



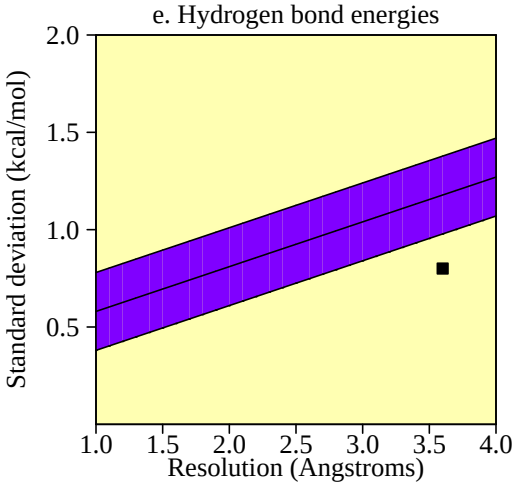
c. Measure of bad non-bonded interactions



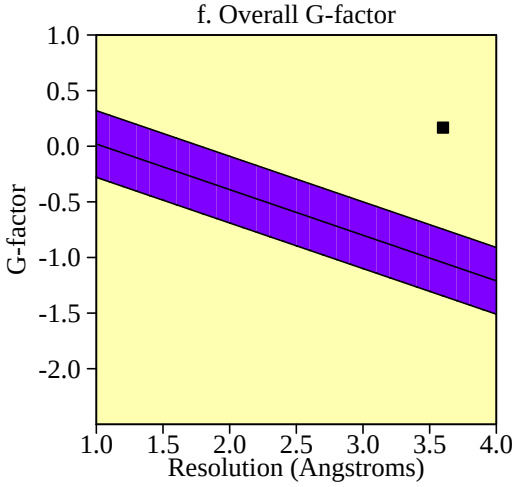
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor



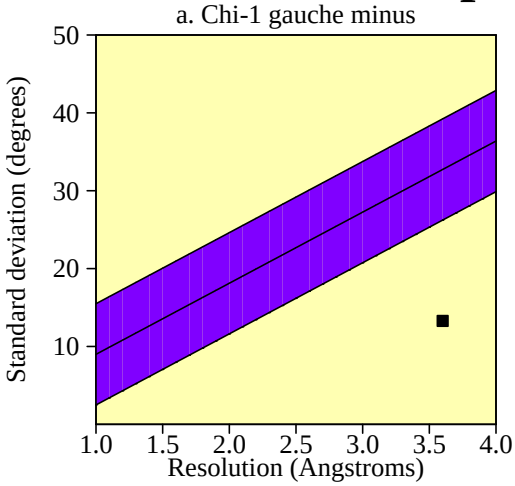
Plot statistics

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	1828	84.5	50.6	10.0	3.4	BETTER
b. Omega angle st dev	2126	1.6	6.0	3.0	-1.5	BETTER
c. Bad contacts / 100 residues	44	2.1	35.5	10.0	-3.3	BETTER
d. Zeta angle st dev	1950	1.3	3.1	1.6	-1.1	BETTER
e. H-bond energy st dev	1412	0.8	1.2	0.2	-1.9	BETTER
f. Overall G-factor	2138	0.2	-1.0	0.3	4.0	BETTER

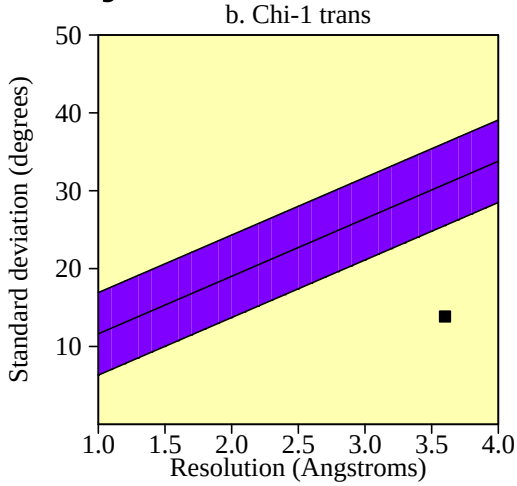
Side-chain parameters

pdb1kfy

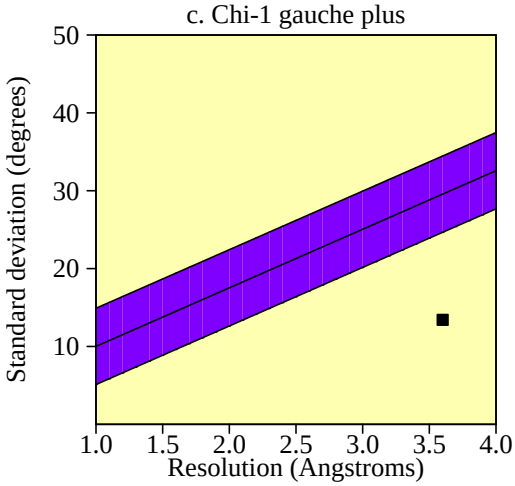
a. Chi-1 gauche minus



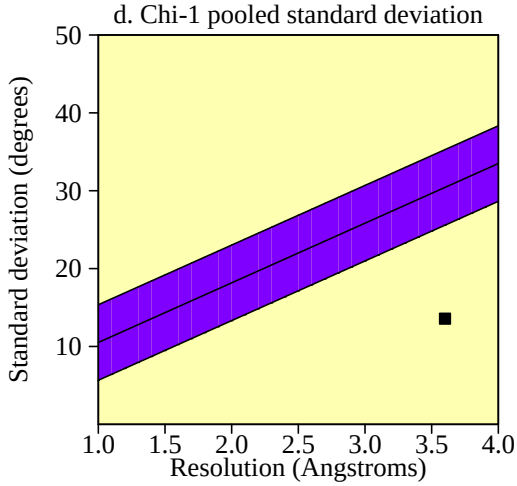
b. Chi-1 trans



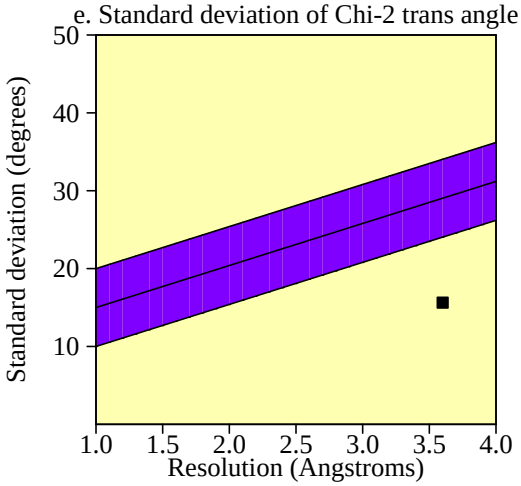
c. Chi-1 gauche plus



d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



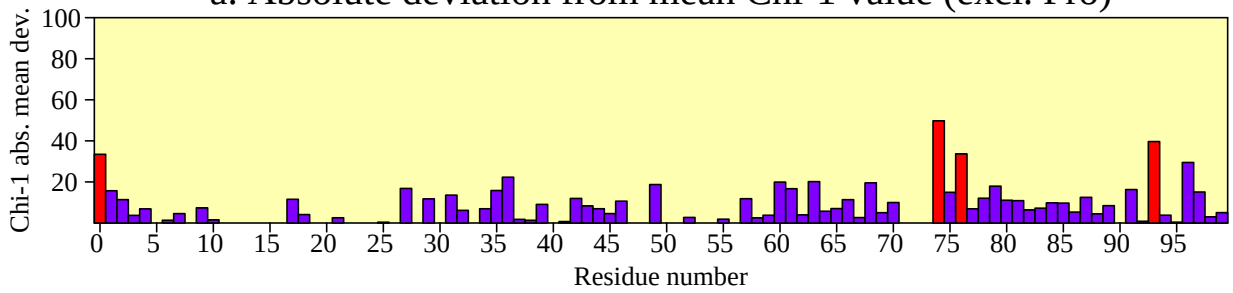
pdb1kfy

Plot statistics

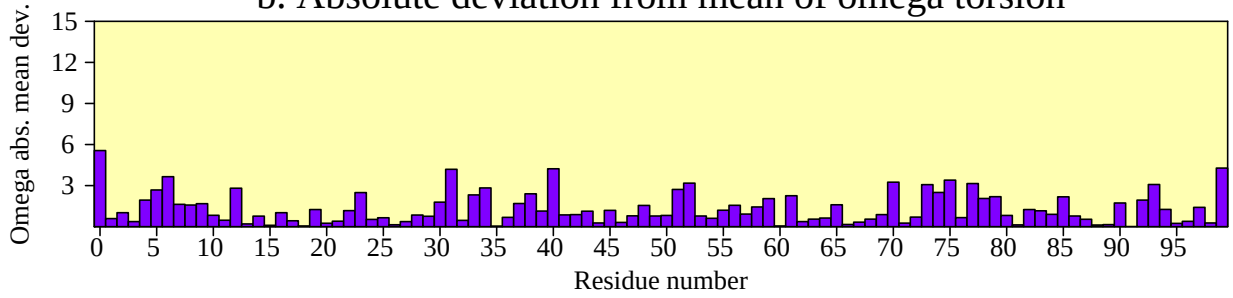
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	221	13.3	32.7	6.5	-3.0	BETTER
b. Chi-1 trans st dev	561	13.9	30.8	5.3	-3.2	BETTER
c. Chi-1 gauche plus st dev	858	13.4	29.6	4.9	-3.3	BETTER
d. Chi-1 pooled st dev	1640	13.6	30.4	4.8	-3.5	BETTER
e. Chi-2 trans st dev	508	15.6	29.0	5.0	-2.7	BETTER

Residue properties
pdb1kfy

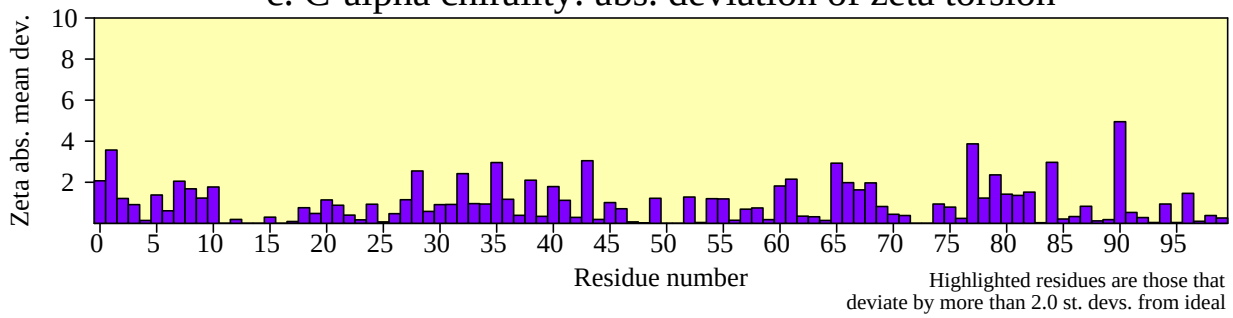
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

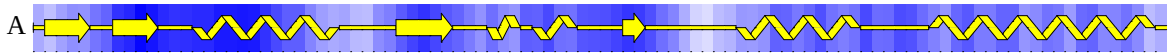


c. C-alpha chirality: abs. deviation of zeta torsion



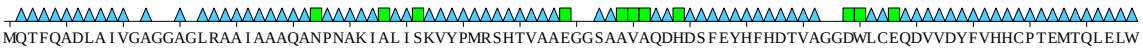
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

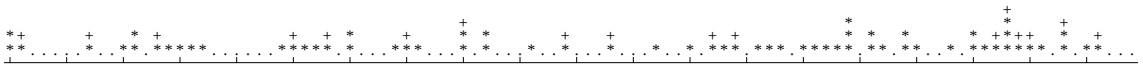


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

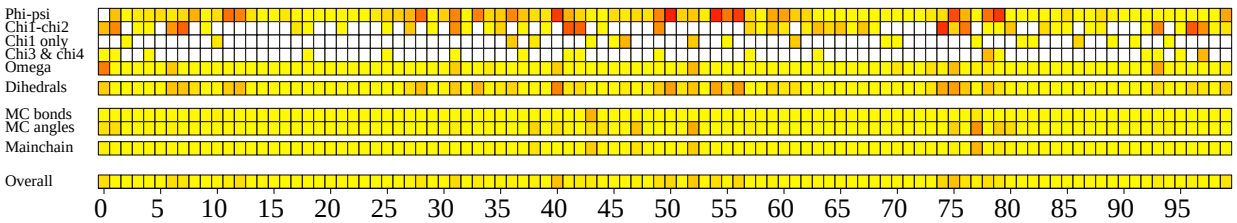
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

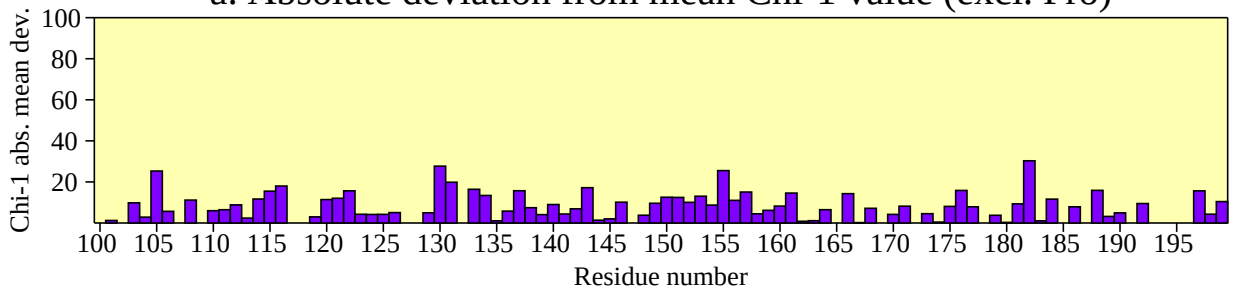


g. G-factors

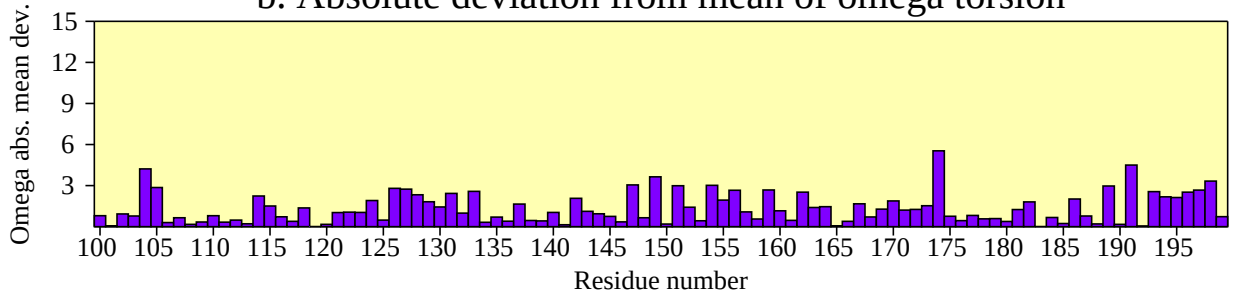


Residue properties
pdb1kfy

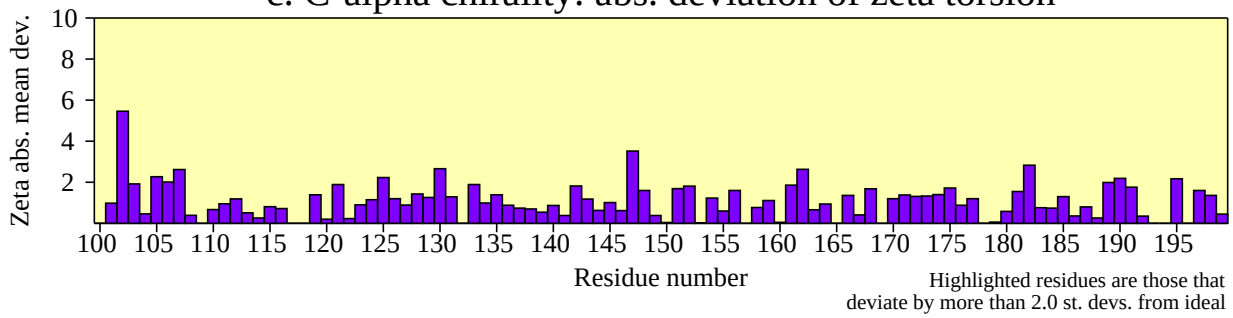
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

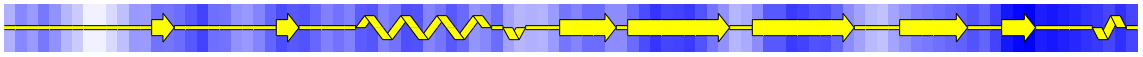


c. C-alpha chirality: abs. deviation of zeta torsion



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

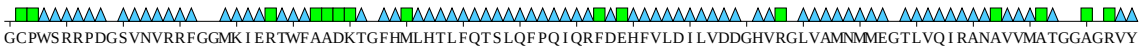
d. Secondary structure & estimated accessibility



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

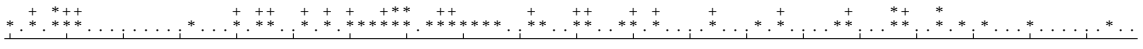
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

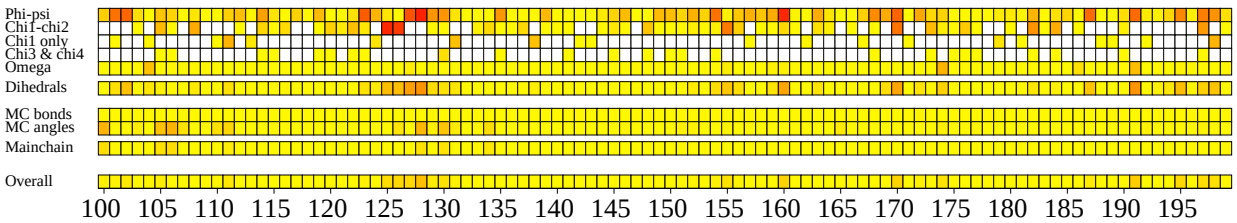


GCPWSRRPDGSVNVRRFGGMKIERTWFAADKTGFHMLHTLFQTSLQFPQIQRFDEHFVLDILVDDGHVRGLVAMNMMEGTLVQIRANAVVMATGGAGRVY

f. Max. deviation (see listing)

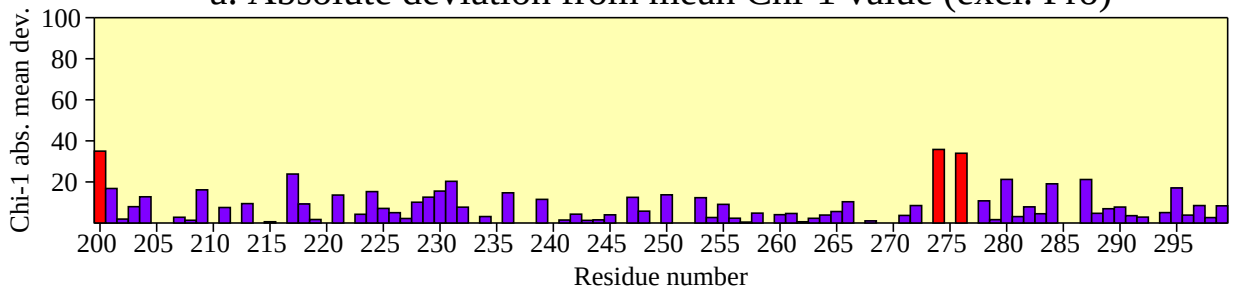


g. G-factors

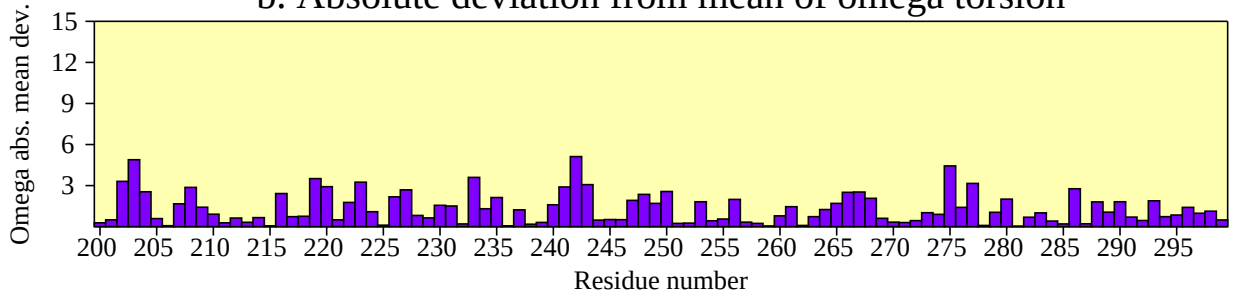


Residue properties
pdb1kfy

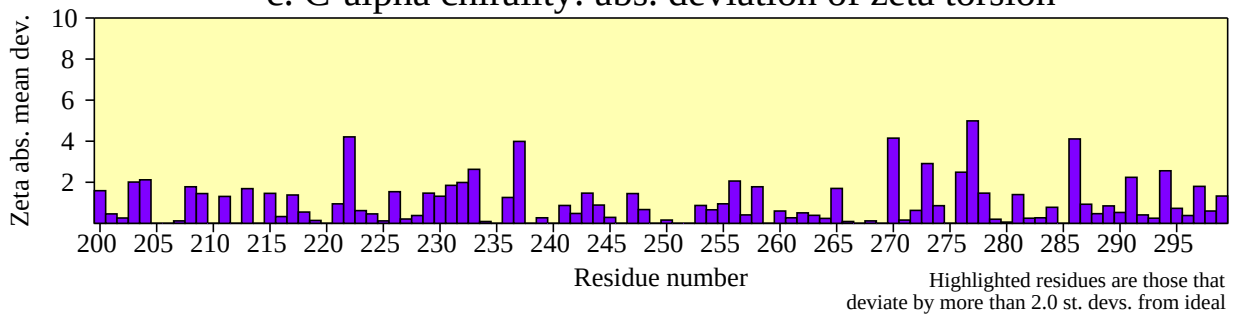
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

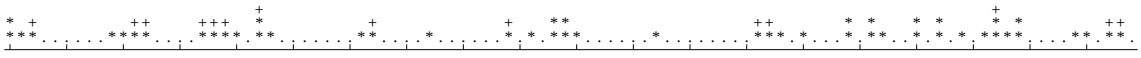
d. Secondary structure & estimated accessibility

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

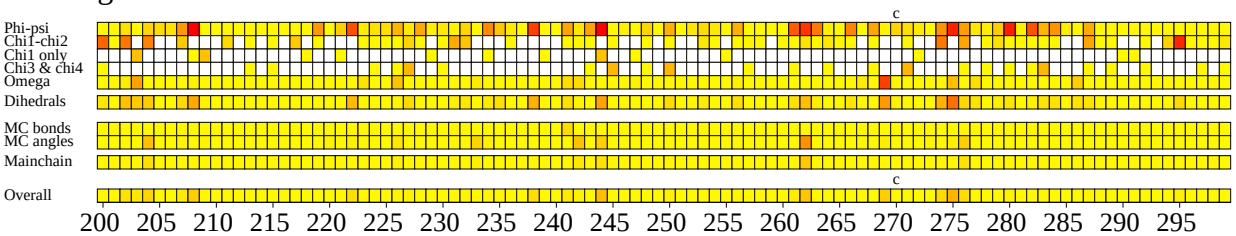
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

RYNTNGG I VTGDGMGMALSHGVPLRDMEFVQYHPTGLPGSG I LMTEGCRGEGG I LVNKNGYRYLQDYGMGPETPLGEPKNKYMELGPRDKVSQAFWHEWR

f. Max. deviation (see listing)



g. G-factors

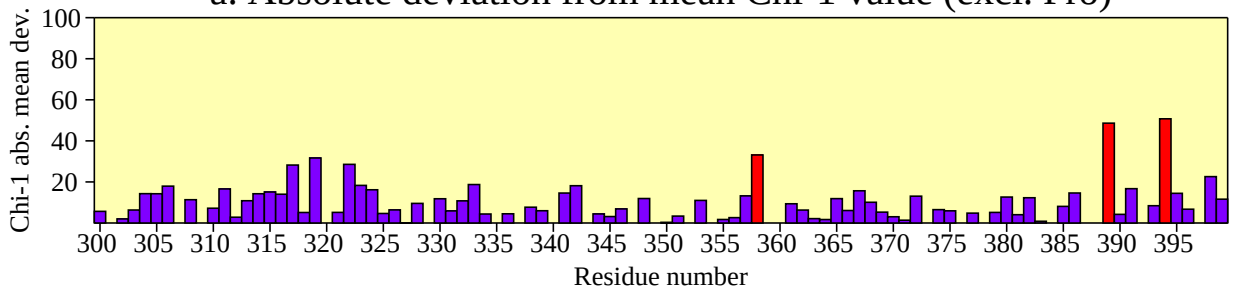


c = cis-peptide

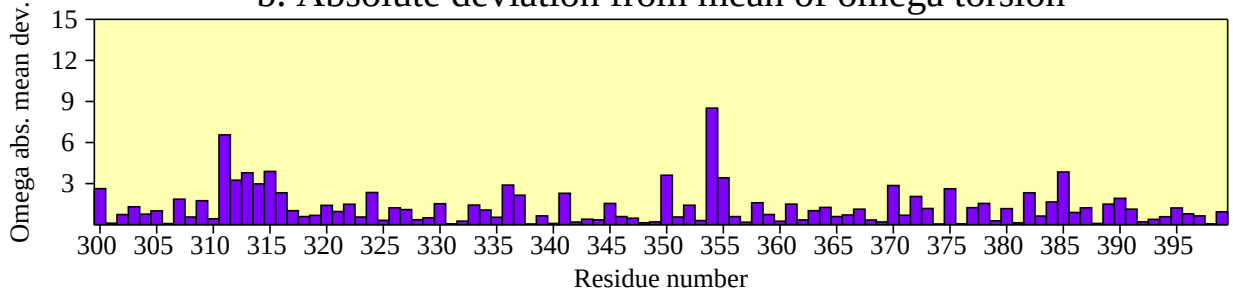
Residue properties

pdb1kfy

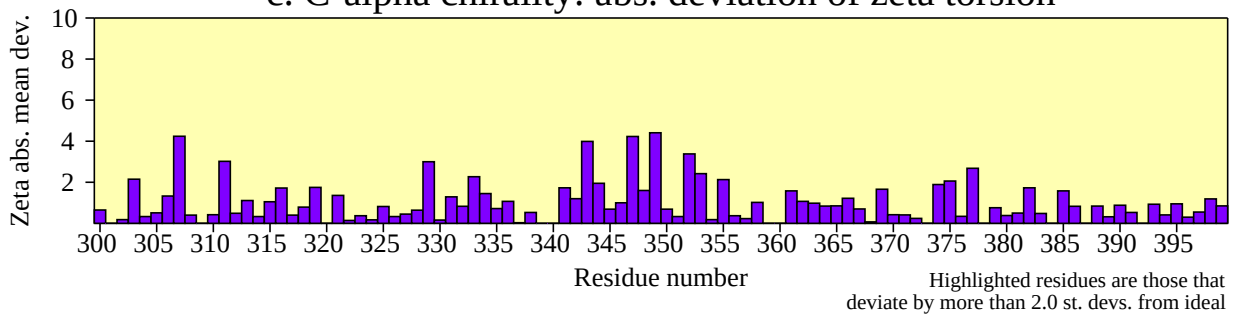
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

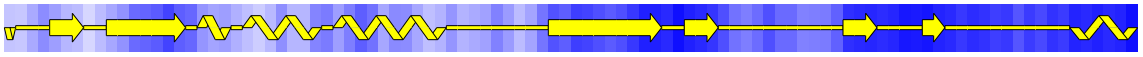


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



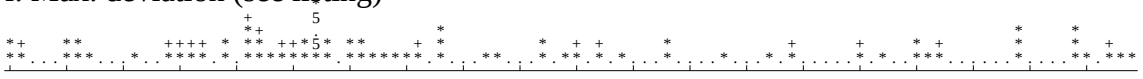
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

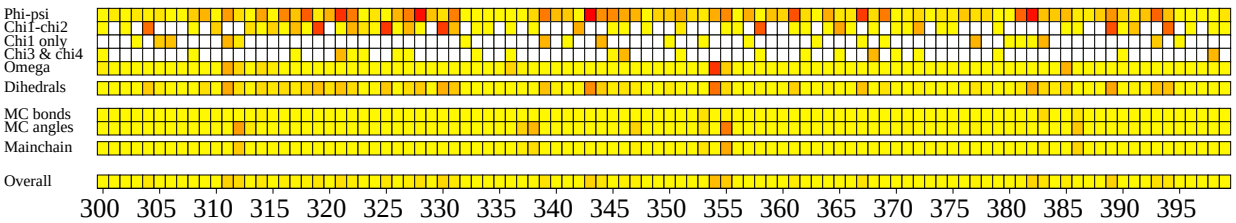
Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)

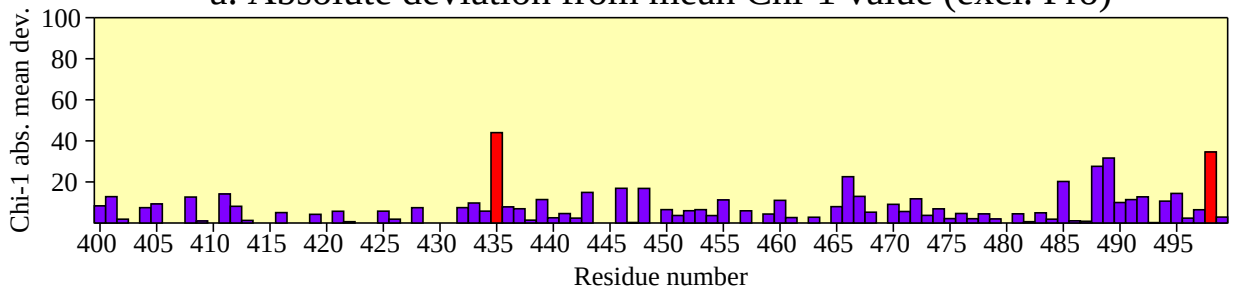


g. G-factors

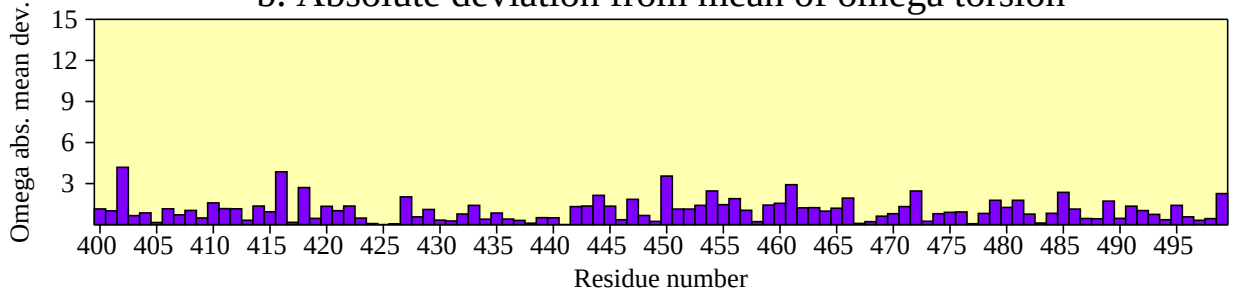


Residue properties
pdb1kfy

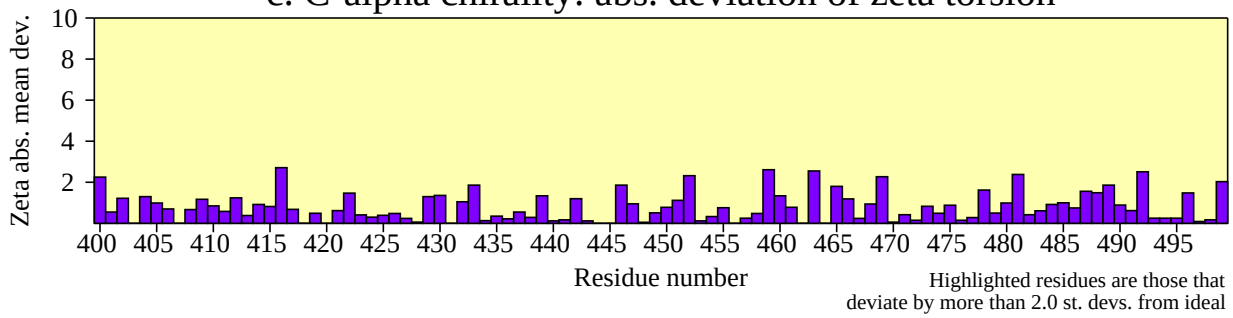
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

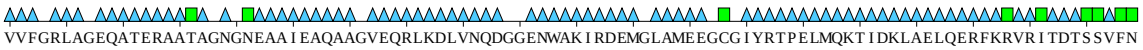


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

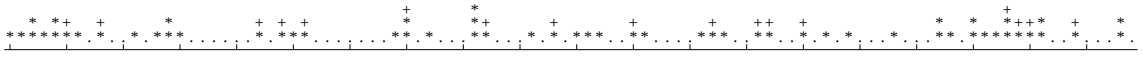
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

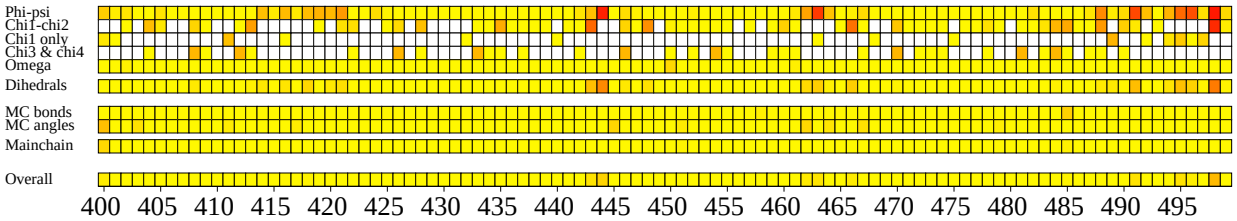


VVFGRLAGEQATERAATAGNGNEAAIEAQAAGVEQRLKDLVNQDGGENWAKIRDEMGLAMEEGCGIYRTPELMQKTIDKLAELQERFKRVRITDTSSVFN

f. Max. deviation (see listing)

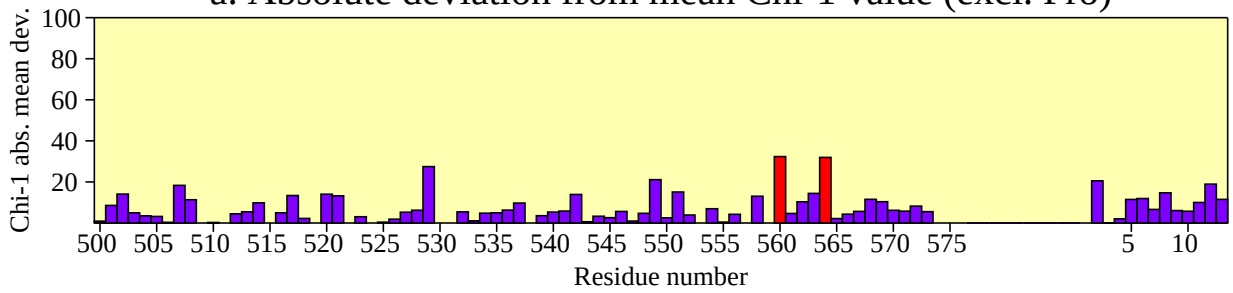


g. G-factors

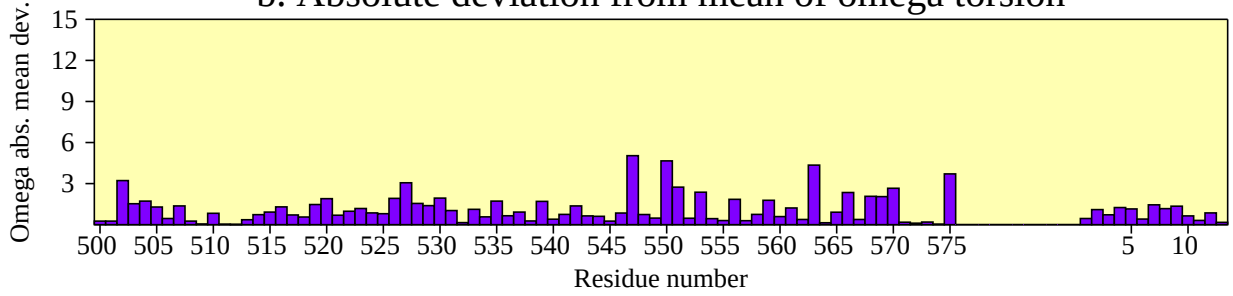


Residue properties
pdb1kfy

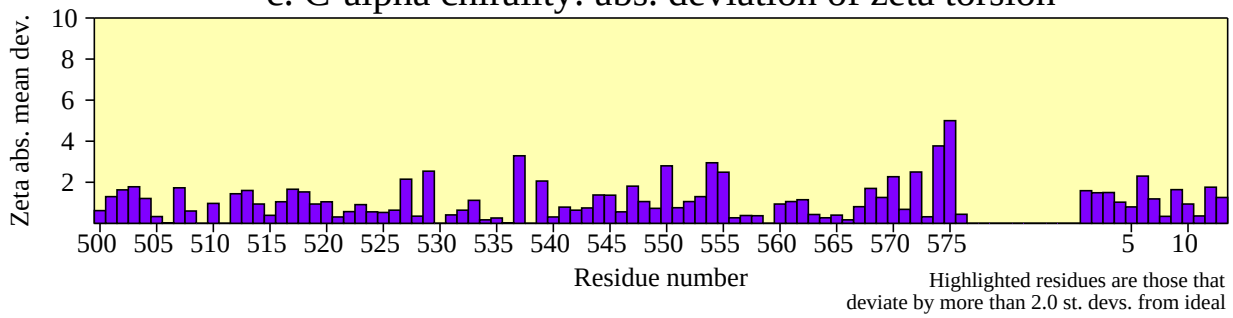
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

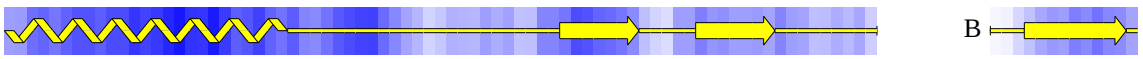


c. C-alpha chirality: abs. deviation of zeta torsion

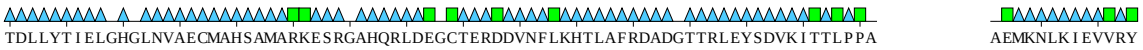


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

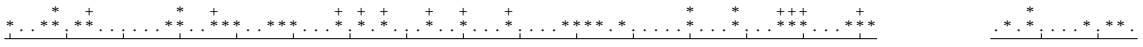
d. Secondary structure & estimated accessibility



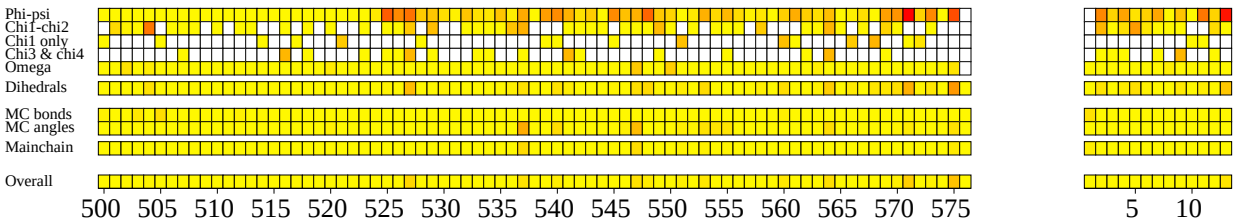
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

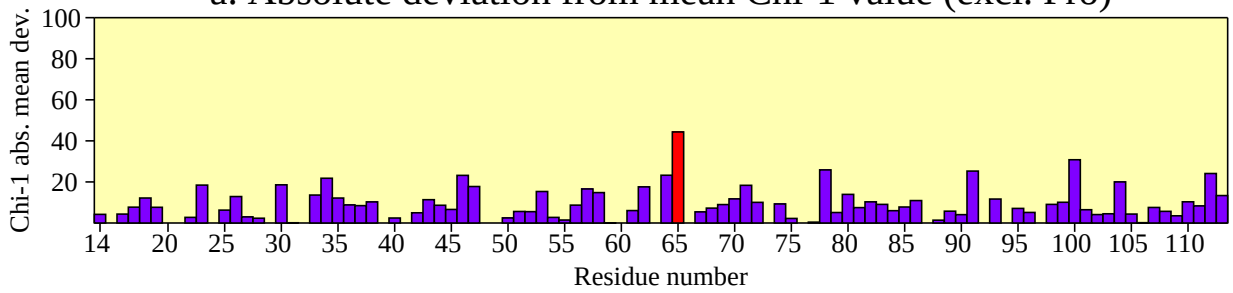


g. G-factors

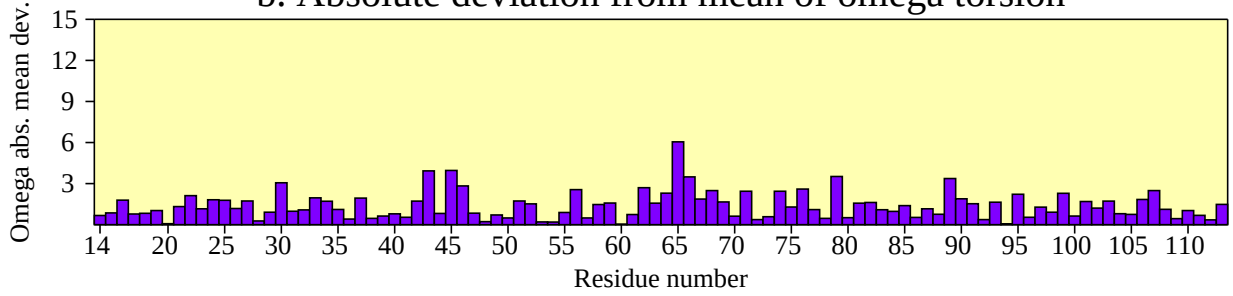


Residue properties
pdb1kfy

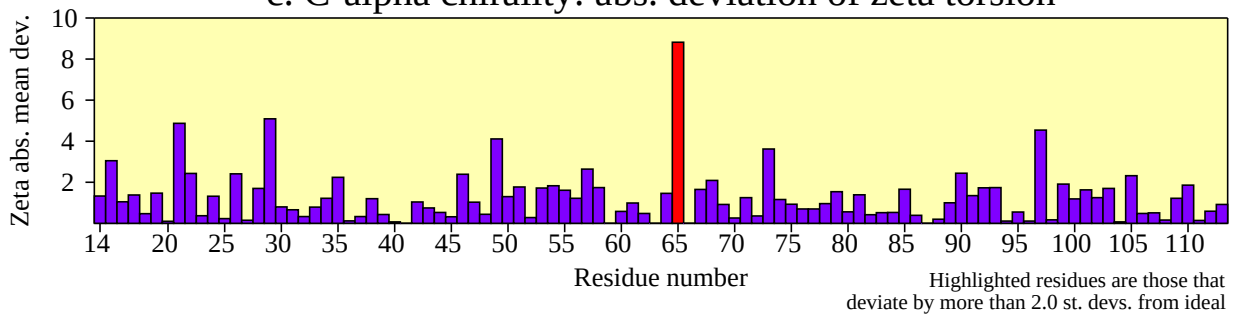
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

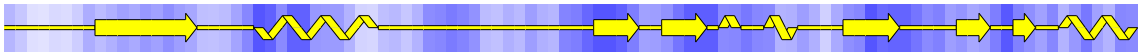


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

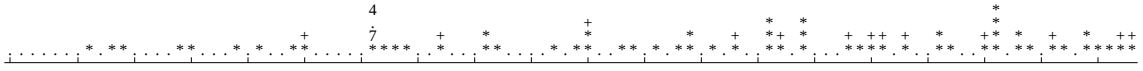


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

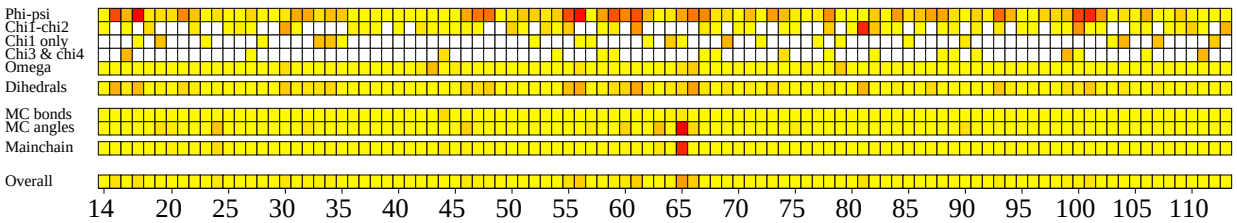
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)

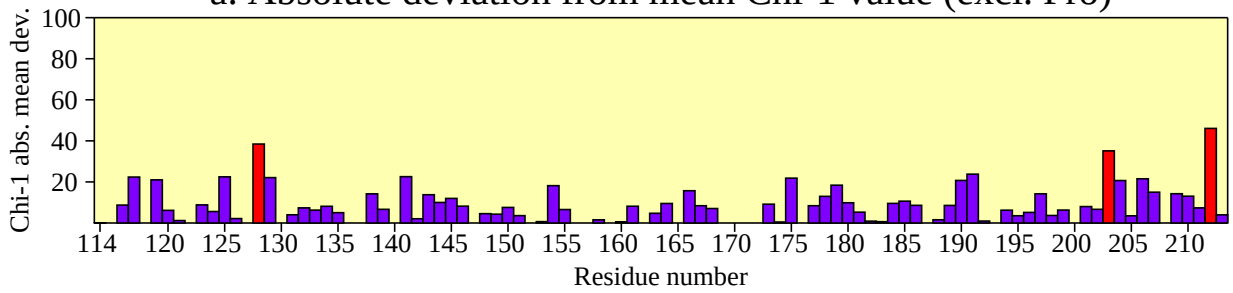


g. G-factors

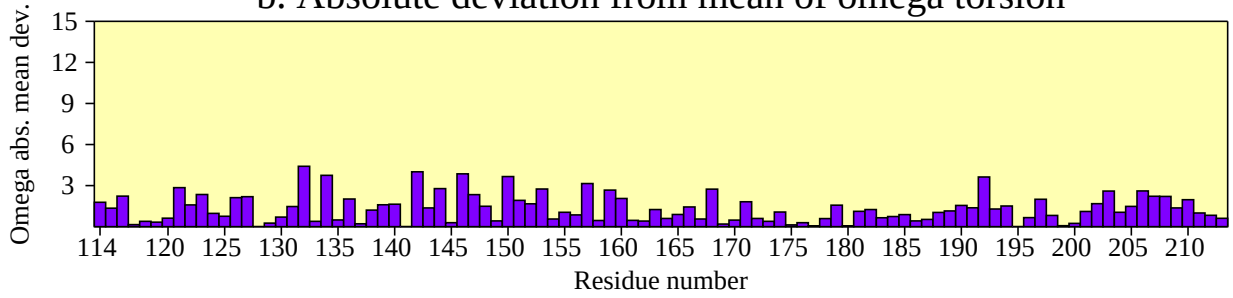


Residue properties
pdb1kfy

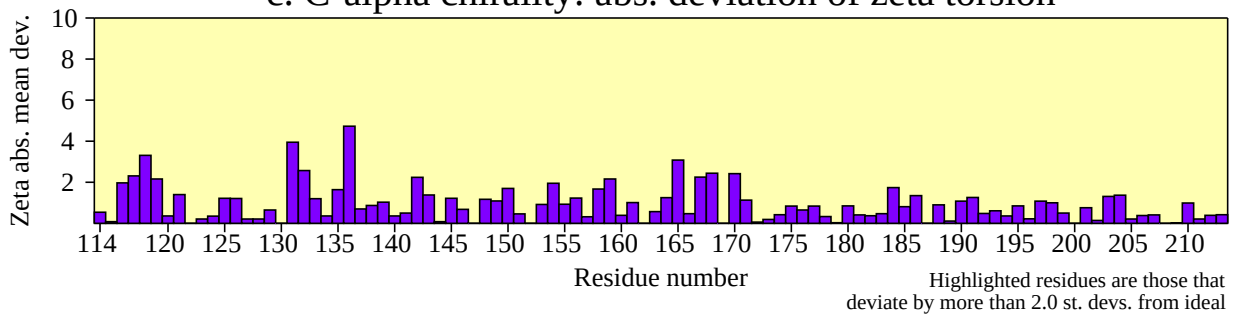
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

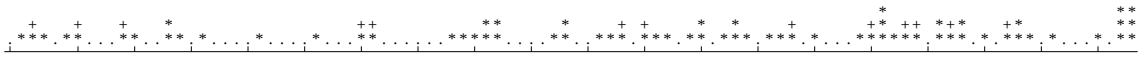
d. Secondary structure & estimated accessibility

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

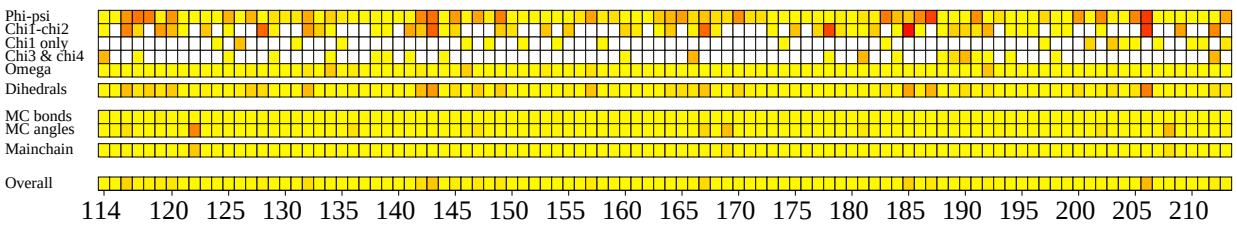
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

EAIKPYIIGNSRTADQGTNIQTPAQMAKYHQFSGCINCGLCYAACPQFGLNPEFIGPAAITLAHRYNEDSRDHGKKERMAQLNSQNGVWSCTFVGYCSEV

f. Max. deviation (see listing)

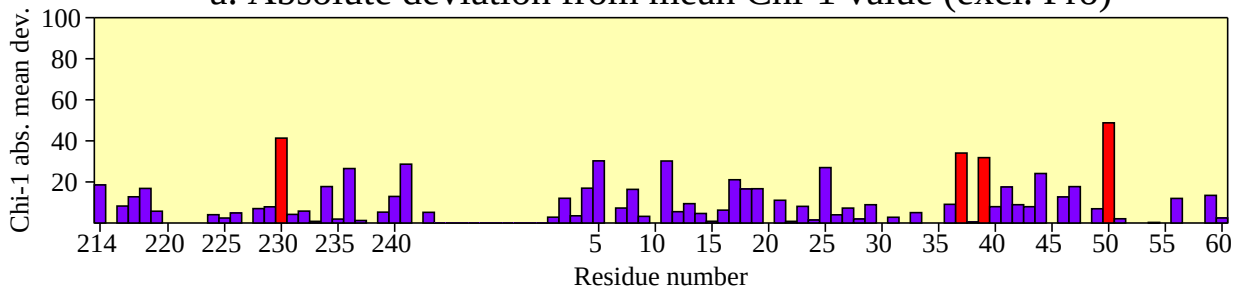


g. G-factors

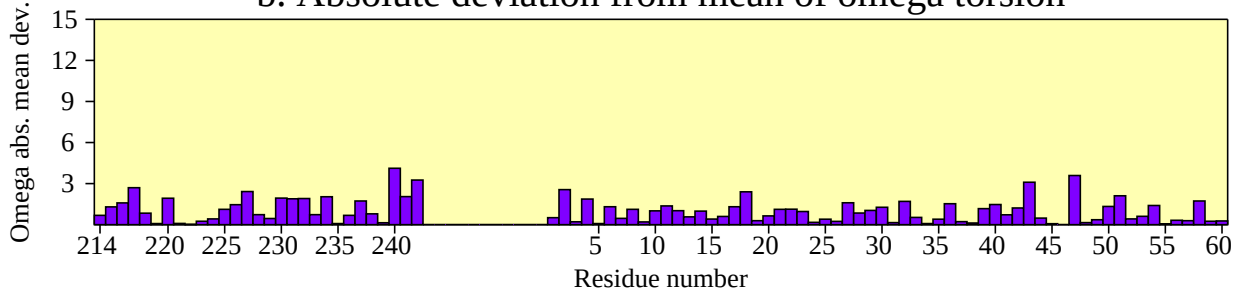


Residue properties
pdb1kfy

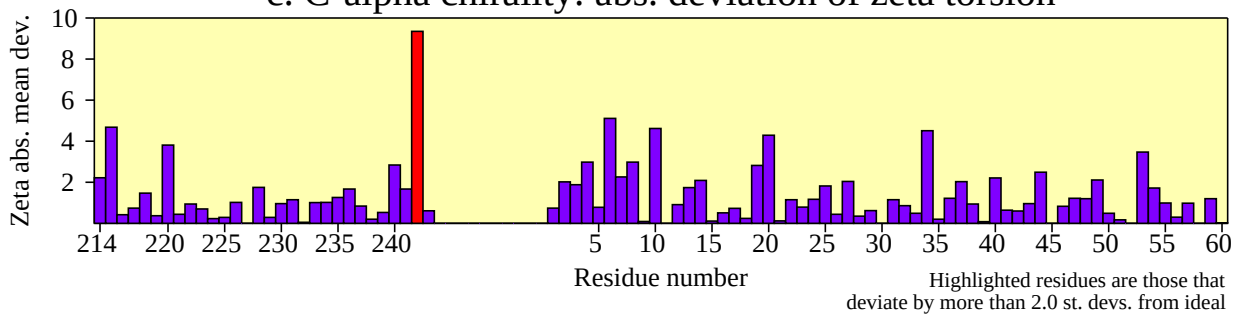
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

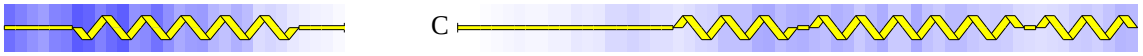


c. C-alpha chirality: abs. deviation of zeta torsion



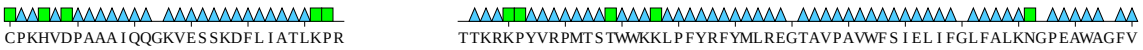
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

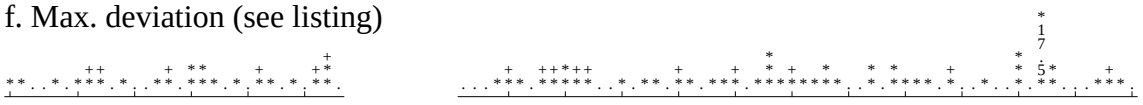


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

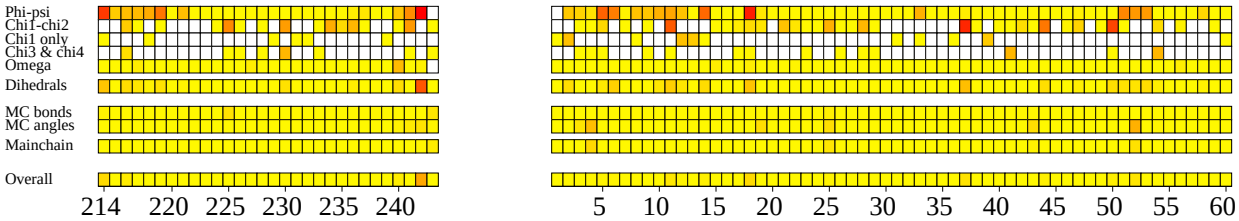
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

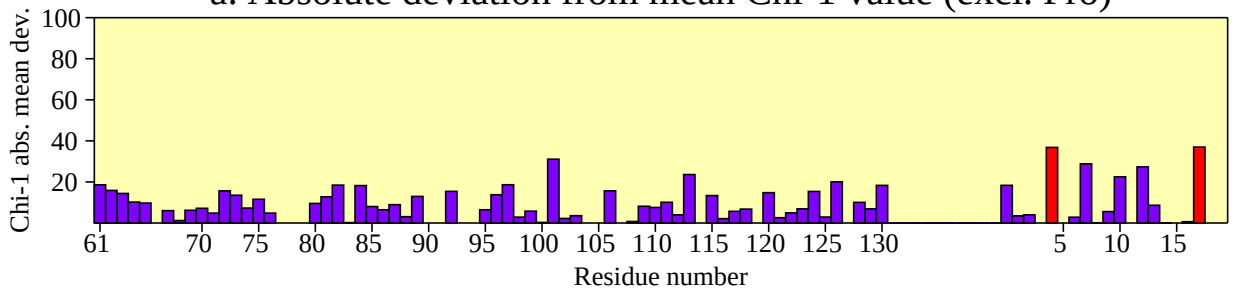


g. G-factors

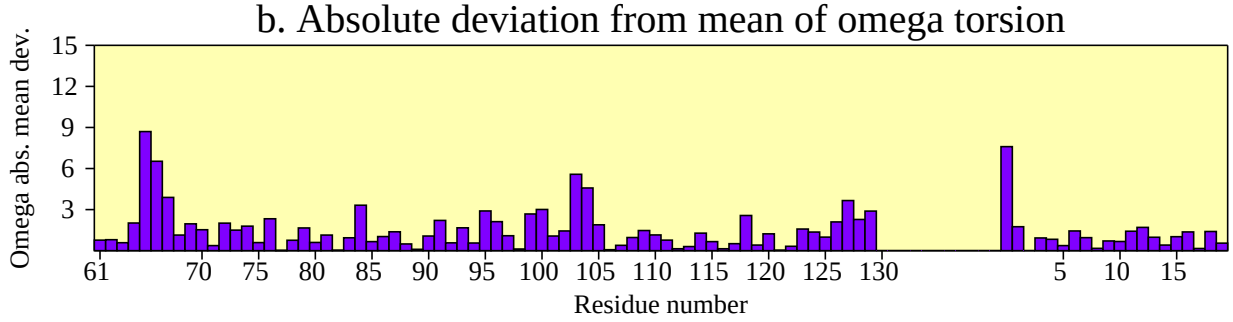


Residue properties
pdb1kfy

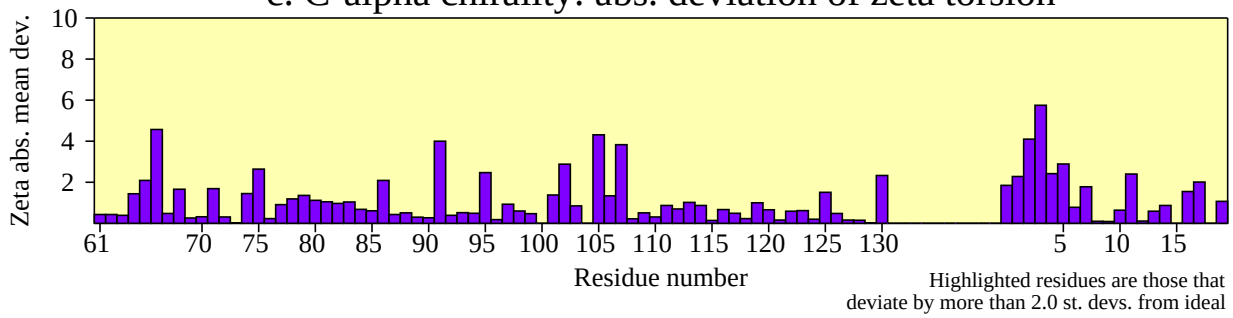
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

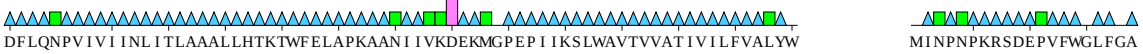


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

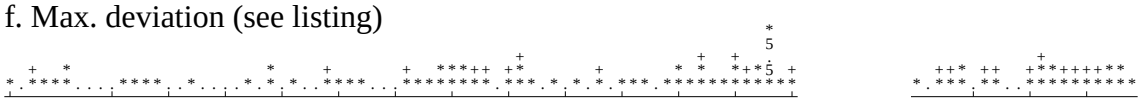
d. Secondary structure & estimated accessibility

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

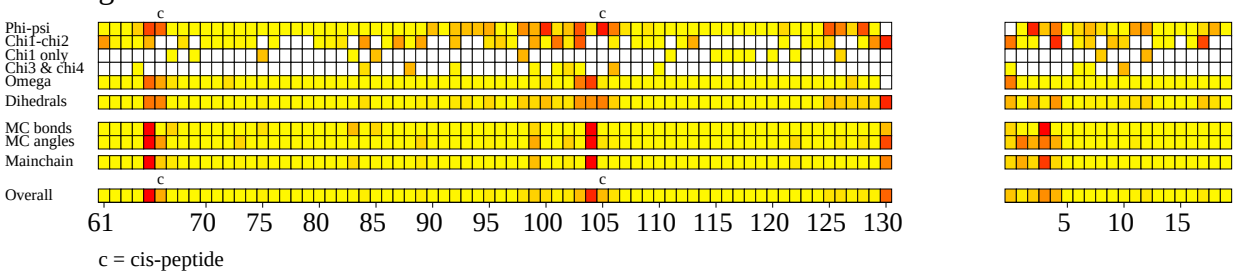
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



g. G-factors

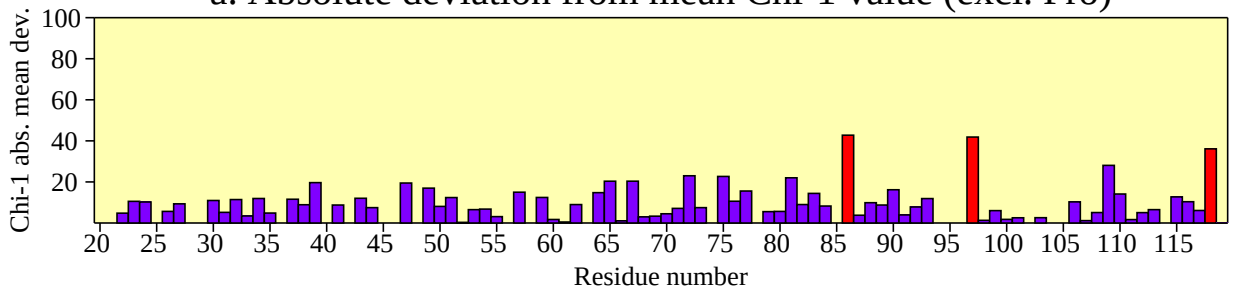


c = cis-peptide

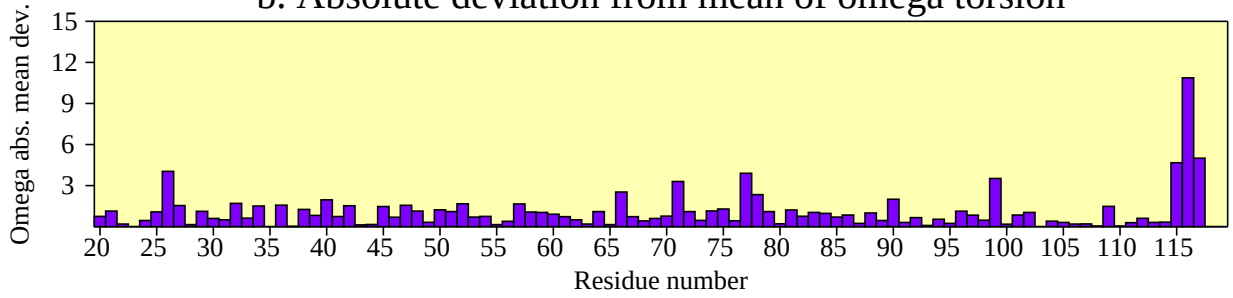
Residue properties

pdb1kfy

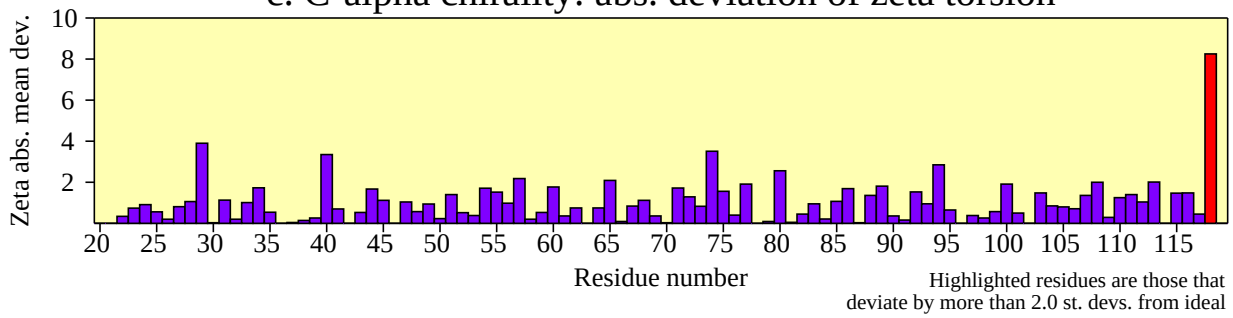
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



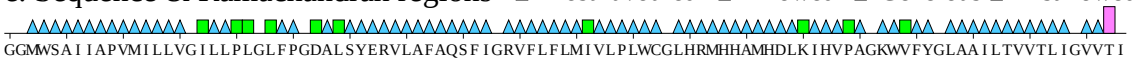
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

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

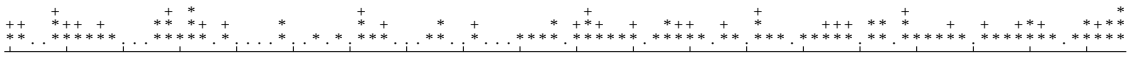
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

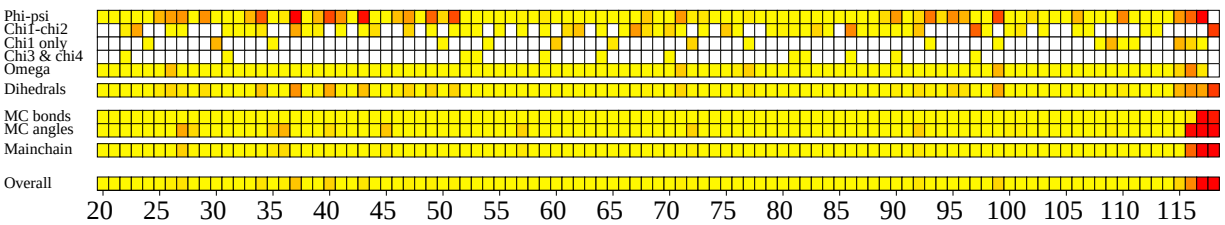


GGMWSA I I APVMI LLVG I LL PLGLF PGDAL SYERVLAFAQSF I GRVF LF LMI VL PLWCGLHRMHHAMHDLK I HVPAGKWVF YGLAA I LTVVTL I GVVT I

f. Max. deviation (see listing)

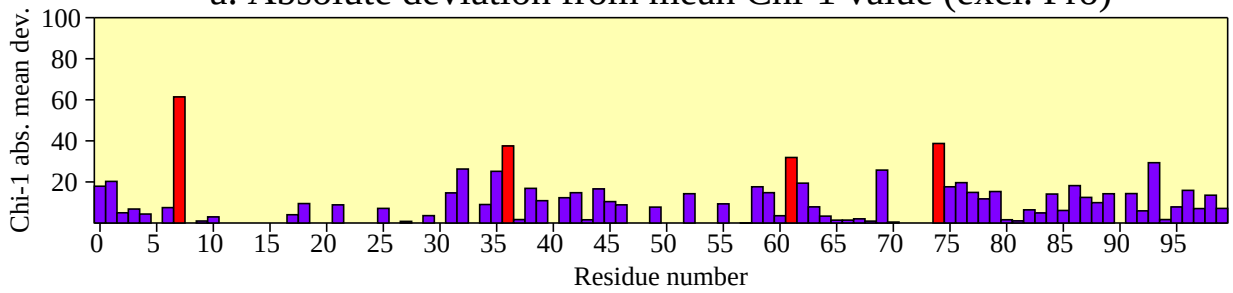


g. G-factors

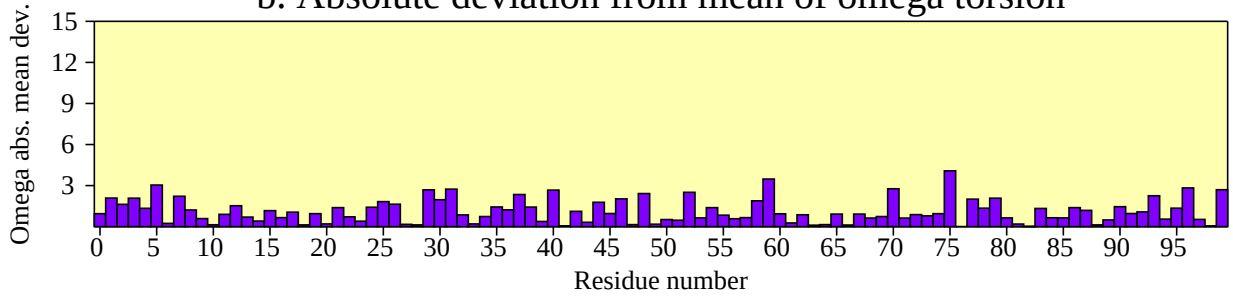


Residue properties
pdb1kfy

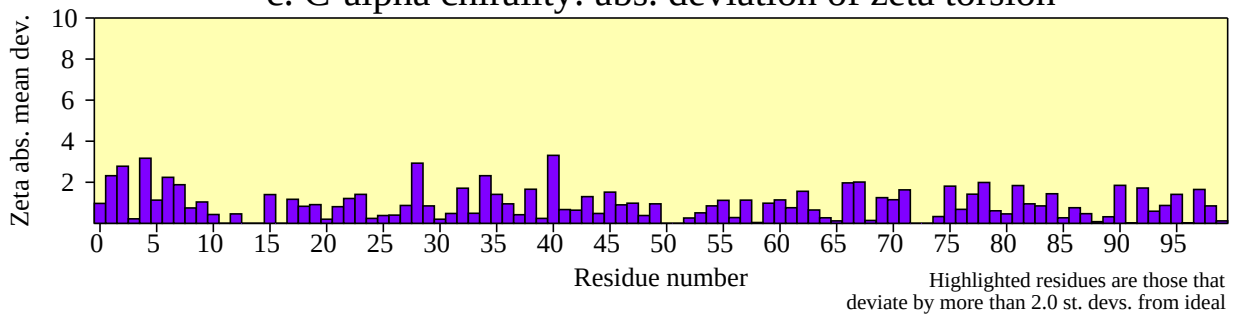
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

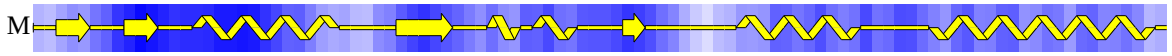


c. C-alpha chirality: abs. deviation of zeta torsion



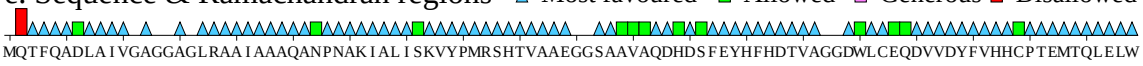
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

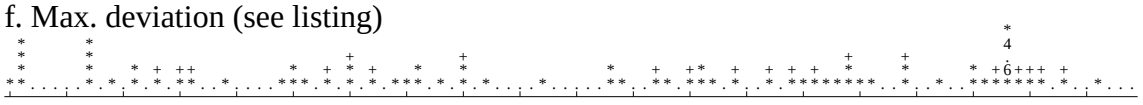


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

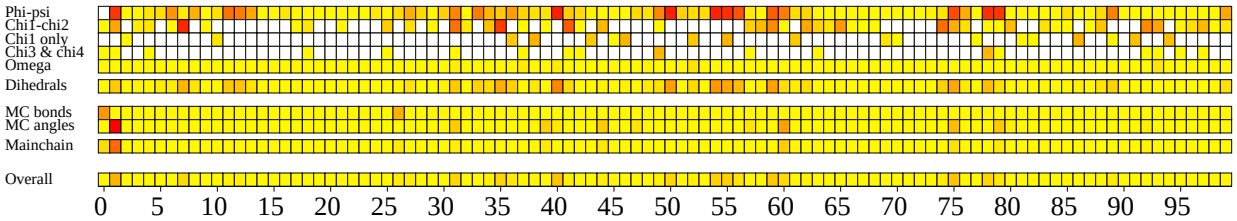
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

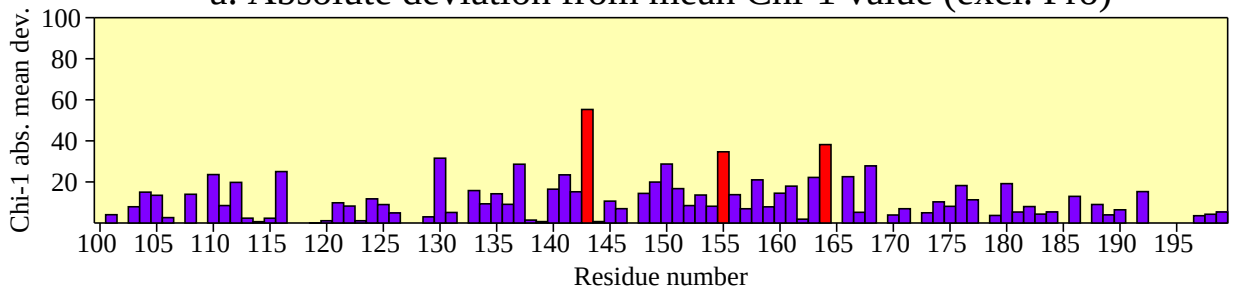


g. G-factors

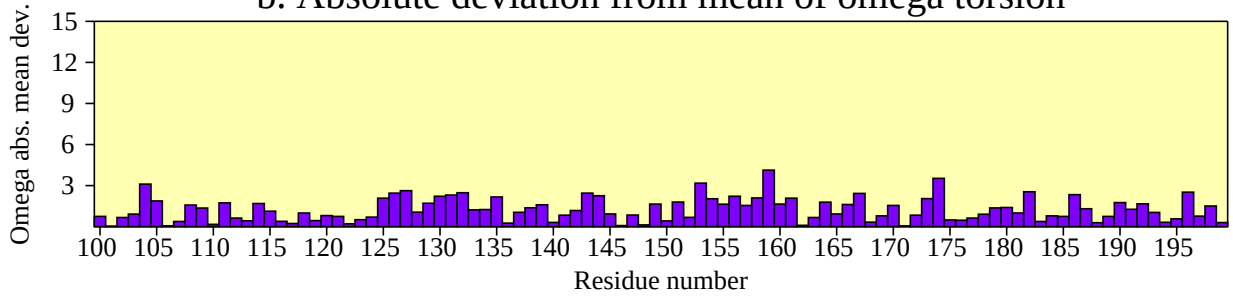


Residue properties
pdb1kfy

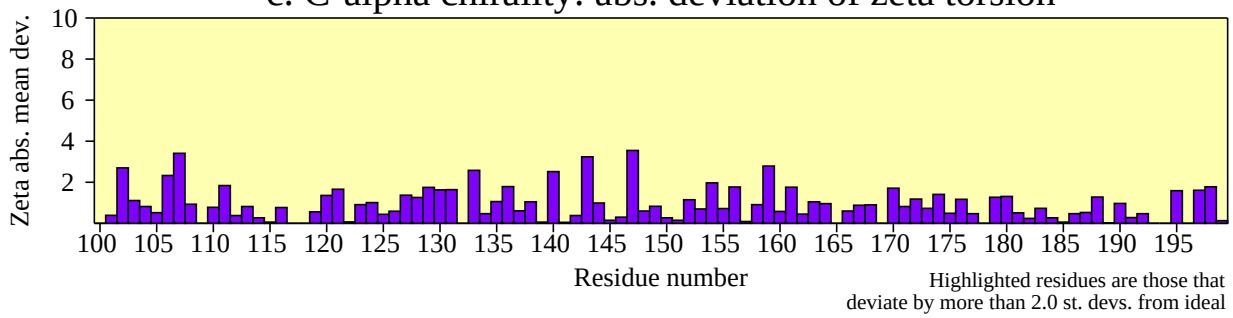
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

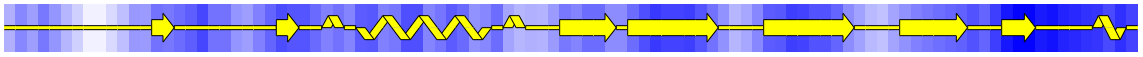


c. C-alpha chirality: abs. deviation of zeta torsion



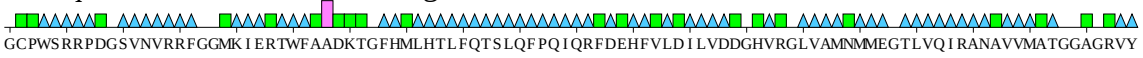
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



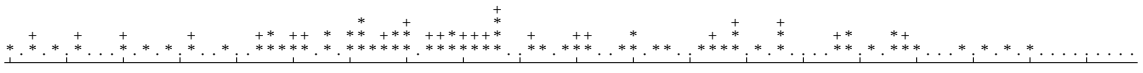
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

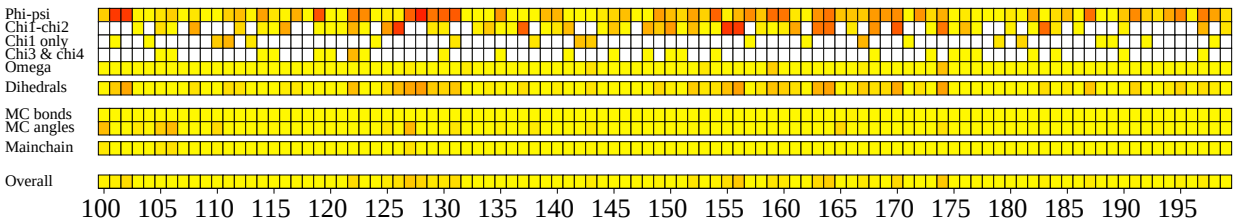


GCPWSRRPDGSVNVRRFGGMKIERTWFAADKTGFHMLHTLFQTSLQFPQIQRFDEHFVLDILVDDGHVRGLVAMNMMEGTLVQIRANAVVMATGGAGRVY

f. Max. deviation (see listing)

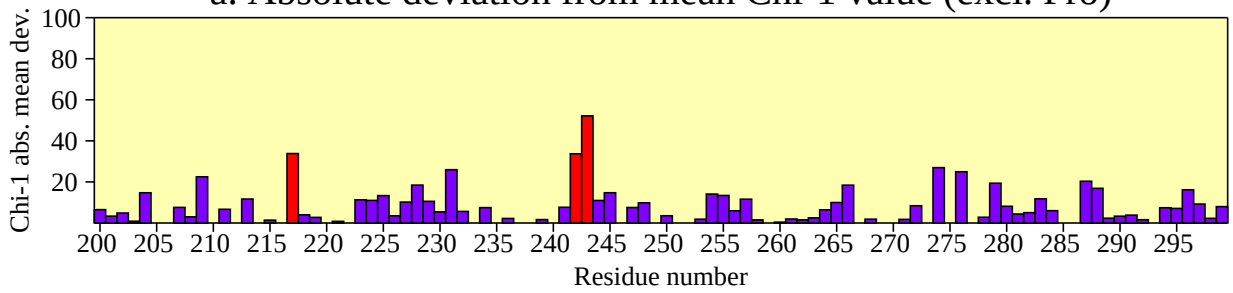


g. G-factors

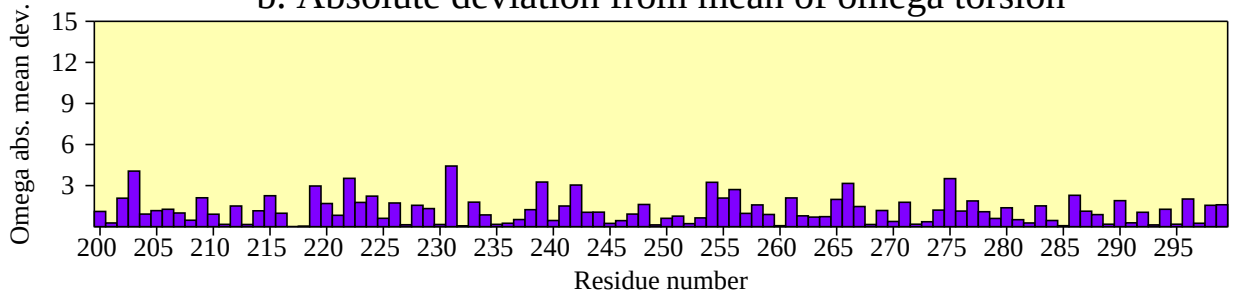


Residue properties
pdb1kfy

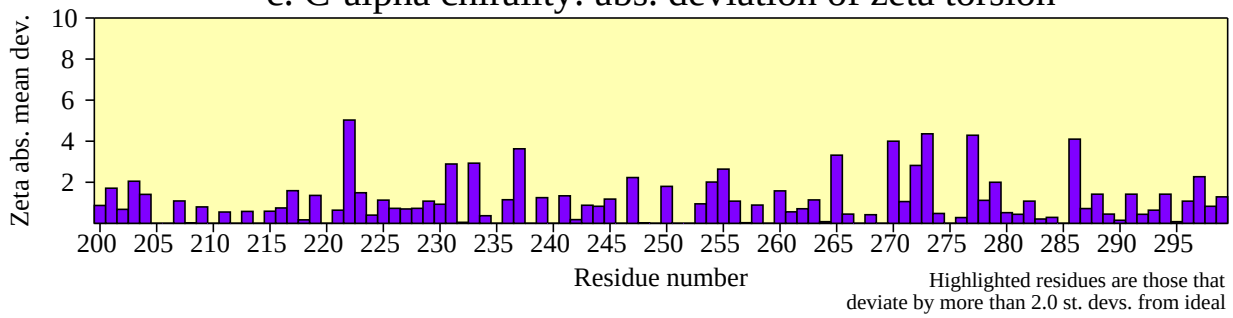
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

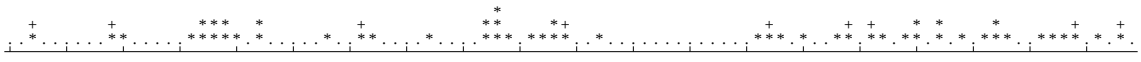
d. Secondary structure & estimated accessibility

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

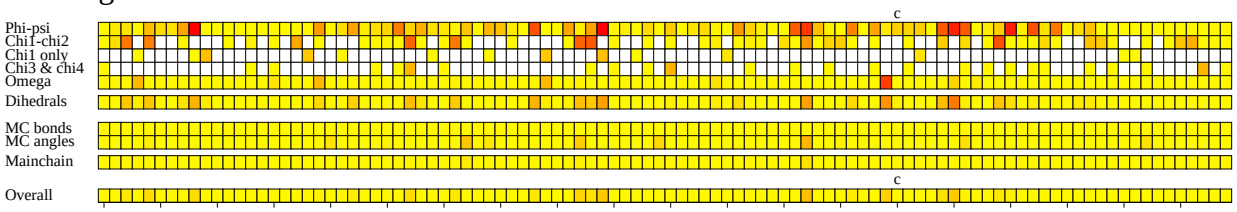
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

RYNTNGG I VTGDGMGMAL SHGVP L RDME F VQYHP TGL PGSG I LMT EGCRGEGG I L VNKNGYRYLQDYGMGP E T P L GE P KNKYME L GP RDKV SQA F WHEWR

f. Max. deviation (see listing)



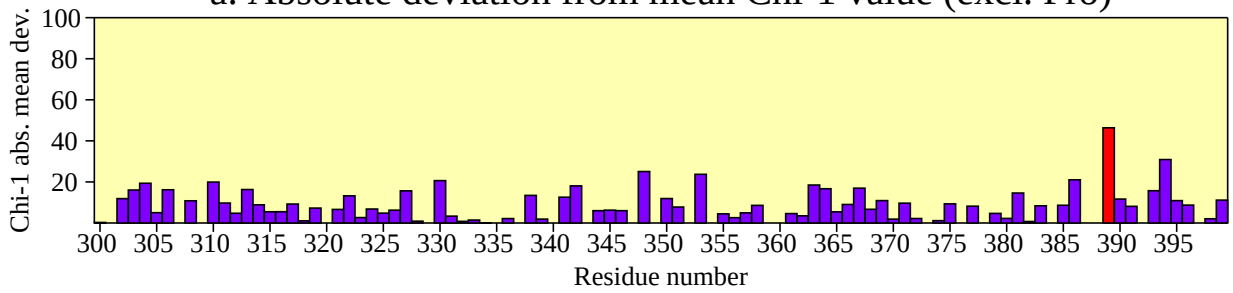
g. G-factors



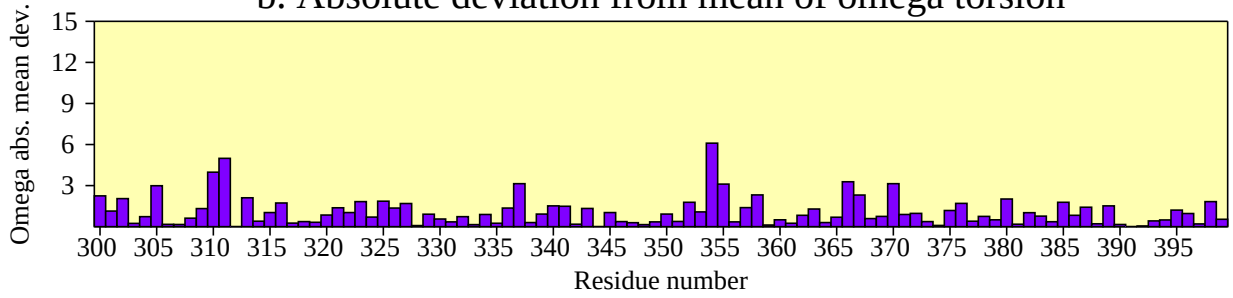
c = cis-peptide

Residue properties
pdb1kfy

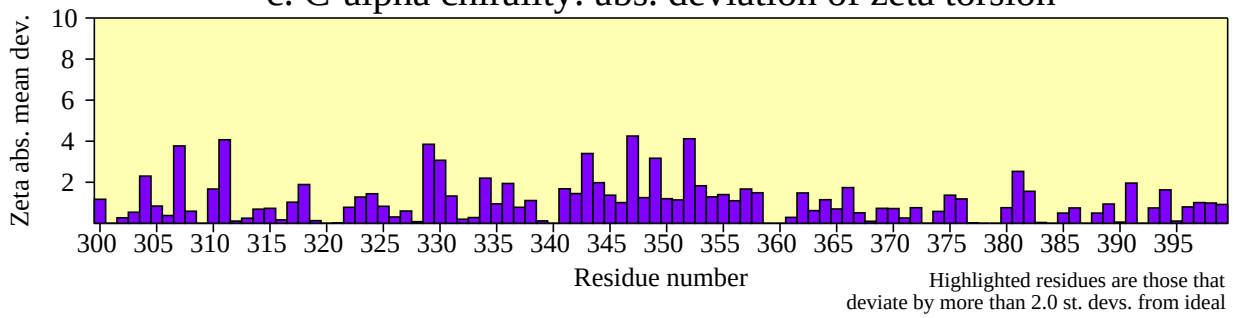
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

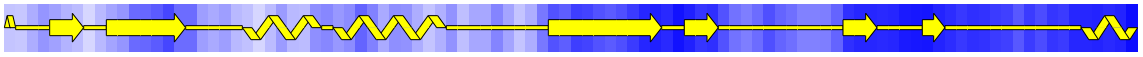


c. C-alpha chirality: abs. deviation of zeta torsion



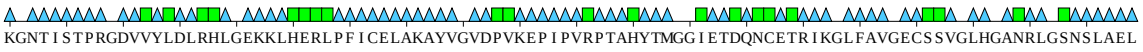
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



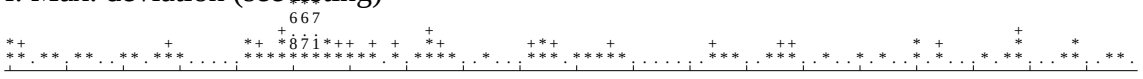
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

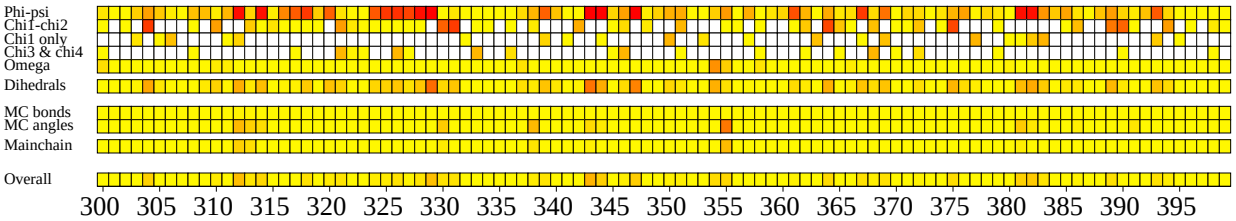


KGNT I S T P R G D V V Y L D L R H L G E K K L H E R L P F I C E L A K A Y V G V D P V K E P I P V R P T A H Y T M G G I E T D Q N C E T R I K G L F A V G E C S S V G L H G A N R L G S N S L A E L

f. Max. deviation (see listing)

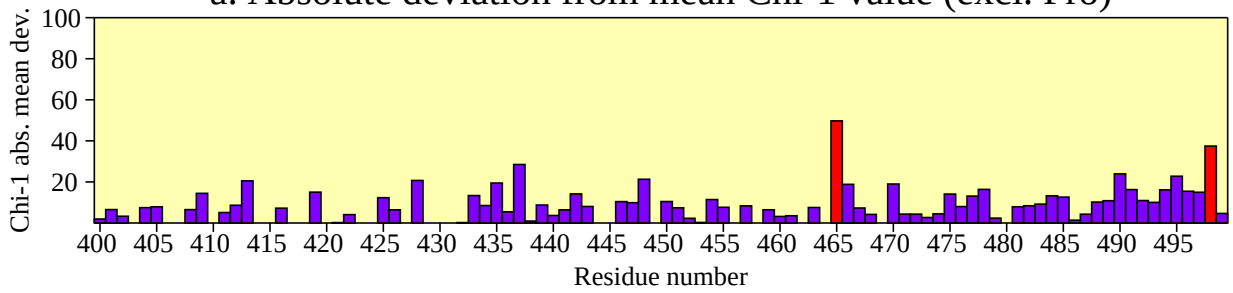


g. G-factors

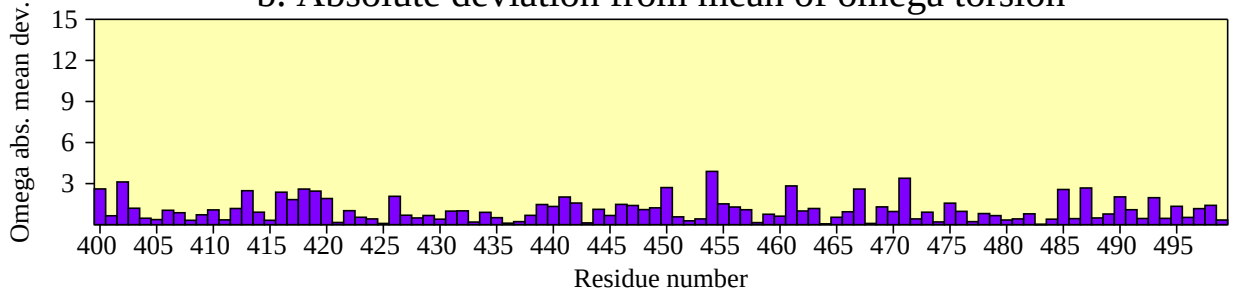


Residue properties
pdb1kfy

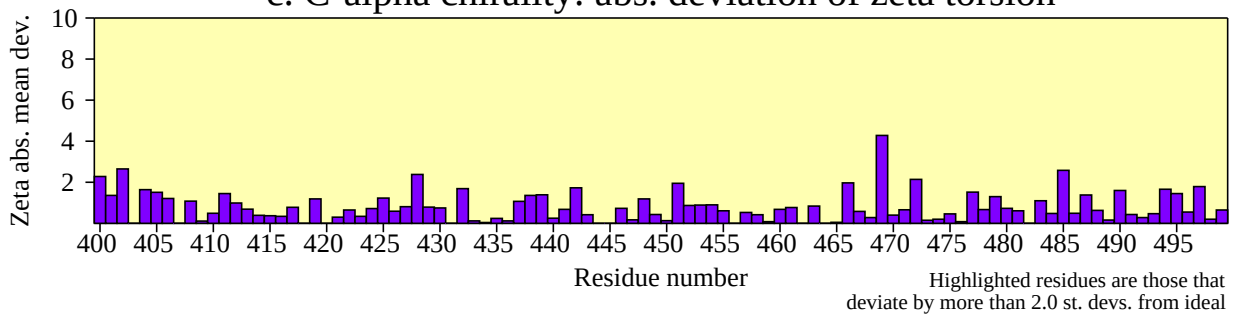
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

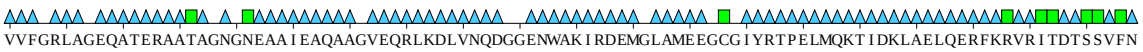


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

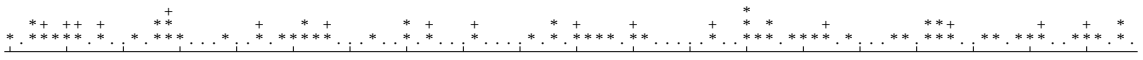
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

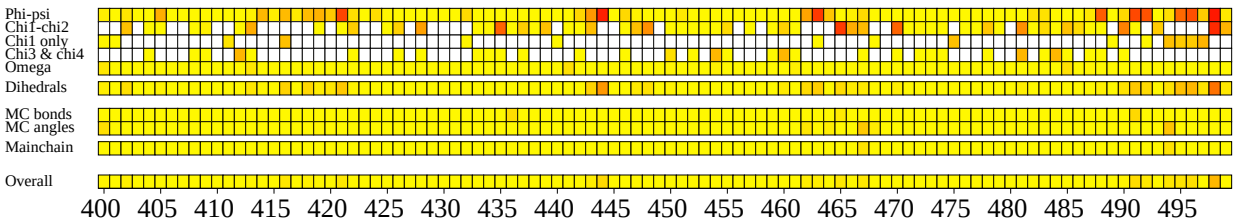


VVFGRLAGEQATERAATAGNGNEAAIEAQAAGVEQRLKDLVNQDGGENWAKIRDEMGLAMEEGCGIYRTPELMQKTIDKLAELQERFKRVRITDTSSVFN

f. Max. deviation (see listing)

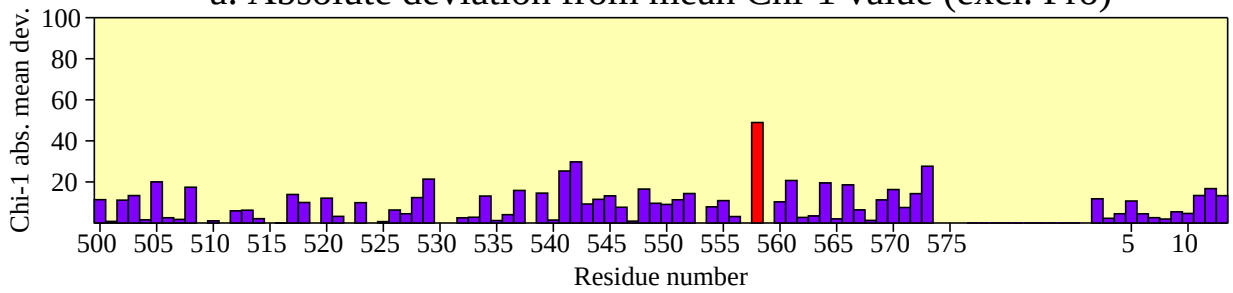


g. G-factors

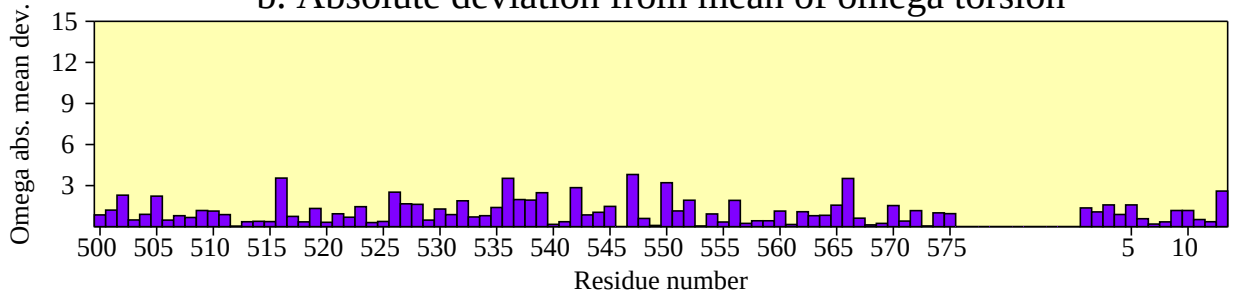


Residue properties
pdb1kfy

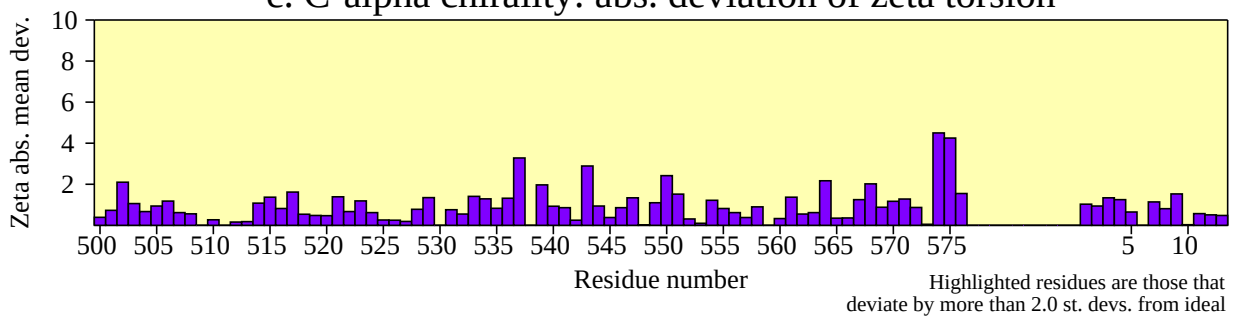
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

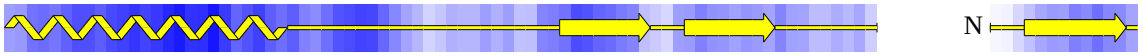


c. C-alpha chirality: abs. deviation of zeta torsion



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

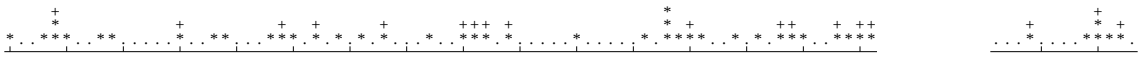
d. Secondary structure & estimated accessibility



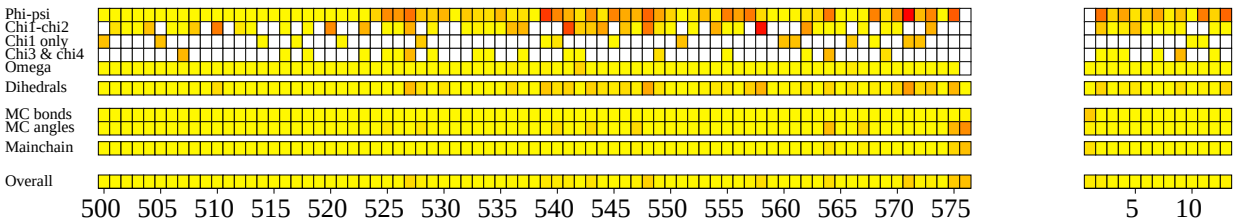
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

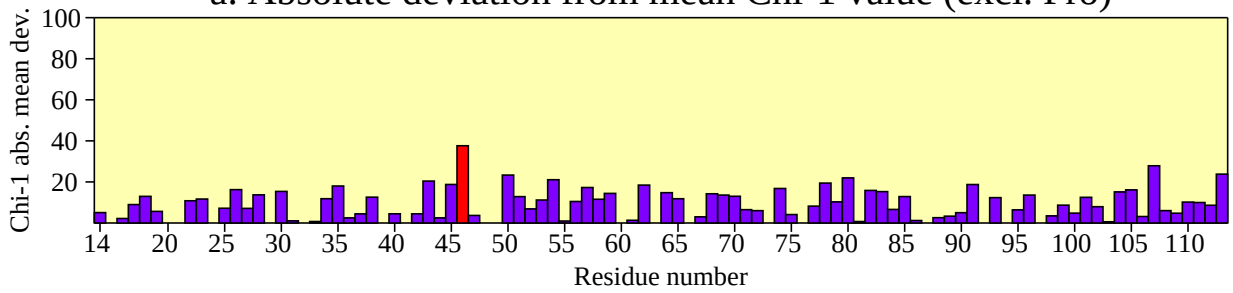


g. G-factors

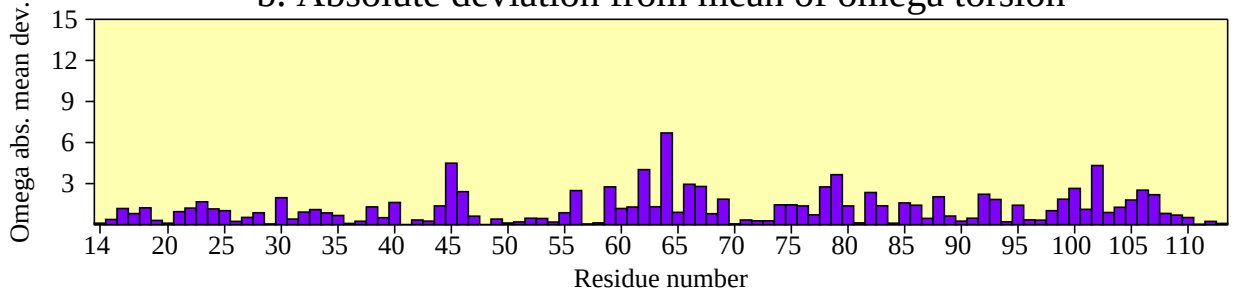


Residue properties
pdb1kfy

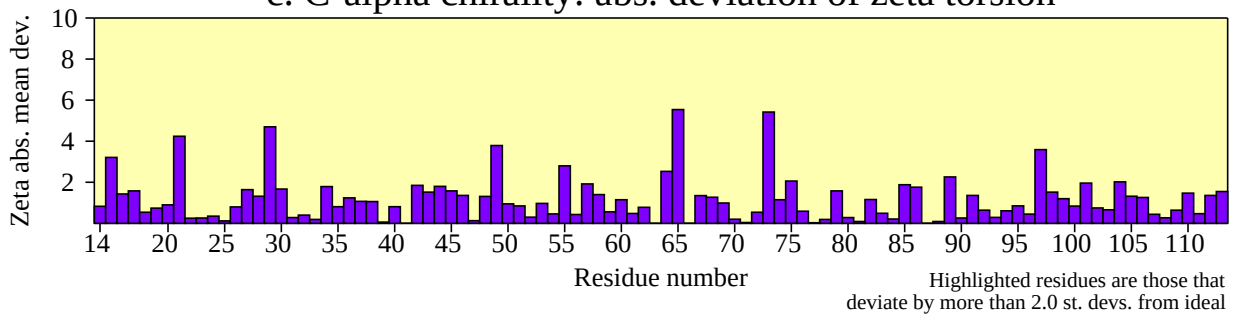
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

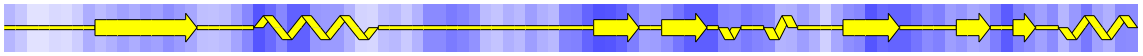


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

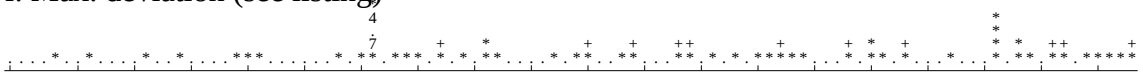


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

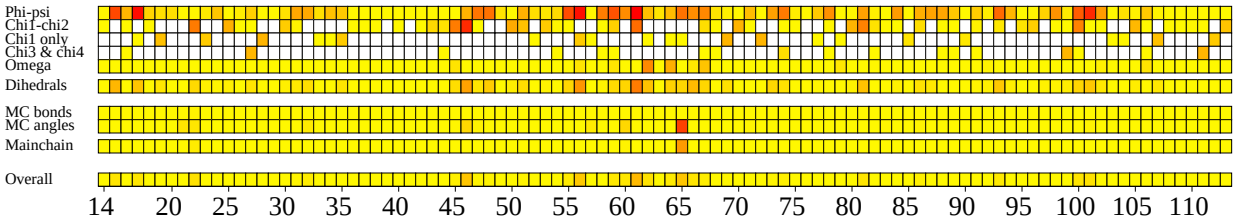
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)

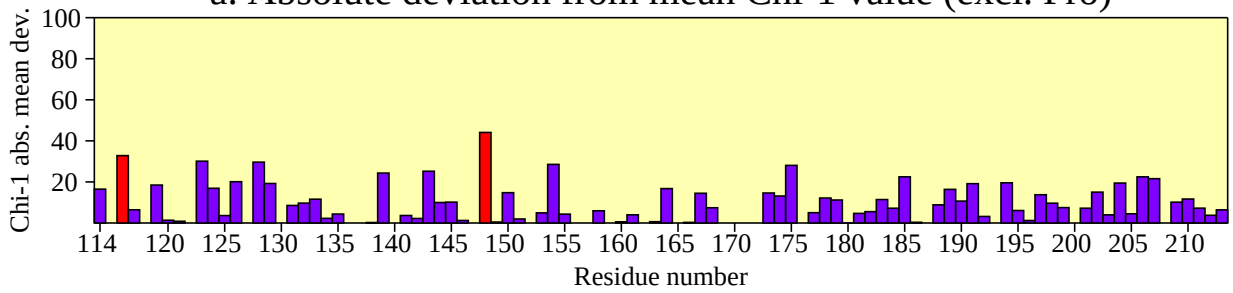


g. G-factors

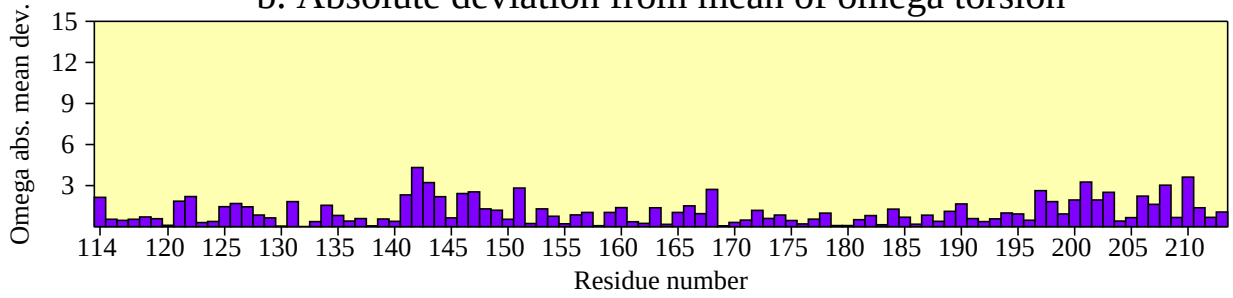


Residue properties
pdb1kfy

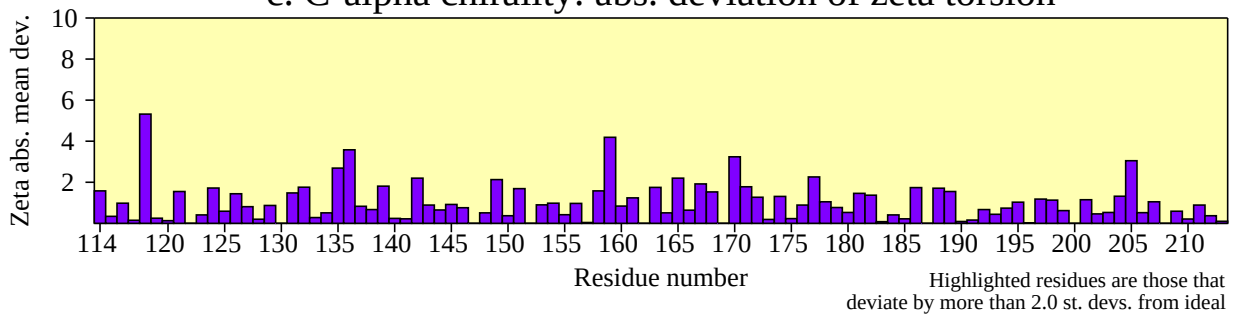
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



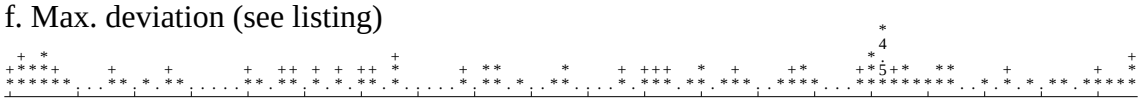
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

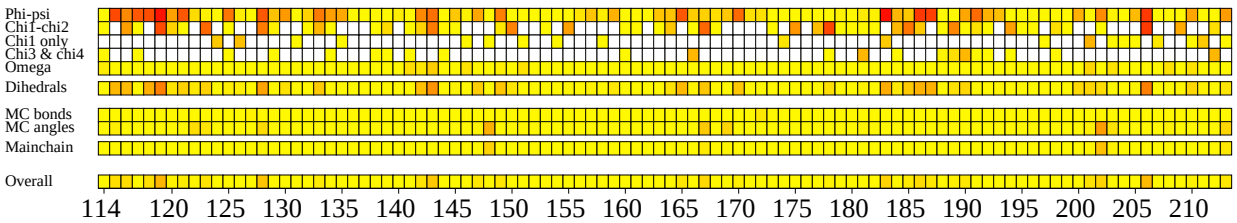
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

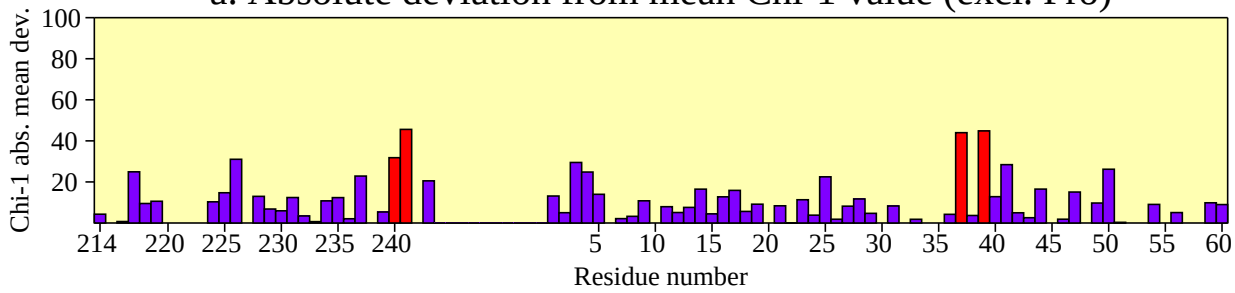


g. G-factors

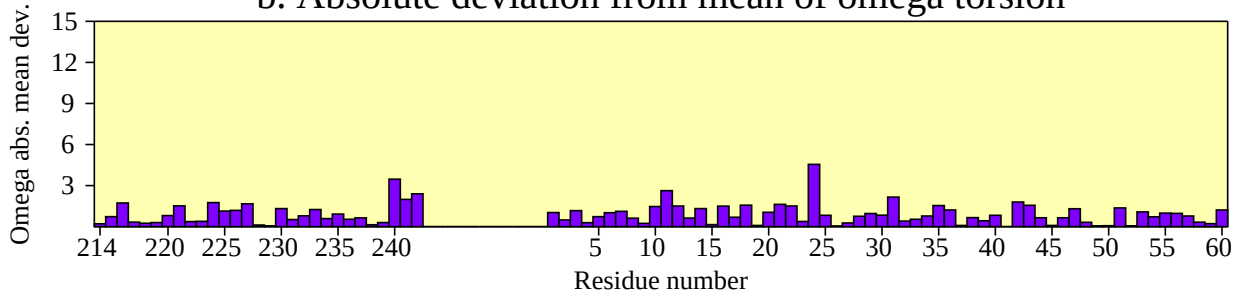


Residue properties
pdb1kfy

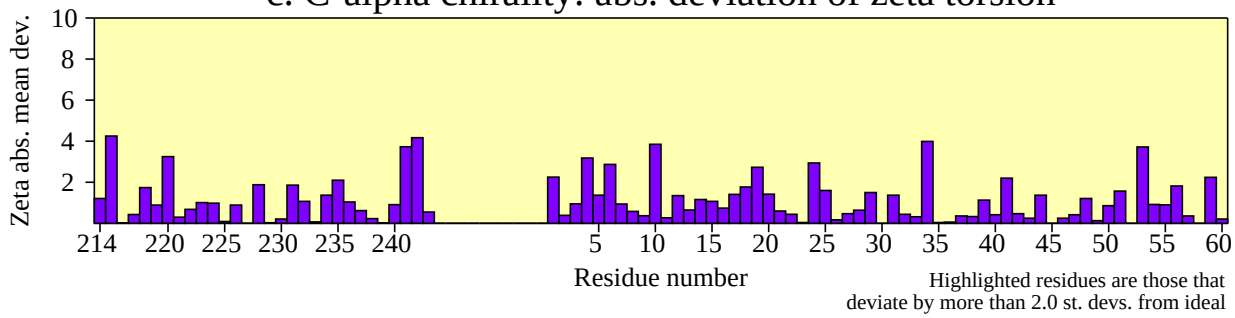
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

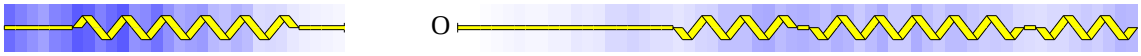


c. C-alpha chirality: abs. deviation of zeta torsion

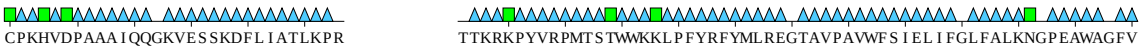


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

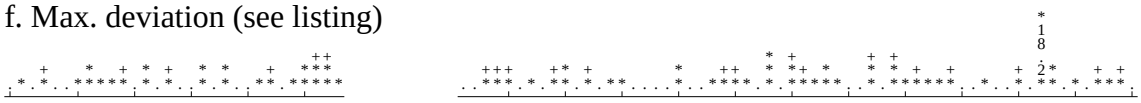
d. Secondary structure & estimated accessibility



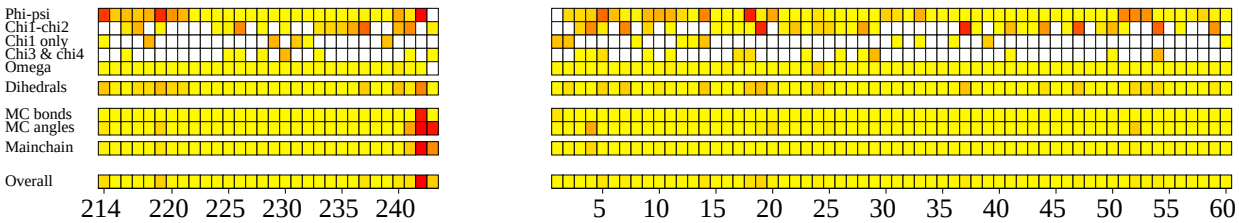
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

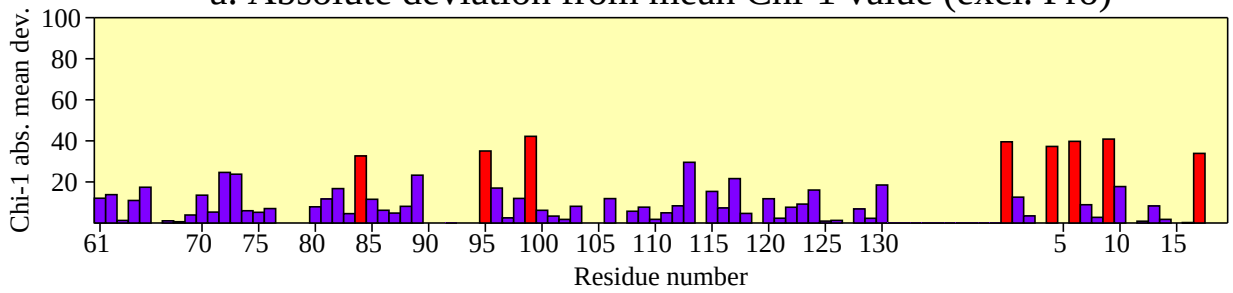


g. G-factors

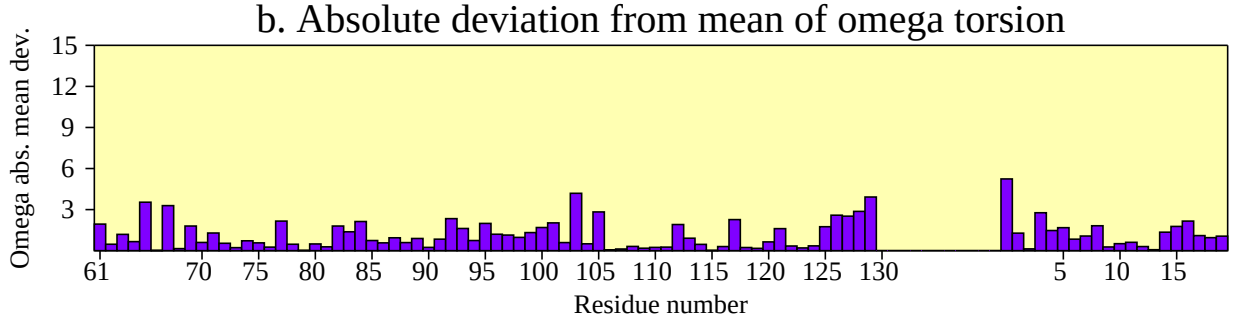


Residue properties
pdb1kfy

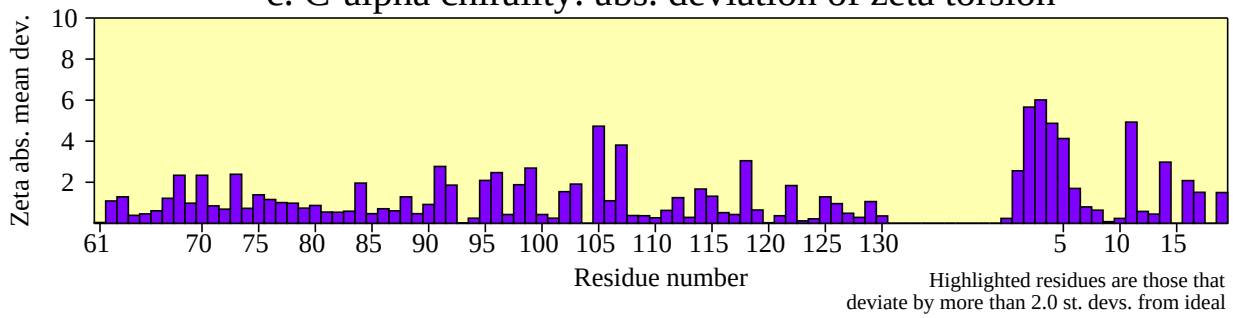
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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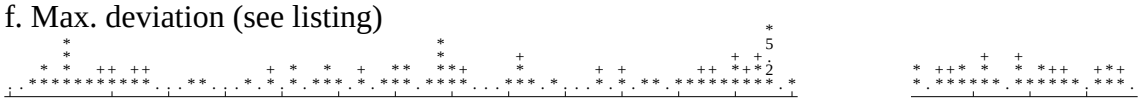
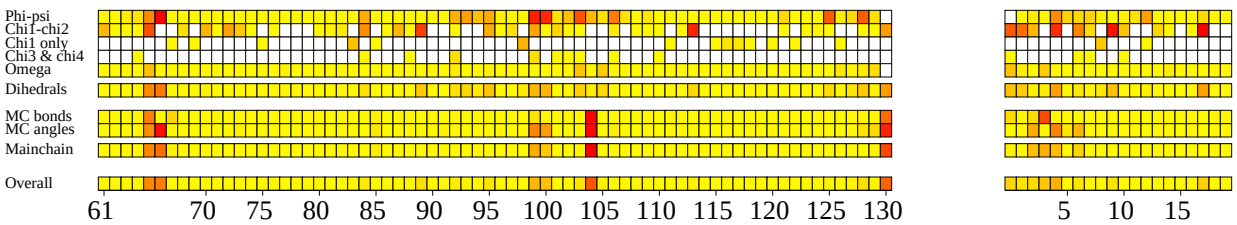
d. Secondary structure & estimated accessibility

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

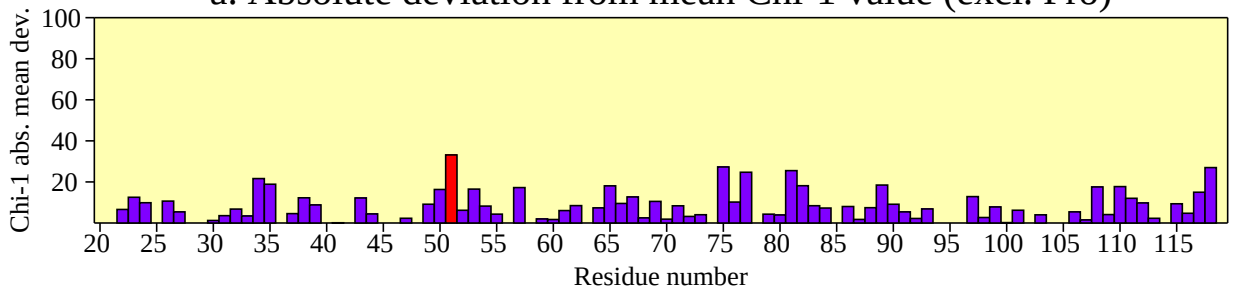


g. G-factors

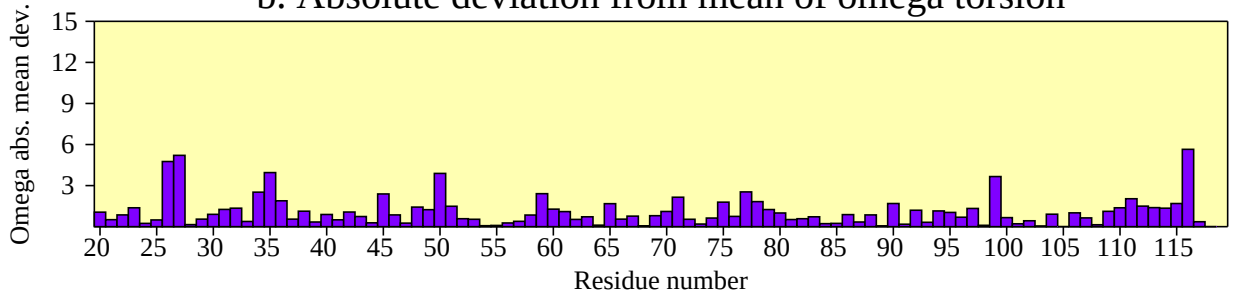


Residue properties
pdb1kfy

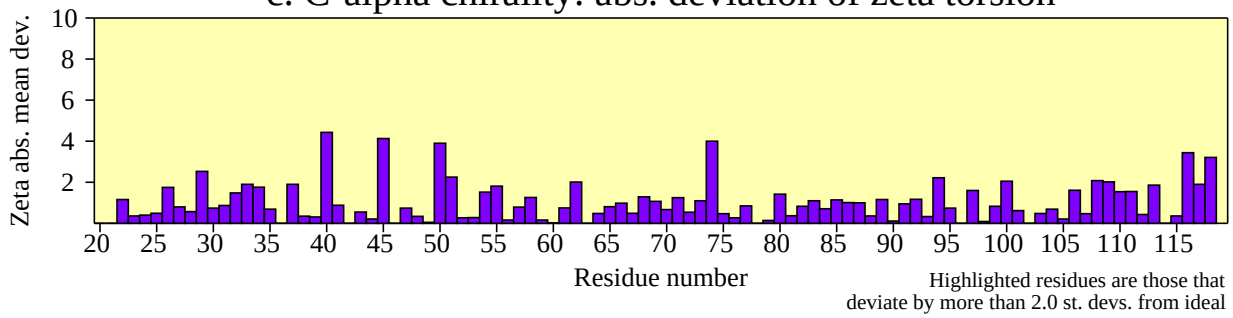
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

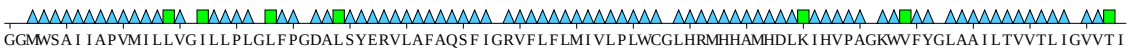


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

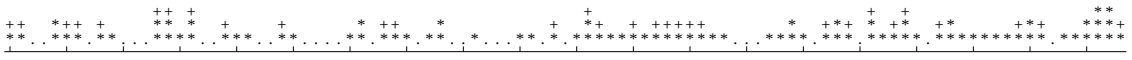
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

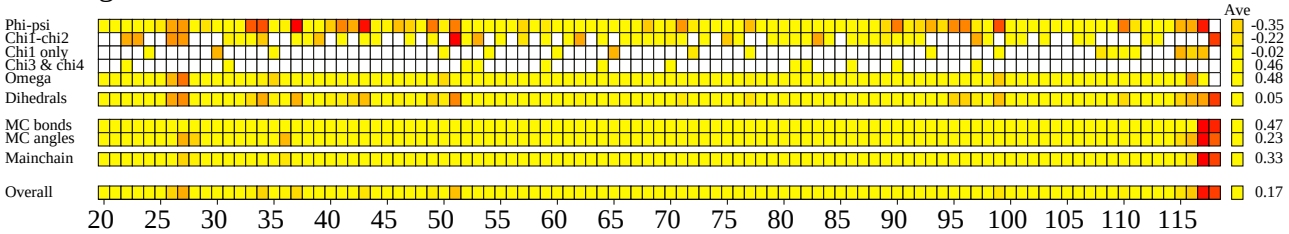


GGMWSA I I APVMI LLVG I LL PLGLF PGDAL SYERVLAFAQSF I GRVF LF LMI VL PLWCGLHRMHHAMHDLK I HVPAGKWVF YGLAA I LTVVTL I GVVT I

f. Max. deviation (see listing)

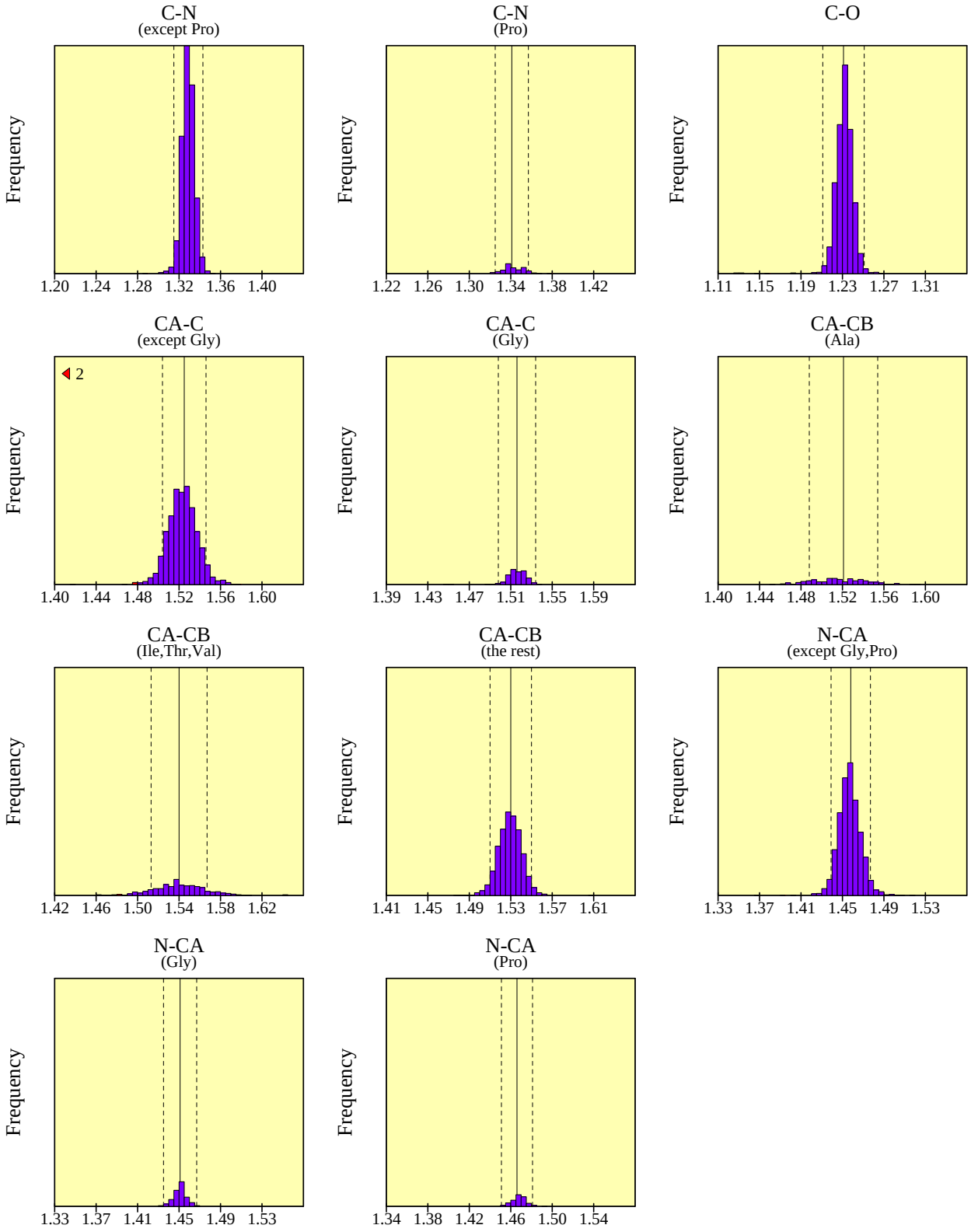


g. G-factors



Main-chain bond lengths

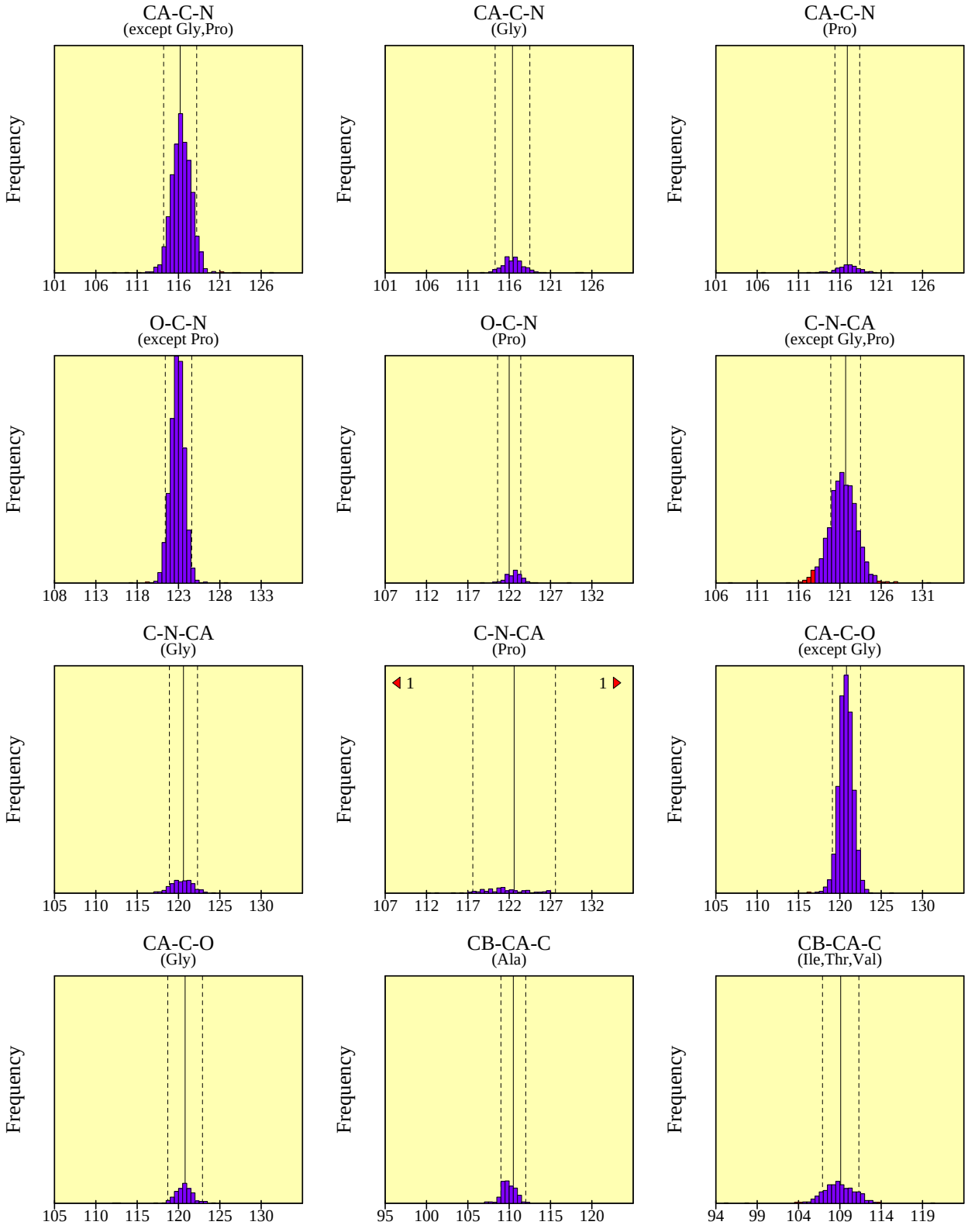
pdb1kfy



Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

Main-chain bond angles

pdb1kfy

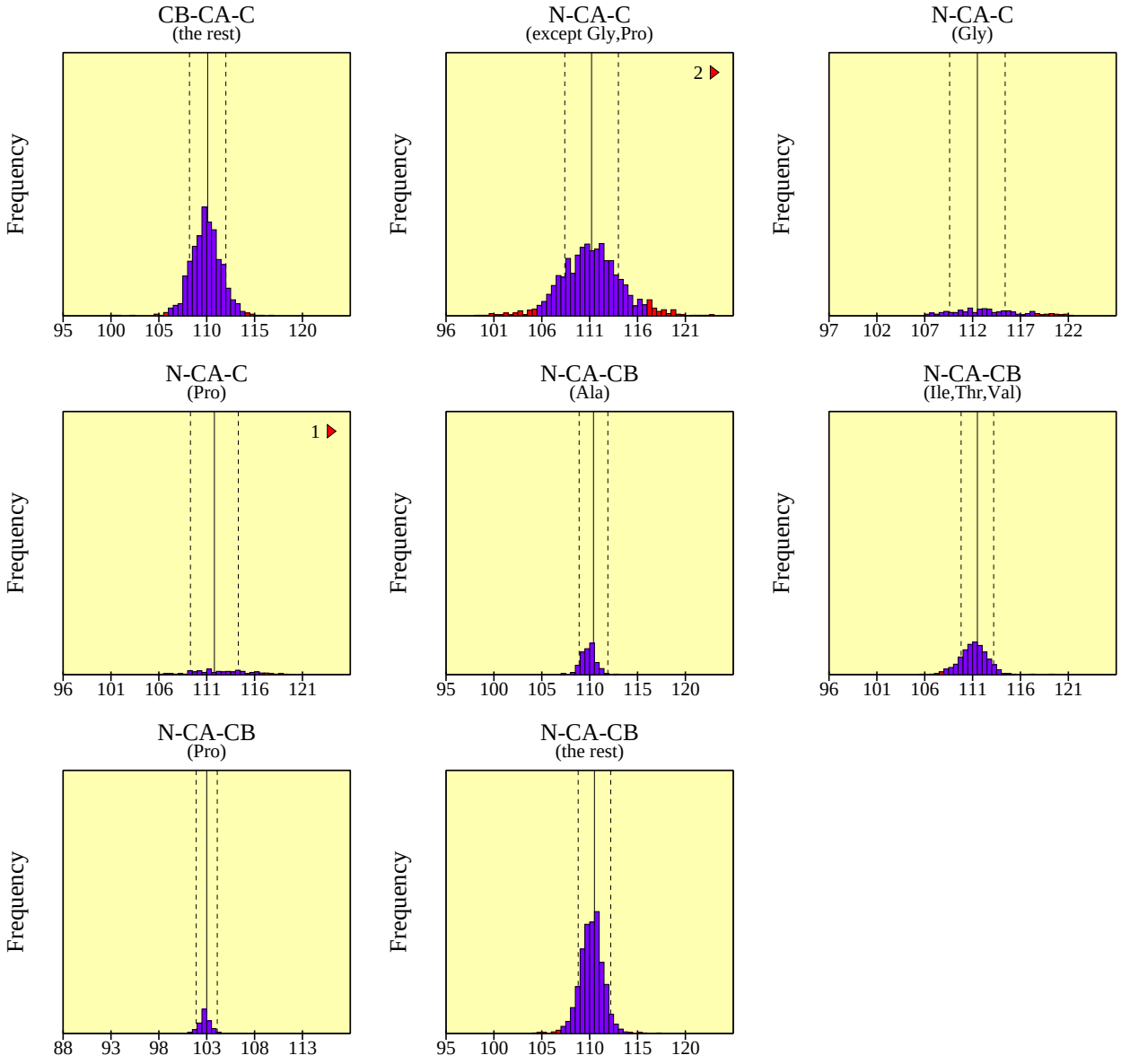


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

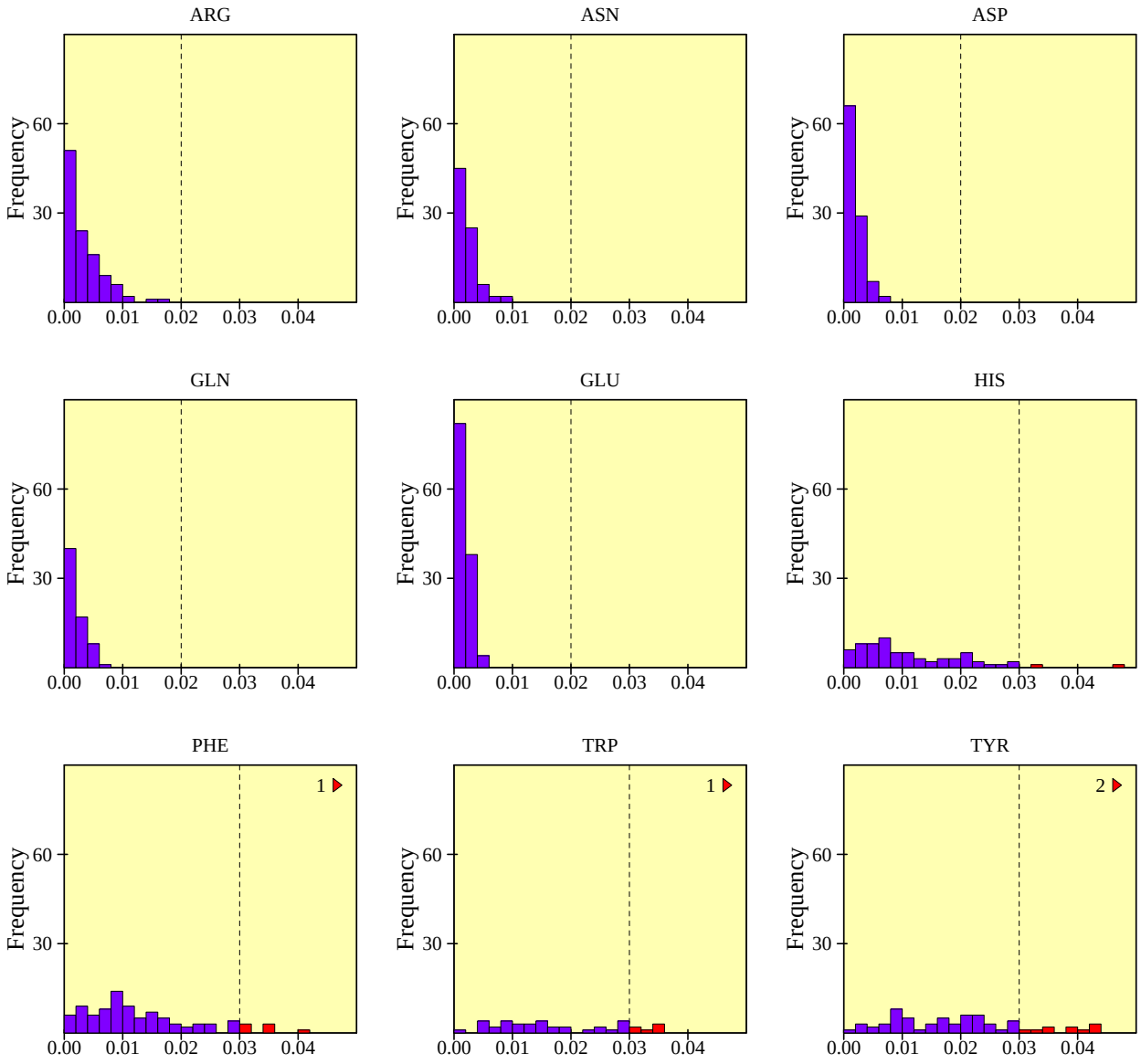
pdb1kfy



Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.
Solid and dashed lines represent the mean and standard deviation values as per Engh & Huber small-molecule data.

RMS distances from planarity

pdb1kfy

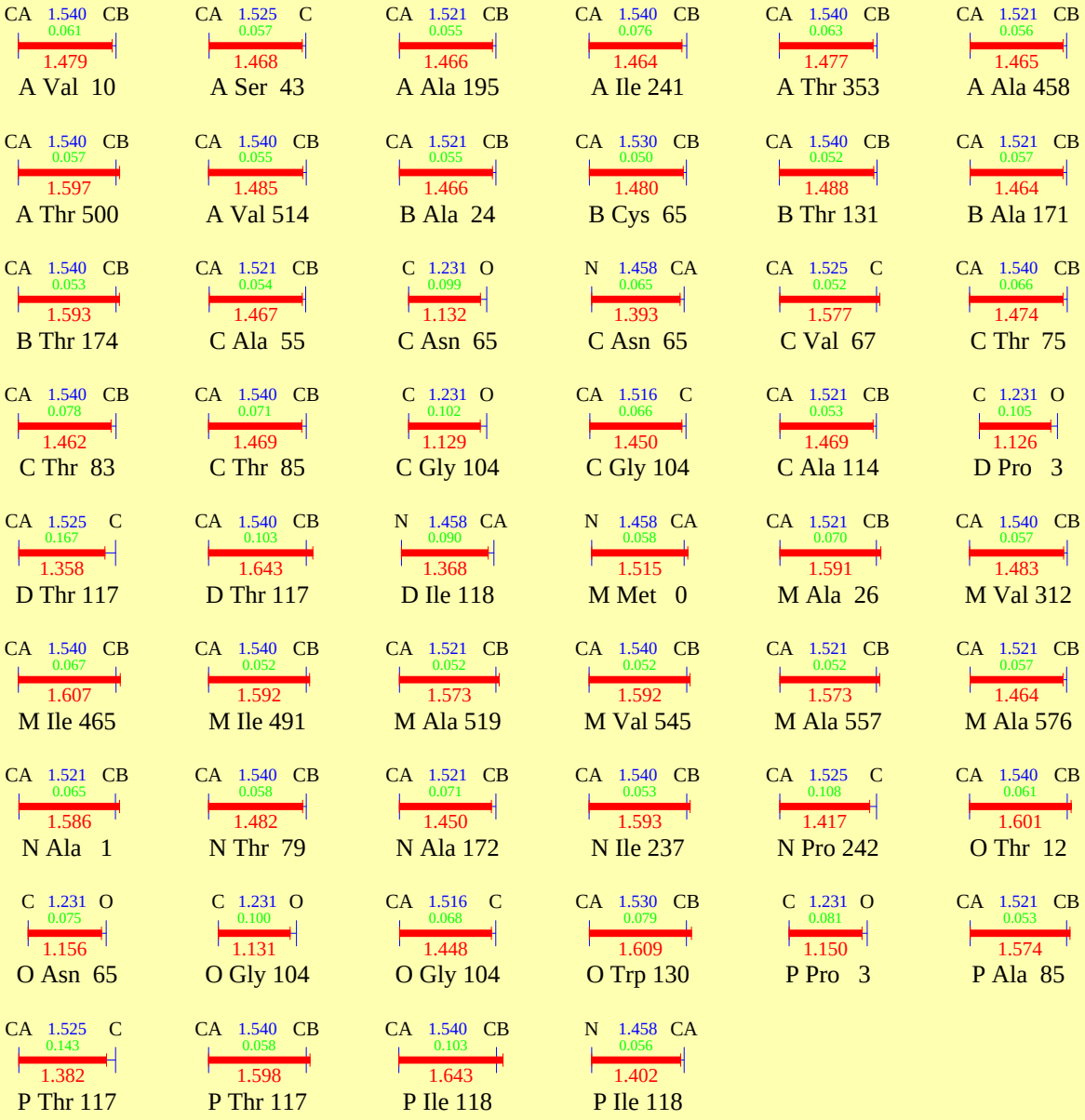


Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

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

Distorted geometry
pdb1kfy

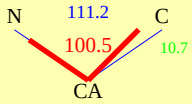
Main-chain bond lengths



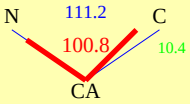
Bonds differing by > 0.05A from small-molecule values. Values shown: "ideal", difference, actual

Distorted geometry
pdb1kfy

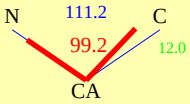
Main-chain bond angles



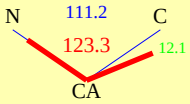
A Arg 106



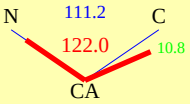
A Ala 128



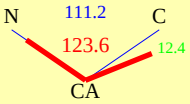
A Val 312



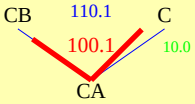
A His 355



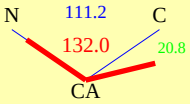
A Phe 547



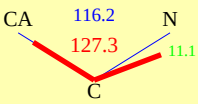
B Cys 65



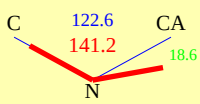
C Asn 65



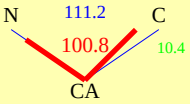
C Asn 65



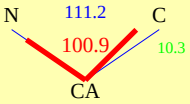
C Asn 65 - C Pro 66



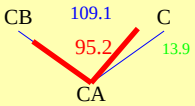
C Asn 65 - C Pro 66



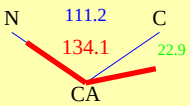
D Ile 1



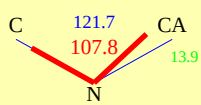
D Asn 4



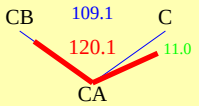
D Thr 117



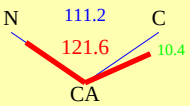
D Thr 117



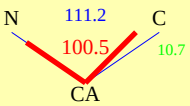
D Thr 117 - D Ile 118



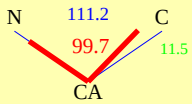
D Ile 118



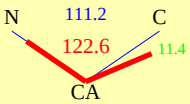
M Trp 75



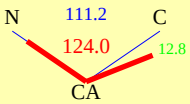
M Arg 106



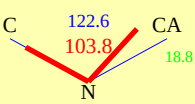
M Ala 127



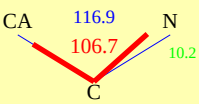
M His 355



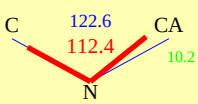
N Cys 65



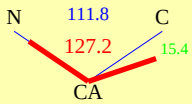
N Lys 241 - N Pro 242



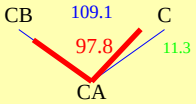
N Pro 242 - N Arg 243



O Asn 65 - O Pro 66



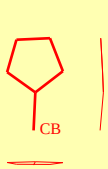
O Pro 66



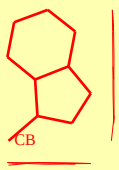
P Thr 117

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

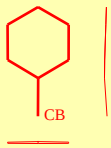
Planar groups



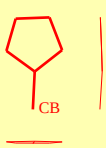
0.047
A His 87



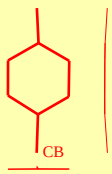
0.032
A Trp 125



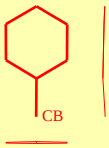
0.036
A Phe 146



0.032
A His 219



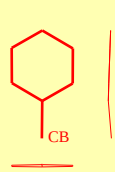
0.043
A Tyr 231



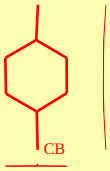
0.031
A Phe 498

Distorted geometry
pdb1kfy

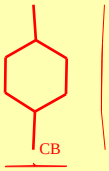
Planar groups (contd)



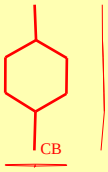
0.041
A Phe 554



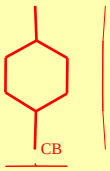
0.039
B Tyr 53



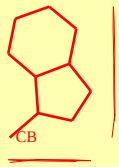
0.053
B Tyr 119



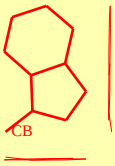
0.040
C Tyr 22



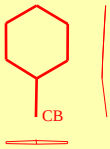
0.044
C Tyr 25



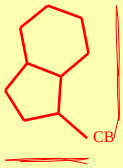
0.034
C Trp 56



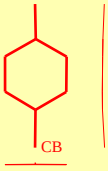
0.035
C Trp 130



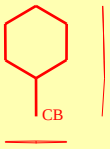
0.064
D Phe 44



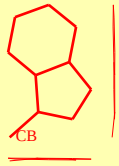
0.064
D Trp 76



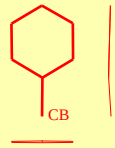
0.033
M Tyr 260



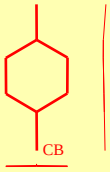
0.031
M Phe 294



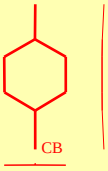
0.032
M Trp 298



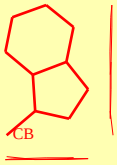
0.032
M Phe 402



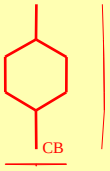
0.034
M Tyr 466



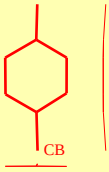
0.031
N Tyr 13



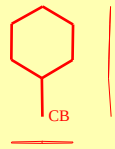
0.036
N Trp 55



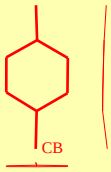
0.034
N Tyr 84



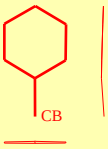
0.042
N Tyr 209



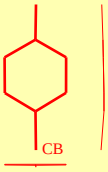
0.035
O Phe 24



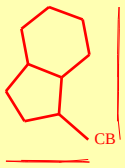
0.064
O Tyr 129



0.036
P Phe 17



0.040
P Tyr 51



0.032
P Trp 76

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