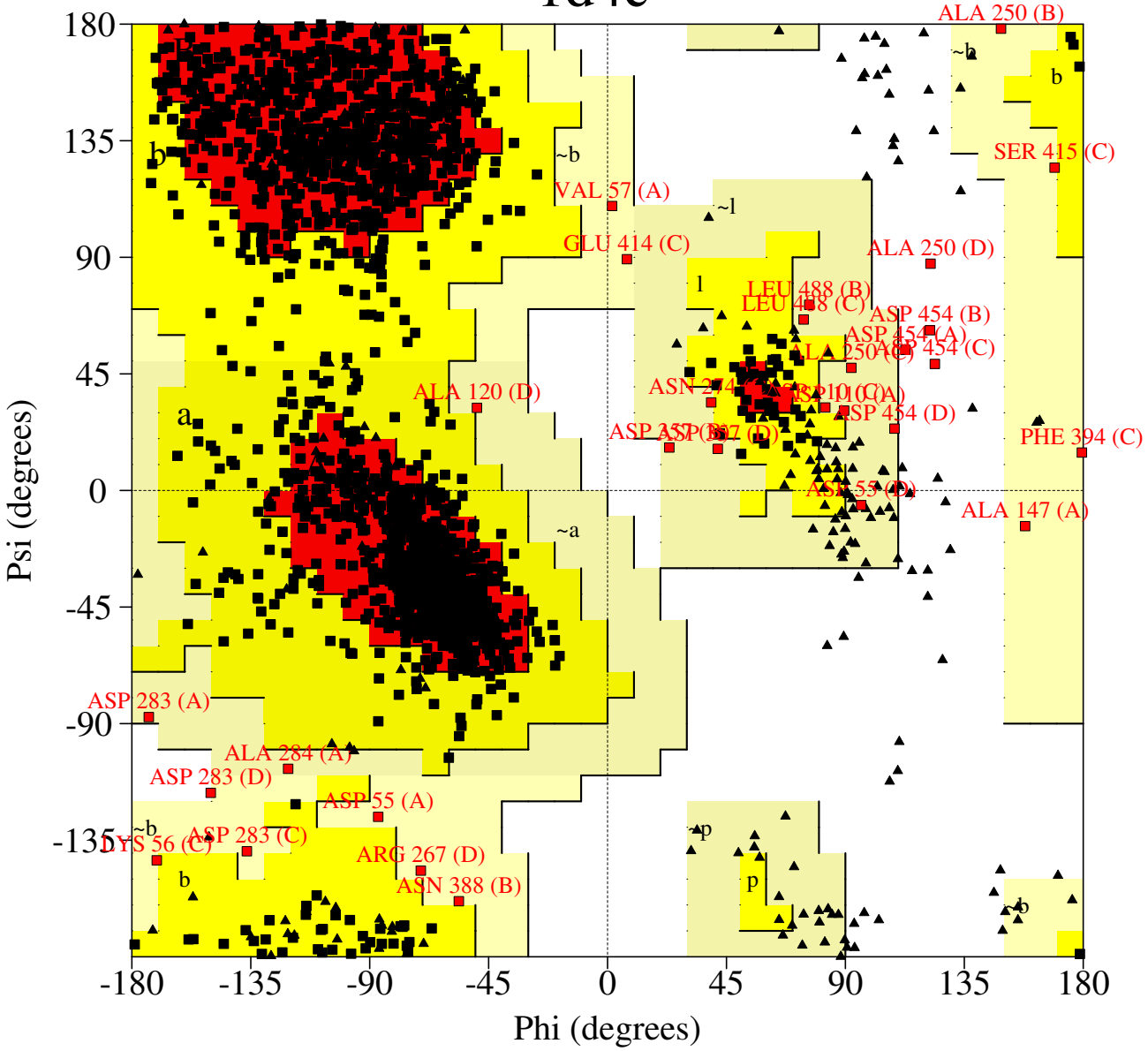
PROCHECK

Ramachandran Plot

1d4c



Plot statistics

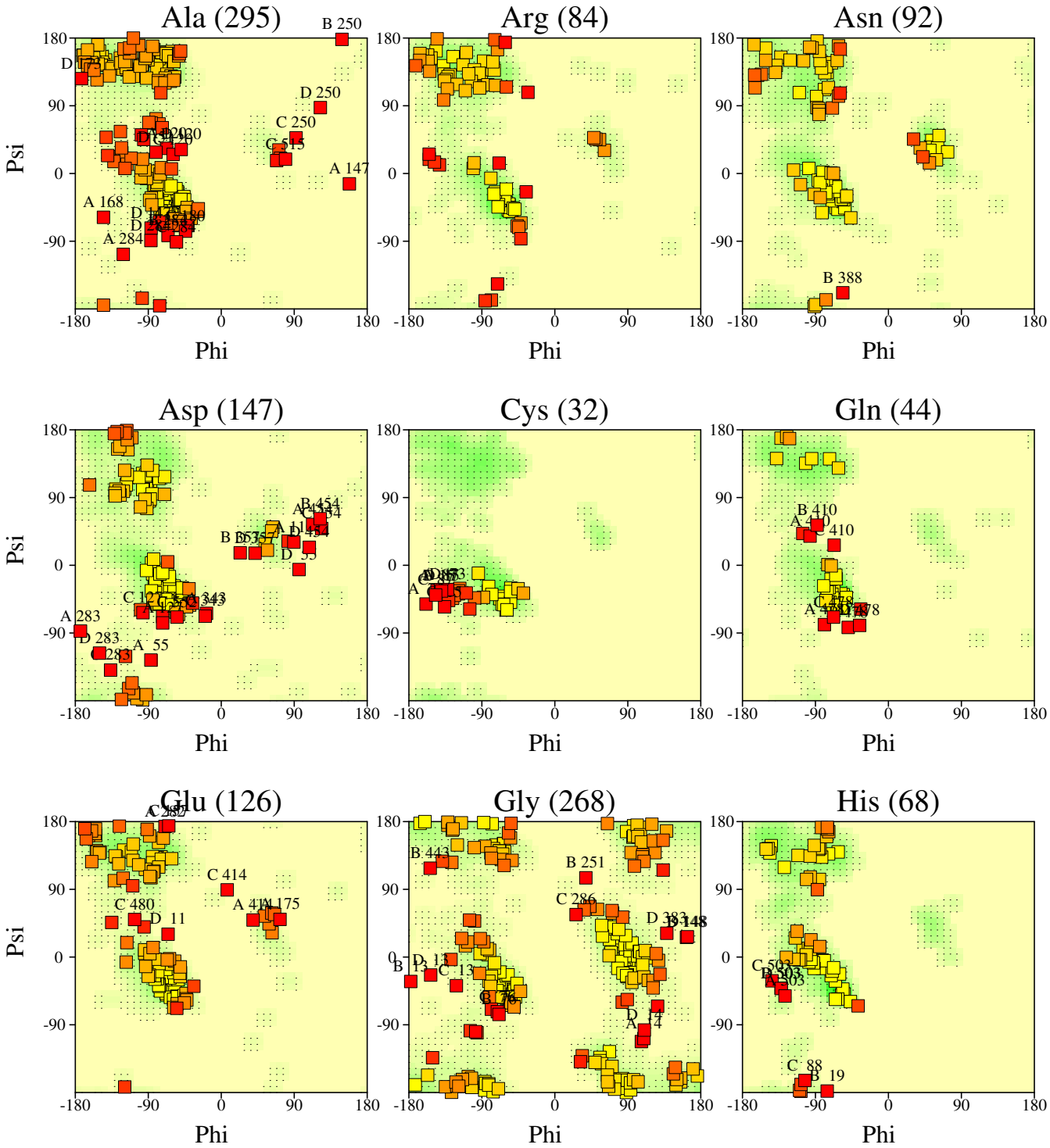
Residues in most favoured regions [A,B,L]	1598	83.4%
Residues in additional allowed regions [a,b,l,p]	290	15.1%
Residues in generously allowed regions [~a,~b,~l,~p]	24	1.3%
Residues in disallowed regions	5	0.3%
	----	------
Number of non-glycine and non-proline residues	1917	100.0%
Number of end-residues (excl. Gly and Pro)	11	
Number of glycine residues (shown as triangles)	268	
Number of proline residues	78	

Total number of residues	2274	

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

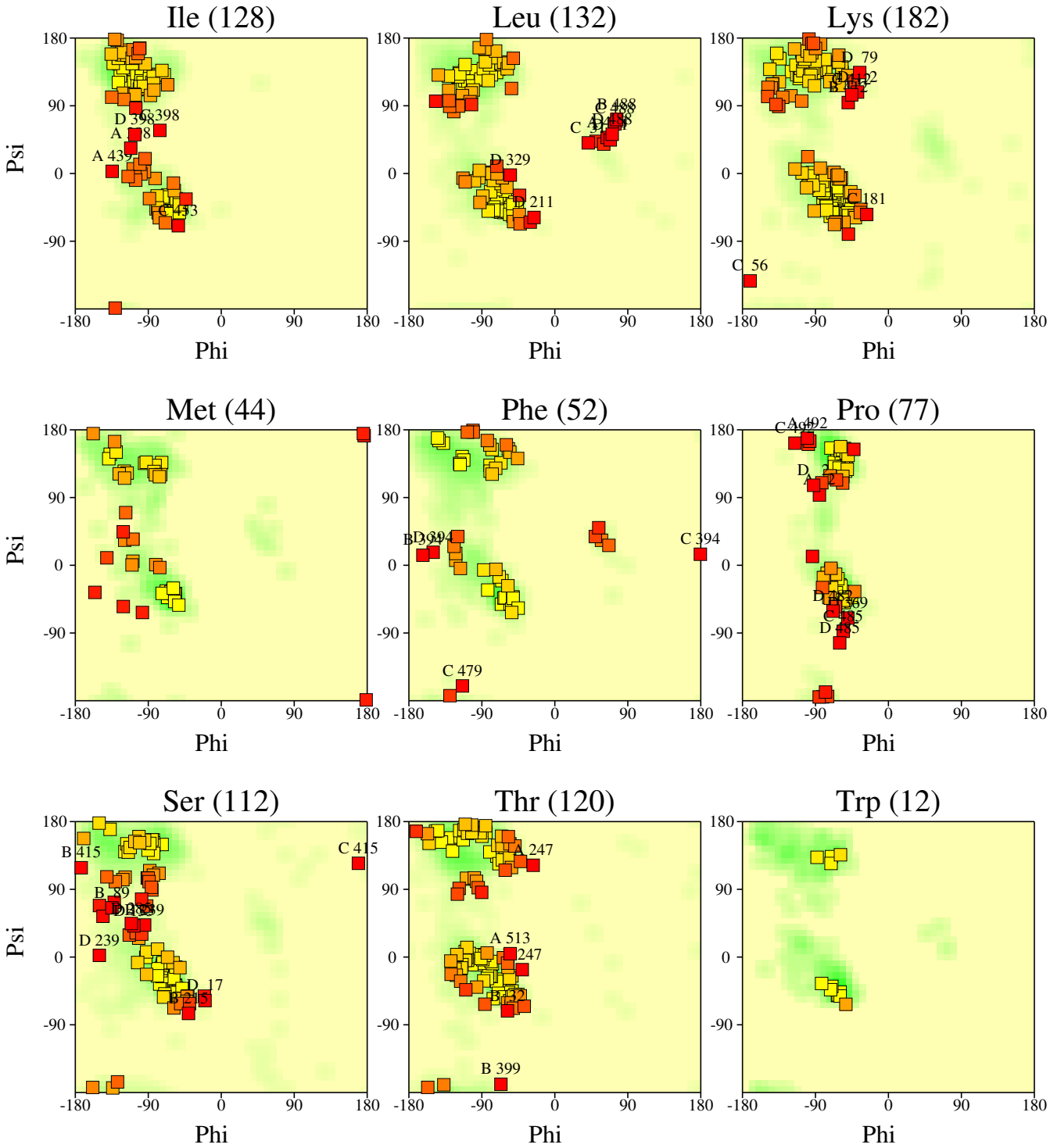
1d4c



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

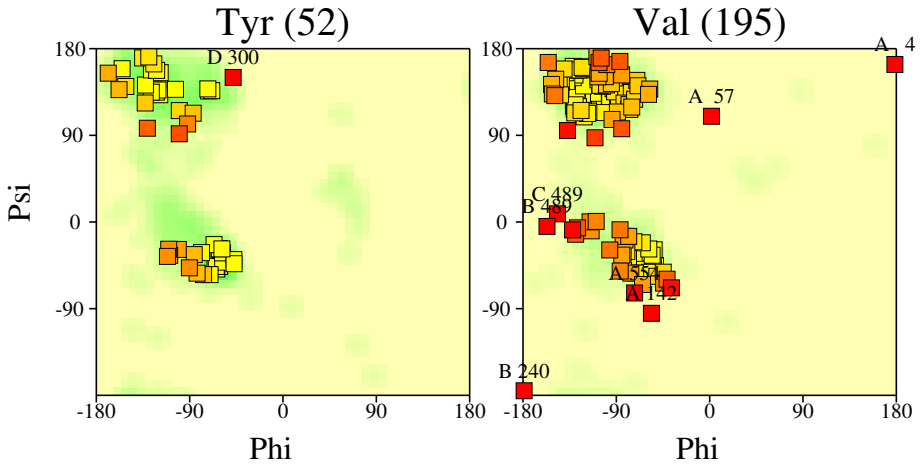
1d4c



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

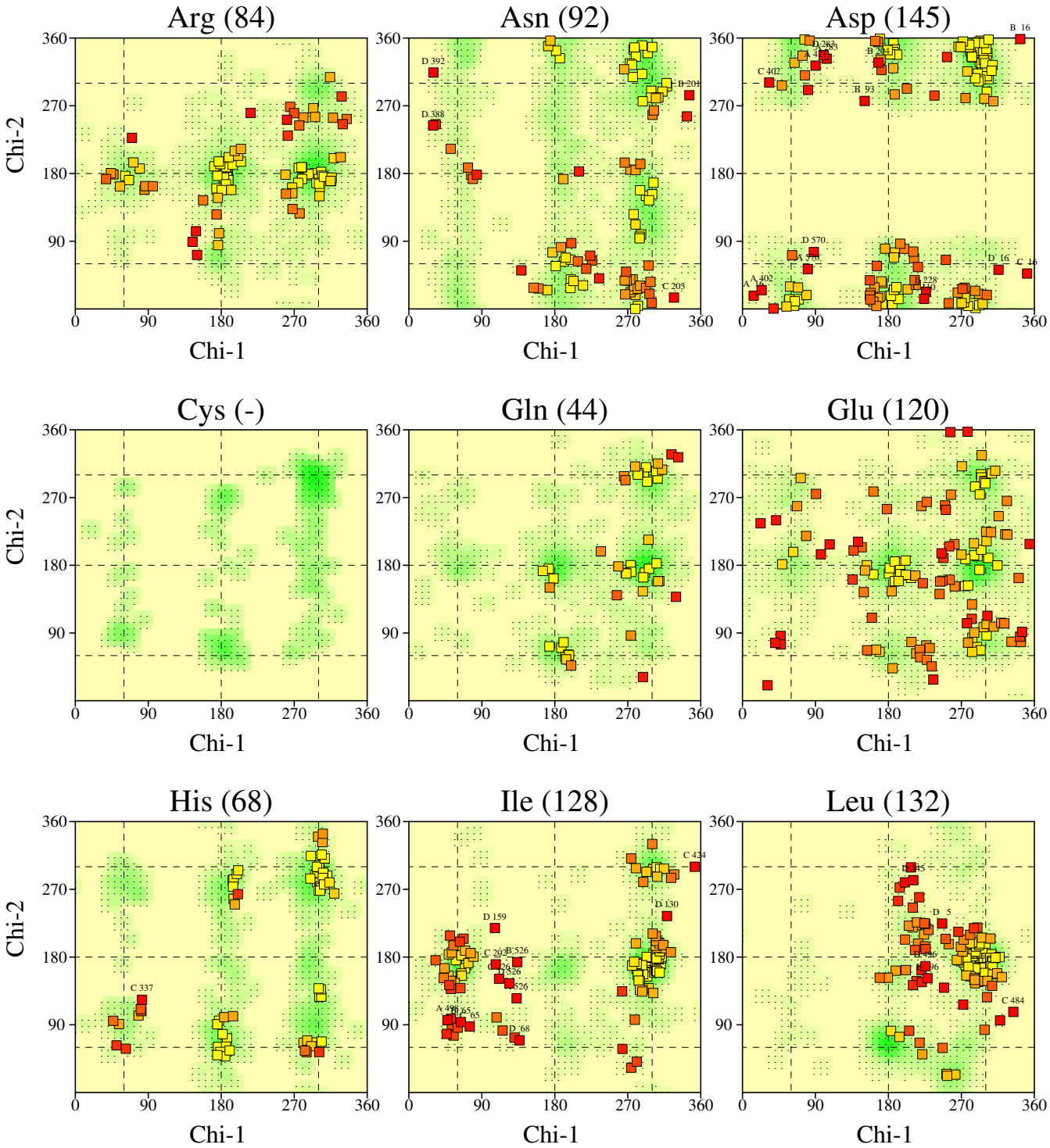
1d4c



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

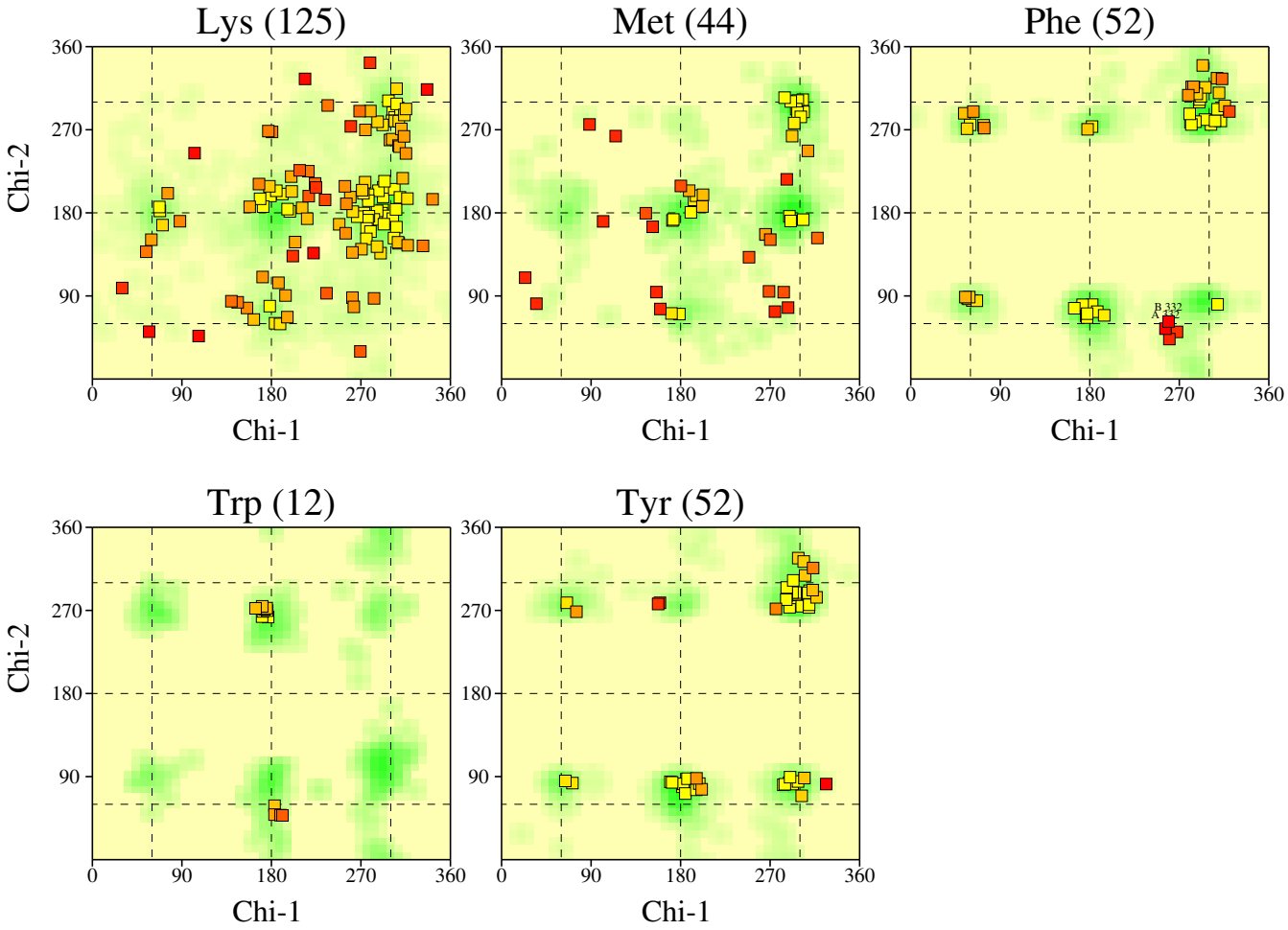
1d4c



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

1d4c



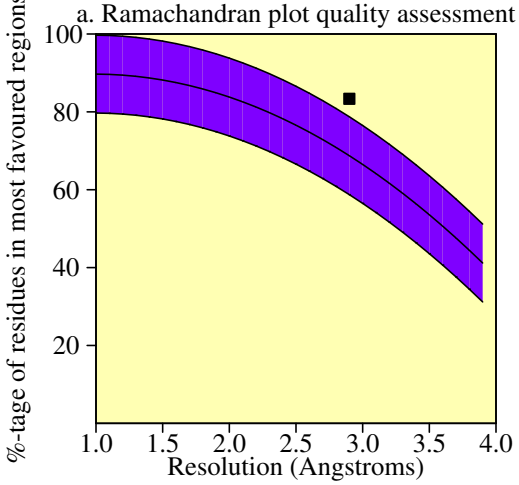
Numbers of residues are shown in brackets. Those in unfavourable conformations (score < -3.00) are labelled.
Shading shows favourable conformations as obtained from an analysis of 163 structures at resolution 2.0A or better.

PROCHECK

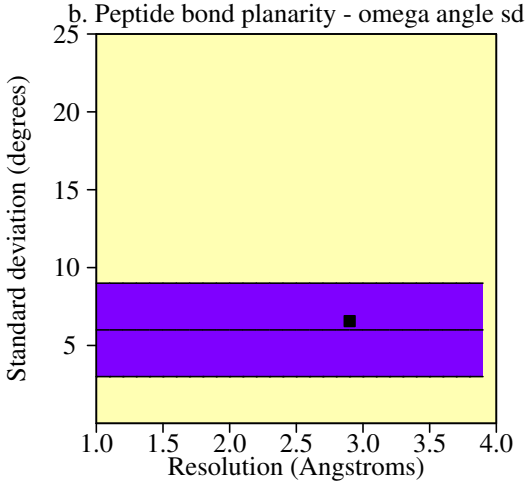
Main-chain parameters

1d4c

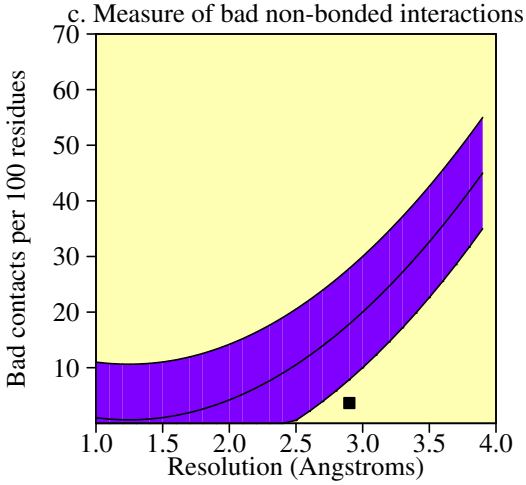
a. Ramachandran plot quality assessment



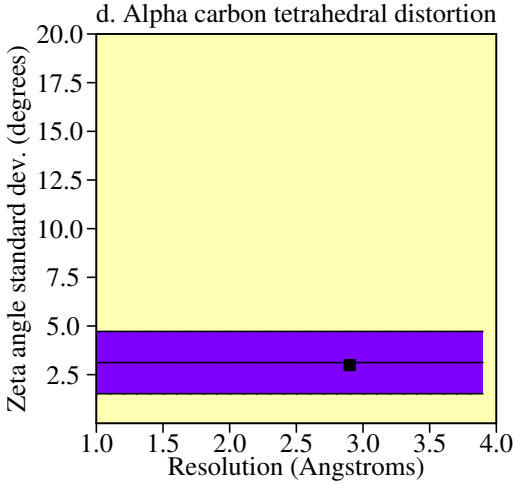
b. Peptide bond planarity - omega angle sd



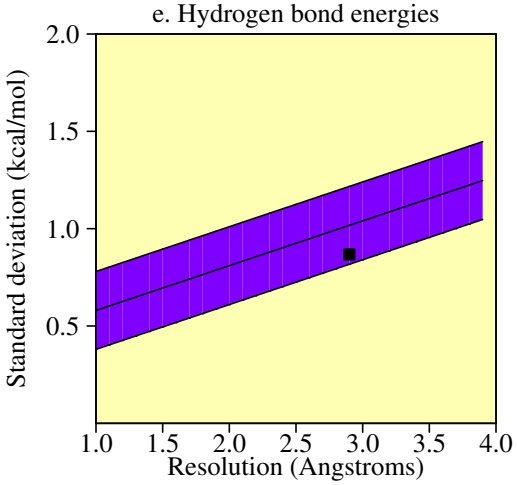
c. Measure of bad non-bonded interactions



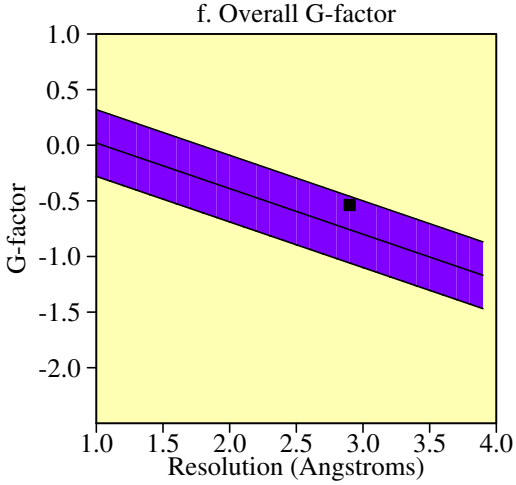
d. Alpha carbon tetrahedral distortion



e. Hydrogen bond energies



f. Overall G-factor



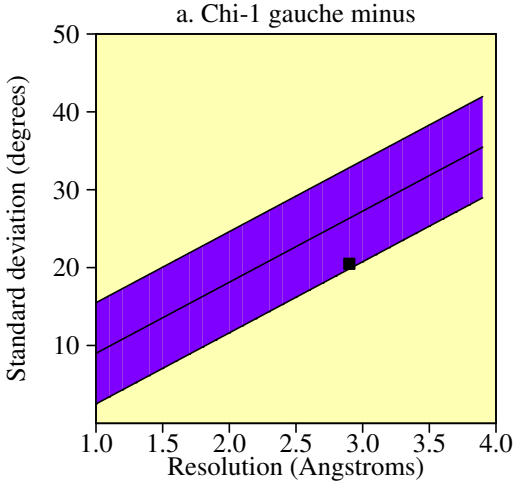
Plot statistics

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	1917	83.4	68.7	10.0	1.5	BETTER
b. Omega angle st dev	2268	6.6	6.0	3.0	0.2	Inside
c. Bad contacts / 100 residues	83	3.6	17.9	10.0	-1.4	BETTER
d. Zeta angle st dev	2004	3.0	3.1	1.6	-0.1	Inside
e. H-bond energy st dev	1367	0.9	1.0	0.2	-0.7	Inside
f. Overall G-factor	2274	-0.5	-0.8	0.3	0.7	Inside

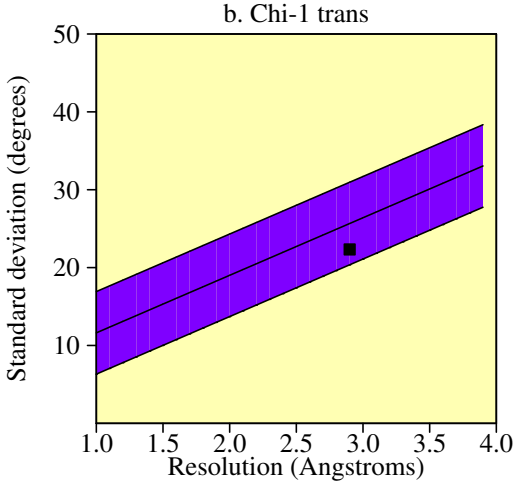
Side-chain parameters

1d4c

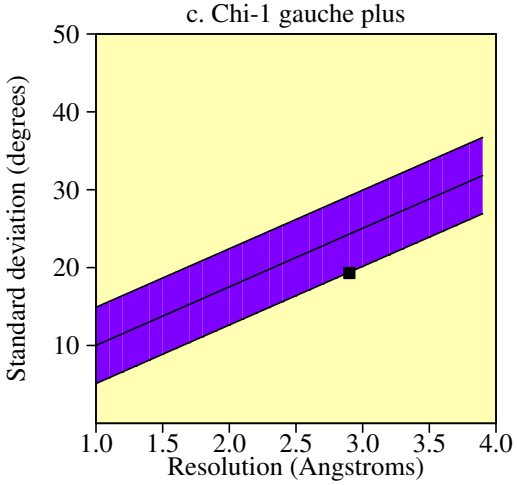
a. Chi-1 gauche minus



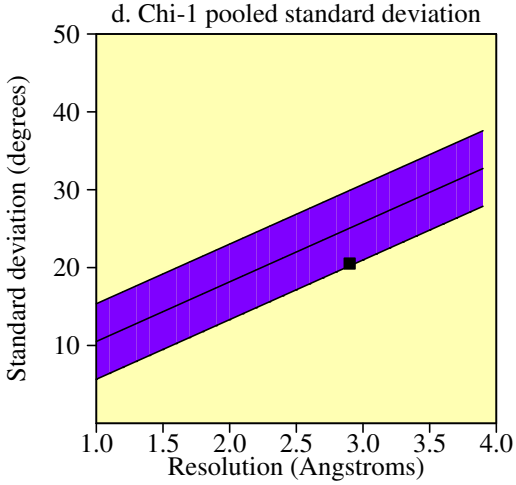
b. Chi-1 trans



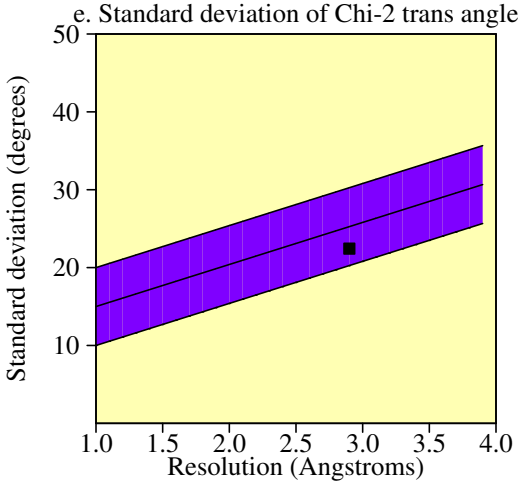
c. Chi-1 gauche plus



d. Chi-1 pooled standard deviation



e. Standard deviation of Chi-2 trans angle



1d4c

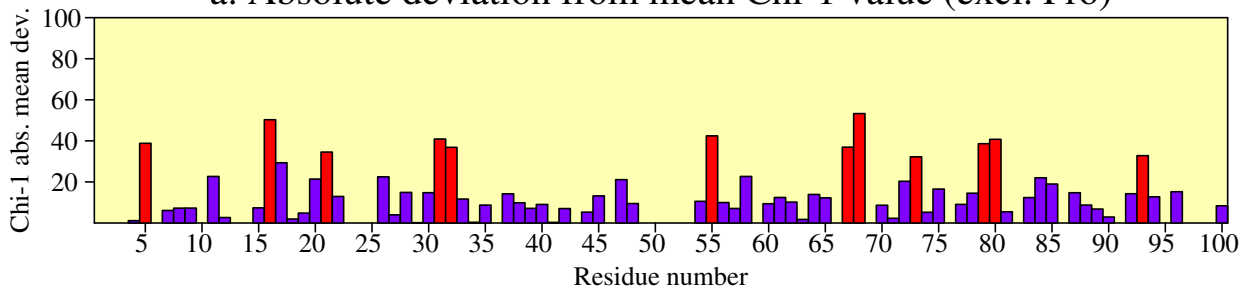
Plot statistics

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	273	20.5	26.3	6.5	-0.9	Inside
b. Chi-1 trans st dev	508	22.3	25.7	5.3	-0.6	Inside
c. Chi-1 gauche plus st dev	769	19.3	24.3	4.9	-1.0	BETTER
d. Chi-1 pooled st dev	1550	20.5	25.1	4.8	-0.9	Inside
e. Chi-2 trans st dev	451	22.4	25.3	5.0	-0.6	Inside

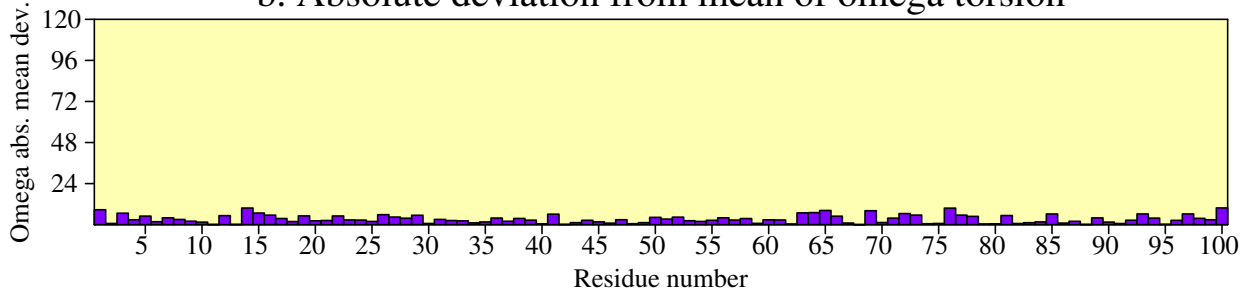
Residue properties

1d4c

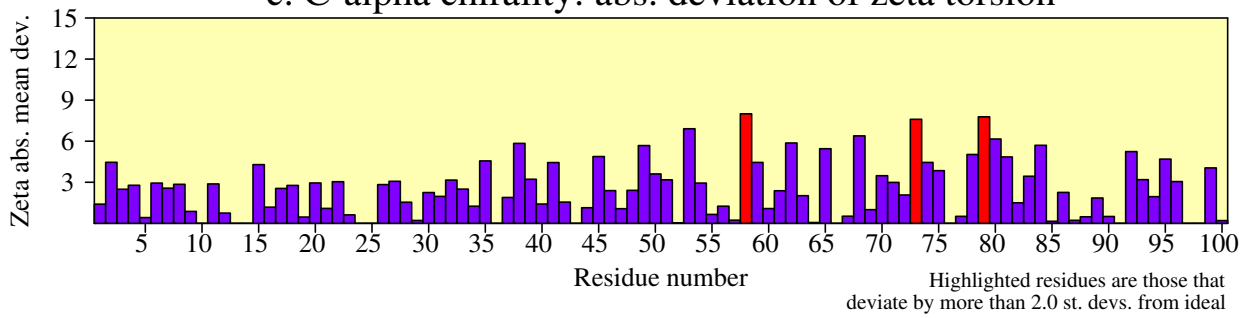
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

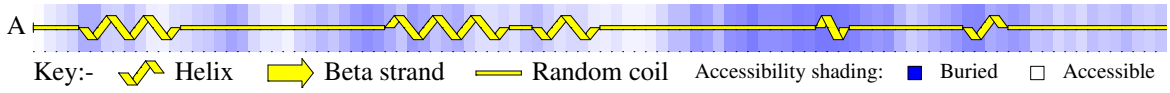


c. C-alpha chirality: abs. deviation of zeta torsion



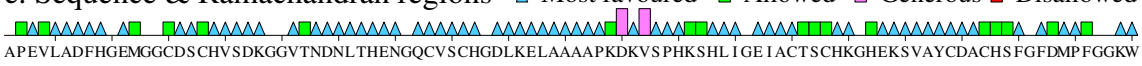
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



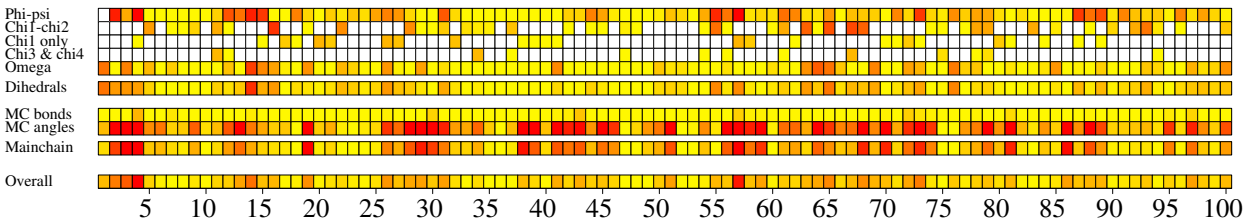
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

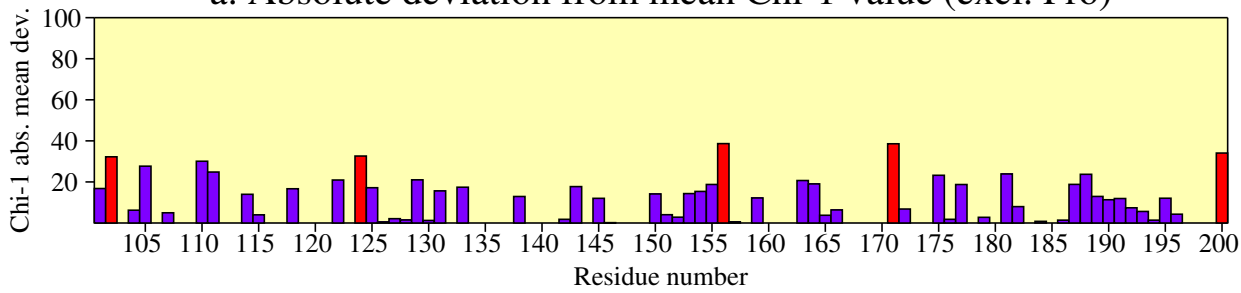
g. G-factors



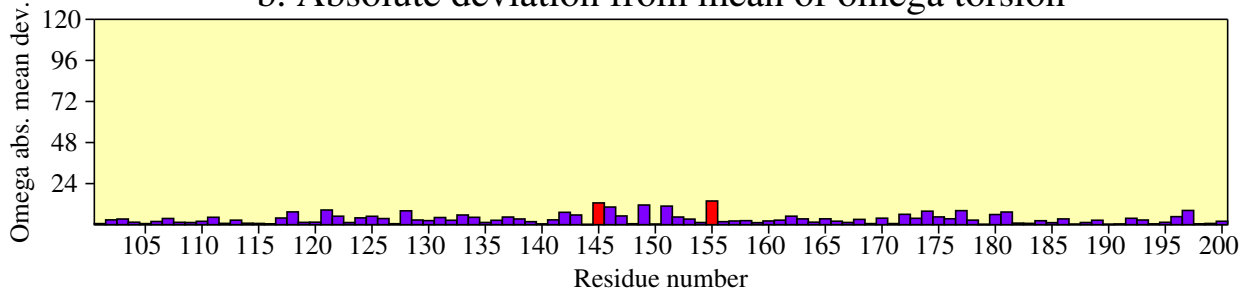
Residue properties

1d4c

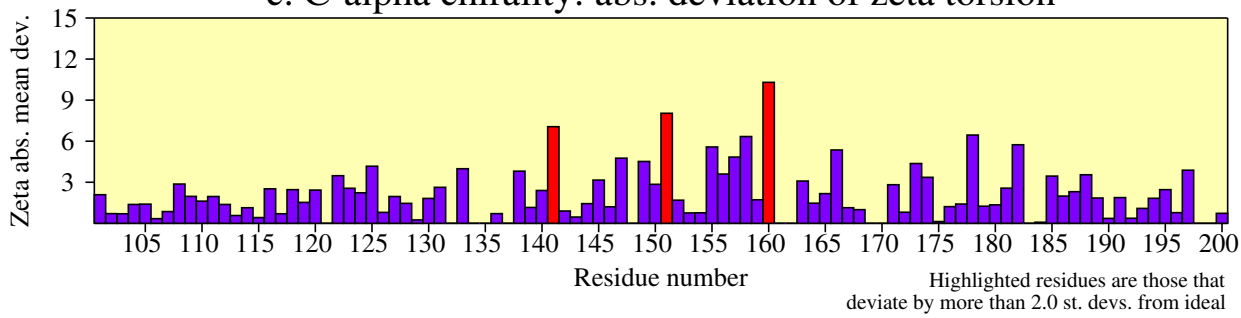
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

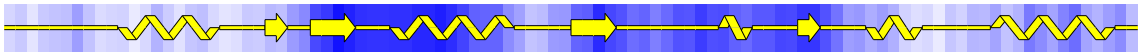


c. C-alpha chirality: abs. deviation of zeta torsion



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

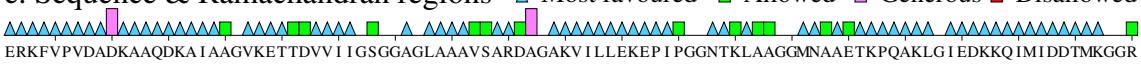
d. Secondary structure & estimated accessibility



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

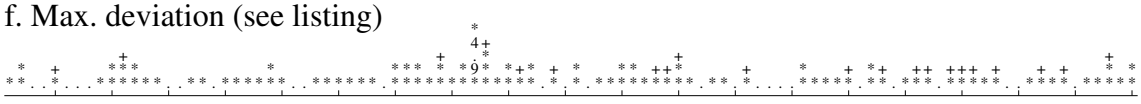
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

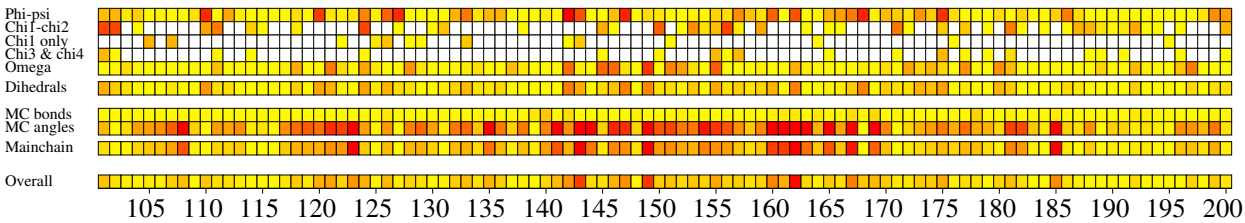


ERKFVPVDADKAAQDKA I AAGVKETTDVV I I GSGGAGLAAAVSARDAGAKV I LLEKEP I PGGNTKLAAGGMNAAETKPQAKLG I EDKKQ IM I DDTMKGGR

f. Max. deviation (see listing)



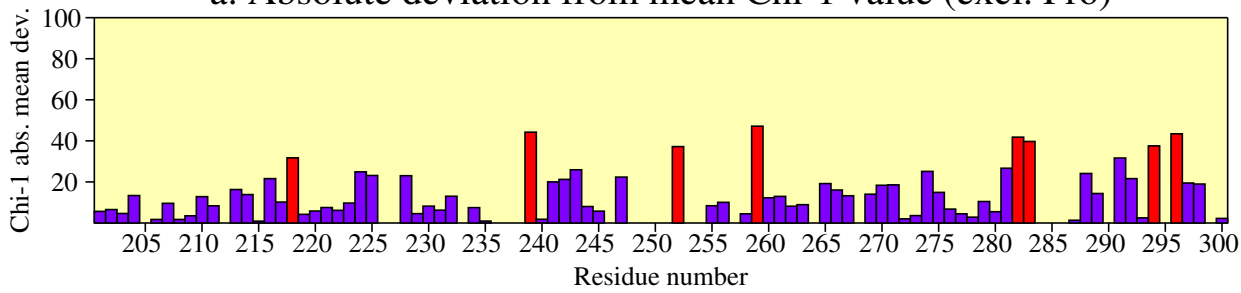
g. G-factors



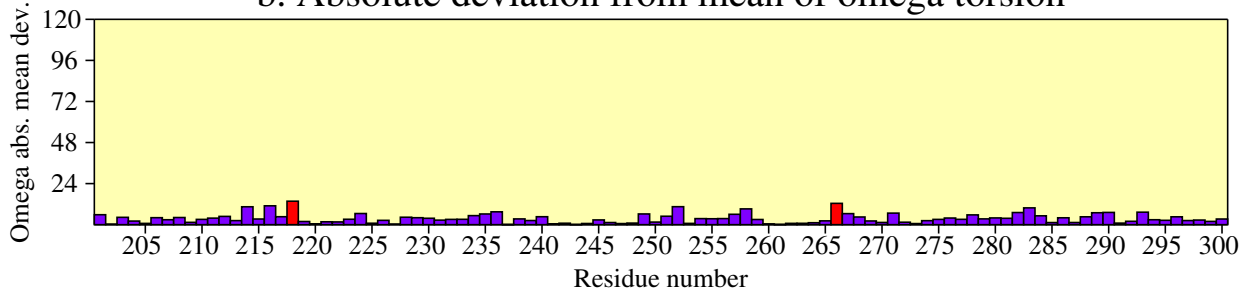
Residue properties

1d4c

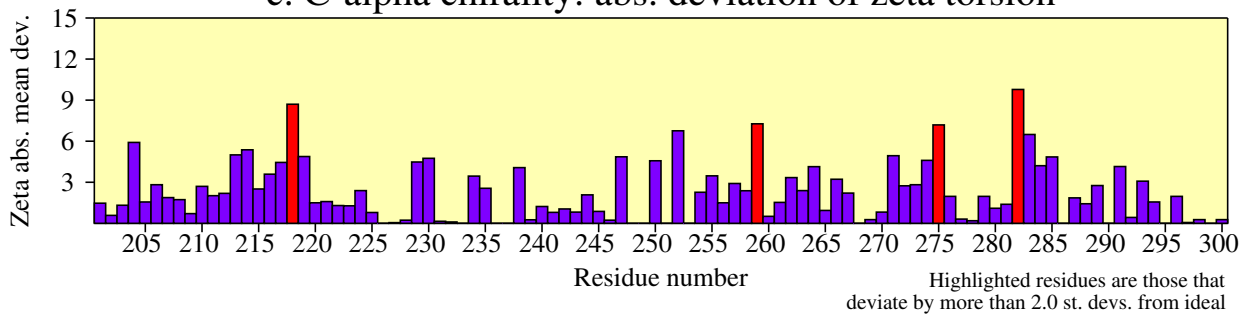
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

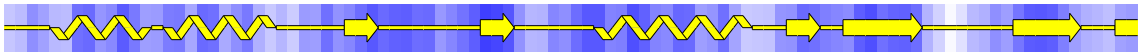


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



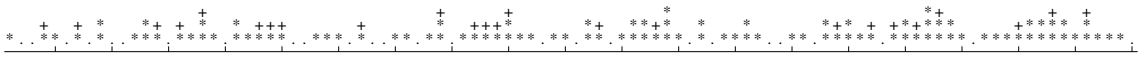
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

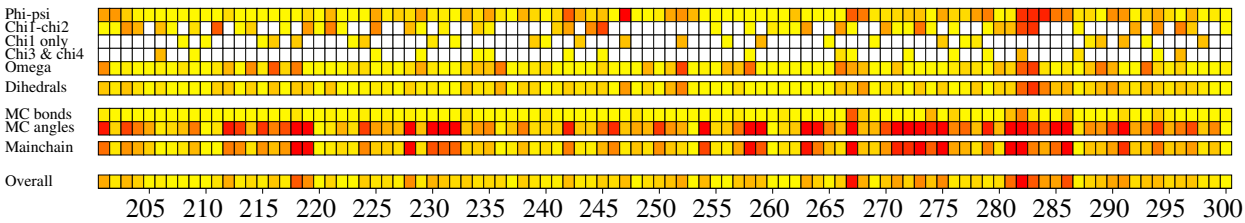
Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)

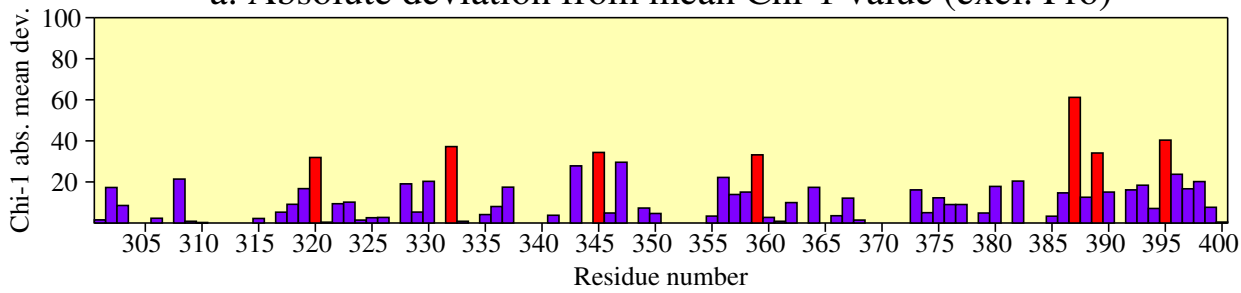


g. G-factors

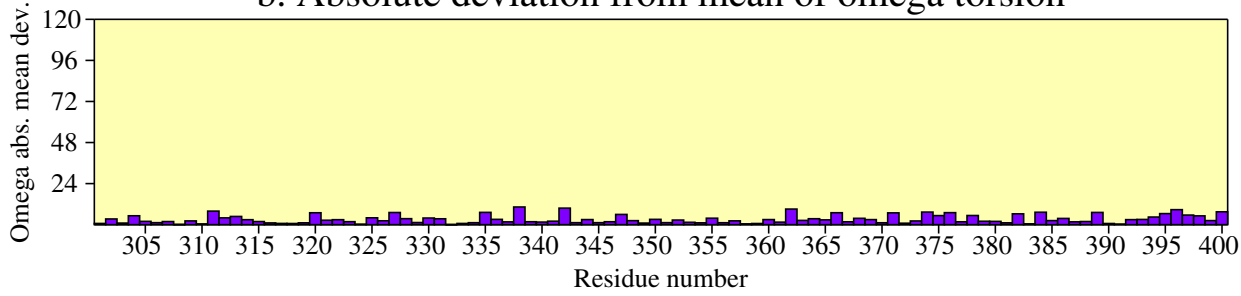


Residue properties
1d4c

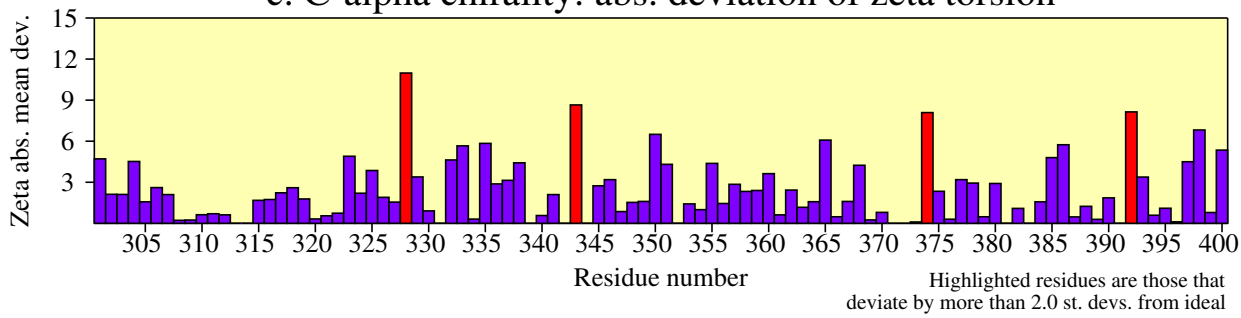
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

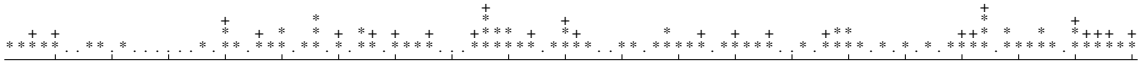
d. Secondary structure & estimated accessibility

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

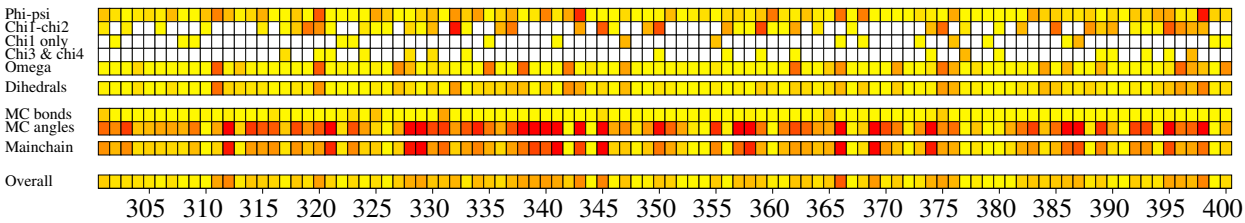
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

YV I KADAVV I AAGGFAKNNERVSKYDPKLKGFKATNHPGATGDGLDVALQAGAATRDLEY I QAHPTYS PAGGVMI TEAVRGNGA I VVNREGNRFMNE I TT

f. Max. deviation (see listing)



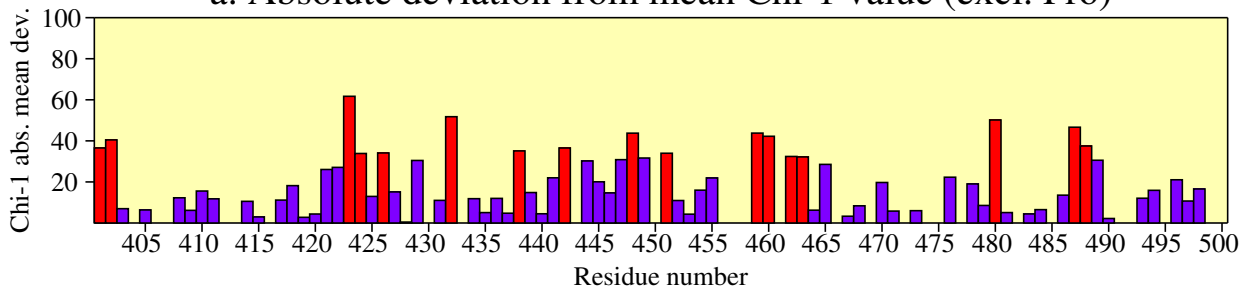
g. G-factors



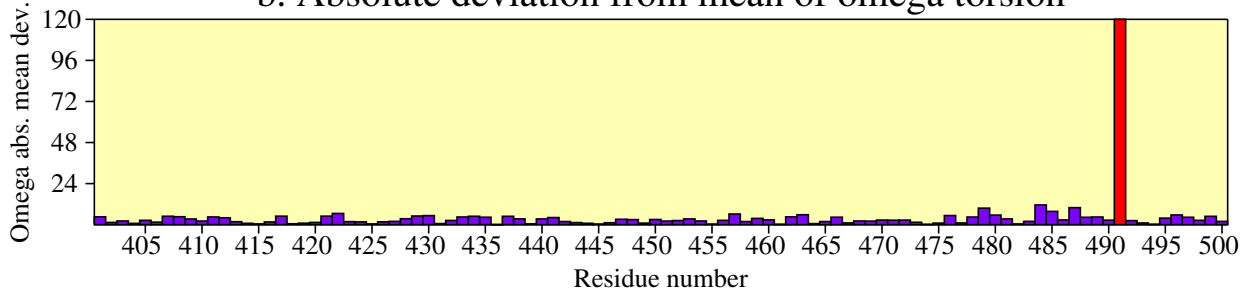
Residue properties

1d4c

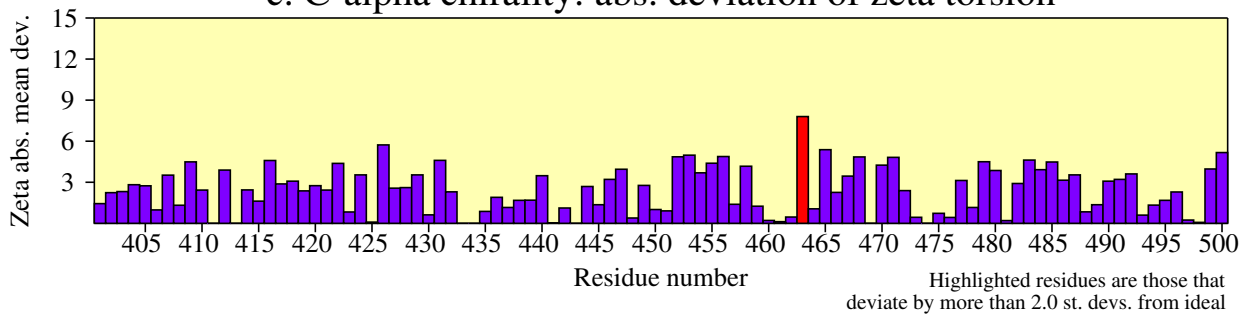
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

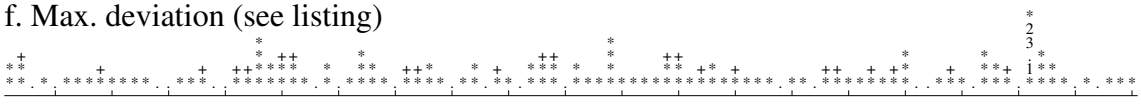
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

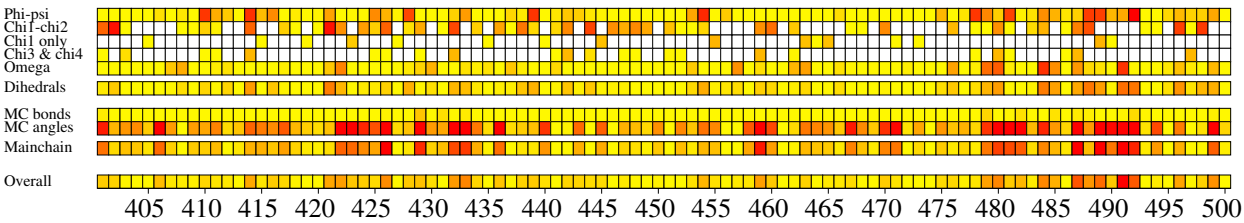
Most favoured Allowed Generous Disallowed

RDKASAAILQQKGESAYLVFDDSIRKSLKAIEGYVHLNIVKEGKTIEELAKQIDVPAAELAKTVTAYNGFVKSGKDAQFERPDLPRELVVAPFYALEIAP

f. Max. deviation (see listing)



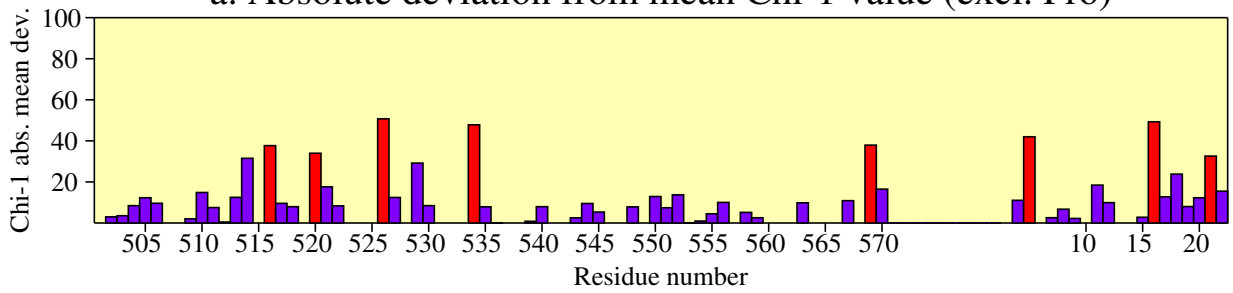
g. G-factors



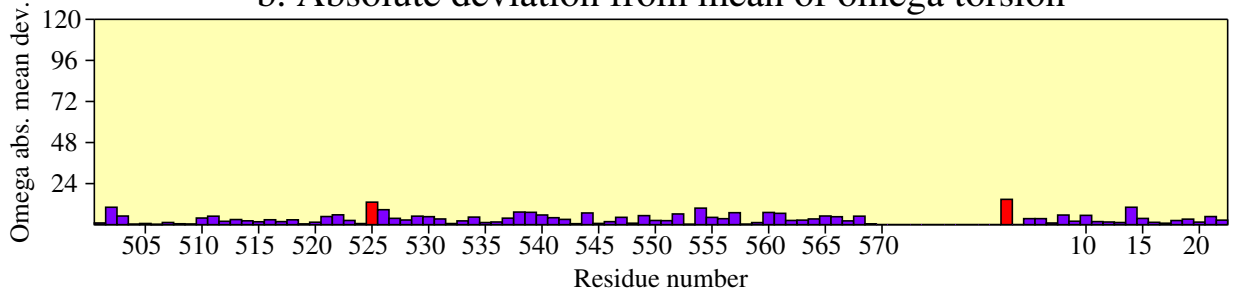
Residue properties

1d4c

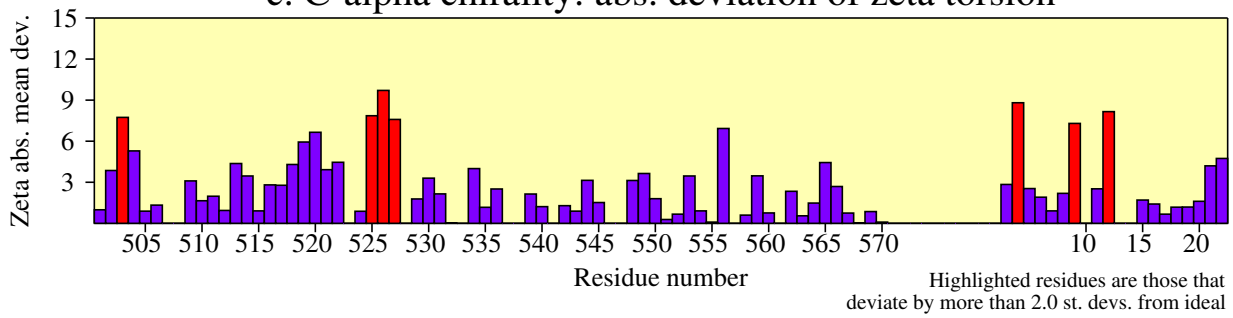
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

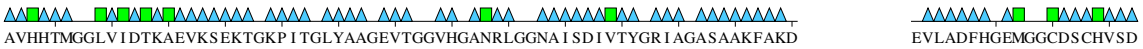


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

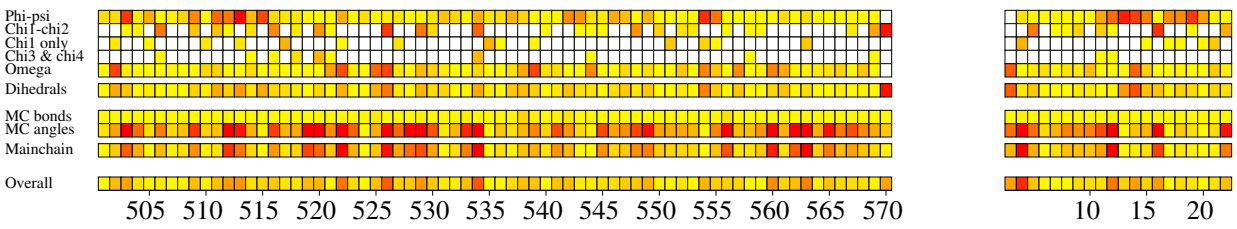
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)

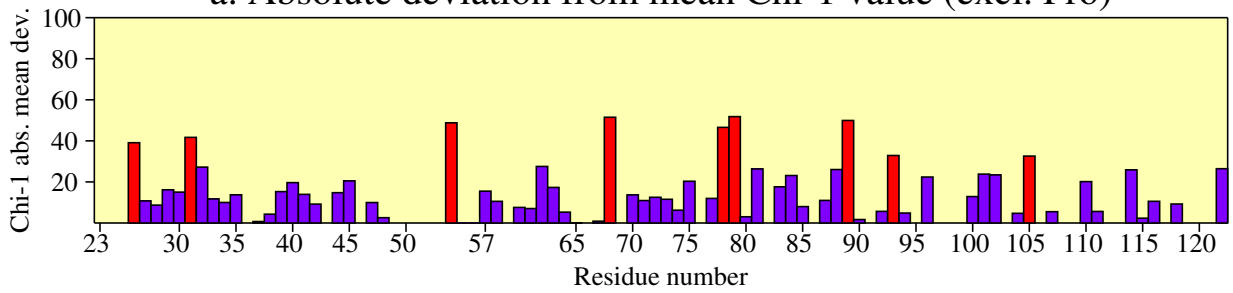
g. G-factors



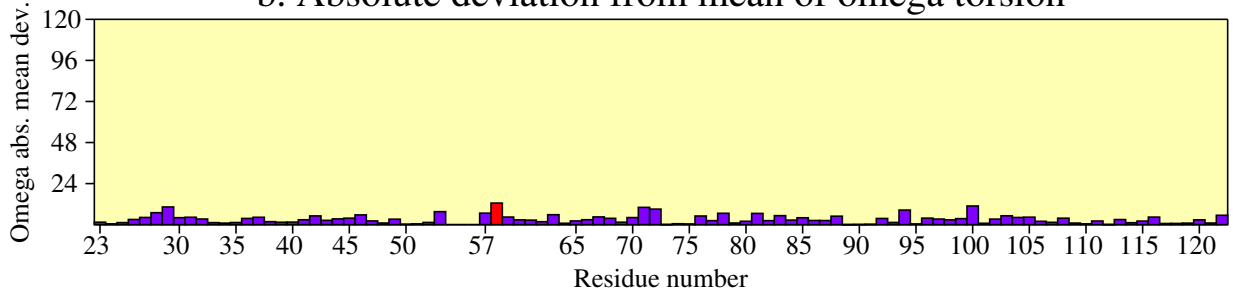
Residue properties

1d4c

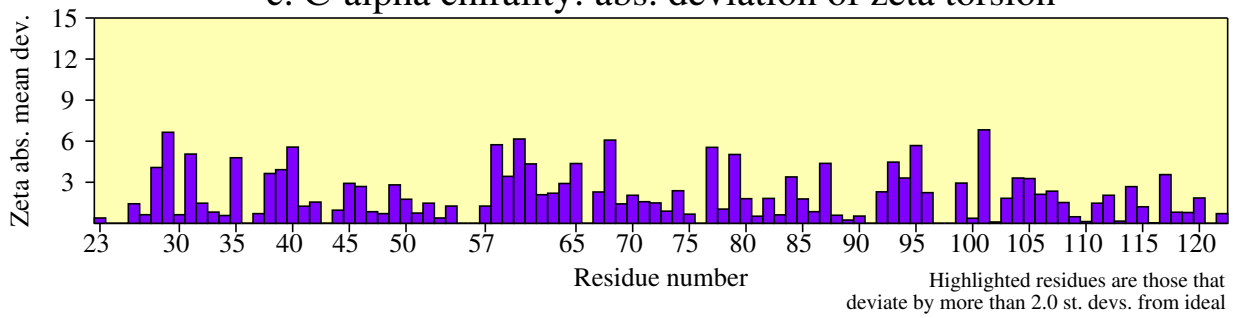
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

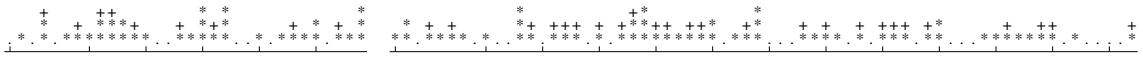
d. Secondary structure & estimated accessibility

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

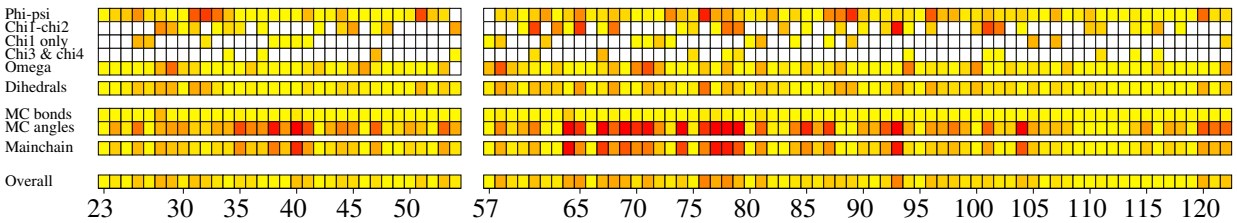
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

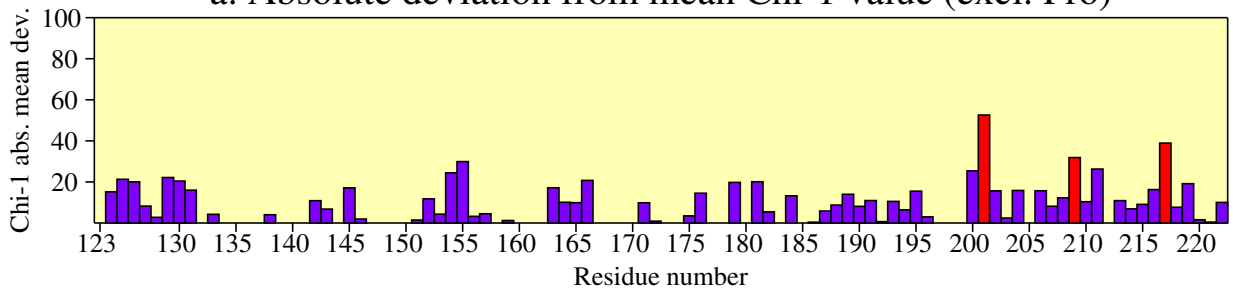


g. G-factors

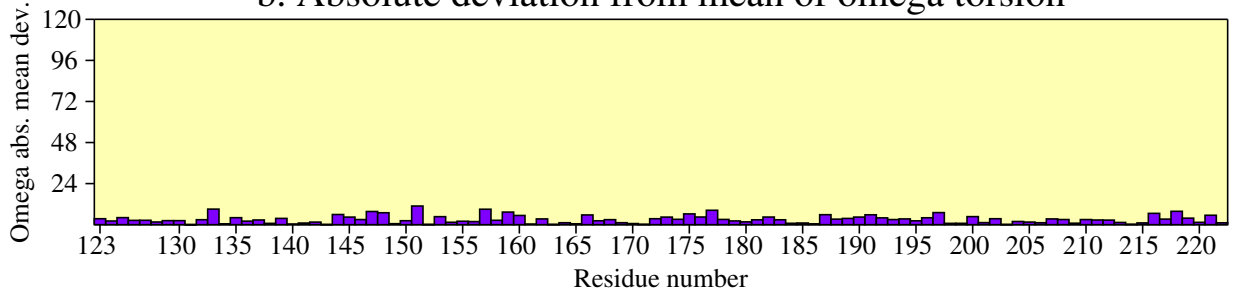


Residue properties
1d4c

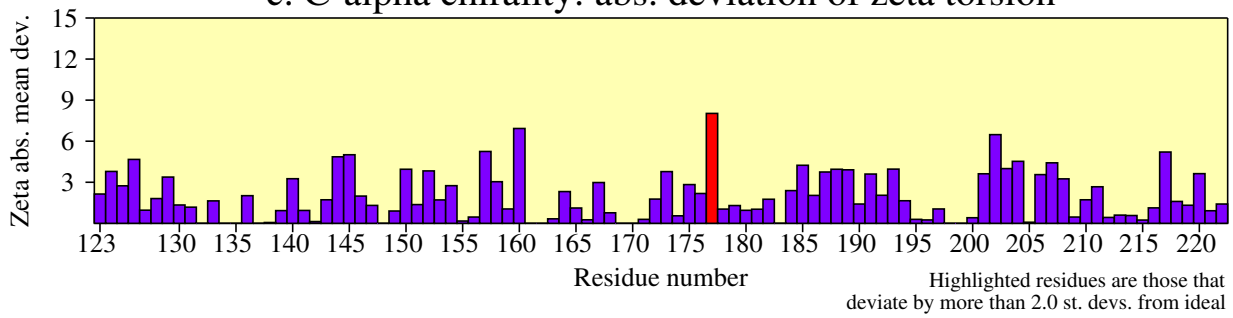
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

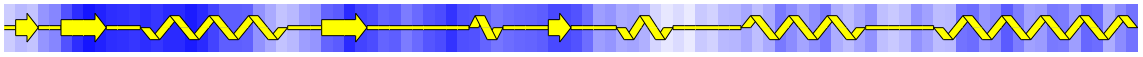


c. C-alpha chirality: abs. deviation of zeta torsion



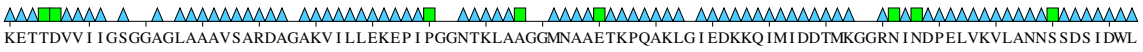
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



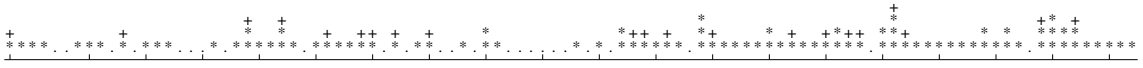
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

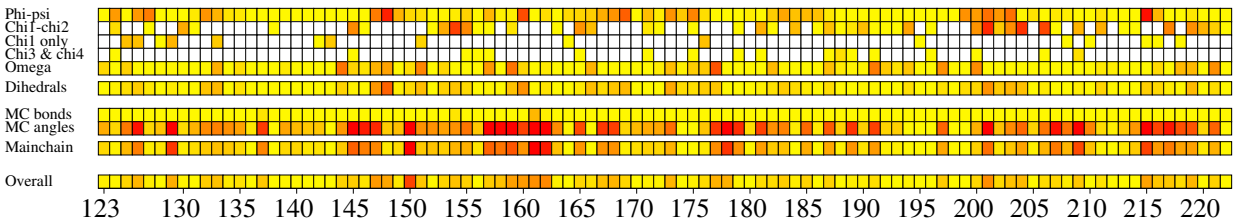


KETTDVVIIGSGGAGLAAAVSARDAGAKVILLEKEPIPGGNTKLAAGGMNAAETKPQAKLGIEDKKQIMIDDTMKGGRNINDPELVKVLANNSSDSIDWL

f. Max. deviation (see listing)

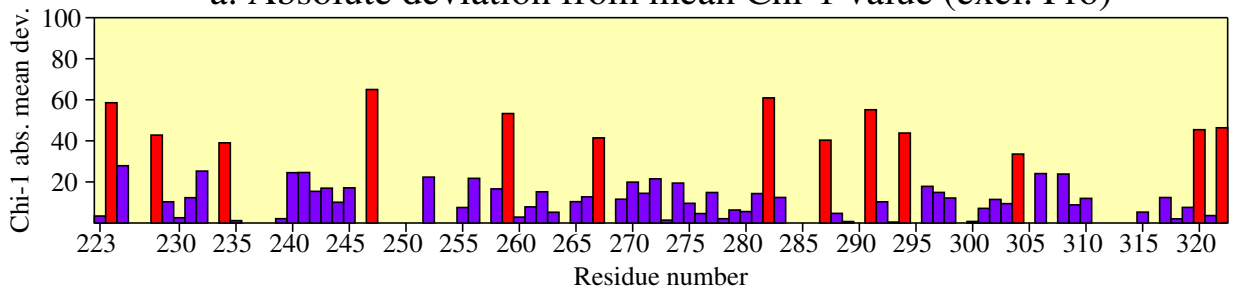


g. G-factors

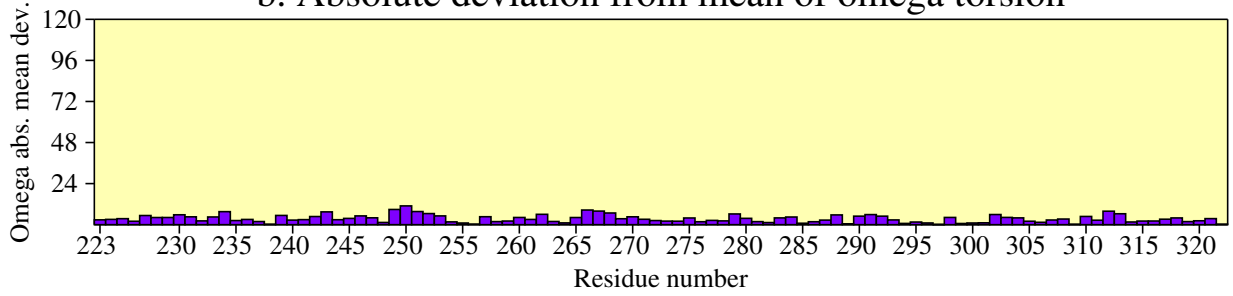


Residue properties
1d4c

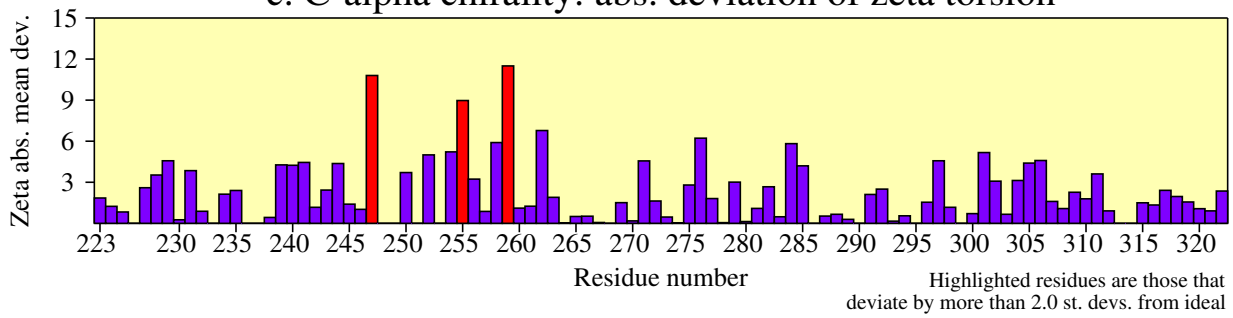
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

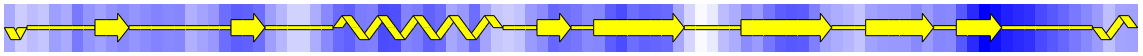


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



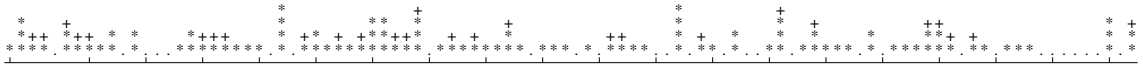
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

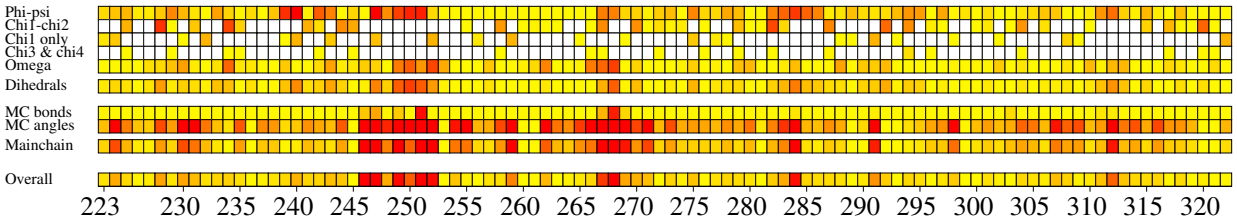
Most favoured Allowed Generous Disallowed

TSMGADMTDVGRMGGASVNRSHRPTGGAGVGAHVAQVLWDNAVKRGTDIRLNSRVVRILEDASGKVTGVLVKGEYTGYYVIKADAVVIAAGGFAKNNERV

f. Max. deviation (see listing)



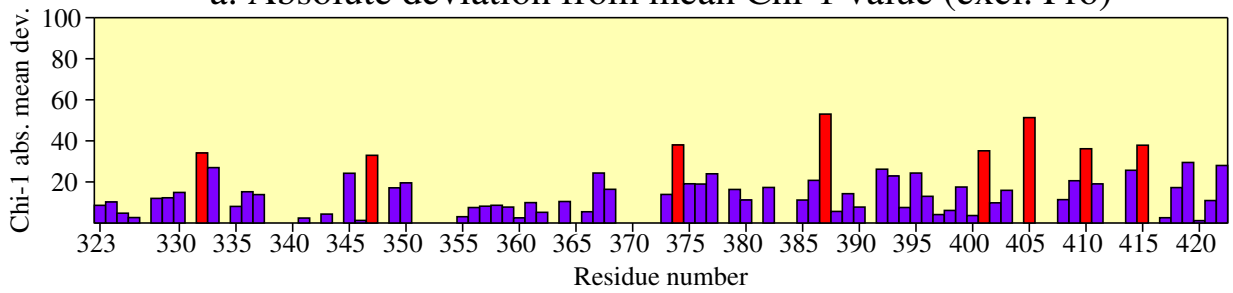
g. G-factors



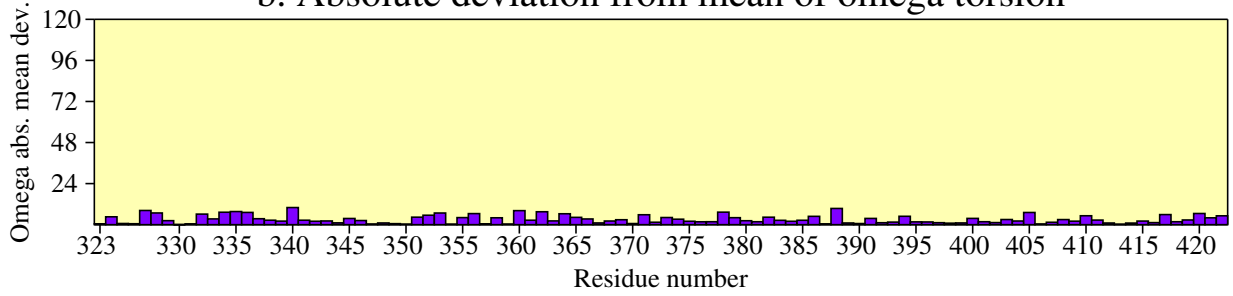
Residue properties

1d4c

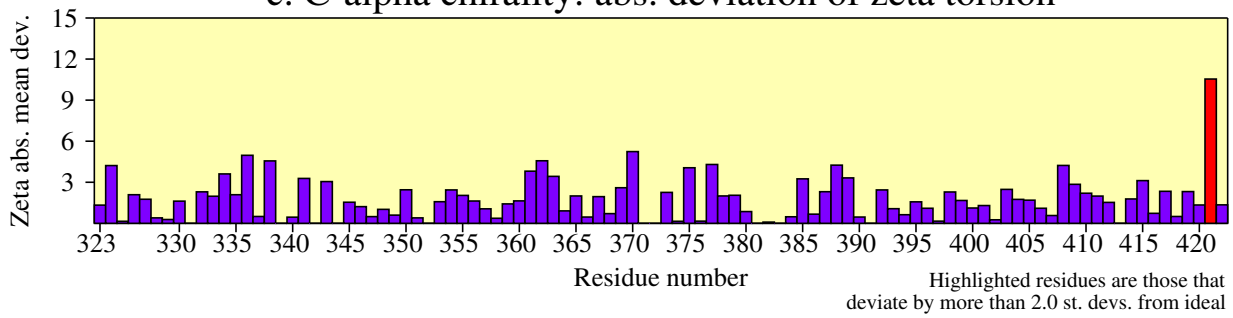
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

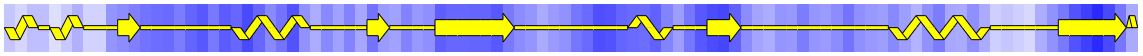


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



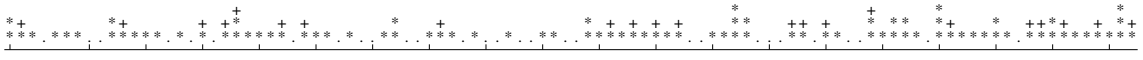
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

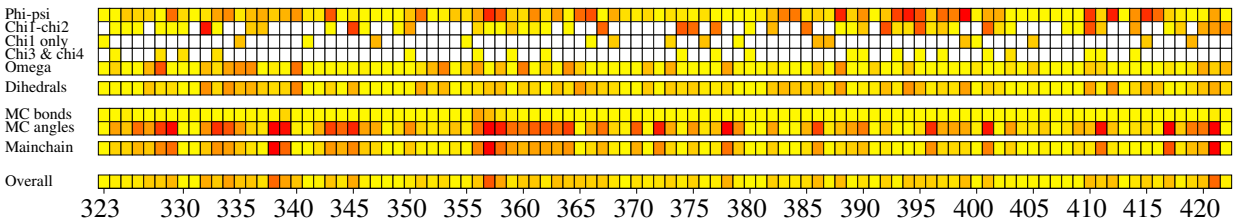
Most favoured Allowed Generous Disallowed

SKYDPKLKGFKATNHPGATGDGLDVALQAGAATRDLEYIQAHPTYSPAGGVMITEAVRGNGAIVVNREGNRFMNEITTRDKASAAILQQKGESAYLVFDD

f. Max. deviation (see listing)



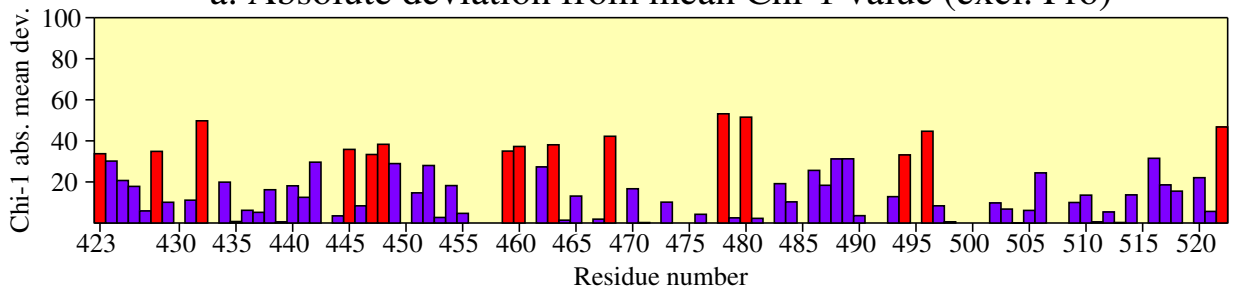
g. G-factors



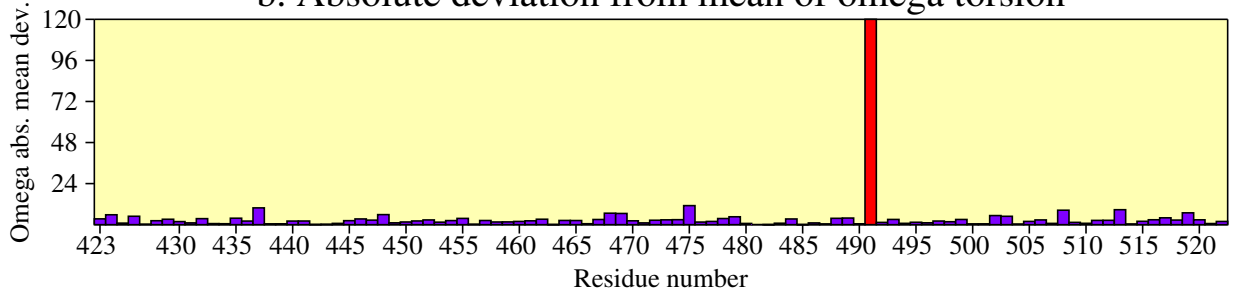
Residue properties

1d4c

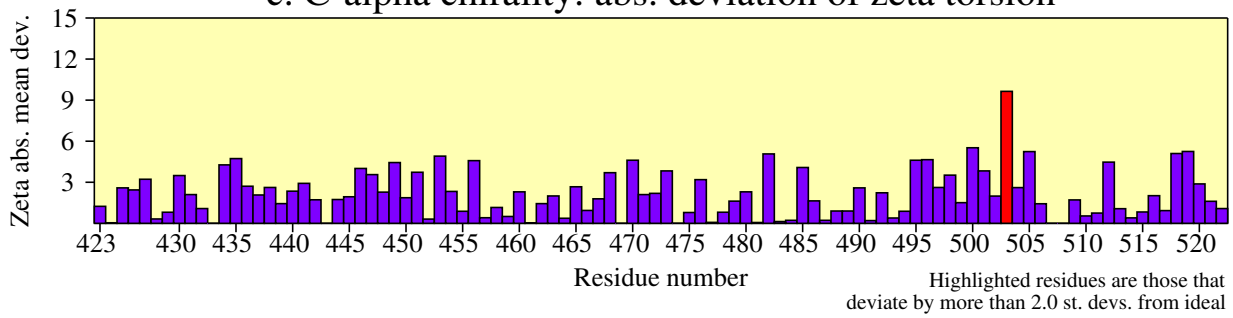
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

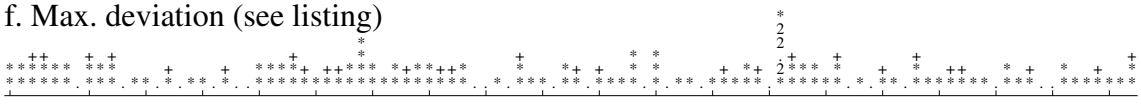
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

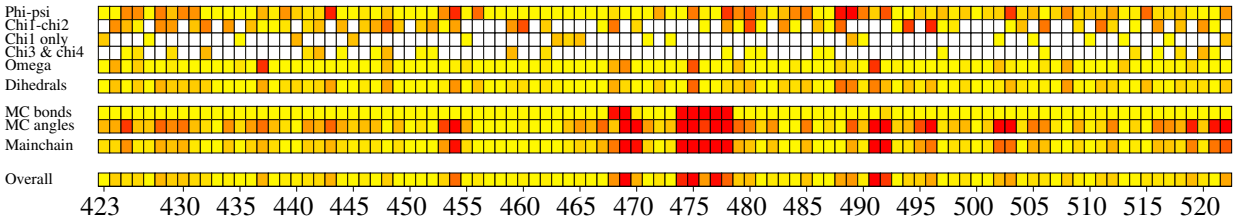
Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)



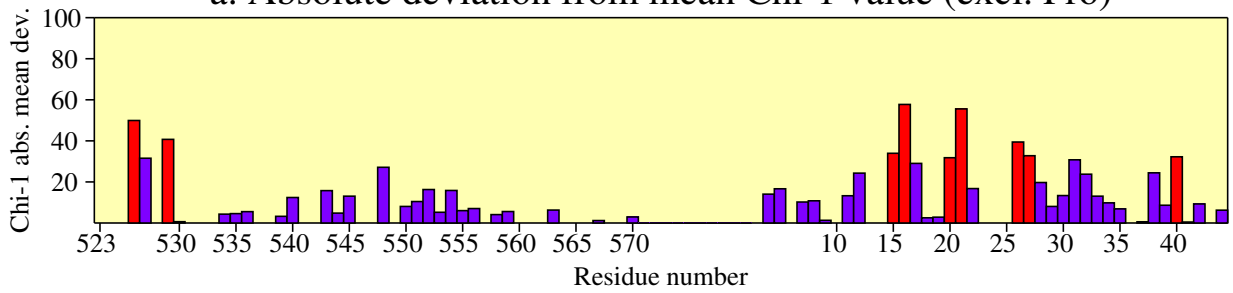
g. G-factors



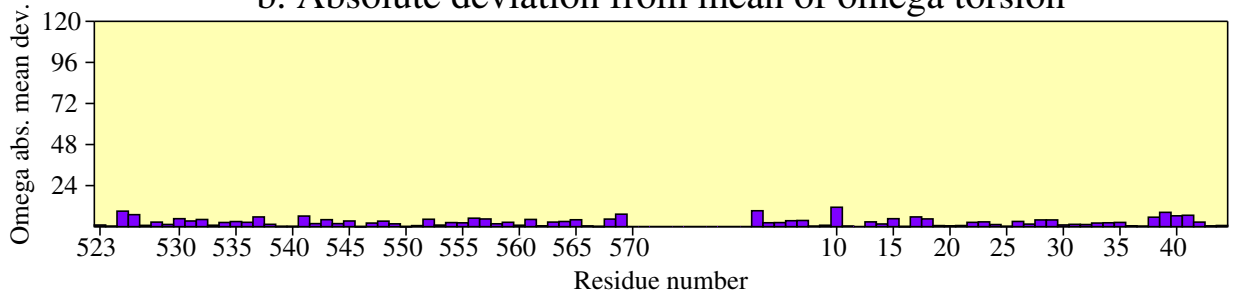
Residue properties

1d4c

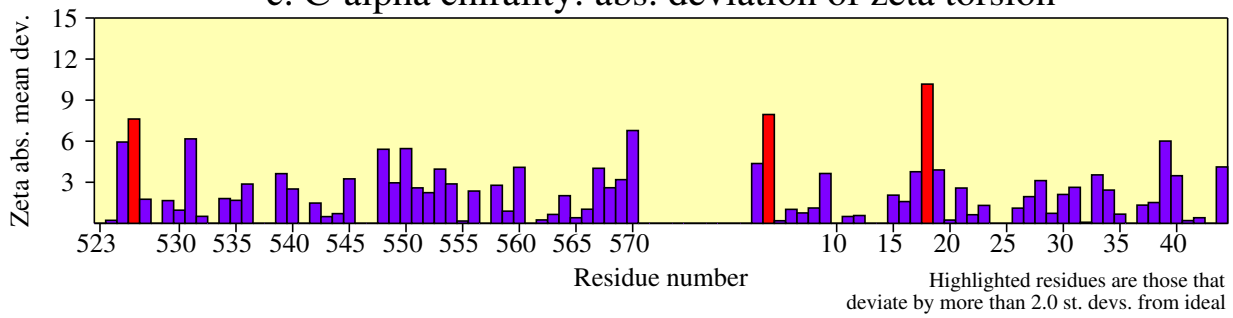
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

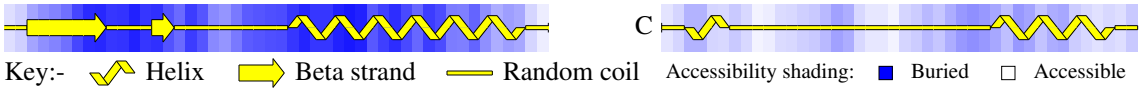


c. C-alpha chirality: abs. deviation of zeta torsion

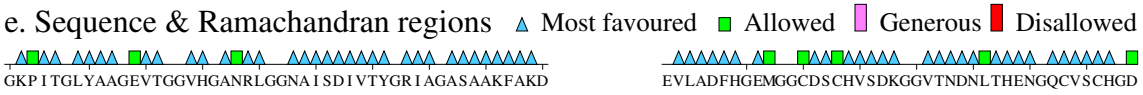


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

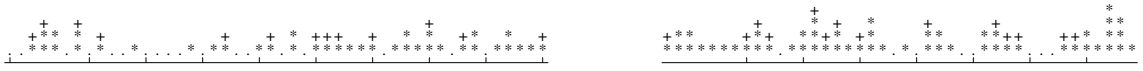
d. Secondary structure & estimated accessibility



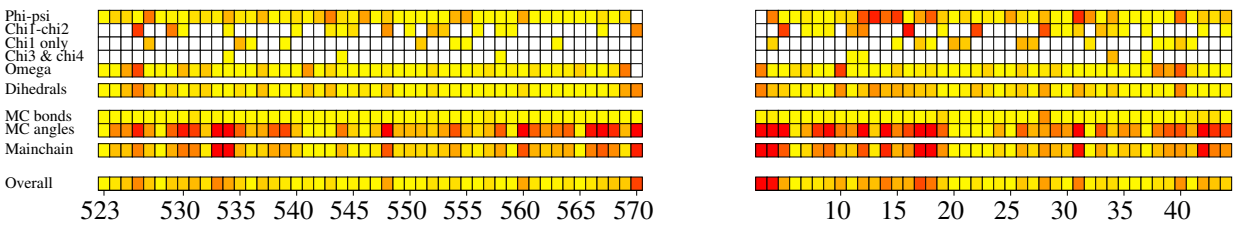
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



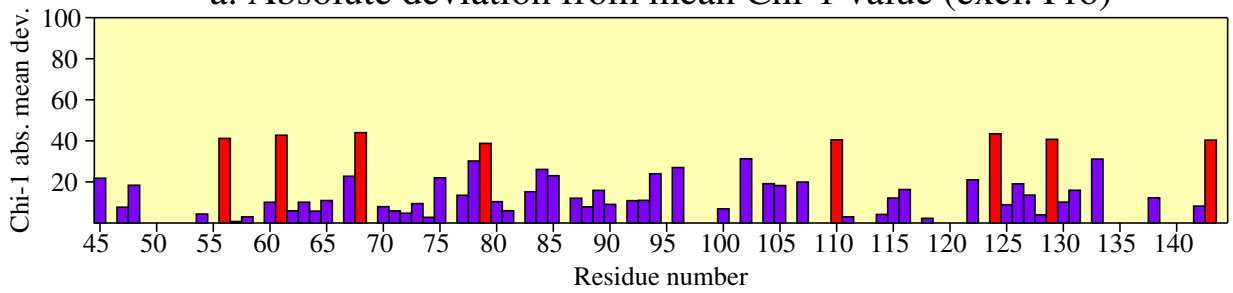
g. G-factors



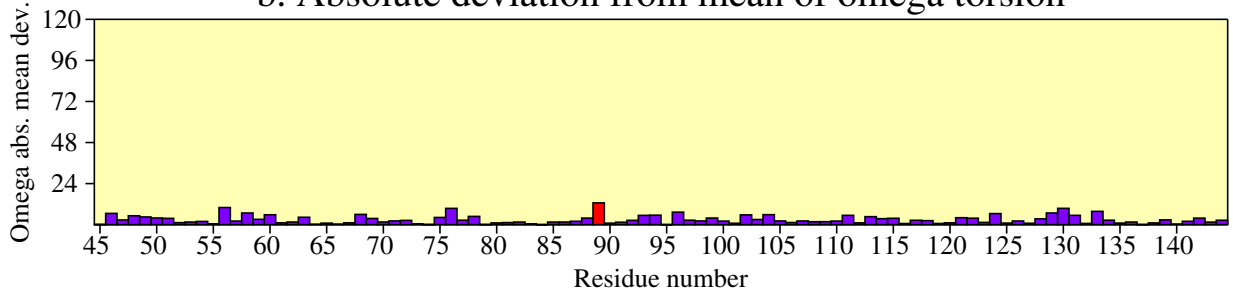
Residue properties

1d4c

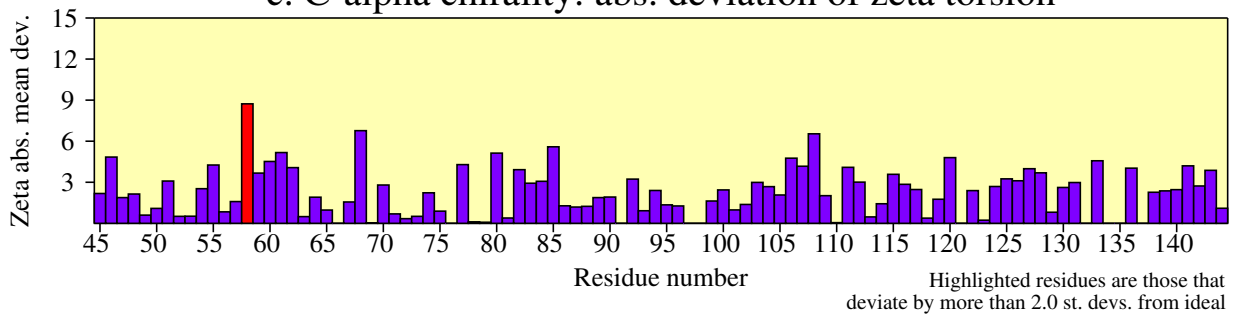
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

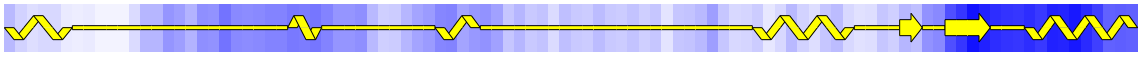


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



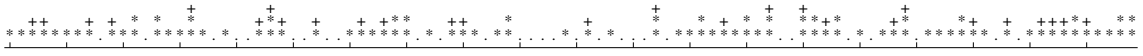
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

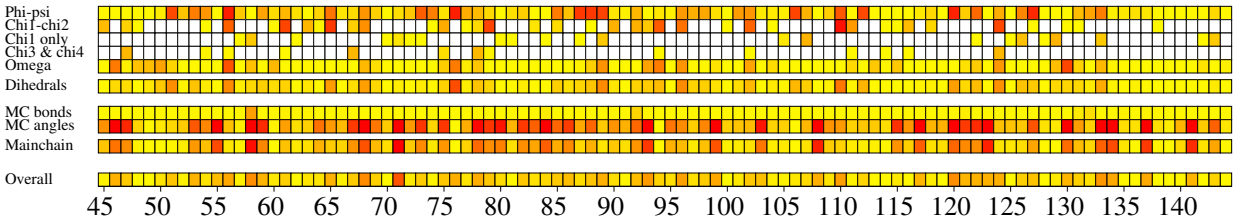
Most favoured Allowed Generous Disallowed

LKELAAAAPKDKVSPHKSHLIGEIACTSCHKGHEKSVAYCDACHSFGFDMPFGGKWERKFVPVDADKAAQDKAIAAGVKETTDVVIIGSGGAGLAAAVSA

f. Max. deviation (see listing)

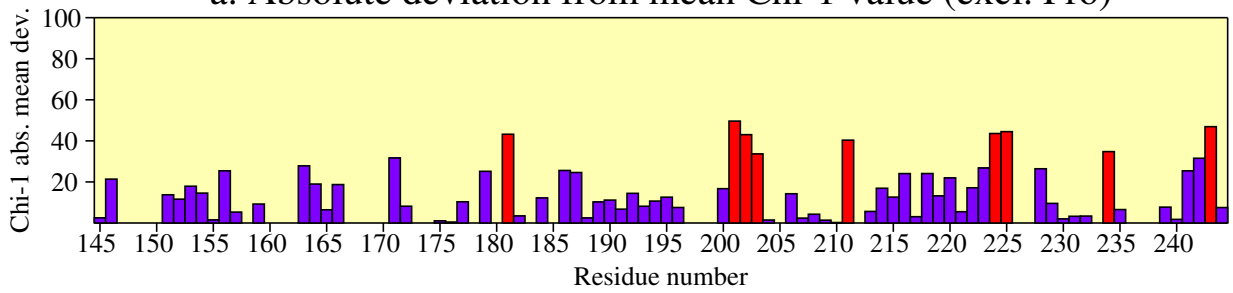


g. G-factors

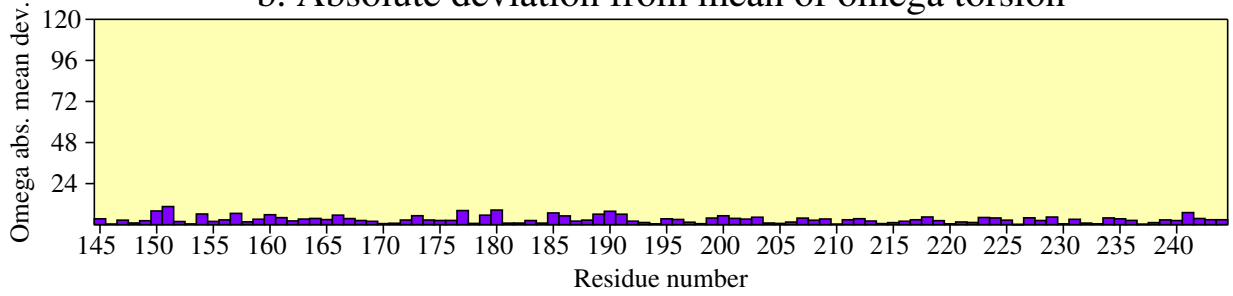


Residue properties
1d4c

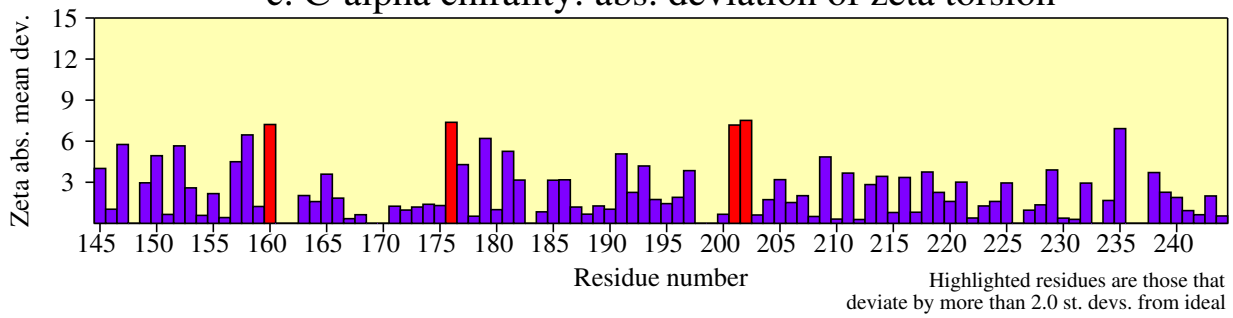
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

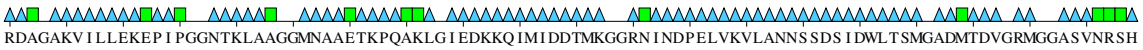


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

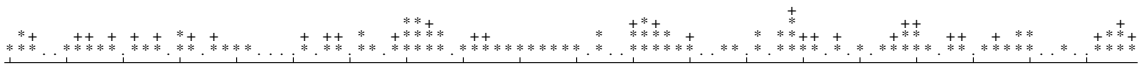
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

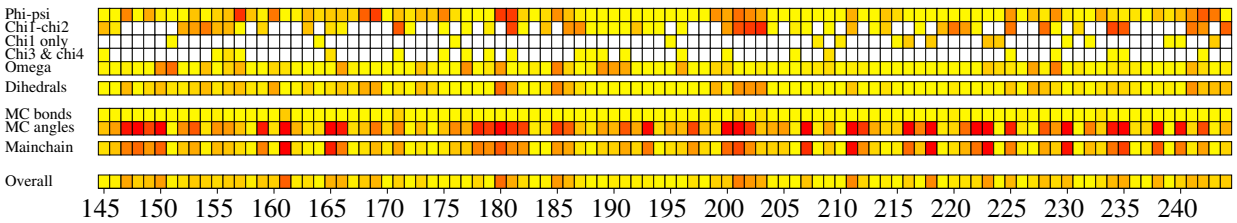


RDAGAKV I LLEKEP I PGGNTKLAAGGMNAAETKPQAKLG I EDKKQ I M I DDTMKGGRN I NDPELVKVLANNSSDS I DWLTSMGADMTDVGRMGGASVNRSH

f. Max. deviation (see listing)



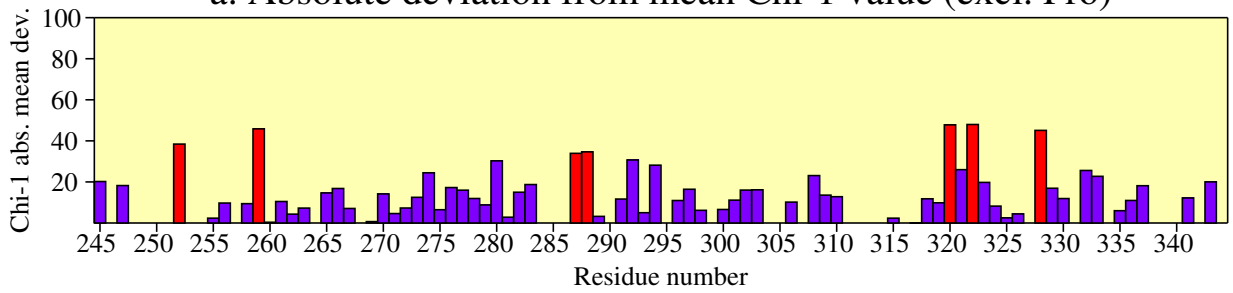
g. G-factors



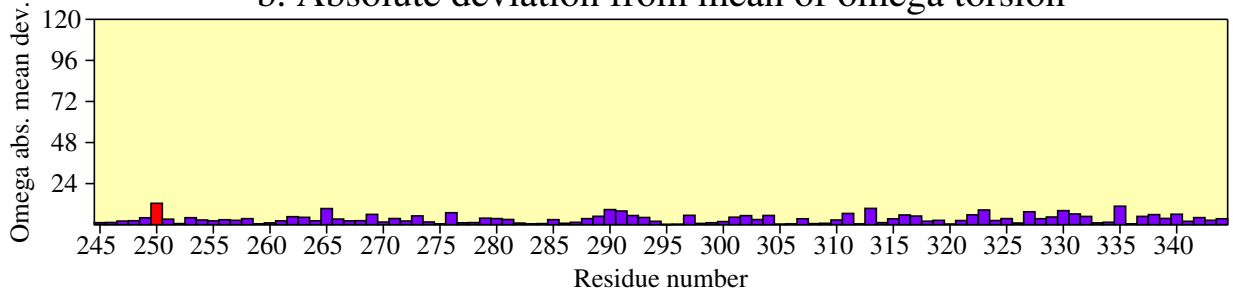
Residue properties

1d4c

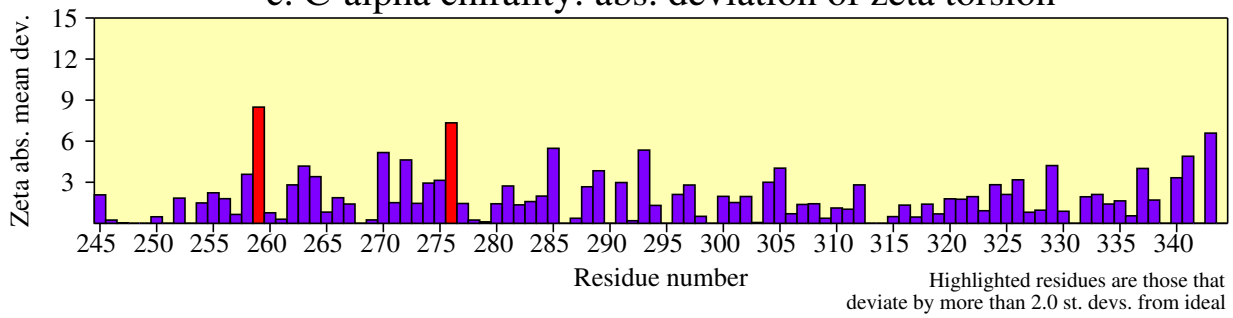
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

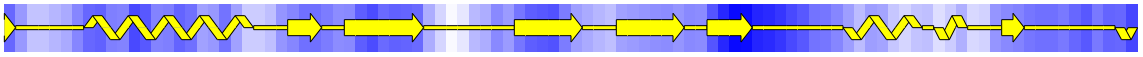


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



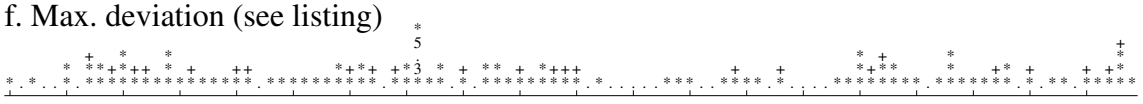
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

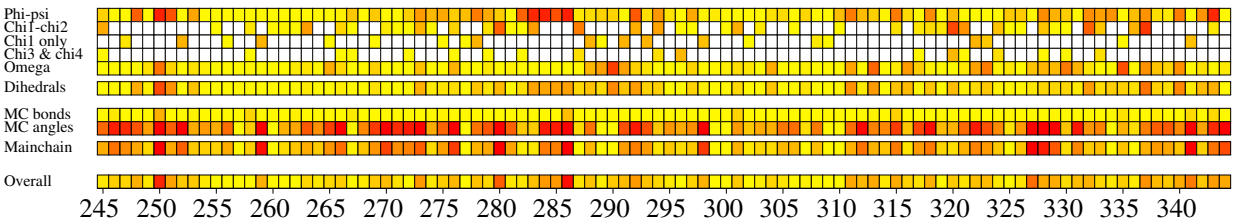
Most favoured Allowed Generous Disallowed

RPTGGAGVGAHVAQVLWDNAVKRGTDIRLNSRVVRILEDASGKVTGVLVKGEYTGYYVIKADAVVIAAGGFAKNNERVSKYDPKLKGFKATNHPGATGDG

f. Max. deviation (see listing)



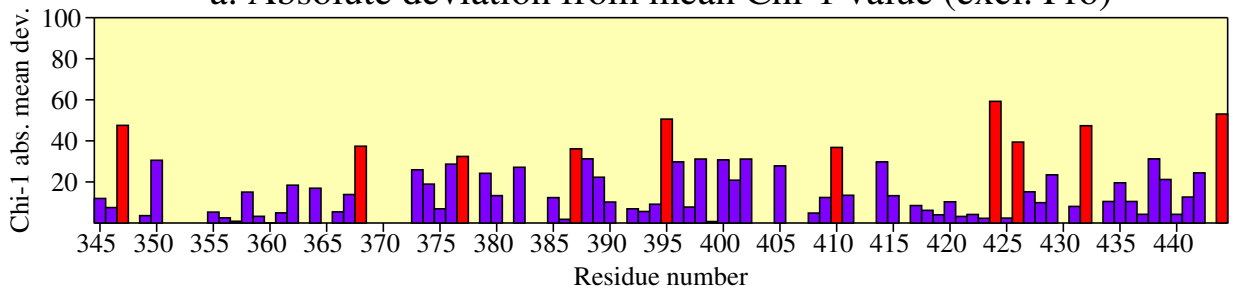
g. G-factors



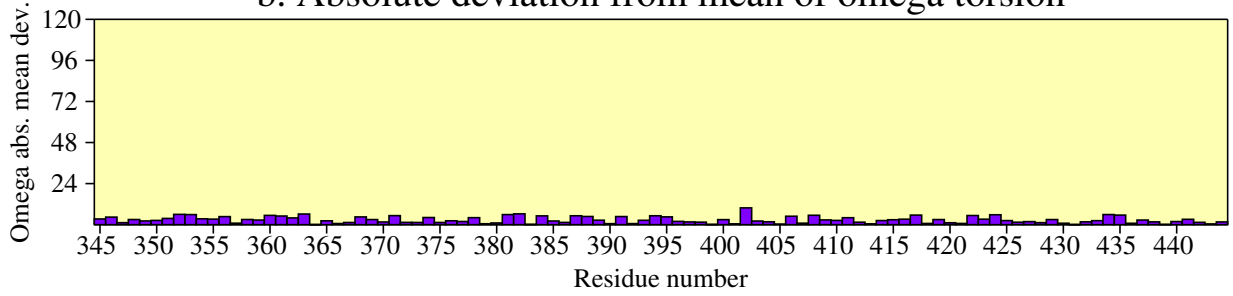
Residue properties

1d4c

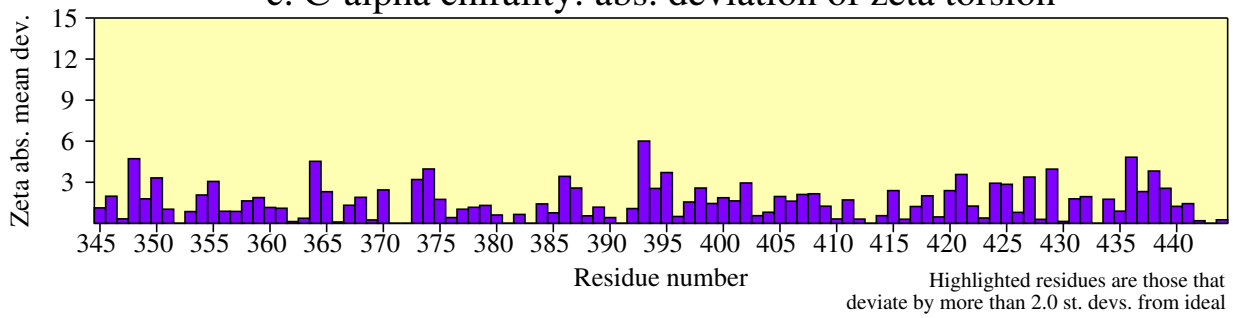
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

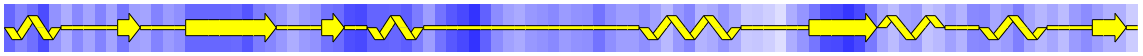


c. C-alpha chirality: abs. deviation of zeta torsion



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

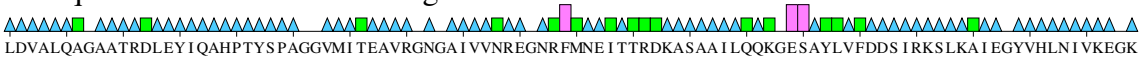
d. Secondary structure & estimated accessibility



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

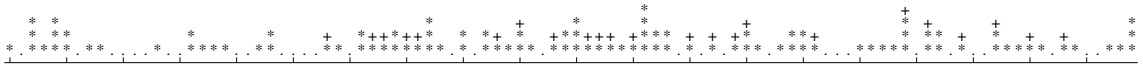
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

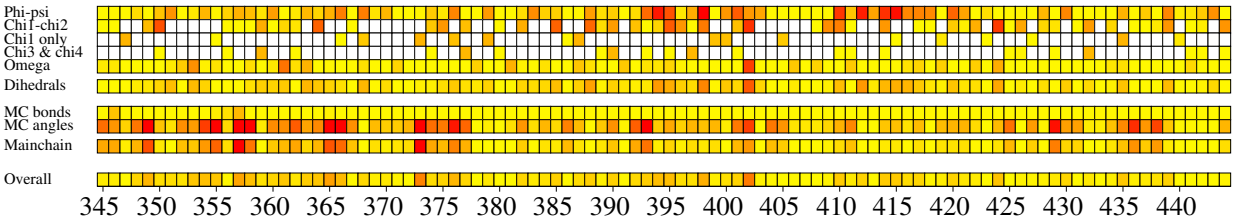


LDVALQAGAATRDLEYIQAHPTYSPAGGVMITEAVRGNGAIVVNREGNRFMNEITTRDKASAAILQQKGESAYLVFDDSIRKSLKAIEGYVHLNIVKEGK

f. Max. deviation (see listing)



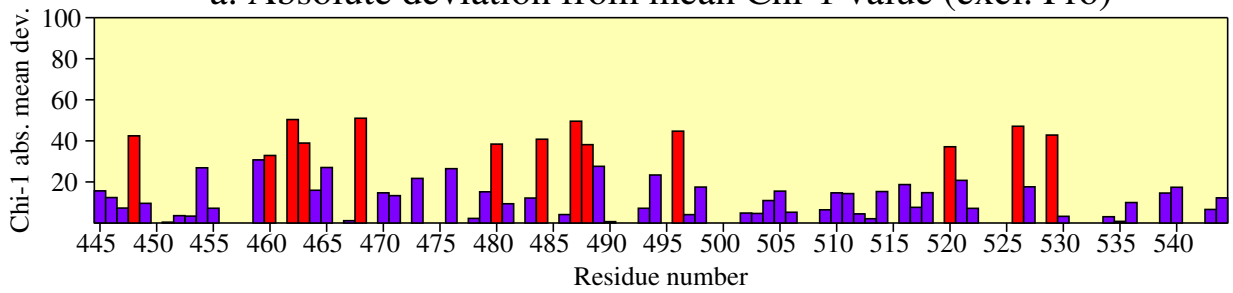
g. G-factors



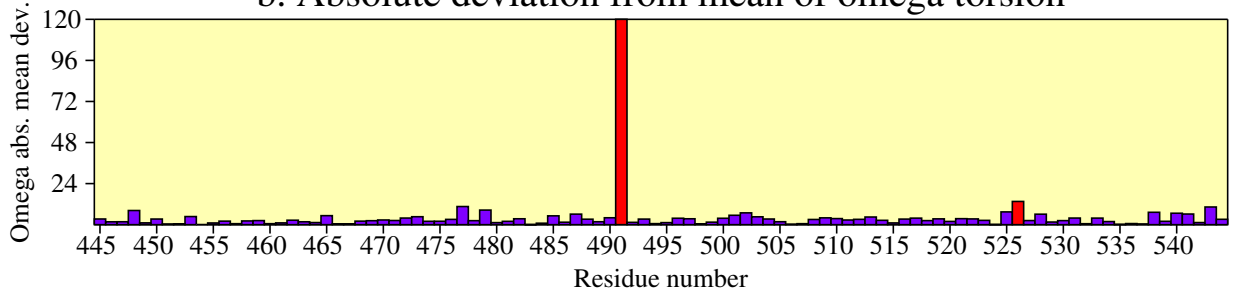
Residue properties

1d4c

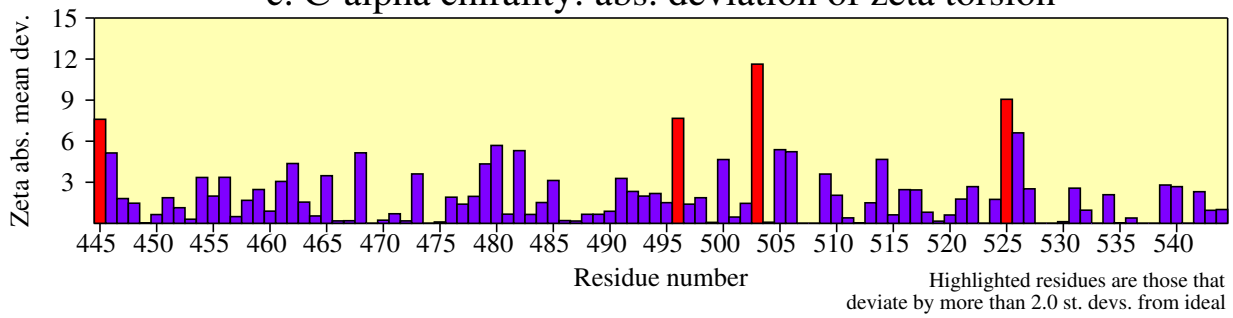
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

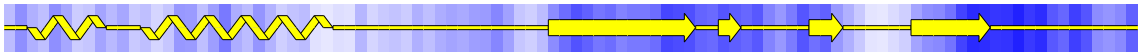


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



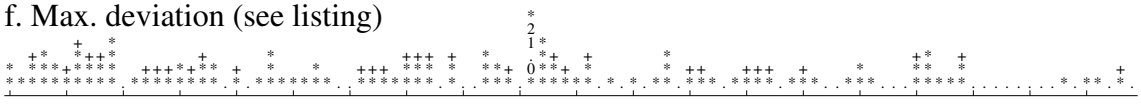
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

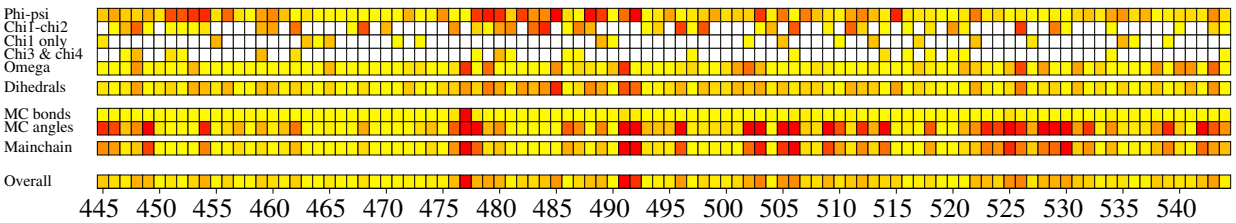
Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)



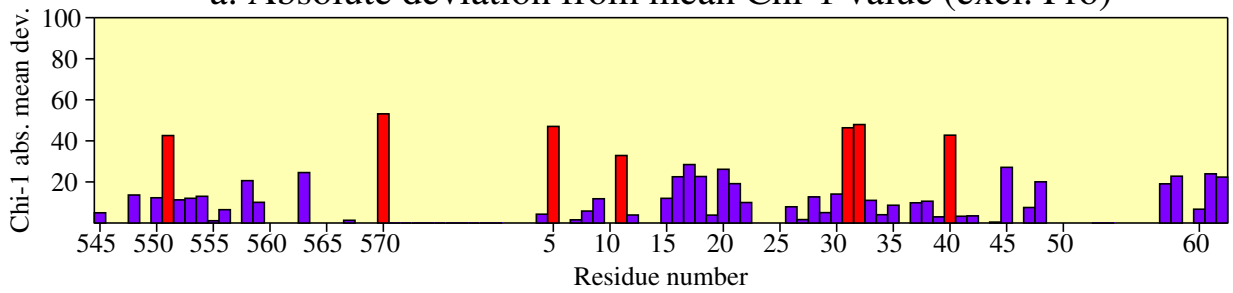
g. G-factors



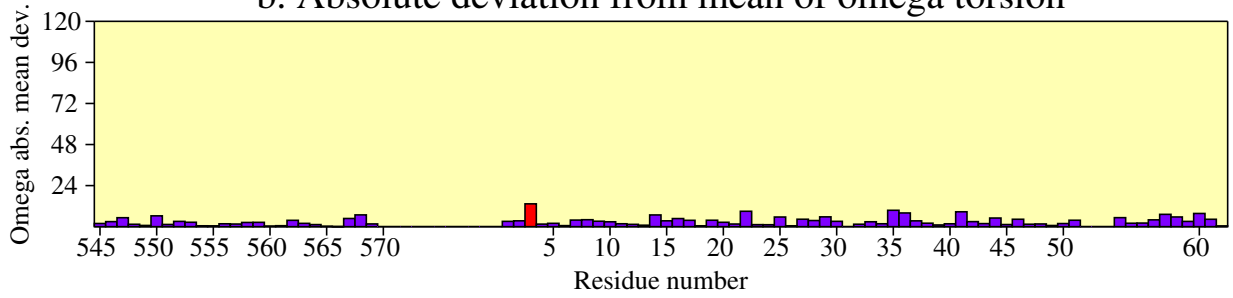
Residue properties

1d4c

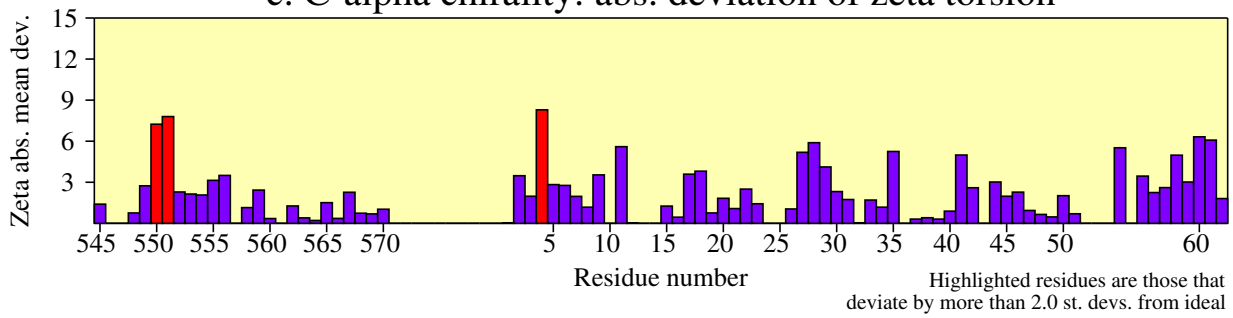
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

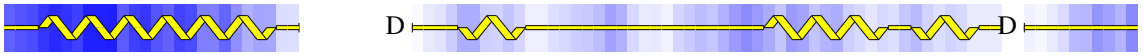


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

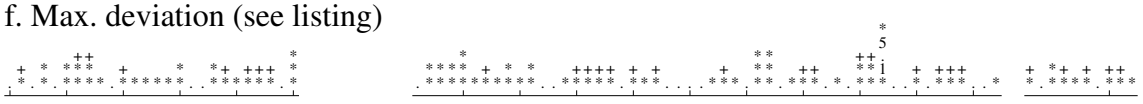


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

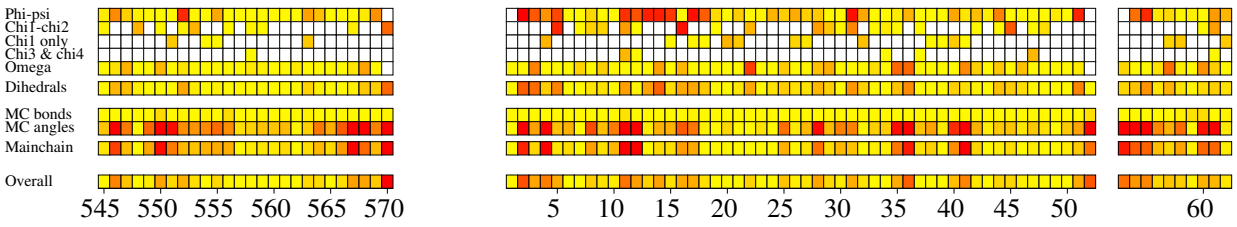
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

f. Max. deviation (see listing)

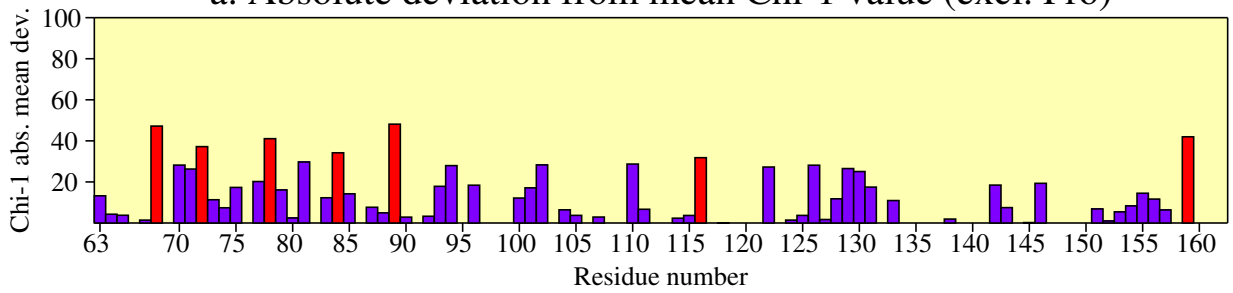


g. G-factors

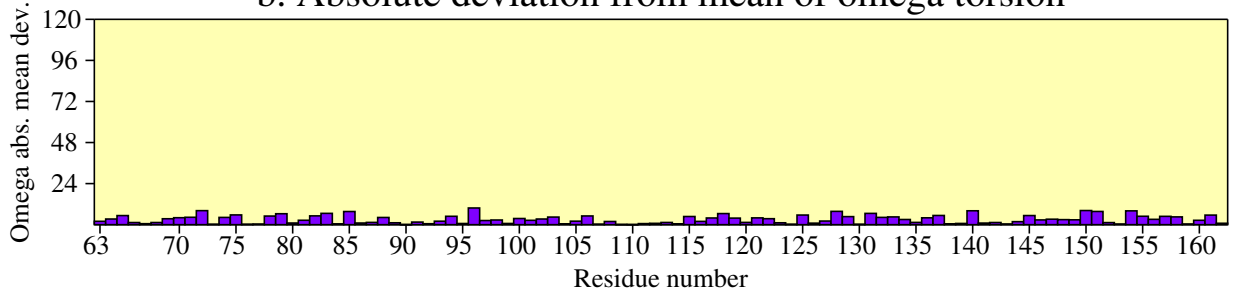


Residue properties
1d4c

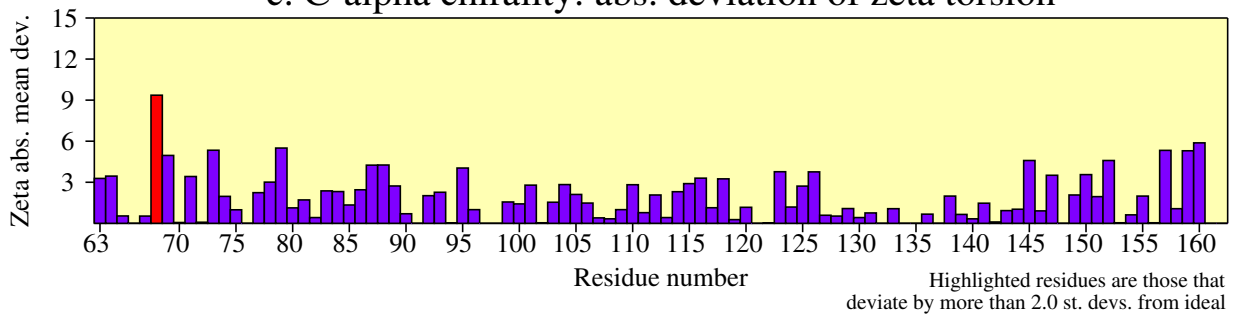
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

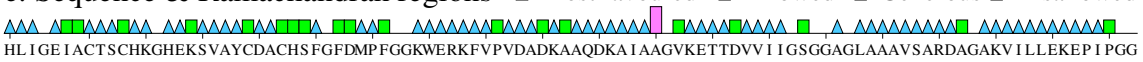


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility

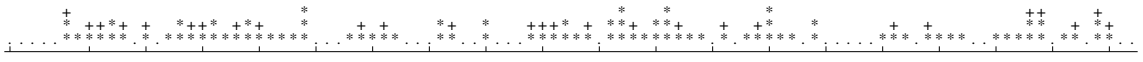
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

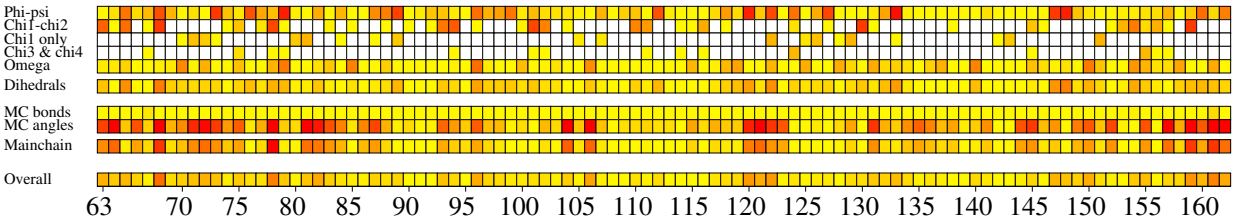


HL I GE I ACT S CHKGHEKS VAYCDACHS FGFDMP FGGKWERKFVPVDADKAAQDKA I AAGVKETTDVV I I GSGGAGLAAAVSARDAGAKV I LLEKEP I PGG

f. Max. deviation (see listing)

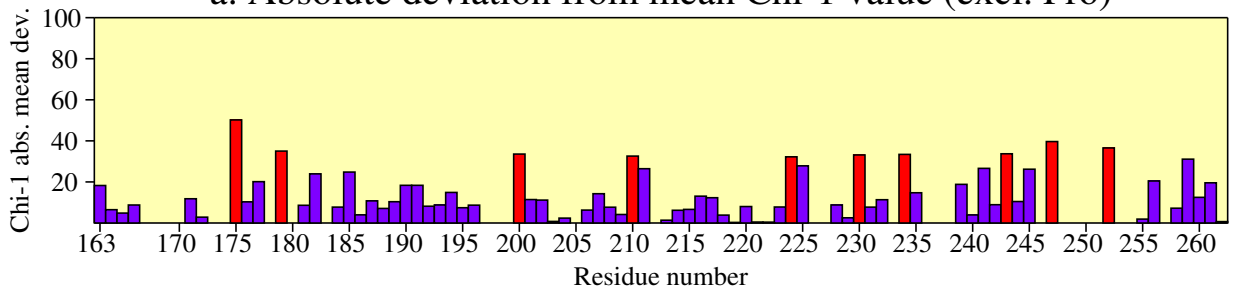


g. G-factors

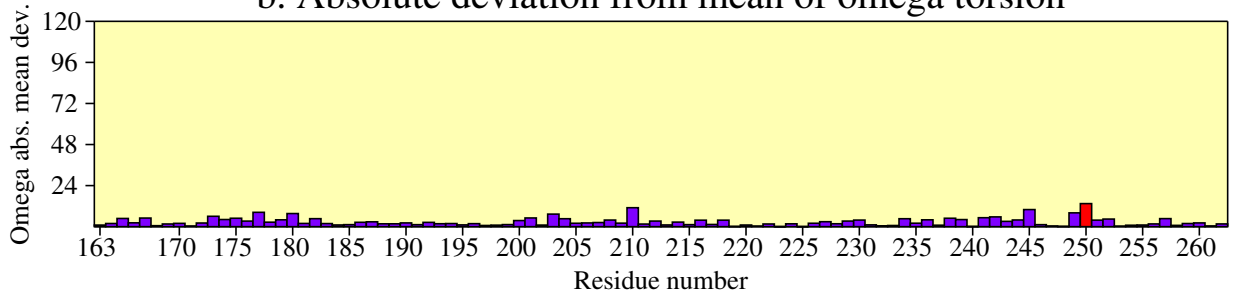


Residue properties
1d4c

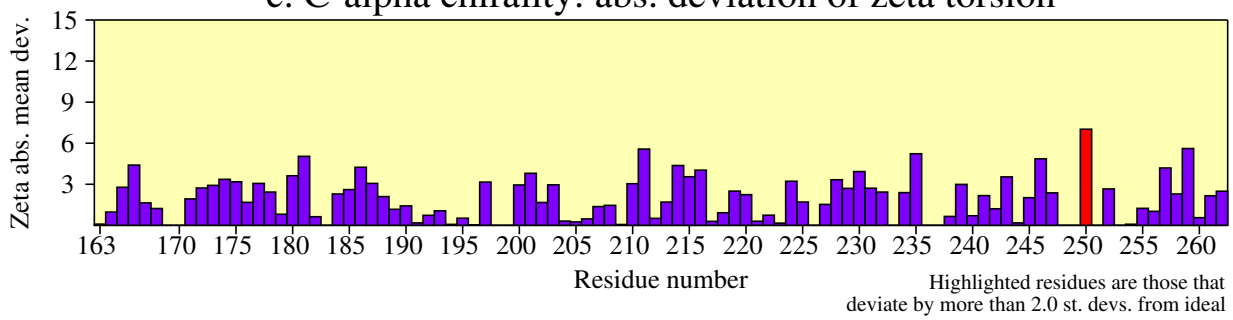
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

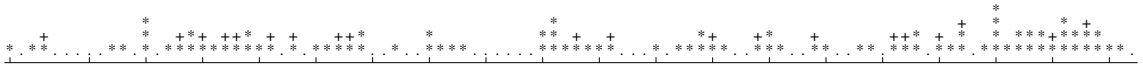
d. Secondary structure & estimated accessibility

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

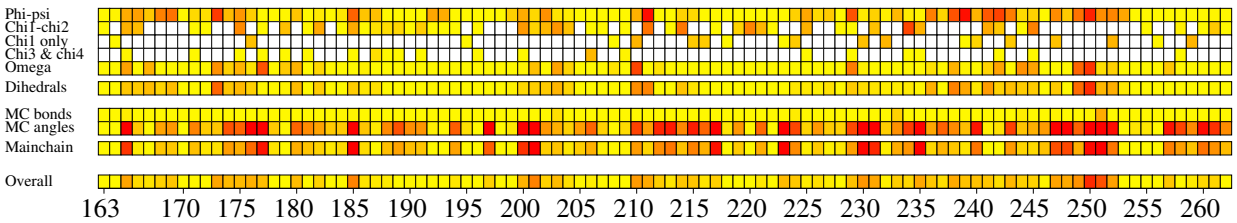
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

NTKLAAGGMNAAETKPQAKLGIEDKKQIMIDDTMKGGRNINDPELVKVLANNSSDSIDWLTSMGADMTDVGRMGGASVNRSHRPTGGAGVGAHVAQVLWD

f. Max. deviation (see listing)

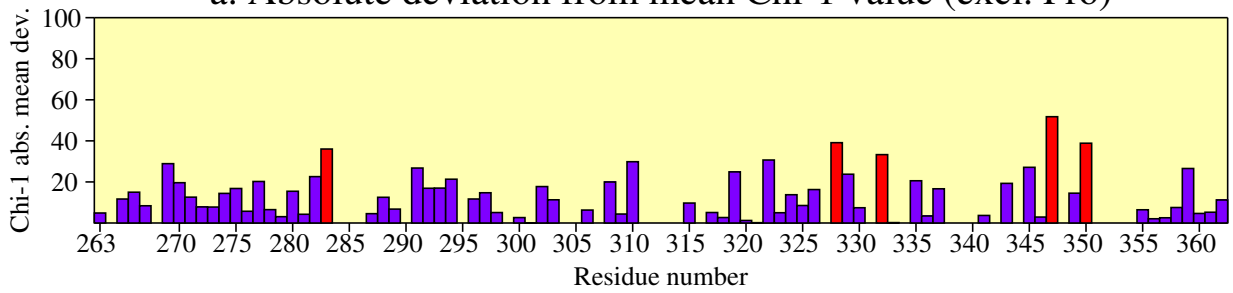


g. G-factors

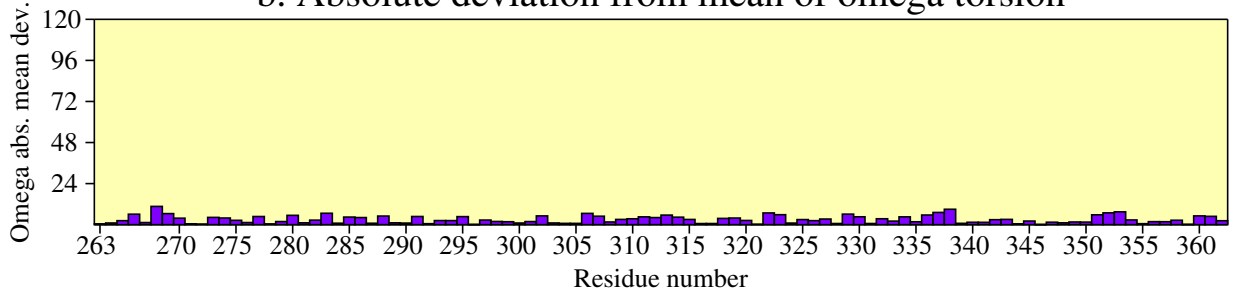


Residue properties
1d4c

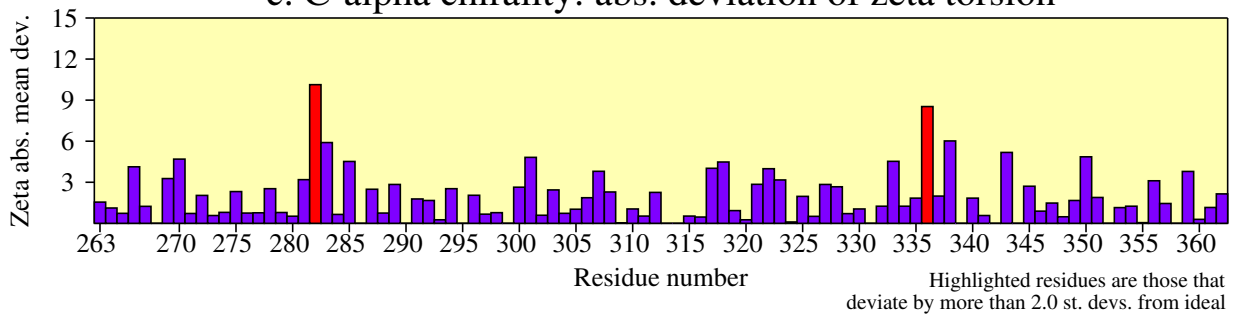
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

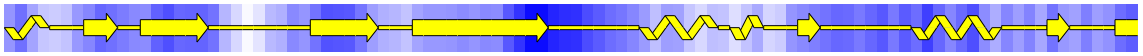


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

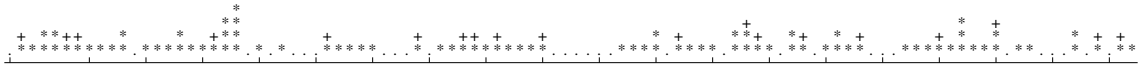


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

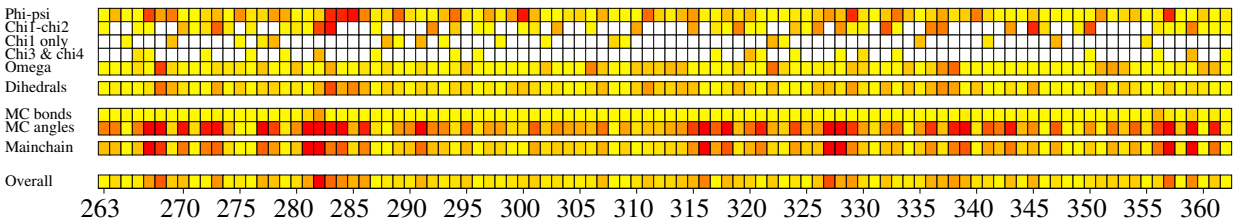
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

NAVKRGTDIRLNSRVVRILEDASGKVTGVLVKGEYTGYYVIKADAVVIAAGGFAKNNERVSKYDPKLKGFKATNHPGATGDGLDVALQAGAATRDLEYIQ

f. Max. deviation (see listing)



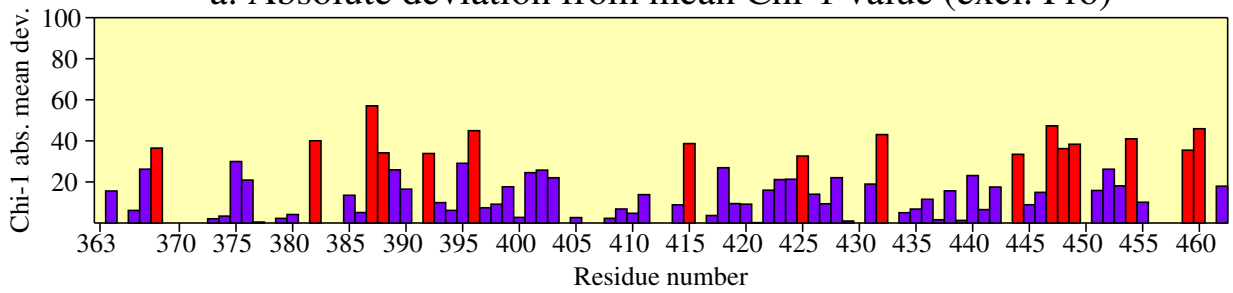
g. G-factors



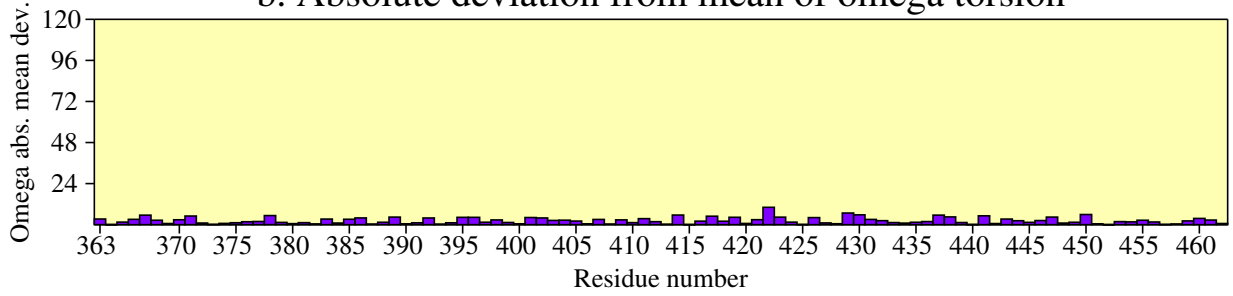
Residue properties

1d4c

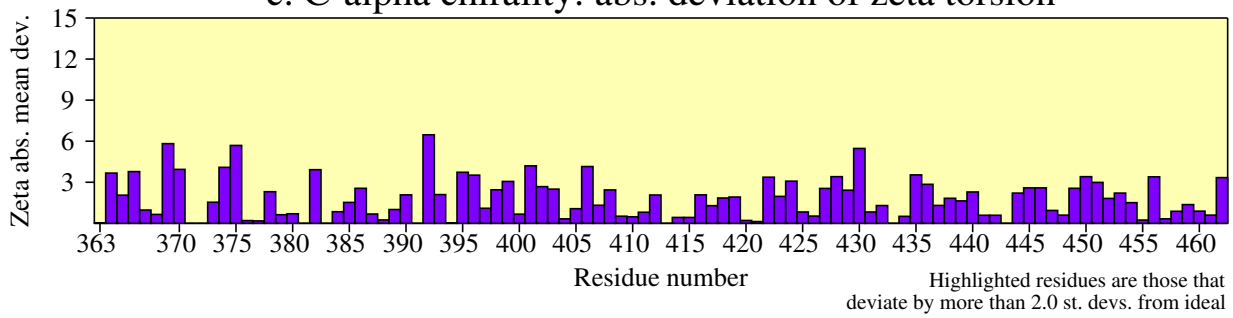
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

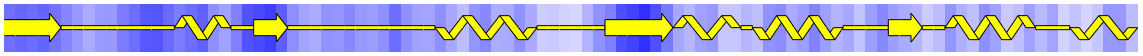


c. C-alpha chirality: abs. deviation of zeta torsion



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

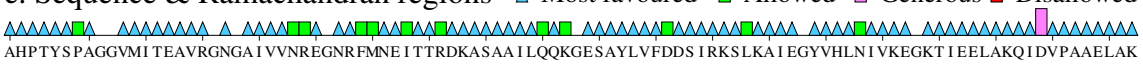
d. Secondary structure & estimated accessibility



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

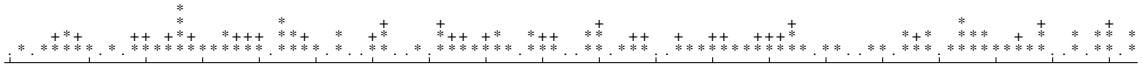
e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

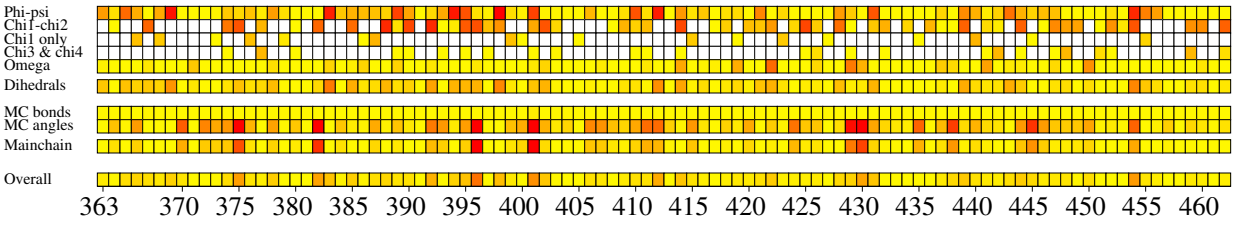


AHPTYSPAGGVMITEAVRGNGAIVVNREGNRFMNEITTRDKASAAILQQKGESAYLVFDDSIRKSLKAIEGYVHLNIVKEGKTIEELAKQIDVPAAELAK

f. Max. deviation (see listing)



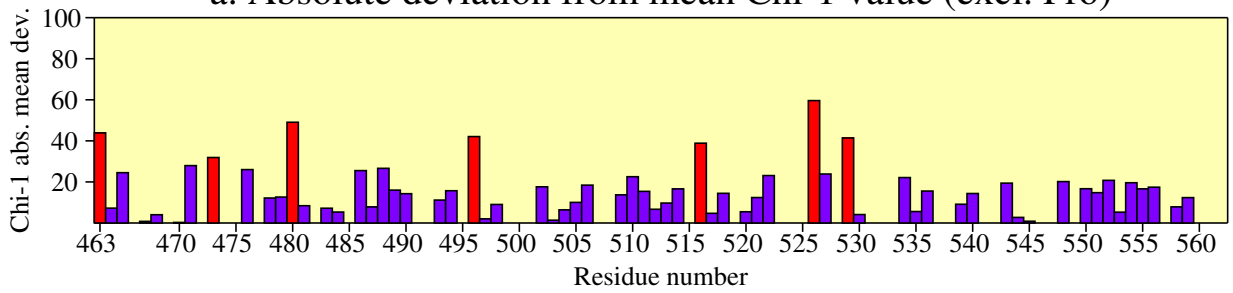
g. G-factors



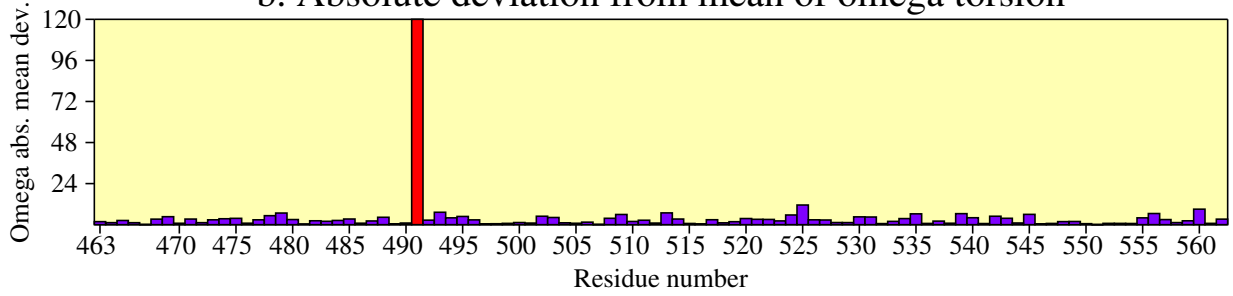
Residue properties

1d4c

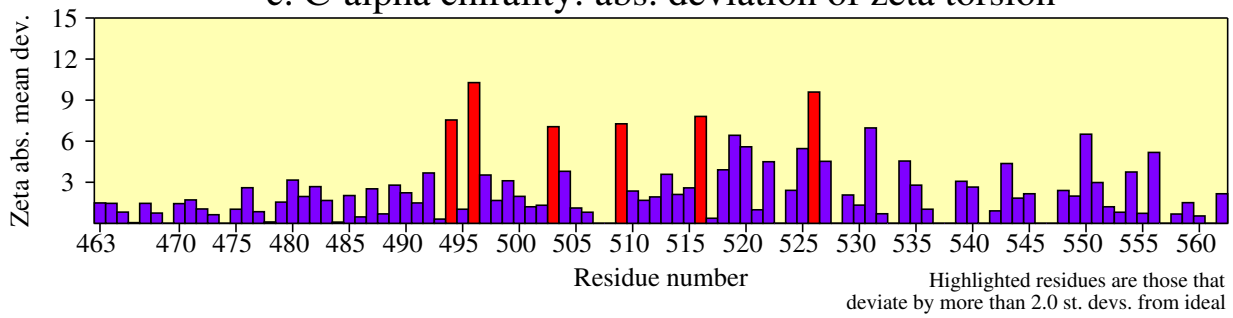
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

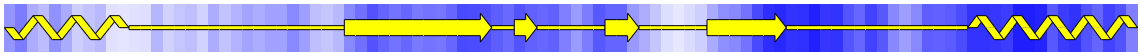


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



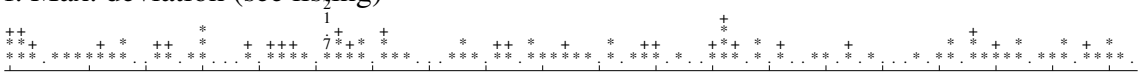
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

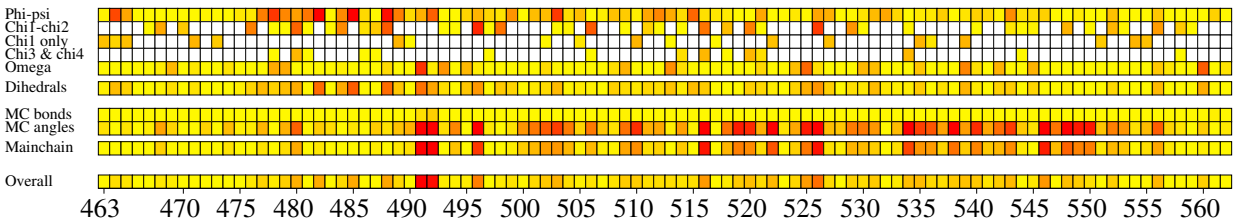
Most favoured Allowed Generous Disallowed

TVTAYNGFVKSGKDAQFERPDLPRELVVAPFYALEIAPAVHHTMGGLVIDTKAEVKSEKTGKPITGLYAAGEVTGGVHGANRLGGNAISDIVTYGRIAGA

f. Max. deviation (see listing)



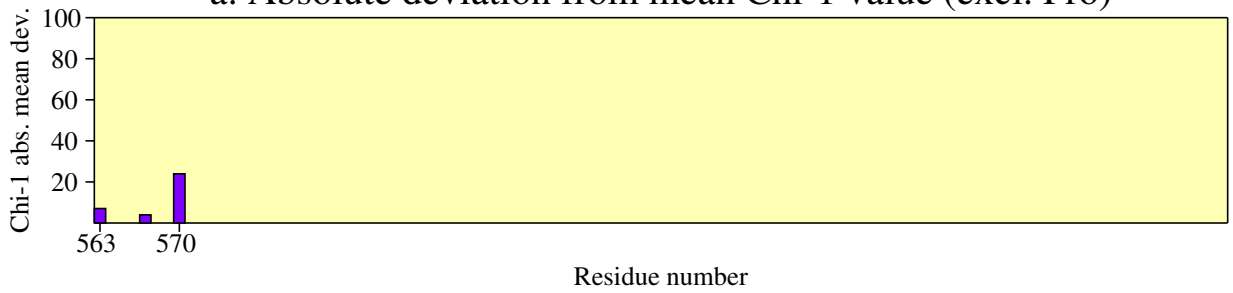
g. G-factors



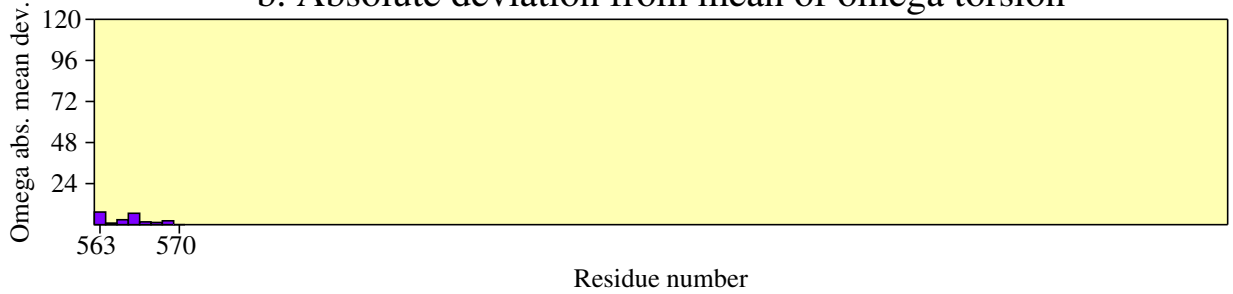
Residue properties

1d4c

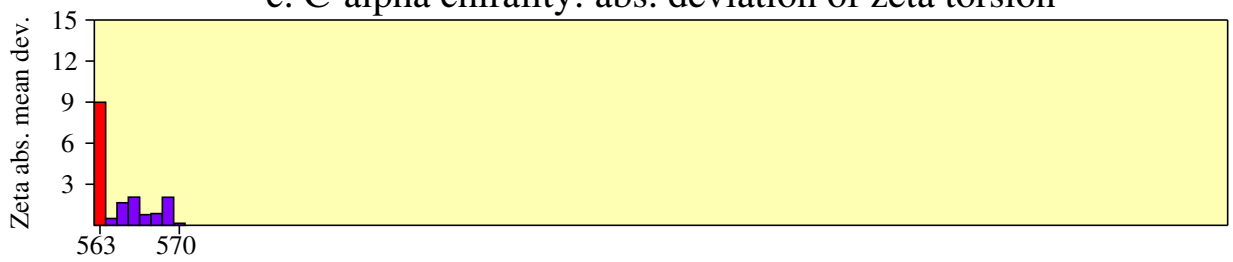
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

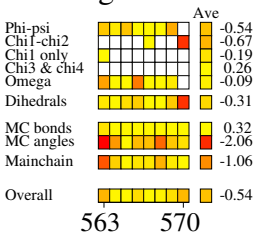
Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

e. Sequence & Ramachandran regions

Most favoured Allowed Generous Disallowed

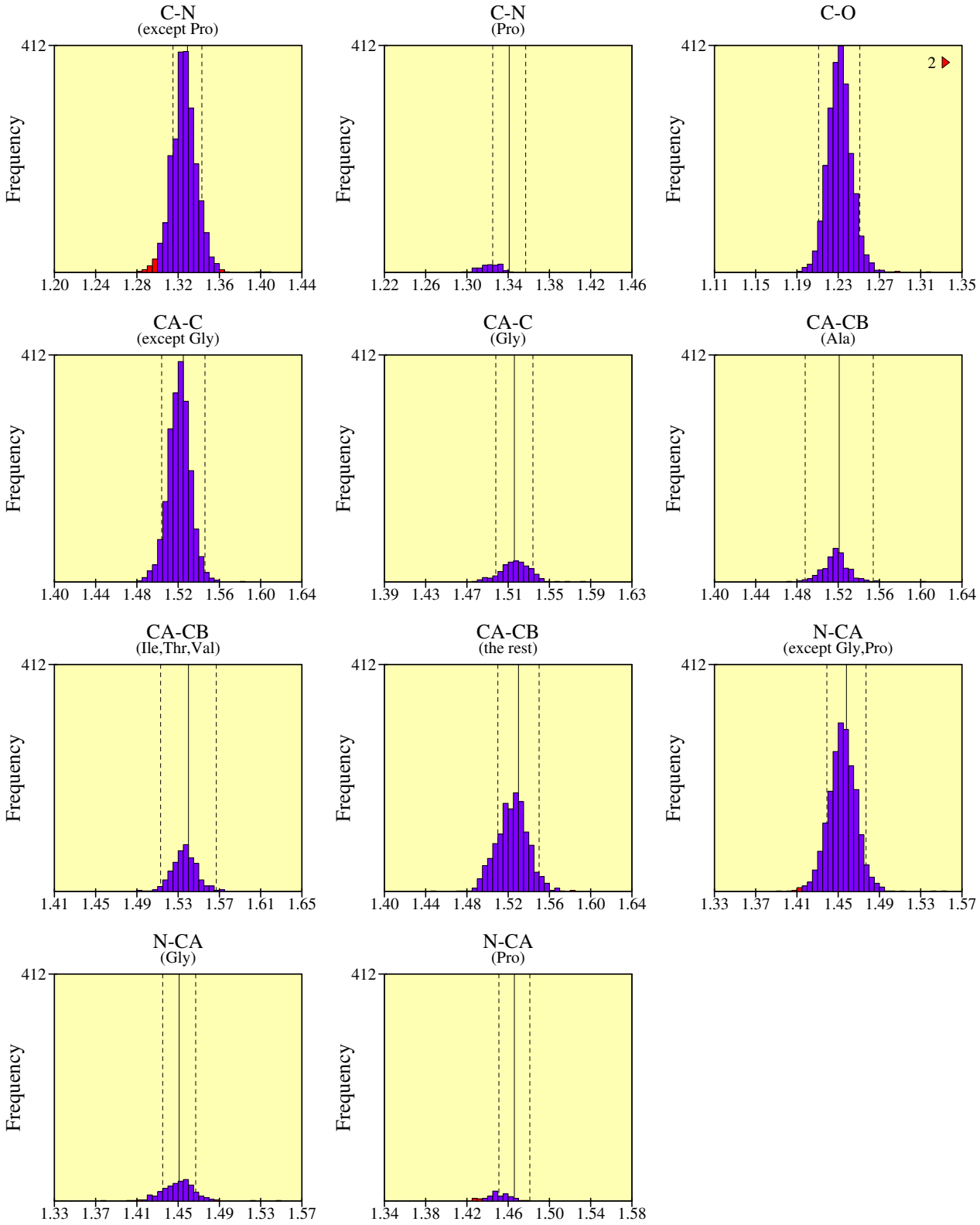
f. Max. deviation (see listing)

g. G-factors



Main-chain bond lengths

1d4c

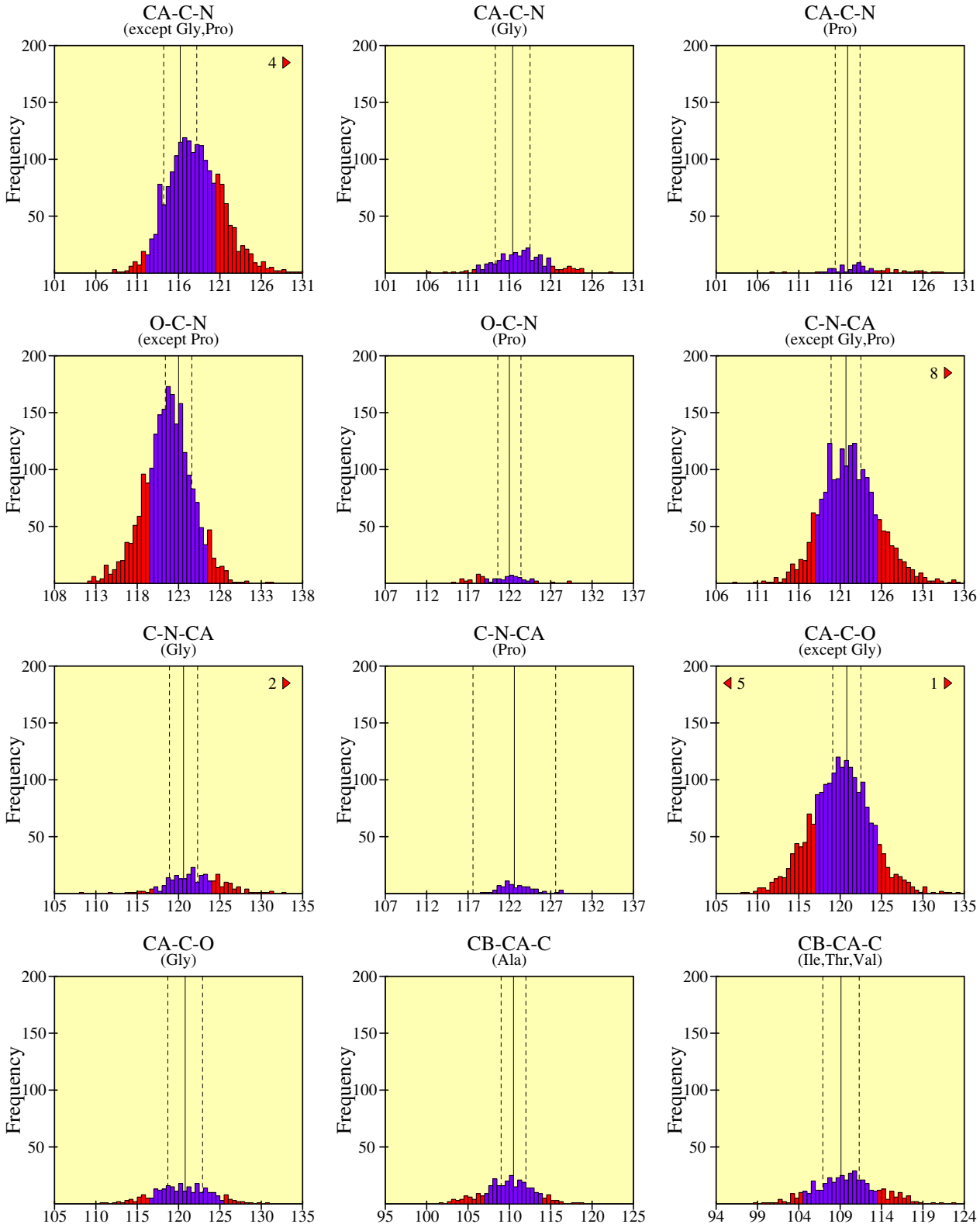


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

1d4c

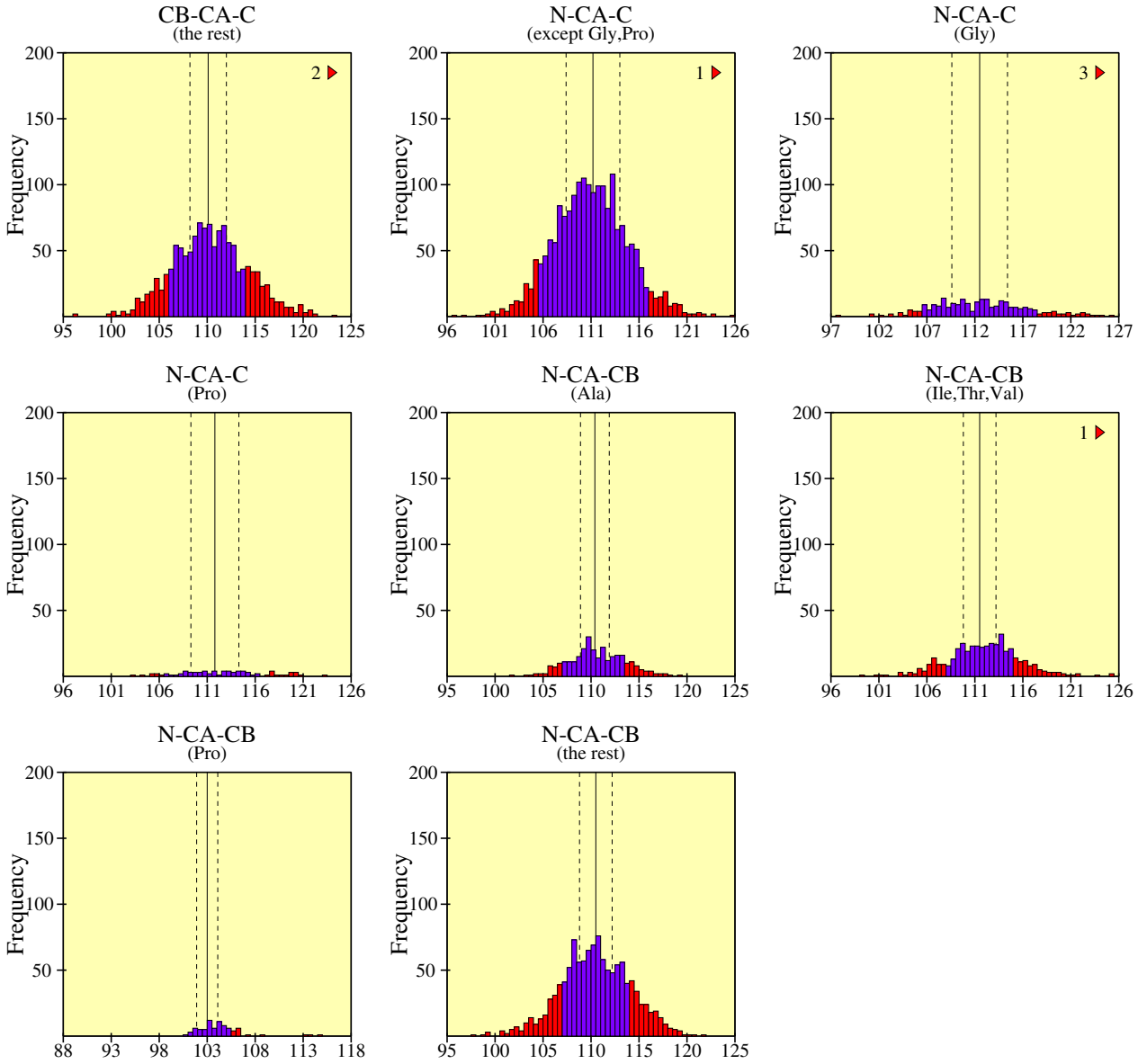


Black bars > 2.0 st. devs. from mean. ◀ or ▶ signifies data points off the graph in the direction shown.

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

Main-chain bond angles

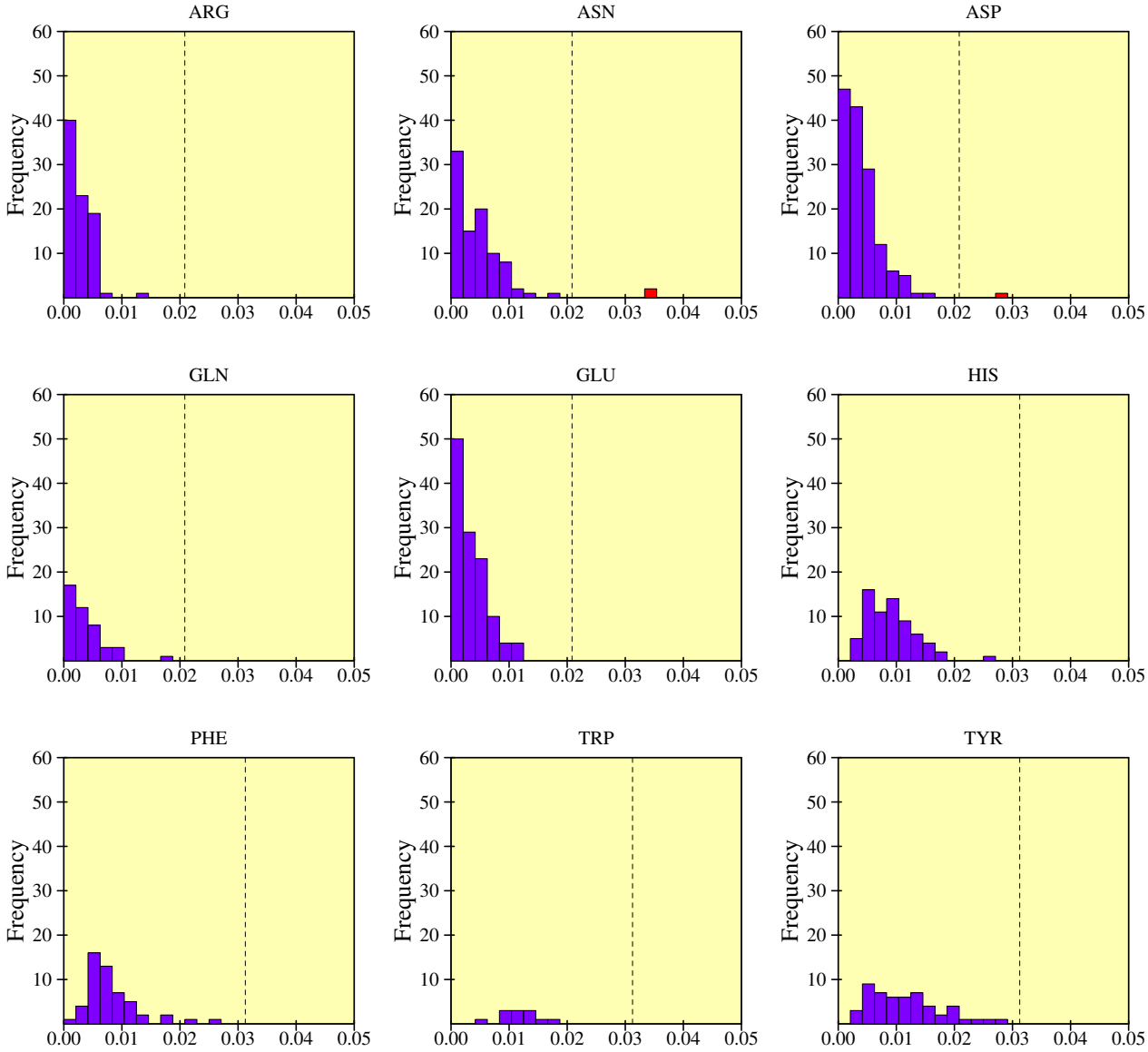
1d4c



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

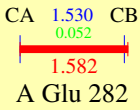
1d4c



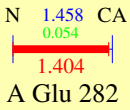
Histograms showing RMS distances of planar atoms from best-fit plane.
Black bars indicate large deviations from planarity: RMS dist > 0.03 for rings, and > 0.02 otherwise.

Distorted geometry
1d4c

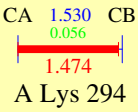
Main-chain bond lengths



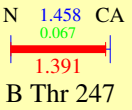
A Glu 282



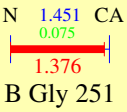
A Glu 282



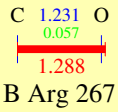
A Lys 294



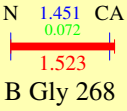
B Thr 247



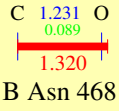
B Gly 251



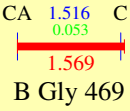
B Arg 267



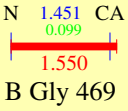
B Gly 268



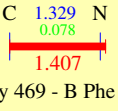
B Asn 468



B Gly 469

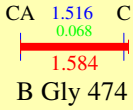


B Gly 469

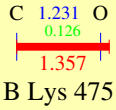


B Gly 469 - B Phe 470

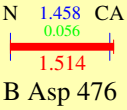
B Gly 474



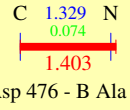
B Gly 474



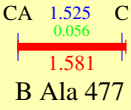
B Lys 475



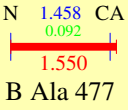
B Asp 476



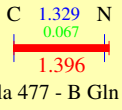
B Asp 476 - B Ala 477



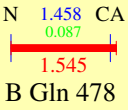
B Ala 477



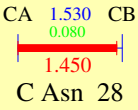
B Ala 477



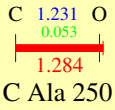
B Ala 477 - B Gln 478



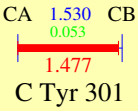
B Gln 478



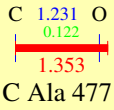
C Asn 28



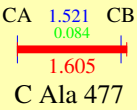
C Ala 250



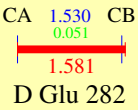
C Tyr 301



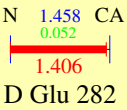
C Ala 477



C Ala 477



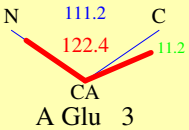
D Glu 282



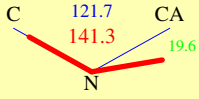
D Glu 282

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

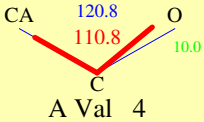
Main-chain bond angles



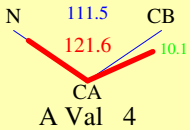
A Glu 3



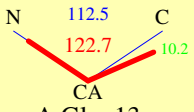
A Glu 3 - A Val 4



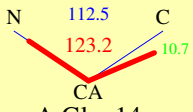
A Val 4



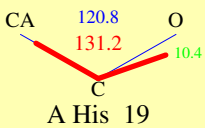
A Val 4



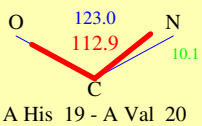
A Gly 13



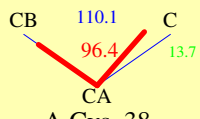
A Gly 14



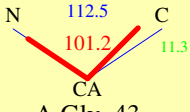
A His 19



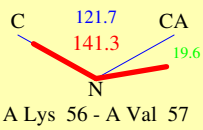
A His 19 - A Val 20



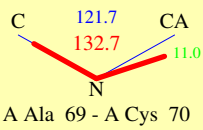
A Cys 38



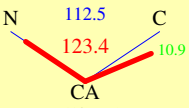
A Gly 43



A Lys 56 - A Val 57



A Ala 69 - A Cys 70



A Gly 97

A Val 107 - A Asp 108

A Lys 123 - A Glu 124

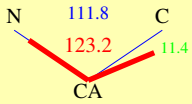
A Ser 143 - A Ala 144

A Gly 148 - A Ala 149

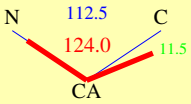
A Lys 150

Distorted geometry
1d4c

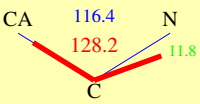
Main-chain bond angles (contd)



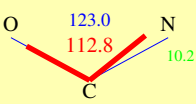
A Pro 160



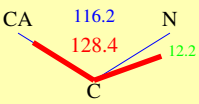
A Gly 161



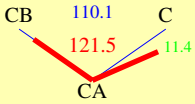
A Gly 162 - A Asn 163



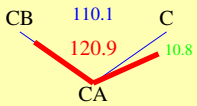
A Gly 162 - A Asn 163



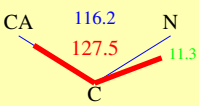
A Ala 167 - A Ala 168



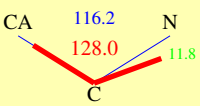
A Glu 185



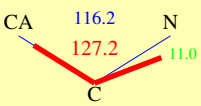
A Ser 218



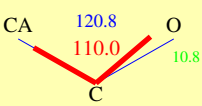
A Ser 218 - A Ile 219



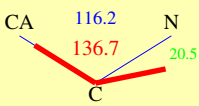
A Gln 258 - A Val 259



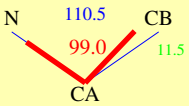
A Asn 263 - A Ala 264



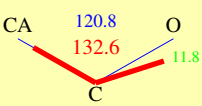
A Arg 267



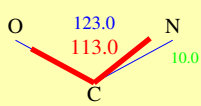
A Arg 267 - A Gly 268



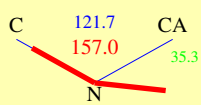
A Ser 275



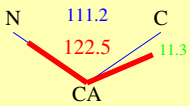
A Leu 281



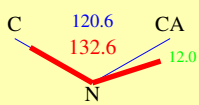
A Leu 281 - A Glu 282



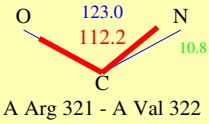
A Leu 281 - A Glu 282



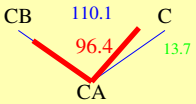
A Glu 282



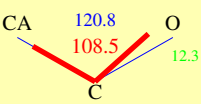
A Ser 285 - A Gly 286



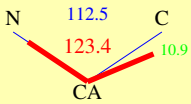
A Arg 321 - A Val 322



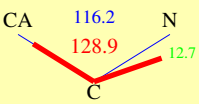
A Lys 328



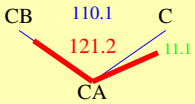
A Leu 329



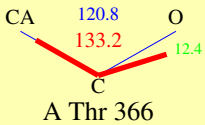
A Gly 331



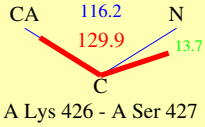
A Thr 341 - A Gly 342



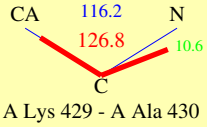
A Leu 345



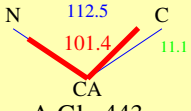
A Thr 366



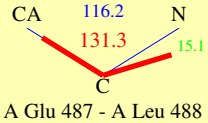
A Lys 426 - A Ser 427



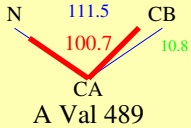
A Lys 429 - A Ala 430



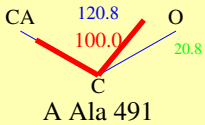
A Gly 443



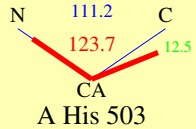
A Glu 487 - A Leu 488



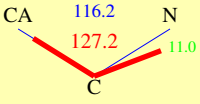
A Val 489



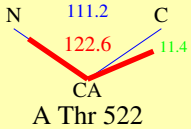
A Ala 491



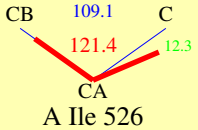
A His 503



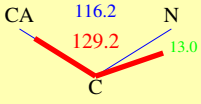
A Asp 512 - A Thr 513



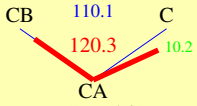
A Thr 522



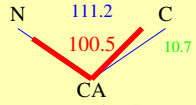
A Ile 526



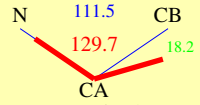
A Glu 534 - A Val 535



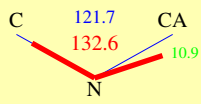
A Ser 563



B Val 4



B Val 4



B Glu 11 - B Met 12

B Met 12

B Met 12

B Ser 40 - B Cys 41

B Gly 76 - B His 77

B Asp 93

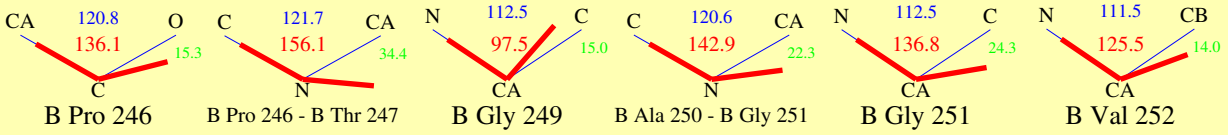
B Lys 150

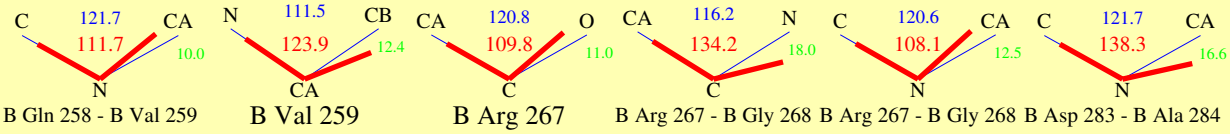
B Gly 161

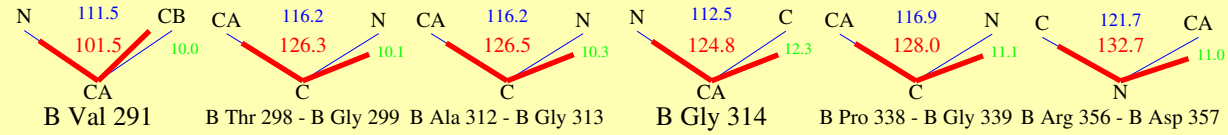
B Gly 161 - B Gly 162

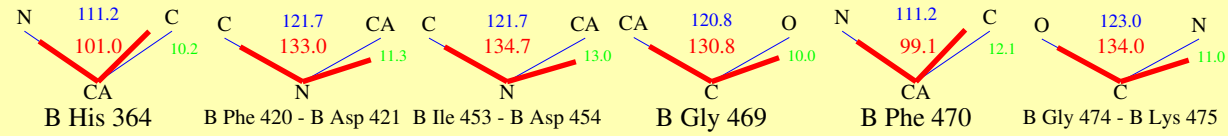
Distorted geometry
1d4c

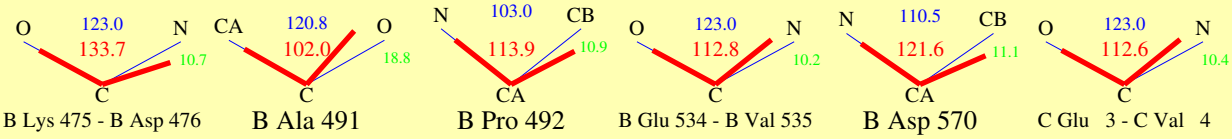
Main-chain bond angles (contd)

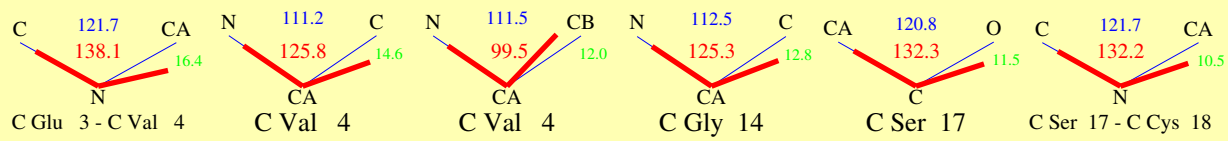


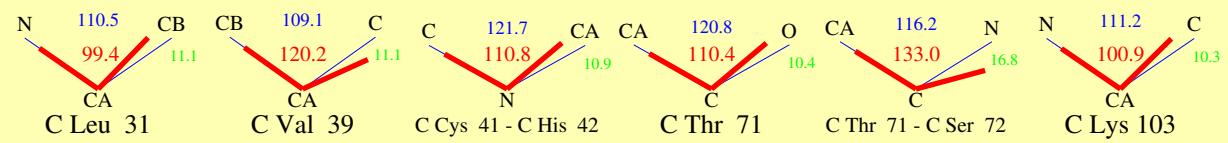


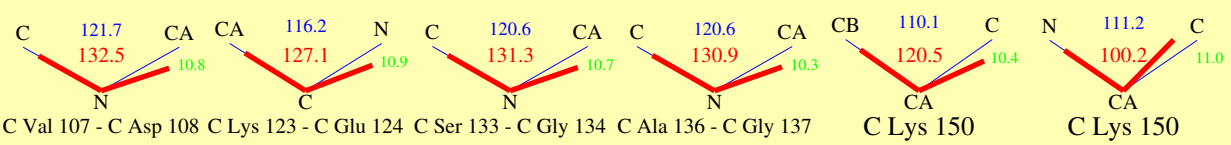






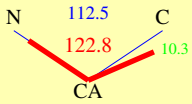




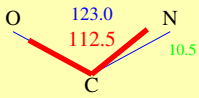


Distorted geometry
1d4c

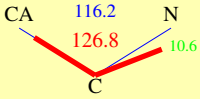
Main-chain bond angles (contd)



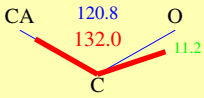
C Gly 161



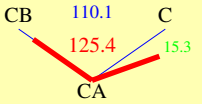
C Gly 161 - C Gly 162



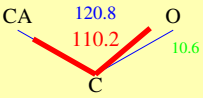
C Leu 207 - C Val 208



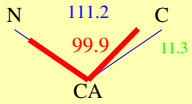
C Leu 211



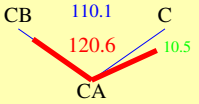
C Ser 218



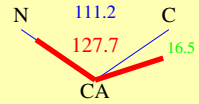
C Thr 230



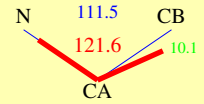
C Met 235



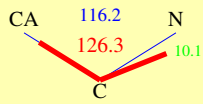
C Pro 246



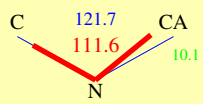
C Ala 250



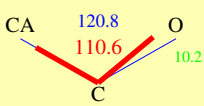
C Val 259



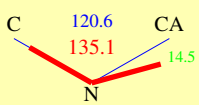
C Lys 266 - C Arg 267



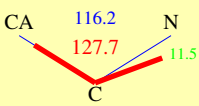
C Arg 279 - C Ile 280



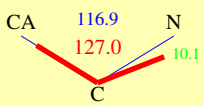
C Ile 280



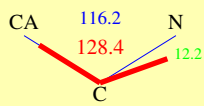
C Ser 285 - C Gly 286



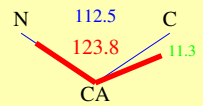
C Thr 298 - C Gly 299



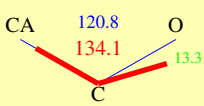
C Pro 327 - C Lys 328



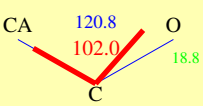
C Thr 341 - C Gly 342



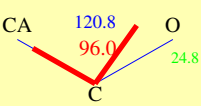
C Gly 352



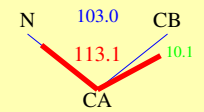
C Val 373



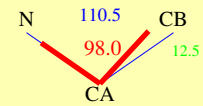
C Ala 477



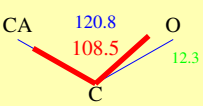
C Ala 491



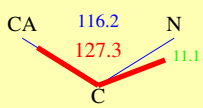
C Pro 492



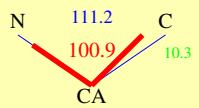
C His 503



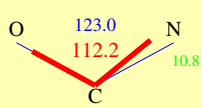
C Met 506



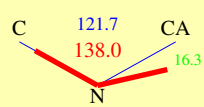
C Met 506 - C Gly 507



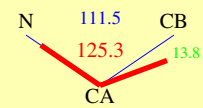
C Asp 512



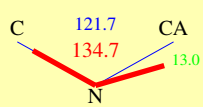
C Tyr 530 - C Ala 531



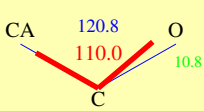
C Lys 569 - C Asp 570



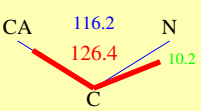
D Val 4



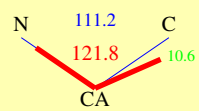
D Gly 10 - D Glu 11



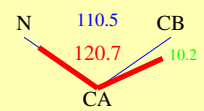
D Cys 41



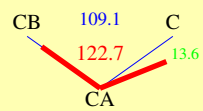
D Cys 41 - D His 42



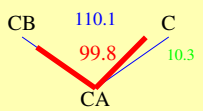
D Lys 56



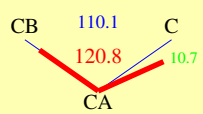
D Lys 61



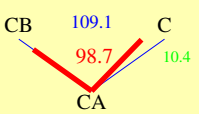
D Ile 68



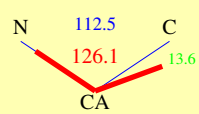
D Cys 73



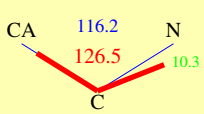
D Glu 78



D Val 81



D Gly 161



D Lys 165 - D Leu 166

D Thr 176 - D Lys 177

D Glu 185

D Arg 200 - D Asn 201

D Asn 201

D Thr 230

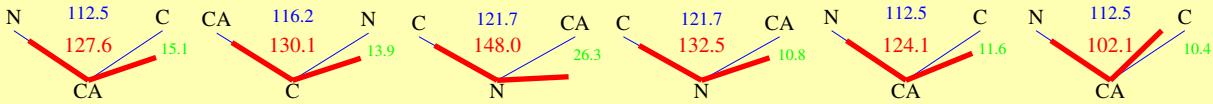
D Asp 231

D Asp 231

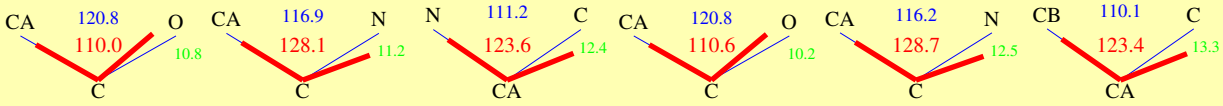
D Met 235

Distorted geometry
1d4c

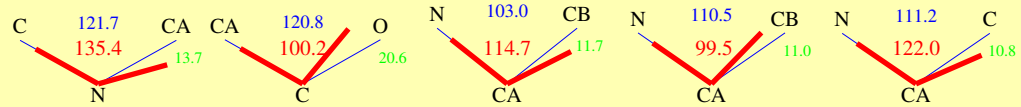
Main-chain bond angles (contd)



D Gly 251 | D Arg 267 - D Gly 268 | D Leu 281 - D Glu 282 | D Asp 283 - D Ala 284 | D Gly 286 | D Gly 295



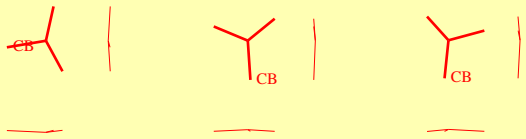
D Pro 327 | D Pro 327 - D Lys 328 | D Asp 357 | D Glu 359 | D Glu 359 - D Tyr 360 | D Asn 396



D Thr 400 - D Arg 401 | D Ala 491 | D Pro 492 | D Glu 516 | D Thr 522

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

Planar groups



0.033 | 0.027 | 0.033

B Asn 468 | B Asp 476 | D Asn 468

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