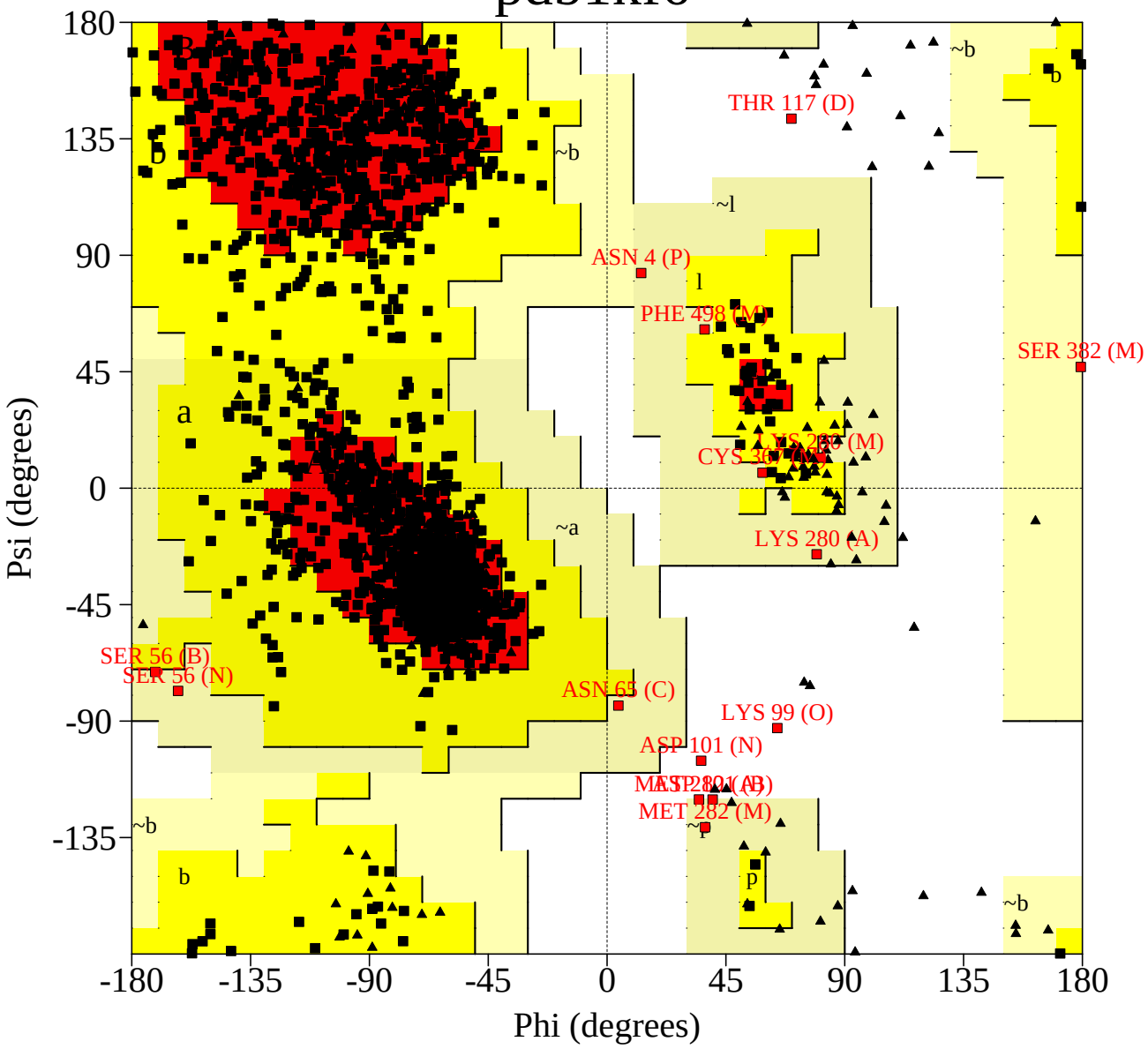
Ramachandran Plot

pdb1kf6



Plot statistics

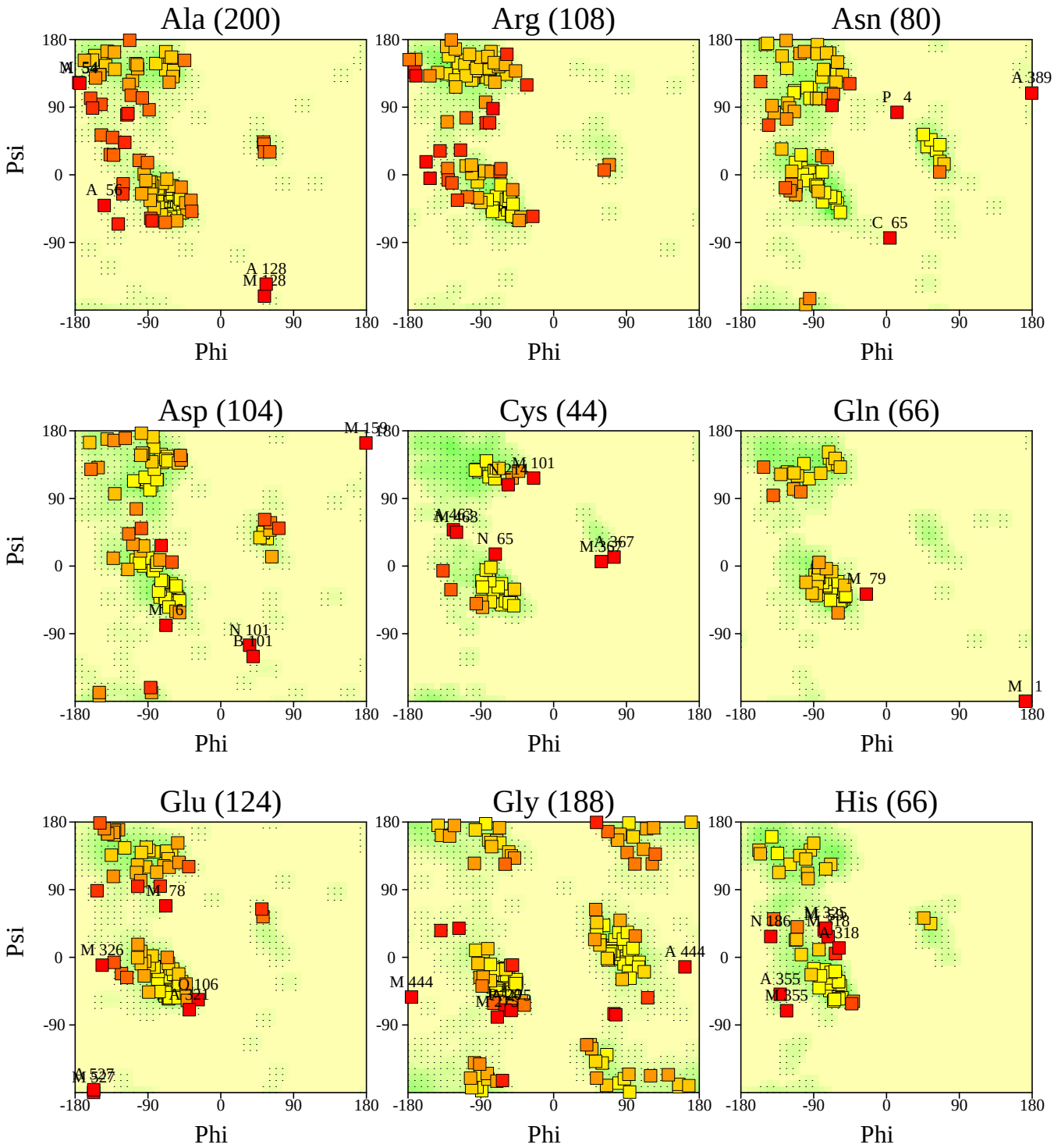
Residues in most favoured regions [A,B,L]	1550	84.8%
Residues in additional allowed regions [a,b,l,p]	263	14.4%
Residues in generously allowed regions [~a,~b,~l,~p]	12	0.7%
Residues in disallowed regions	3	0.2%
	----	------
Number of non-glycine and non-proline residues	1828	100.0%
Number of end-residues (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

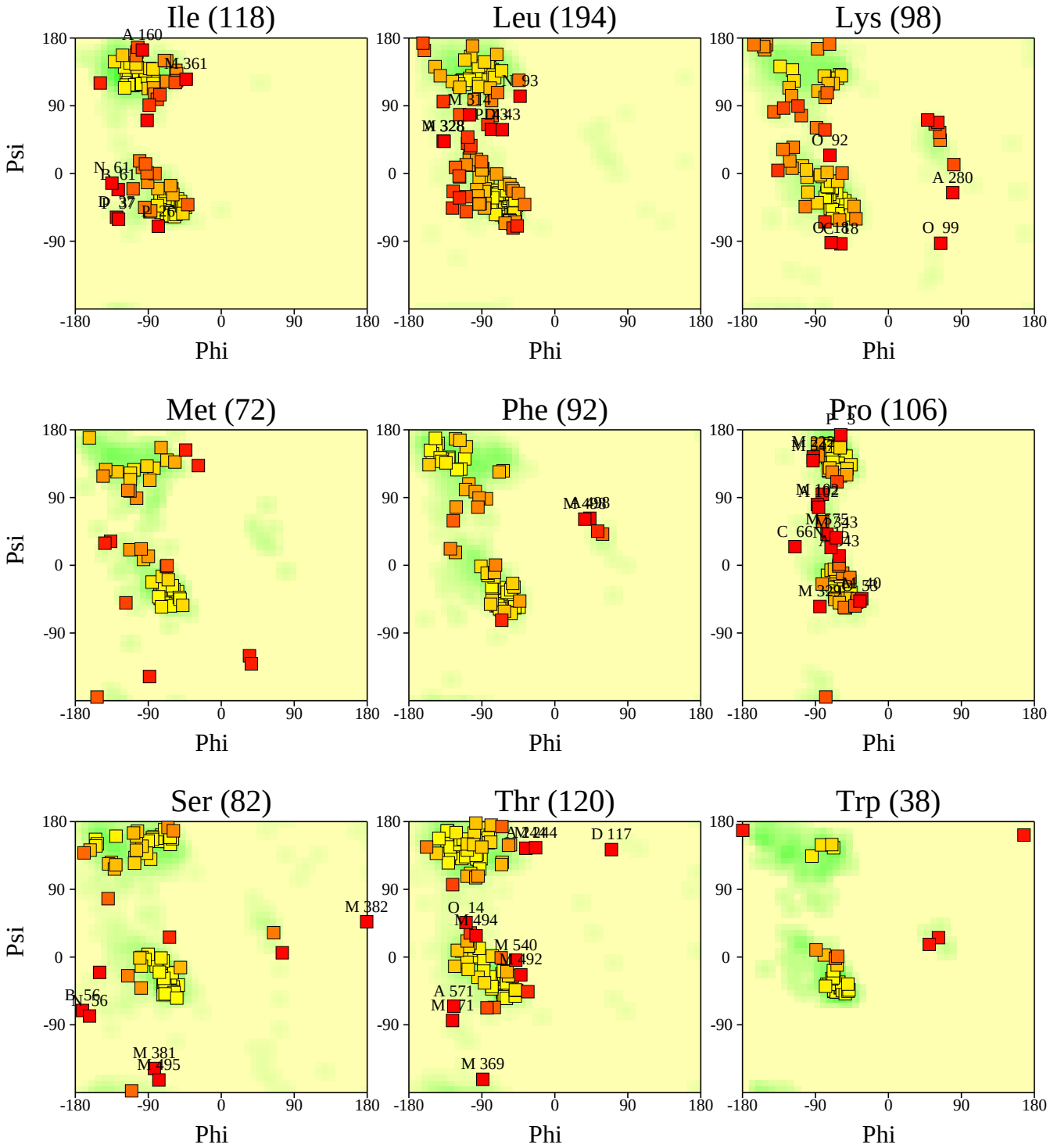
pdb1kf6



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

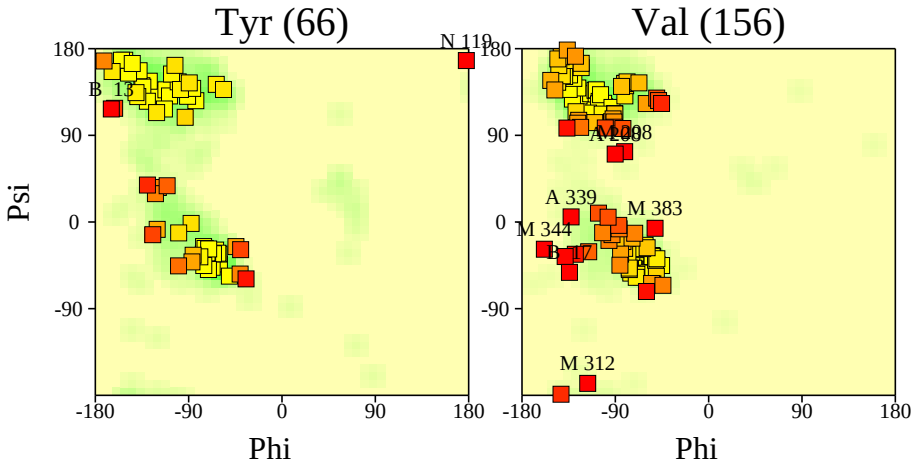
pdb1kf6



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

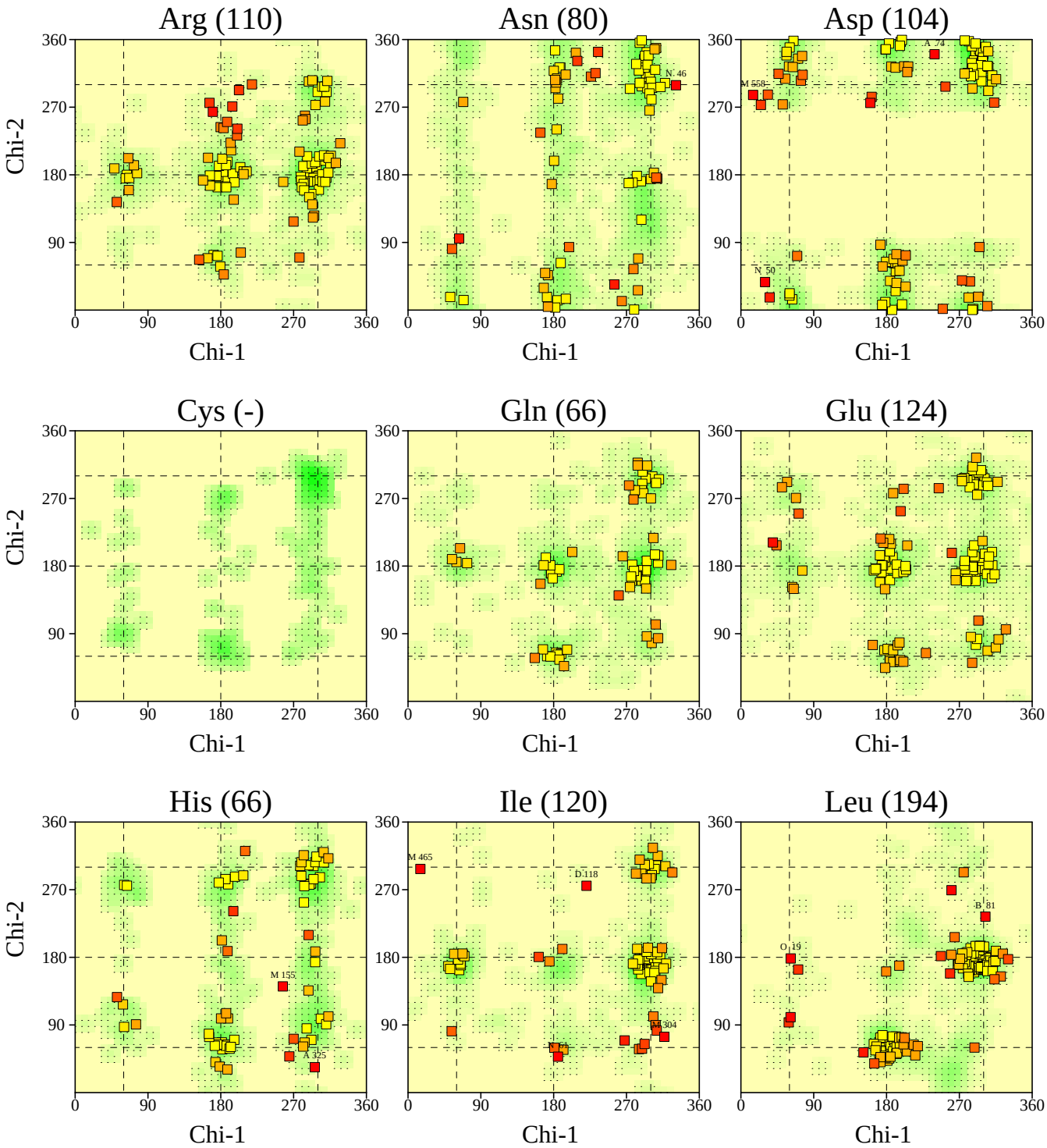
pdb1kf6



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

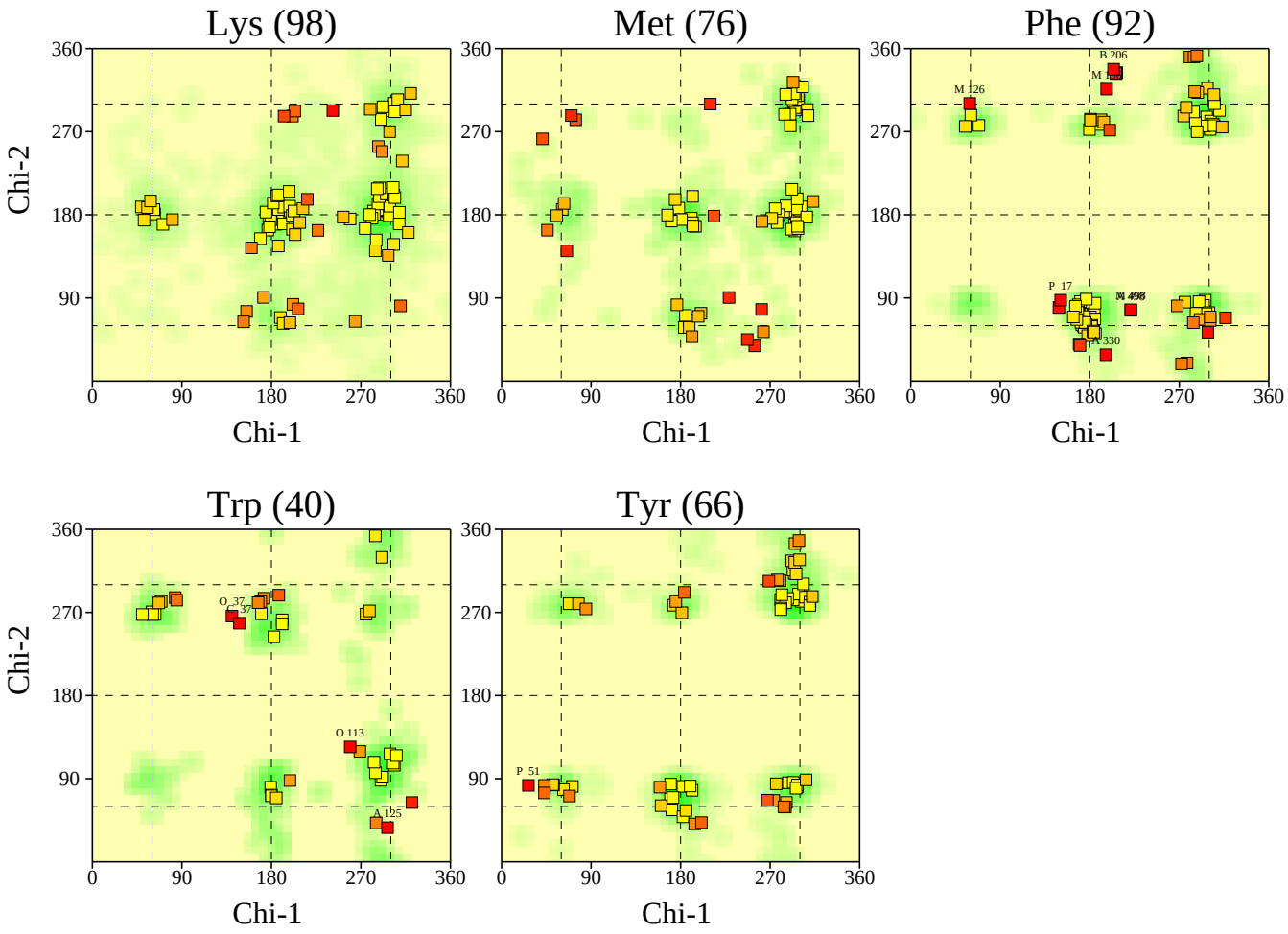
pdb1kf6



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

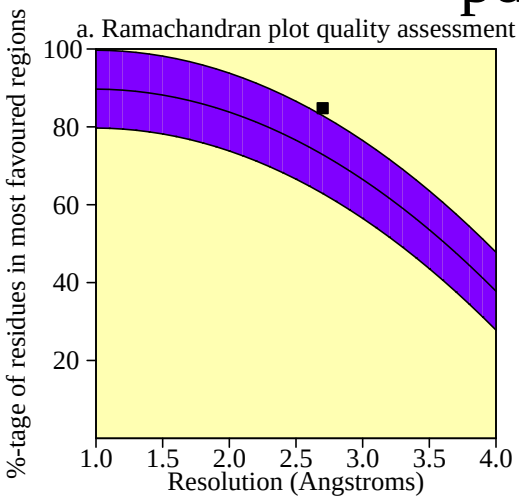
pdb1kf6



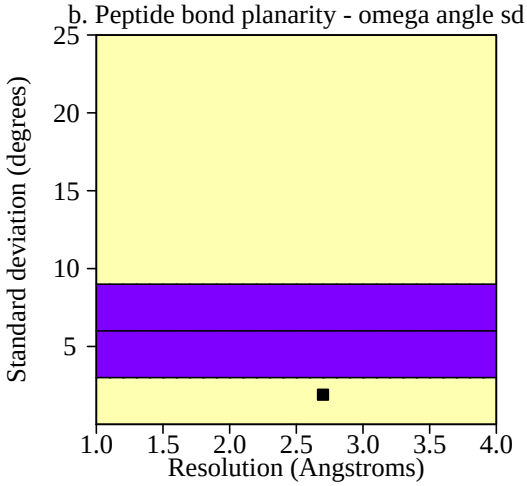
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

Main-chain parameters
pdb1kf6

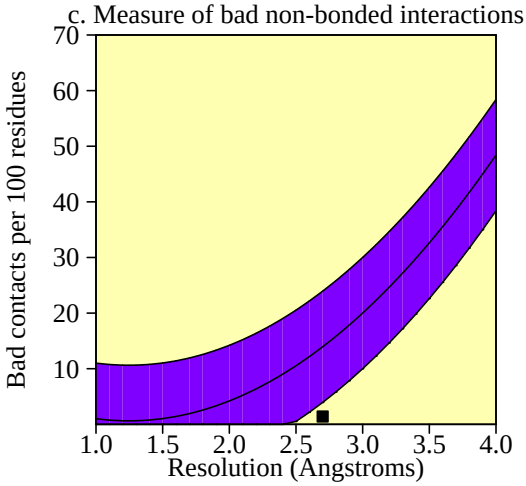
a. Ramachandran plot quality assessment



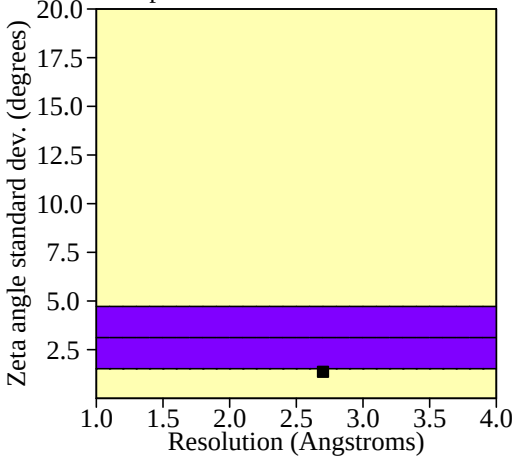
b. Peptide bond planarity - omega angle sd



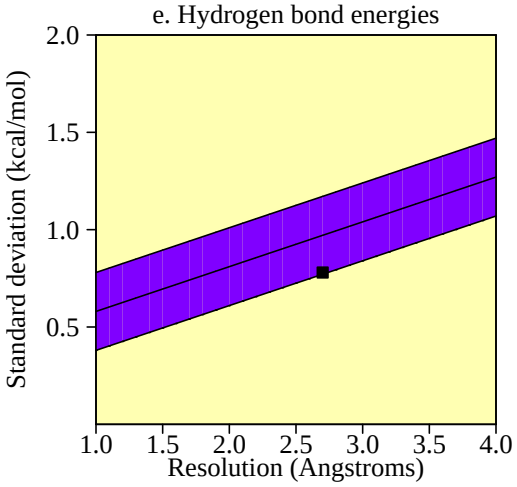
c. Measure of bad non-bonded interactions



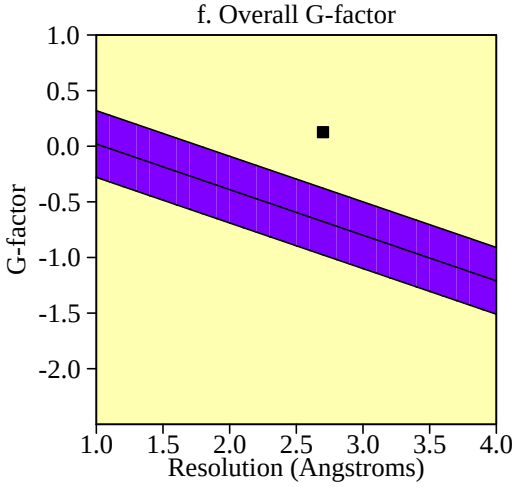
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor

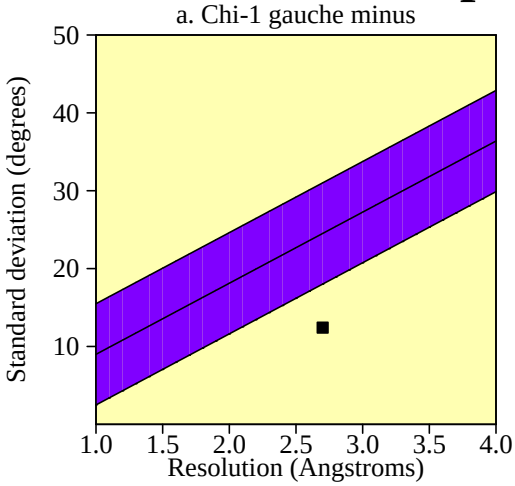


Plot statistics

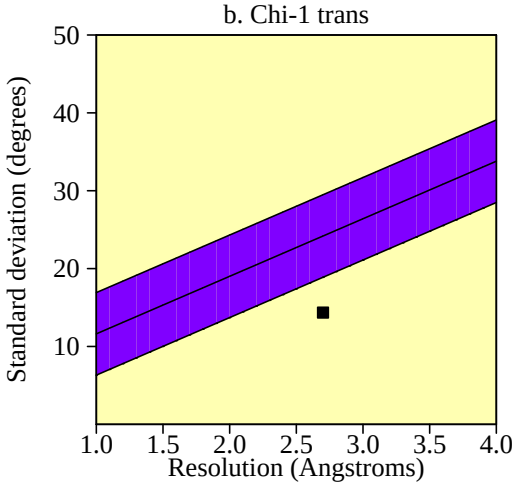
Stereochemical parameter	No. of data pts	Parameter value	Comparison values: Typical value	Comparison values: Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	1828	84.8	72.9	10.0	1.2	BETTER
b. Omega angle st dev	2126	1.9	6.0	3.0	-1.4	BETTER
c. Bad contacts / 100 residues	30	1.4	13.9	10.0	-1.3	BETTER
d. Zeta angle st dev	1950	1.4	3.1	1.6	-1.1	BETTER
e. H-bond energy st dev	1399	0.8	1.0	0.2	-1.0	Inside
f. Overall G-factor	2138	0.1	-0.7	0.3	2.7	BETTER

Side-chain parameters
pdb1kf6

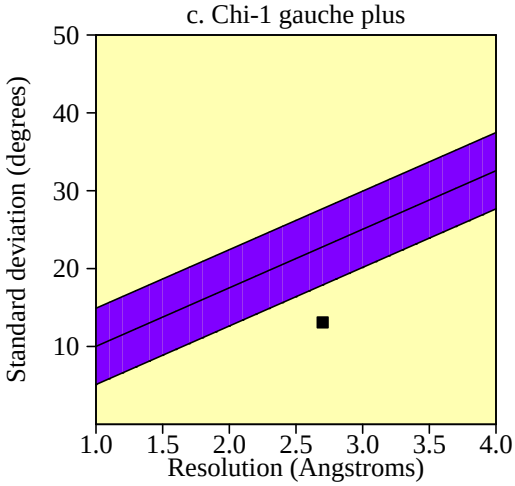
a. Chi-1 gauche minus



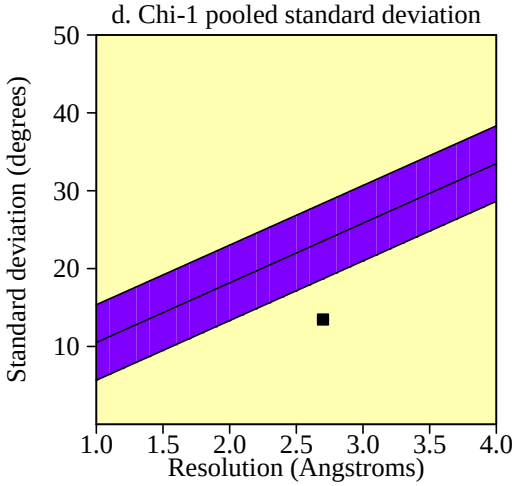
b. Chi-1 trans



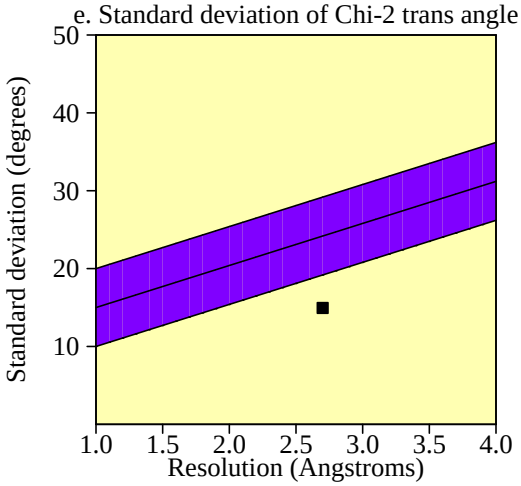
c. Chi-1 gauche plus



d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



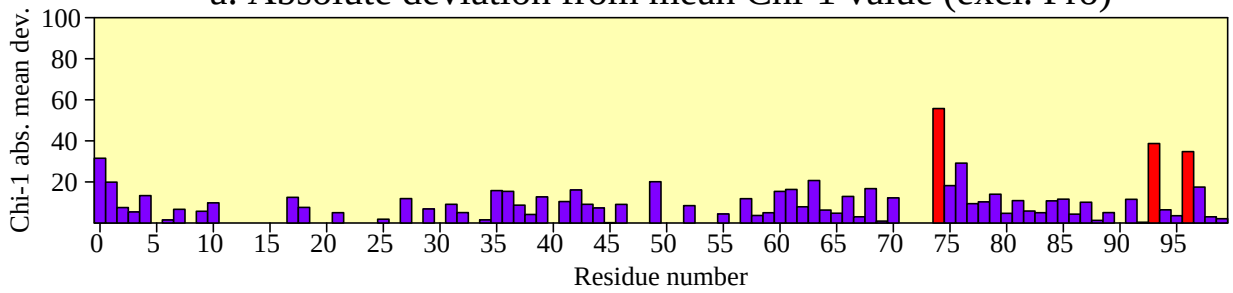
pdb1kf6

Plot statistics

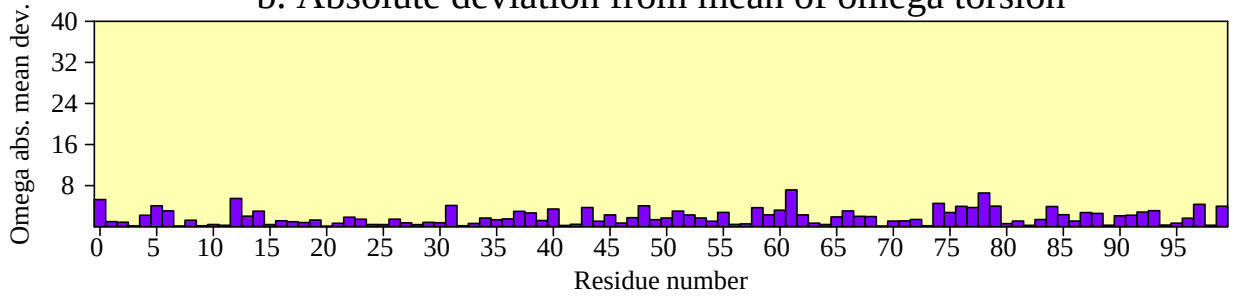
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	220	12.4	24.5	6.5	-1.9	BETTER
b. Chi-1 trans st dev	568	14.3	24.2	5.3	-1.9	BETTER
c. Chi-1 gauche plus st dev	852	13.1	22.8	4.9	-2.0	BETTER
d. Chi-1 pooled st dev	1640	13.5	23.5	4.8	-2.1	BETTER
e. Chi-2 trans st dev	505	14.9	24.2	5.0	-1.8	BETTER

Residue properties
pdb1kf6

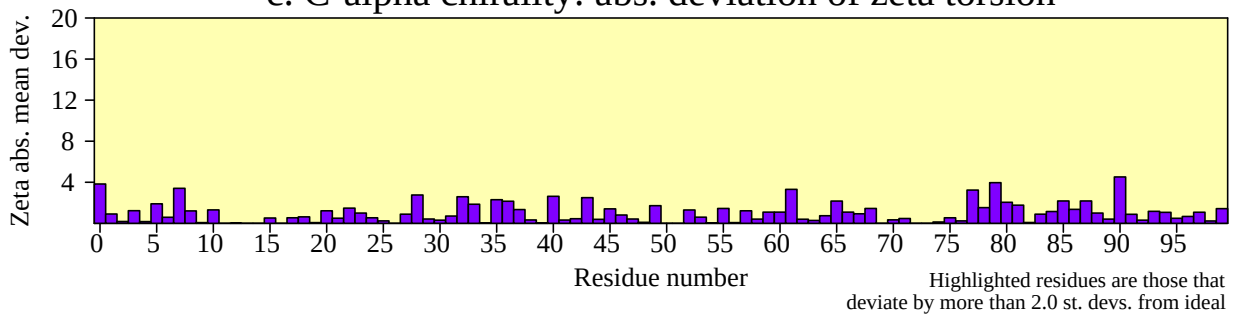
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

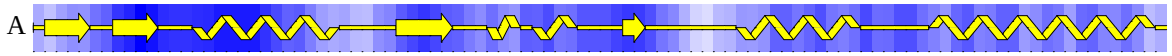


c. C-alpha chirality: abs. deviation of zeta torsion



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

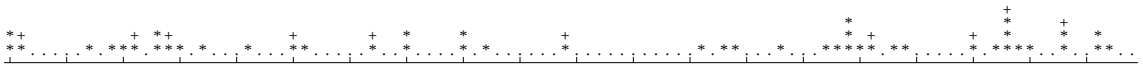
d. Secondary structure & estimated accessibility



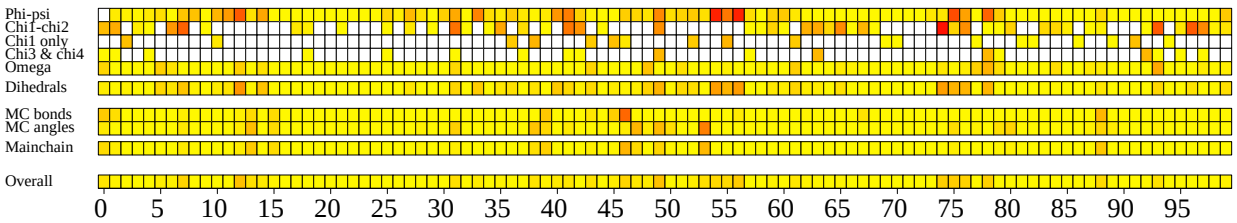
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

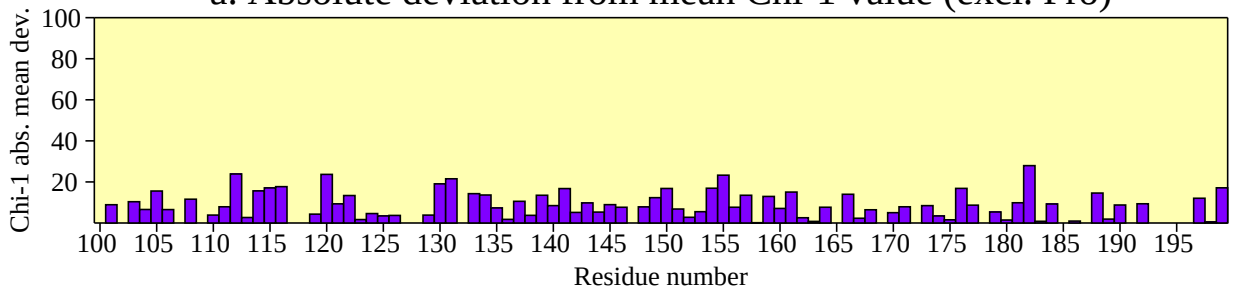


g. G-factors

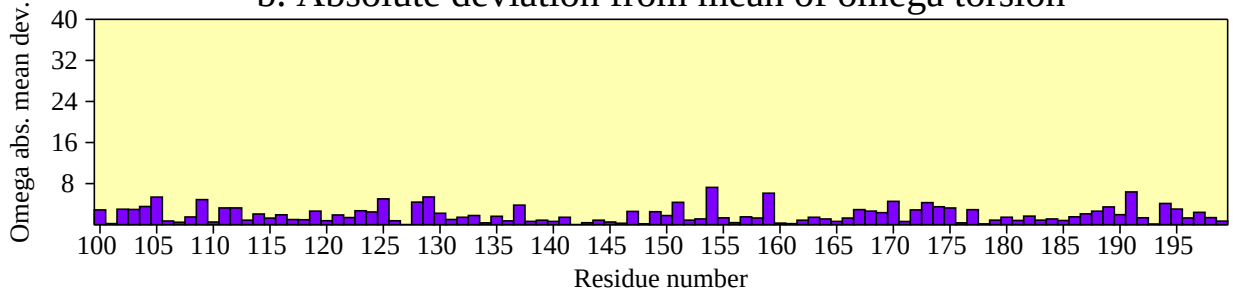


Residue properties
pdb1kf6

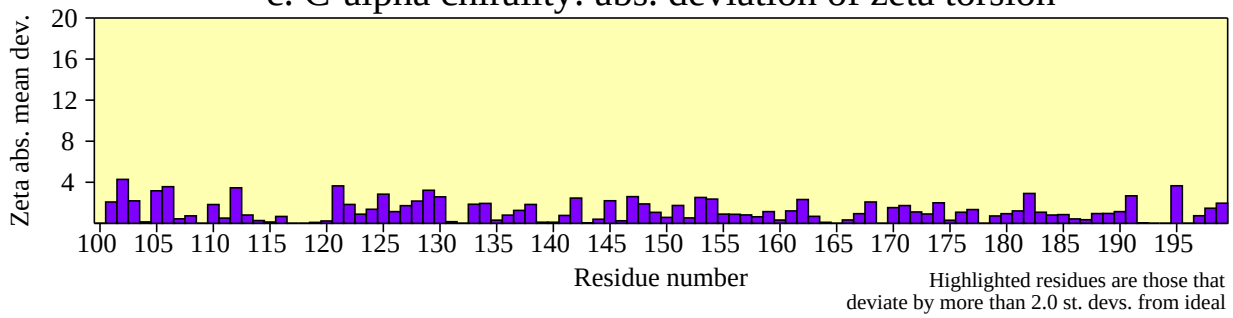
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

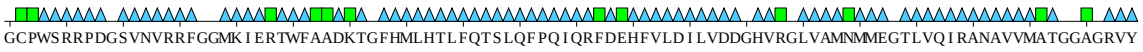


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

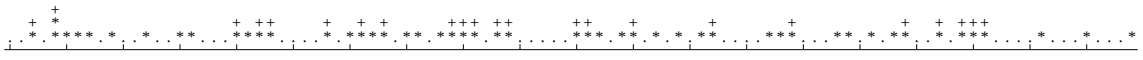
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

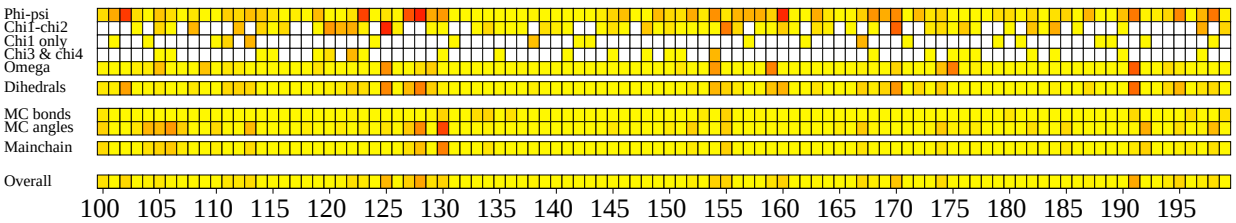


GCPWSRRPDGSVNVRRFGGMKIERTWFAADKTGFHMLHTLFQTSLQFPQIQRFDEHFVLDILVDDGHVRGLVAMNMMEGTLVQIRANAVVMATGGAGRVY

f. Max. deviation (see listing)

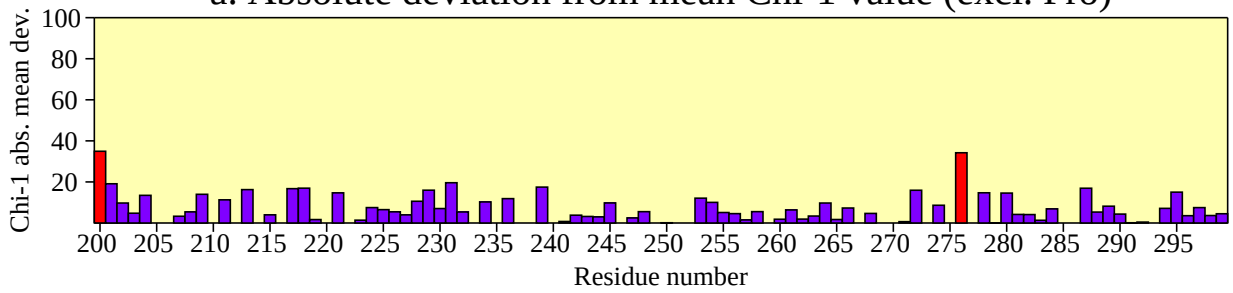


g. G-factors

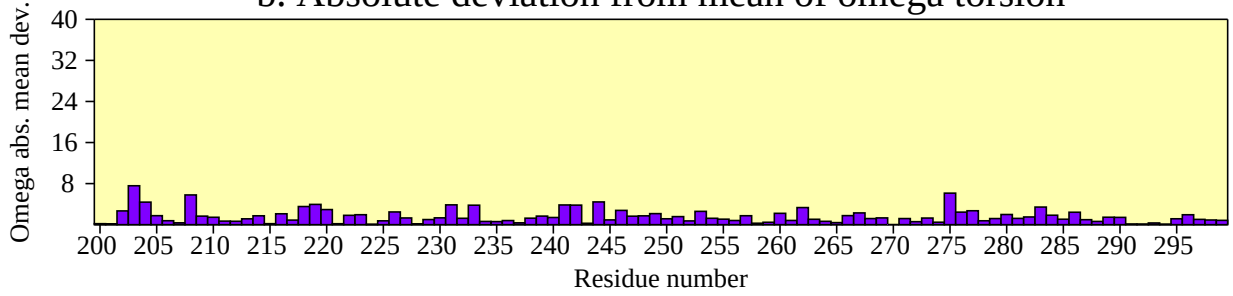


Residue properties
pdb1kf6

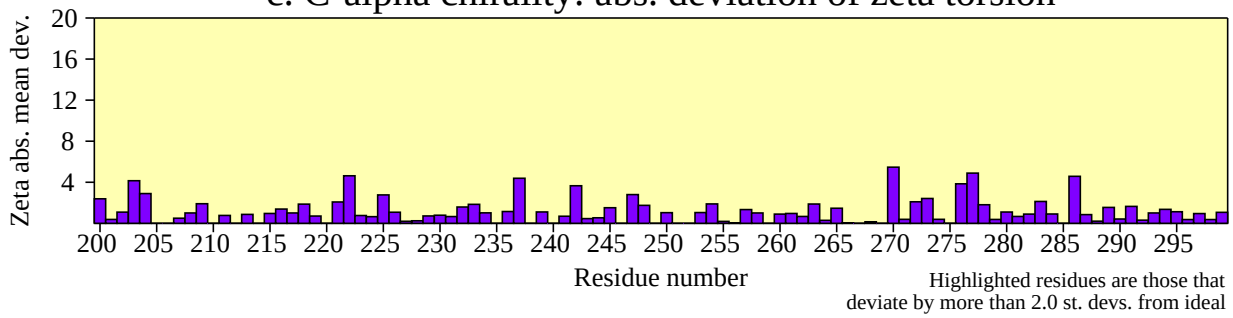
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

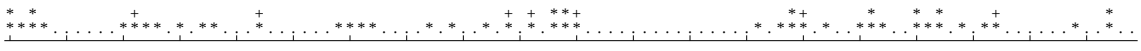
d. Secondary structure & estimated accessibility

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

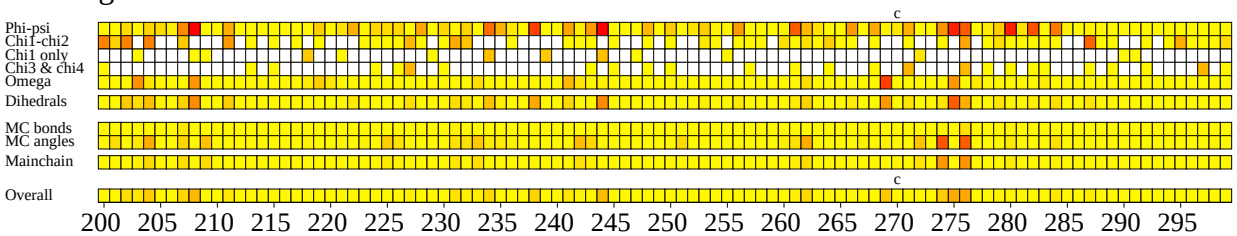
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

RYNTNGGIVTGDGMGMALSHGVPLRDMEFVQYHPTGLPGSGILMTEGCRGEGGILVNKNGYRYLQDYGMGPETPLGEPKNKYMELGPRDKVSQAFWHEWR

f. Max. deviation (see listing)



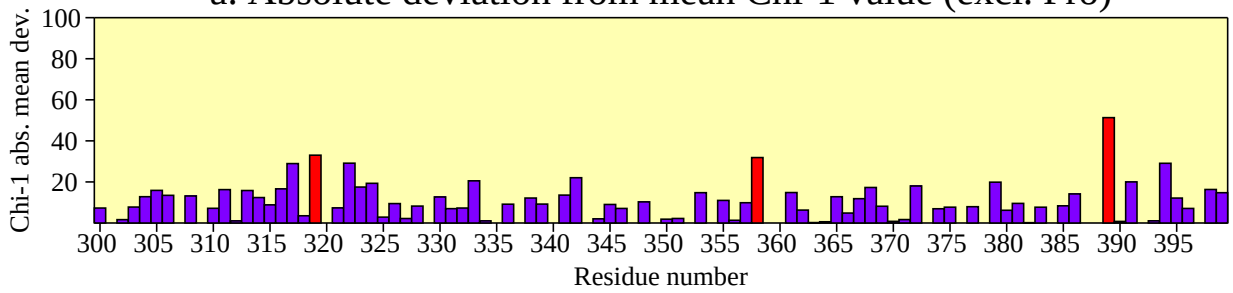
g. G-factors



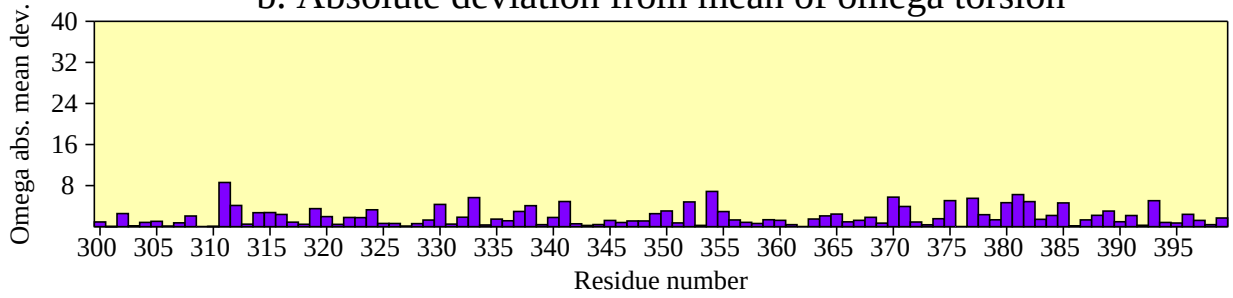
c = cis-peptide

Residue properties
pdb1kf6

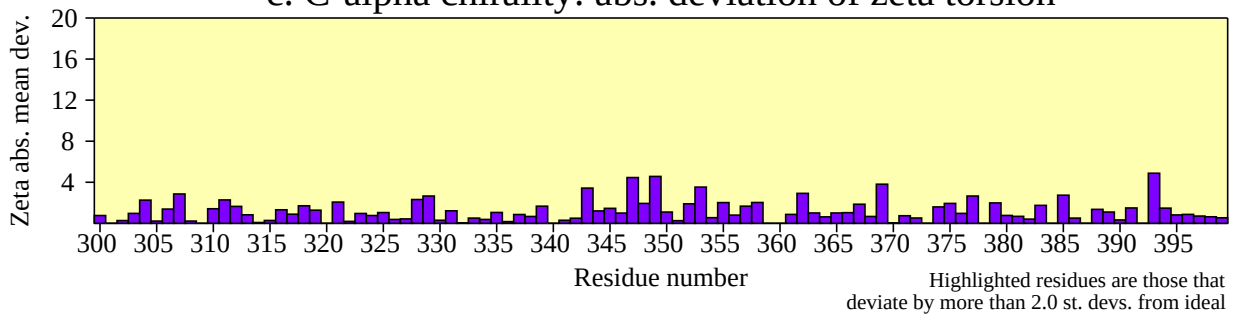
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

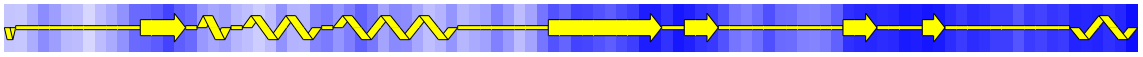


c. C-alpha chirality: abs. deviation of zeta torsion



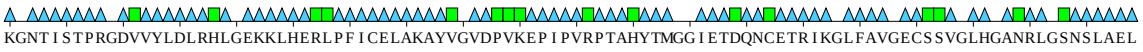
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



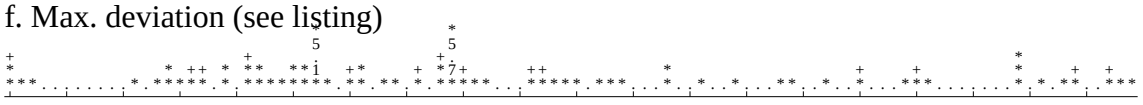
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

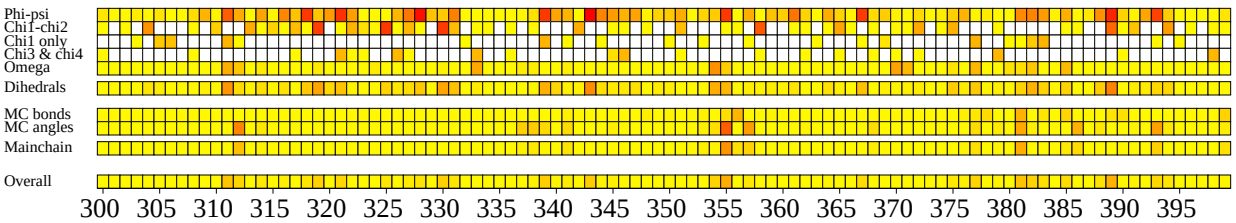


KGNT I S T P R G D V V Y L D L R H L G E K K L H E R L P F I C E L A K A Y V G V D P V K E P I P V R P T A H Y T M G G I E T D Q N C E T R I K G L F A V G E C S S V G L H G A N R L G S N S L A E L

f. Max. deviation (see listing)

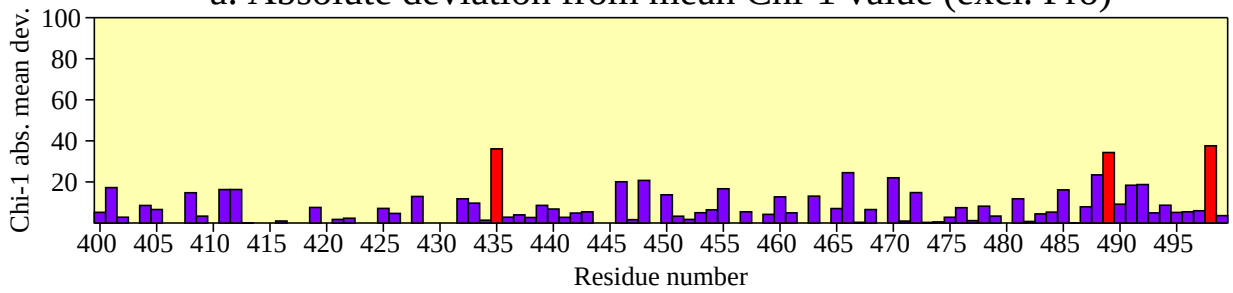


g. G-factors

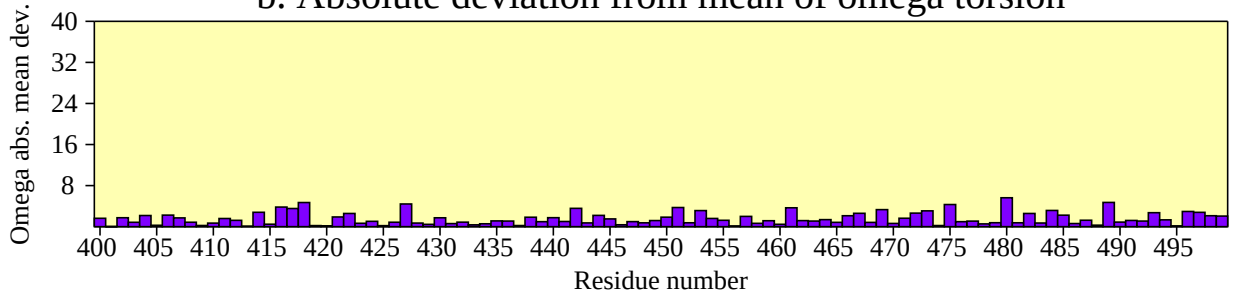


Residue properties
pdb1kf6

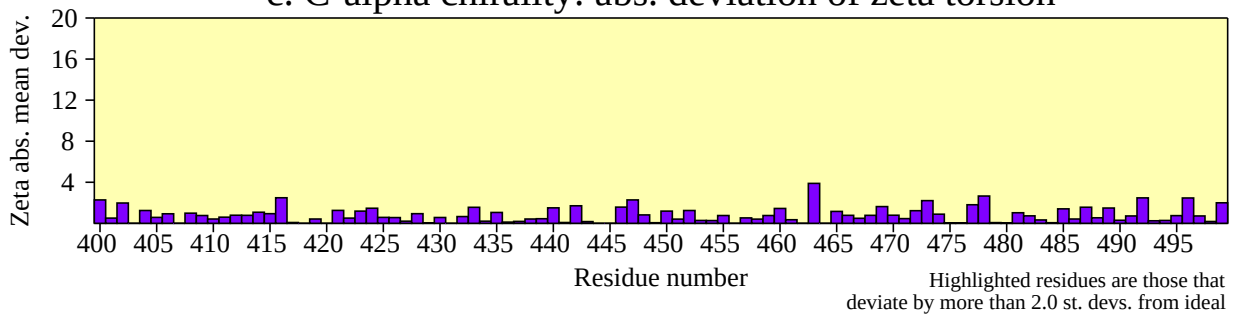
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



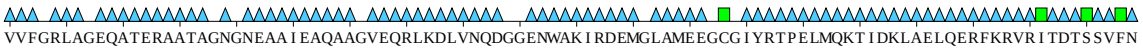
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

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

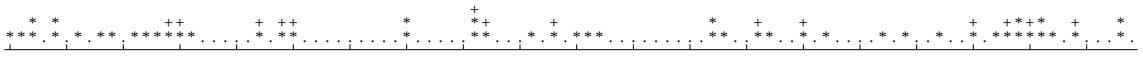
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

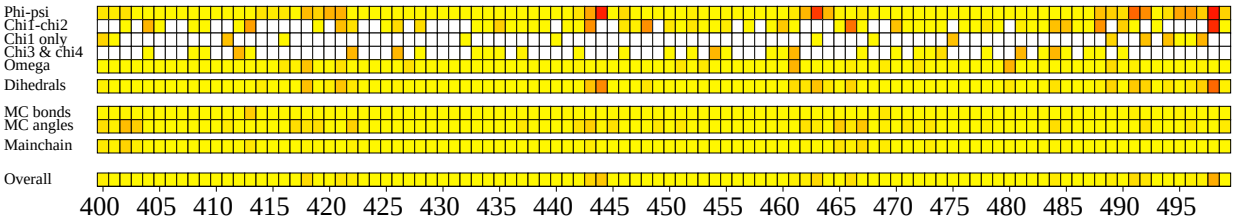


VVFGRLAGEQATERAATAGNGNEAAIEAQAAGVEQRLKDLVNQDGGENWAKIRDEMGLAMEEGCGIYRTPELMQKTIDKLAELQERFKRVRITDTSSVFN

f. Max. deviation (see listing)

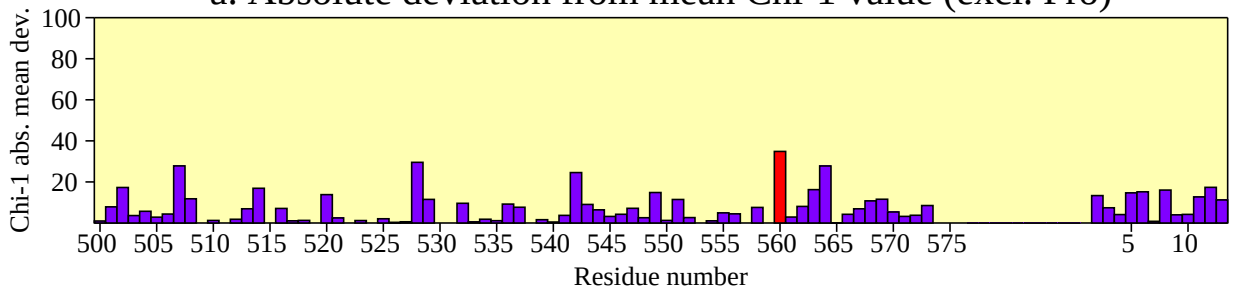


g. G-factors

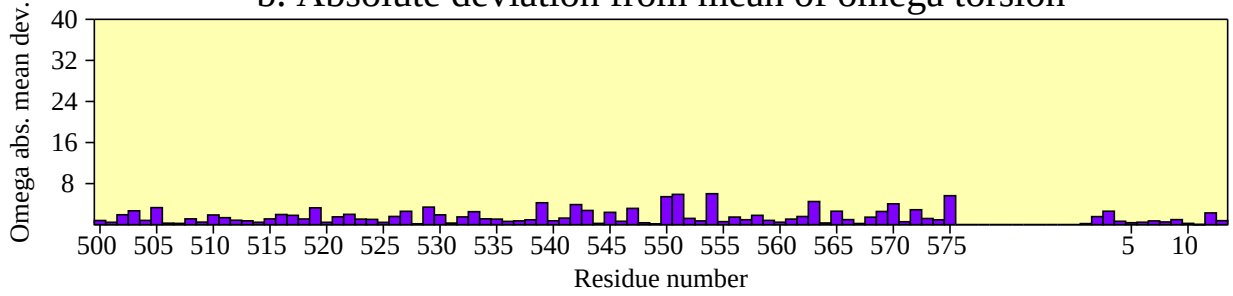


Residue properties
pdb1kf6

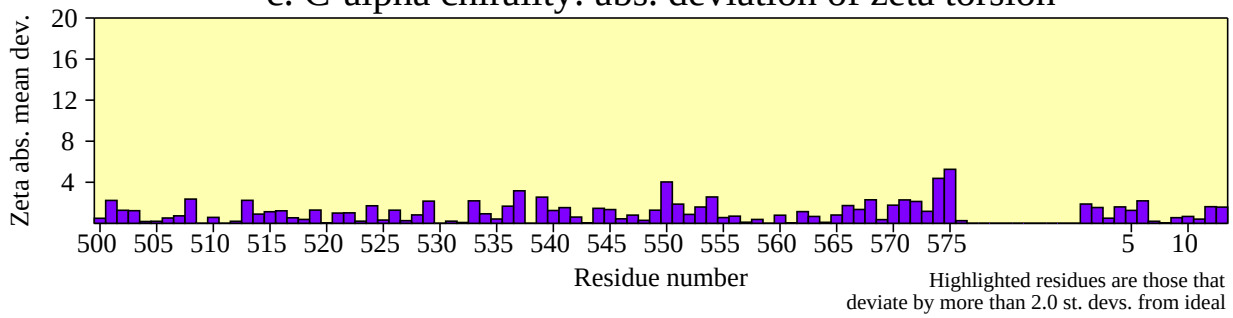
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

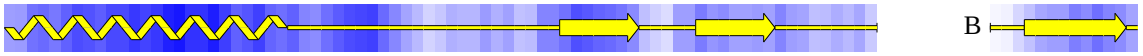


c. C-alpha chirality: abs. deviation of zeta torsion



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

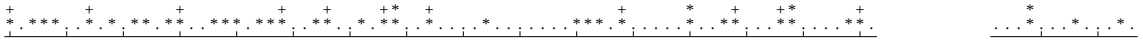
d. Secondary structure & estimated accessibility



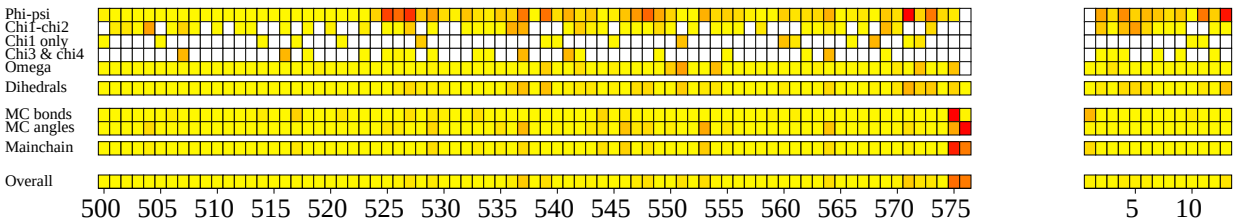
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

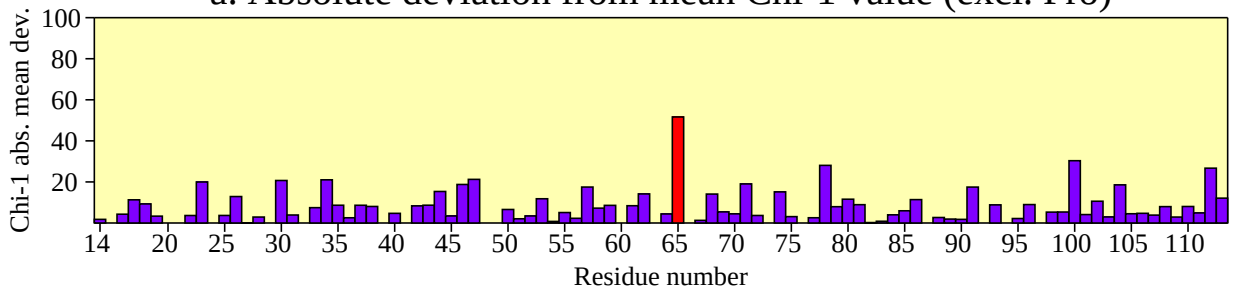


g. G-factors

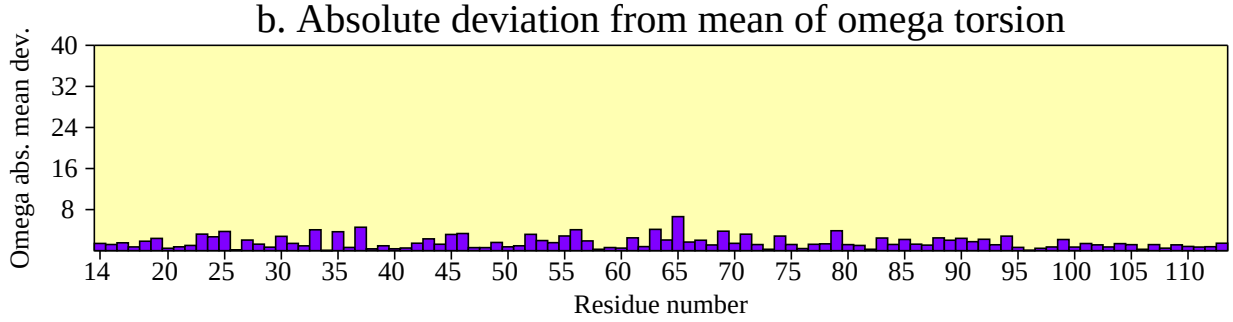


Residue properties
pdb1kf6

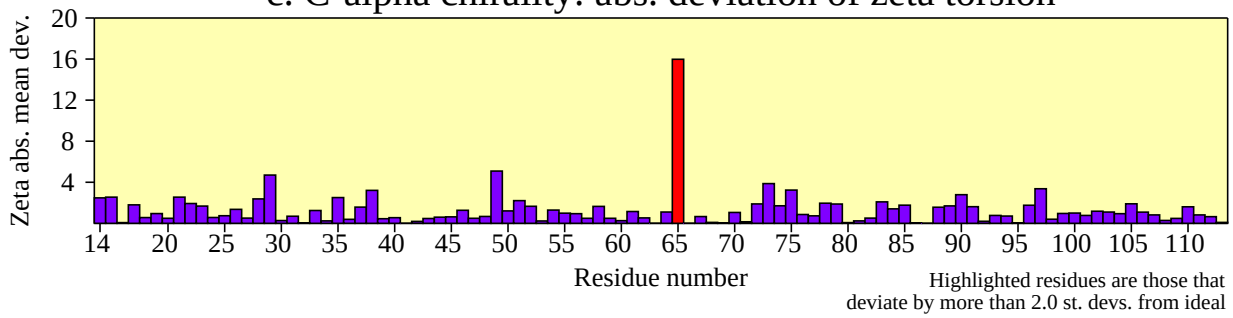
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

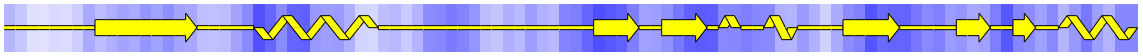


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



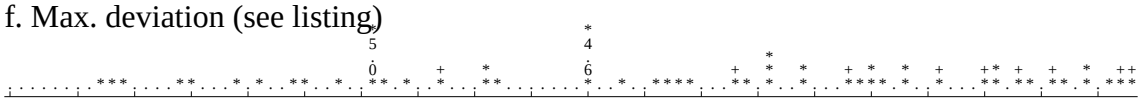
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

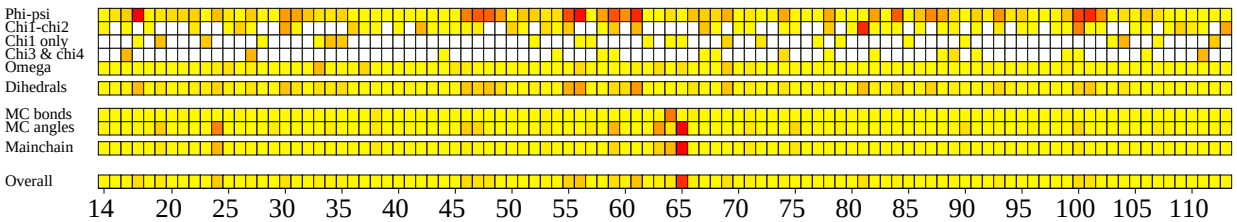
Most favoured Allowed Generous Disallowed

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)

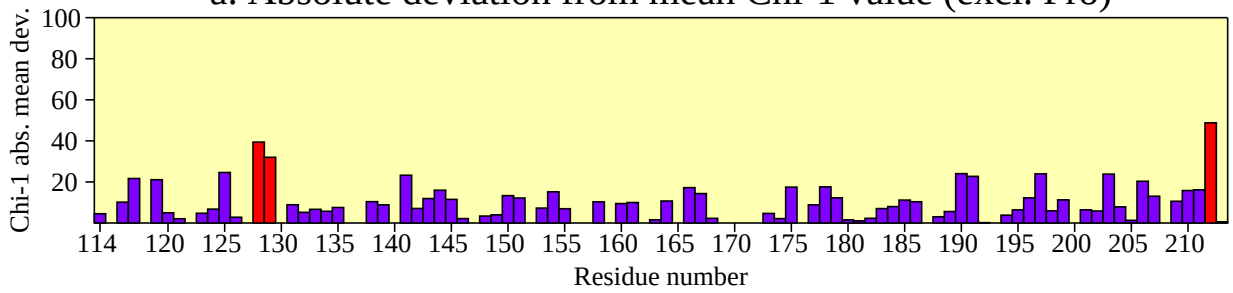


g. G-factors

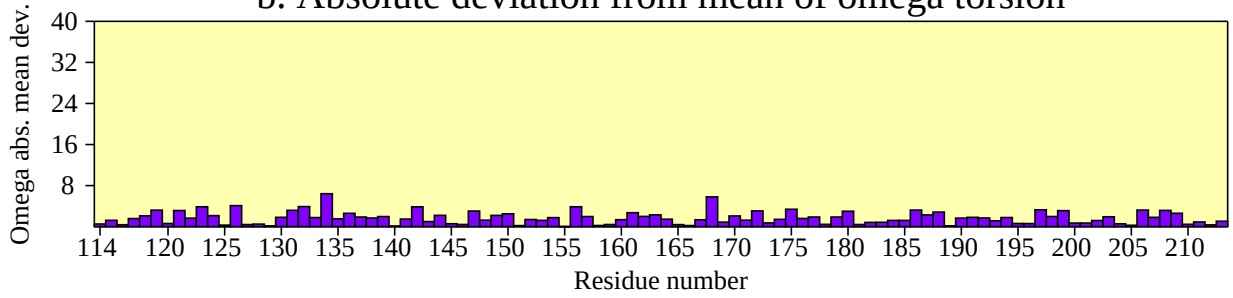


Residue properties
pdb1kf6

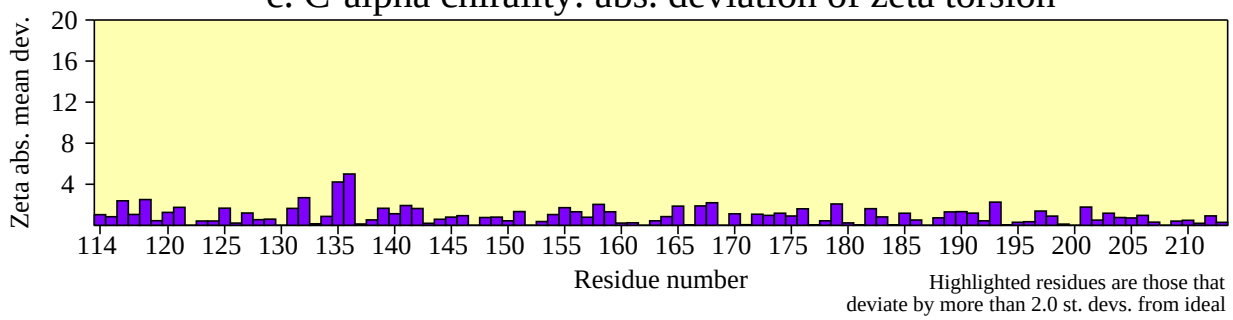
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

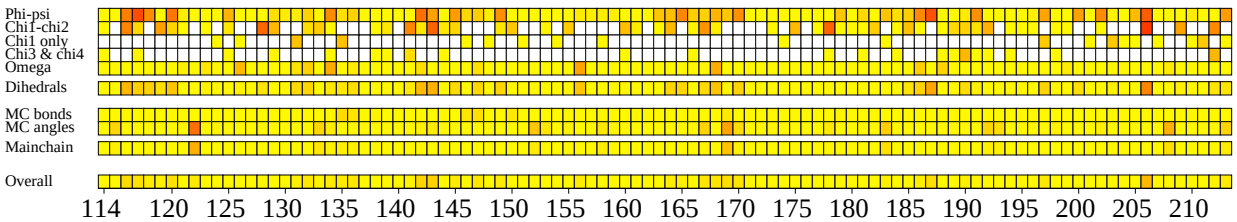
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

EAIKPYIIGNSRTADQGTNIQTPAQMAKYHQFSGCINCGLCYAACPQFGLNPEFIGPAAITLAHRYNEDSRDHGKKERMAQLNSQNGVWSCTFVGYCSEV

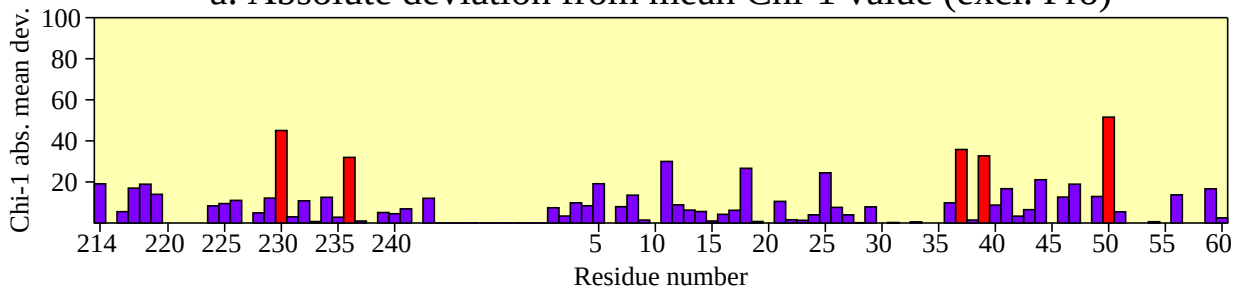
f. Max. deviation (see listing)

g. G-factors

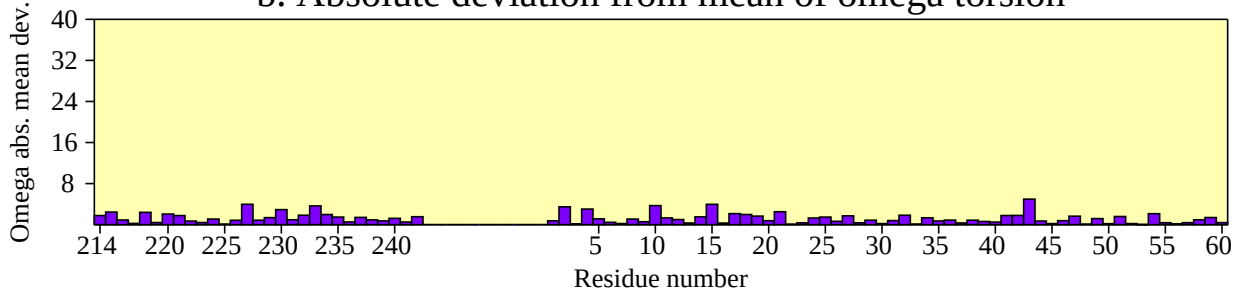


Residue properties
pdb1kf6

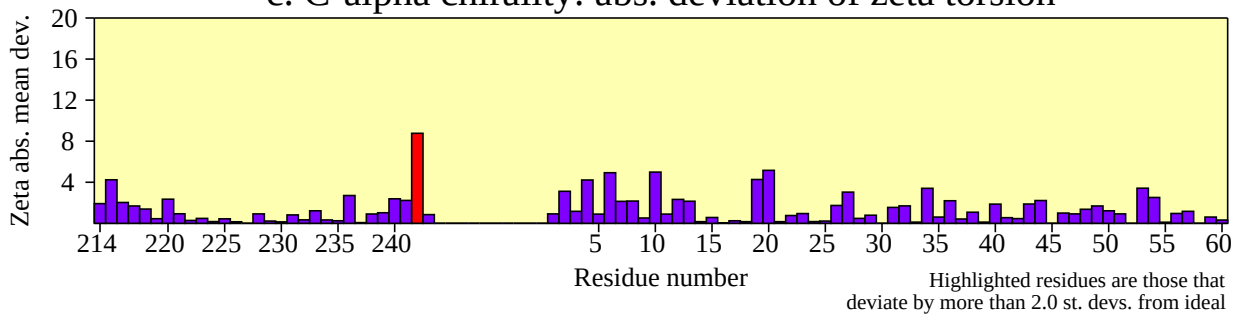
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

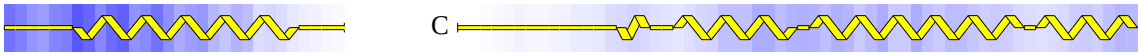


c. C-alpha chirality: abs. deviation of zeta torsion



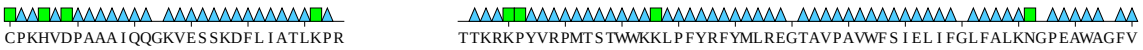
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

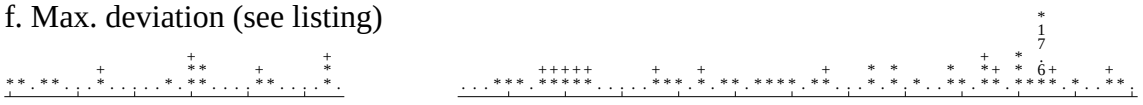


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

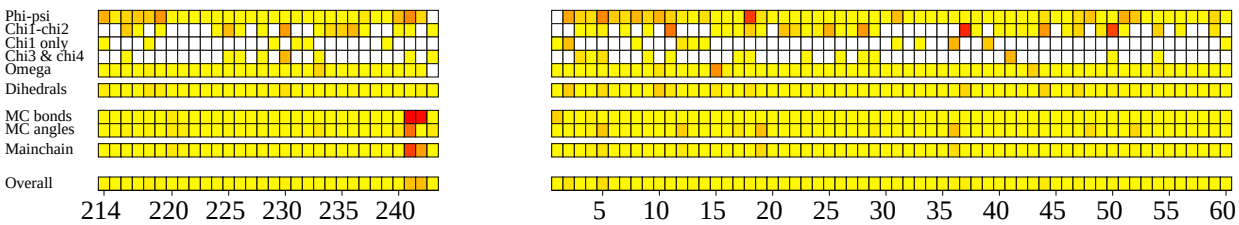
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

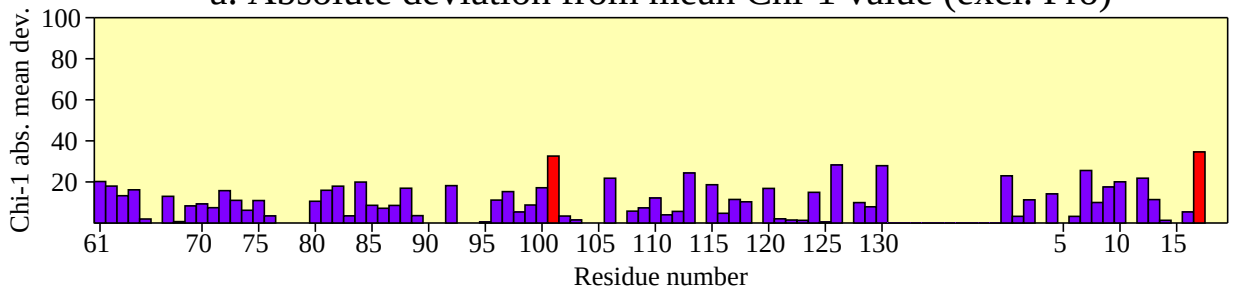


g. G-factors

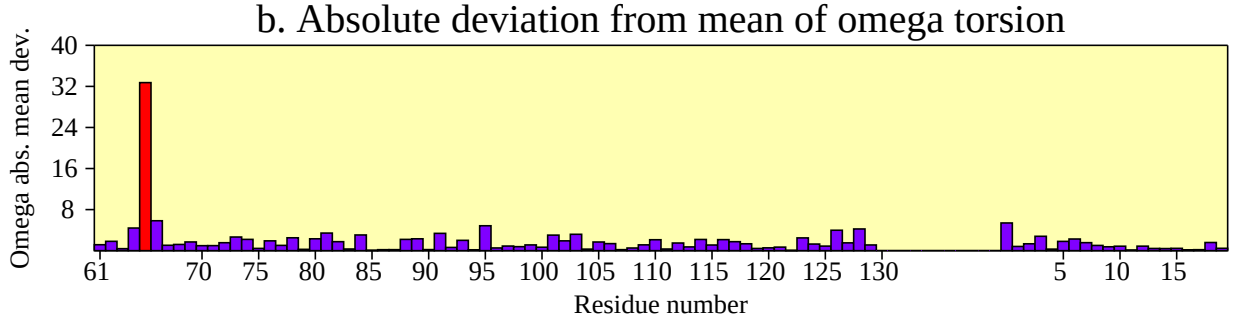


Residue properties
pdb1kf6

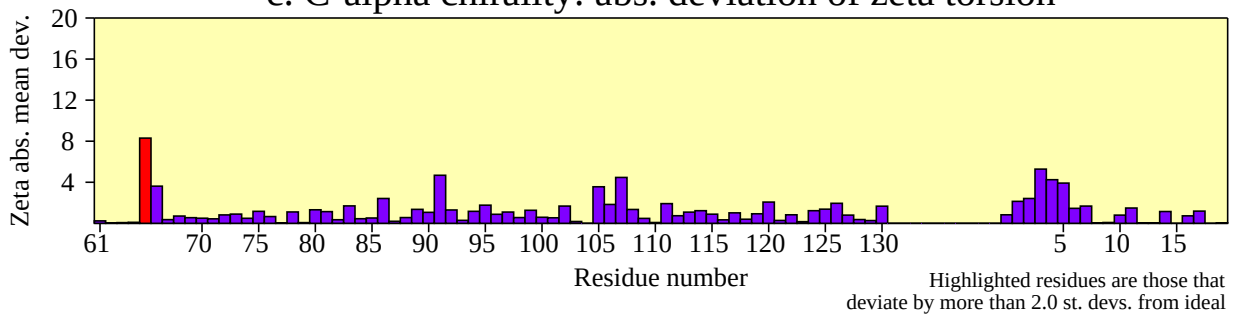
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



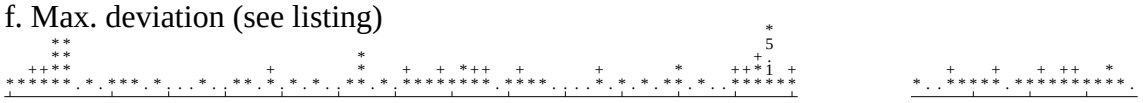
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

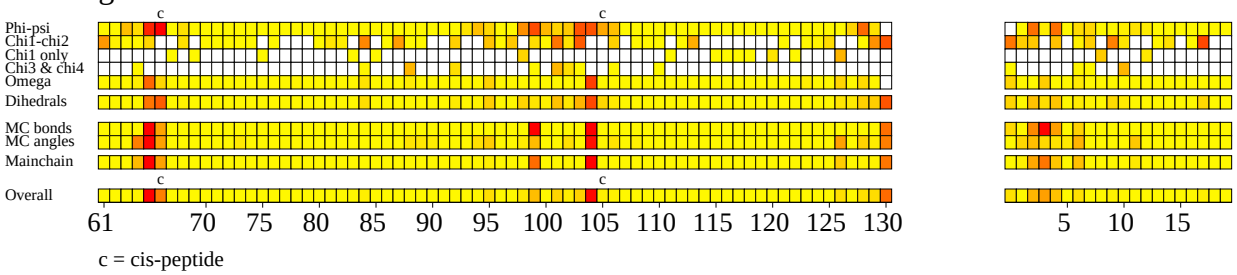
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)



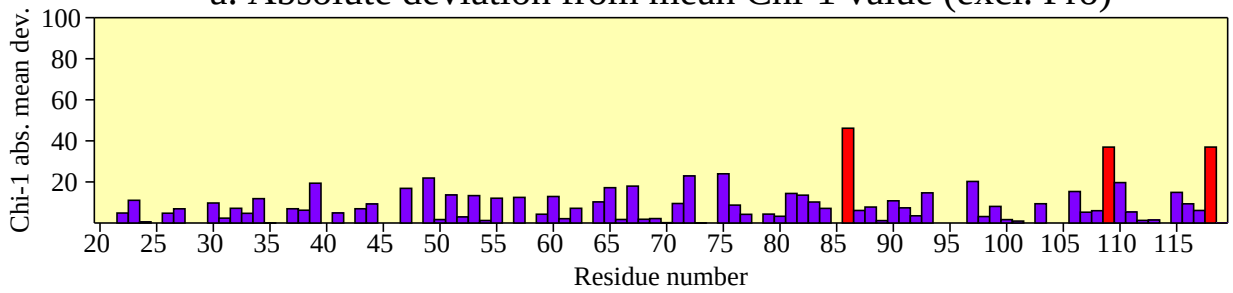
g. G-factors



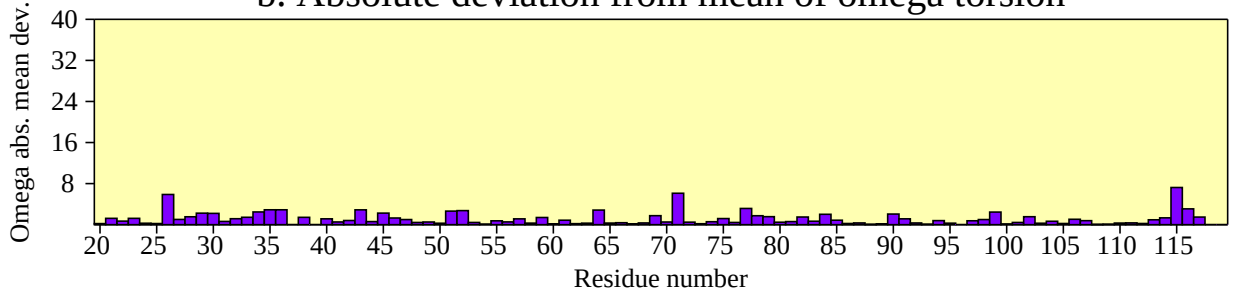
c = cis-peptide

Residue properties
pdb1kf6

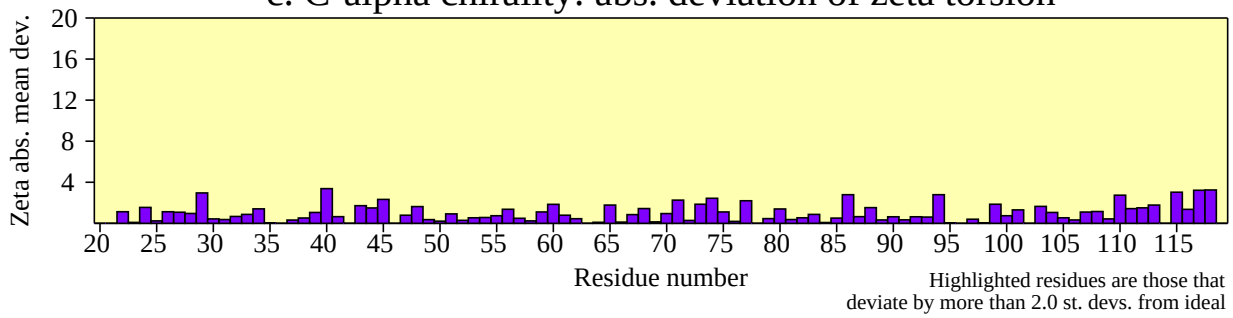
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

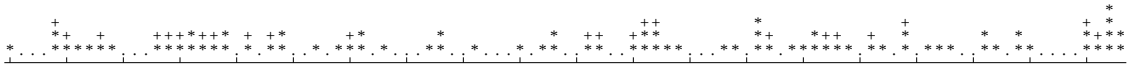
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

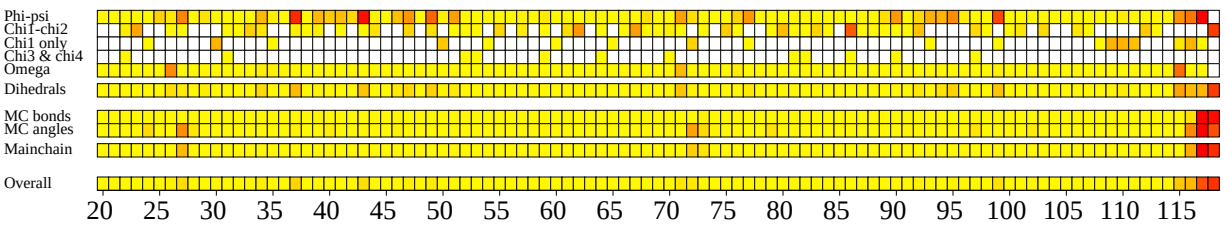
Most favoured Allowed Generous Disallowed

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)

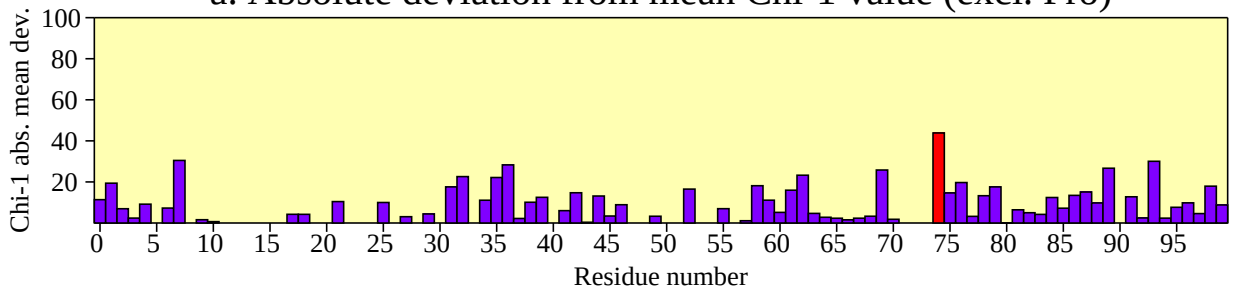


g. G-factors

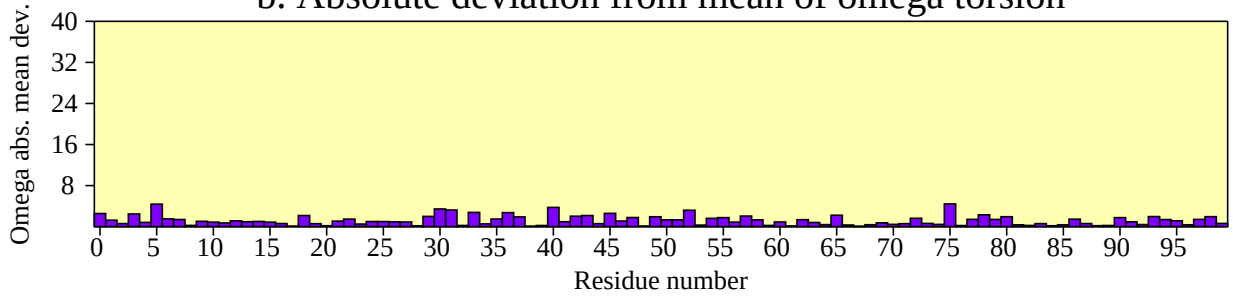


Residue properties
pdb1kf6

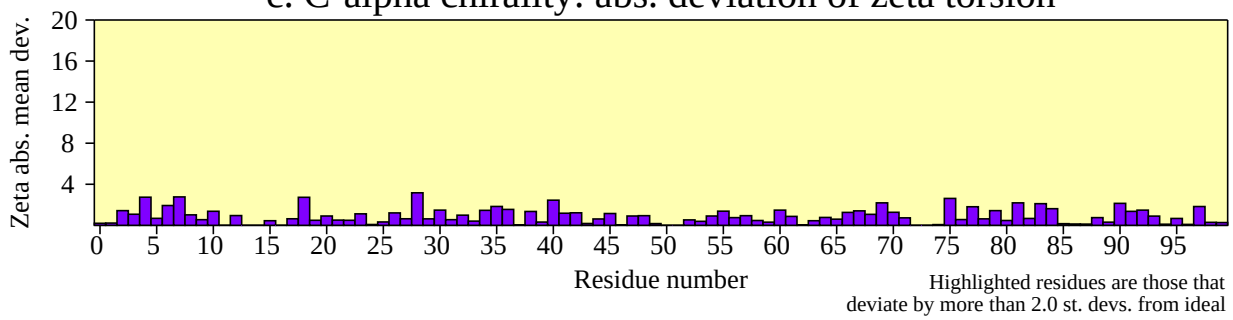
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

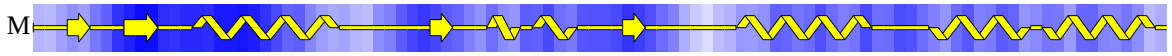


c. C-alpha chirality: abs. deviation of zeta torsion



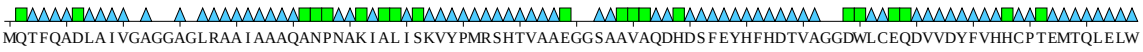
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

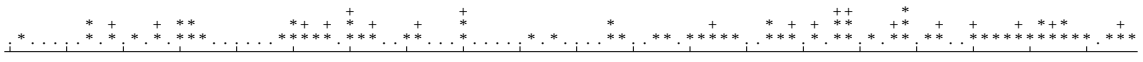


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

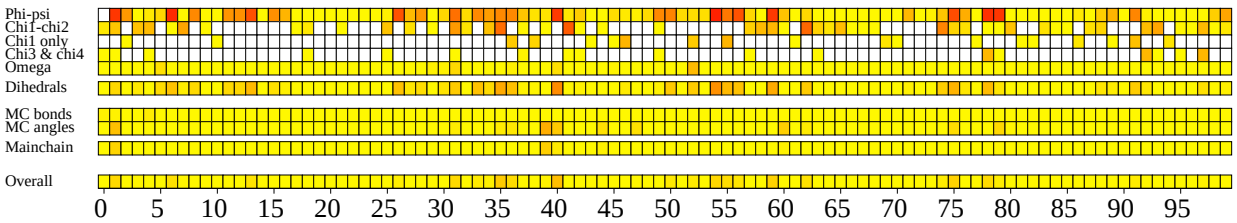
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

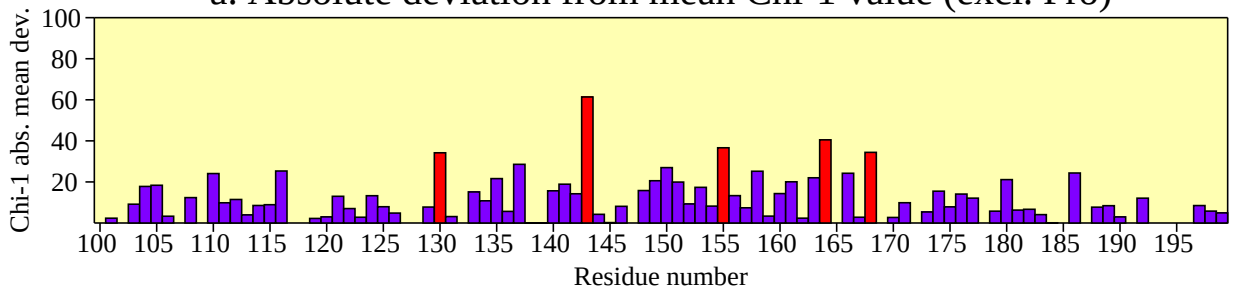


g. G-factors

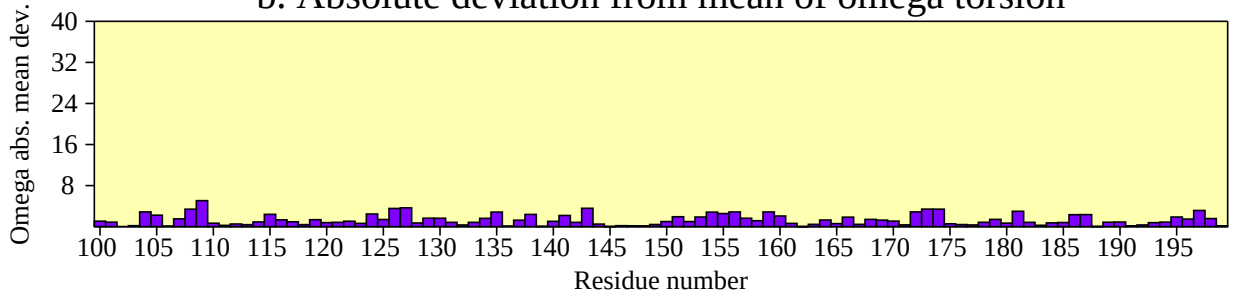


Residue properties
pdb1kf6

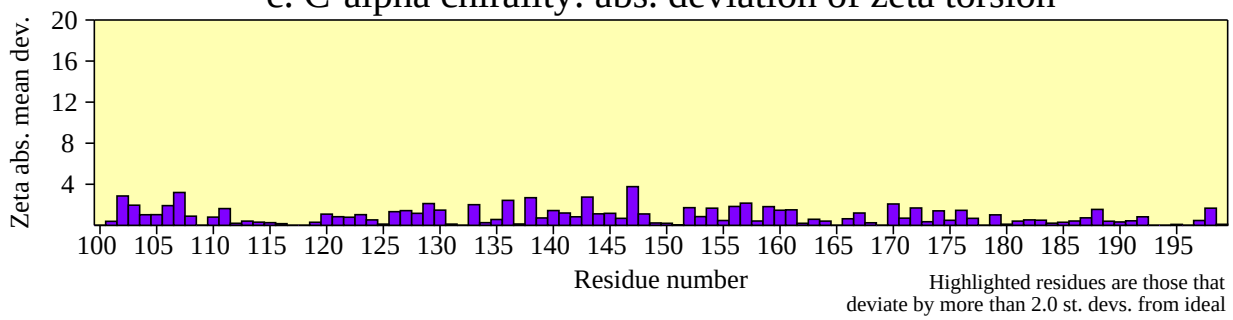
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

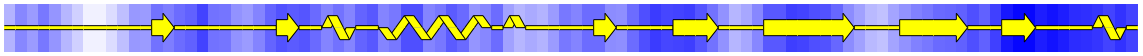


c. C-alpha chirality: abs. deviation of zeta torsion



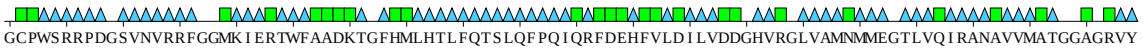
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

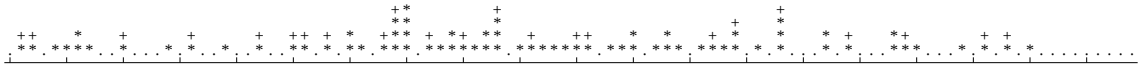


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

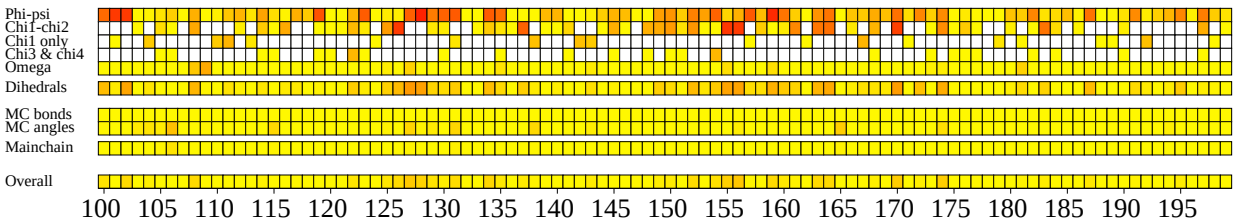
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

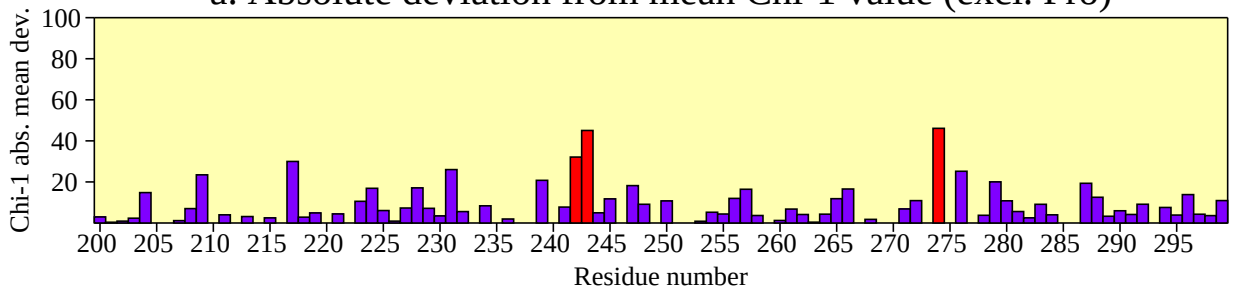


g. G-factors

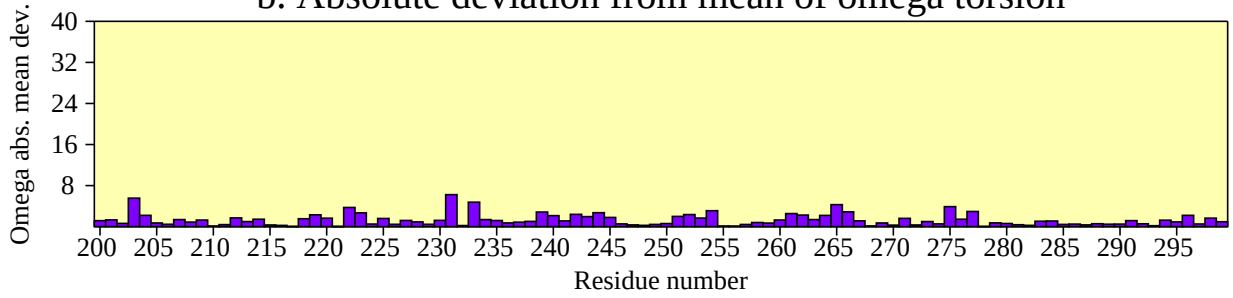


Residue properties
pdb1kf6

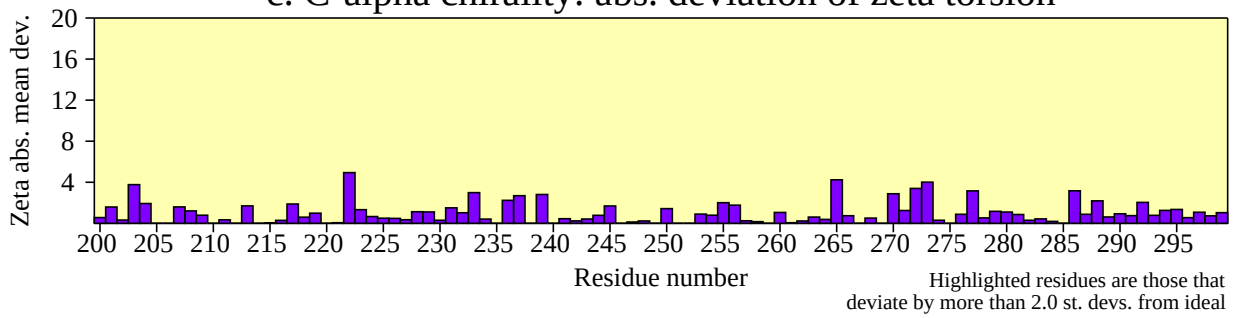
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

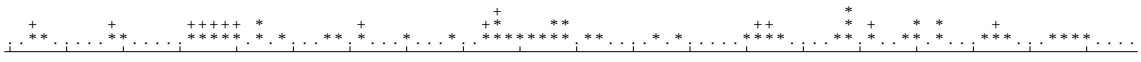
d. Secondary structure & estimated accessibility

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

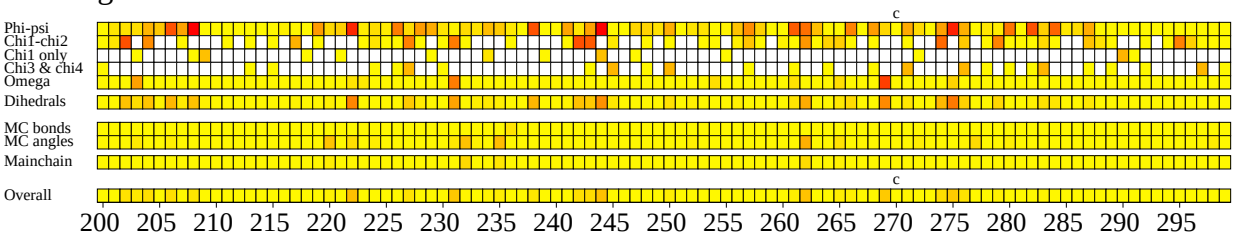
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

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 FWHEWR

f. Max. deviation (see listing)



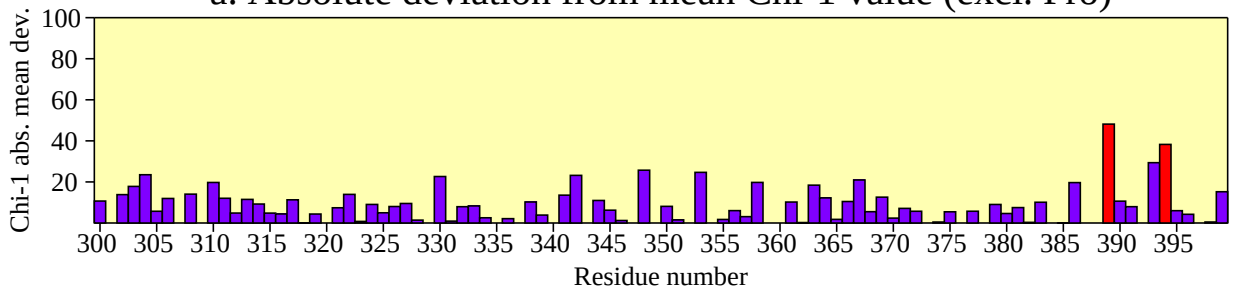
g. G-factors



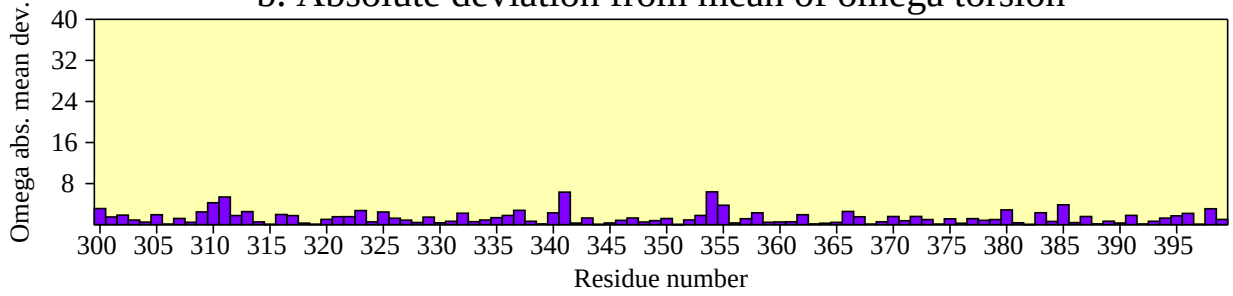
c = cis-peptide

Residue properties
pdb1kf6

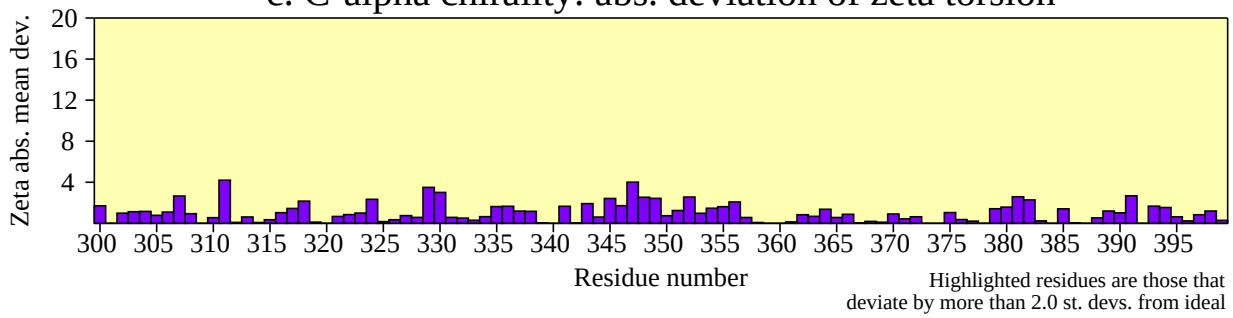
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

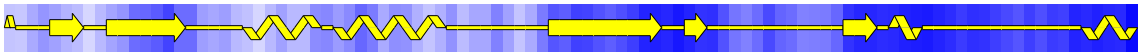


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

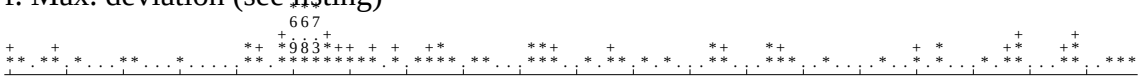


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

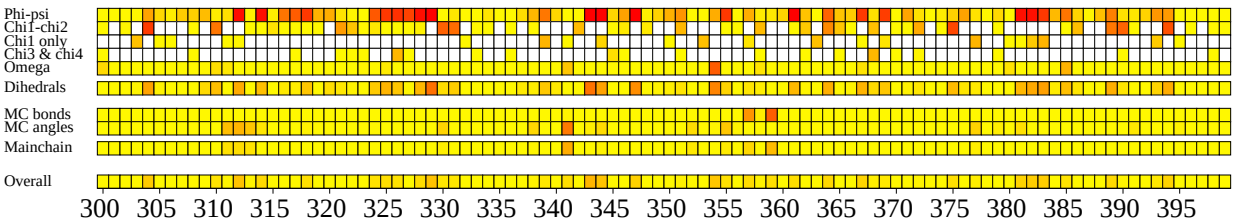
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

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)

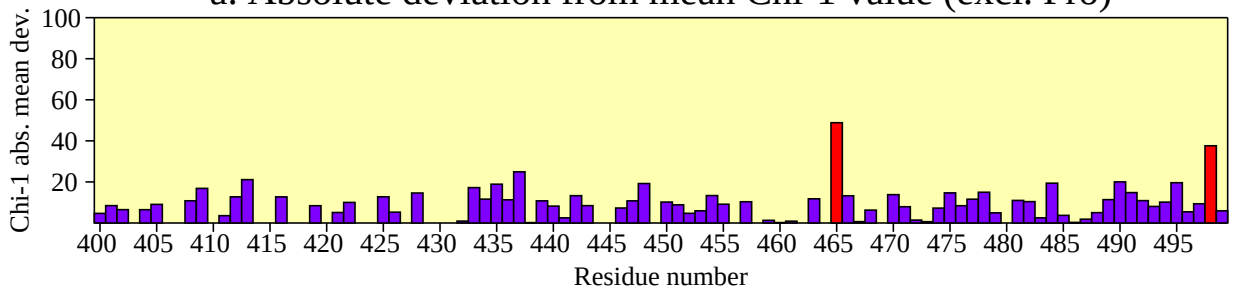


g. G-factors

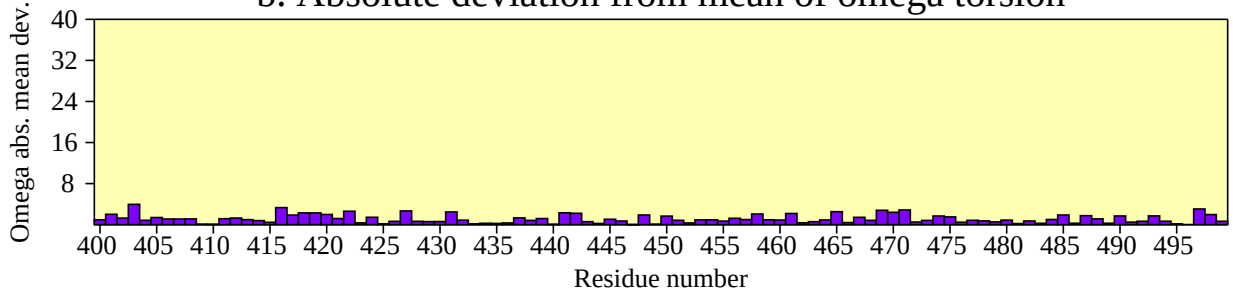


Residue properties
pdb1kf6

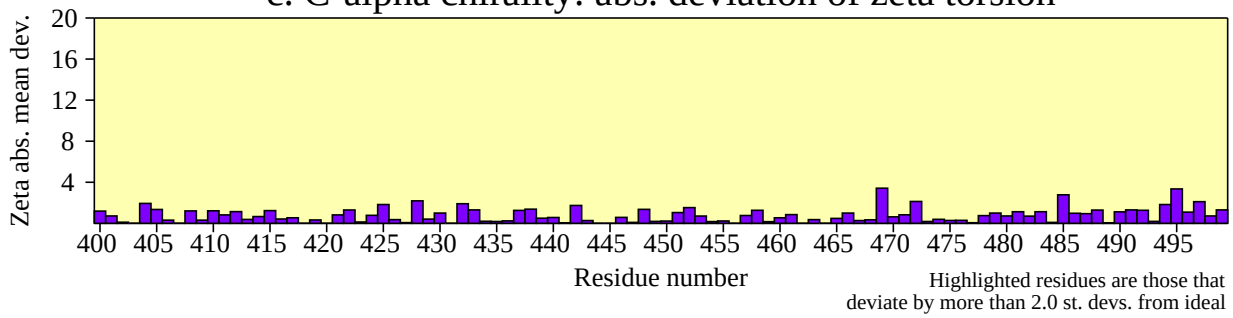
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

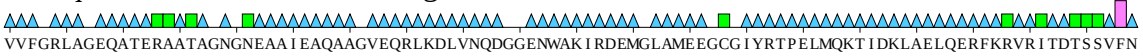


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

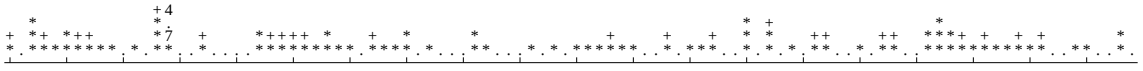
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

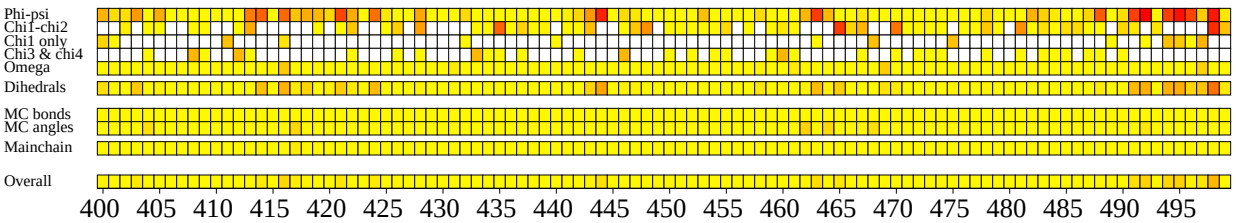


VVFGRLAGEQATERAATAGNGNEAAIEAQAAGVEQRLKDLVNQDGGENWAKIRDEMGLAMEEGCGIYRTPELMQKTIDKLAELQERFKRVRITDTSSVFN

f. Max. deviation (see listing)

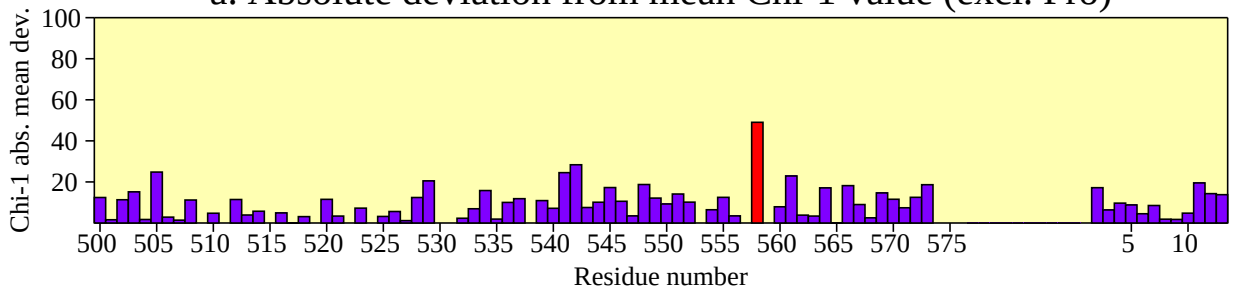


g. G-factors

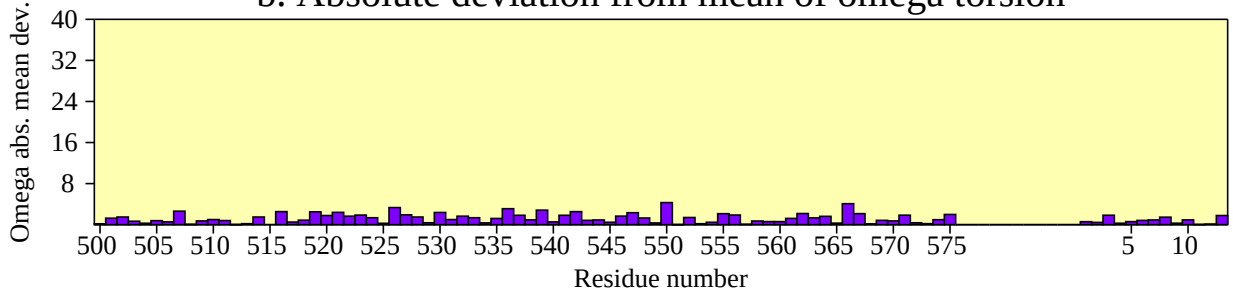


Residue properties
pdb1kf6

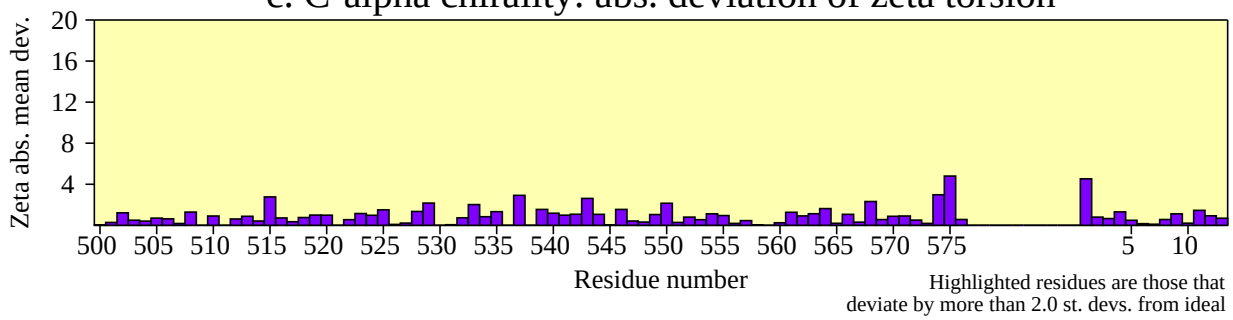
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



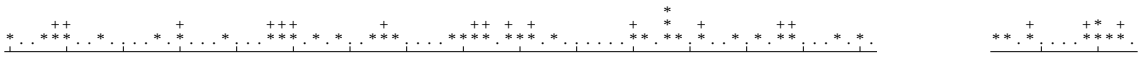
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

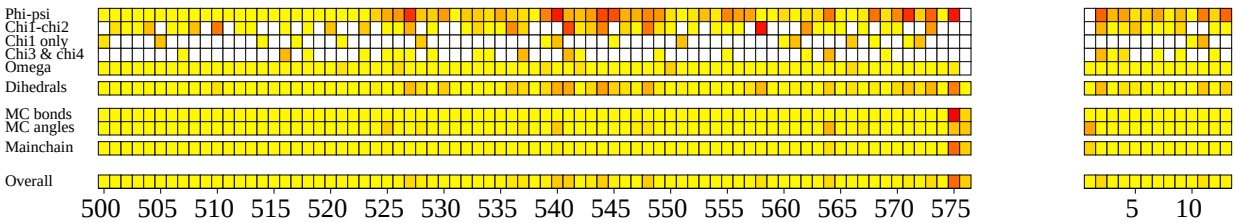
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

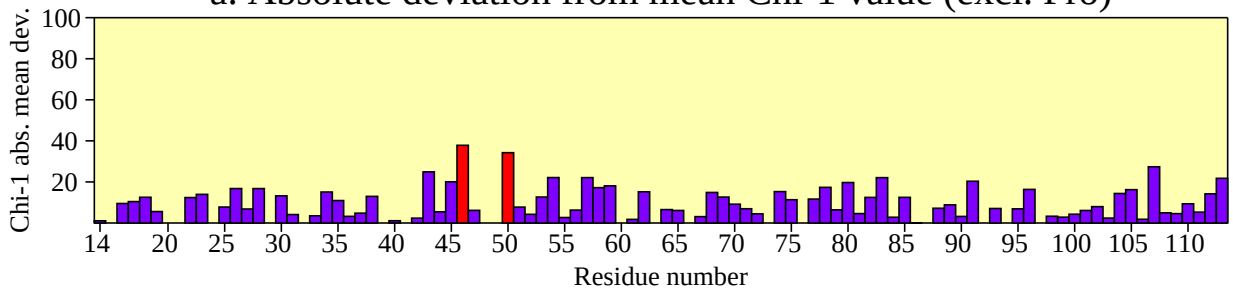


g. G-factors

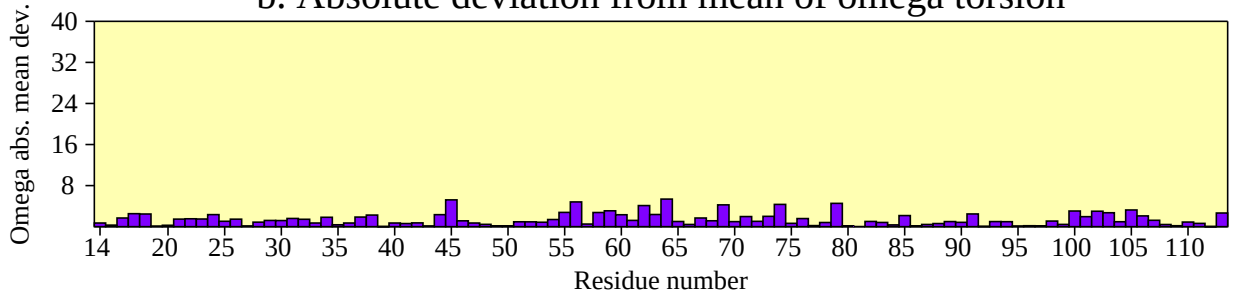


Residue properties
pdb1kf6

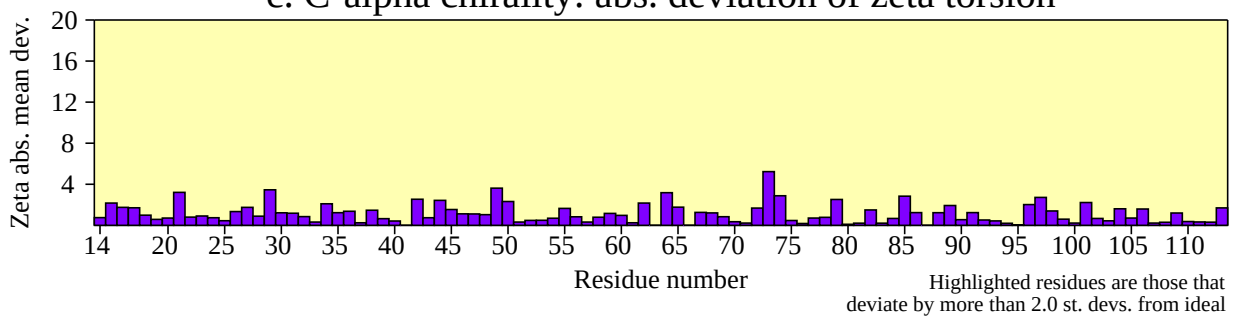
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

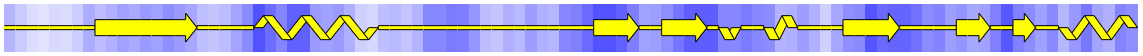


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

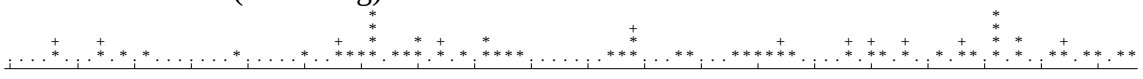


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

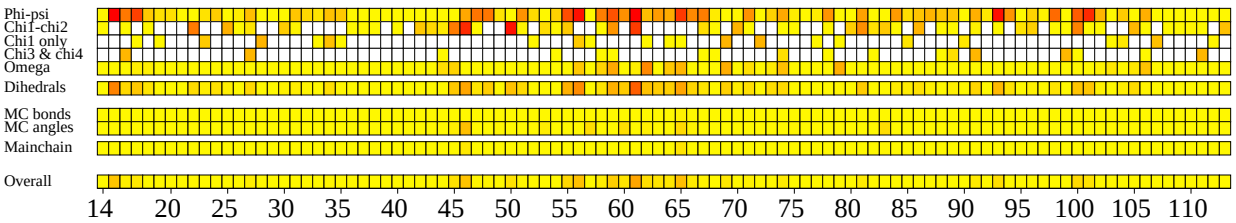
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

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)

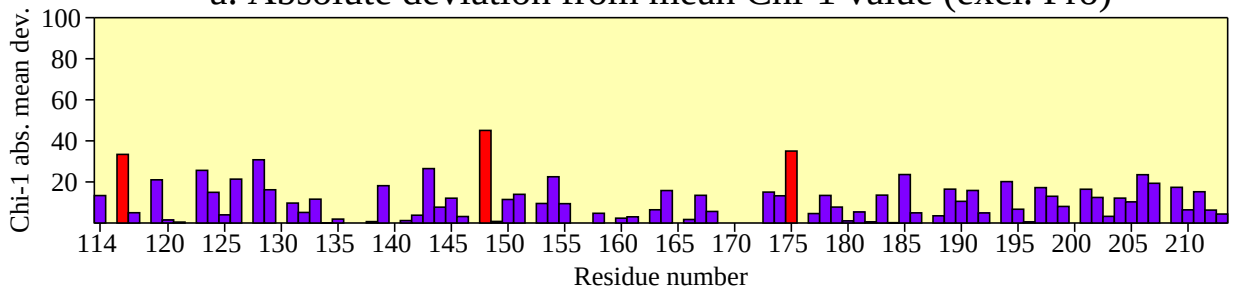


g. G-factors

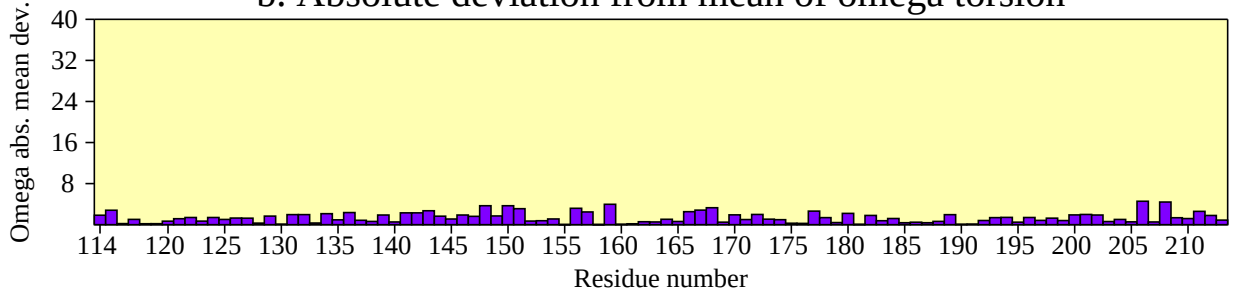


Residue properties
pdb1kf6

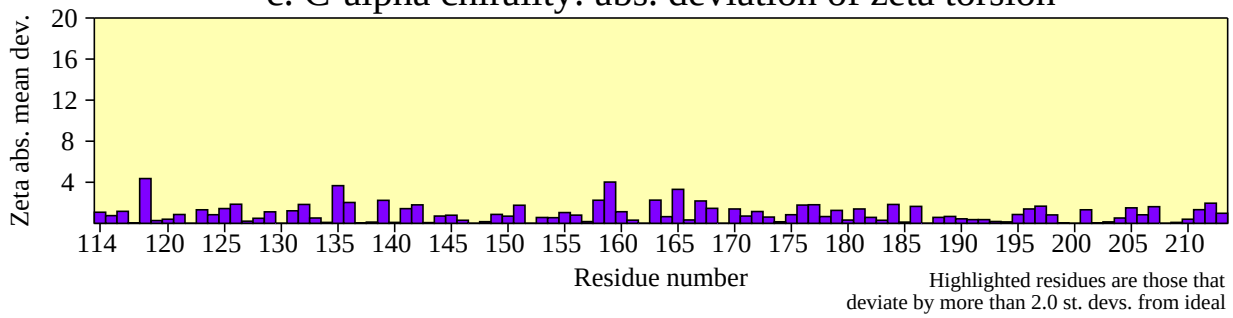
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

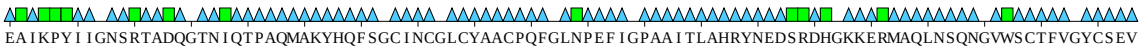


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

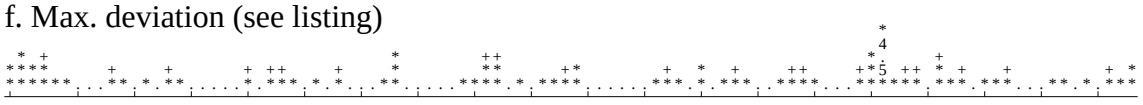
d. Secondary structure & estimated accessibility

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

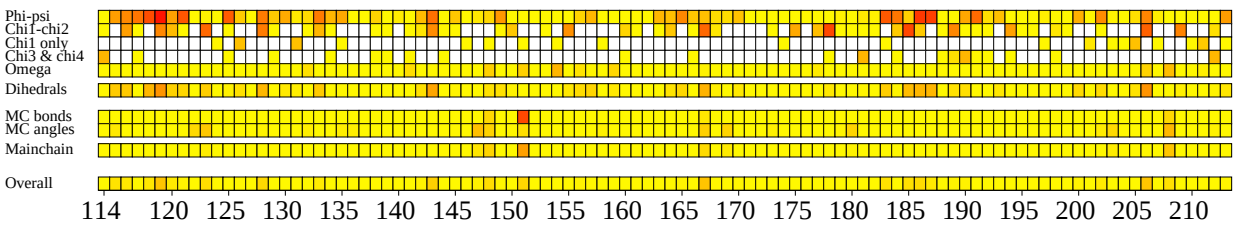
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

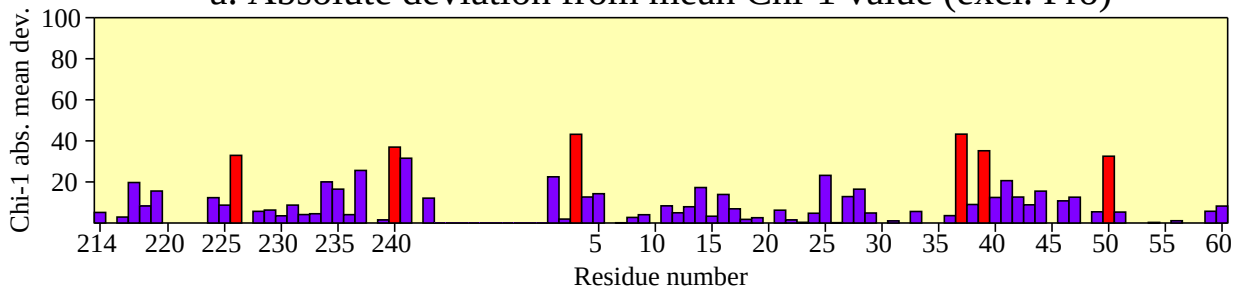


g. G-factors

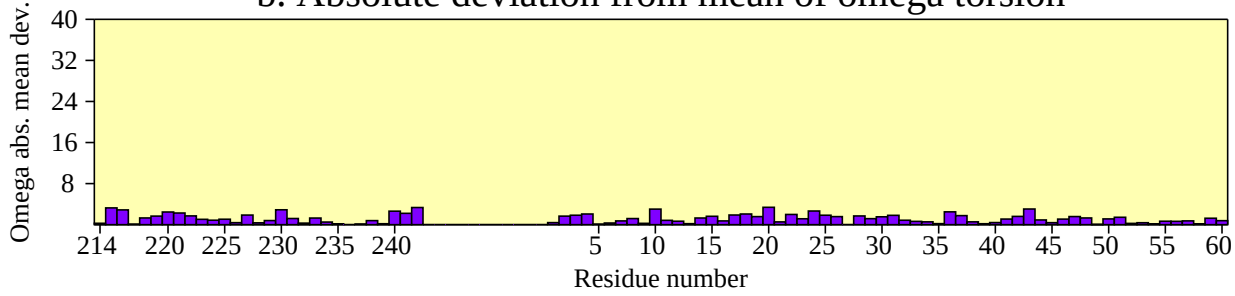


Residue properties
pdb1kf6

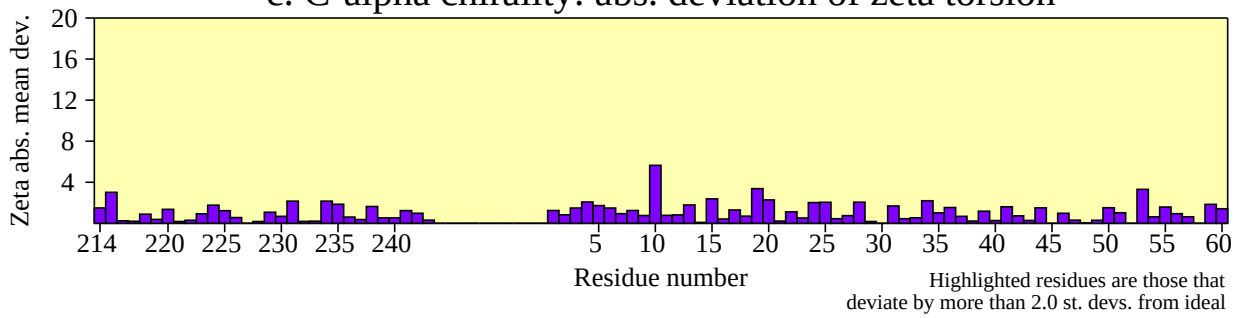
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

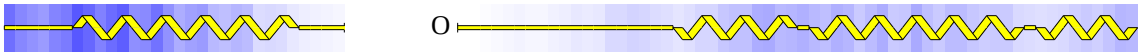


c. C-alpha chirality: abs. deviation of zeta torsion

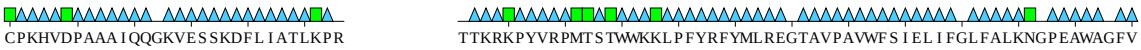


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

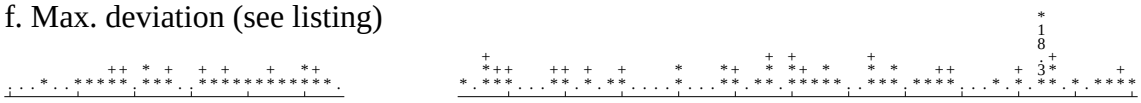
d. Secondary structure & estimated accessibility



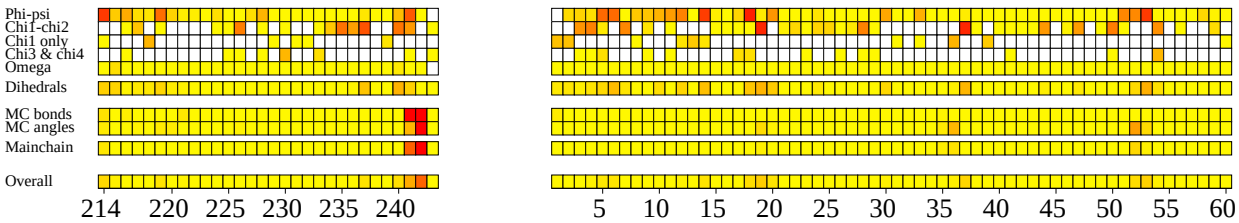
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

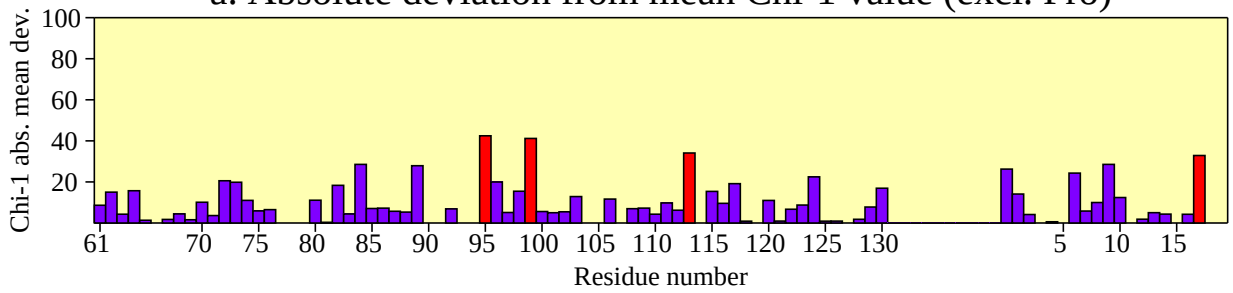


g. G-factors

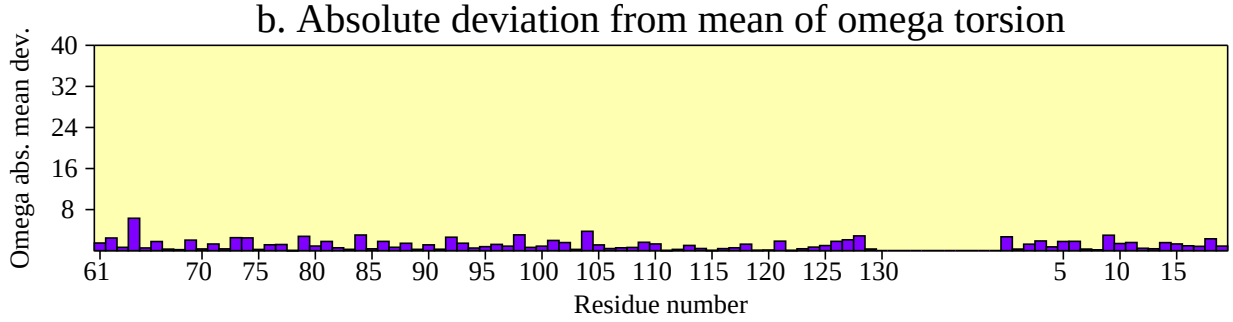


Residue properties
pdb1kf6

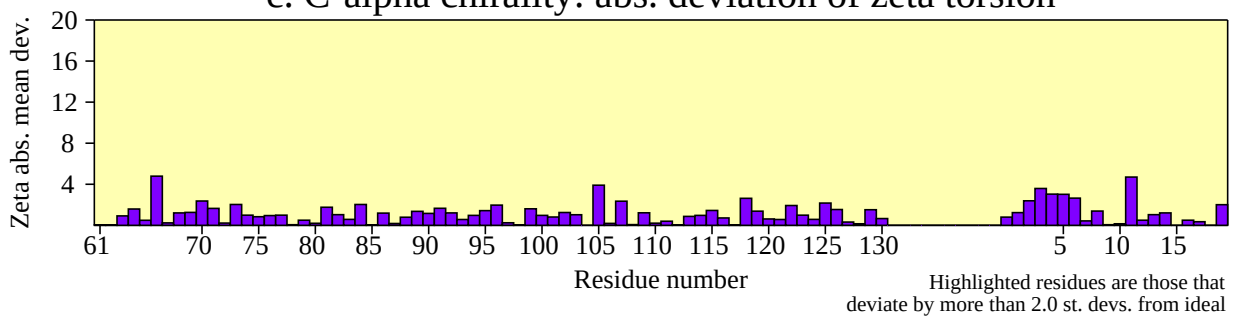
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



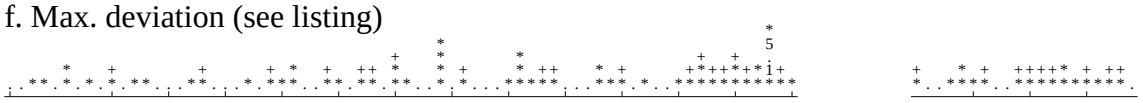
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

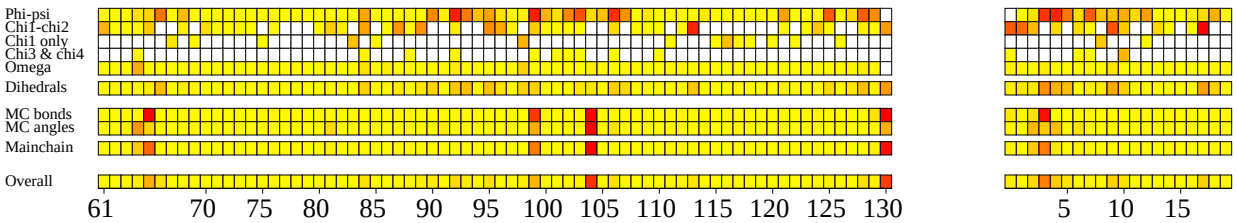
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

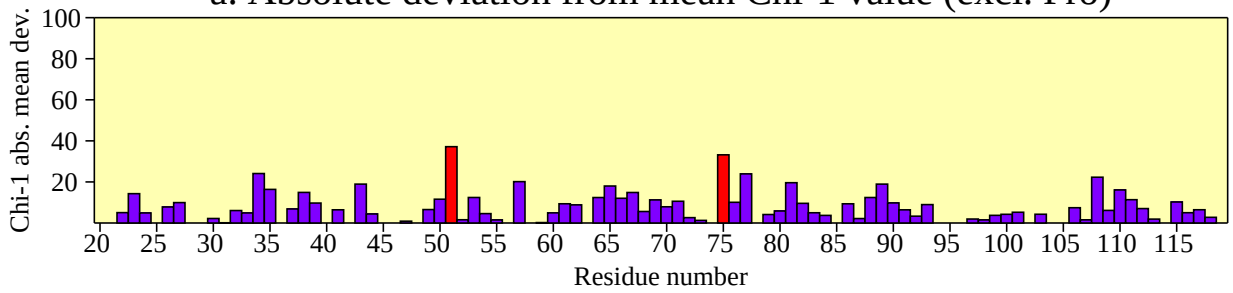


g. G-factors

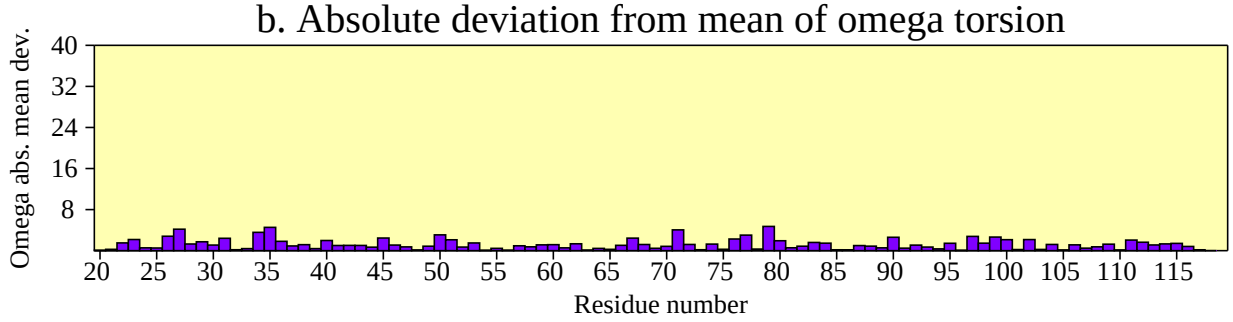


Residue properties
pdb1kf6

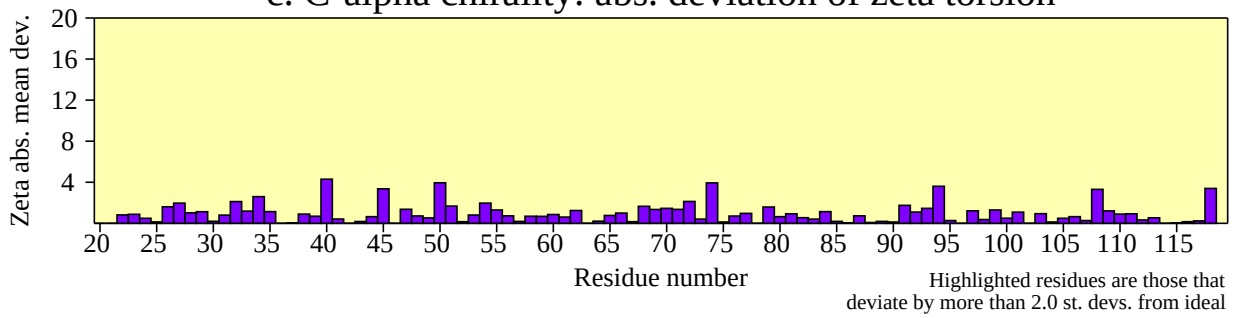
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



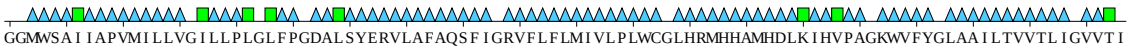
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

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

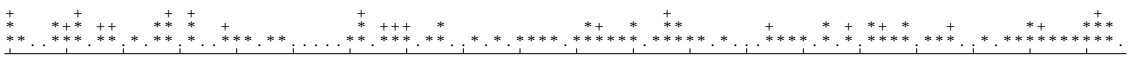
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

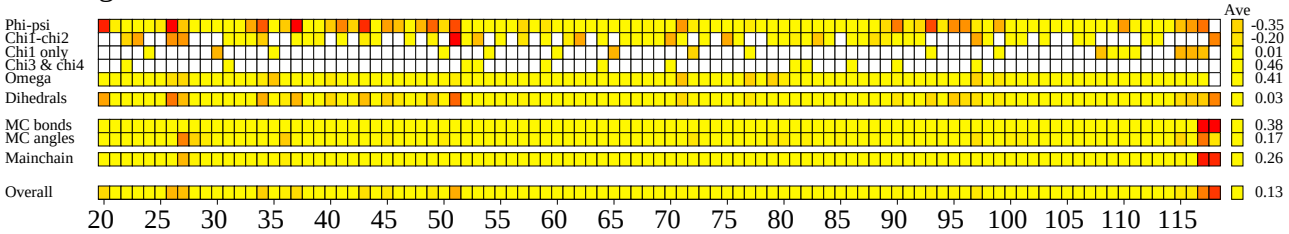


GGMWSA I I APVMI LLVG I LL PLGLF PGDAL SYERVLAFAQSF I GRVF LF LMI VL PLWCGLHRMHHAMHDLK I HVPAGKWVF YGLAA I LTVVTL I GVVT I

f. Max. deviation (see listing)

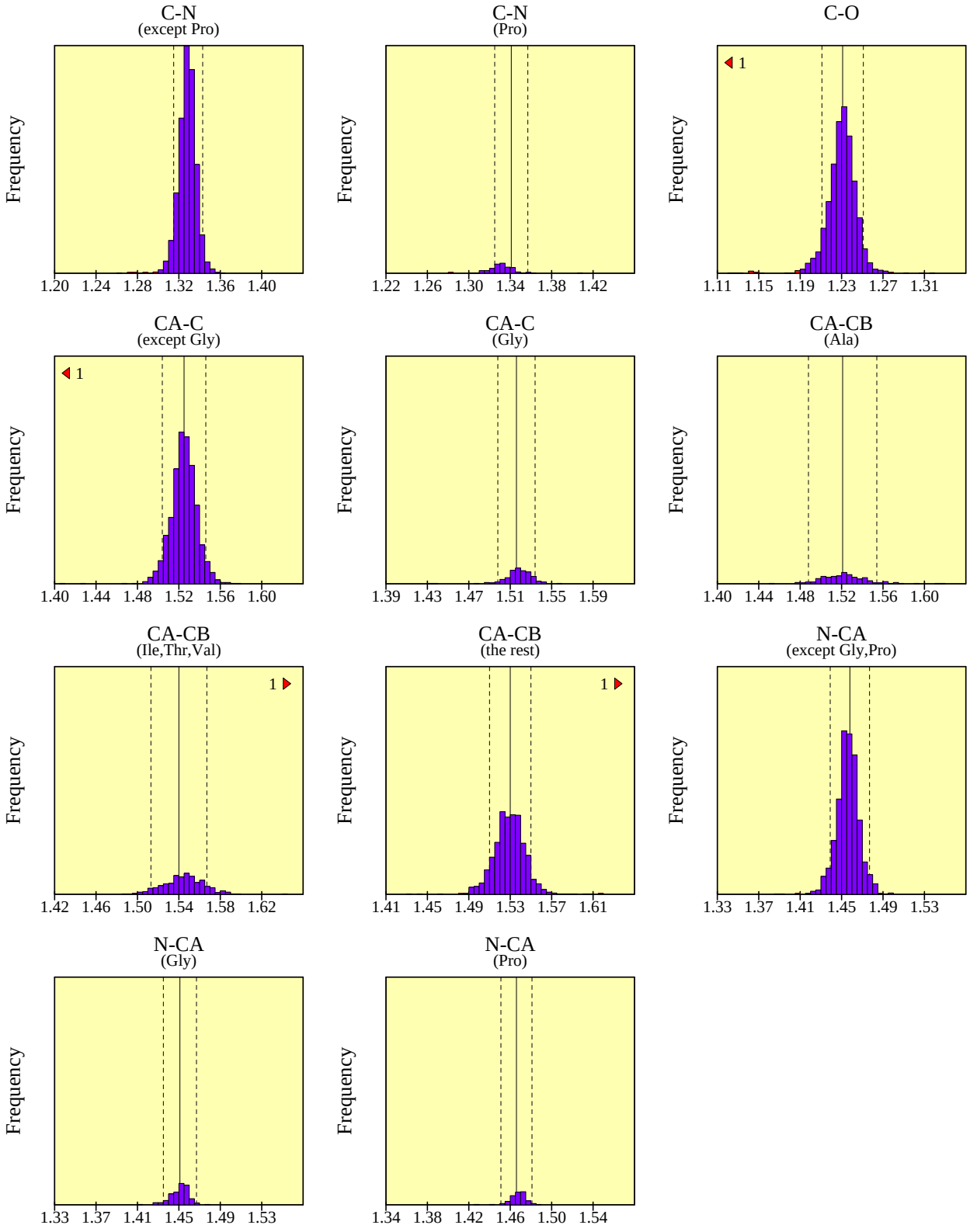


g. G-factors



Main-chain bond lengths

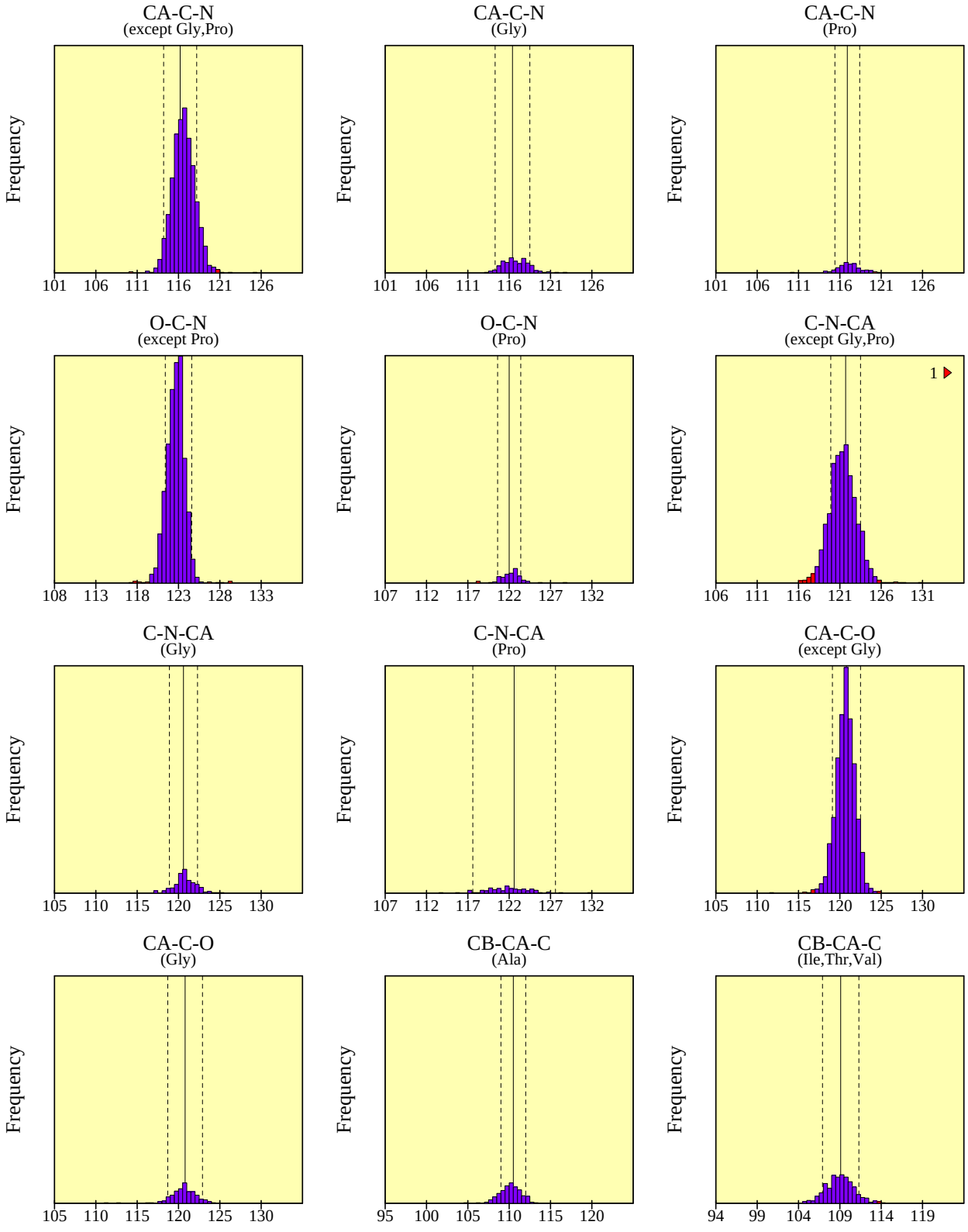
pdb1kf6



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

pdb1kf6



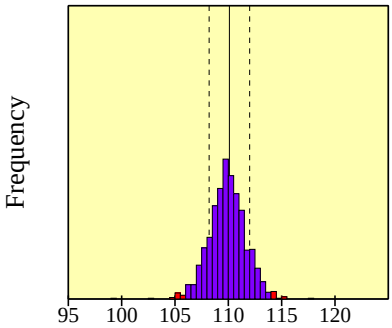
Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

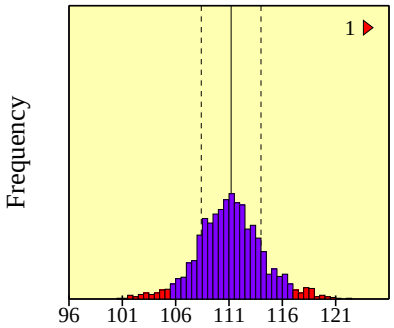
Main-chain bond angles

pdb1kf6

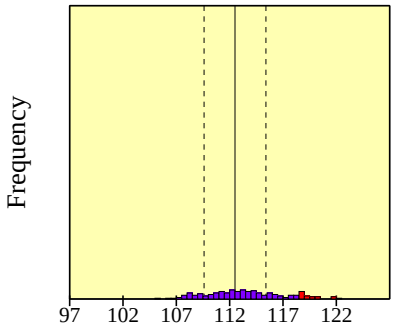
CB-CA-C
(the rest)



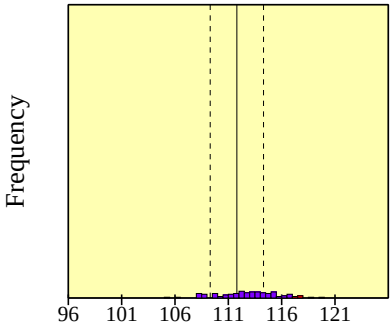
N-CA-C
(except Gly,Pro)



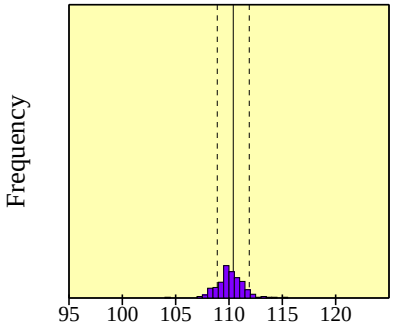
N-CA-C
(Gly)



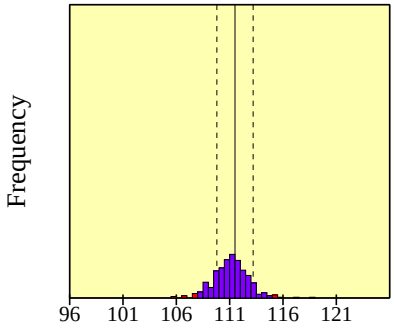
N-CA-C
(Pro)



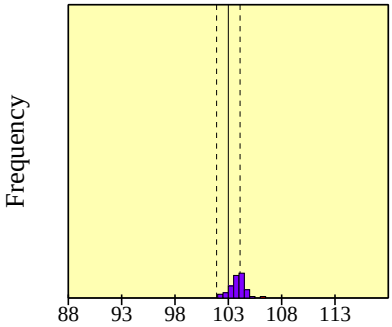
N-CA-CB
(Ala)



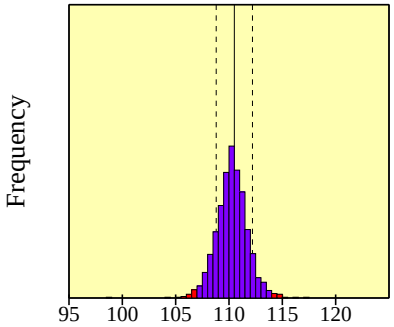
N-CA-CB
(Ile,Thr,Val)



N-CA-CB
(Pro)



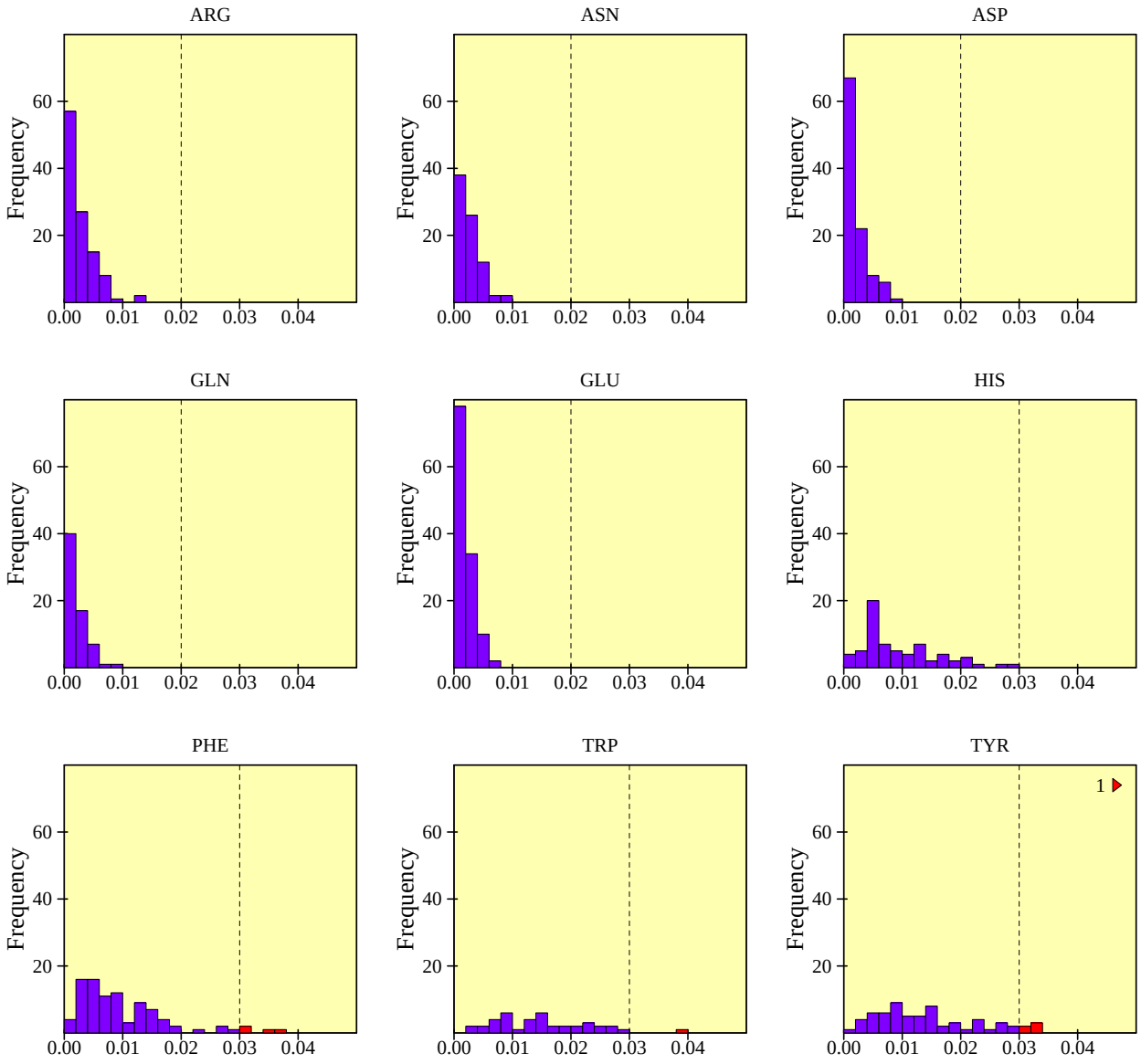
N-CA-CB
(the rest)



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

pdb1kf6



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
pdb1kf6

Main-chain bond lengths

C 1.329 N 0.051 1.278 — A Val 46 - A Ala 47
CA 1.521 CB 0.073 1.594 — A Ala 56
CA 1.530 CB 0.067 1.463 — A His 88
CA 1.521 CB 0.055 1.576 — A Ala 185
CA 1.521 CB 0.053 1.574 — A Ala 195
CA 1.540 CB 0.051 1.591 — A Val 350

C 1.231 O 0.061 1.292 — A Tyr 356
C 1.231 O 0.053 1.178 — A Leu 385
CA 1.540 CB 0.050 1.490 — A Ile 506
C 1.231 O 0.099 1.132 — A Pro 575
C 1.329 N 0.067 1.262 — A Pro 575 - A Ala 576
CA 1.521 CB 0.068 1.453 — A Ala 576

CA 1.521 CB 0.096 1.617 — B Ala 1
CA 1.540 CB 0.060 1.600 — B Val 10
C 1.329 N 0.055 1.274 — B Ser 64 - B Cys 65
CA 1.530 CB 0.053 1.583 — B Pro 136
CA 1.521 CB 0.051 1.572 — B Ala 222
C 1.231 O 0.090 1.141 — B Lys 241

C 1.341 N 0.057 1.284 — B Lys 241 - B Pro 242
CA 1.525 C 0.059 1.466 — B Pro 242
CA 1.530 CB 0.086 1.616 — B Pro 242
C 1.231 O 0.143 1.088 — C Asn 65
CA 1.530 CB 0.097 1.433 — C Asn 65
C 1.341 N 0.065 1.406 — C Asn 65 - C Pro 66

CA 1.525 C 0.054 1.579 — C Pro 66
C 1.231 O 0.082 1.149 — C Lys 99
C 1.329 N 0.056 1.273 — C Lys 99 - C Asp 100
C 1.231 O 0.078 1.153 — C Gly 104
CA 1.516 C 0.083 1.433 — C Gly 104
CA 1.530 CB 0.087 1.443 — C Trp 130

CA 1.530 CB 0.074 1.604 — D Asn 2
C 1.231 O 0.090 1.141 — D Pro 3
CA 1.530 CB 0.064 1.594 — D Asn 4
CA 1.525 C 0.115 1.410 — D Thr 117
CA 1.540 CB 0.103 1.643 — D Ile 118
N 1.458 CA 0.067 1.391 — D Ile 118

C 1.231 O 0.078 1.309 — M Thr 357
C 1.231 O 0.085 1.316 — M Gly 359
C 1.231 O 0.086 1.145 — M Pro 575
C 1.329 N 0.051 1.278 — M Pro 575 - M Ala 576
CA 1.521 CB 0.090 1.611 — M Ala 576
CA 1.530 CB 0.056 1.586 — N Cys 148

CA 1.530 CB 0.088 1.618 — N Cys 151
C 1.231 O 0.088 1.143 — N Lys 241
C 1.341 N 0.056 1.285 — N Lys 241 - N Pro 242
CA 1.525 C 0.095 1.430 — N Pro 242
CA 1.530 CB 0.079 1.609 — N Pro 242
C 1.231 O 0.107 1.124 — O Asn 65

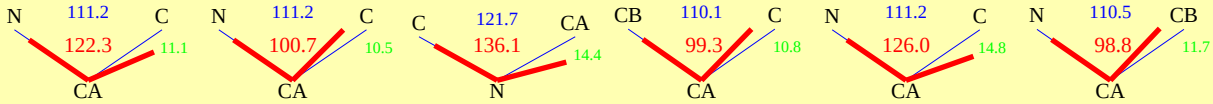
C 1.231 O 0.082 1.149 — O Lys 99
C 1.231 O 0.104 1.127 — O Gly 104
CA 1.516 C 0.080 1.436 — O Gly 104
CA 1.530 CB 0.141 1.671 — O Trp 130
C 1.231 O 0.087 1.144 — P Pro 3
CA 1.525 C 0.129 1.396 — P Thr 117

CA 1.540 CB 0.149 1.689 — P Ile 118
N 1.458 CA 0.072 1.386 — P Ile 118

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

Distorted geometry
pdb1kf6

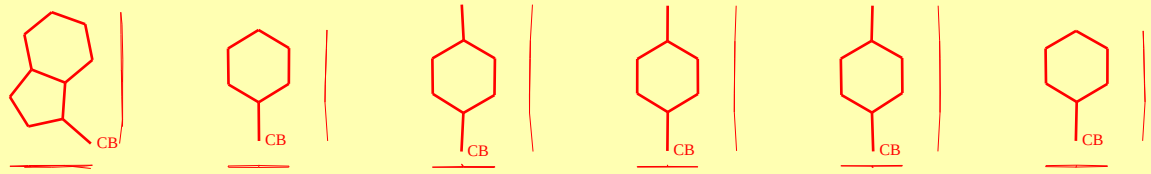
Main-chain bond angles



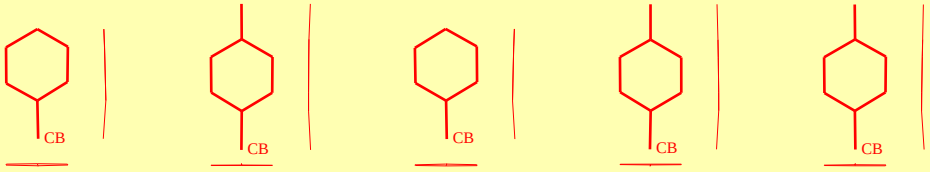
A Glu 276 | A Val 312 | B Ser 64 - B Cys 65 | B Cys 65 | B Cys 65 | B Cys 65

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

Planar groups



0.038 A Trp 75 | 0.037 A Phe 140 | 0.051 A Tyr 260 | 0.032 B Tyr 142 | 0.033 B Tyr 155 | 0.031 B Phe 167



0.034 M Phe 294 | 0.030 M Tyr 565 | 0.031 N Phe 80 | 0.030 N Tyr 84 | 0.033 O Tyr 25

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