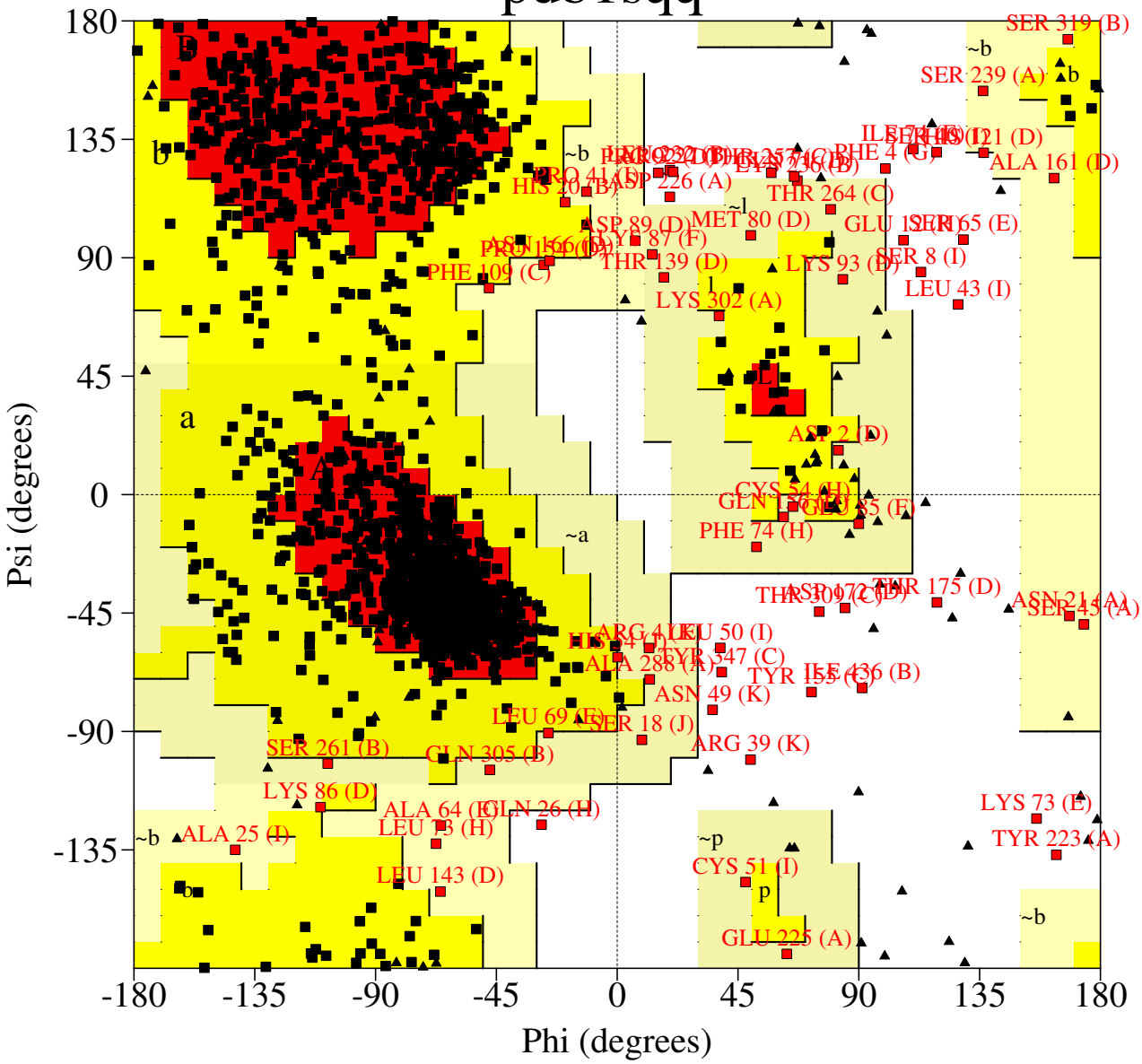
Ramachandran Plot

pdb1sqq



Plot statistics

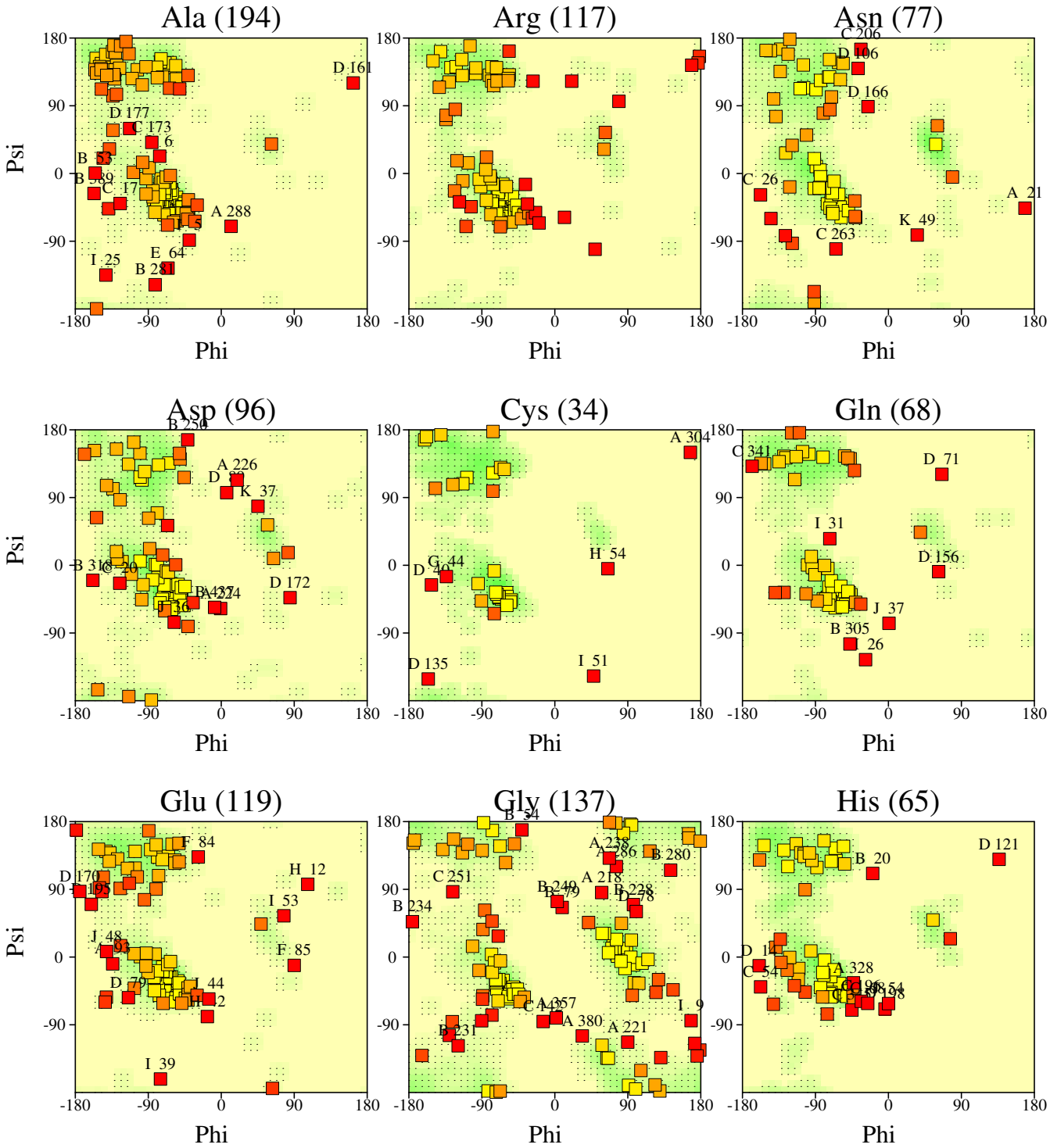
Residues in most favoured regions [A,B,L]	1526	83.1%
Residues in additional allowed regions [a,b,l,p]	251	13.7%
Residues in generously allowed regions [~a,~b,~l,~p]	35	1.9%
Residues in disallowed regions	25	1.4%
	----	------
Number of non-glycine and non-proline residues	1837	100.0%
Number of end-residues (excl. Gly and Pro)	18	
Number of glycine residues (shown as triangles)	140	
Number of proline residues	109	

Total number of residues	2104	

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

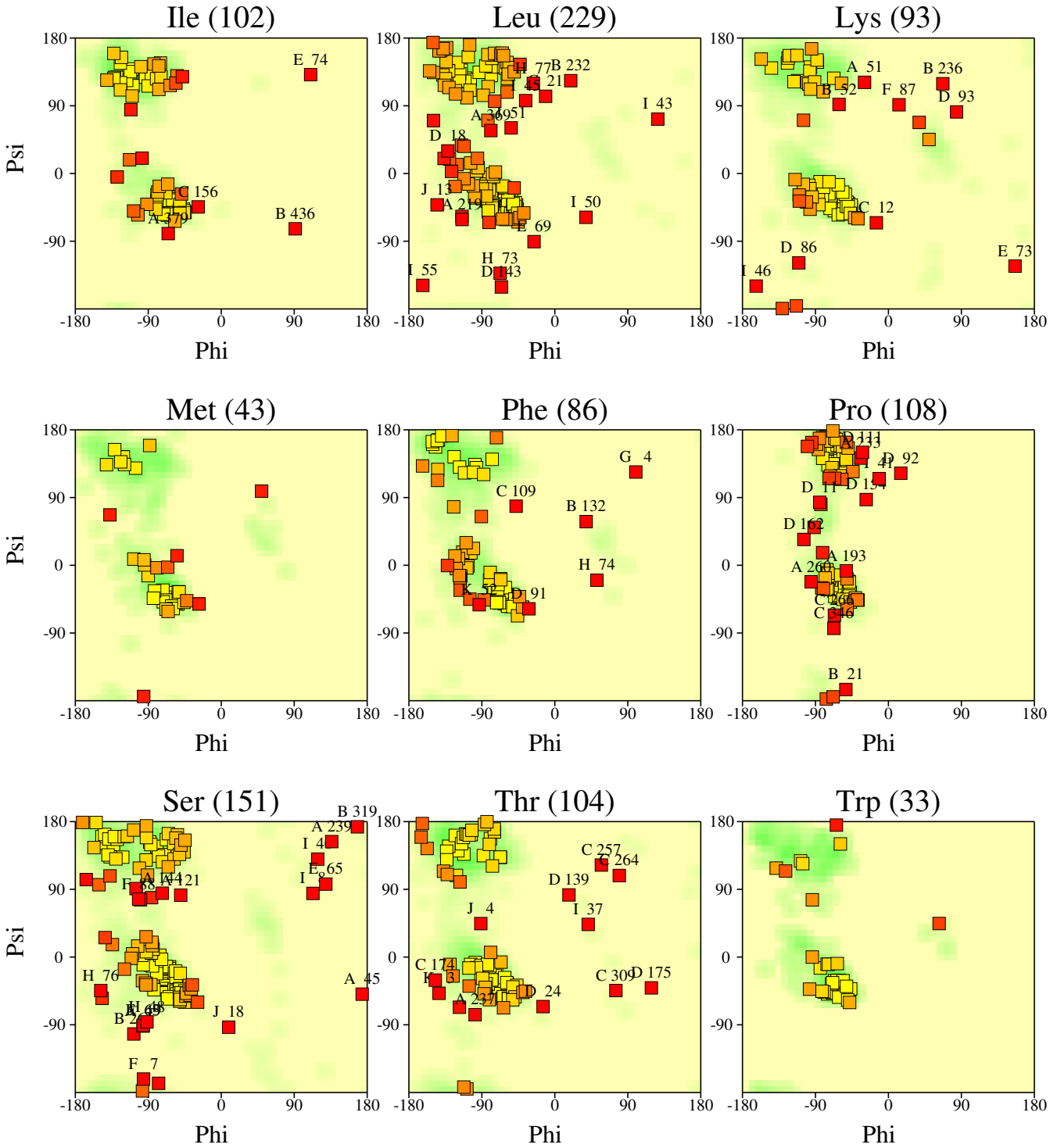
pdb1sqq



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

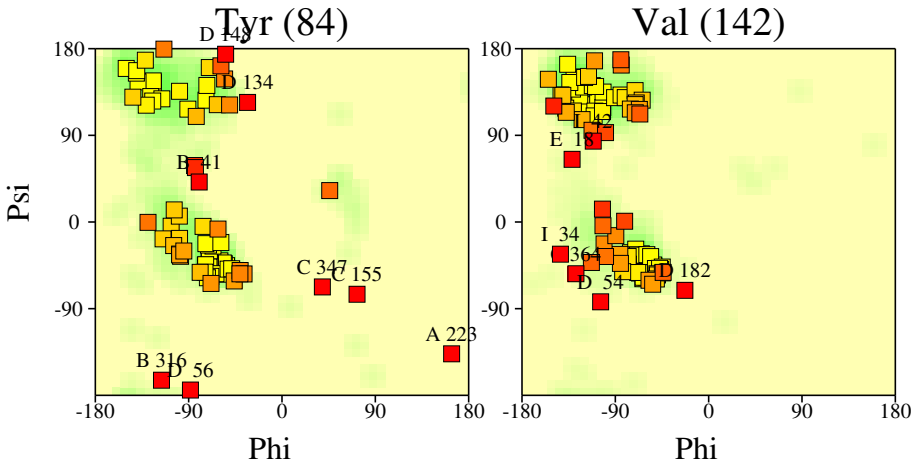
pdb1sqq



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

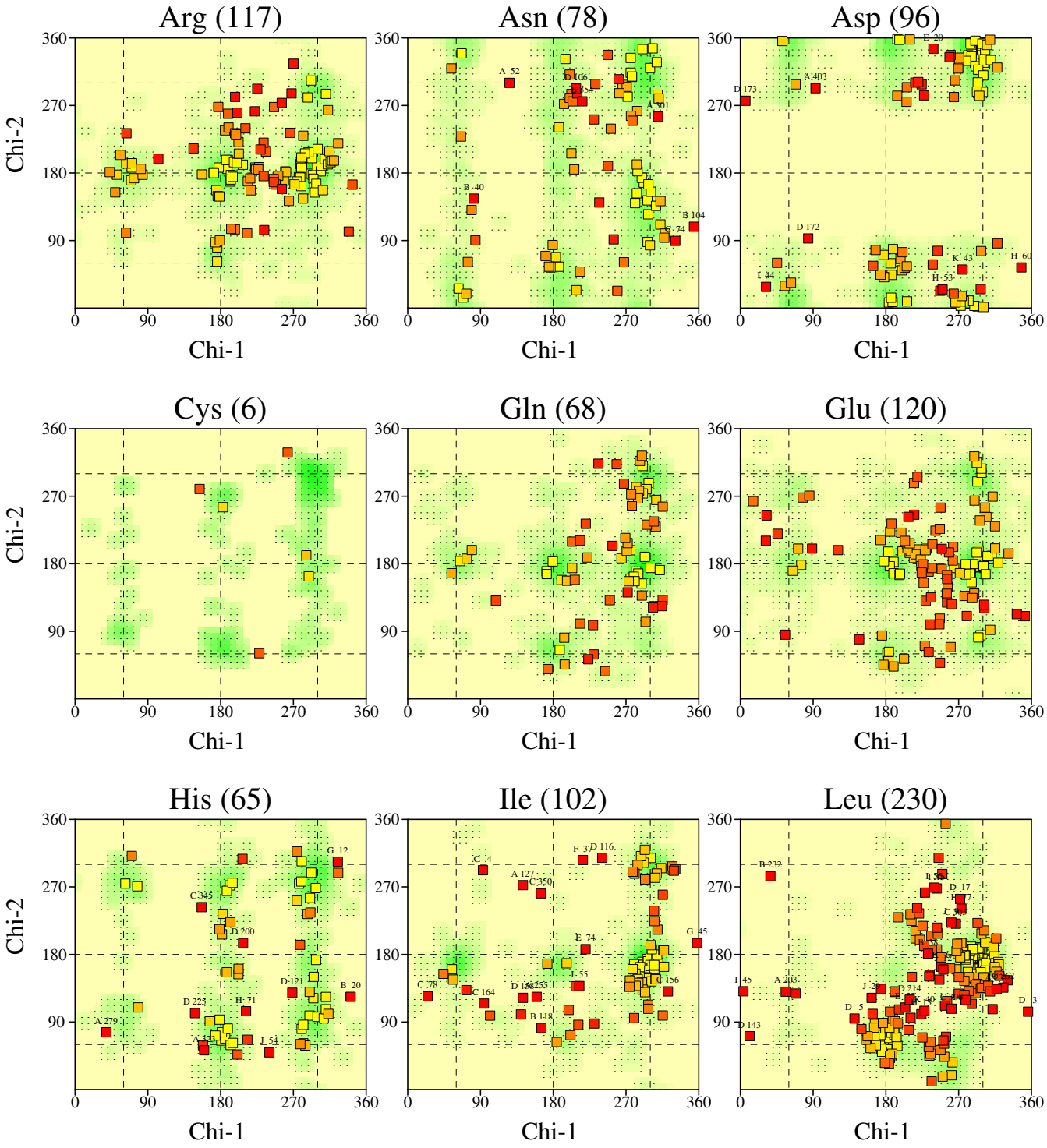
pdb1sqq



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

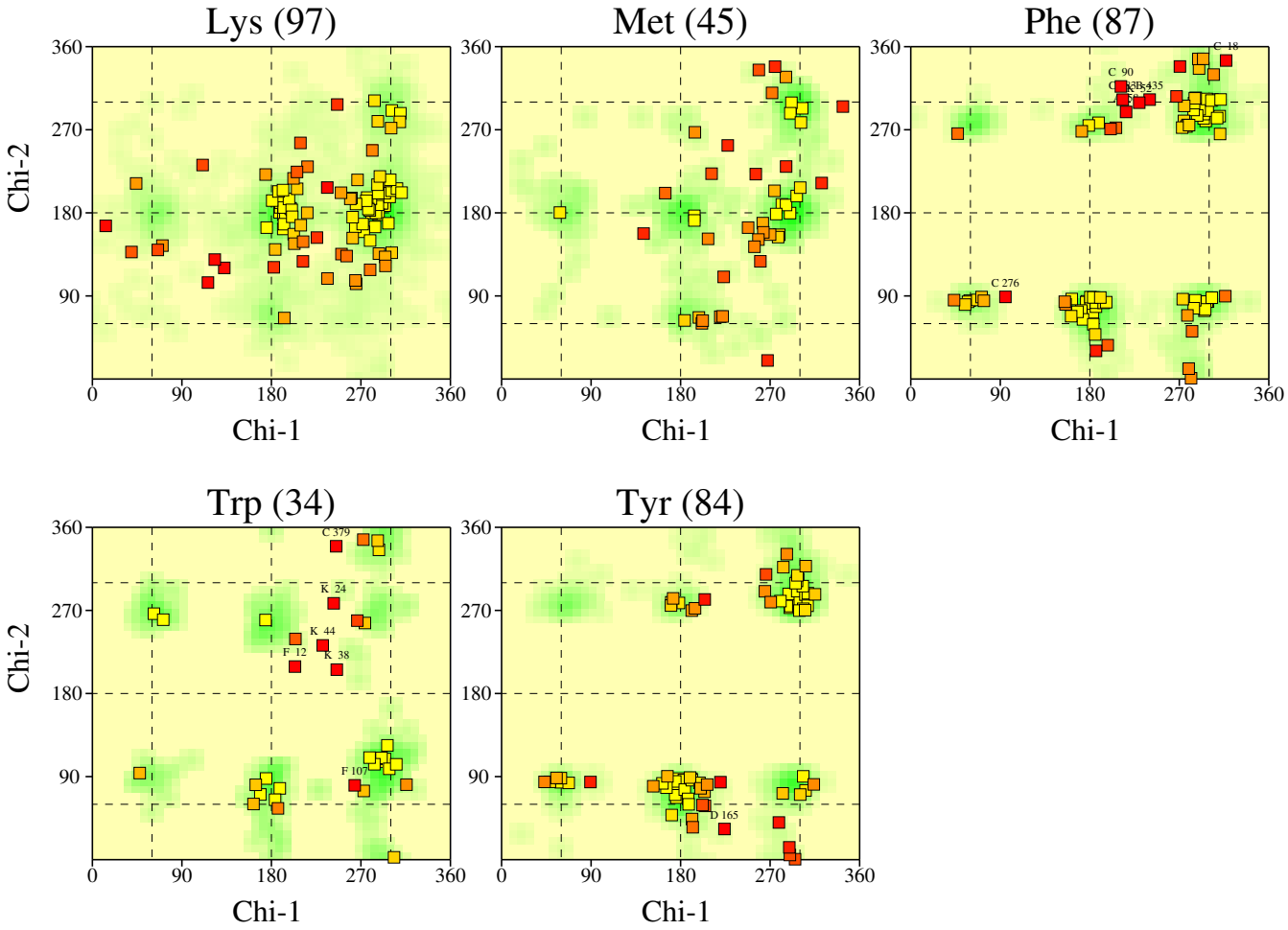
pdb1sqq



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

pdb1sqq



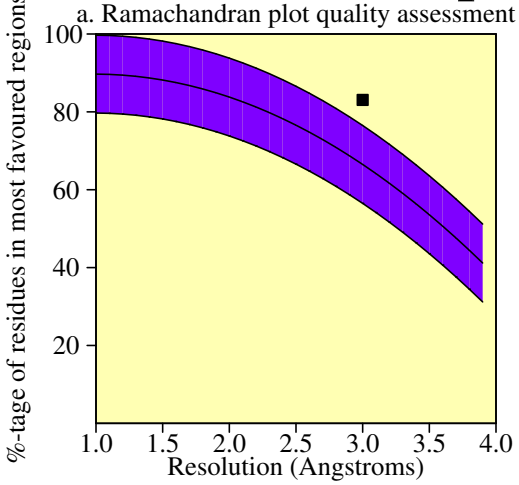
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

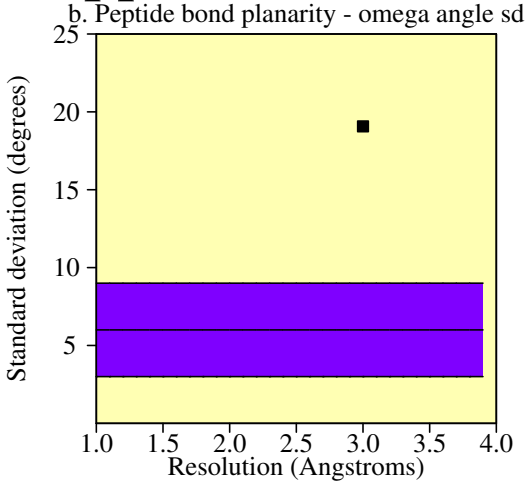
Main-chain parameters

pdb1sqq

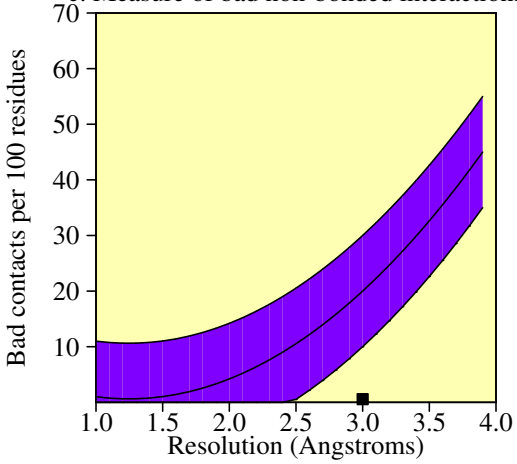
a. Ramachandran plot quality assessment



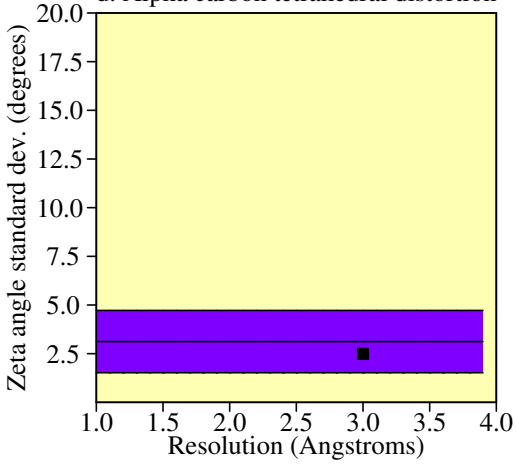
b. Peptide bond planarity - omega angle sd



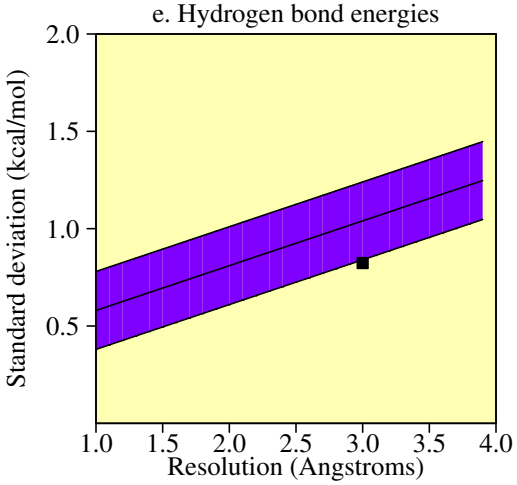
c. Measure of bad non-bonded interactions



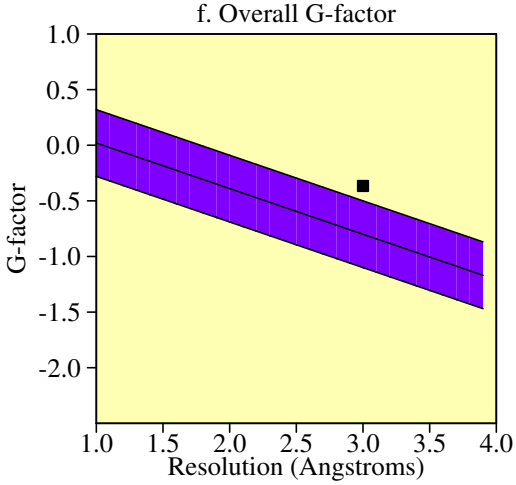
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor



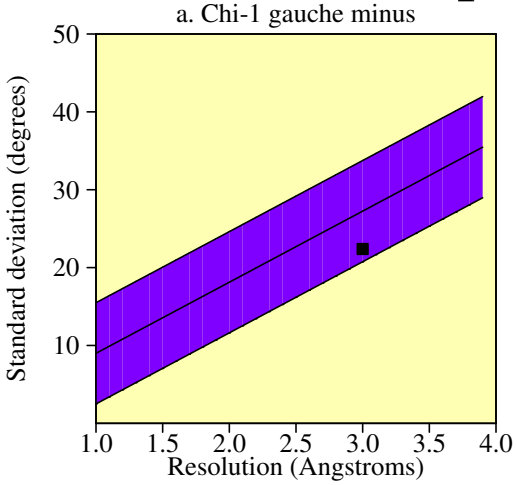
Plot statistics

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	1837	83.1	66.5	10.0	1.7	BETTER
b. Omega angle st dev	2092	19.1	6.0	3.0	4.4	WORSE
c. Bad contacts / 100 residues	12	0.6	20.0	10.0	-1.9	BETTER
d. Zeta angle st dev	1964	2.5	3.1	1.6	-0.4	Inside
e. H-bond energy st dev	1372	0.8	1.0	0.2	-1.1	BETTER
f. Overall G-factor	2104	-0.4	-0.8	0.3	1.4	BETTER

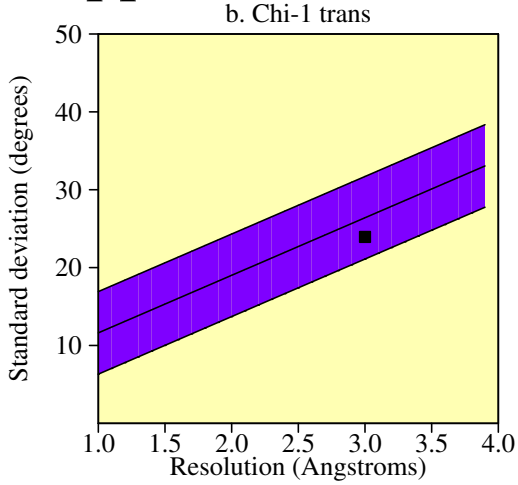
Side-chain parameters

pdb1sqq

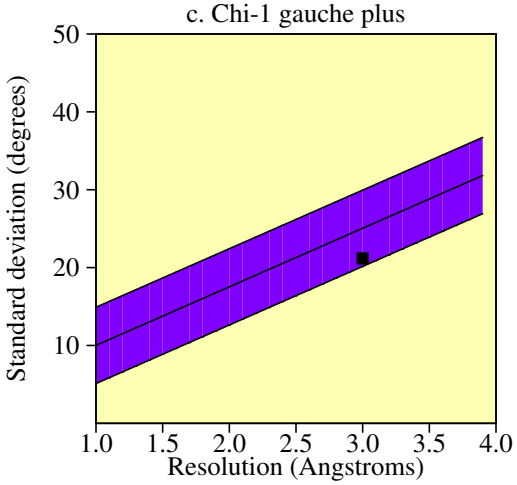
a. Chi-1 gauche minus



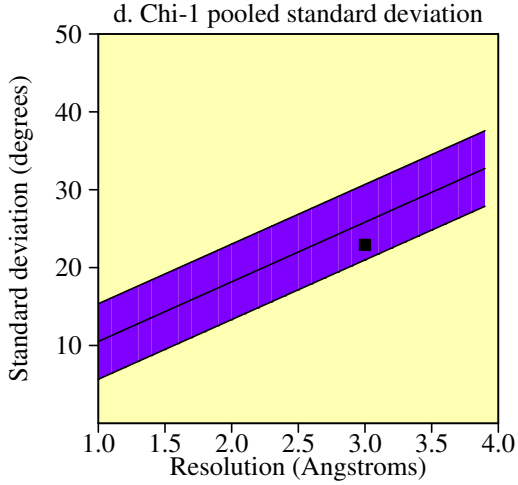
b. Chi-1 trans



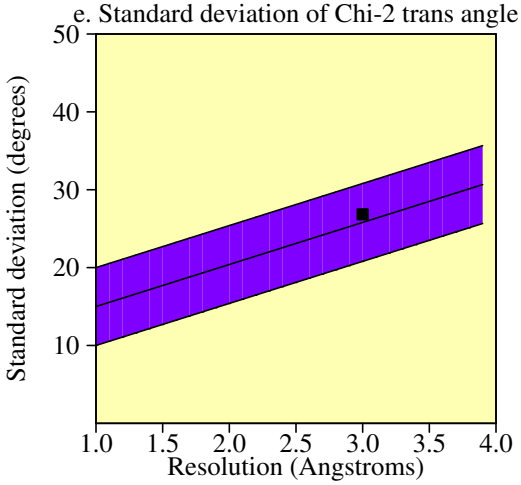
c. Chi-1 gauche plus



d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



pdb1sqq

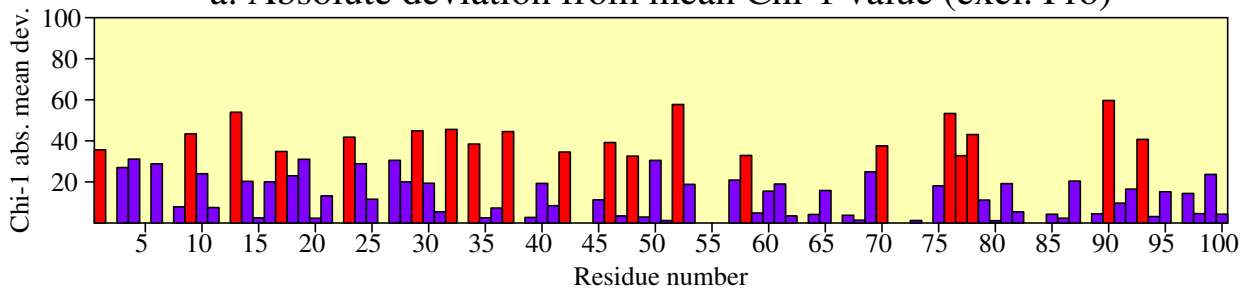
Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. Chi-1 gauche minus st dev	221	22.4	27.2	6.5	-0.7	Inside
b. Chi-1 trans st dev	615	23.9	26.4	5.3	-0.5	Inside
c. Chi-1 gauche plus st dev	824	21.2	25.0	4.9	-0.8	Inside
d. Chi-1 pooled st dev	1660	22.9	25.8	4.8	-0.6	Inside
e. Chi-2 trans st dev	536	26.8	25.8	5.0	0.2	Inside

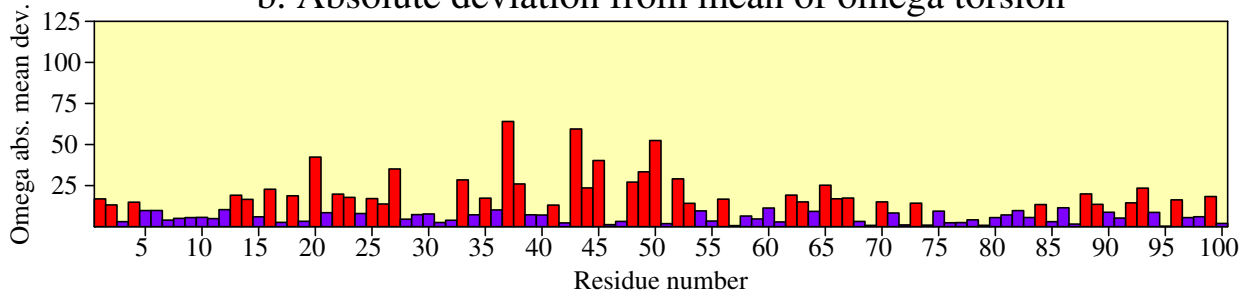
Residue properties

pdb1sqq

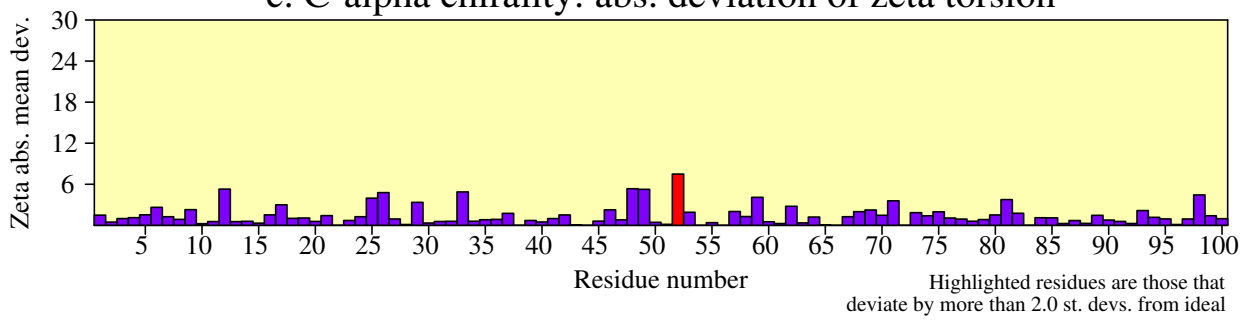
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

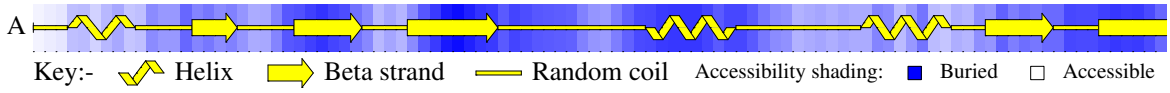


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

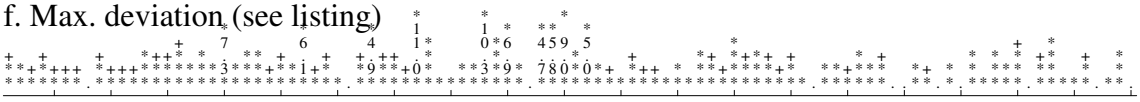


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

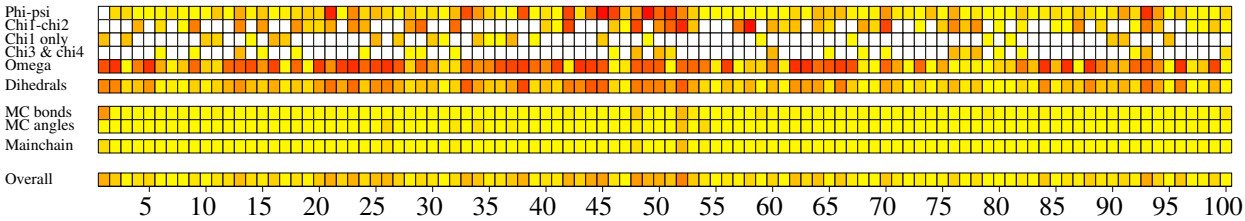
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)



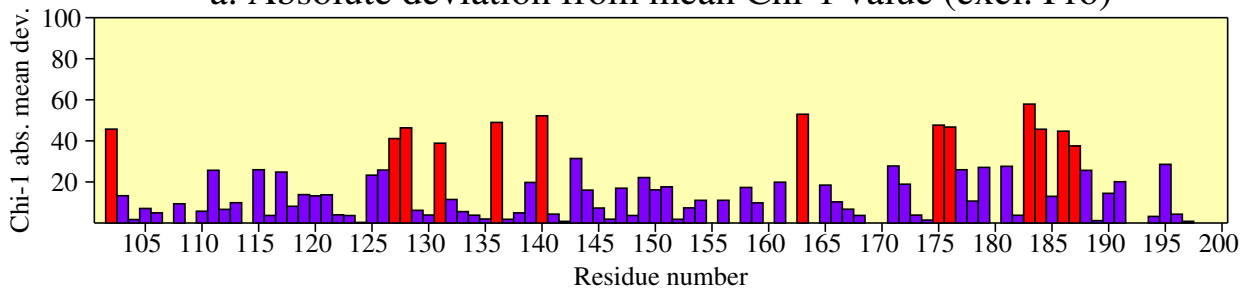
g. G-factors



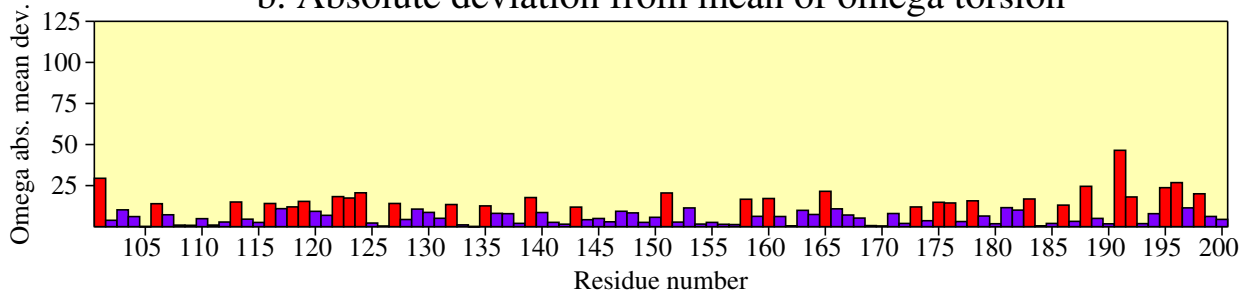
Residue properties

pdb1sqq

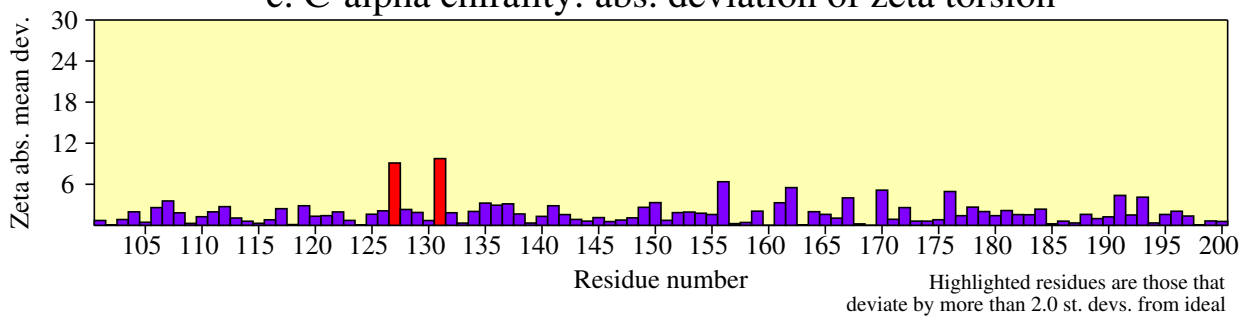
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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

d. Secondary structure & estimated accessibility

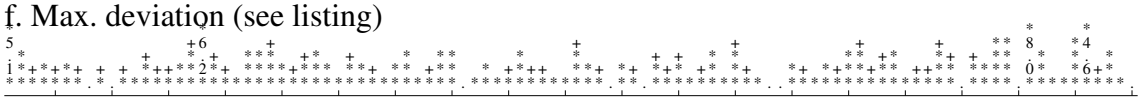
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

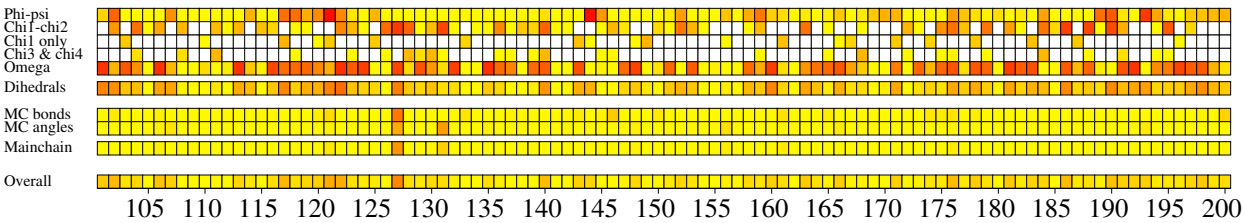
Most favoured Allowed Generous Disallowed

ALSKDLPKAVELLADIVQNCSLEDSQIEKERDVILQELQENDTSMRDVVFNYLHATAFQGTPLAQSVEGPSENVRKLSRADLTEYLSRHYKAPRMVLAAA

f. Max. deviation (see listing)



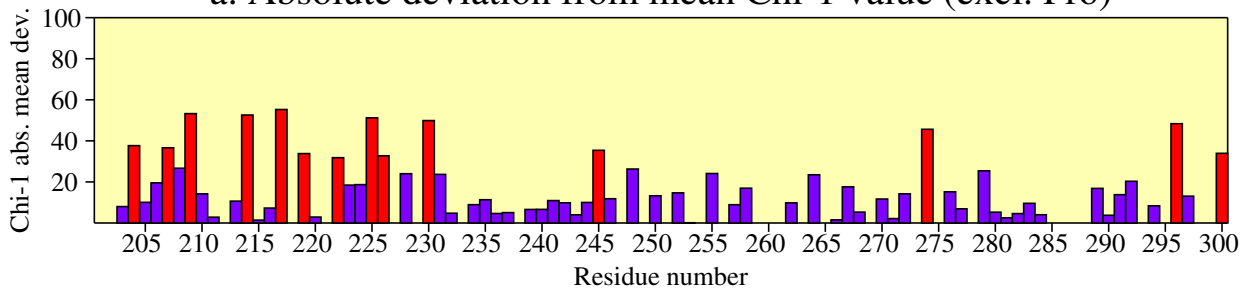
g. G-factors



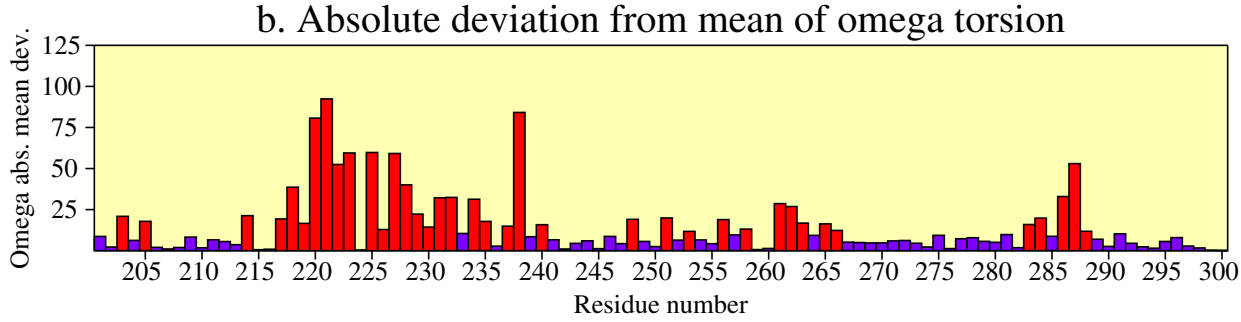
Residue properties

pdb1sqq

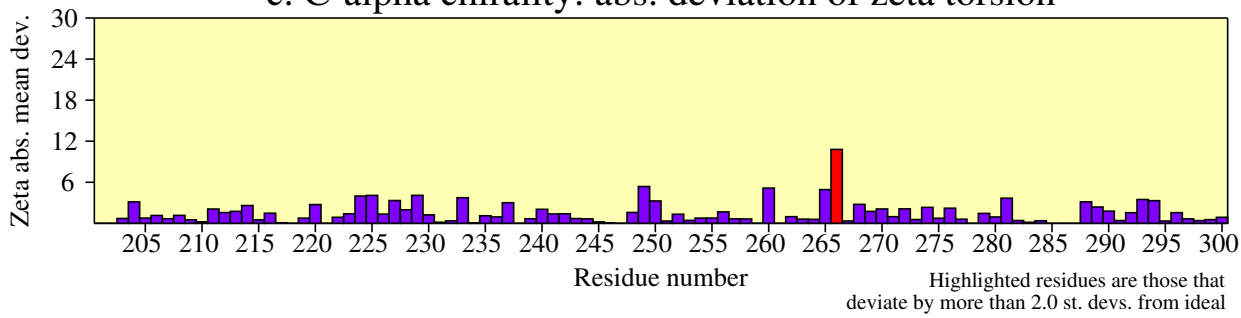
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

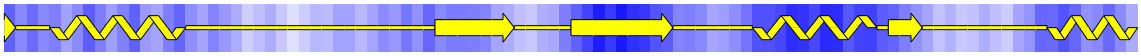


c. C-alpha chirality: abs. deviation of zeta torsion



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

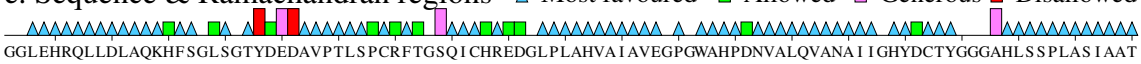
d. Secondary structure & estimated accessibility



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

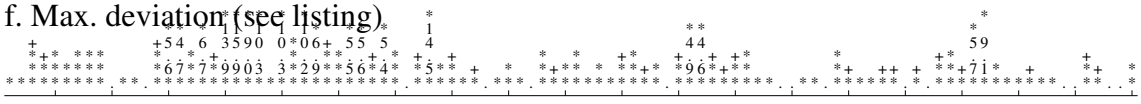
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

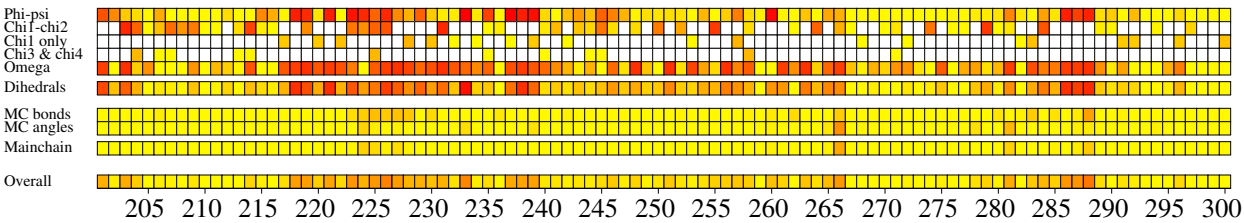


GGLEHRQLLDLAQKHFSGLSGTYDEDAVPTLSPCRFTGSQICHREDGLPLAHVAIAVEGPGWAHPDNVALQVANAIIGHYDCTYGGGAHLSSPLASIAAT

f. Max. deviation (see listing)

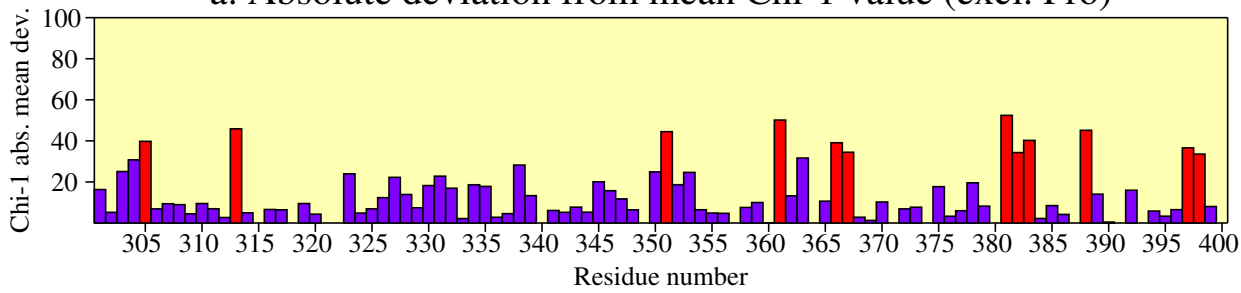


g. G-factors

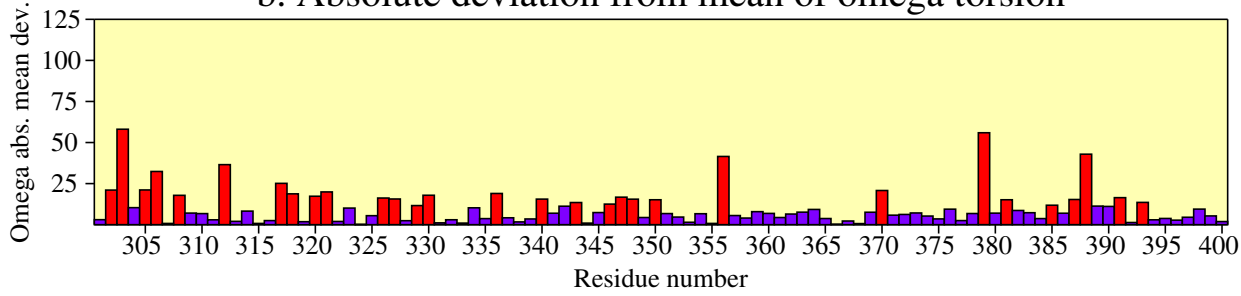


Residue properties
pdb1sqq

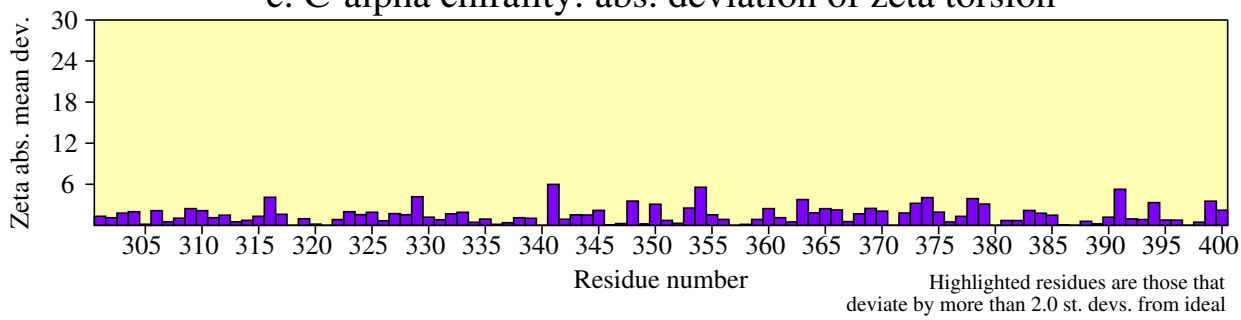
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

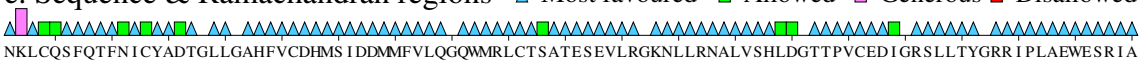


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

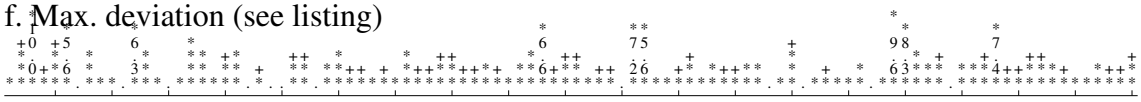
d. Secondary structure & estimated accessibility

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

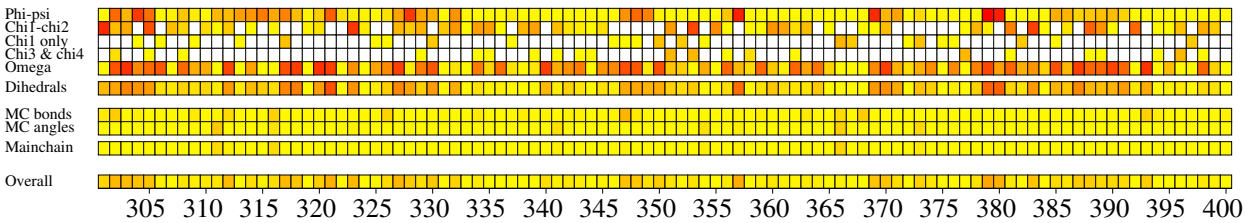
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



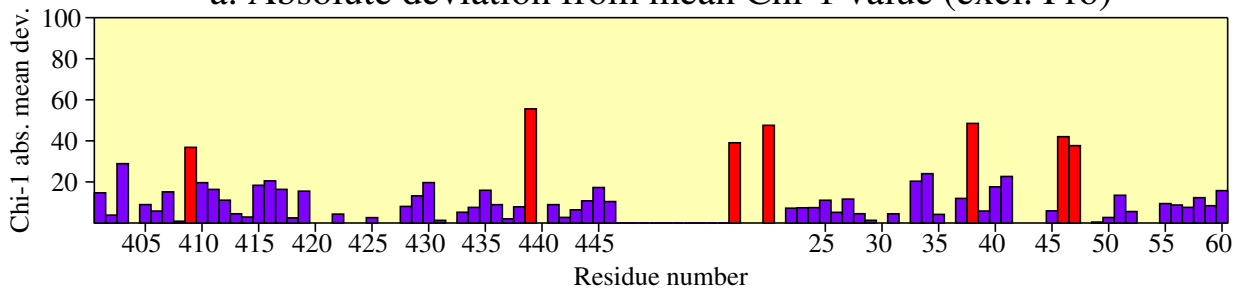
g. G-factors



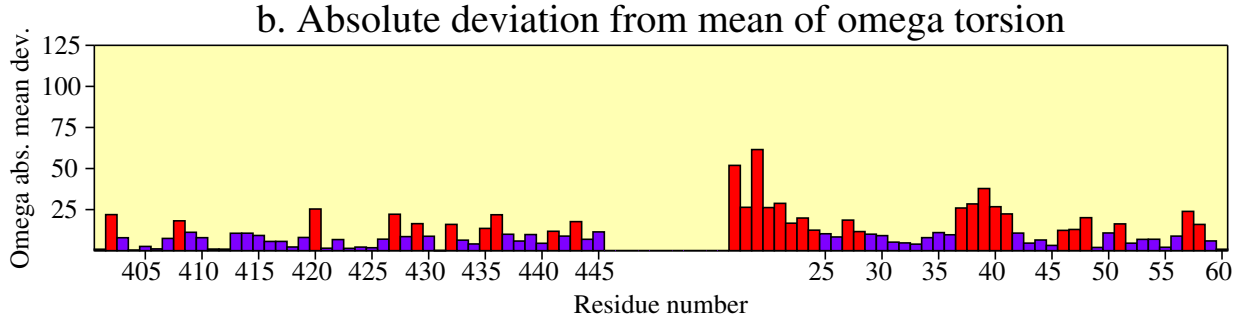
Residue properties

pdb1sqq

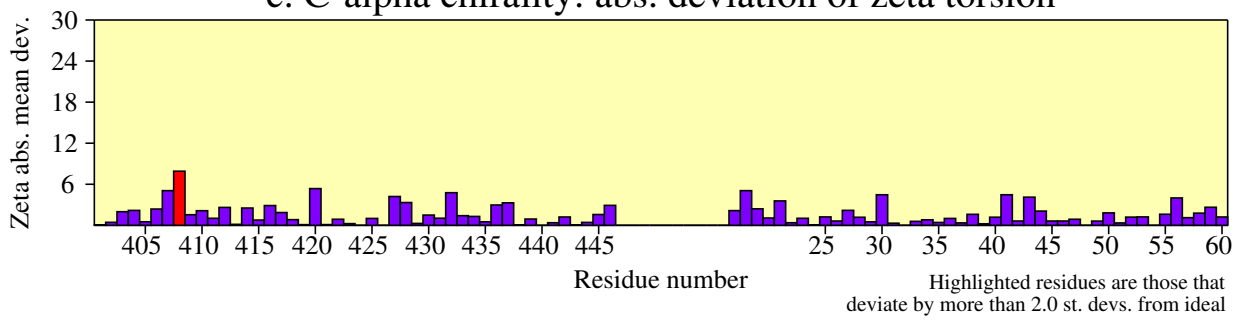
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

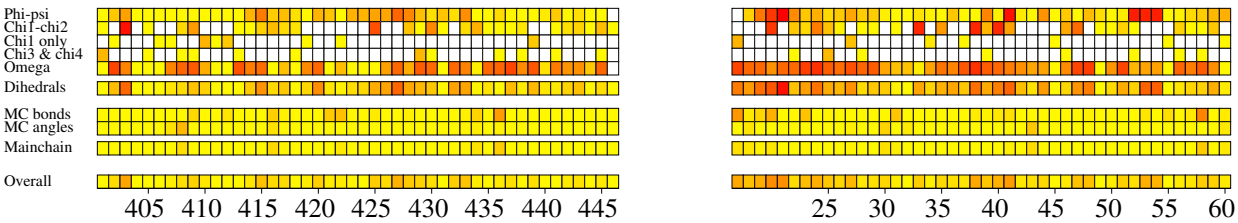
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

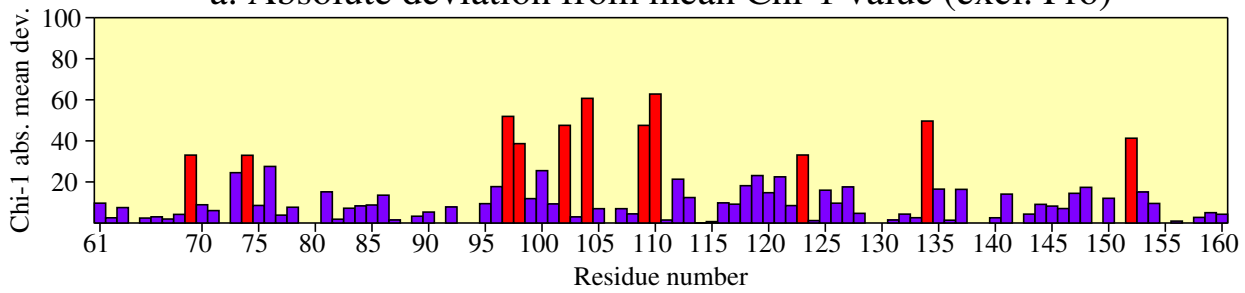
g. G-factors



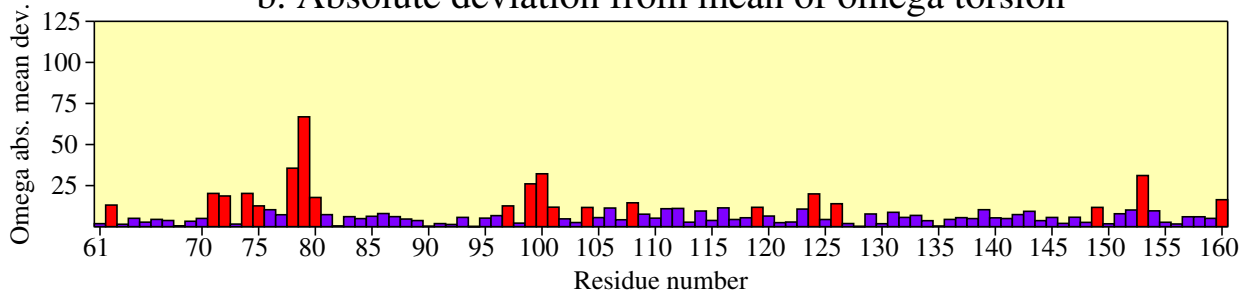
Residue properties

pdb1sqq

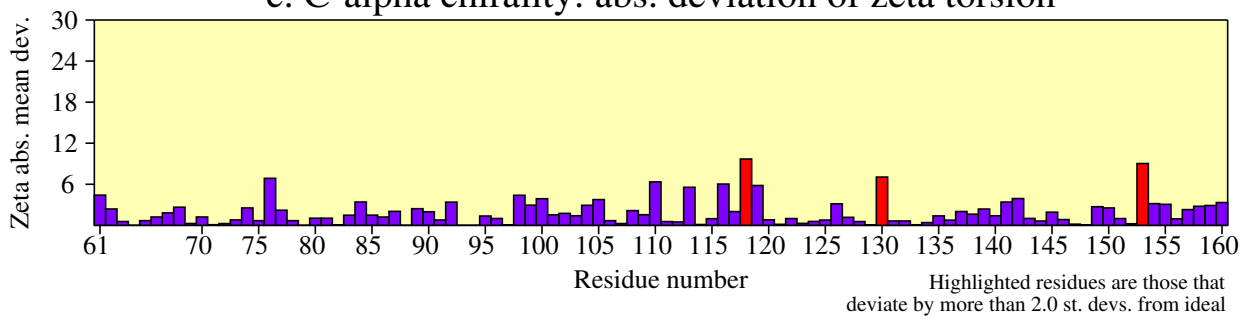
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

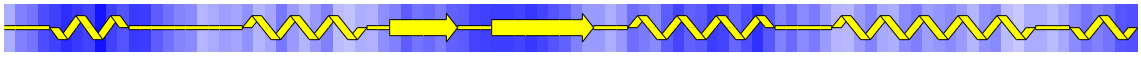


c. C-alpha chirality: abs. deviation of zeta torsion



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

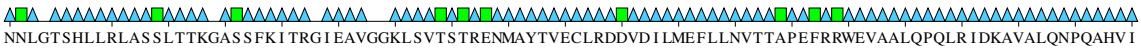
d. Secondary structure & estimated accessibility



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

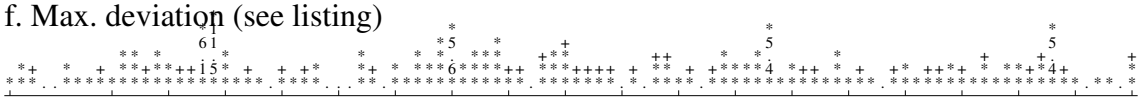
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

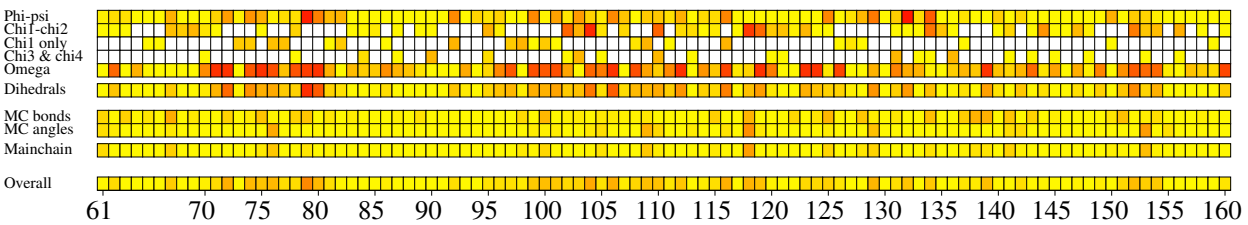


NNLGTSHLLRLASSLTTKGASSFKITRGIEAVGGKLSVTSTRENMAYTVECLRDDVDILMEFLLNVTTAPEFRRWEVAALQPQLRIDKAVALQNPQAHVI

f. Max. deviation (see listing)



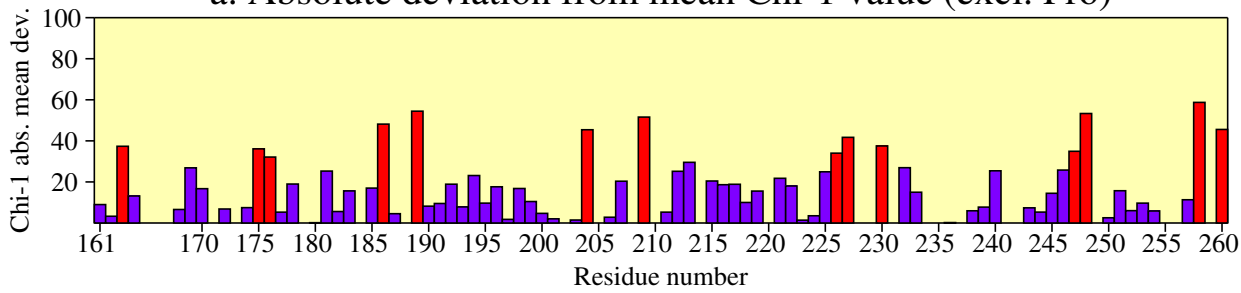
g. G-factors



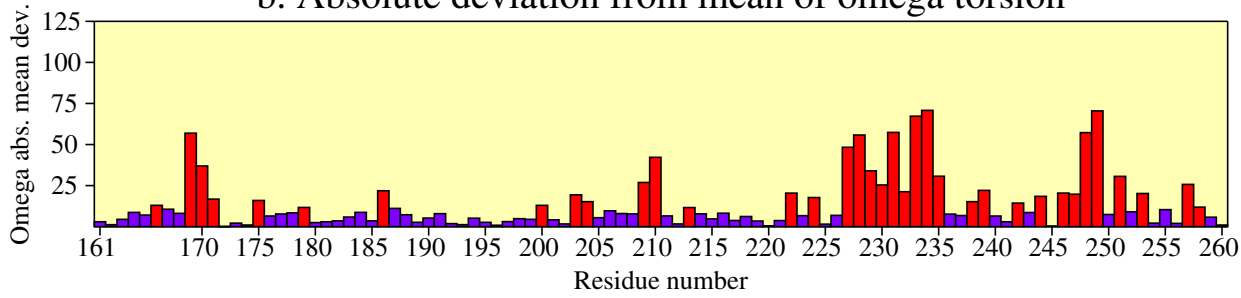
Residue properties

pdb1sqq

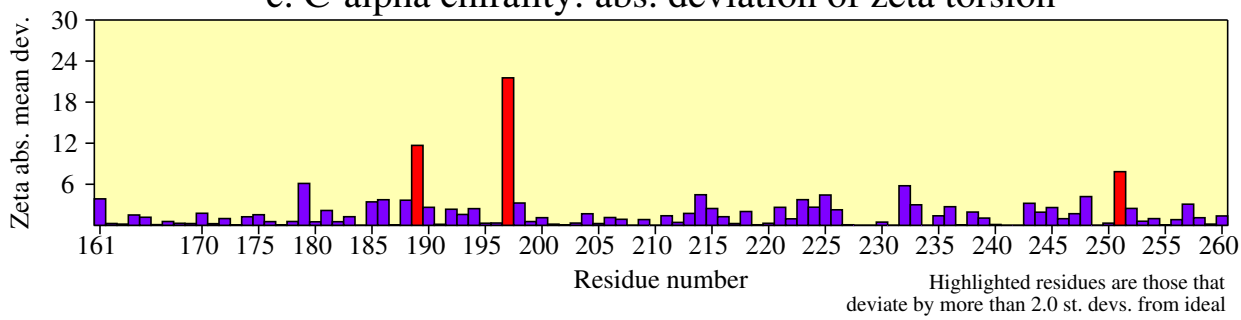
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

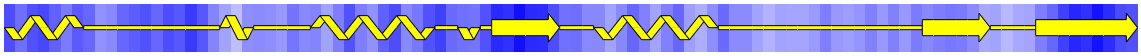


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



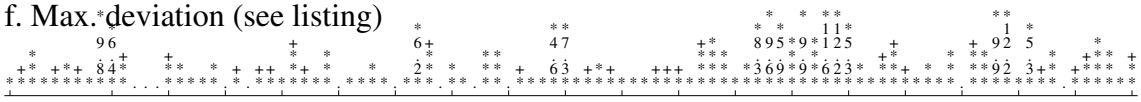
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

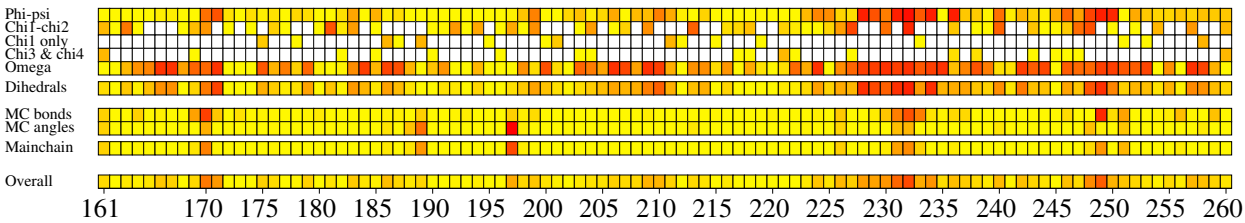
Most favoured Allowed Generous Disallowed

ENLHAAAYRNALANSLYCPDYRIGKVTPVELHDYVQNHFTSARMALIGLGVSHPVLKQVAEQFLNIRGGLGLSGAKAKYHGGEIREQNGDSLVHAALVAE

f. Max. deviation (see listing)



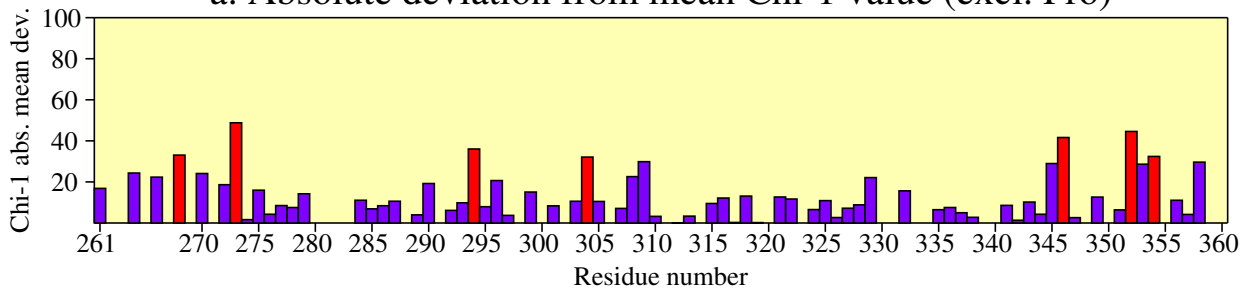
g. G-factors



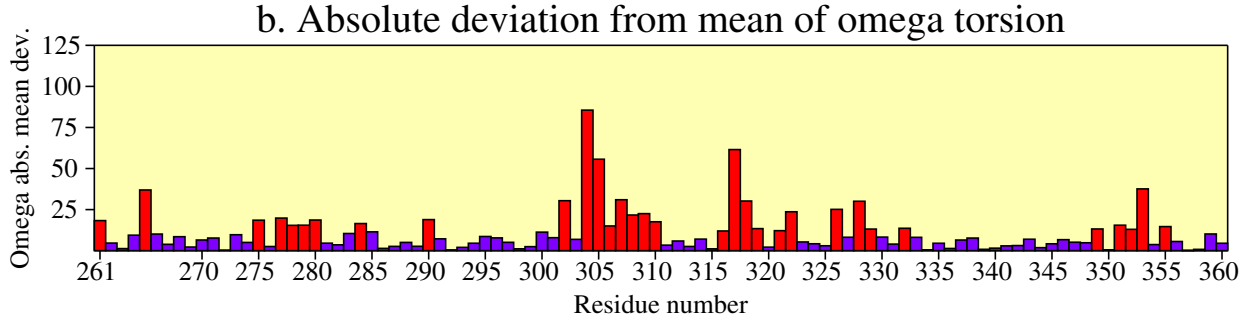
Residue properties

pdb1sqq

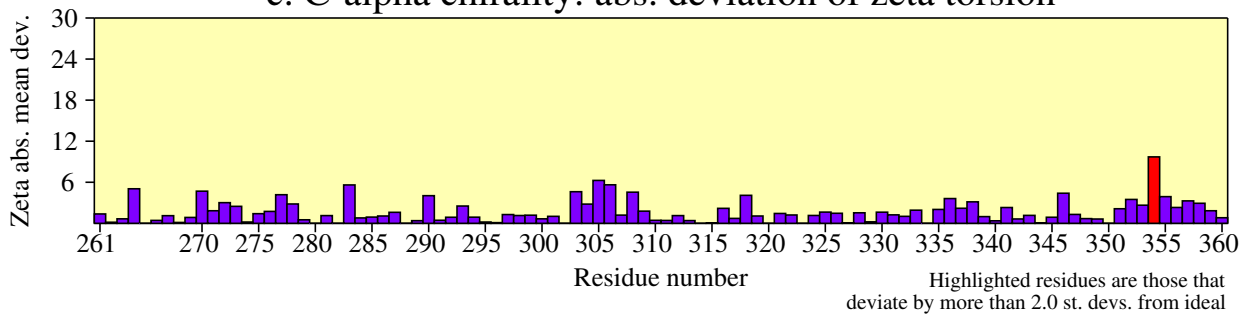
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



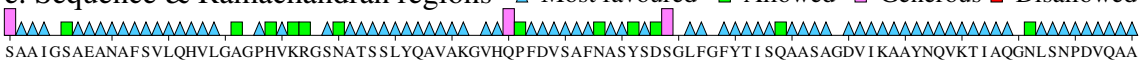
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

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

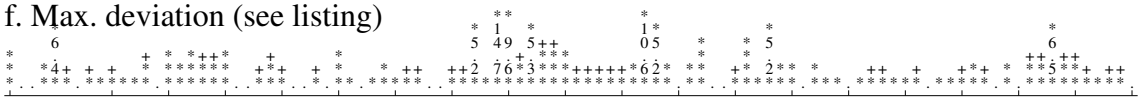
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

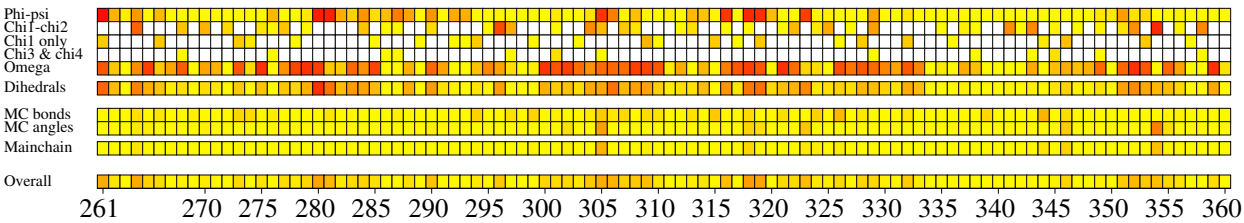


SAAIGSAEANAFSVLQHVLGAGPHVKRGSNATSSLYQAVAKGVHQPFDVSAFNASYSDSGLFGFYTISQAASAGDVIKAAYNQVKTIAQGNLSNPDVQAA

f. Max. deviation (see listing)



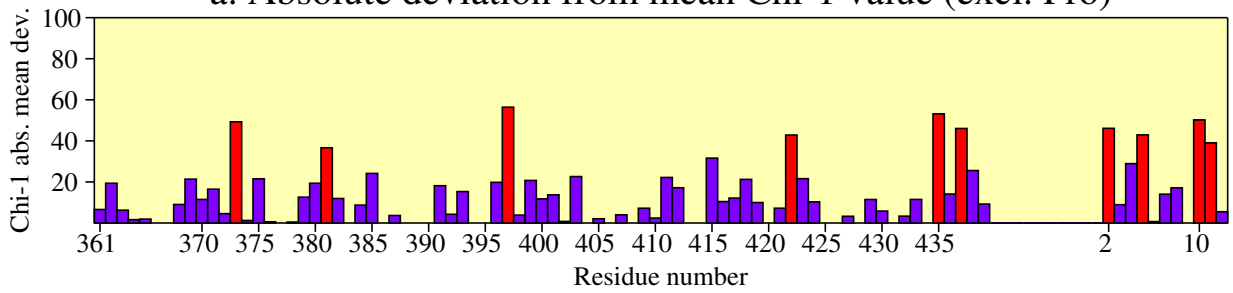
g. G-factors



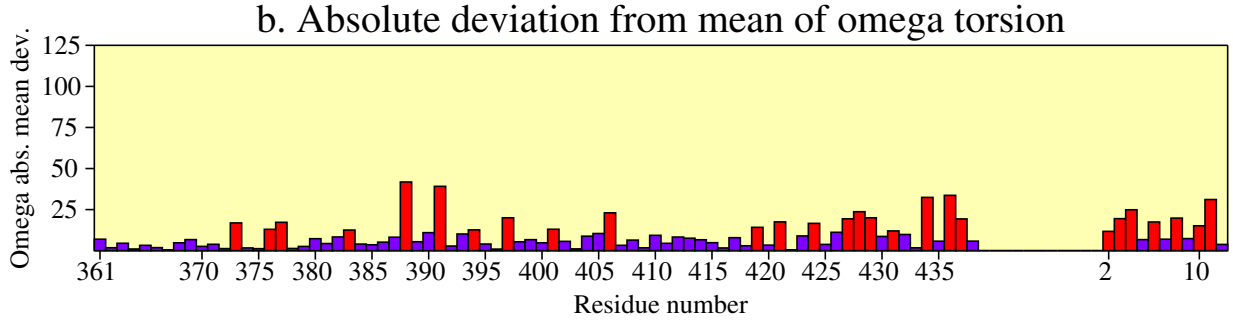
Residue properties

pdb1sqq

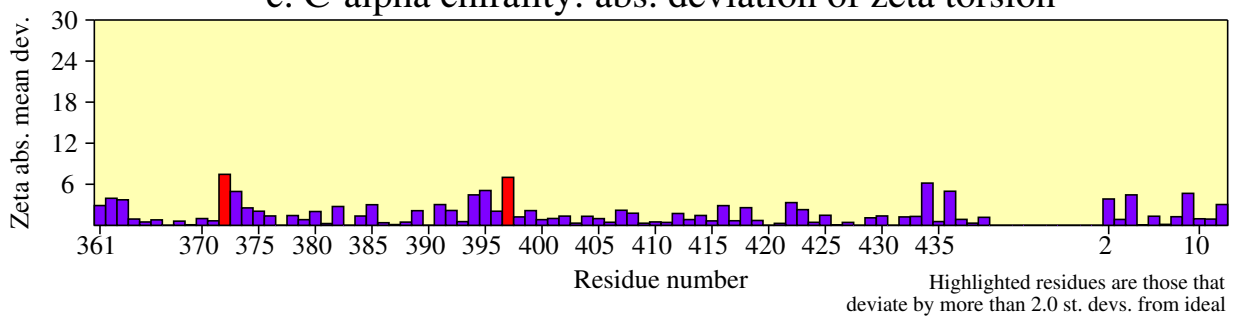
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

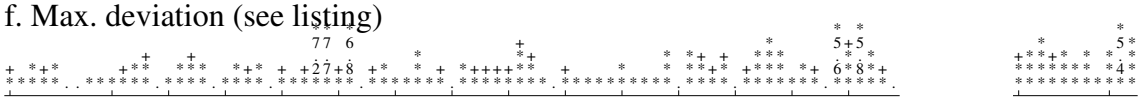
d. Secondary structure & estimated accessibility

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

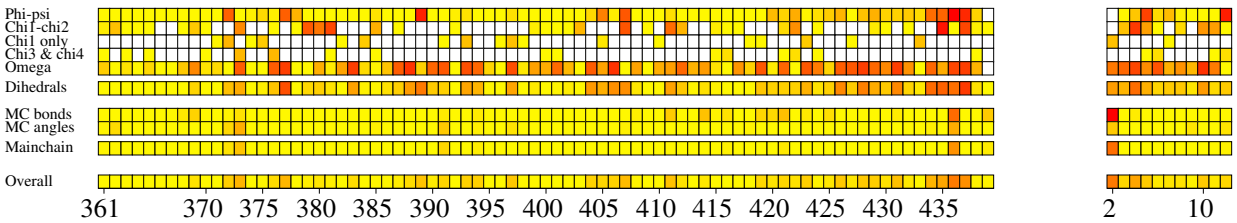
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)



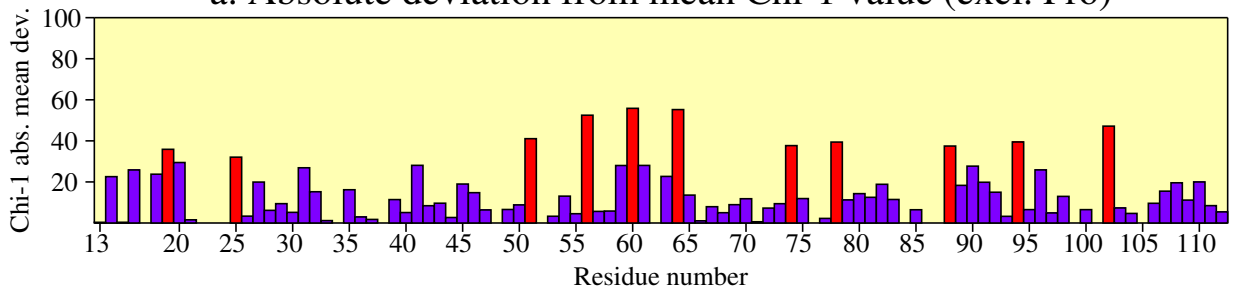
g. G-factors



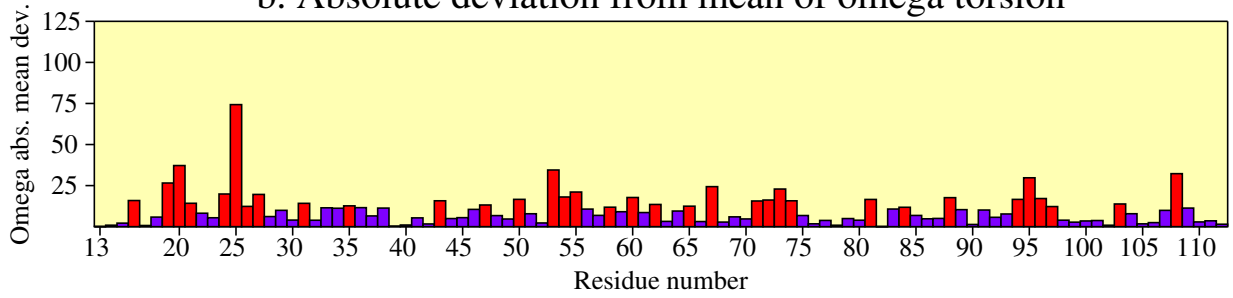
Residue properties

pdb1sqq

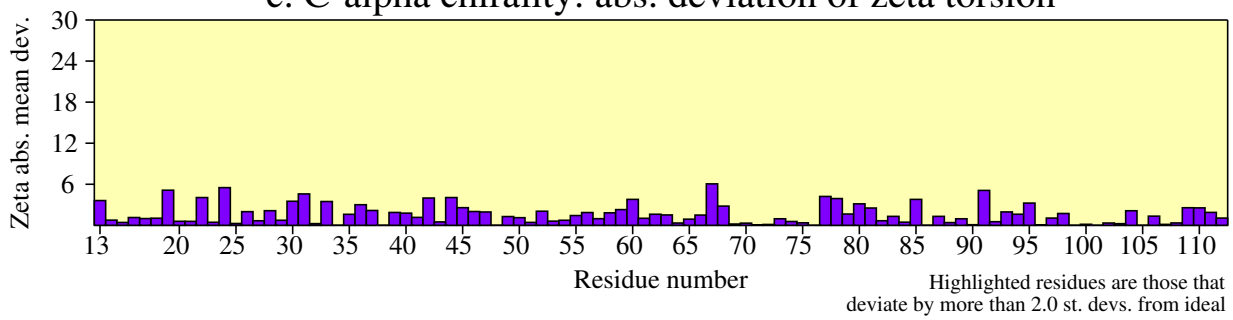
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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

d. Secondary structure & estimated accessibility

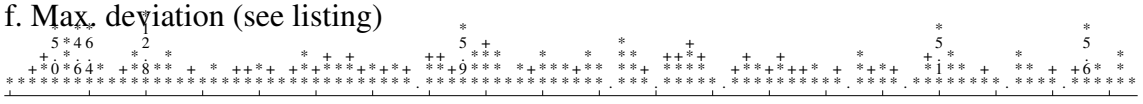
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

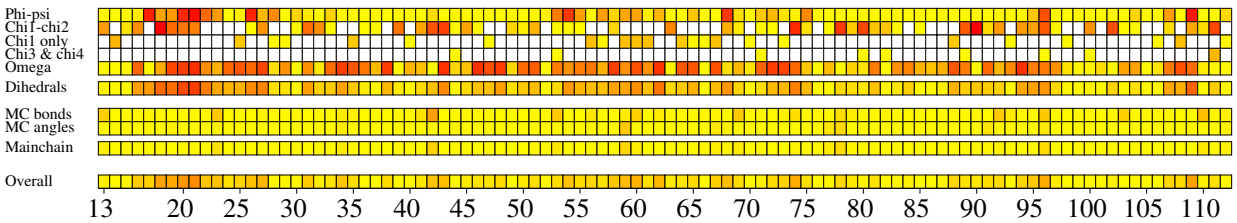
Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)



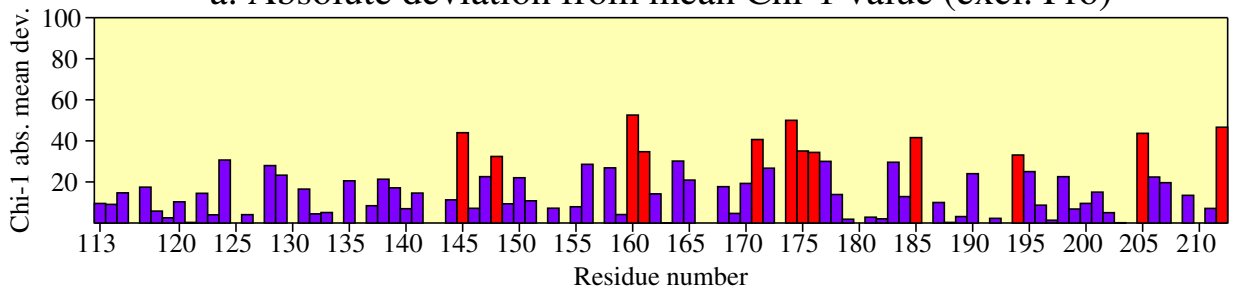
g. G-factors



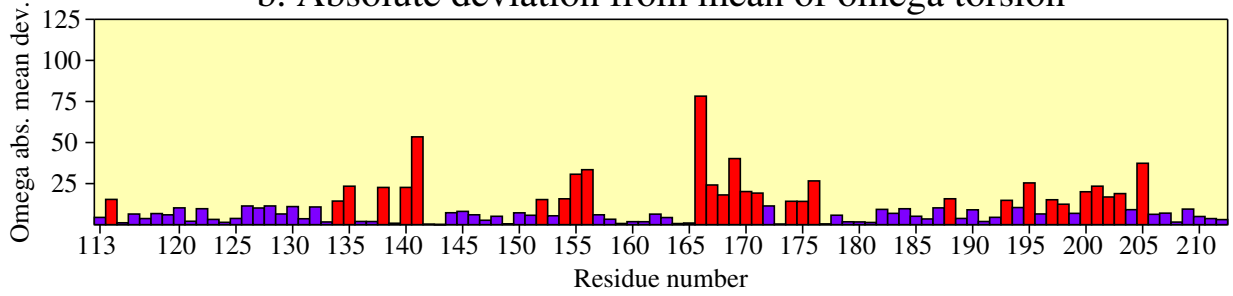
Residue properties

pdb1sqq

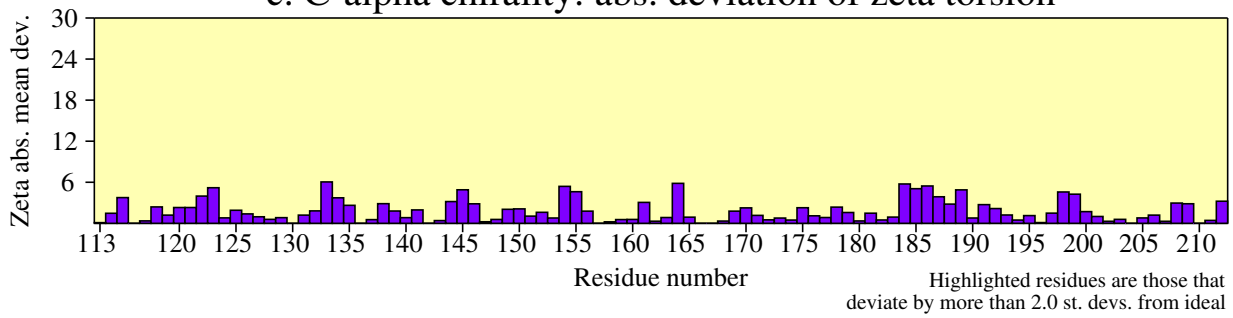
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



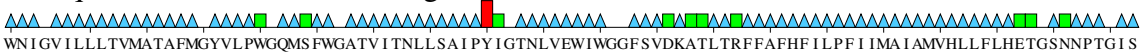
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

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

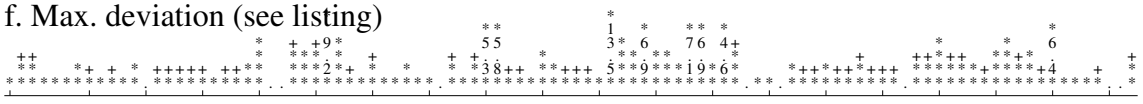
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

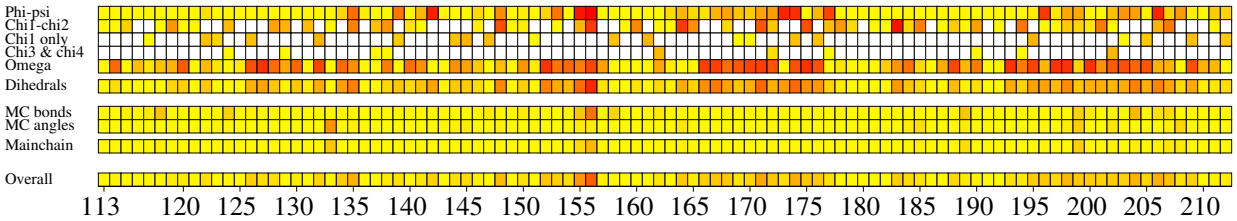


WN I GV I LLL TVMA TA FMGYVL PWGQMS FWGA TV I TNLL SA I PY I GTNL VEW I WGGF SVDKA TL TRF FA FHF I LPF I IMA I AMVHLL FLHETGSNNPTG I S

f. Max. deviation (see listing)



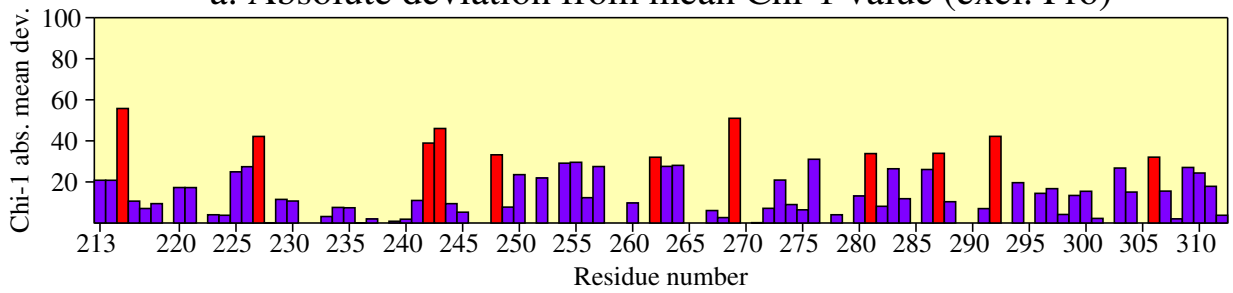
g. G-factors



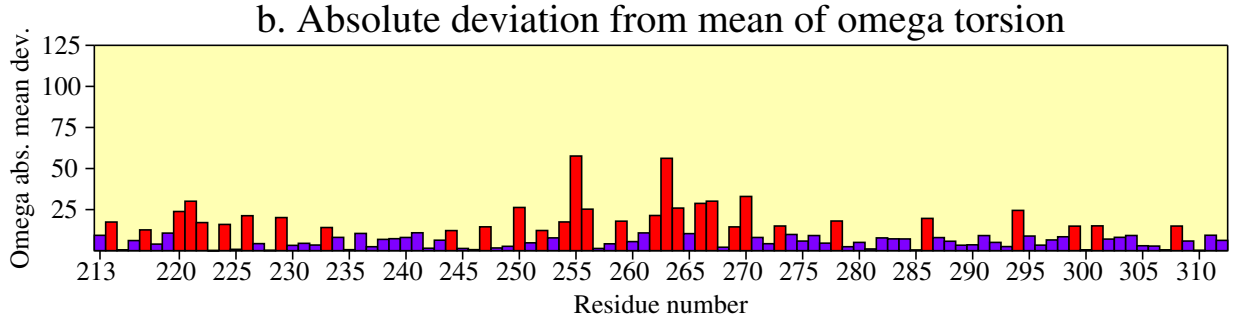
Residue properties

pdb1sqq

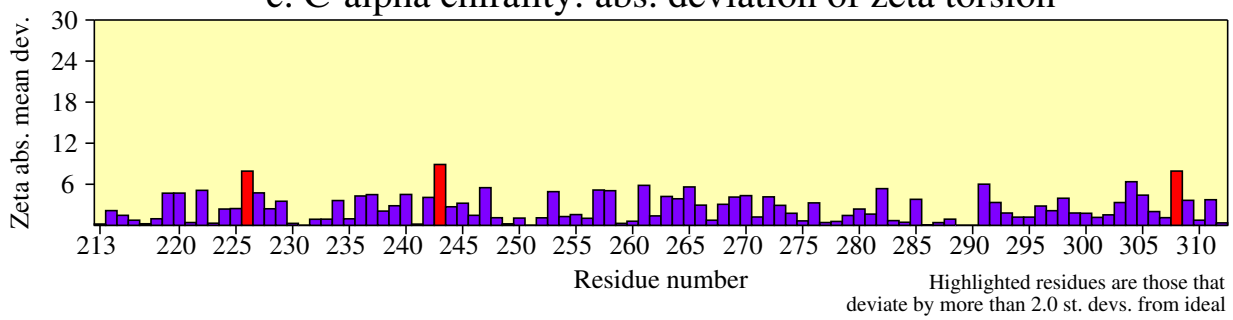
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

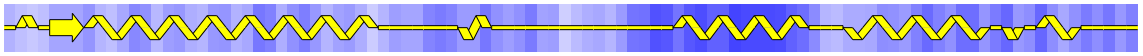


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



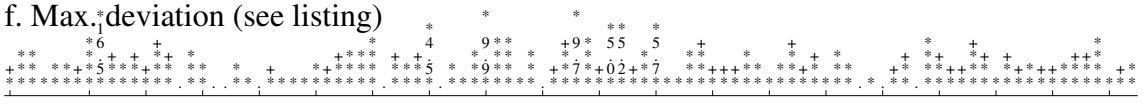
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

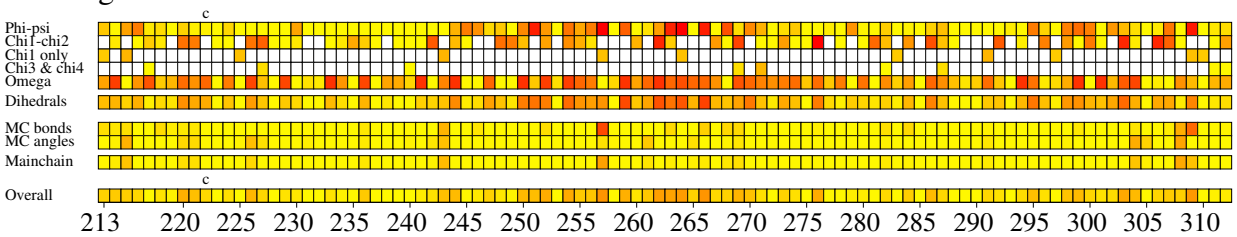
Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)



g. G-factors

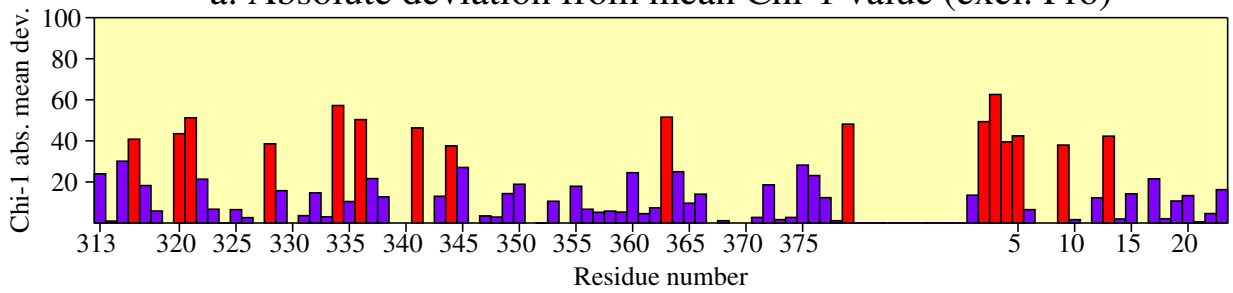


c = cis-peptide

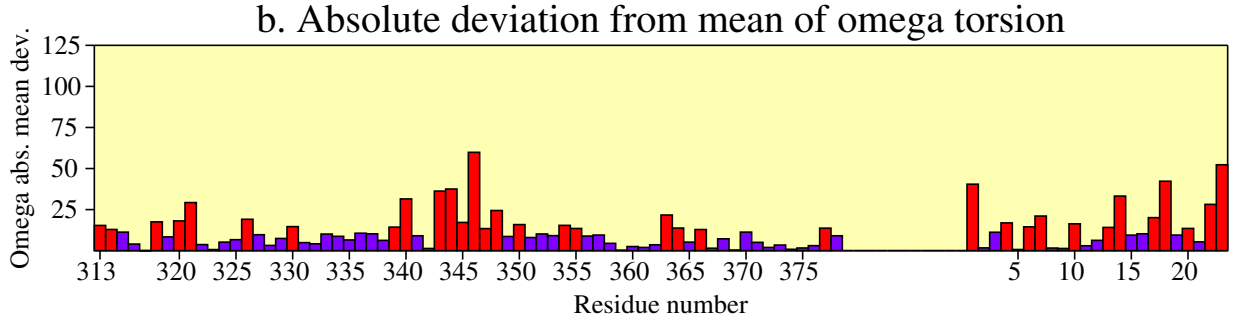
Residue properties

pdb1sqq

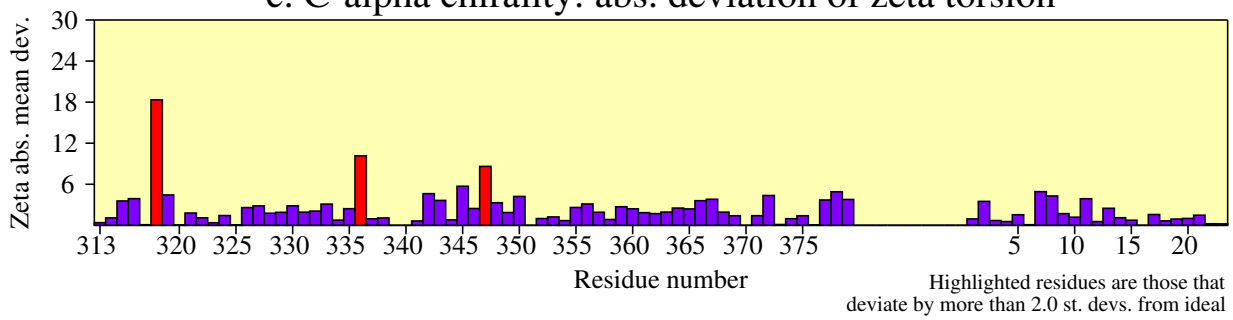
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

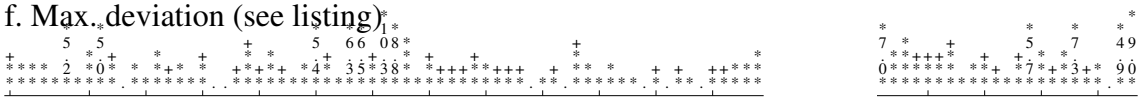
d. Secondary structure & estimated accessibility

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

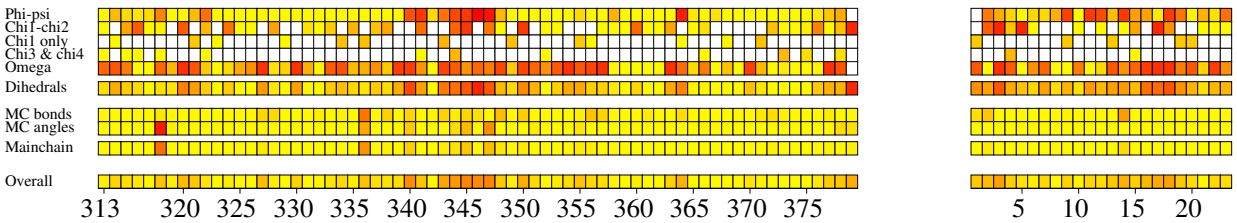
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

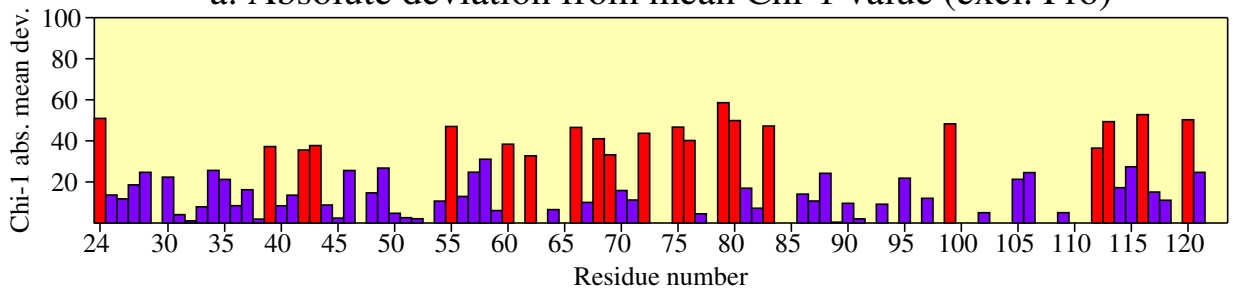


g. G-factors

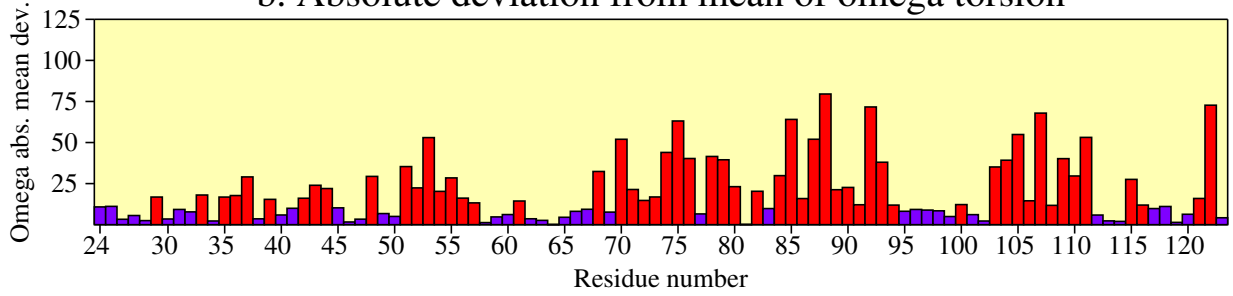


Residue properties
pdb1sqq

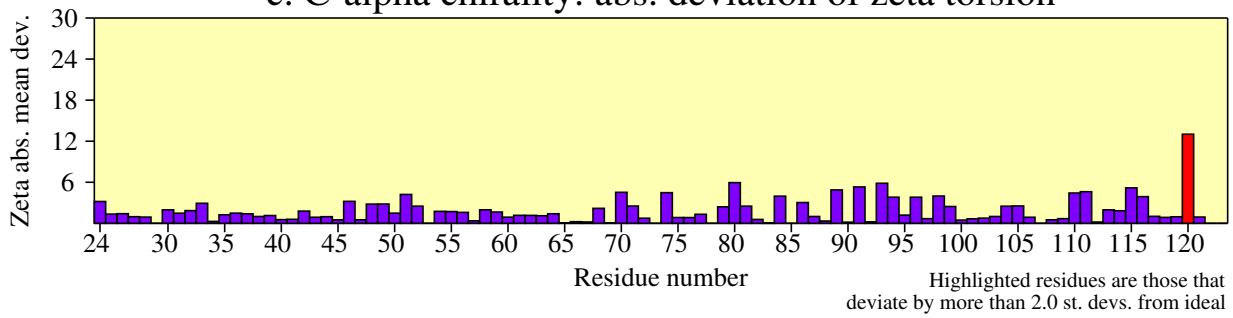
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

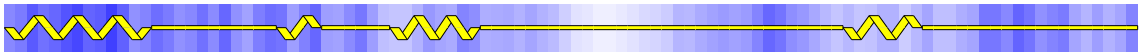


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

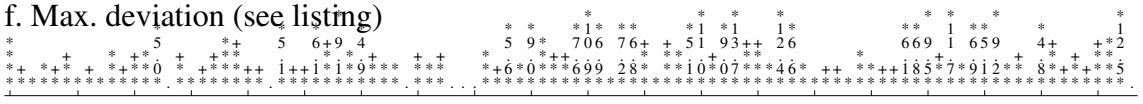


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

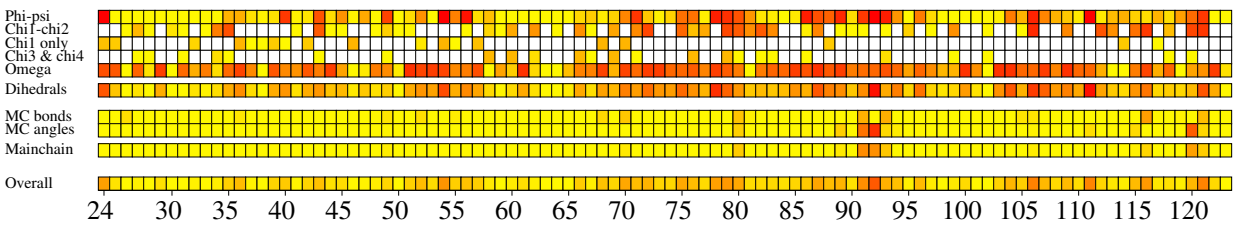
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)

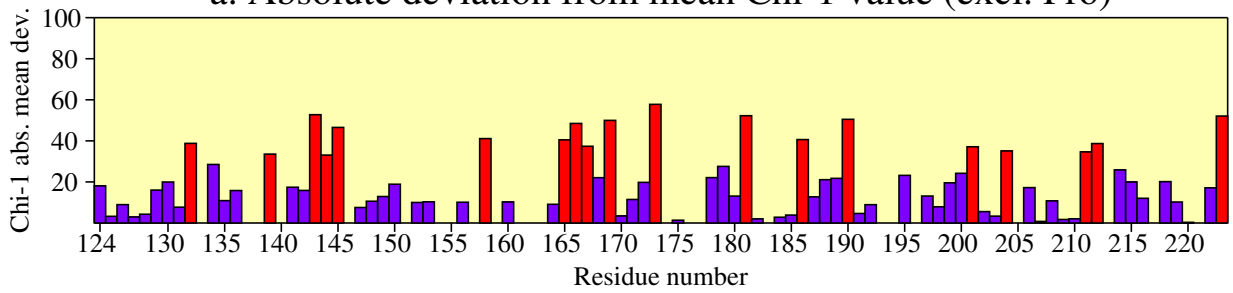


g. G-factors

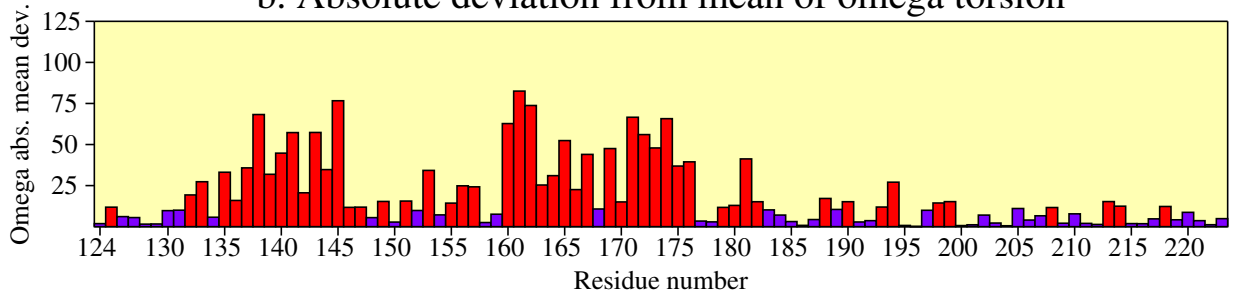


Residue properties
pdb1sqq

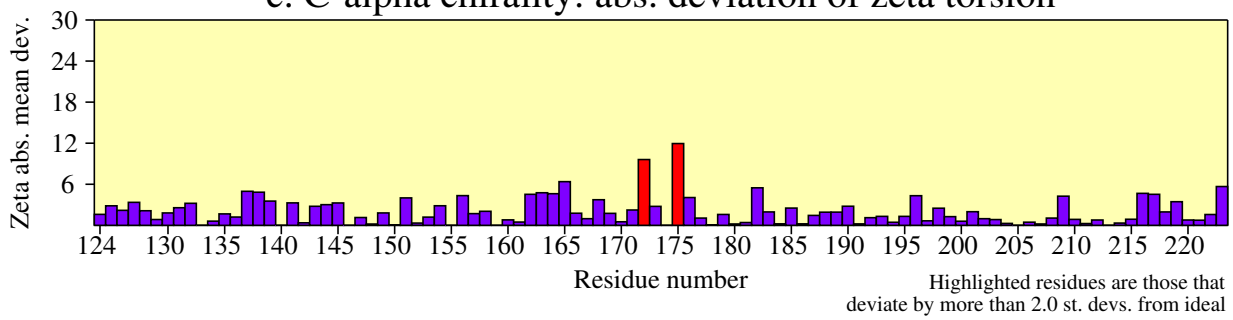
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

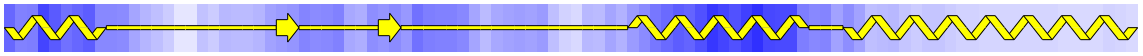


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

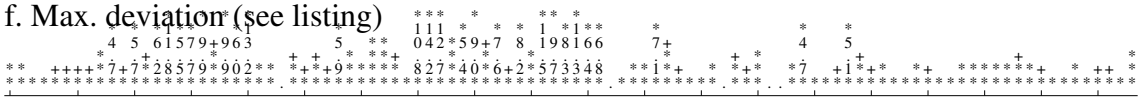


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

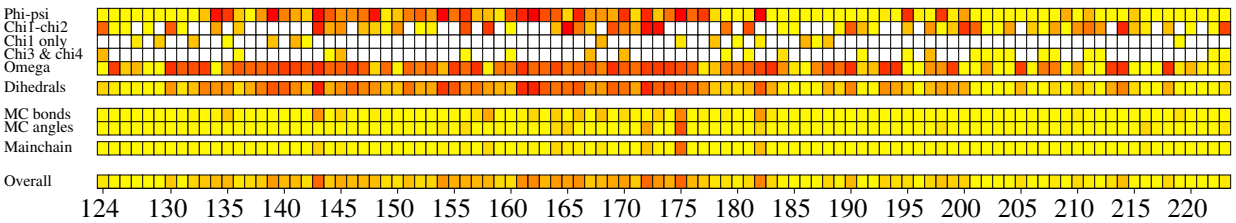
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

EDYVFSLLTGYCEPPTGVSLREGLYFNPYFPGQAIGMAPPIYNEVLEFDDGTPATMSQVAKDVCTFLRWAAEPEHDHRKRMGLKMLLMMGLLLPLVYAMK

f. Max. deviation (see listing)



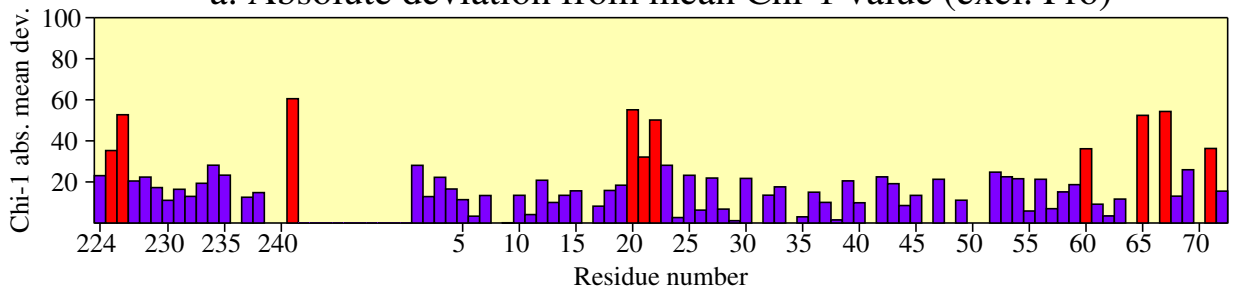
g. G-factors



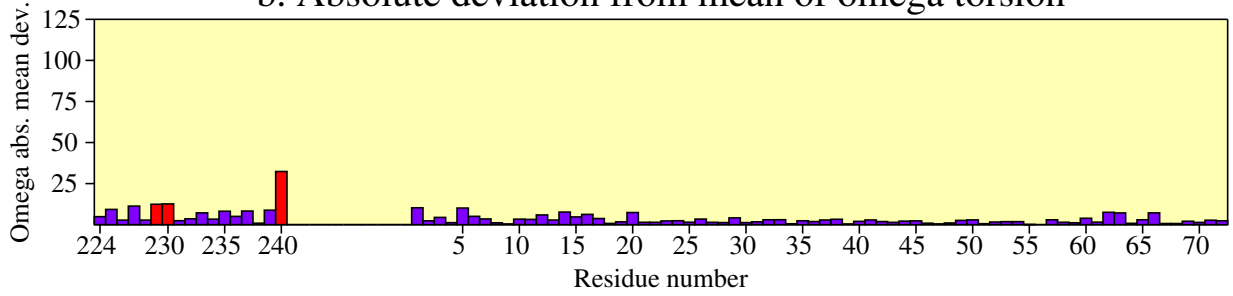
Residue properties

pdb1sqq

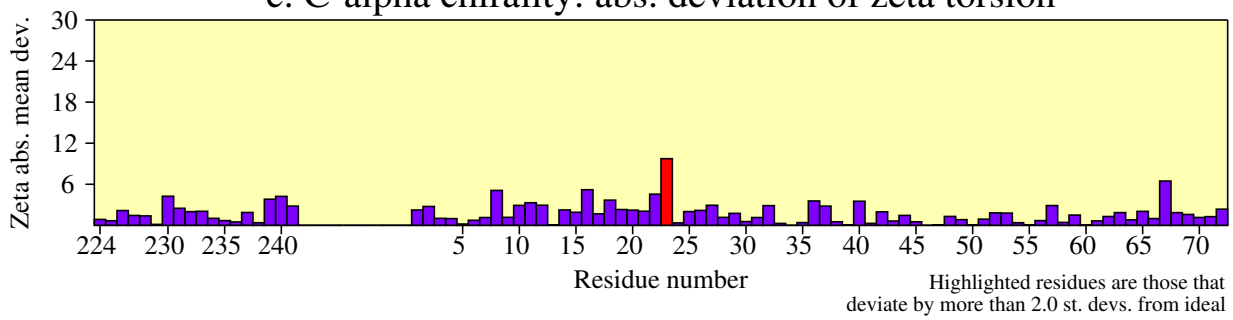
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

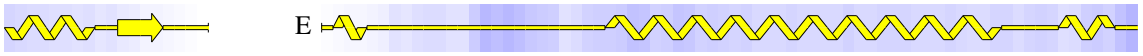


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

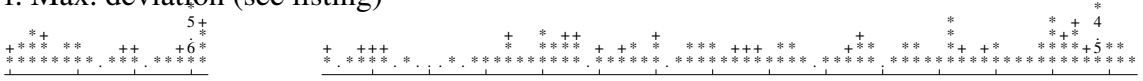


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

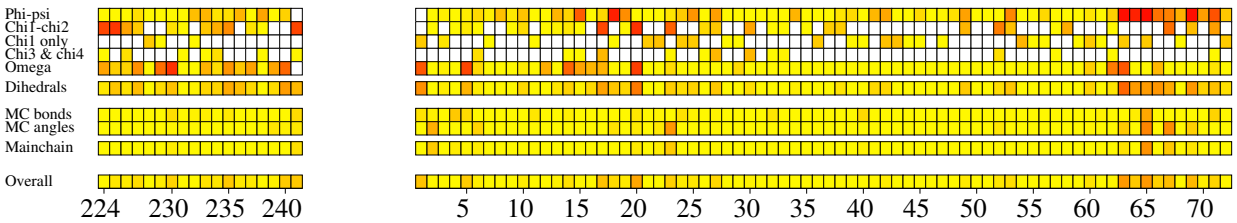
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)



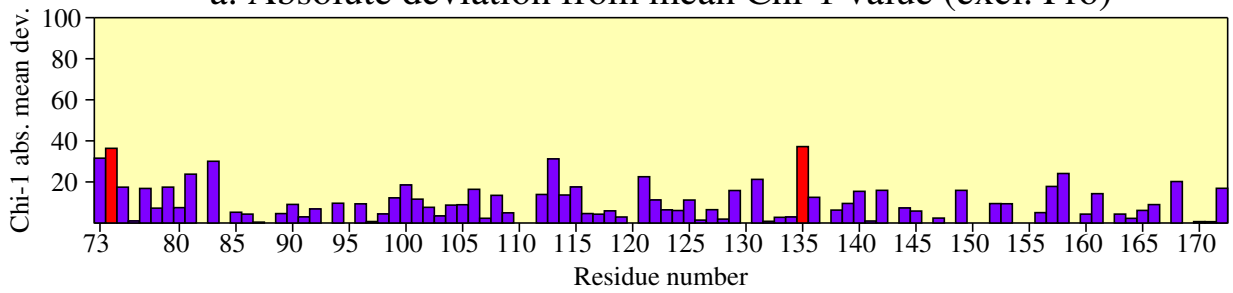
g. G-factors



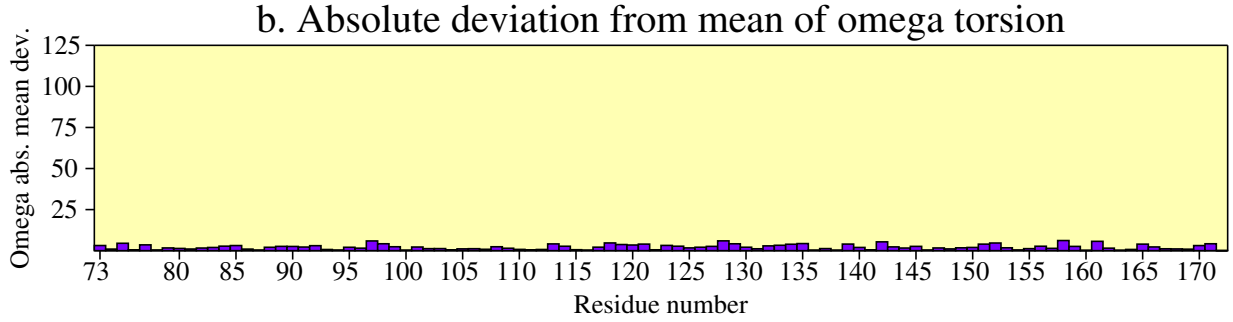
Residue properties

pdb1sqq

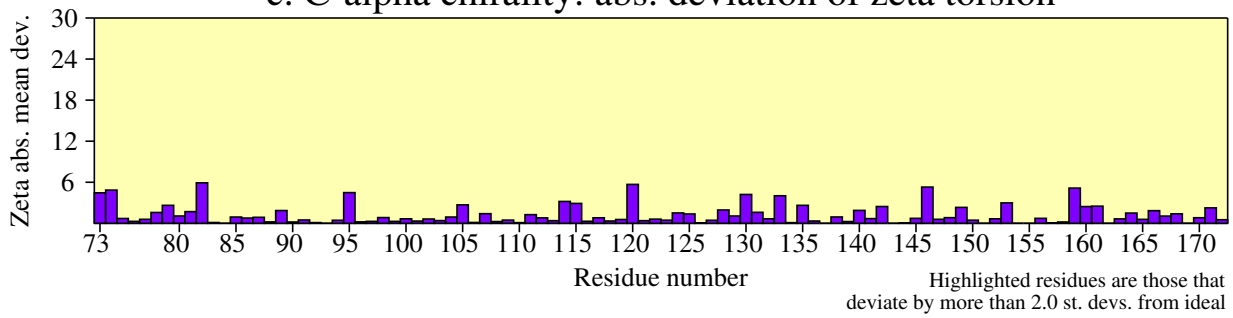
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



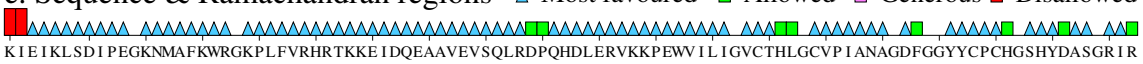
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

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

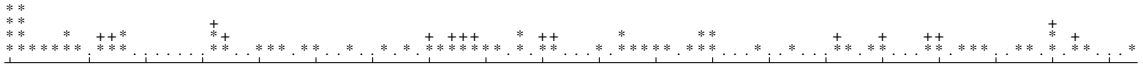
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

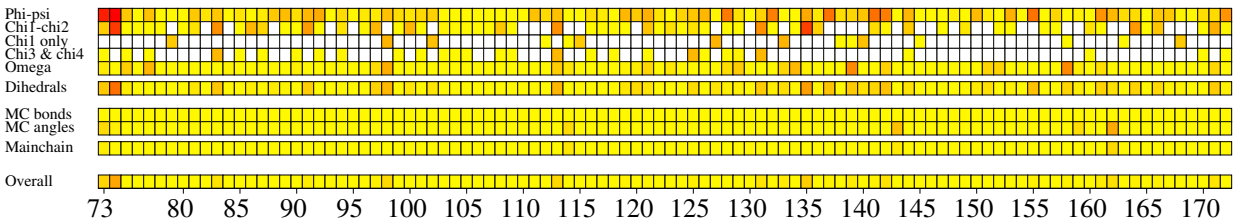


K I E I K L S D I P E G K N M A F K W R G K P L F V R H R T K K E I D Q E A A V E V S Q L R D P Q H D L E R V K K P E W V I L I G V C T H L G C V P I A N A G D F G G Y Y C P C H G S H Y D A S G R I R

f. Max. deviation (see listing)



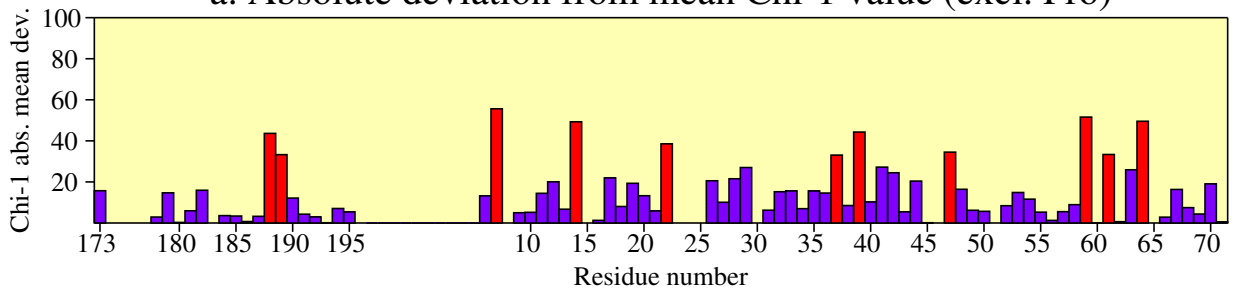
g. G-factors



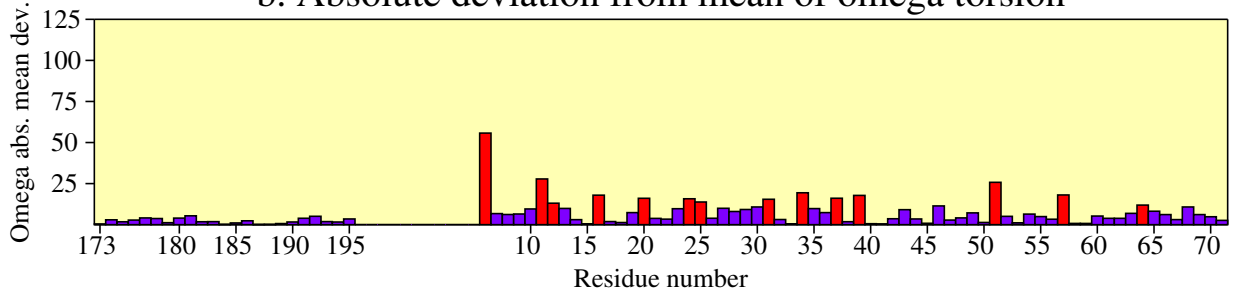
Residue properties

pdb1sqq

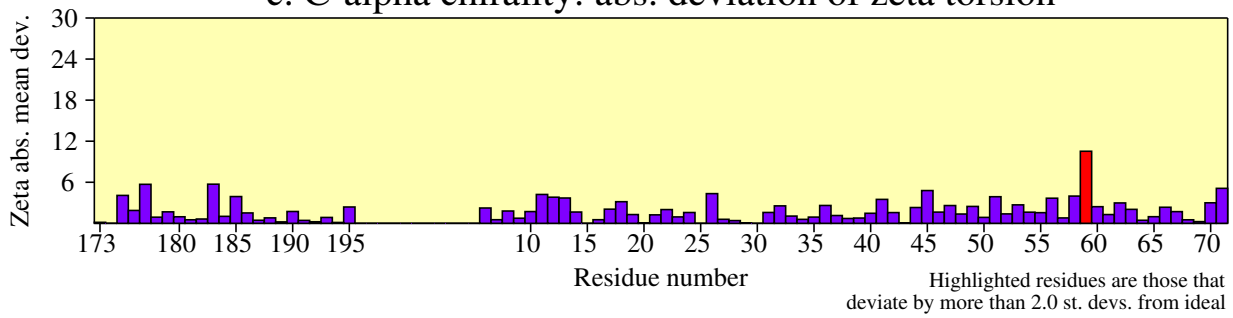
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

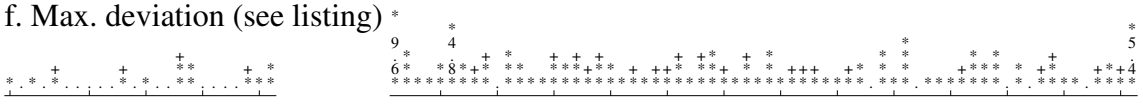
d. Secondary structure & estimated accessibility

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

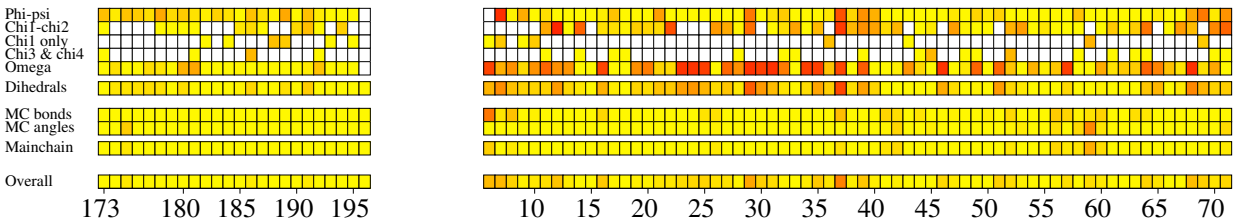
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)



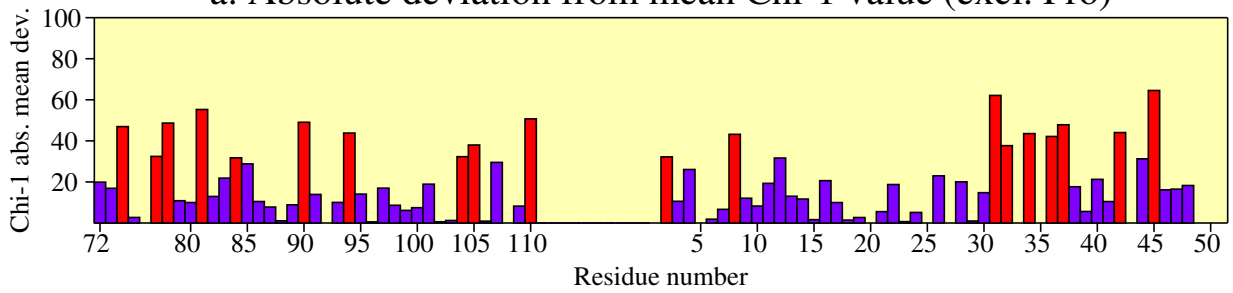
g. G-factors



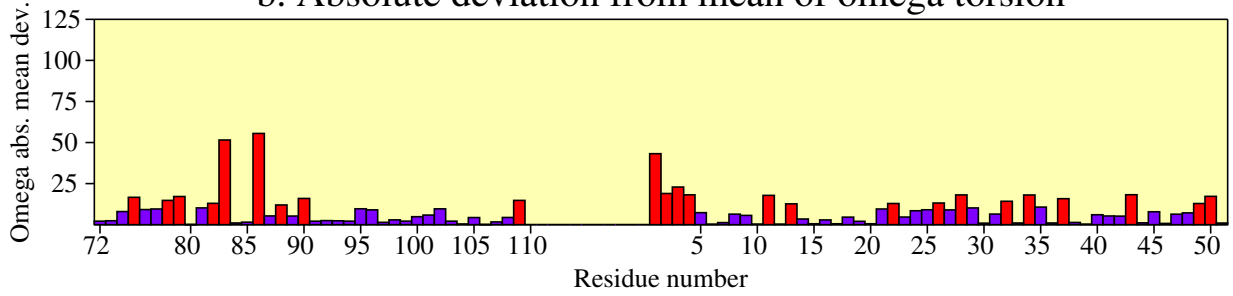
Residue properties

pdb1sqq

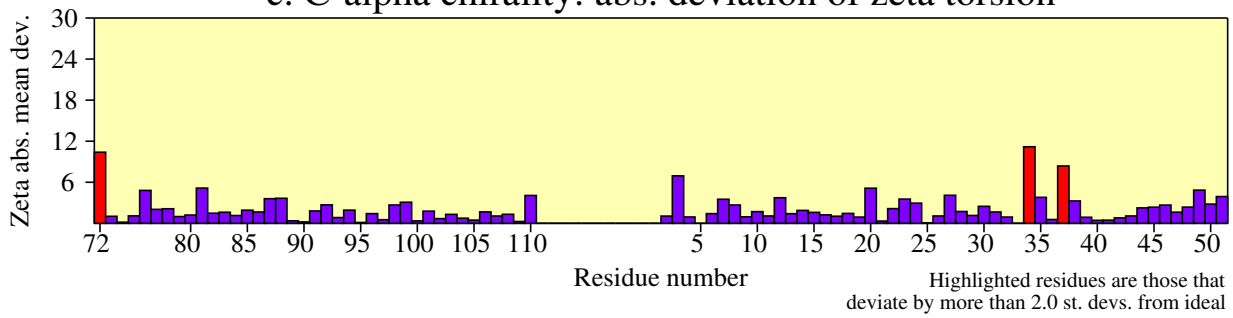
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

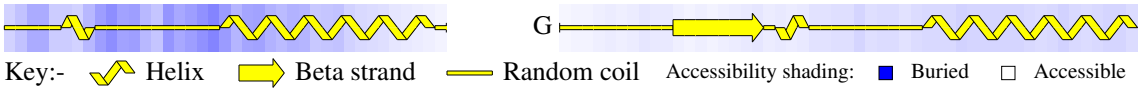


c. C-alpha chirality: abs. deviation of zeta torsion



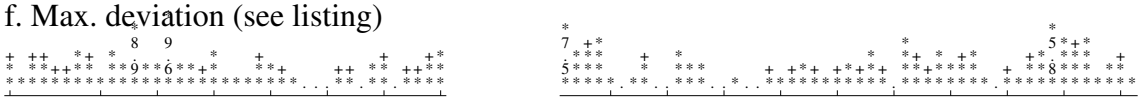
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

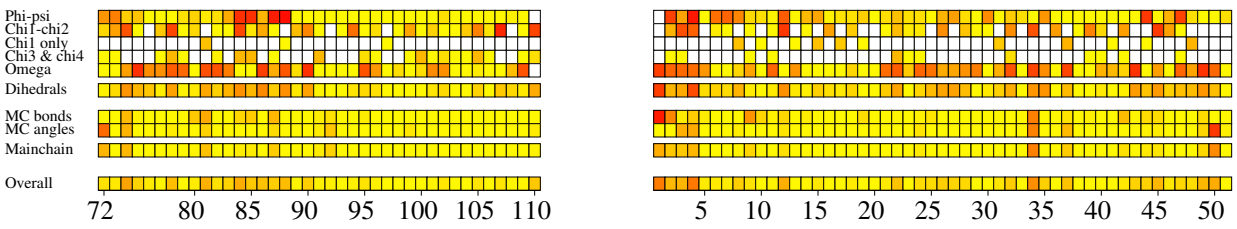


e. Sequence & Ramachandran regions

f. Max. deviation (see listing)



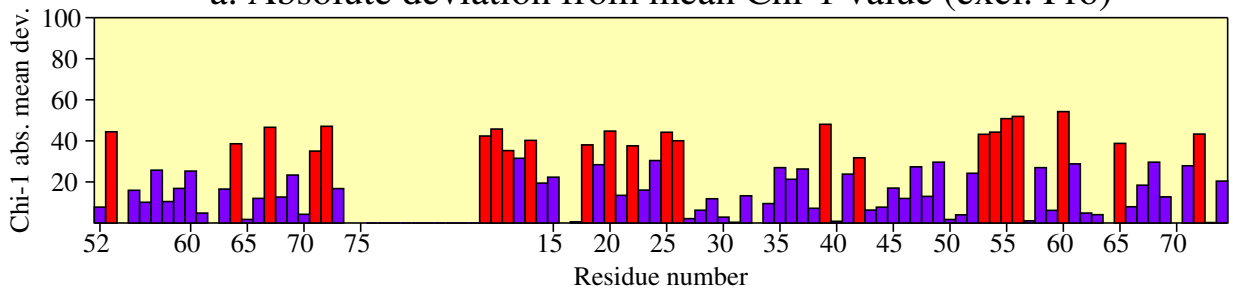
g. G-factors



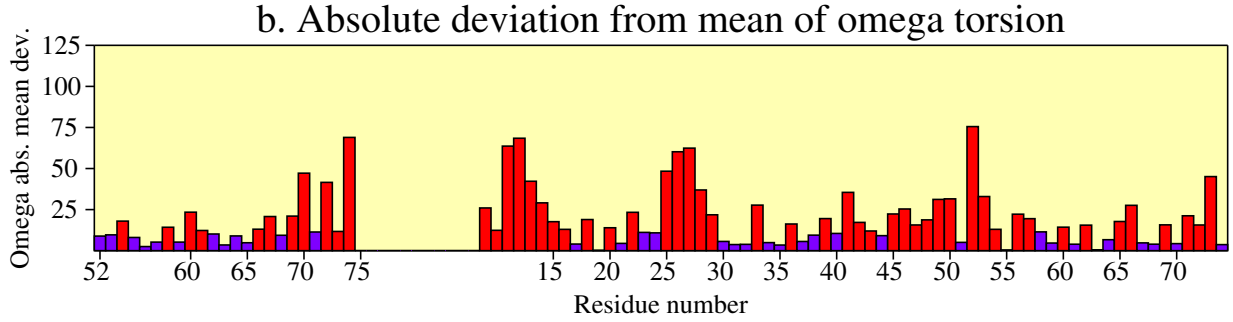
Residue properties

pdb1sqq

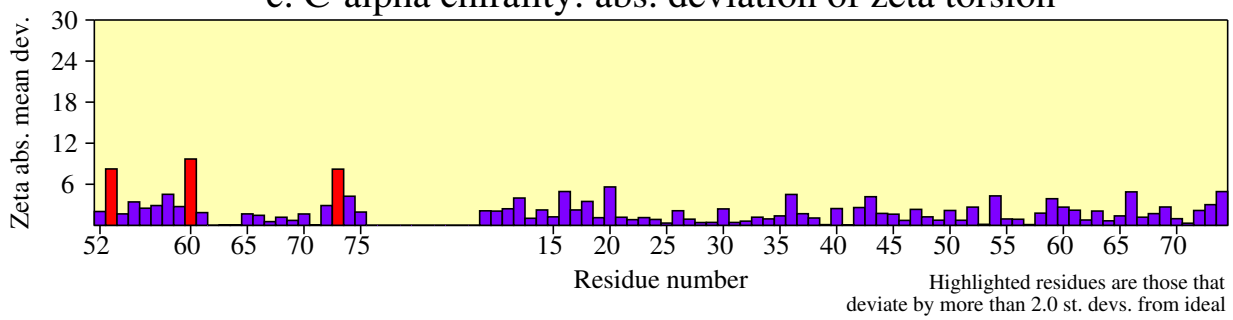
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

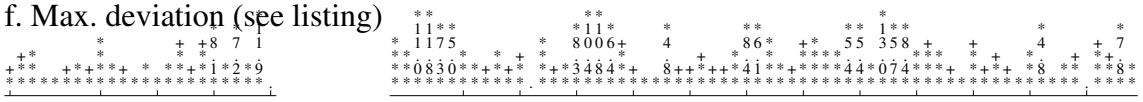
d. Secondary structure & estimated accessibility

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

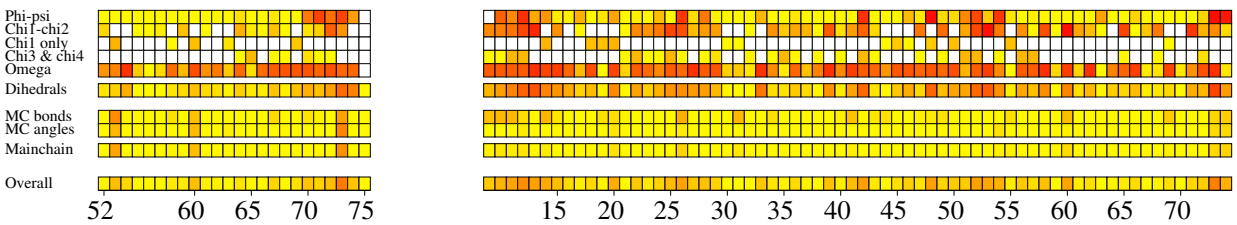
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)



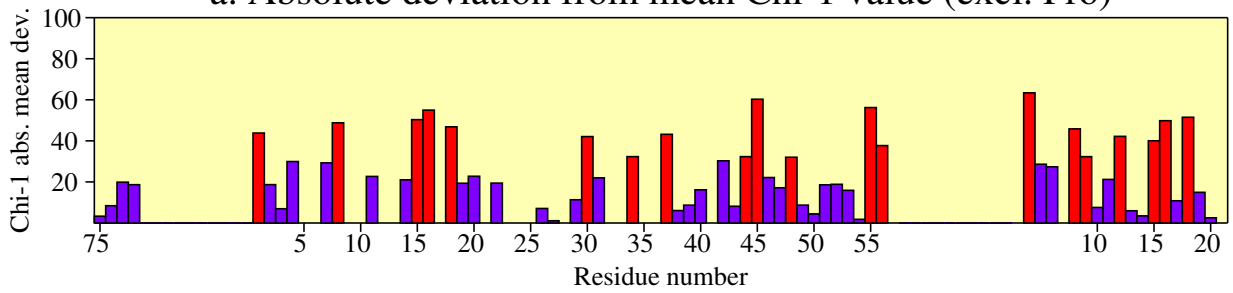
g. G-factors



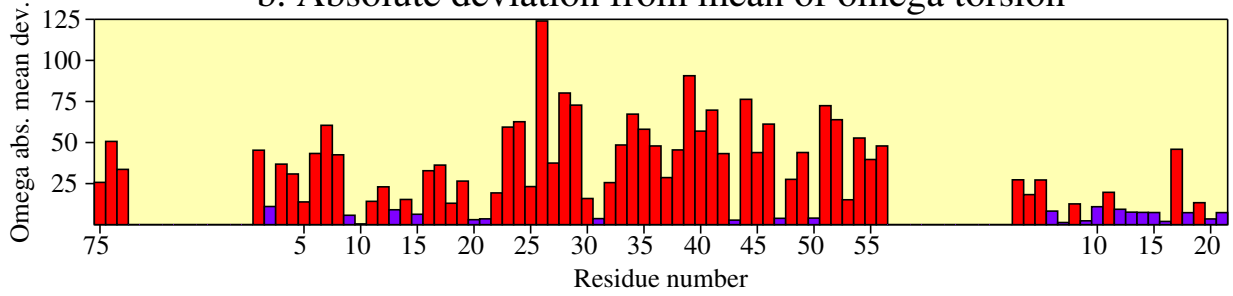
Residue properties

pdb1sqq

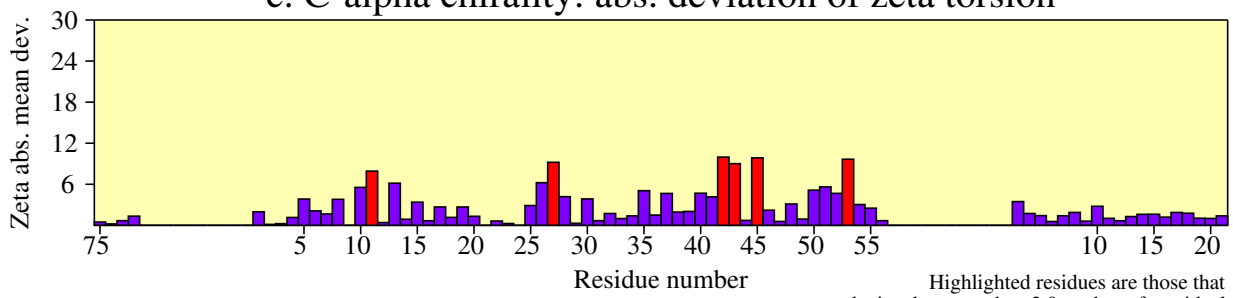
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

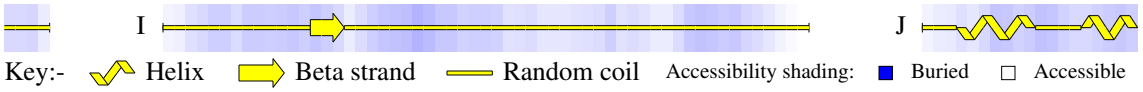


c. C-alpha chirality: abs. deviation of zeta torsion



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

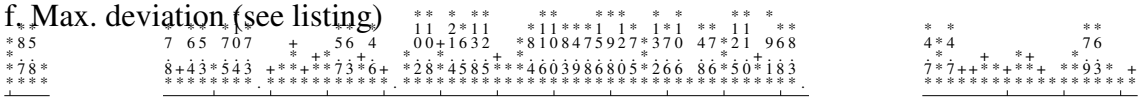
d. Secondary structure & estimated accessibility



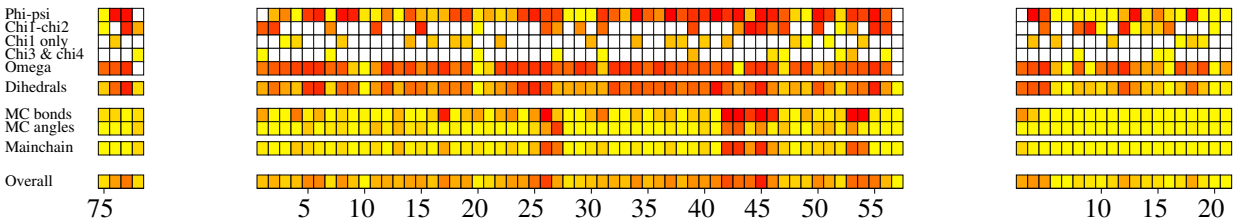
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)



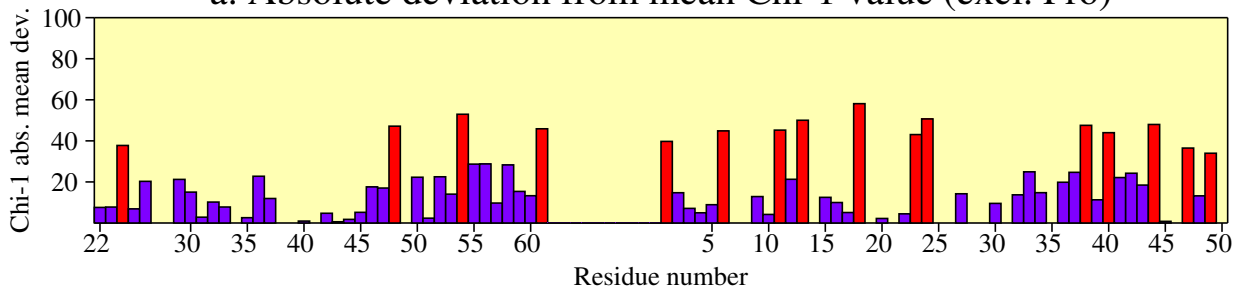
g. G-factors



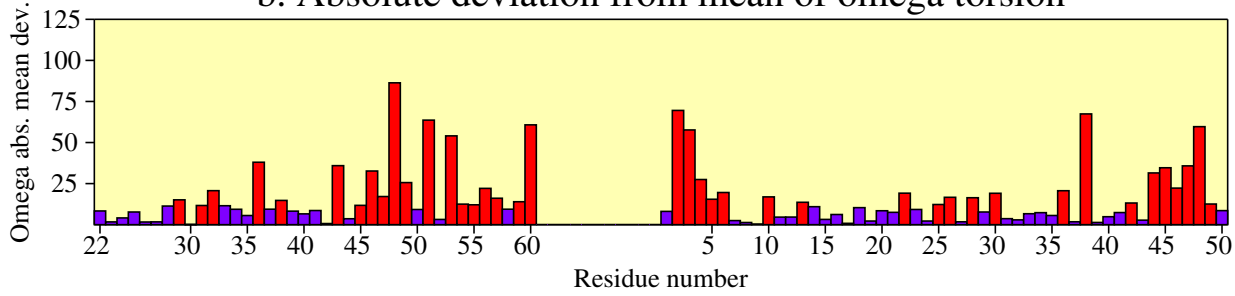
Residue properties

pdb1sqq

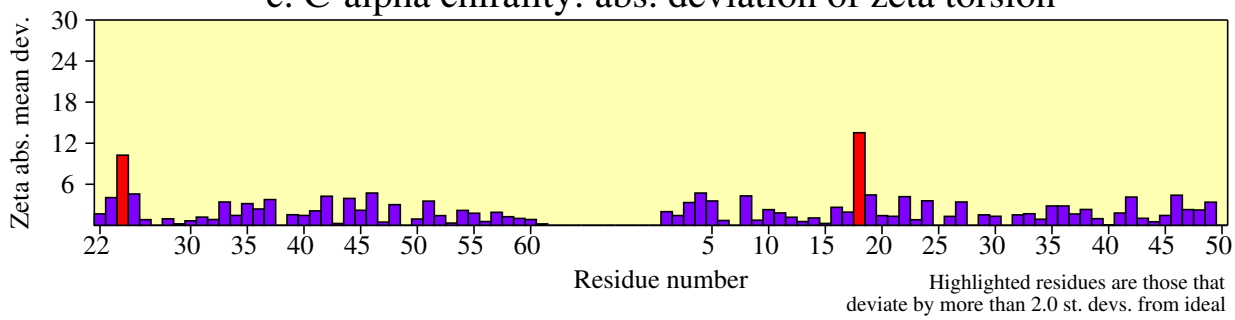
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

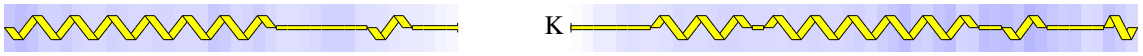


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

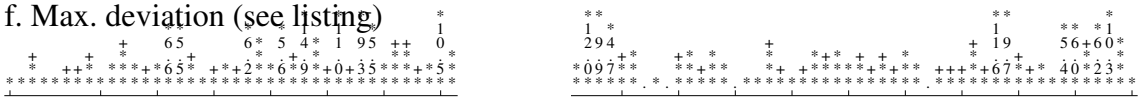


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

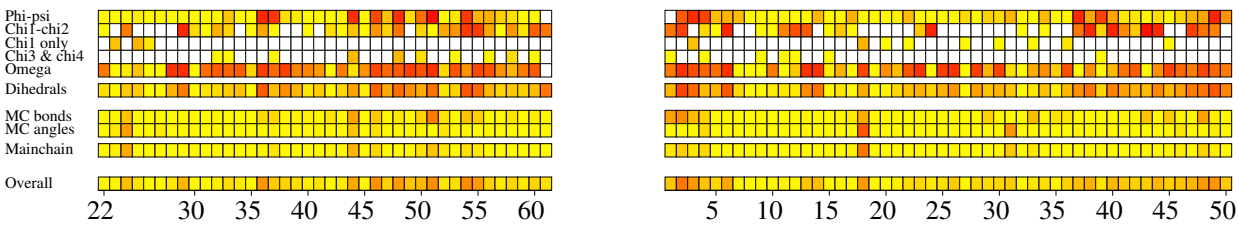
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

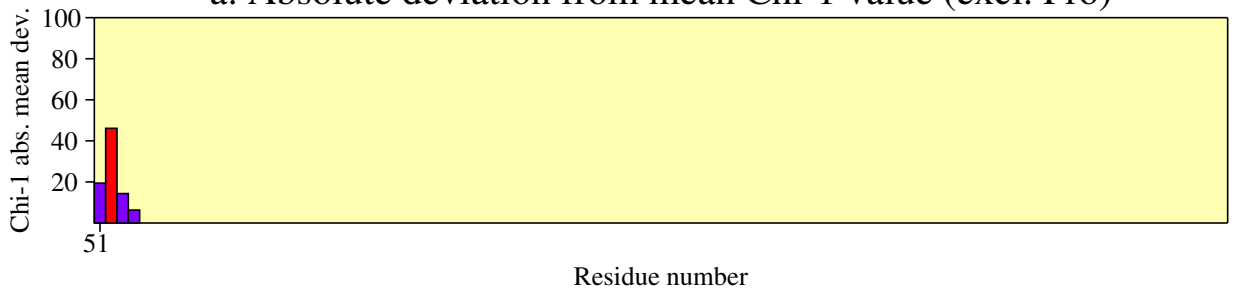


g. G-factors

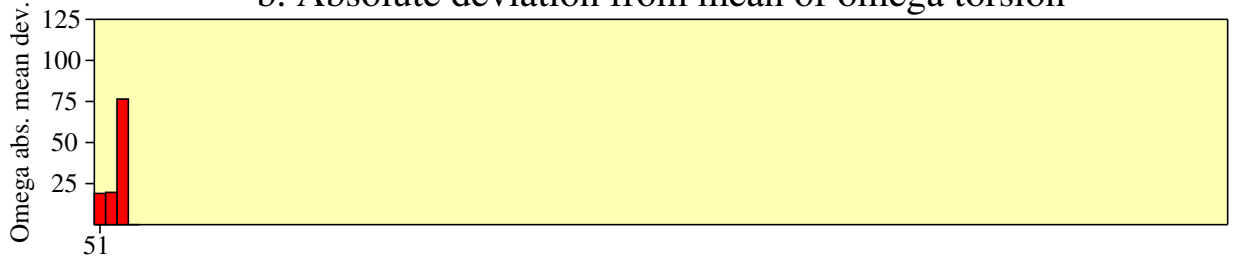


Residue properties
pdb1sqq

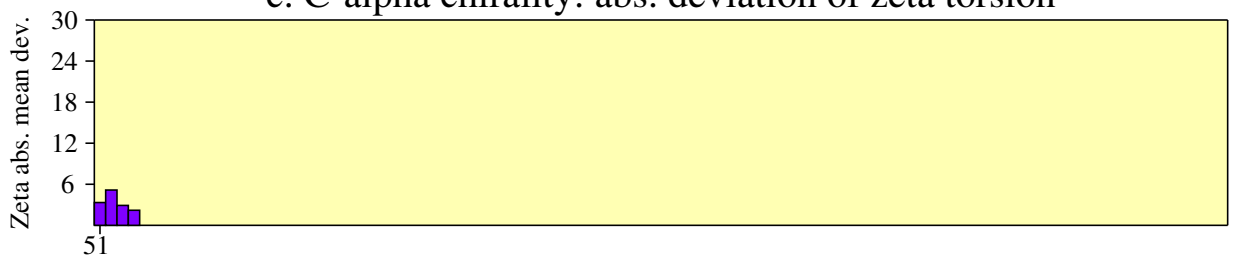
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



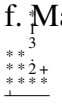
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

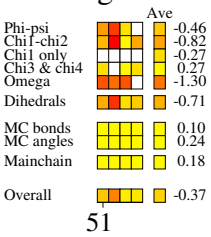
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

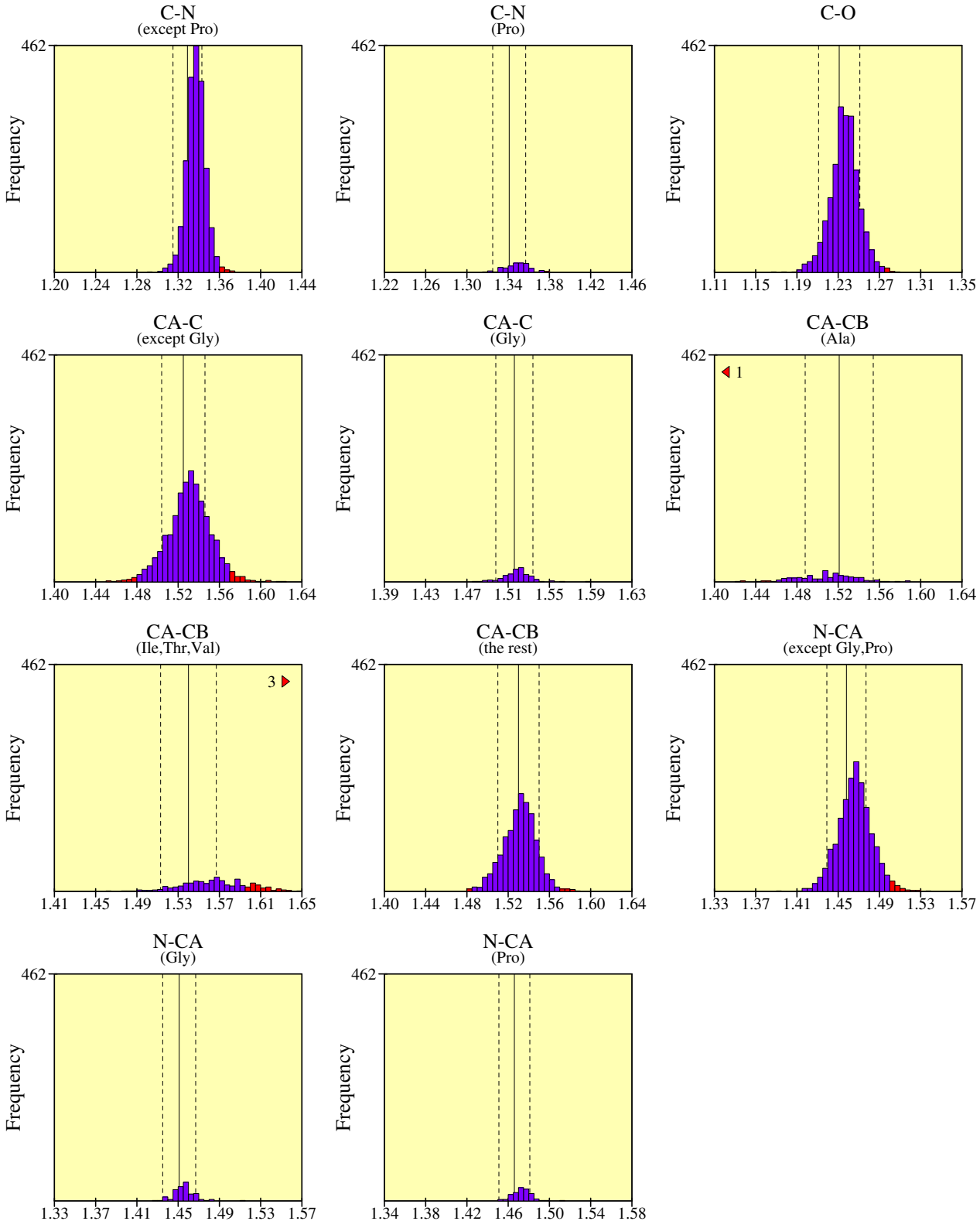


g. G-factors



Main-chain bond lengths

pdb1sqq

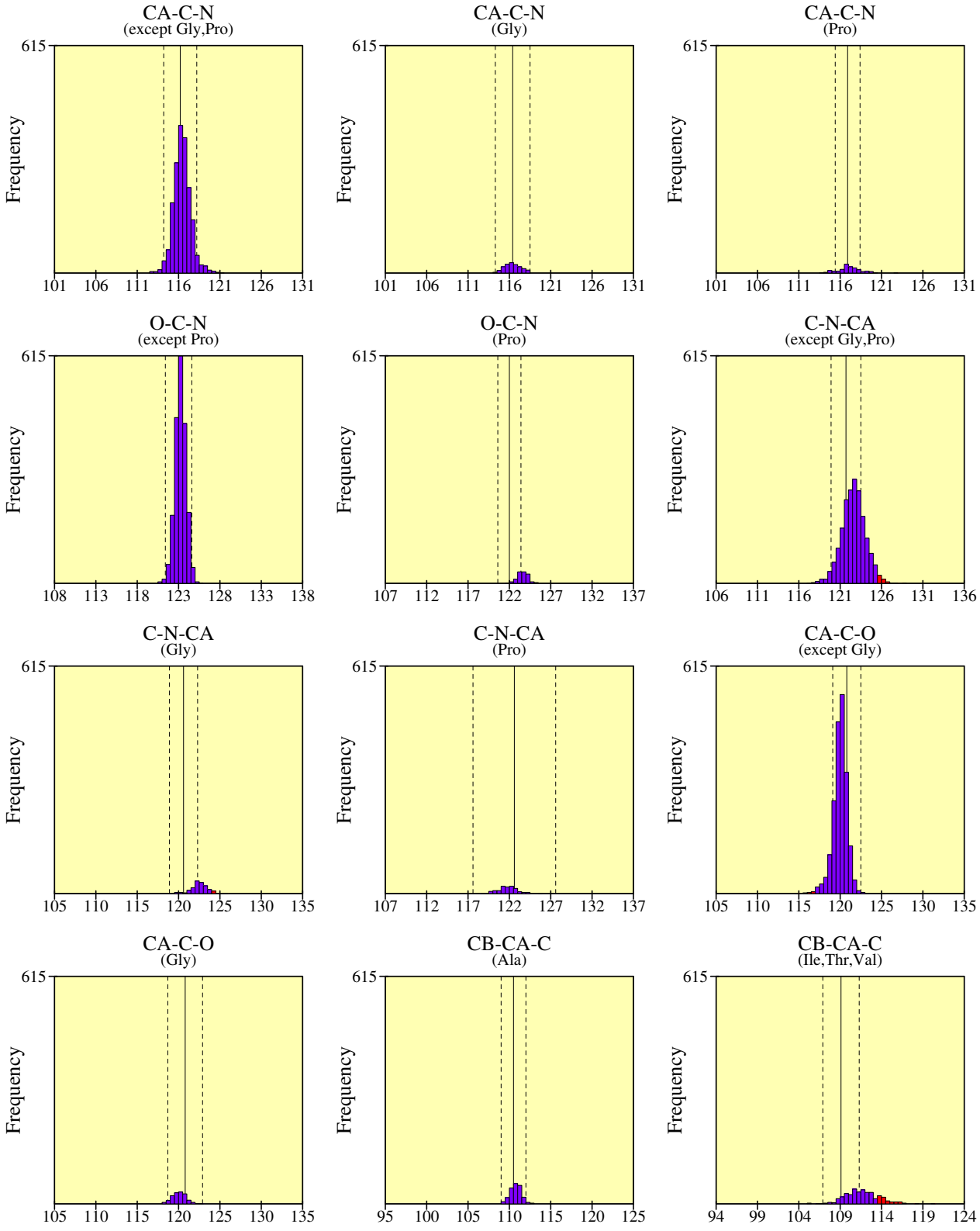


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

pdb1sqq

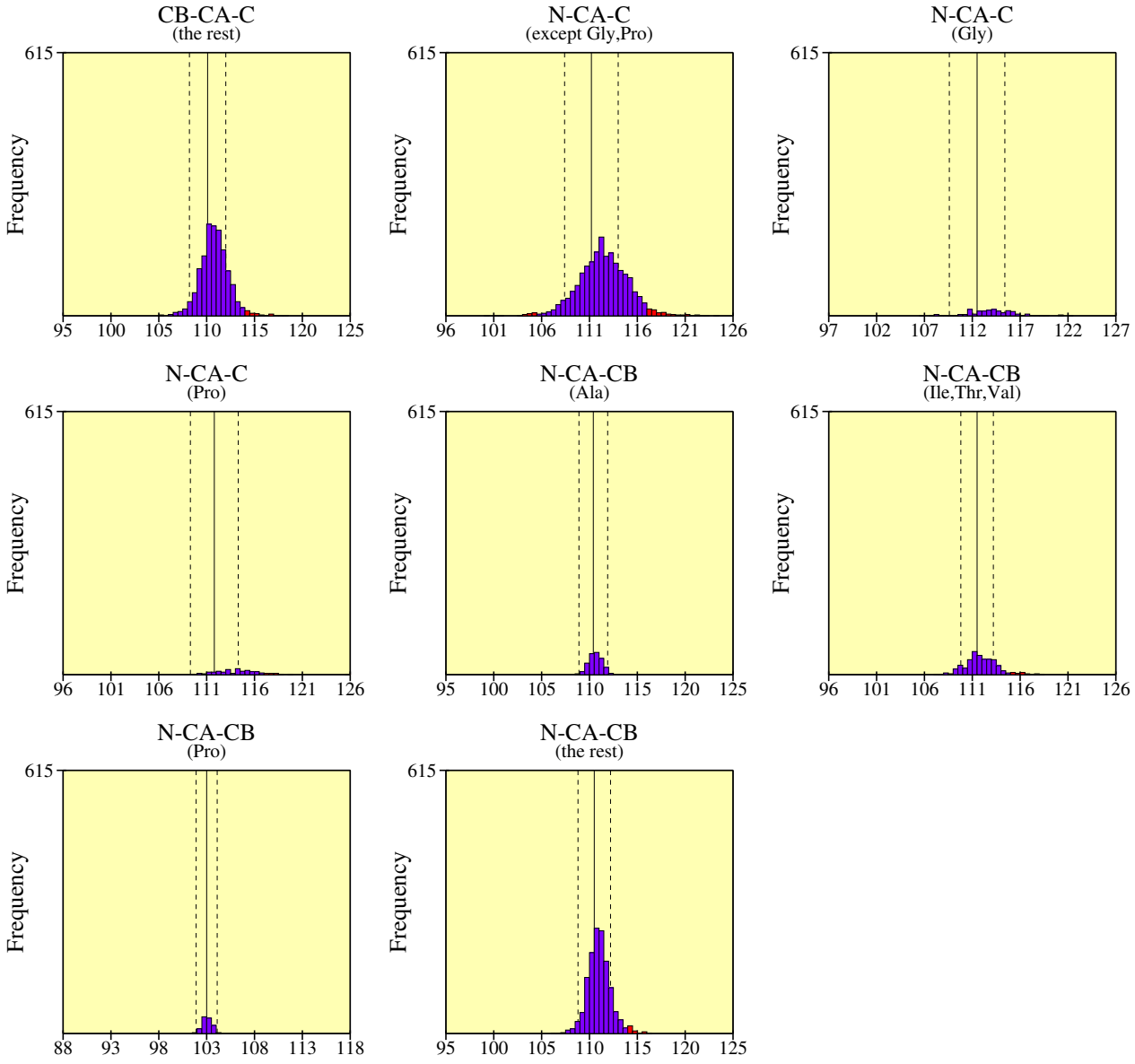


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

pdb1sqq

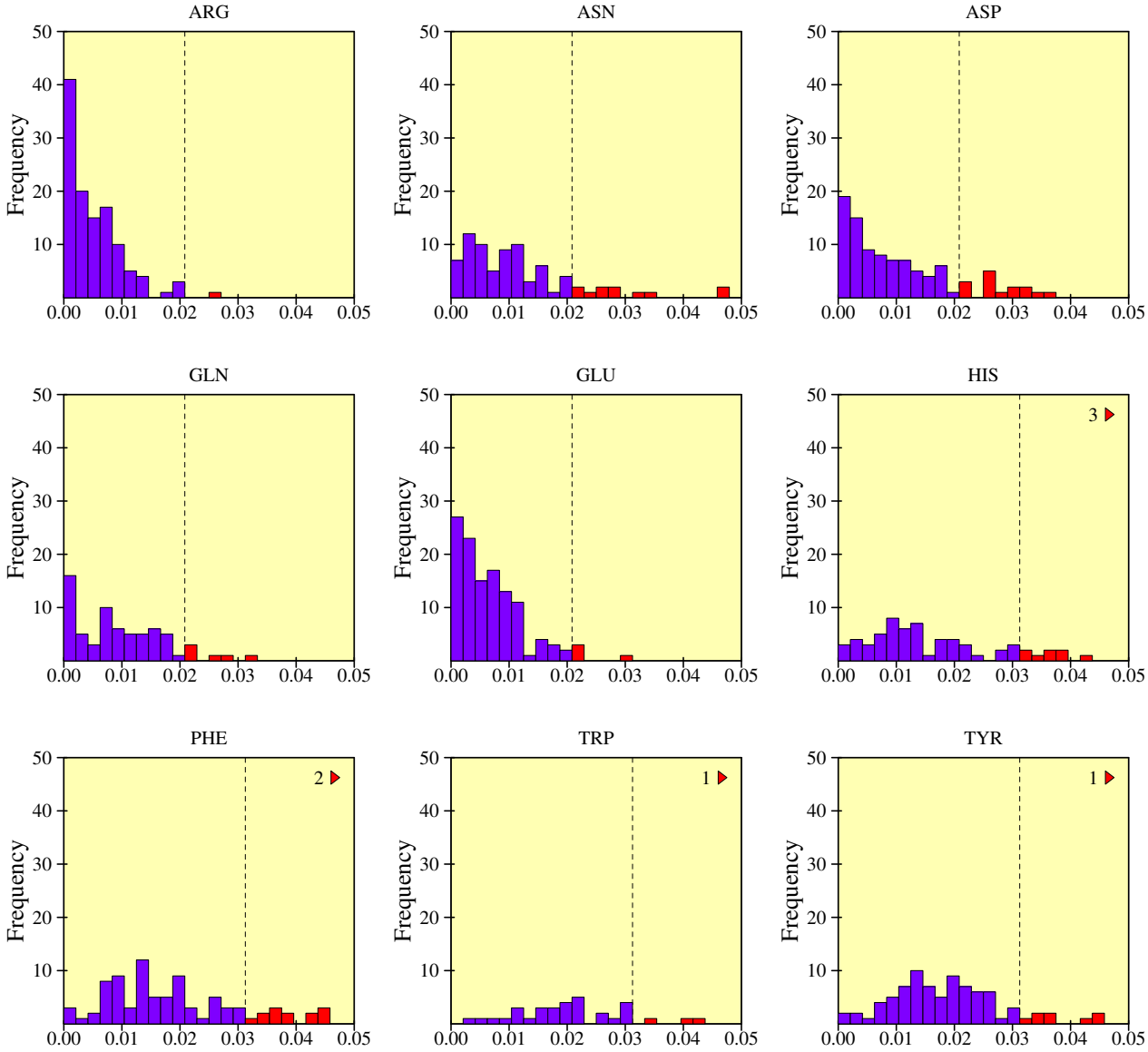


Black bars > 2.0 st. devs. from mean.

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

RMS distances from planarity

pdb1sqq



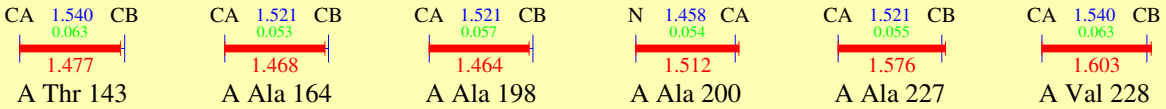
Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

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

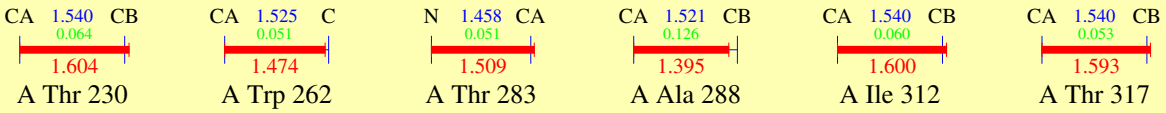
Distorted geometry
pdb1sqq

Main-chain bond lengths

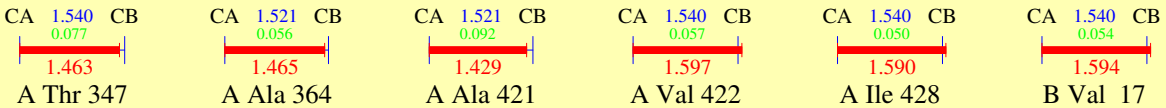
A Thr 1 | A Ala 7 | A Asn 52 | A Ala 84 | A Lys 100 | A Ile 127



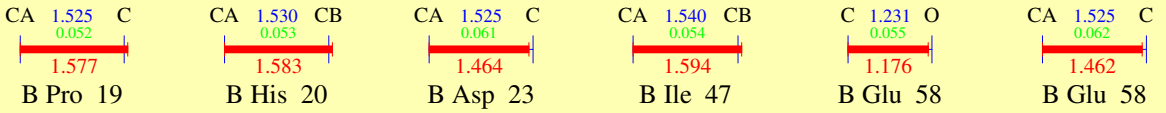
A Thr 143 | A Ala 164 | A Ala 198 | A Ala 200 | A Ala 227 | A Val 228



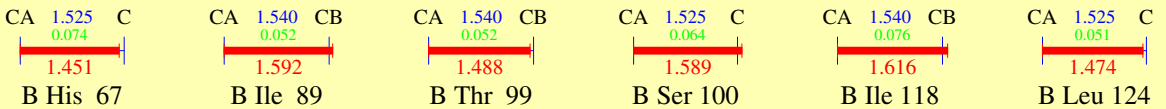
A Thr 230 | A Trp 262 | A Thr 283 | A Ala 288 | A Ile 312 | A Thr 317



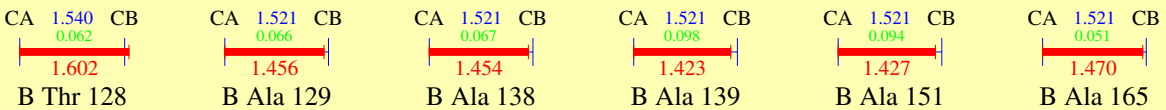
A Thr 347 | A Ala 364 | A Ala 421 | A Val 422 | A Ile 428 | B Val 17



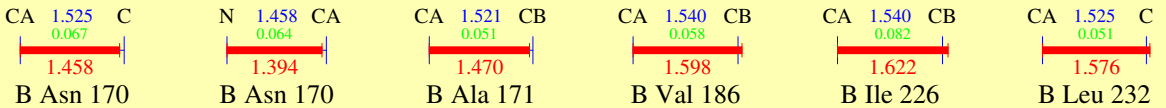
B Pro 19 | B His 20 | B Asp 23 | B Ile 47 | B Glu 58 | B Glu 58



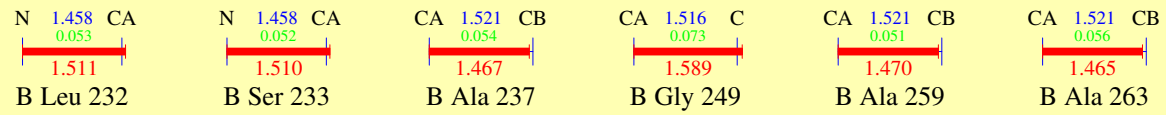
B His 67 | B Ile 89 | B Thr 99 | B Ser 100 | B Ile 118 | B Leu 124



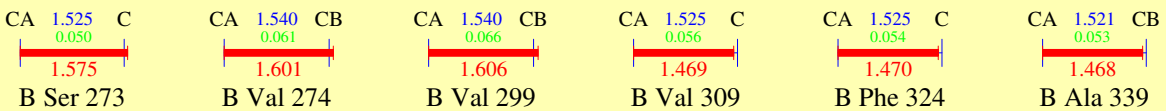
B Thr 128 | B Ala 129 | B Ala 138 | B Ala 139 | B Ala 151 | B Ala 165



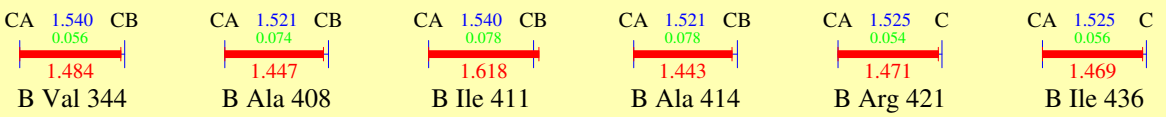
B Asn 170 | B Asn 170 | B Ala 171 | B Val 186 | B Ile 226 | B Leu 232



B Leu 232 | B Ser 233 | B Ala 237 | B Gly 249 | B Ala 259 | B Ala 263



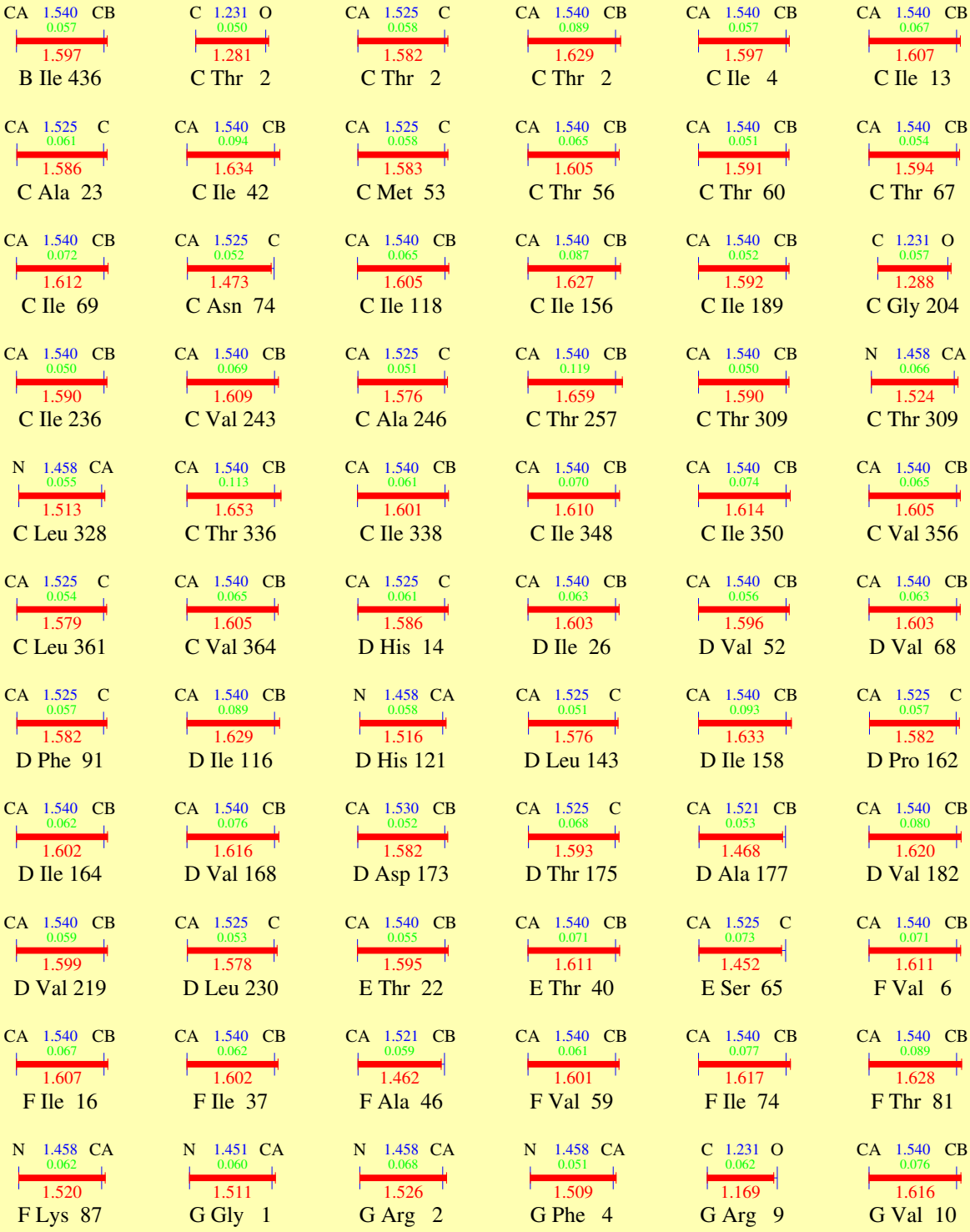
B Ser 273 | B Val 274 | B Val 299 | B Val 309 | B Phe 324 | B Ala 339



B Val 344 | B Ala 408 | B Ile 411 | B Ala 414 | B Arg 421 | B Ile 436

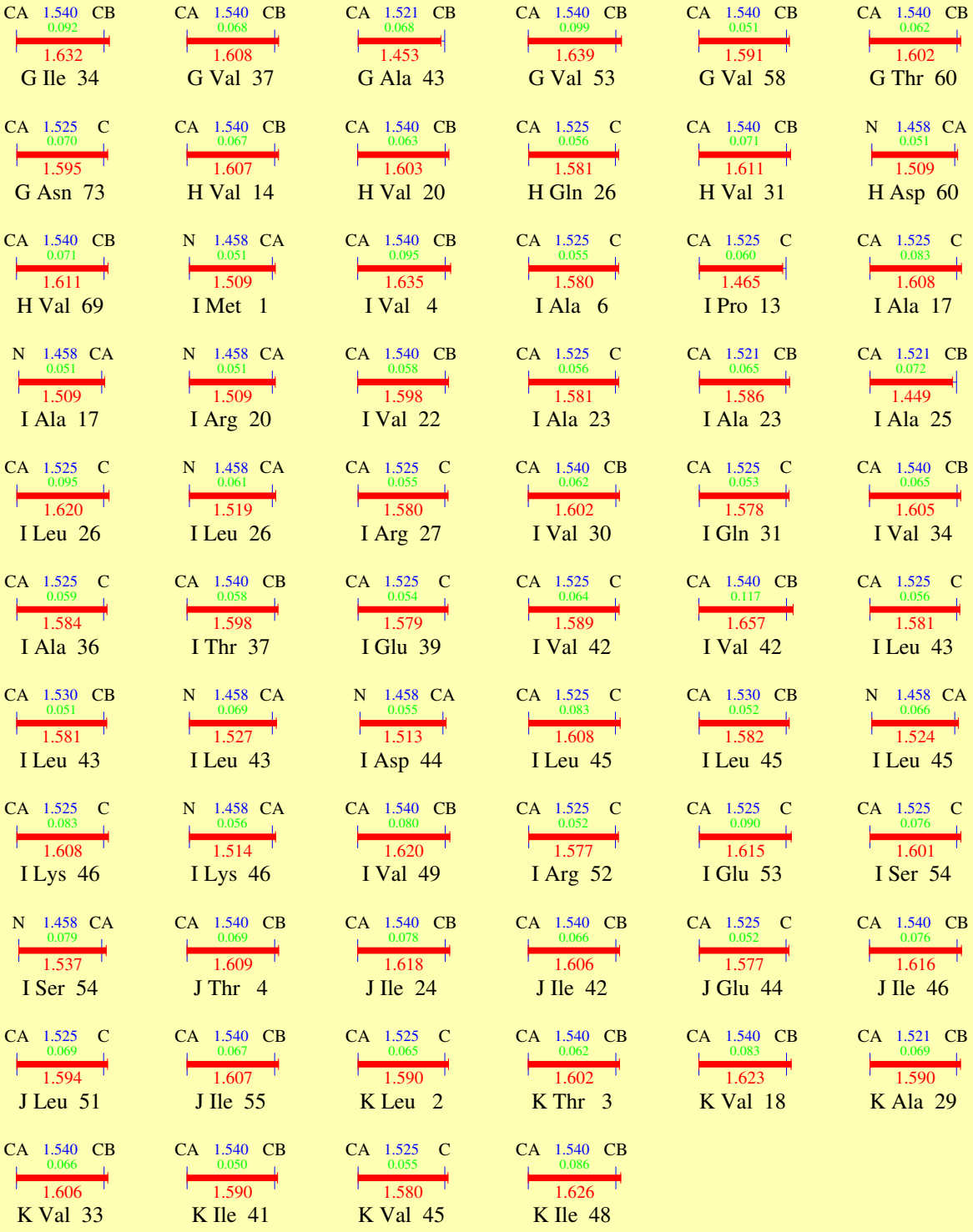
Distorted geometry
pdb1sqq

Main-chain bond lengths (contd)



Distorted geometry
pdb1sqq

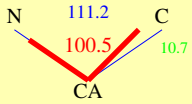
Main-chain bond lengths (contd)



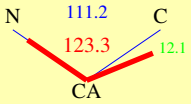
Bonds differing by > 0.05A from small-molecule values. Values shown: "ideal", difference, actual

Distorted geometry
pdb1sqq

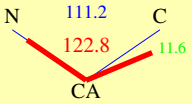
Main-chain bond angles



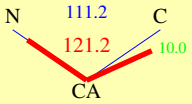
B Asn 170



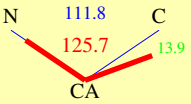
B Asn 197



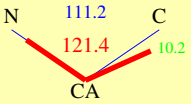
C Arg 318



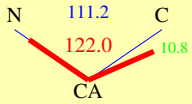
D Phe 91



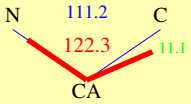
D Pro 92



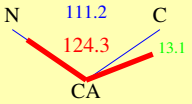
D Arg 120



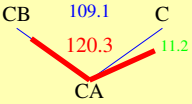
D Thr 175



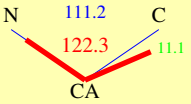
I Leu 26



I Arg 27



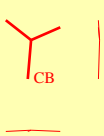
I Val 42



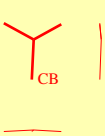
I Leu 45

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

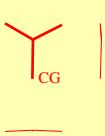
Planar groups



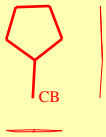
0.020
A Asp 20



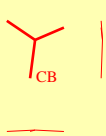
0.025
A Asn 52



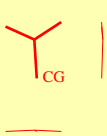
0.020
A Glu 80



0.035
A His 85

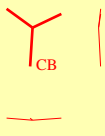


0.023
A Asn 87

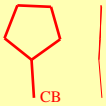


0.021
A Glu 93

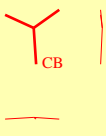
0.022
A Gln 159



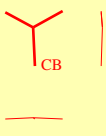
0.035
A Asp 181



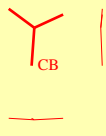
0.041
A His 243



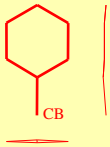
0.029
A Asp 281



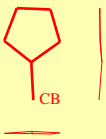
0.021
A Asn 301



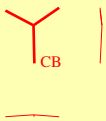
0.026
A Asp 332



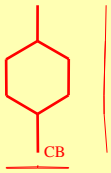
0.037
A Phe 336



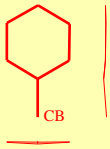
0.036
A His 368



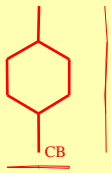
0.032
A Asp 378



0.041
A Tyr 414



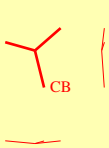
0.032
A Phe 415



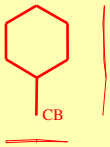
0.032
A Tyr 434

Distorted geometry
pdb1sqq

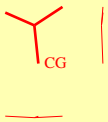
Planar groups (contd)



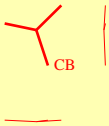
0.046
B Asn 104



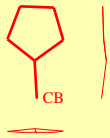
0.040
B Phe 122



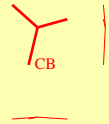
0.025
B Gln 143



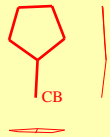
0.025
B Asn 154



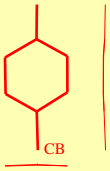
0.058
B His 158



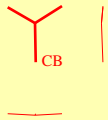
0.032
B Asn 162



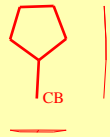
0.061
B His 164



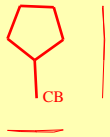
0.034
B Tyr 177



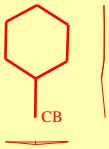
0.025
B Asp 180



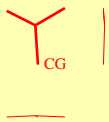
0.037
B His 192



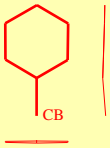
0.033
B His 198



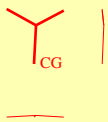
0.042
B Phe 199



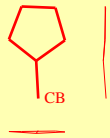
0.021
B Gln 222



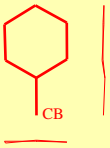
0.037
B Phe 223



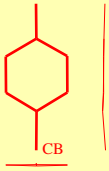
0.028
B Gln 247



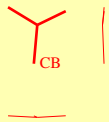
0.034
B His 254



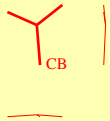
0.032
B Phe 324



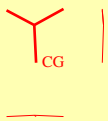
0.034
B Tyr 341



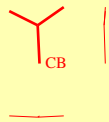
0.027
B Asn 354



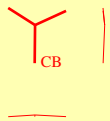
0.032
B Asp 380



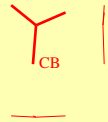
0.022
B Gln 400



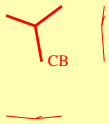
0.022
B Asp 409



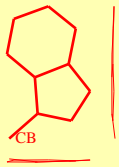
0.028
B Asn 429



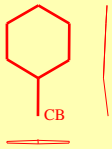
0.021
C Asp 20



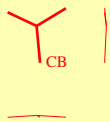
0.046
C Asn 26



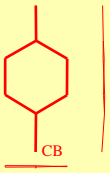
0.039
C Trp 31



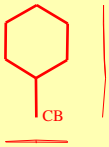
0.060
C Phe 33



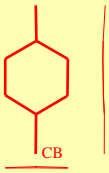
0.030
C Asn 74



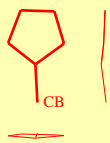
0.035
C Tyr 75



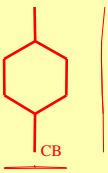
0.035
C Phe 90



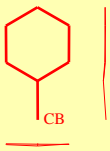
0.031
C Tyr 95



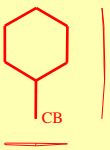
0.060
C His 97



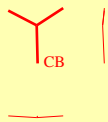
0.044
C Tyr 104



0.030
C Phe 168



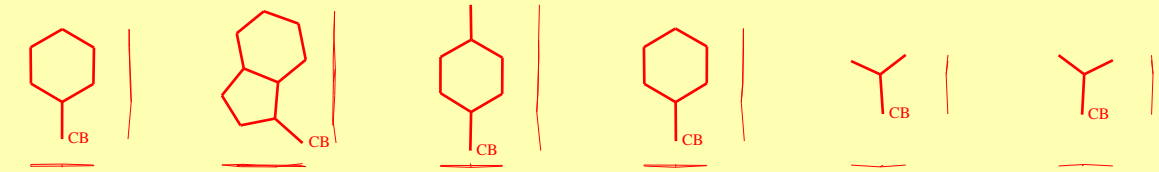
0.042
C Phe 187



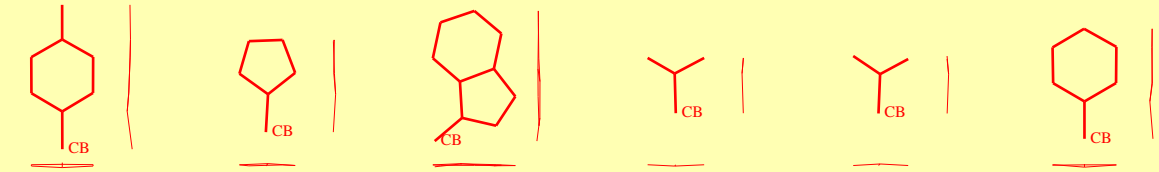
0.029
C Asp 331

Distorted geometry
pdb1sqq

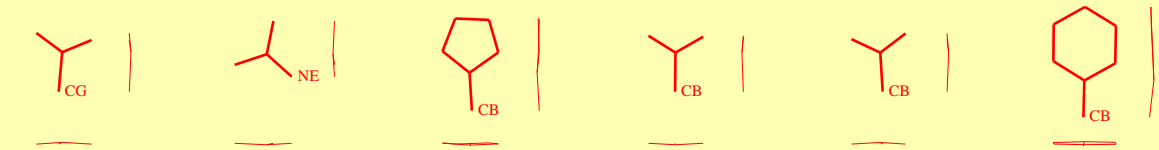
Planar groups (contd)



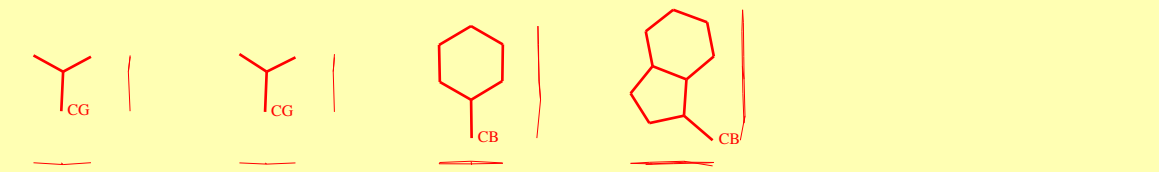
0.040 C Phe 359 | 0.040 C Trp 379 | 0.044 D Tyr 33 | 0.034 D Phe 81 | 0.030 D Asp 172 | 0.025 D Asp 173



0.054 D Tyr 220 | 0.031 D His 225 | 0.034 D Trp 227 | 0.022 F Asn 40 | 0.026 F Asp 42 | 0.035 F Phe 60



0.029 F Glu 96 | 0.025 F Arg 101 | 0.031 G His 6 | 0.024 H Asp 41 | 0.026 H Asp 60 | 0.056 I Phe 11



0.030 I Gln 31 | 0.020 I Glu 53 | 0.043 J Phe 20 | 0.049 K Trp 24

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