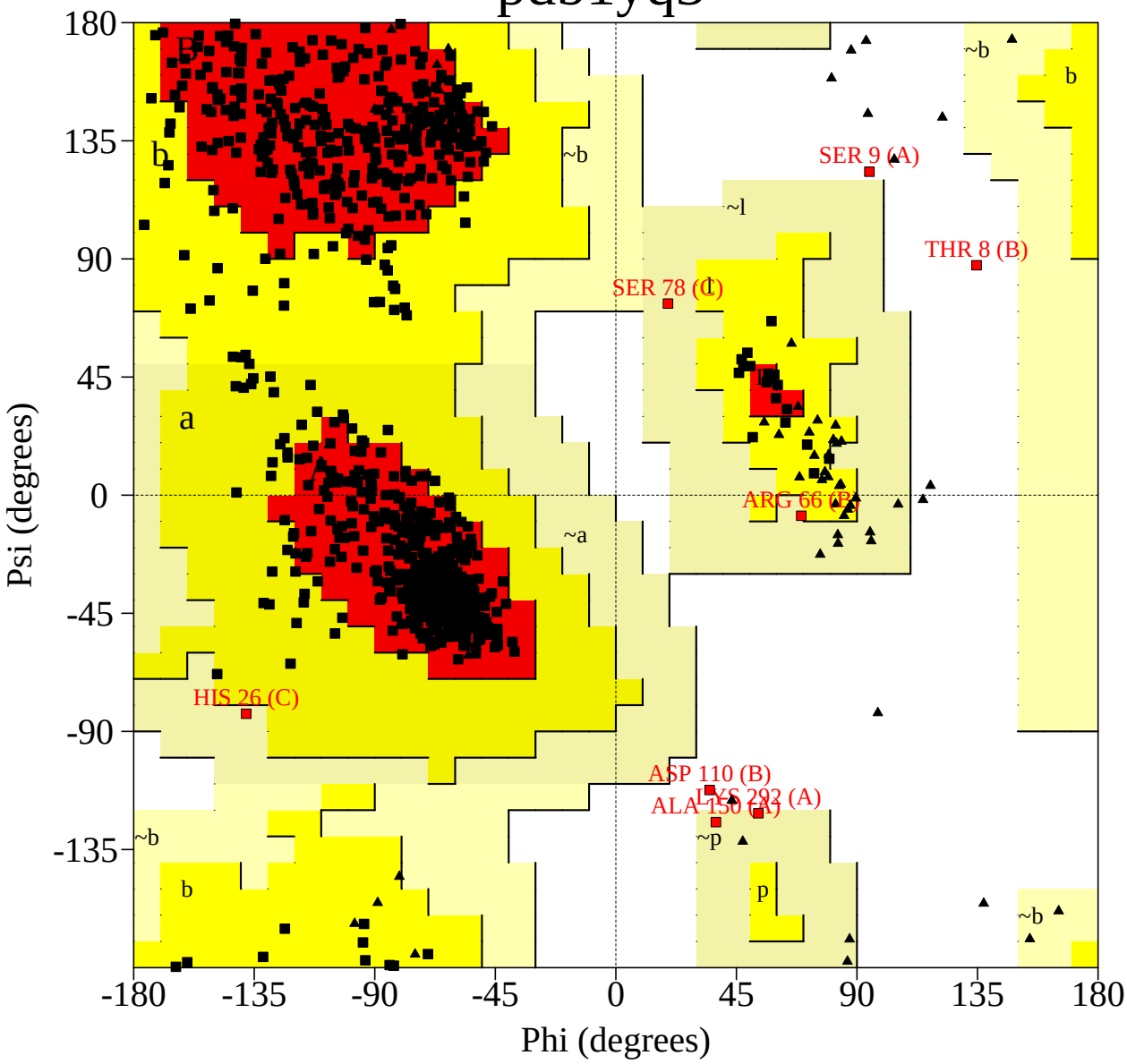
PROCHECK

Ramachandran Plot

pdb1yq3



Plot statistics

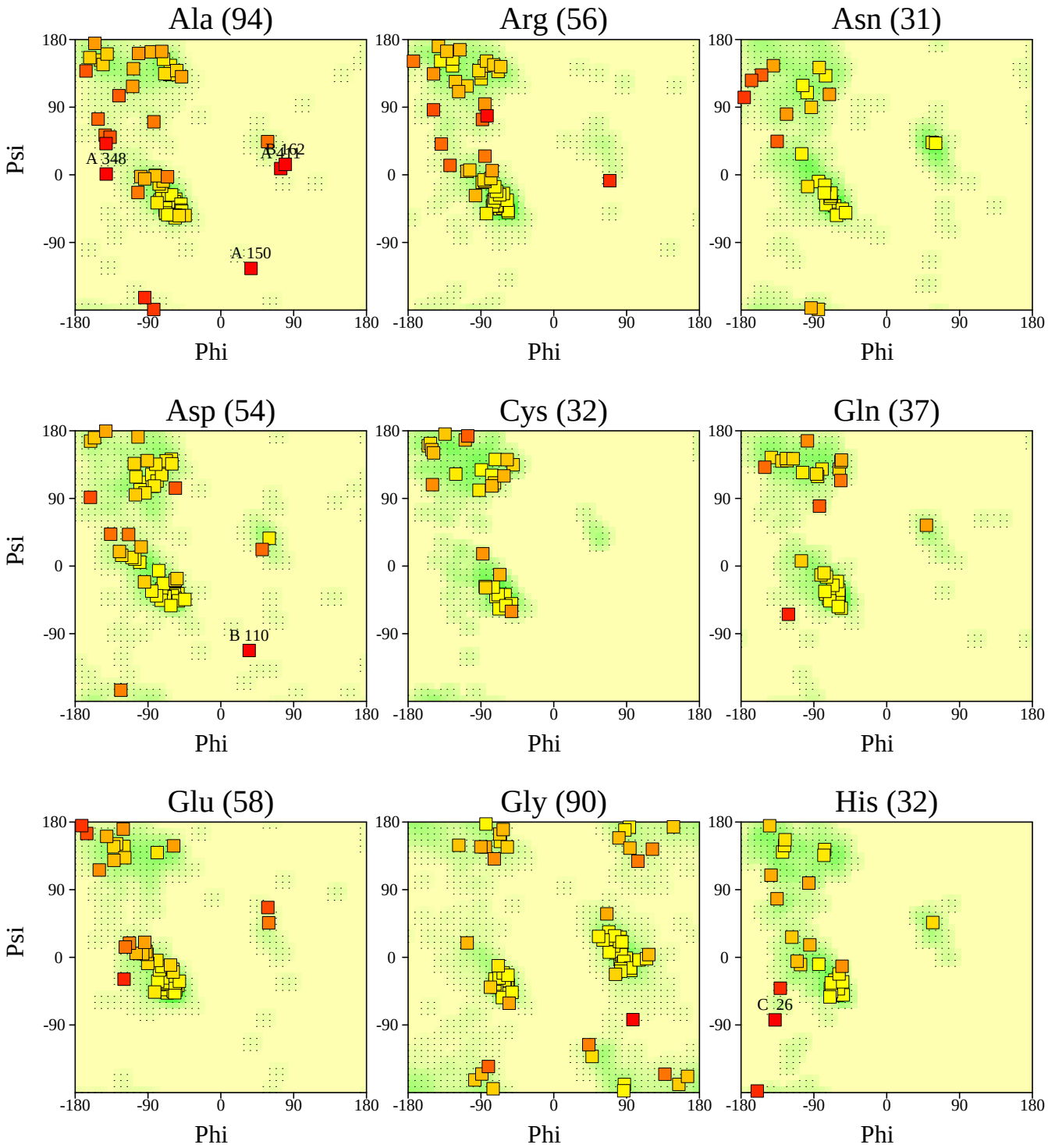
Residues in most favoured regions [A,B,L]	842	88.6%
Residues in additional allowed regions [a,b,l,p]	100	10.5%
Residues in generously allowed regions [~a,~b,~l,~p]	5	0.5%
Residues in disallowed regions	3	0.3%
	----	------
Number of non-glycine and non-proline residues	950	100.0%
Number of end-residues (excl. Gly and Pro)	8	
Number of glycine residues (shown as triangles)	90	
Number of proline residues	50	

Total number of residues	1098	

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

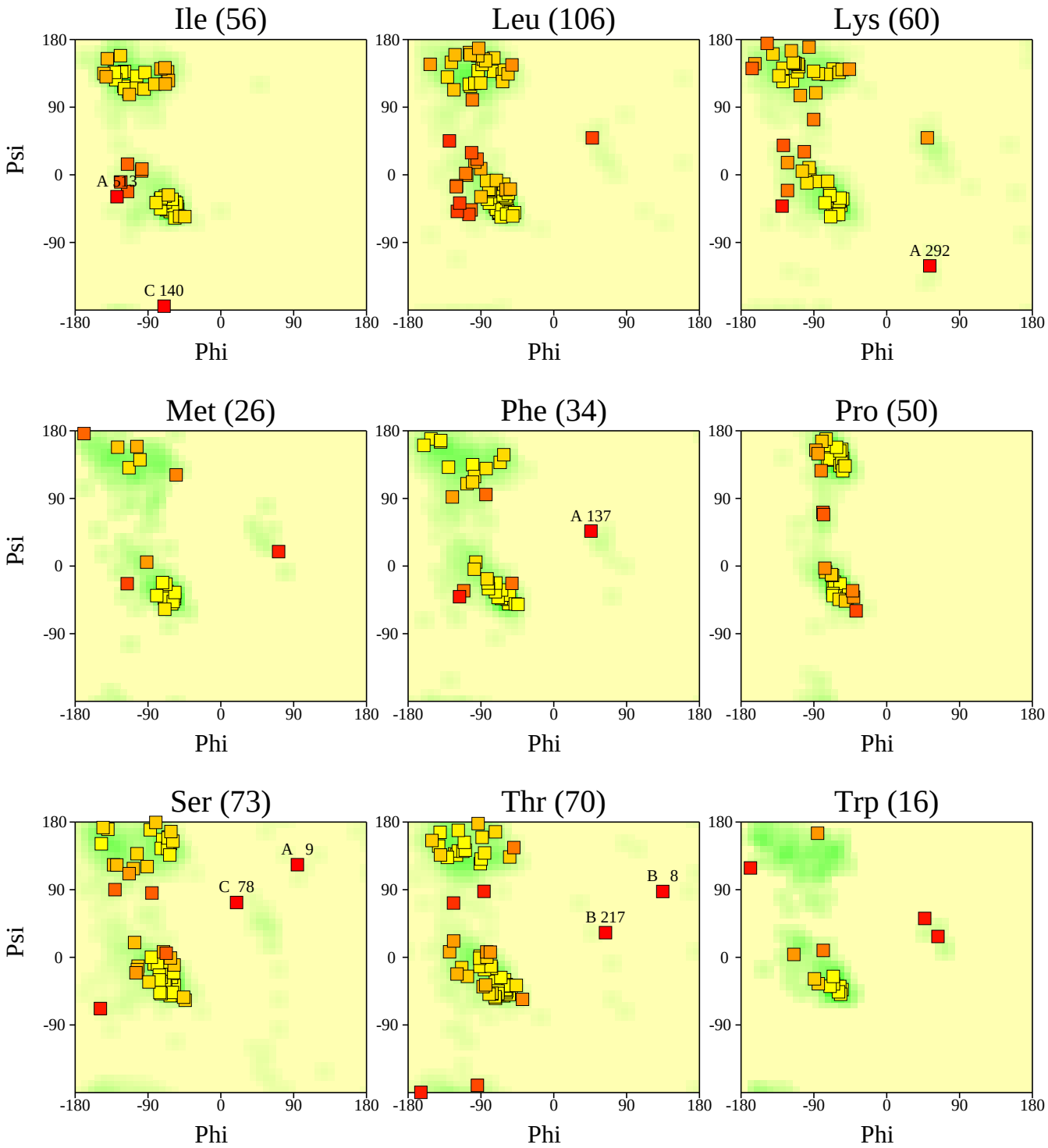
pdb1yq3



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

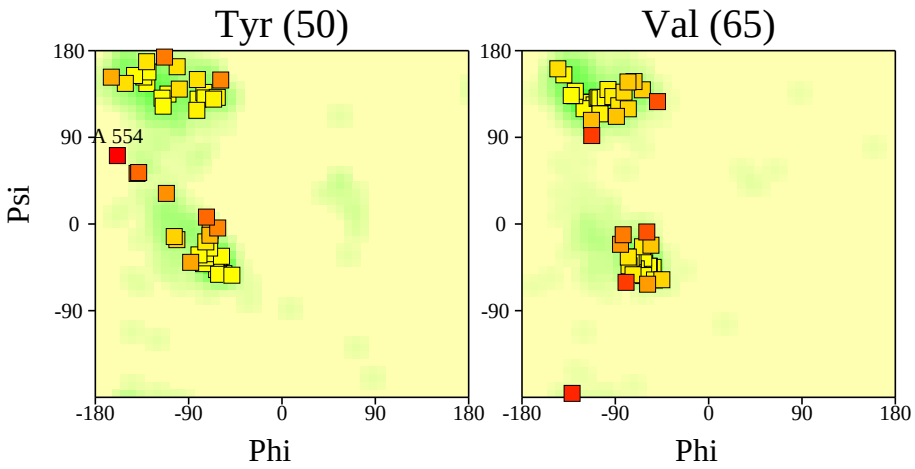
pdb1yq3



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

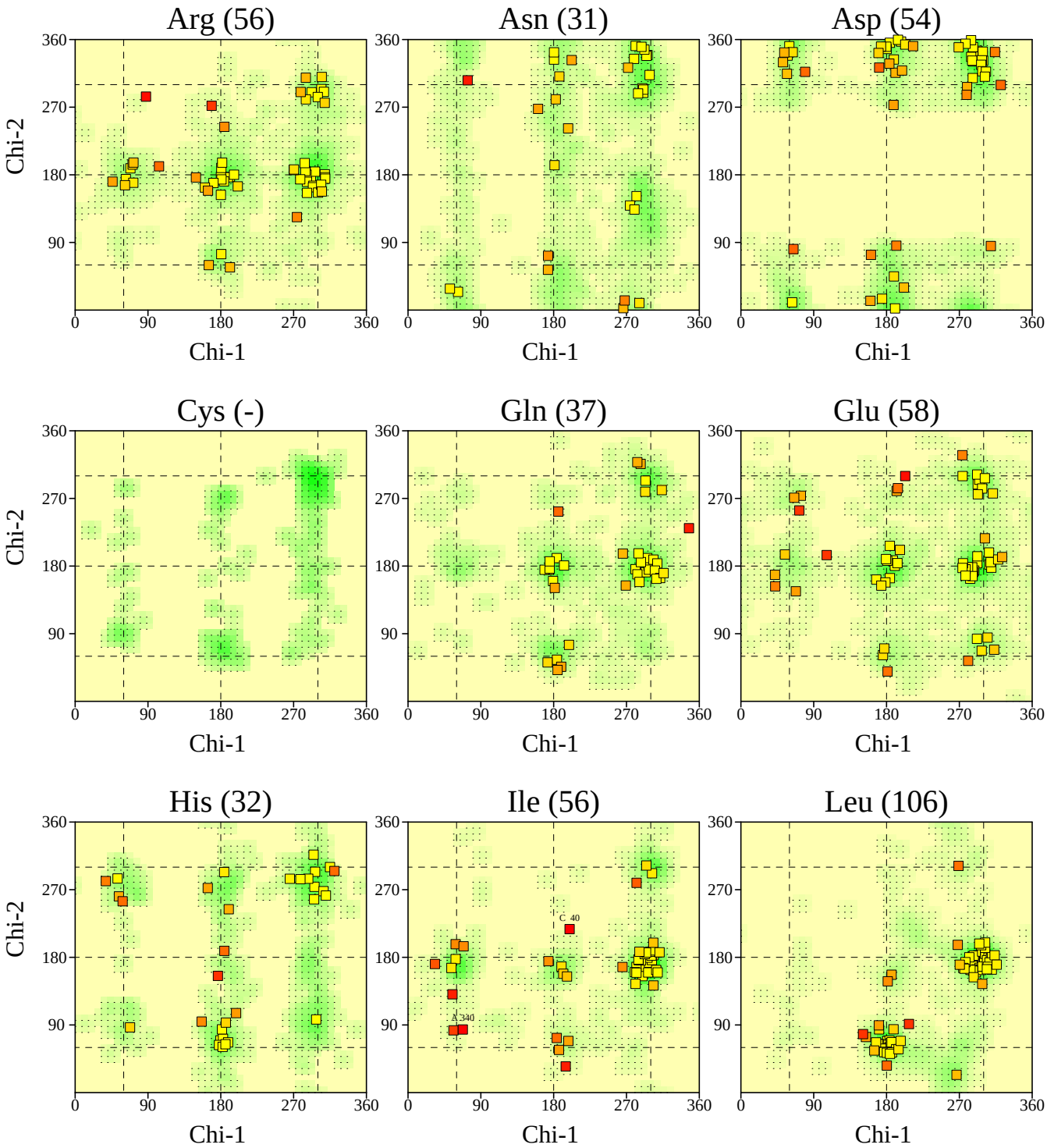
pdb1yq3



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

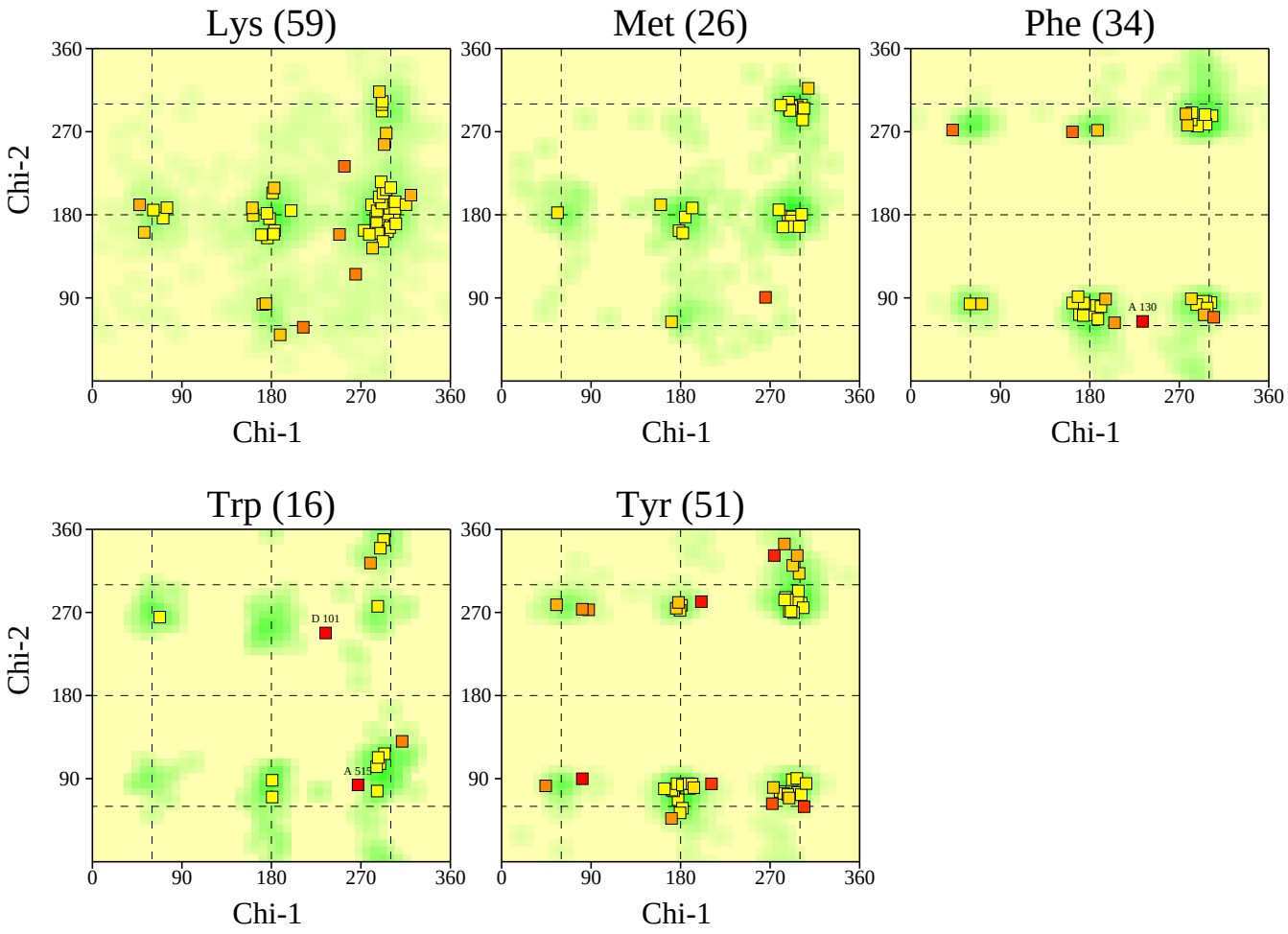
pdb1yq3



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

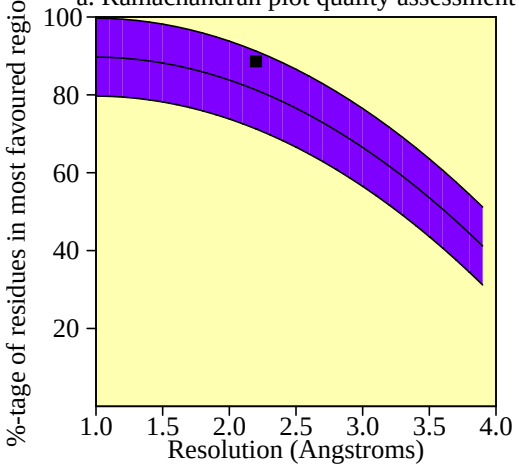
pdb1yq3



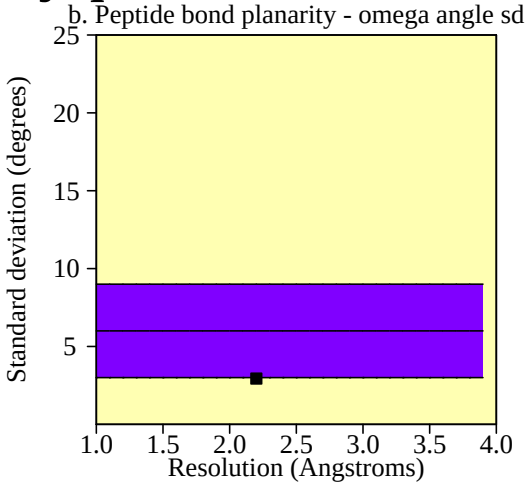
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

Main-chain parameters
pdb1yq3

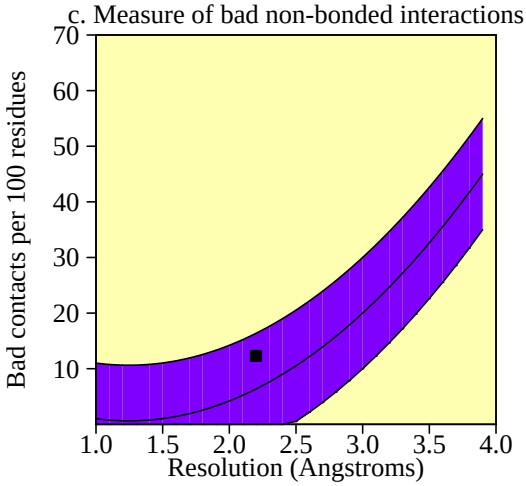
a. Ramachandran plot quality assessment



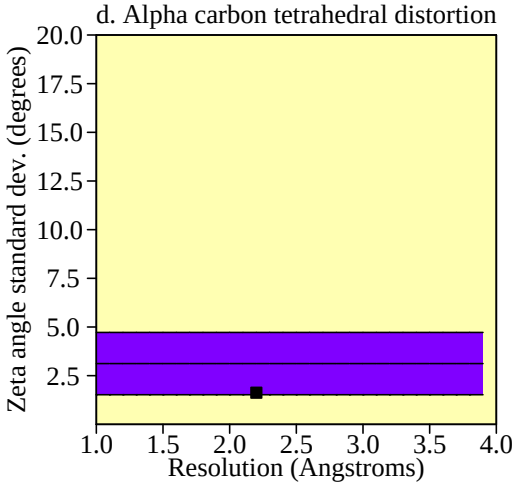
b. Peptide bond planarity - omega angle sd



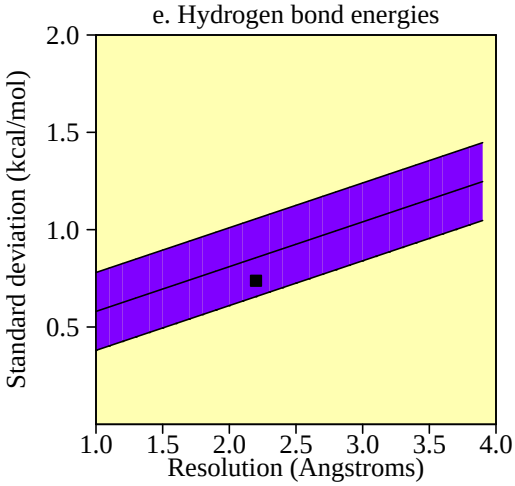
c. Measure of bad non-bonded interactions



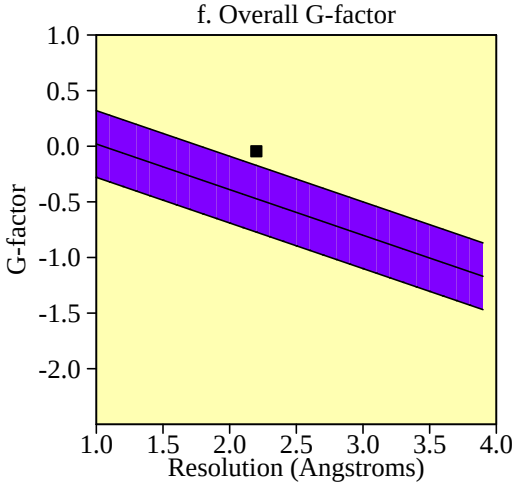
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor



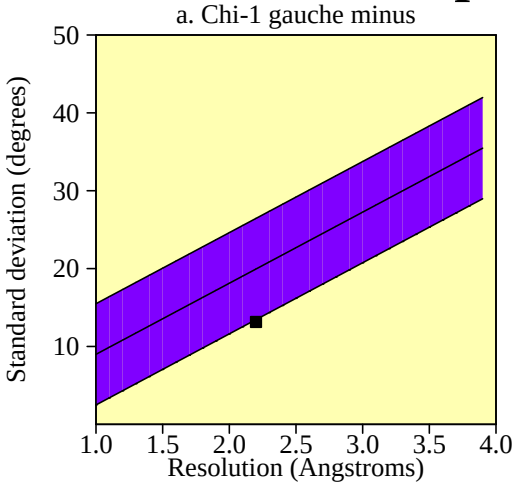
Plot statistics

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	950	88.6	81.3	10.0	0.7	Inside
b. Omega angle st dev	1092	2.9	6.0	3.0	-1.0	BETTER
c. Bad contacts / 100 residues	135	12.3	6.4	10.0	0.6	Inside
d. Zeta angle st dev	1007	1.6	3.1	1.6	-0.9	Inside
e. H-bond energy st dev	717	0.7	0.9	0.2	-0.6	Inside
f. Overall G-factor	1098	0.0	-0.5	0.3	1.4	BETTER

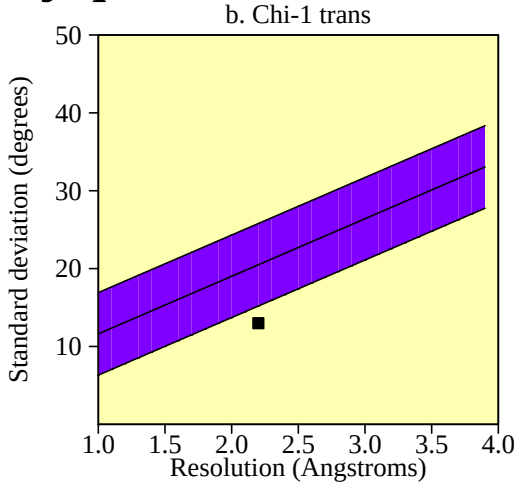
Side-chain parameters

pdb1yq3

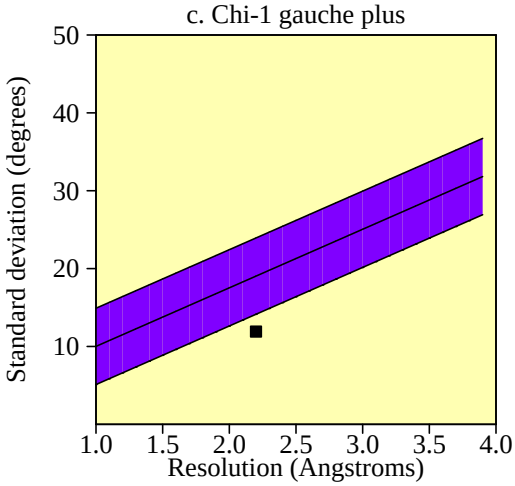
a. Chi-1 gauche minus



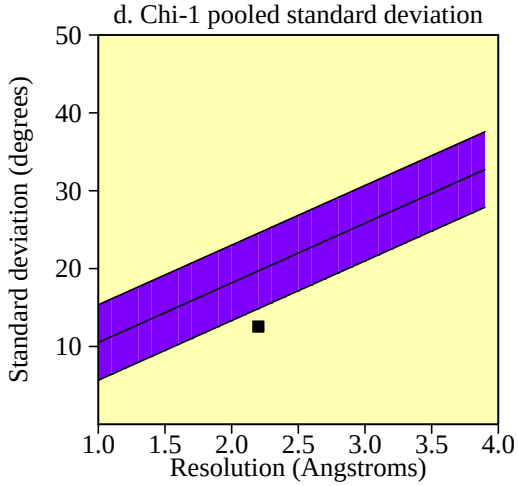
b. Chi-1 trans



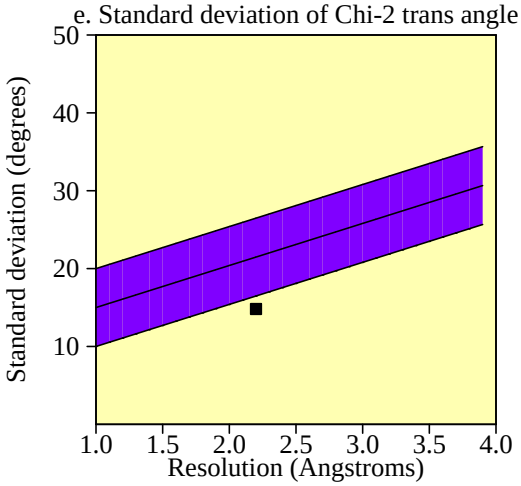
c. Chi-1 gauche plus

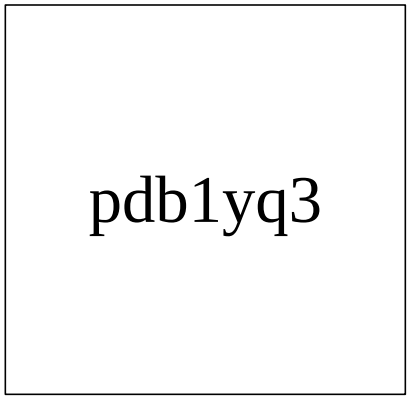


d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



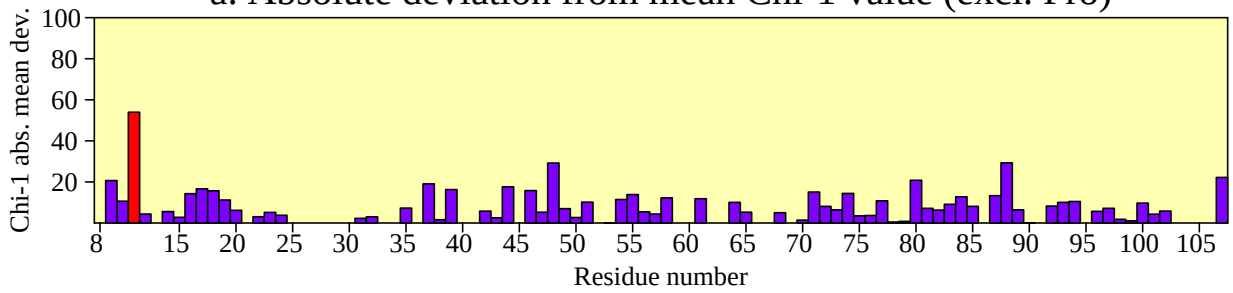


Plot statistics

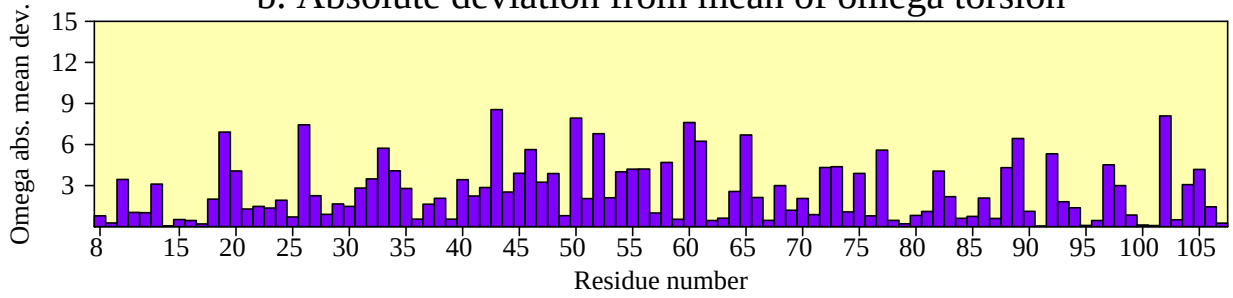
Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	129	13.1	19.9	6.5	-1.0	BETTER
b. Chi-1 trans st dev	274	13.0	20.5	5.3	-1.4	BETTER
c. Chi-1 gauche plus st dev	453	11.9	19.0	4.9	-1.5	BETTER
d. Chi-1 pooled st dev	856	12.5	19.7	4.8	-1.5	BETTER
e. Chi-2 trans st dev	287	14.8	21.5	5.0	-1.3	BETTER

Residue properties
pdb1yq3

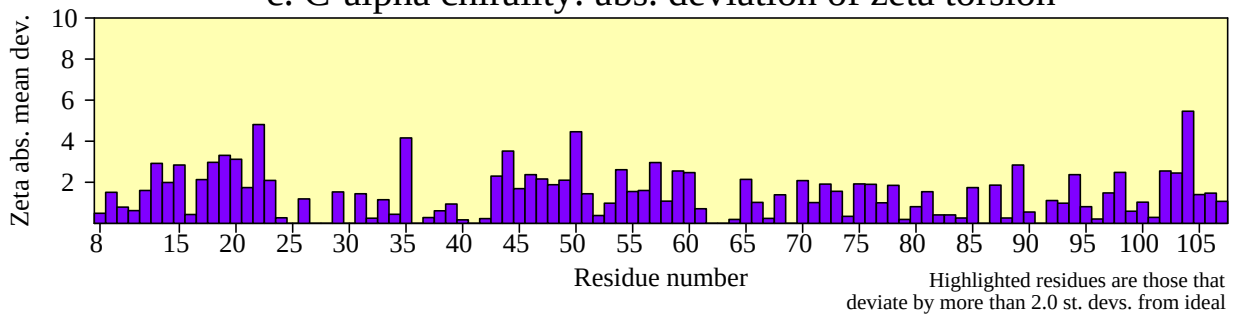
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

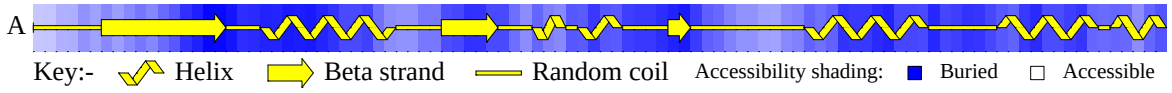


c. C-alpha chirality: abs. deviation of zeta torsion



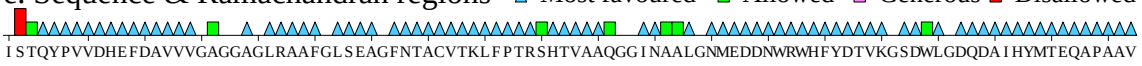
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

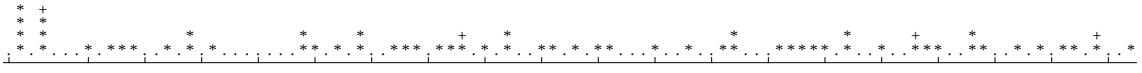


e. Sequence & Ramachandran regions

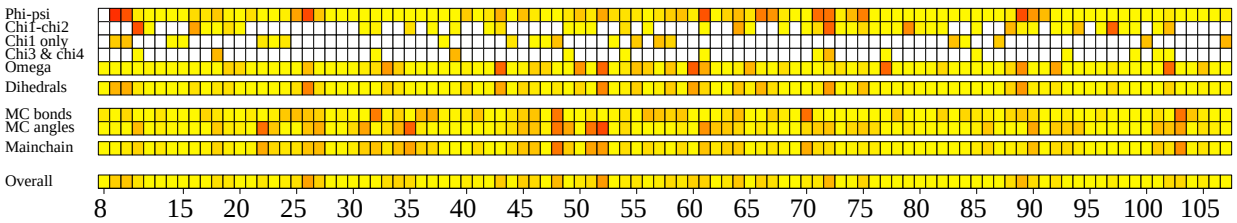
Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

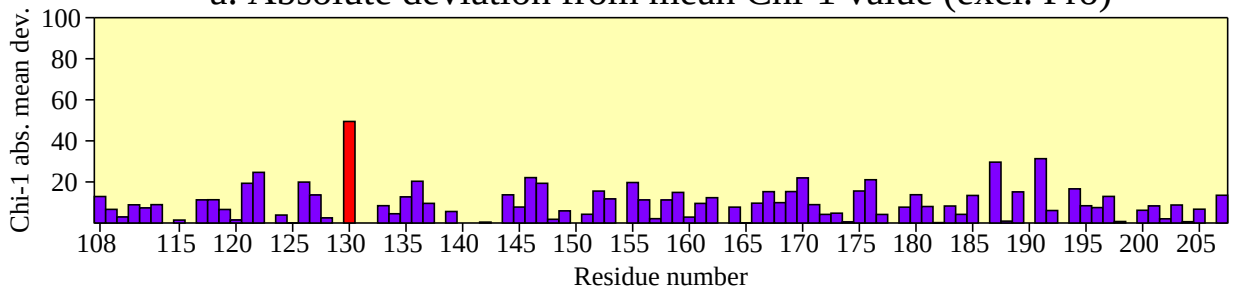


g. G-factors

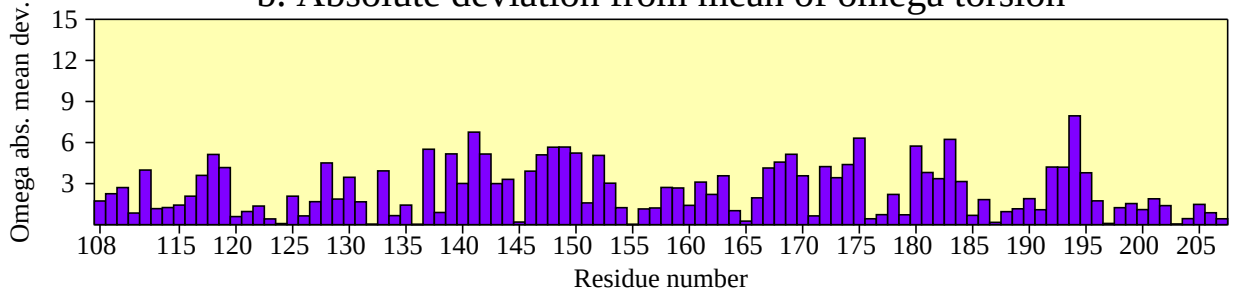


Residue properties
pdb1yq3

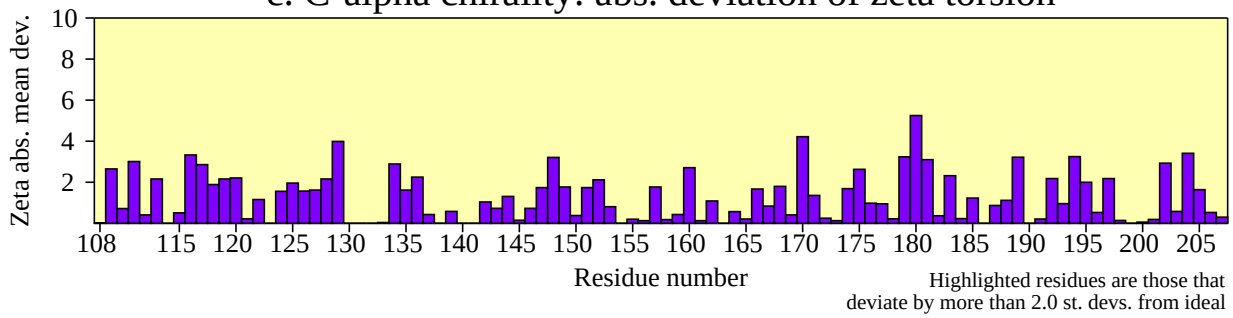
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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

d. Secondary structure & estimated accessibility

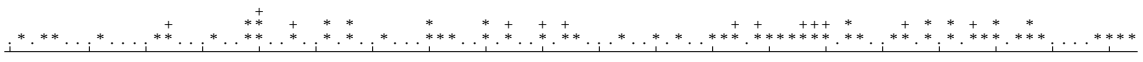
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

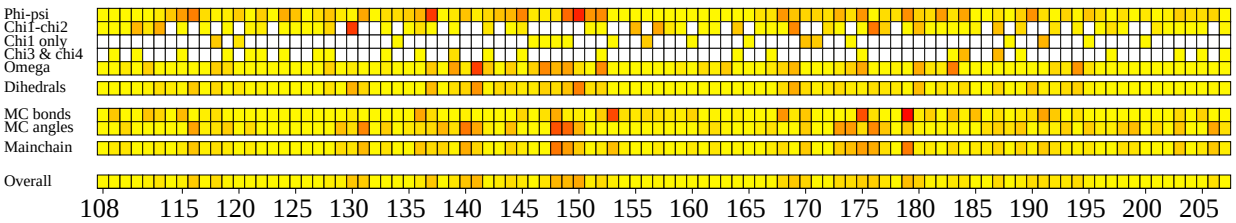
Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)

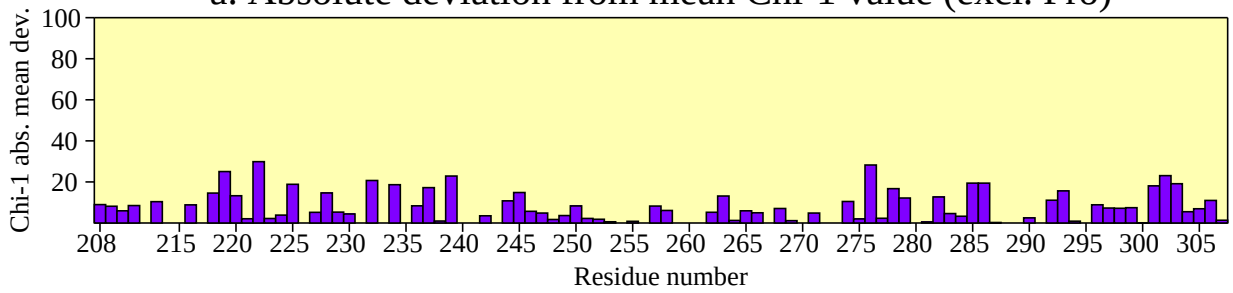


g. G-factors

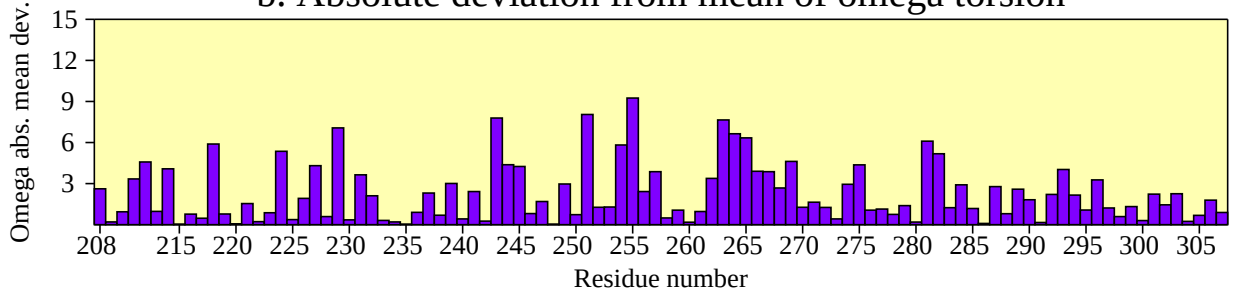


Residue properties
pdb1yq3

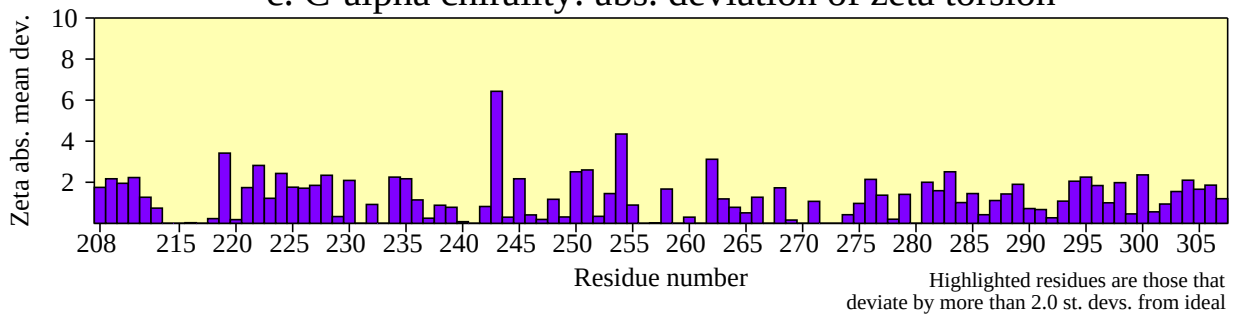
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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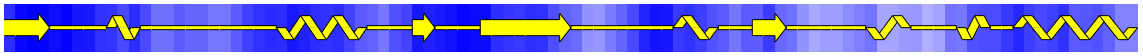
d. Secondary structure & estimated accessibility



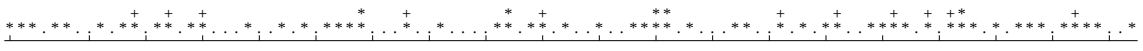
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

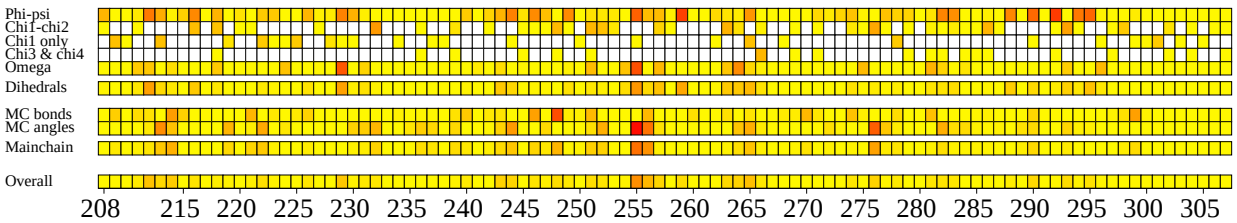
Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)

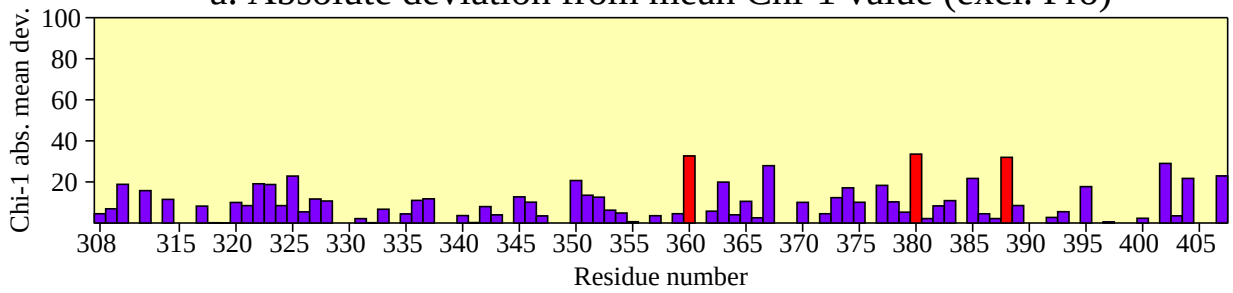


g. G-factors

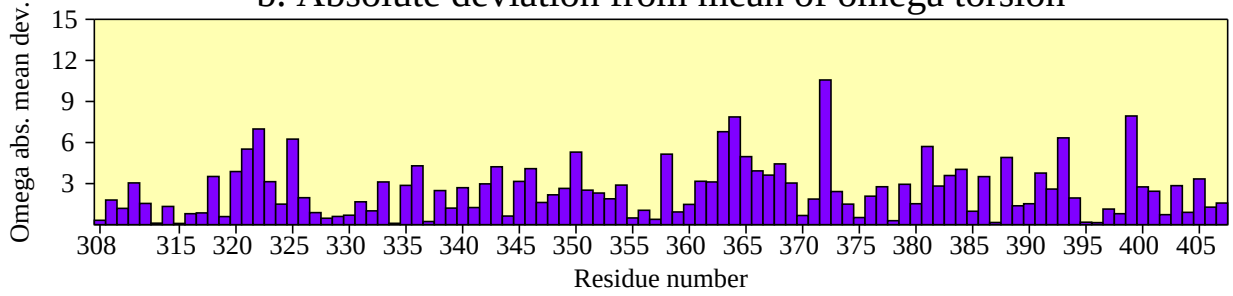


Residue properties
pdb1yq3

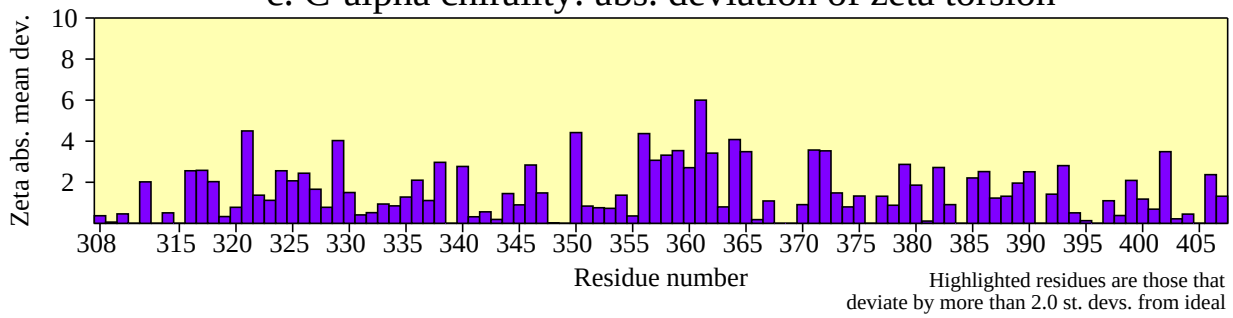
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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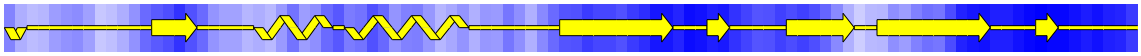
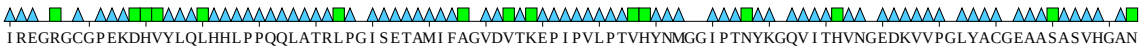
d. Secondary structure & estimated accessibility



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

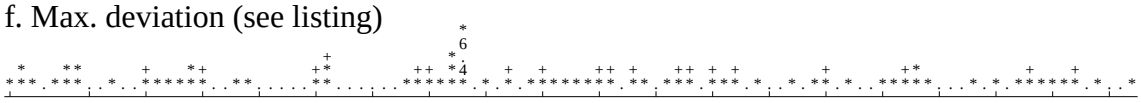
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

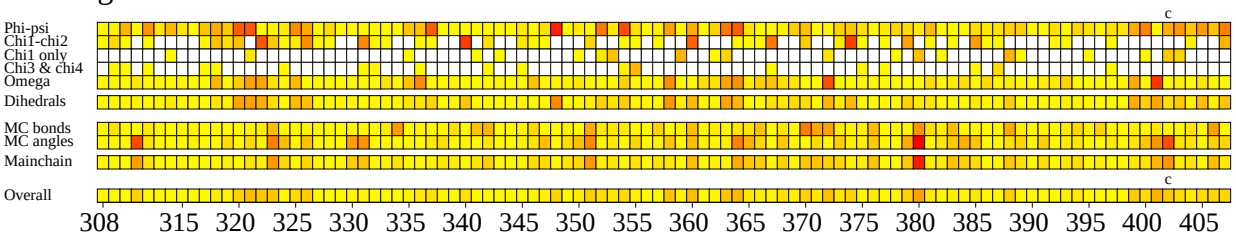


I REGRGCGPEKDHVYLQLHHLPPQQLATRLPGISETAMIFAGVDVTKEPIPVLPTVHYNMGGIPTNYKGQVITHVNGEDKVVPGLYACGEAASASVHGAN

f. Max. deviation (see listing)



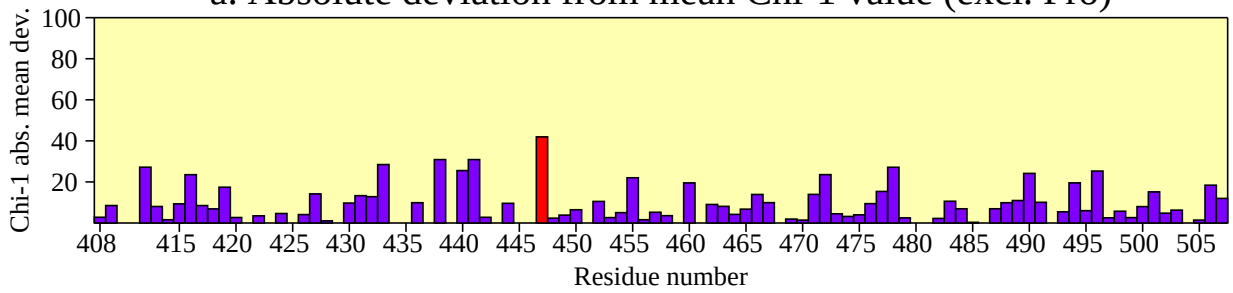
g. G-factors



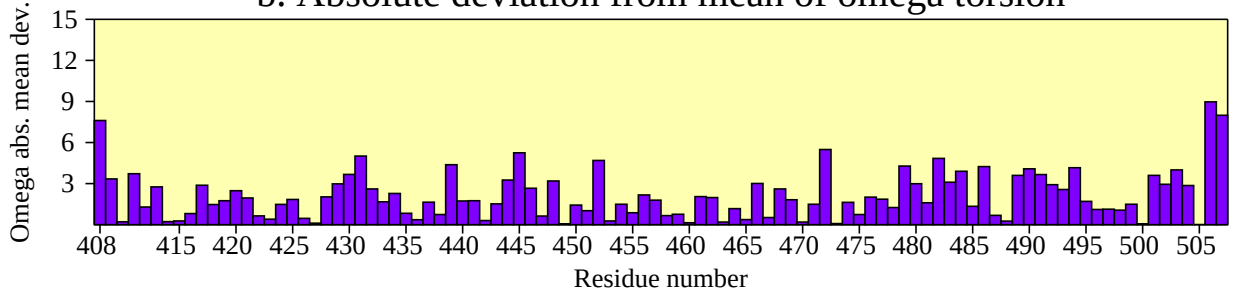
c = cis-peptide

Residue properties
pdb1yq3

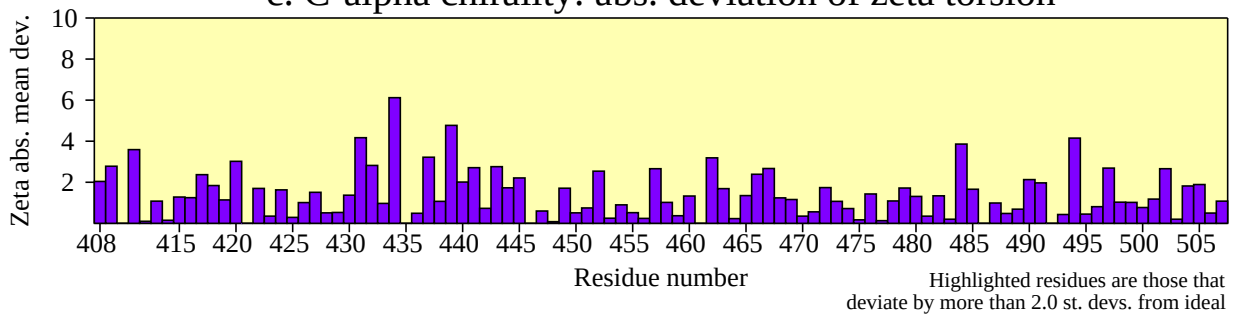
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

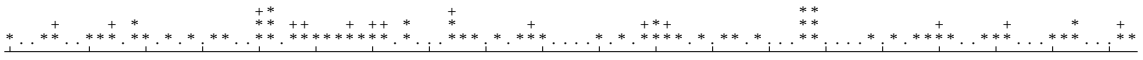
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

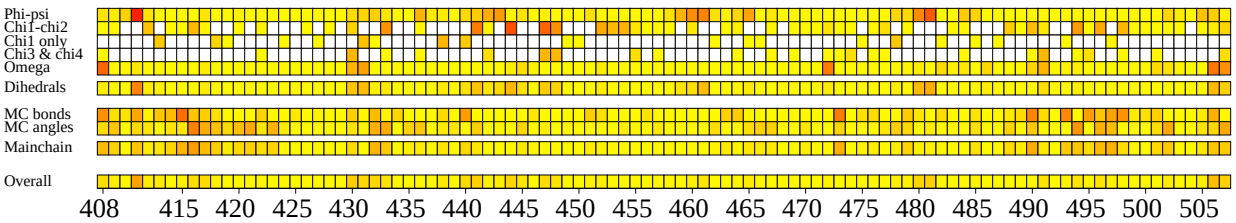
Most favoured Allowed Generous Disallowed

RLGANSLLDLVVFGRACALTIAETCKPGEPVPSIKPNAGEESVANLDKLRFADGTIRTSEARLNMQKTMQSHAAVFRTGSILQEGCEKLSQIYRDLAHLK

f. Max. deviation (see listing)

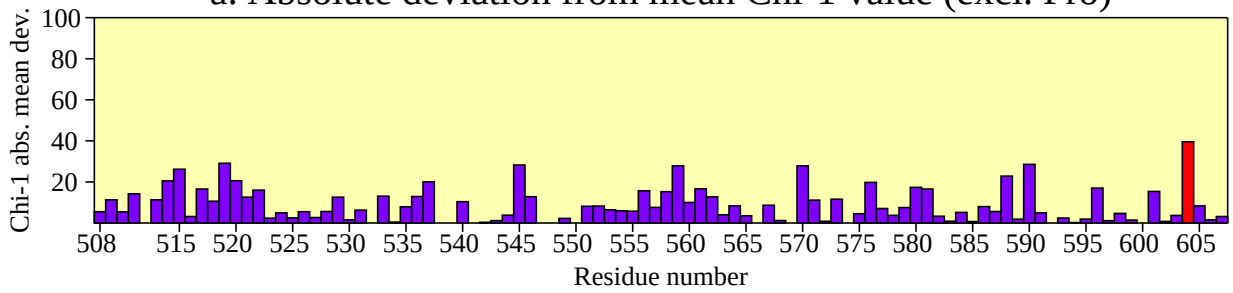


g. G-factors

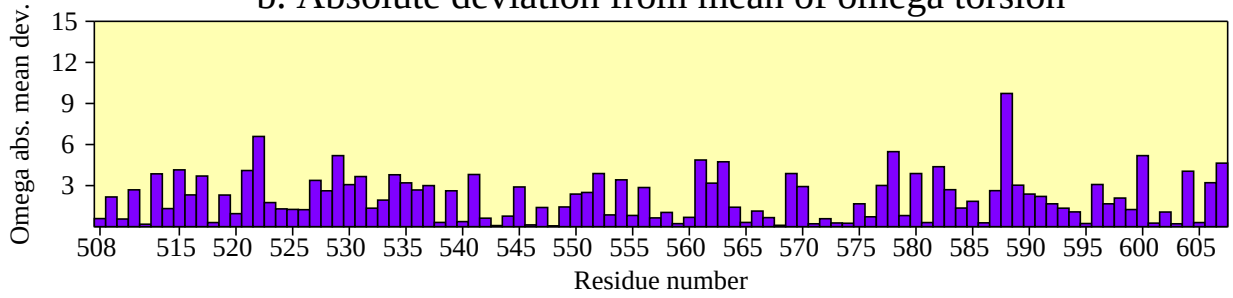


Residue properties
pdb1yq3

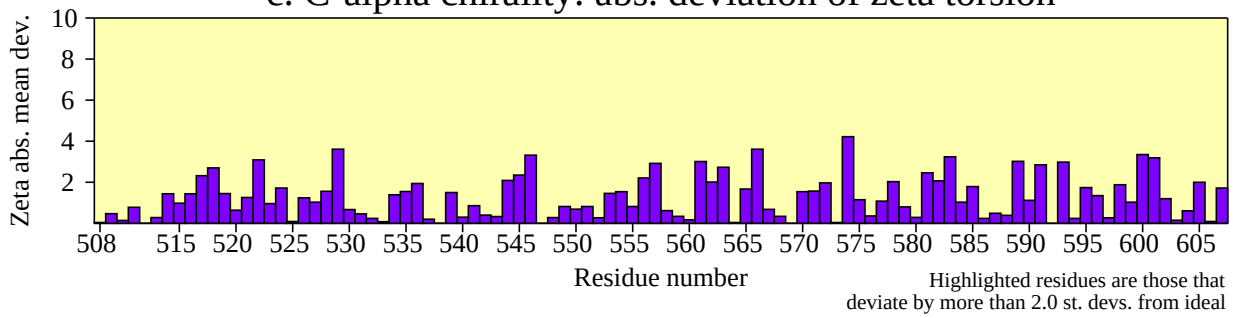
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

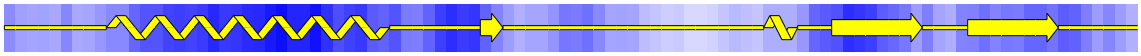


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



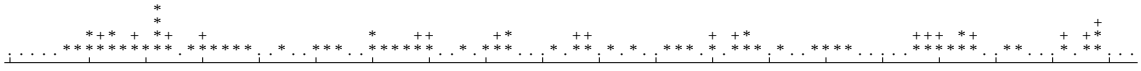
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

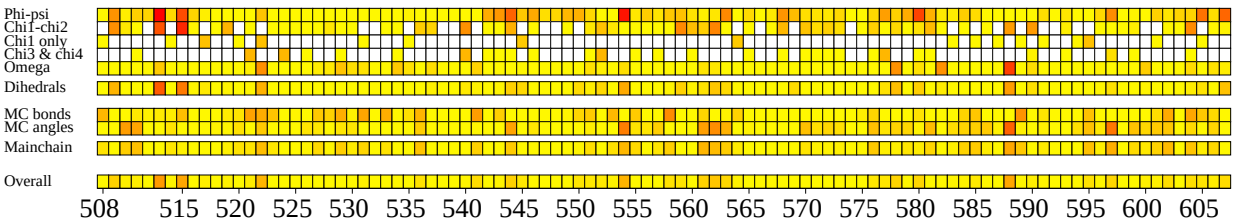
Most favoured Allowed Generous Disallowed

TFDRGIVWNTDLVETLELQNLMLCALQTIYGAEARKESRGAHAREDYKLRIDEFDYSKPLQGQQKRPFEEHWRKHTLSYVDVKSGKVTLKYRPVIDRTLN

f. Max. deviation (see listing)

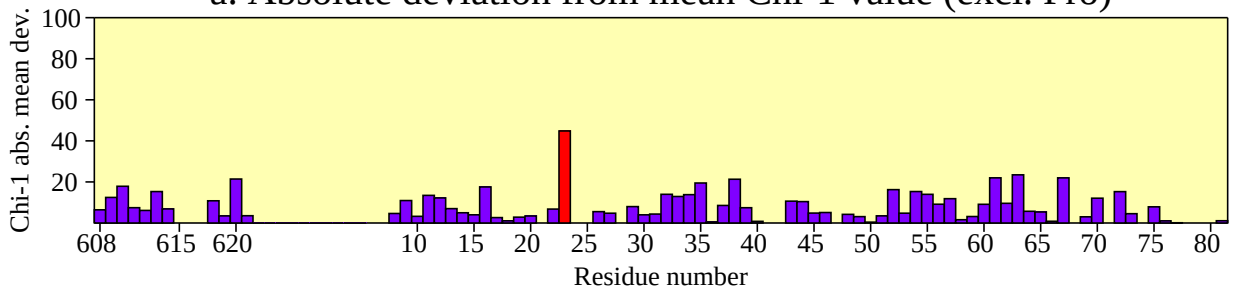


g. G-factors

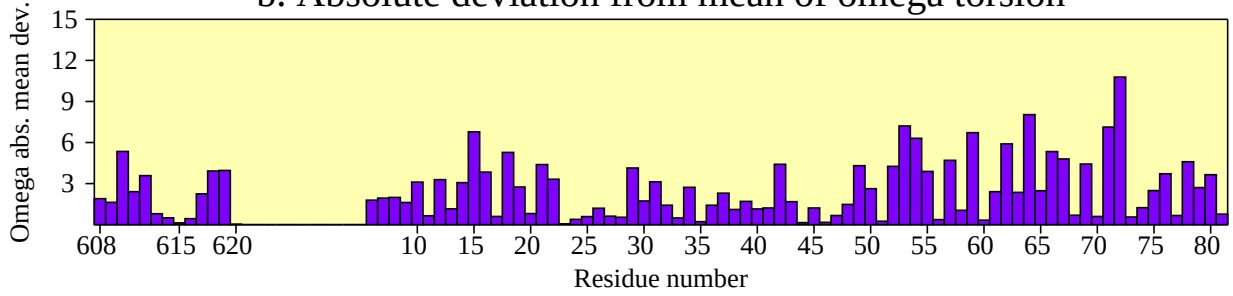


Residue properties
pdb1yq3

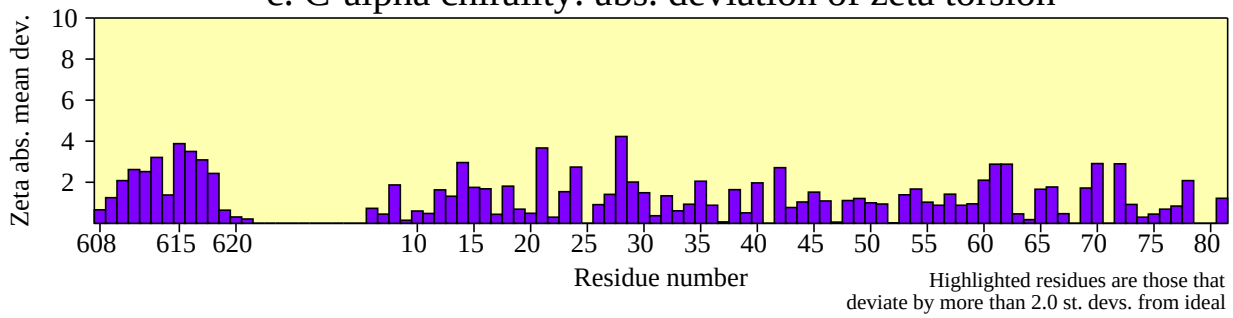
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

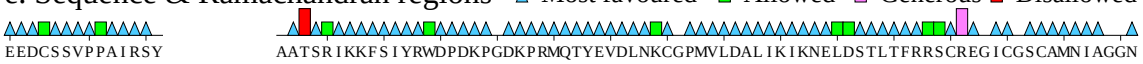


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

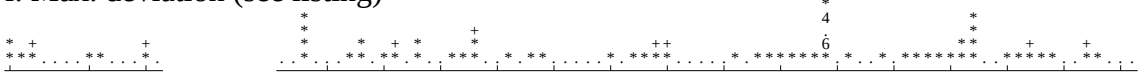
d. Secondary structure & estimated accessibility

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

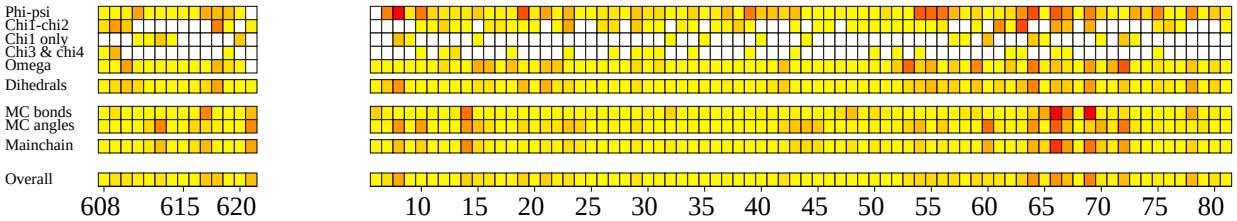
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

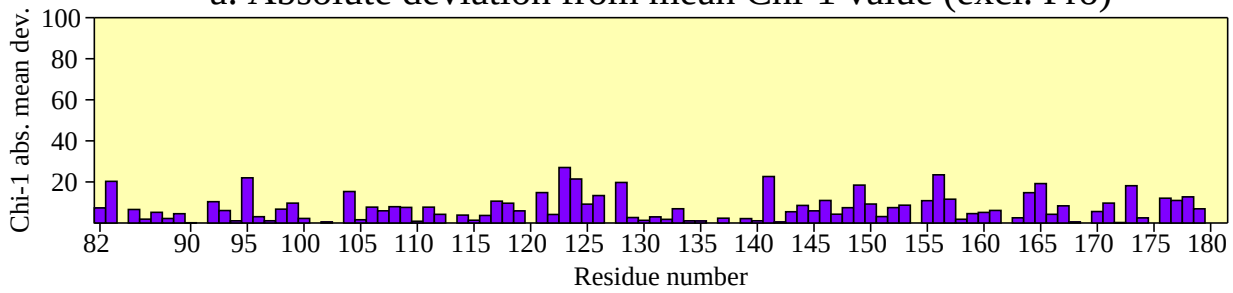


g. G-factors

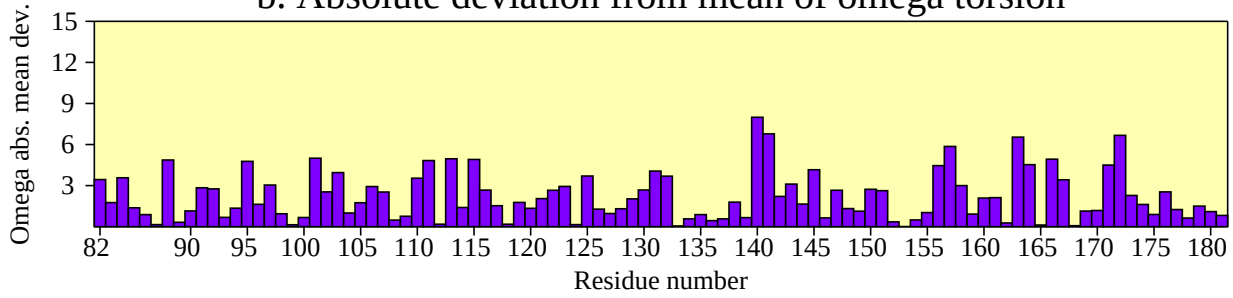


Residue properties
pdb1yq3

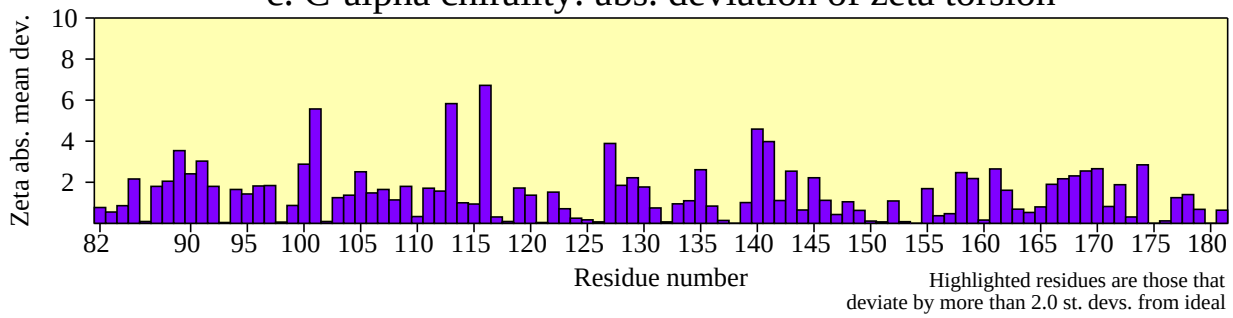
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

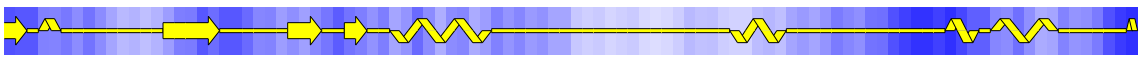


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



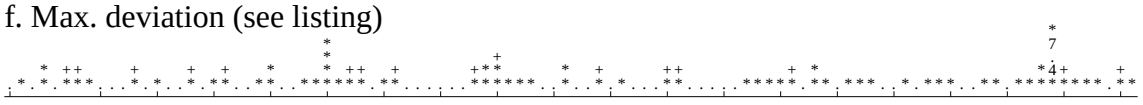
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

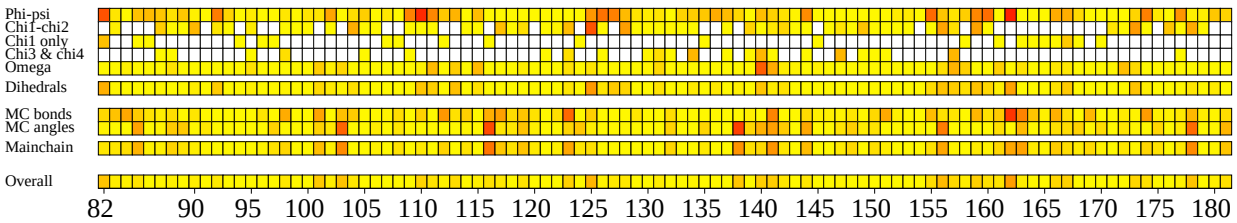
Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)

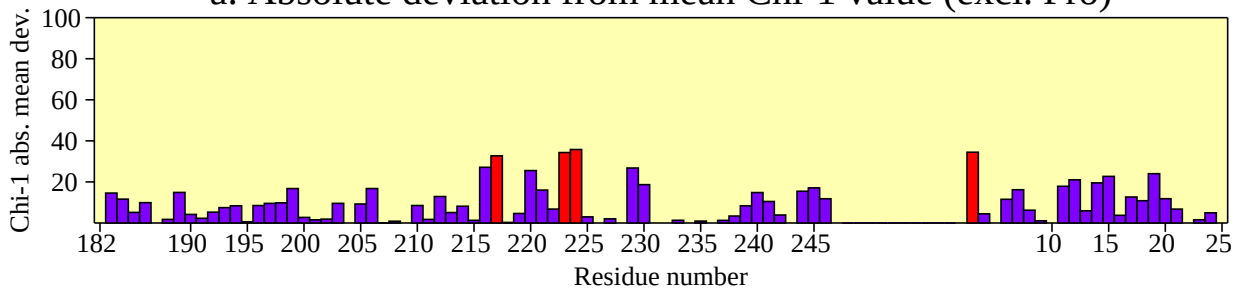


g. G-factors

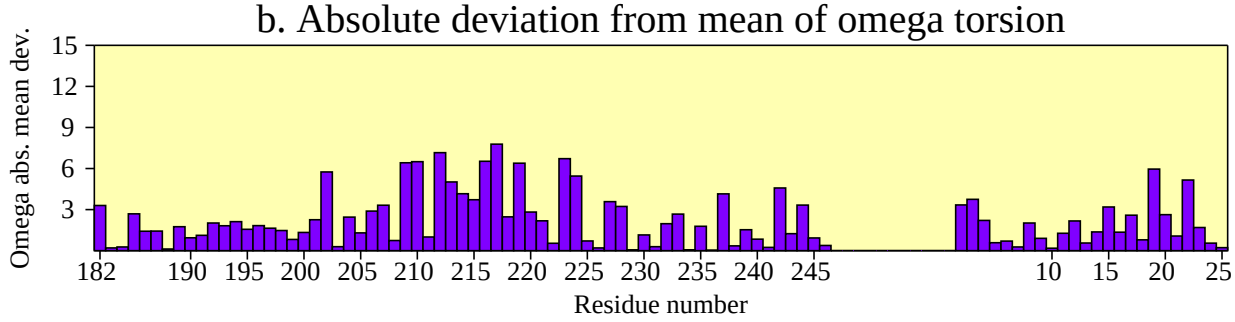


Residue properties
pdb1yq3

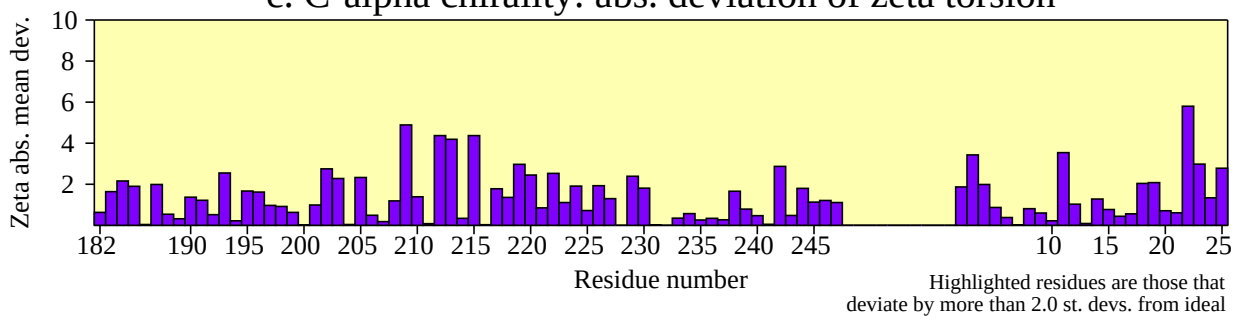
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

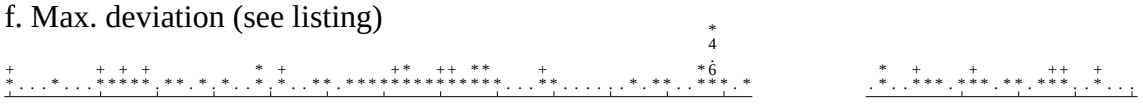
d. Secondary structure & estimated accessibility

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

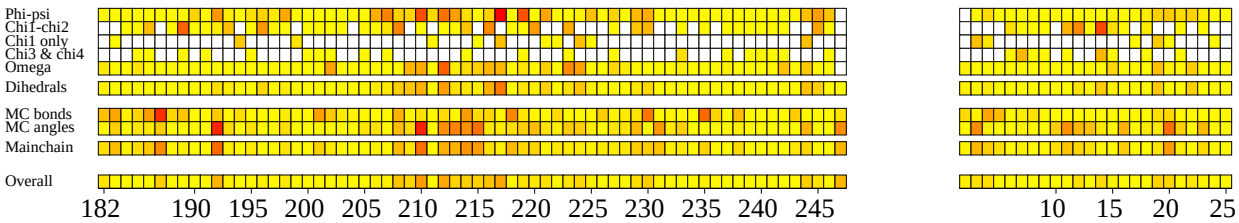
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

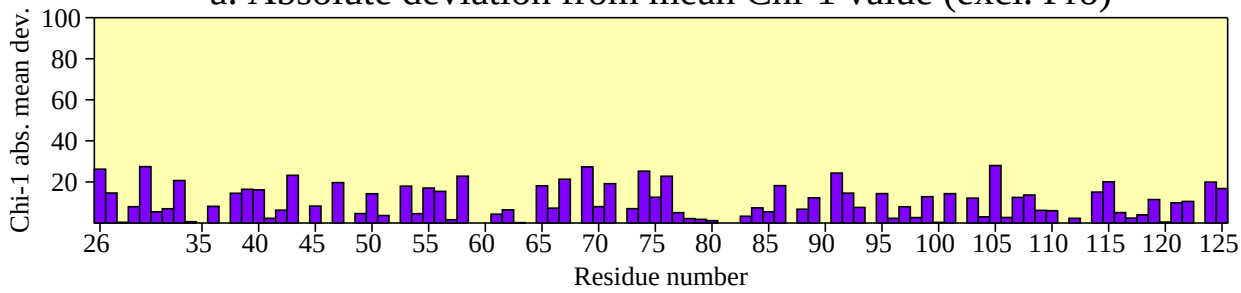


g. G-factors

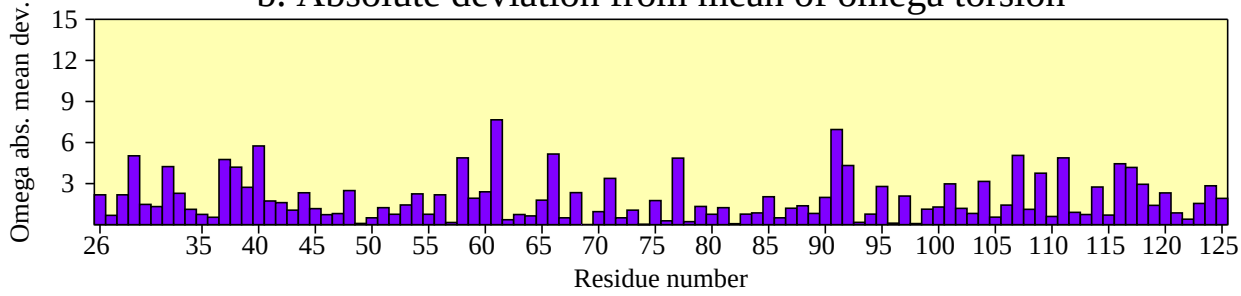


Residue properties
pdb1yq3

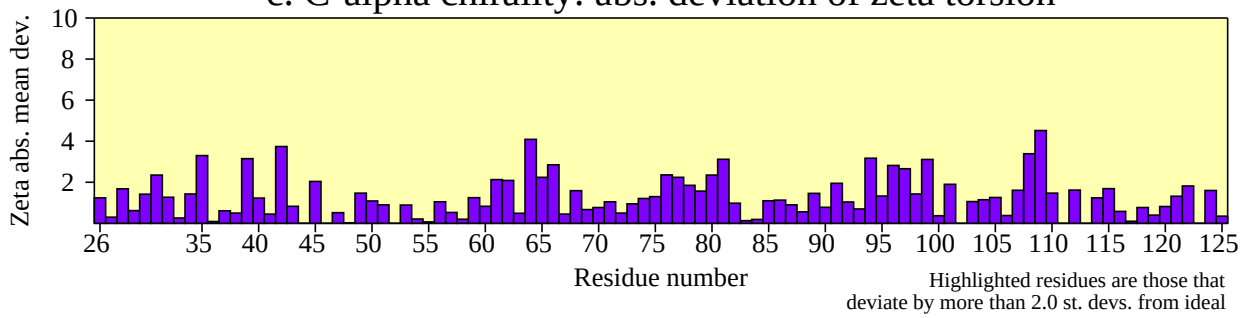
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

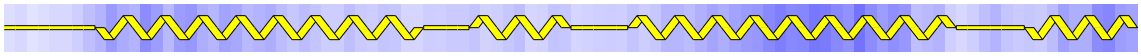


c. C-alpha chirality: abs. deviation of zeta torsion



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

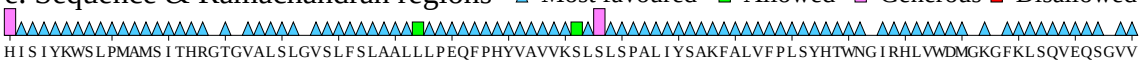
d. Secondary structure & estimated accessibility



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

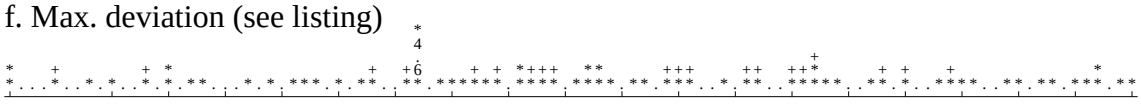
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

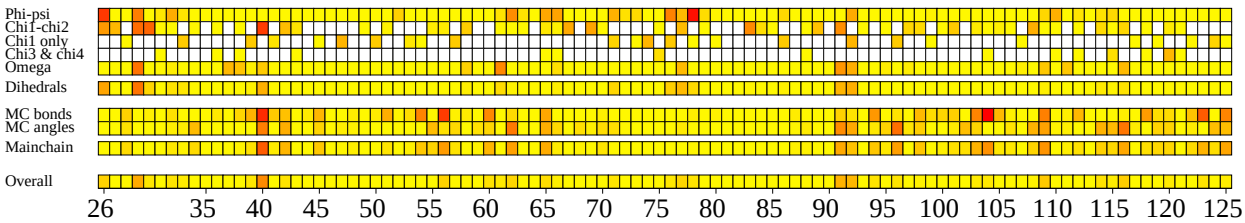


H I S I Y K W S L P M A M S I T H R G T G V A L S L G V S L F S L A A L L L P E Q F P H Y V A V V K S L S L S P A L I Y S A K F A L V F P L S Y H T W N G I R H L V W D M G K G F K L S Q V E Q S G V V

f. Max. deviation (see listing)

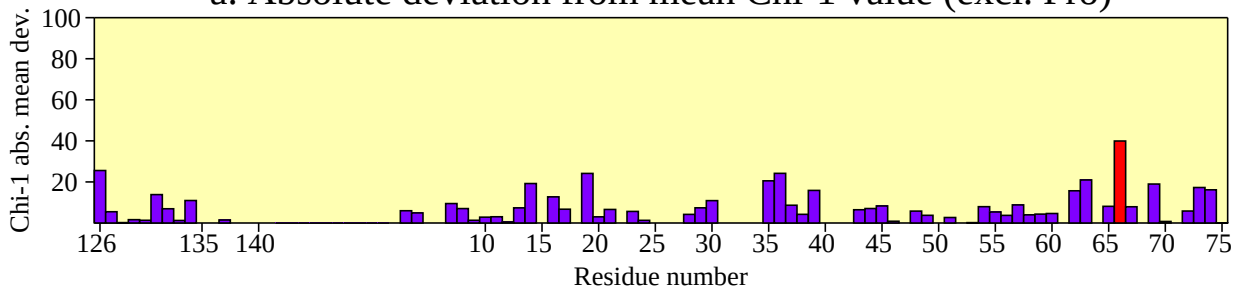


g. G-factors

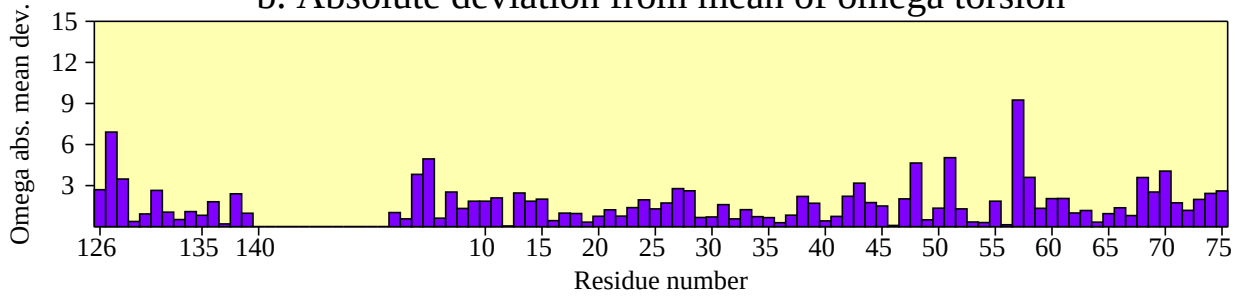


Residue properties
pdb1yq3

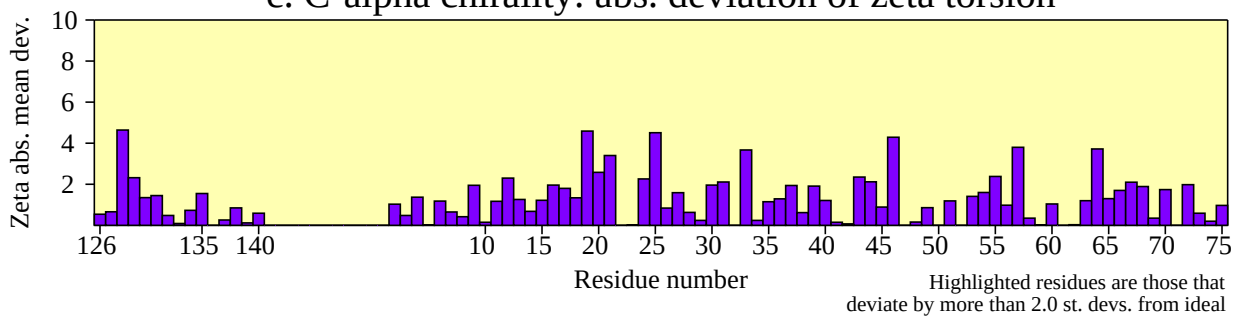
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



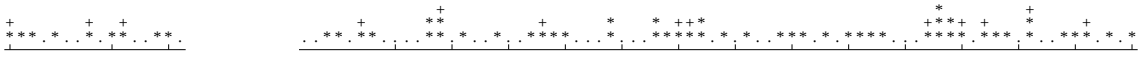
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

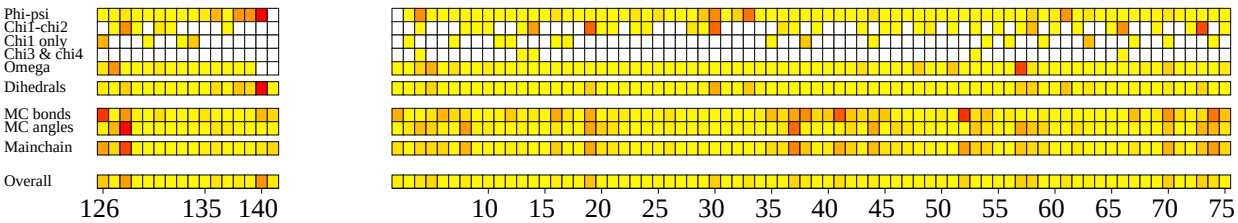
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

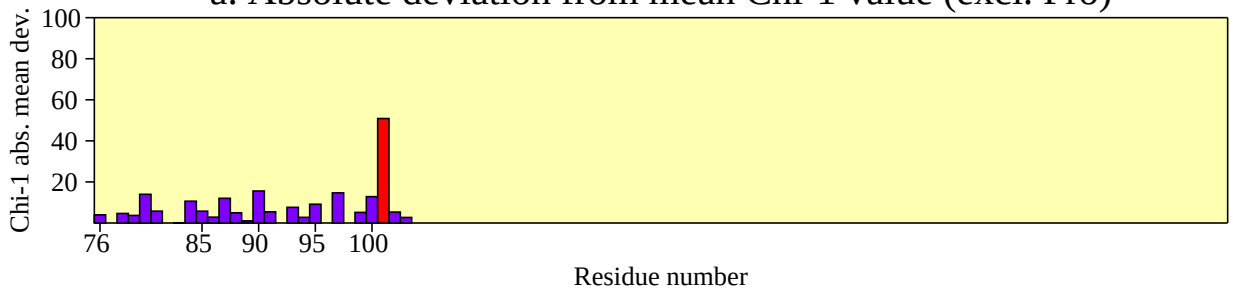


g. G-factors

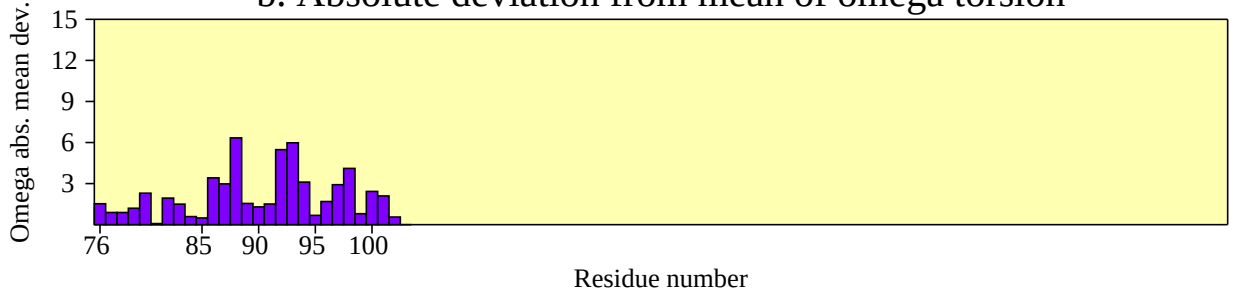


Residue properties
pdb1yq3

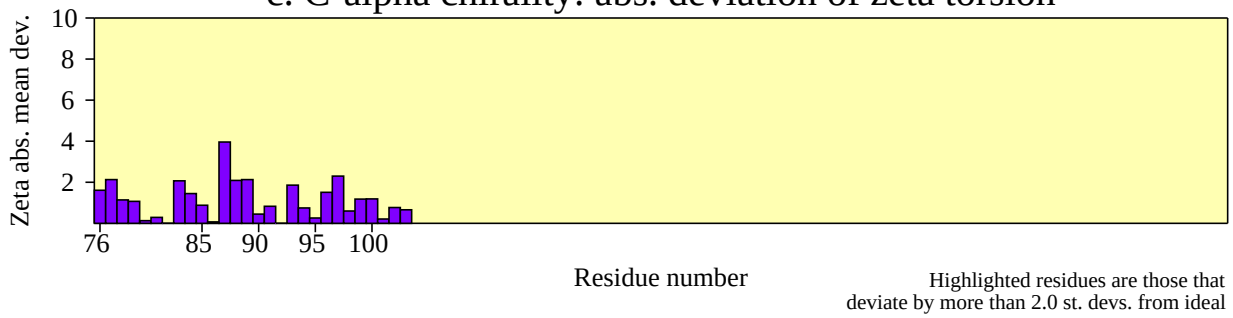
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



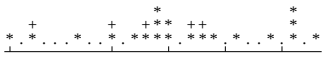
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

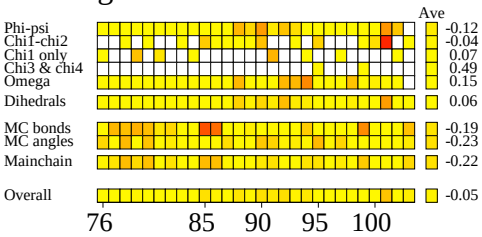
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

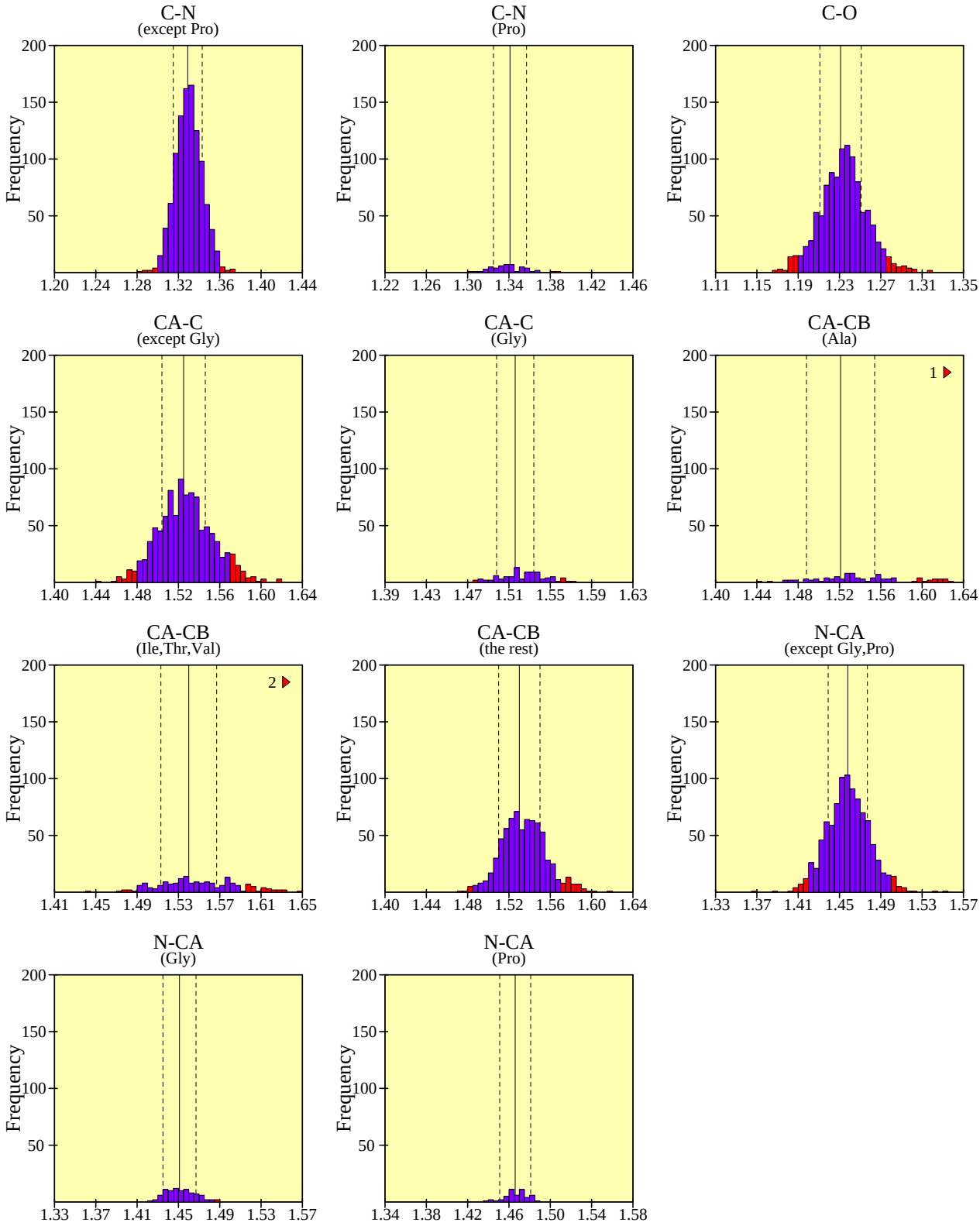


g. G-factors



Main-chain bond lengths

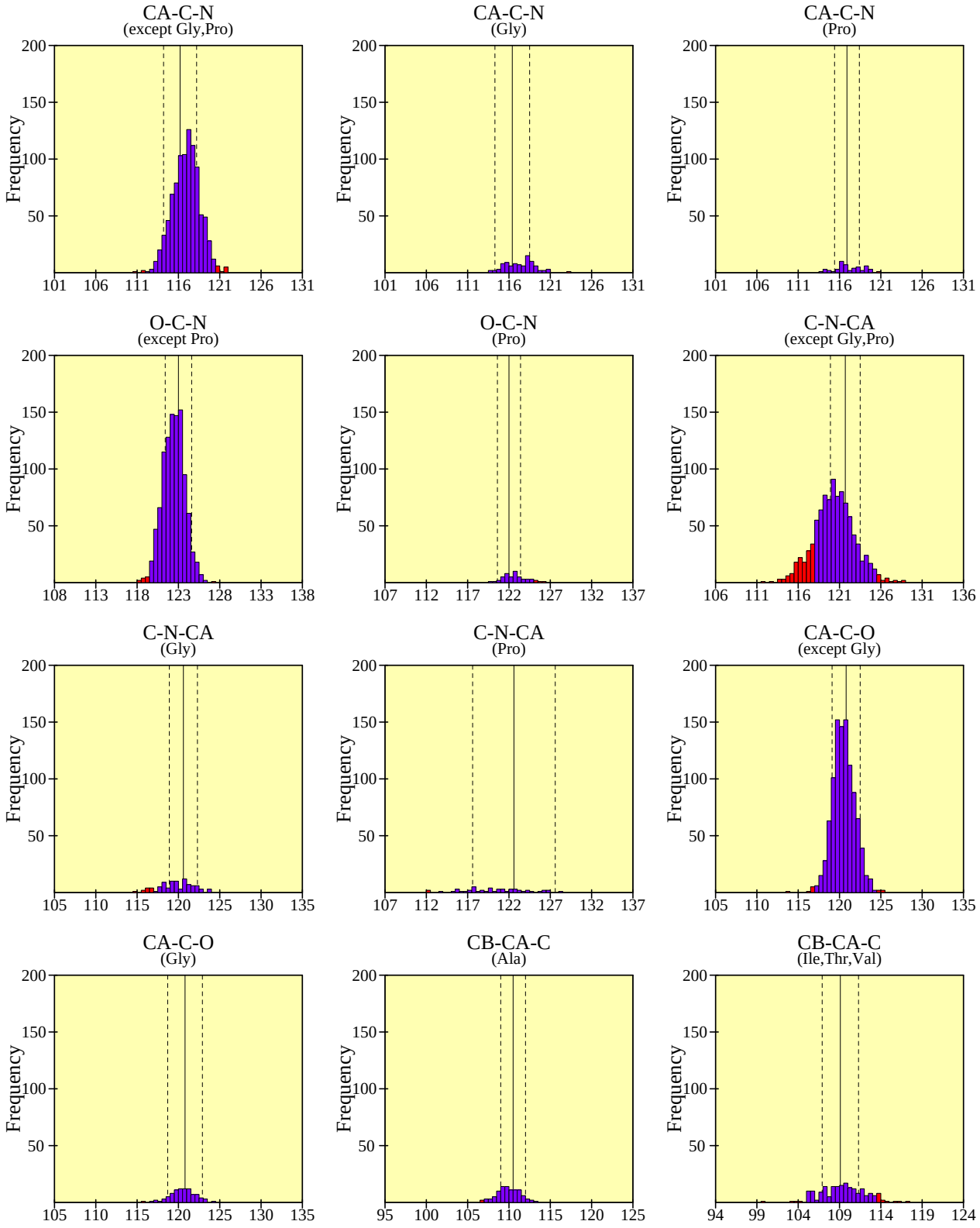
pdb1yq3



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

pdb1yq3



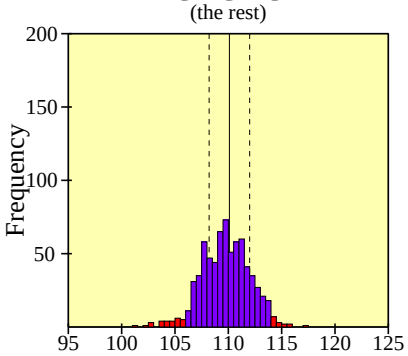
Black bars > 2.0 st. devs. from mean.

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

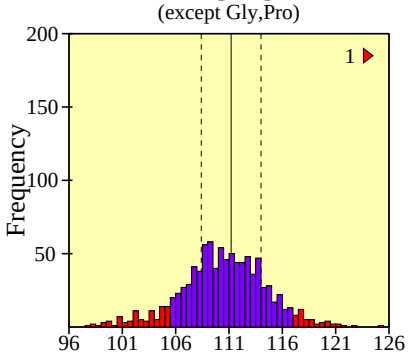
Main-chain bond angles

pdb1yq3

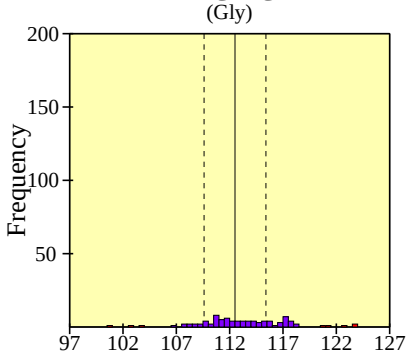
CB-CA-C
(the rest)



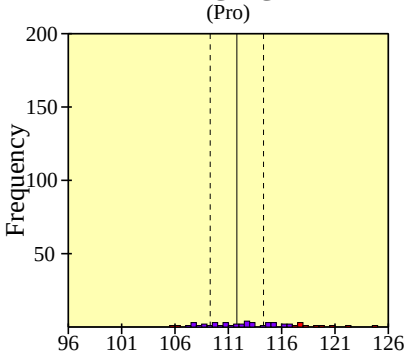
N-CA-C
(except Gly,Pro)



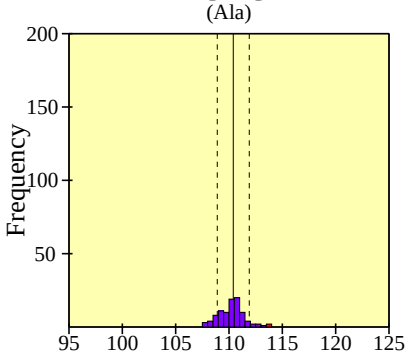
N-CA-C
(Gly)



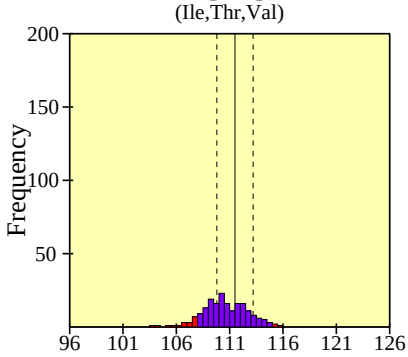
N-CA-C
(Pro)



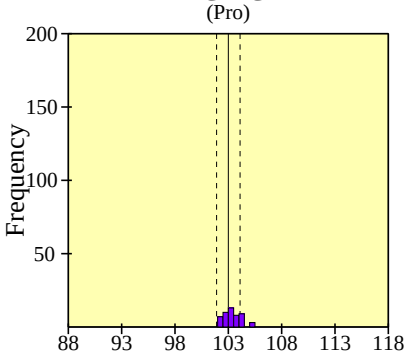
N-CA-CB
(Ala)



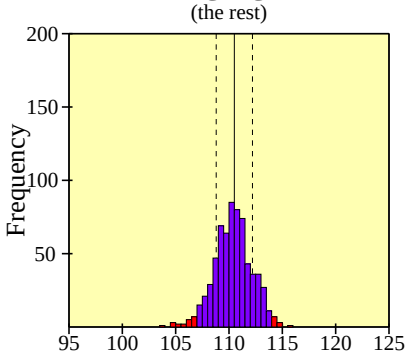
N-CA-CB
(Ile,Thr,Val)



N-CA-CB
(Pro)



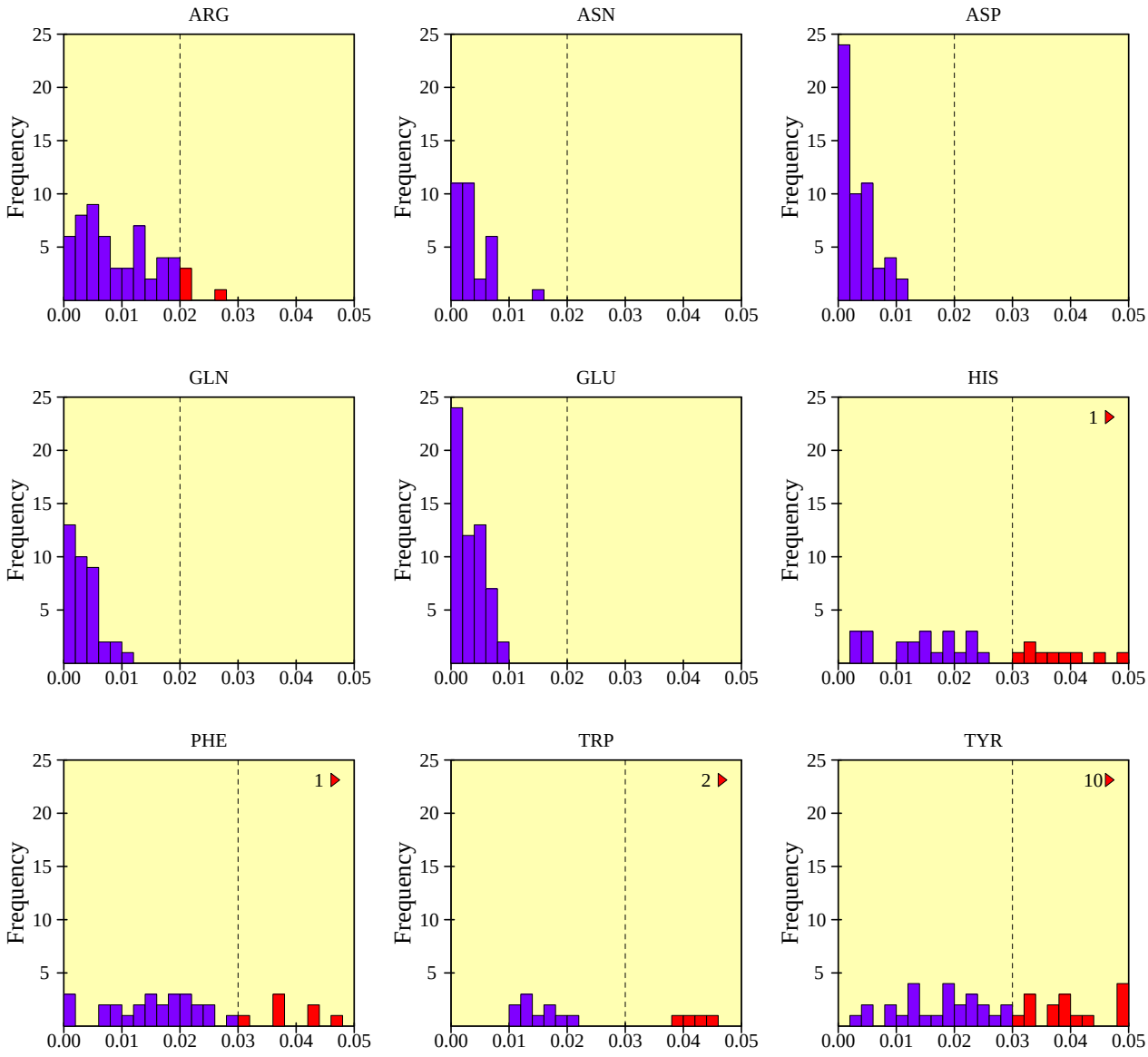
N-CA-CB
(the rest)



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

pdb1yq3

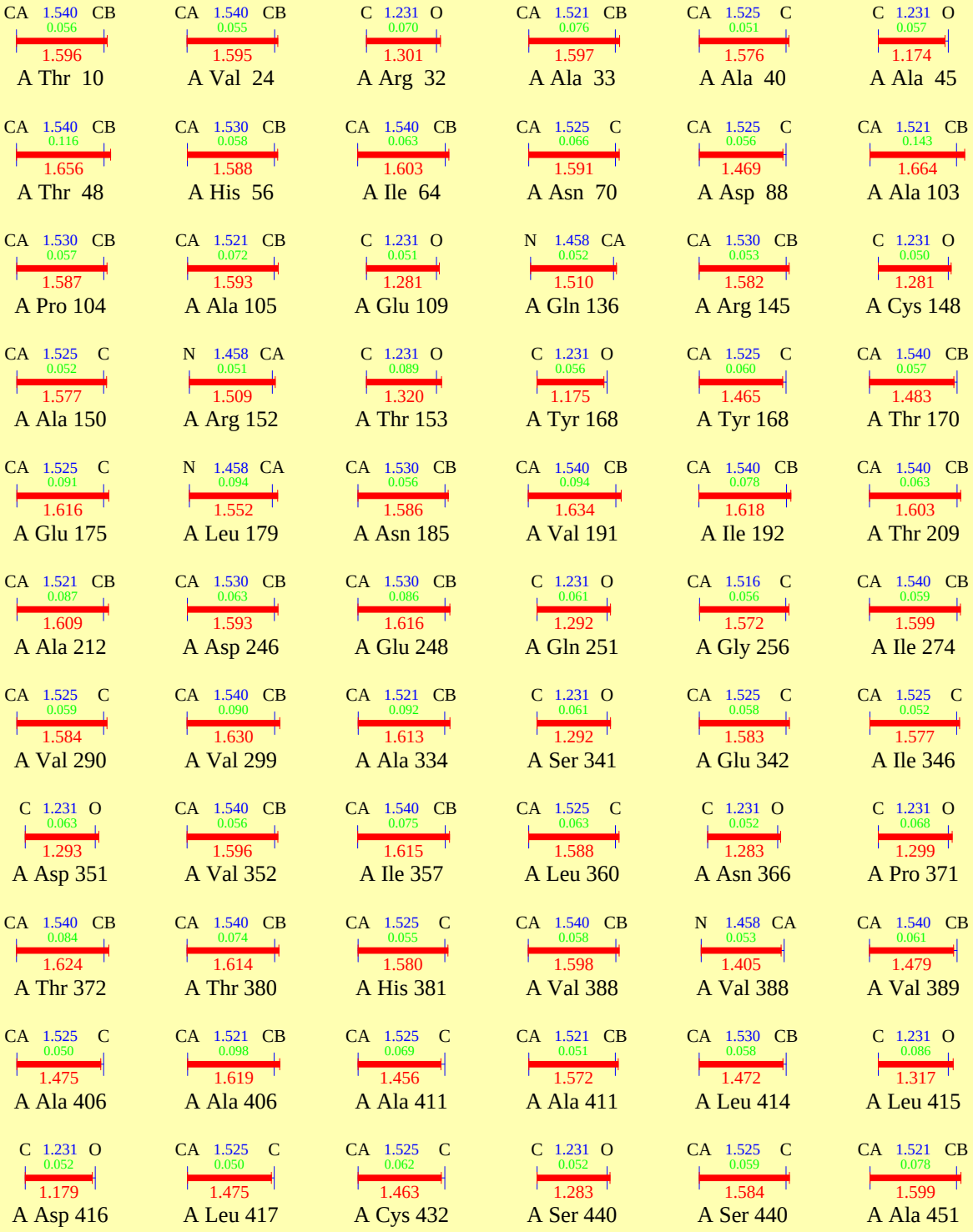


Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

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

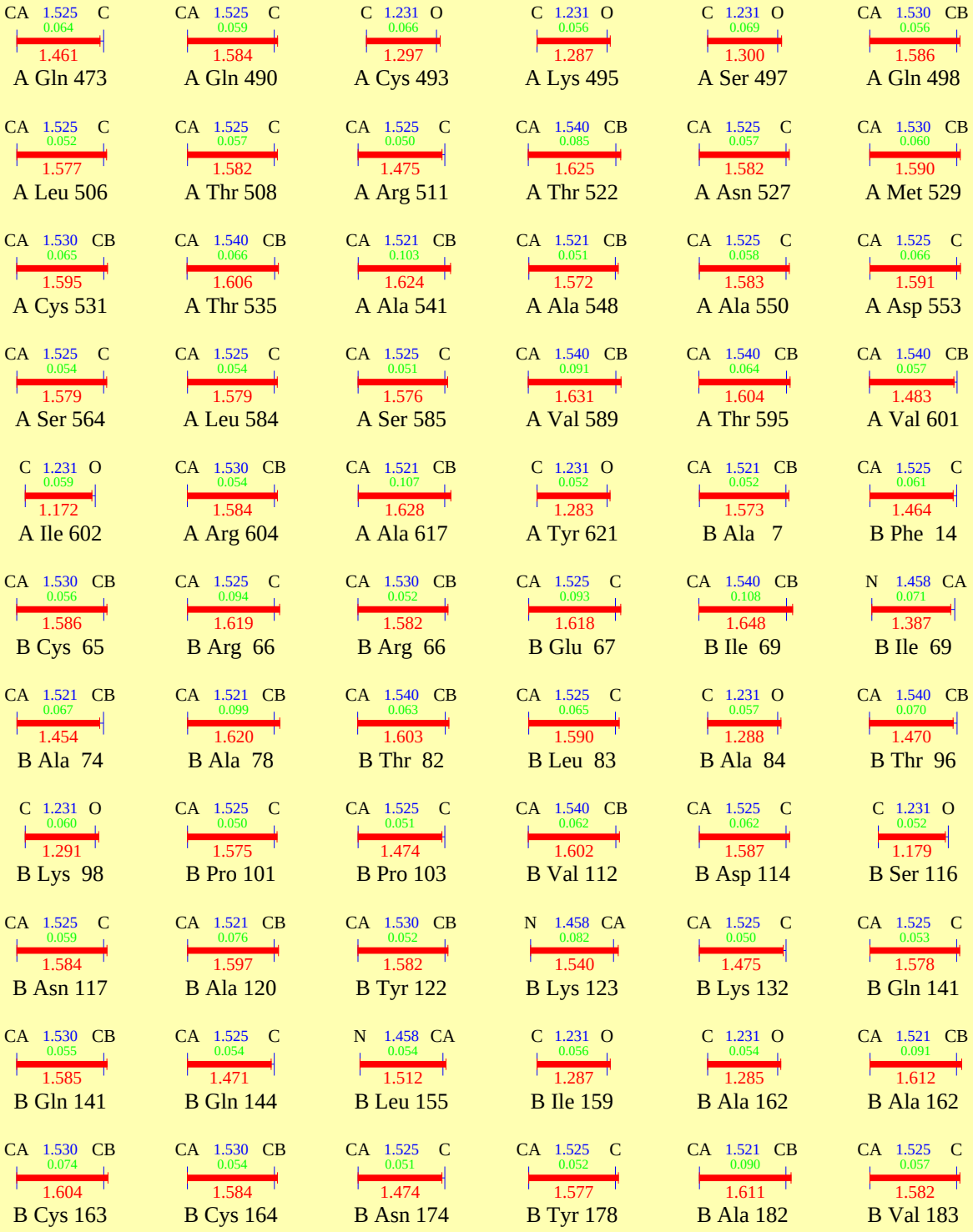
Distorted geometry
pdb1yq3

Main-chain bond lengths



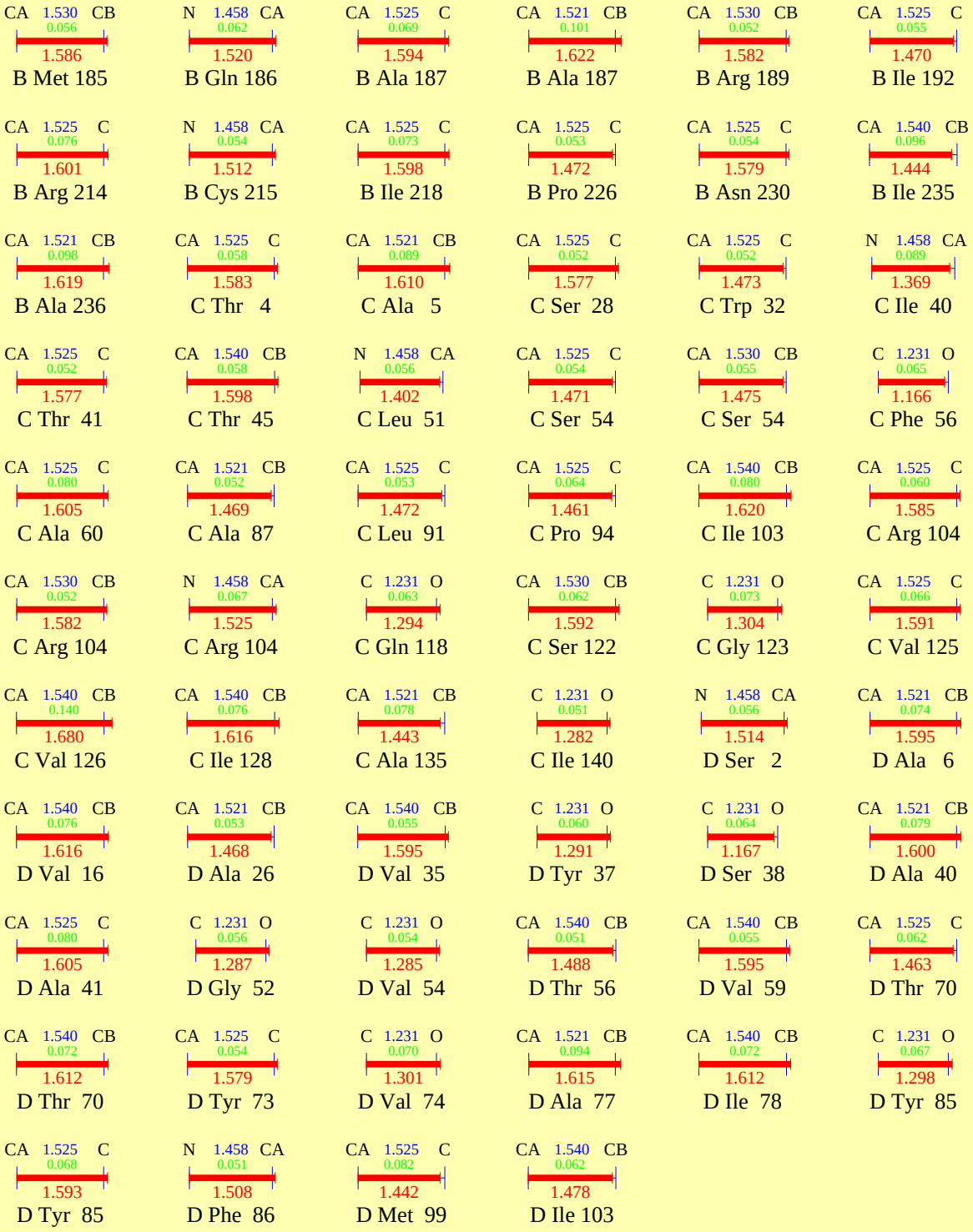
Distorted geometry
pdb1yq3

Main-chain bond lengths (contd)



Distorted geometry
pdb1yq3

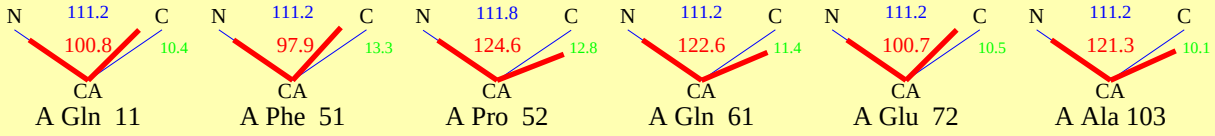
Main-chain bond lengths (contd)



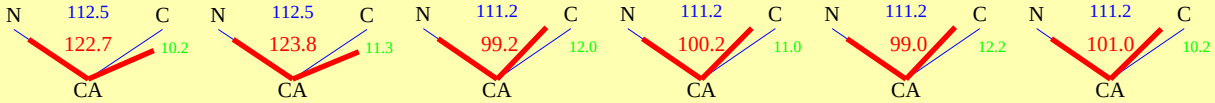
Bonds differing by > 0.05A from small-molecule values. Values shown: "ideal", difference, actual

Distorted geometry
pdb1yq3

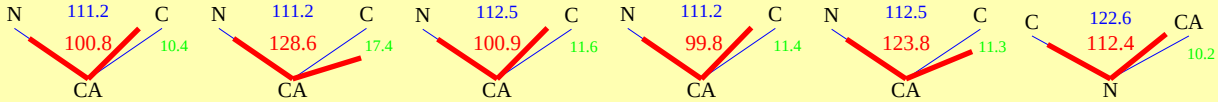
Main-chain bond angles



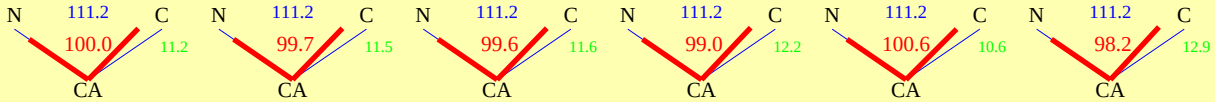
A Gln 11 | A Phe 51 | A Pro 52 | A Gln 61 | A Glu 72 | A Ala 103



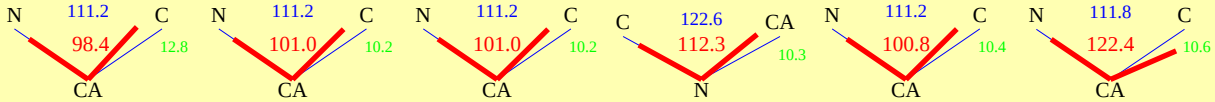
A Gly 131 | A Gly 140 | A Val 149 | A Phe 173 | A Tyr 176 | A Thr 219



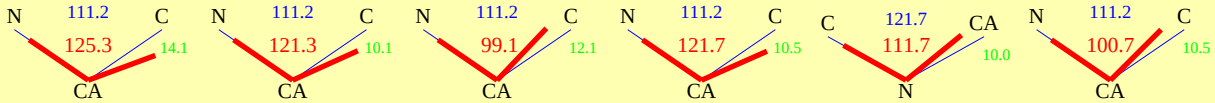
A Cys 244 | A Thr 255 | A Gly 256 | A Arg 282 | A Gly 311 | A Pro 329 - A Pro 330



A Asp 351 | A Thr 380 | A Glu 544 | A Tyr 554 | A Gln 570 | A Asp 588



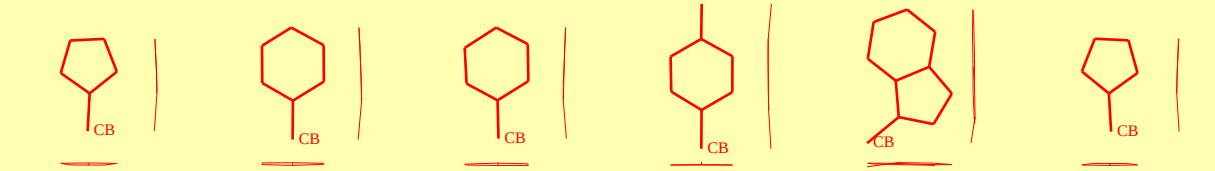
A Ser 613 | B Arg 10 | B Phe 14 | B Asp 20 - B Pro 21 | B Lys 23 | B Pro 103



B Phe 210 | B Tyr 213 | C Thr 3 | C Leu 62 | C Leu 127 - C Ile 128 | D Leu 8

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

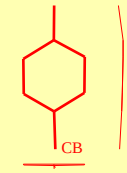
Planar groups



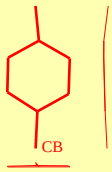
0.039 A His 17 | 0.047 A Phe 35 | 0.043 A Phe 51 | 0.050 A Tyr 81 | 0.046 A Trp 89 | 0.036 A His 97

Distorted geometry
pdb1yq3

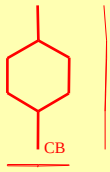
Planar groups (contd)



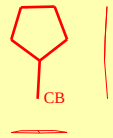
0.065
A Tyr 98



0.060
A Tyr 113

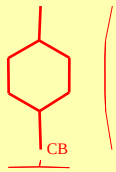


0.033
A Tyr 126

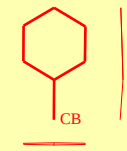


0.045
A His 144

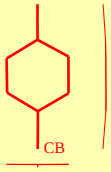
0.021
A Arg 164



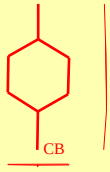
0.119
A Tyr 172



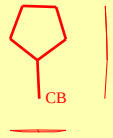
0.038
A Phe 173



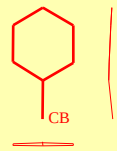
0.048
A Tyr 176



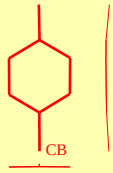
0.038
A Tyr 216



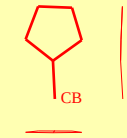
0.035
A His 227



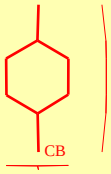
0.055
A Phe 252



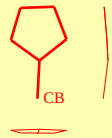
0.051
A Tyr 287



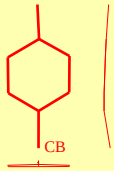
0.033
A His 320



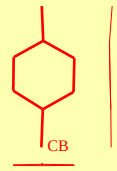
0.071
A Tyr 322



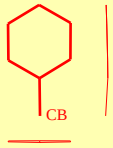
0.069
A His 364



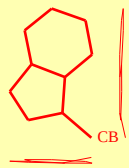
0.083
A Tyr 365



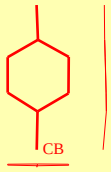
0.033
A Tyr 374



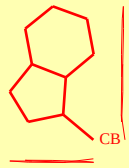
0.030
A Phe 509



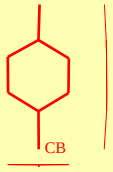
0.069
A Trp 515



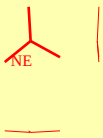
0.040
A Tyr 554



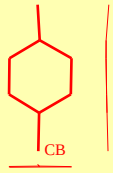
0.043
A Trp 579



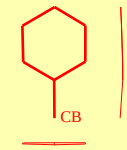
0.039
B Tyr 17



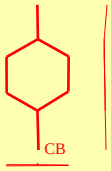
0.027
B Arg 18



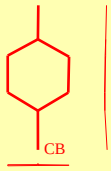
0.037
B Tyr 33



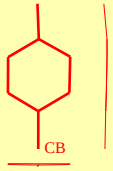
0.037
B Phe 61



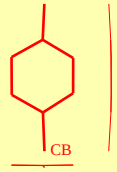
0.036
B Tyr 119



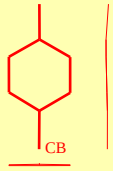
0.032
B Tyr 128



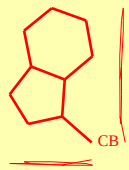
0.042
B Tyr 142



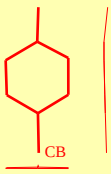
0.040
B Tyr 156



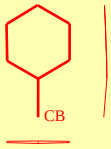
0.031
B Tyr 171



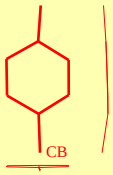
0.066
B Trp 173



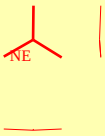
0.049
B Tyr 198



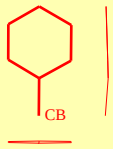
0.043
C Phe 12



0.079
C Tyr 30



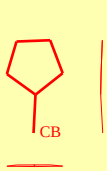
0.021
C Arg 43



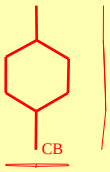
0.037
C Phe 67

Distorted geometry
pdb1yq3

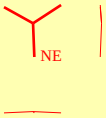
Planar groups (contd)



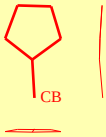
0.030
C His 69



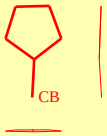
0.049
C Tyr 97



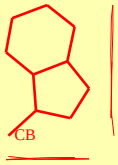
0.022
C Arg 104



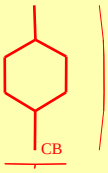
0.050
C His 105



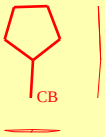
0.033
D His 48



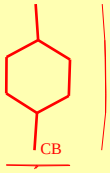
0.039
D Trp 49



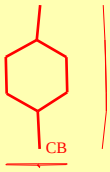
0.077
D Tyr 58



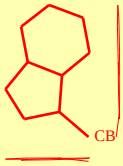
0.041
D His 60



0.060
D Tyr 73



0.056
D Tyr 85



0.041
D Trp 101

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