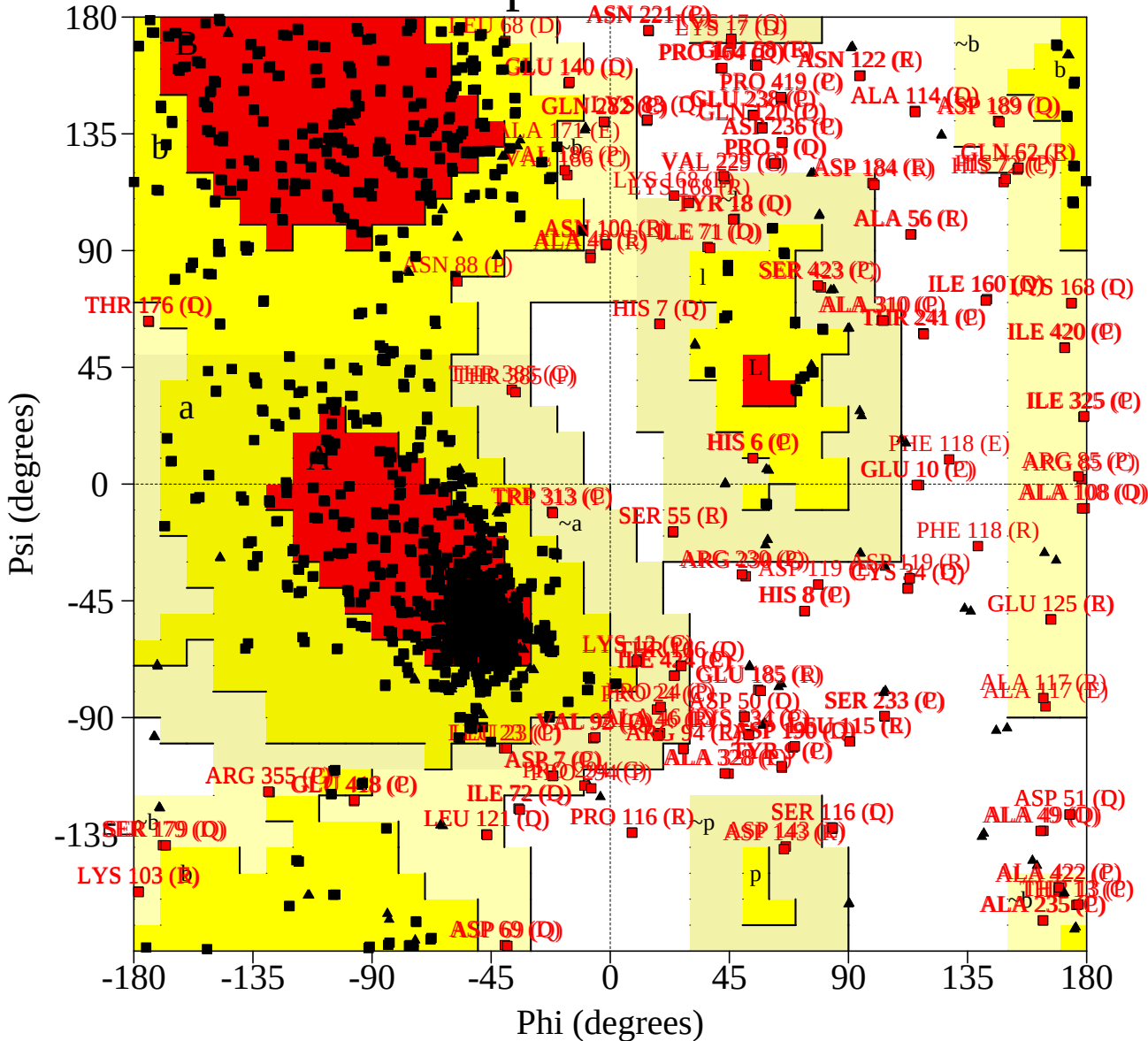


Ramachandran Plot

pdb1zrt



Plot statistics

Residues in most favoured regions [A,B,L]	899	62.3%
Residues in additional allowed regions [a,b,l,p]	388	26.9%
Residues in generously allowed regions [~a,~b,~l,~p]	91	6.3%
Residues in disallowed regions	64	4.4%

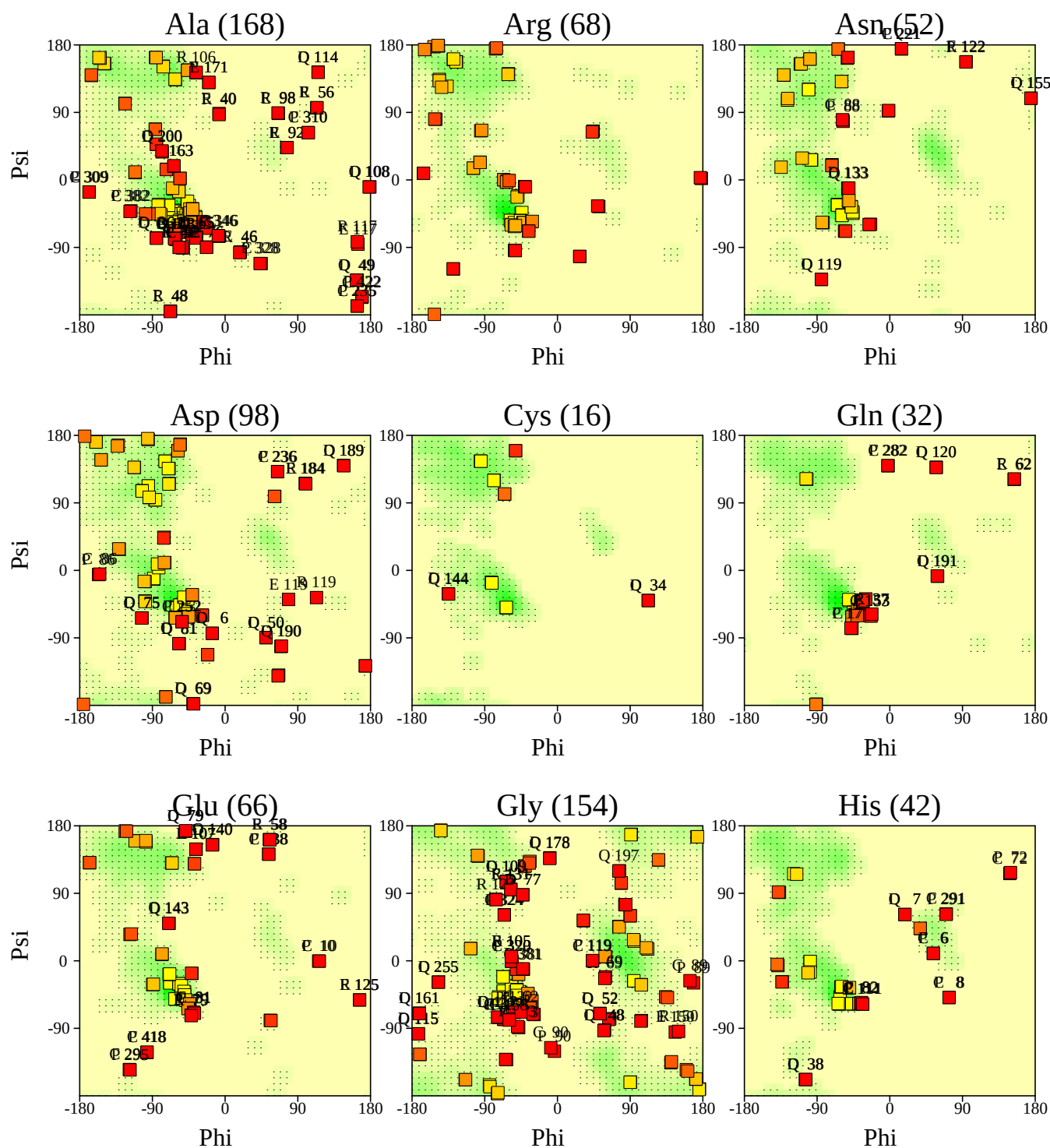
Number of non-glycine and non-proline residues	1442	100.0%
Number of end-residues (excl. Gly and Pro)	10	
Number of glycine residues (shown as triangles)	156	
Number of proline residues	112	

Total number of residues	1720	

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

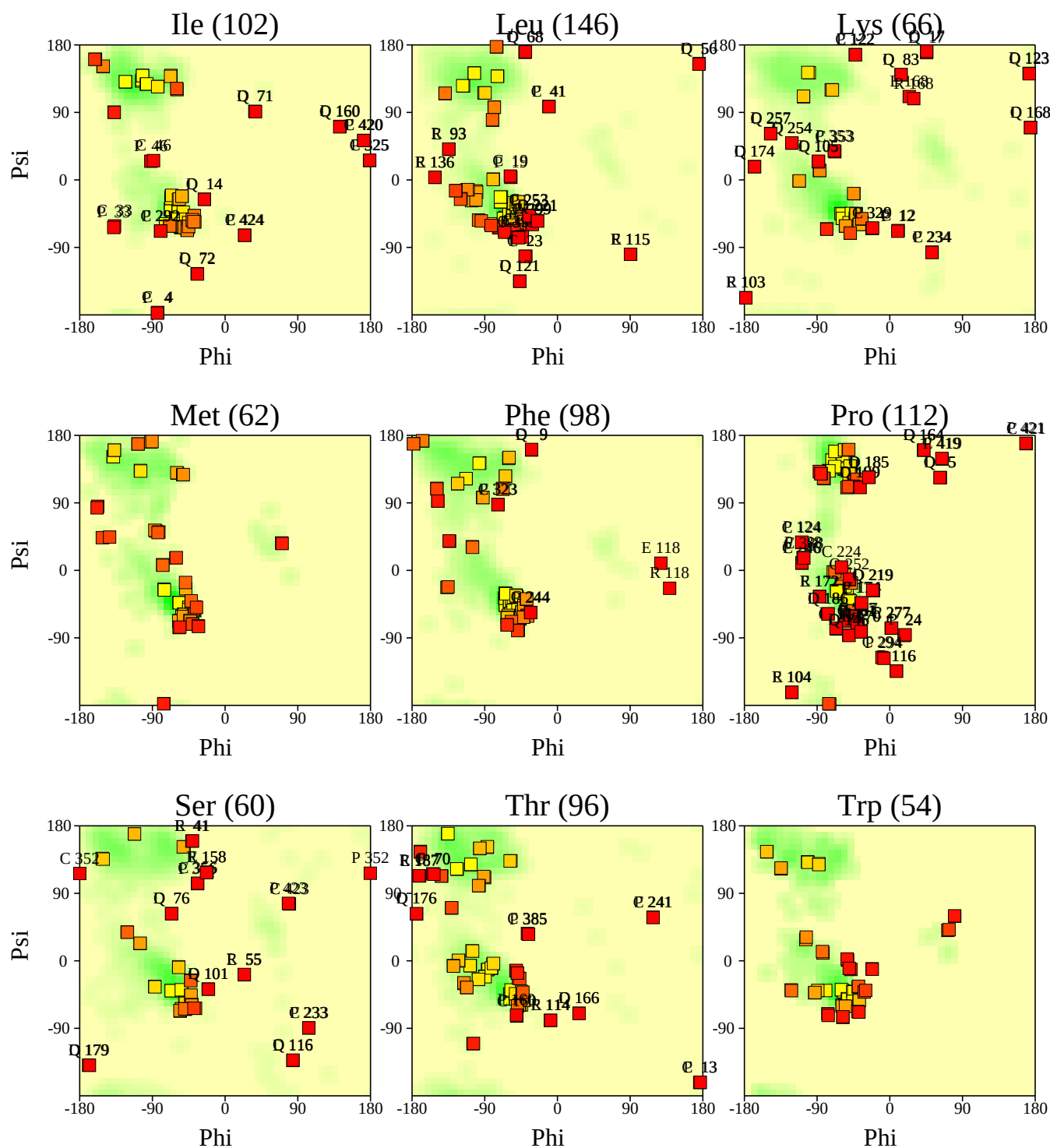
pdb1zrt



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 2.0Å or better.

Ramachandran plots for all residue types

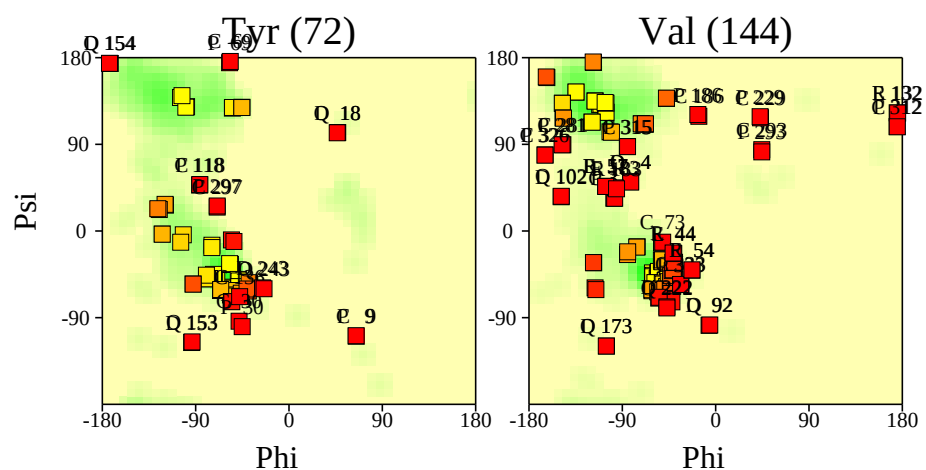
pdb1zrt



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 2.0Å or better.

Ramachandran plots for all residue types

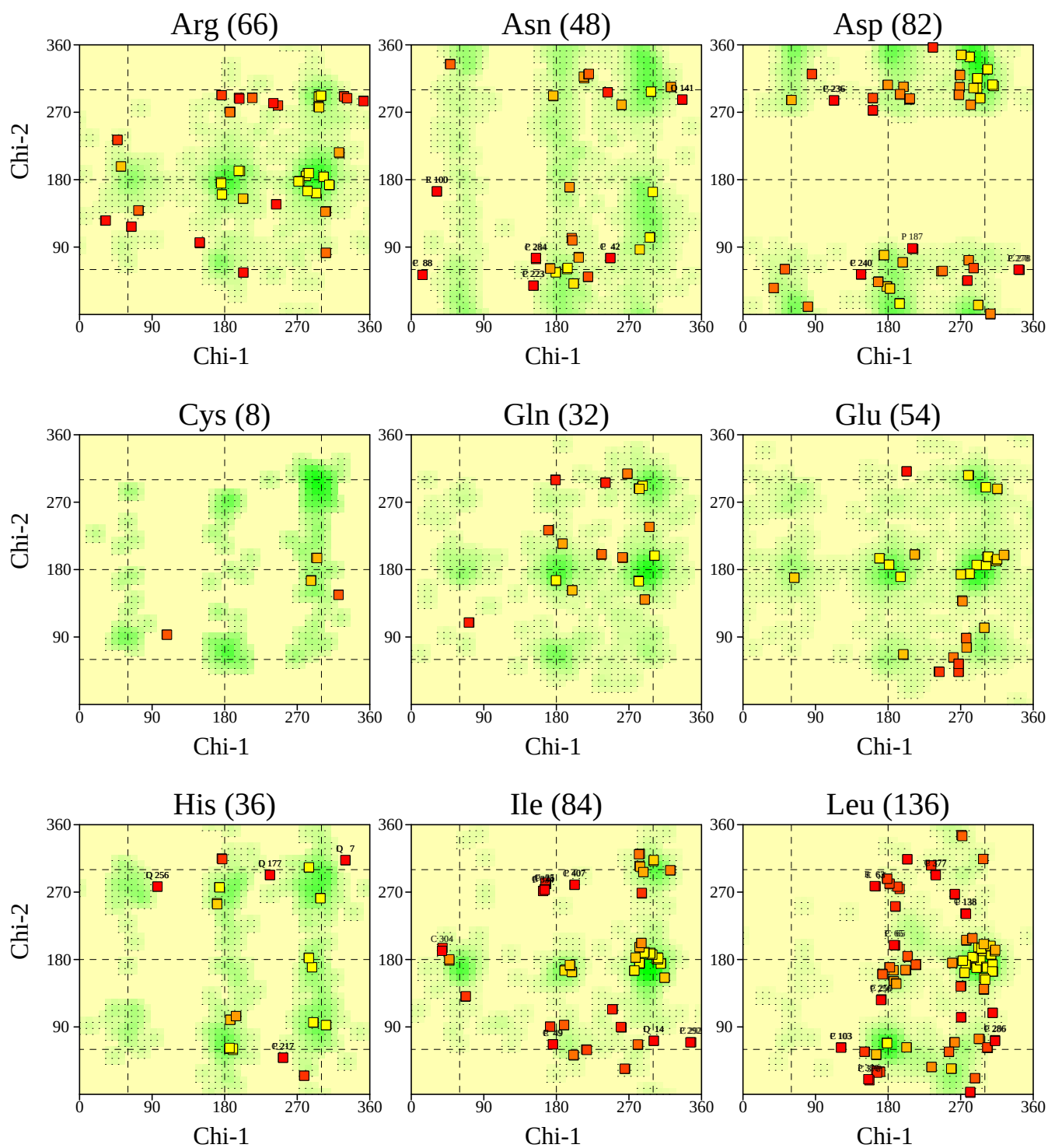
pdb1zrt



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 2.0Å or better.

Chi1-Chi2 plots

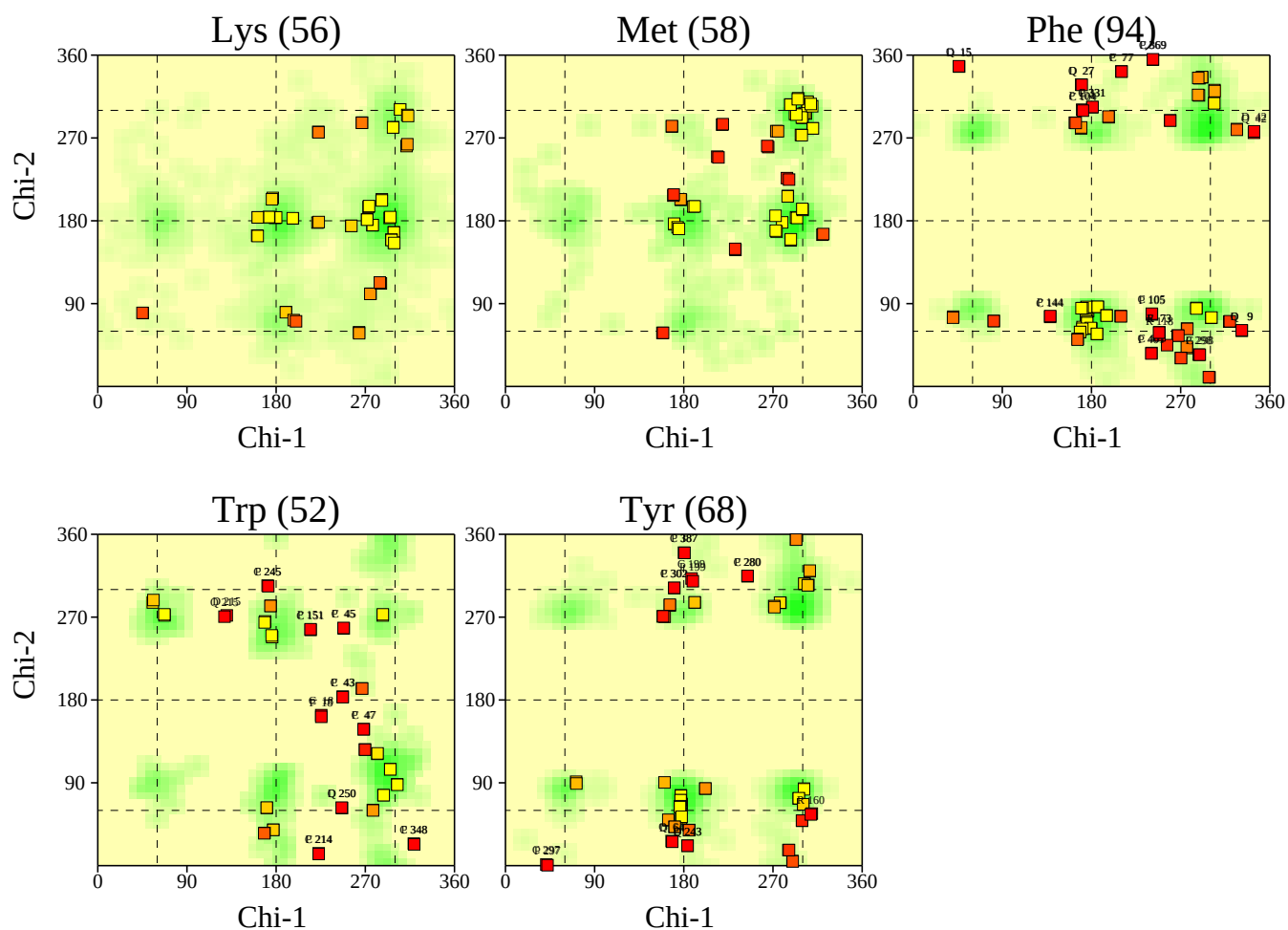
pdb1zrt



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 2.0Å or better.

Chi1-Chi2 plots

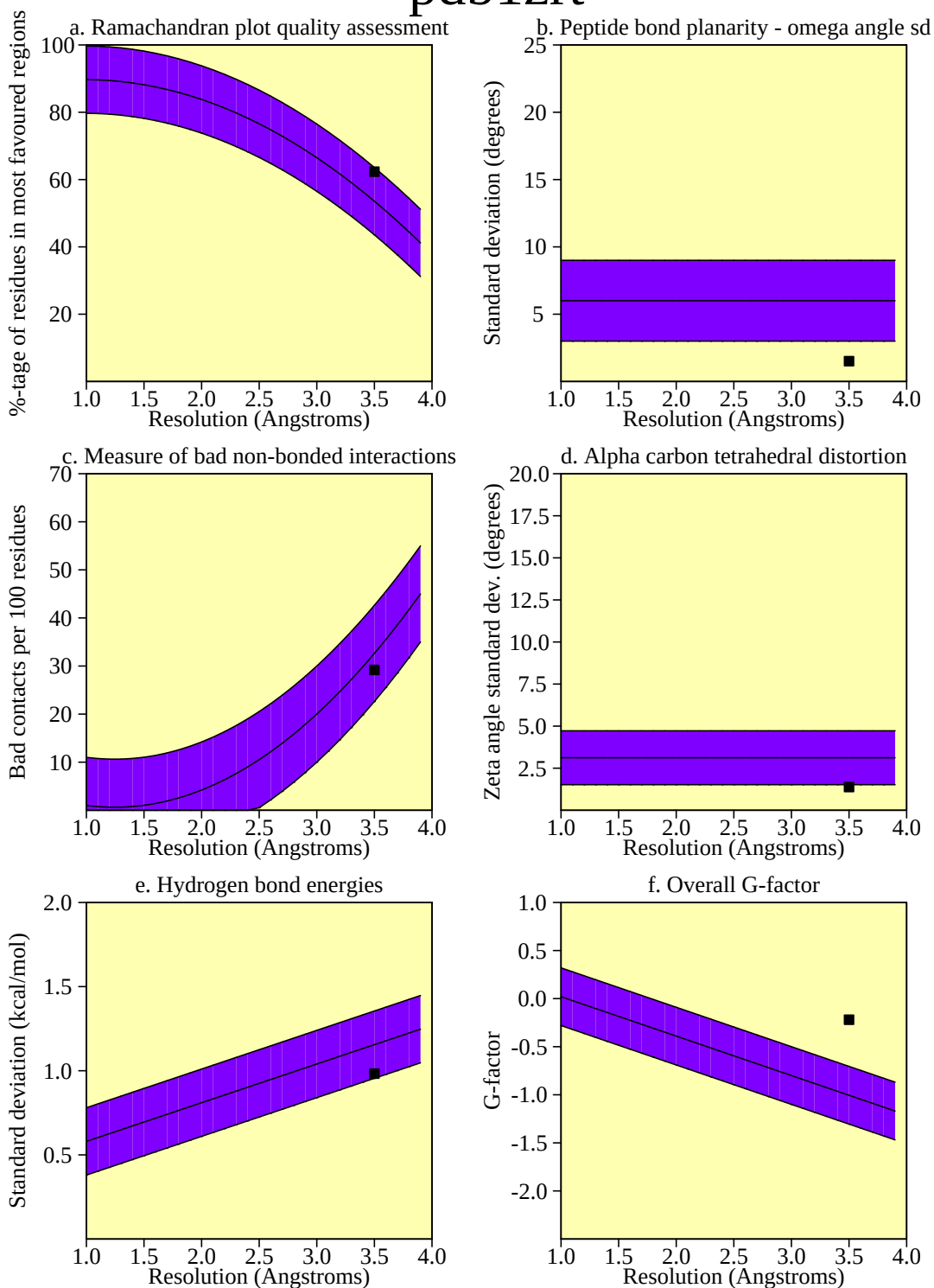
pdb1zrt



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 2.0Å or better.

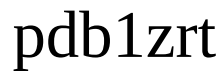
Main-chain parameters

pdb1zrt



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	1442	62.3	53.6	10.0	0.9	Inside
b. Omega angle st dev	1708	1.5	6.0	3.0	-1.5	BETTER
c. Bad contacts / 100 residues	502	29.2	32.6	10.0	-0.3	Inside
d. Zeta angle st dev	1560	1.4	3.1	1.6	-1.1	BETTER
e. H-bond energy st dev	977	1.0	1.2	0.2	-0.9	Inside
f. Overall G-factor	1720	-0.2	-1.0	0.3	2.6	BETTER

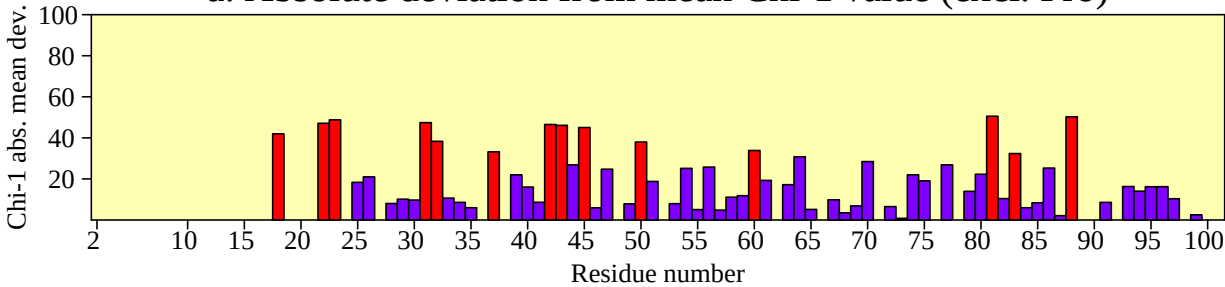


Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. Chi-1 gauche minus st dev	138	22.9	31.8	6.5	-1.4	BETTER
b. Chi-1 trans st dev	472	21.9	30.1	5.3	-1.6	BETTER
c. Chi-1 gauche plus st dev	564	22.9	28.8	4.9	-1.2	BETTER
d. Chi-1 pooled st dev	1174	22.6	29.7	4.8	-1.5	BETTER
e. Chi-2 trans st dev	268	21.0	28.5	5.0	-1.5	BETTER

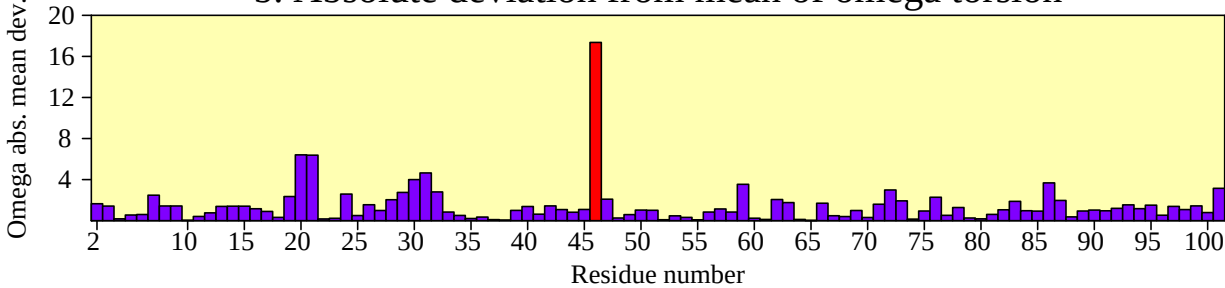
Residue properties

pdb1zrt

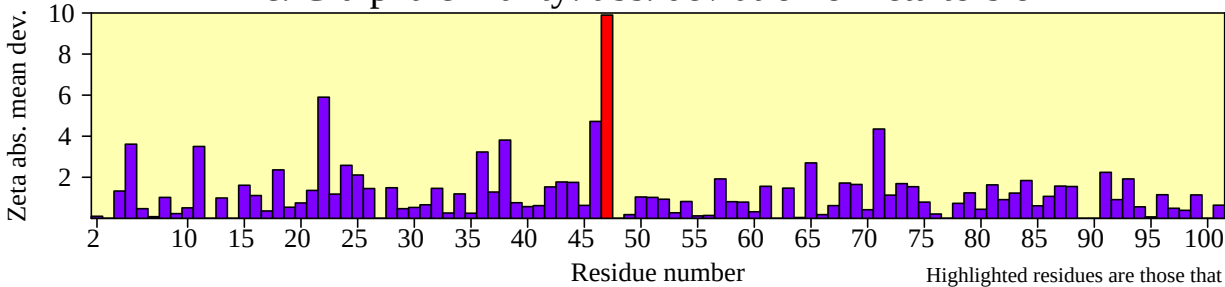
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

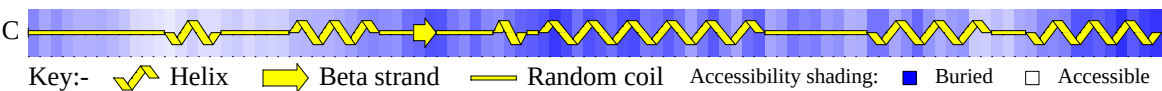


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



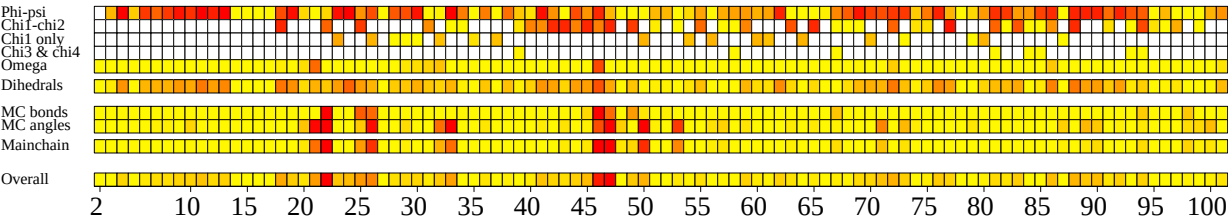
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



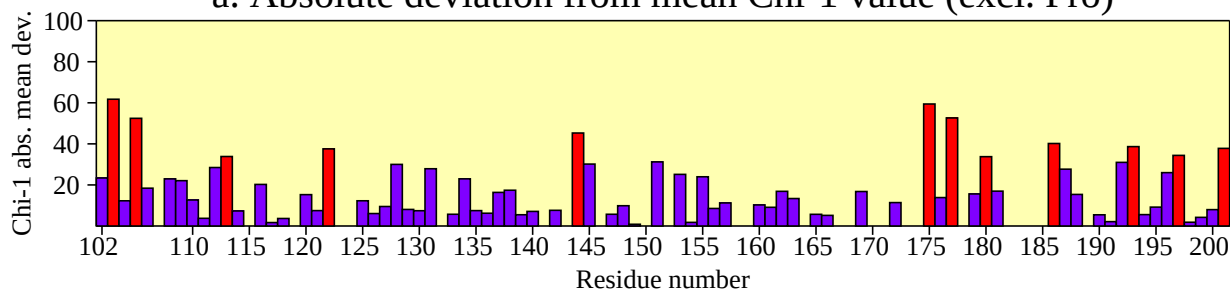
g. G-factors



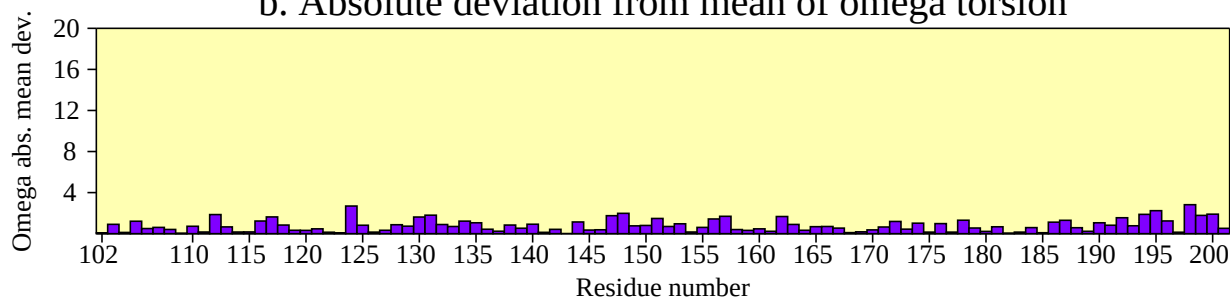
Residue properties

pdb1zrt

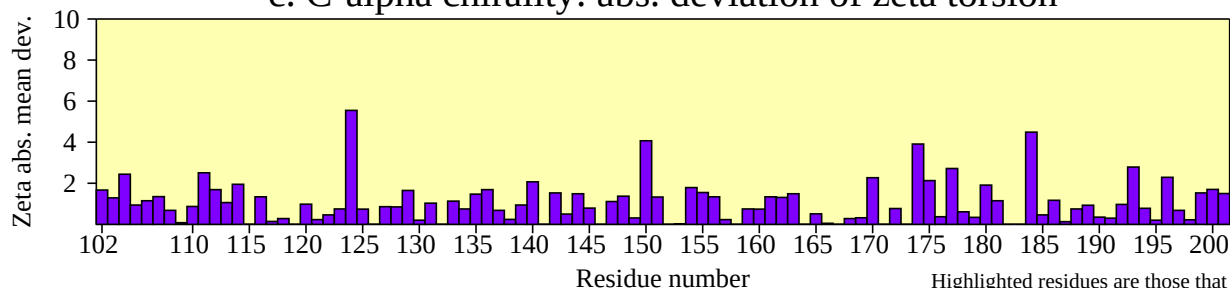
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

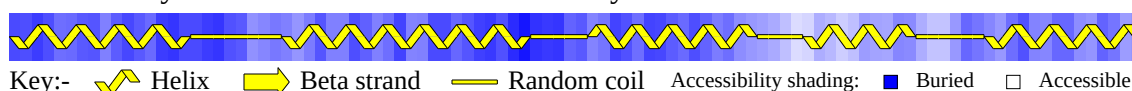


c. C-alpha chirality: abs. deviation of zeta torsion



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

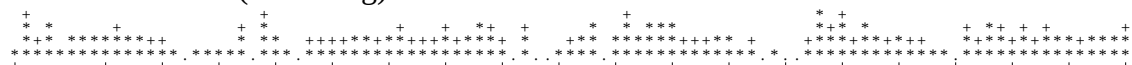
d. Secondary structure & estimated accessibility



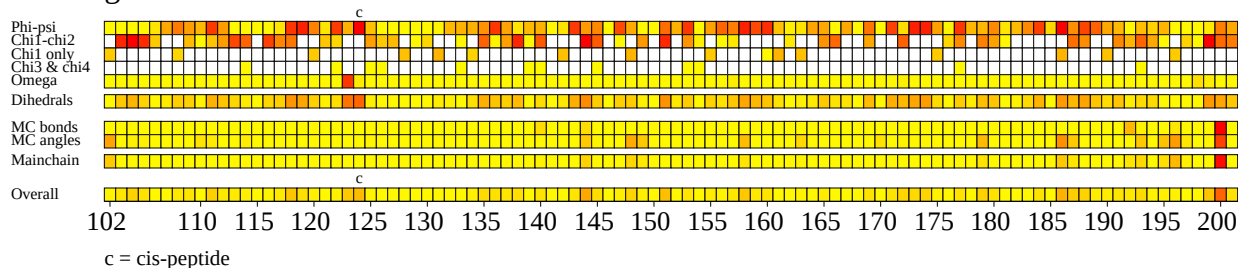
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



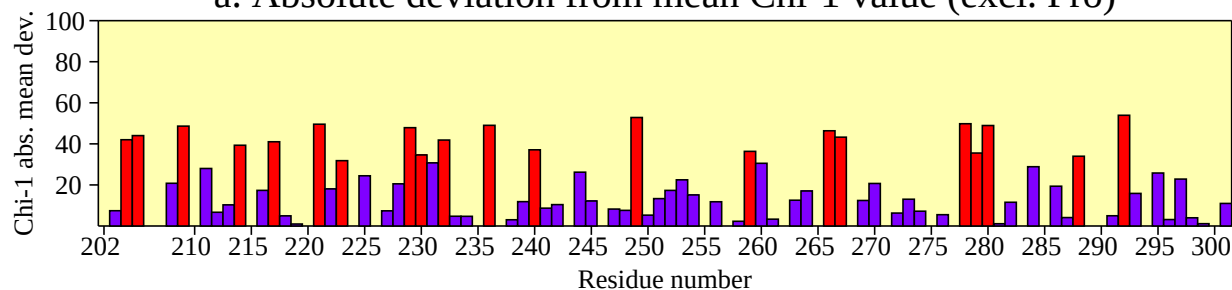
g. G-factors



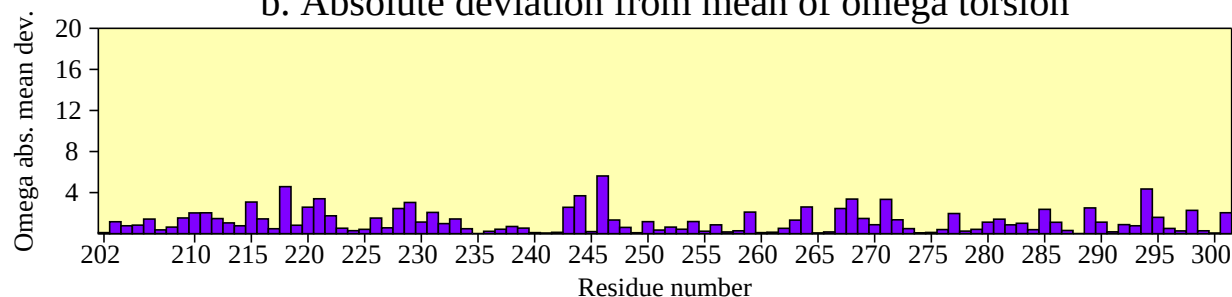
Residue properties

pdb1zrt

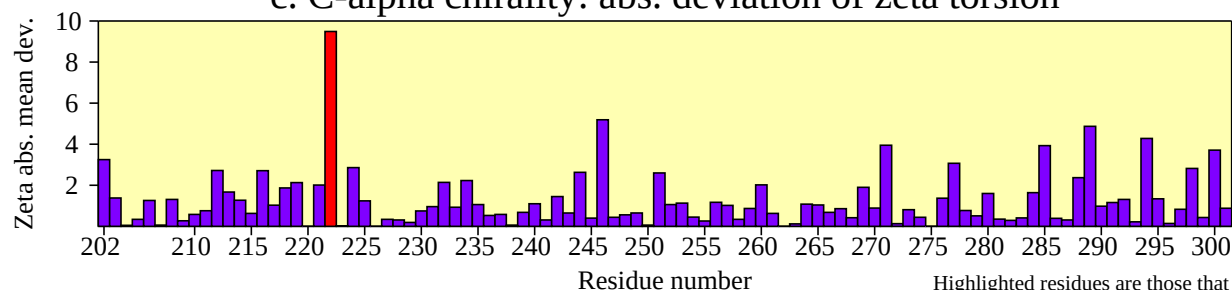
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

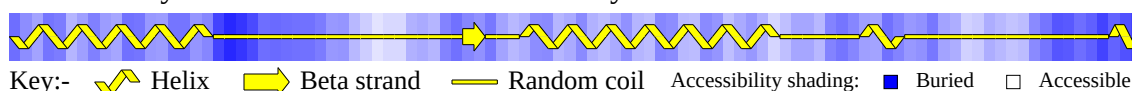


c. C-alpha chirality: abs. deviation of zeta torsion

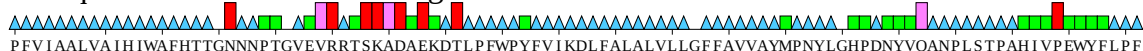


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

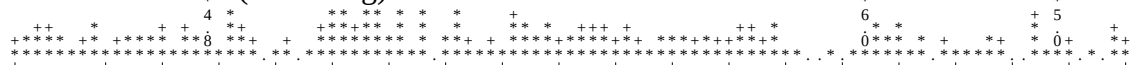
d. Secondary structure & estimated accessibility



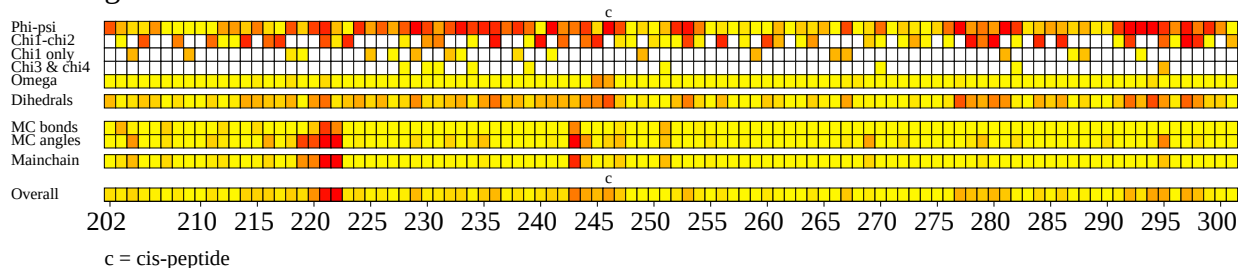
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



g. G-factors

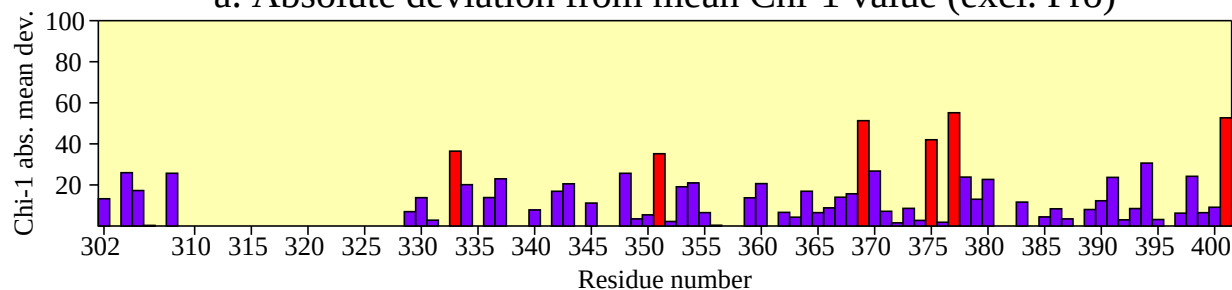


c = cis-peptide

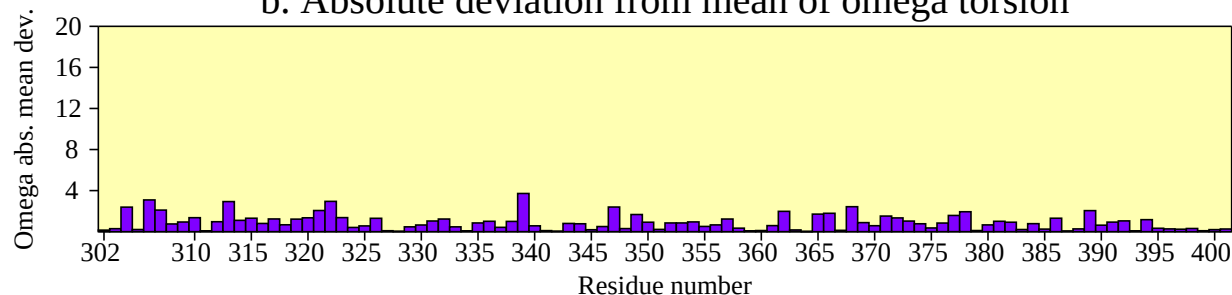
Residue properties

pdb1zrt

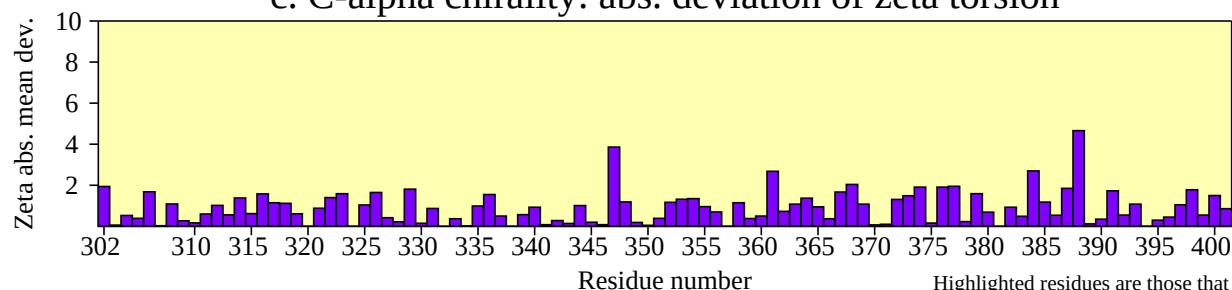
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

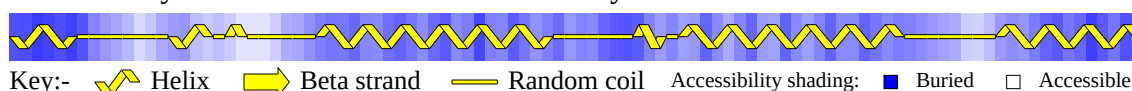


c. C-alpha chirality: abs. deviation of zeta torsion



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

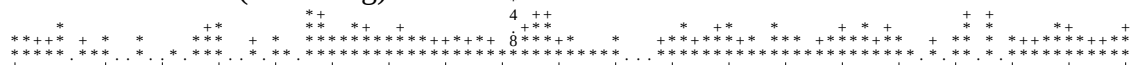
d. Secondary structure & estimated accessibility



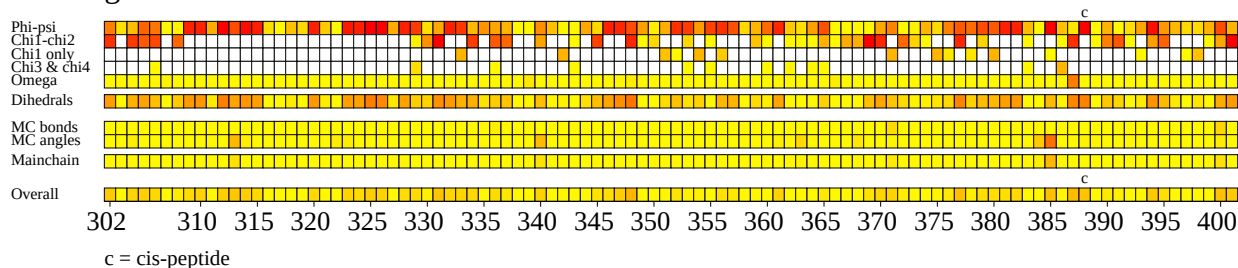
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



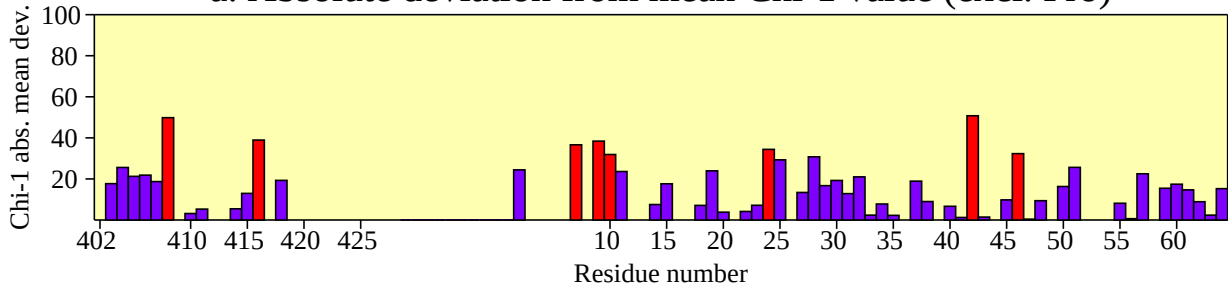
g. G-factors



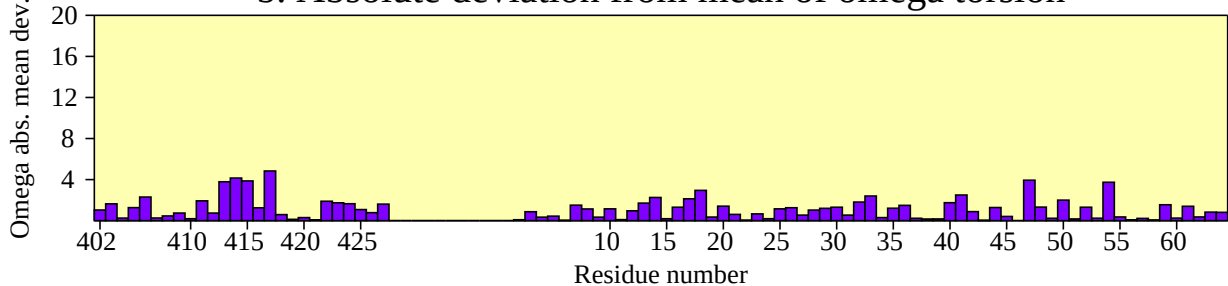
Residue properties

pdb1zrt

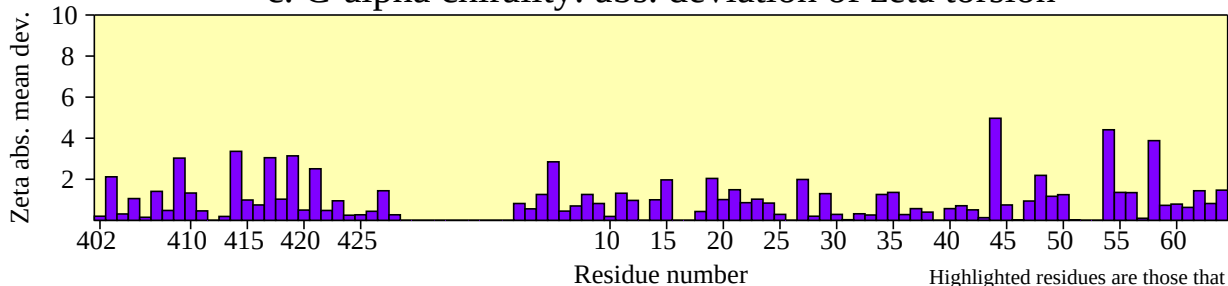
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

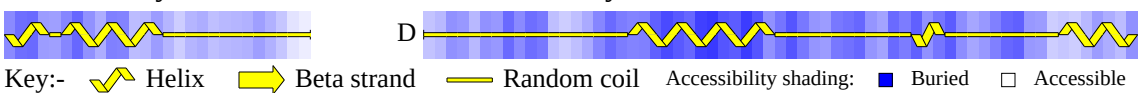


c. C-alpha chirality: abs. deviation of zeta torsion

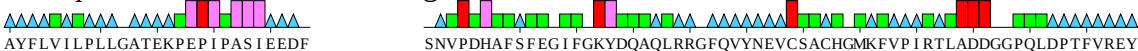


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



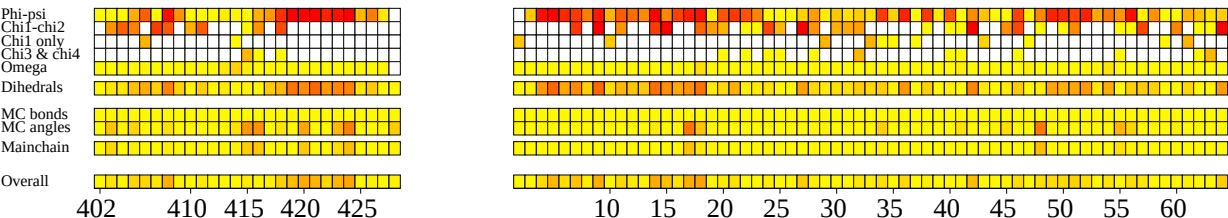
e. Sequence & Ramachandran regions



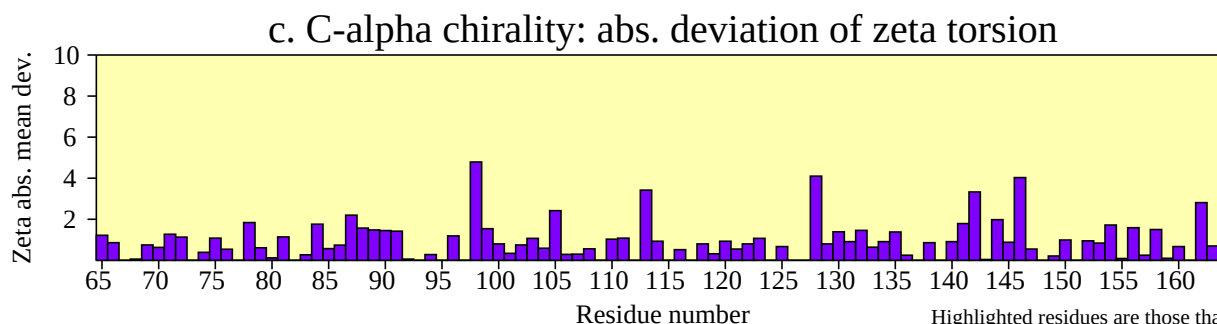
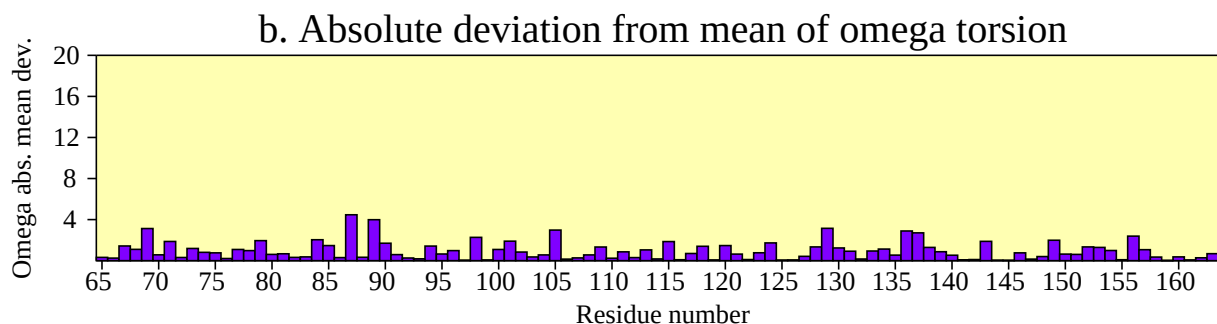
f. Max. deviation₂ (see listing)



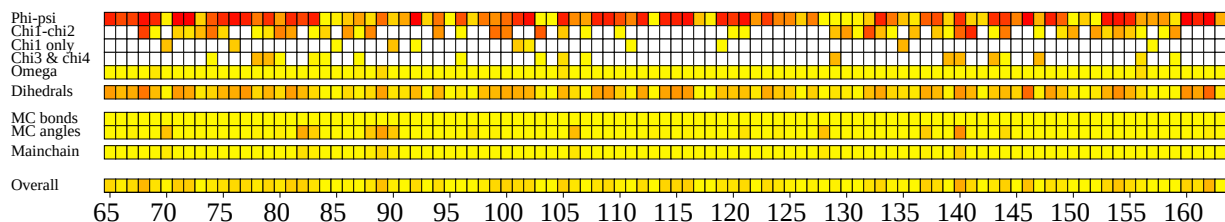
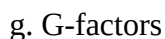
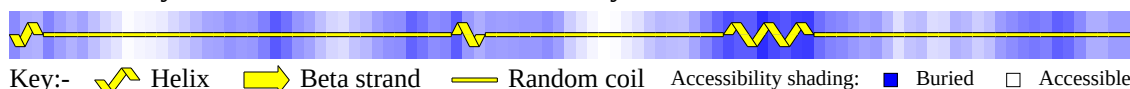
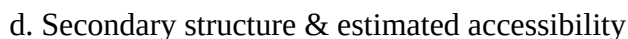
g. G-factors



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



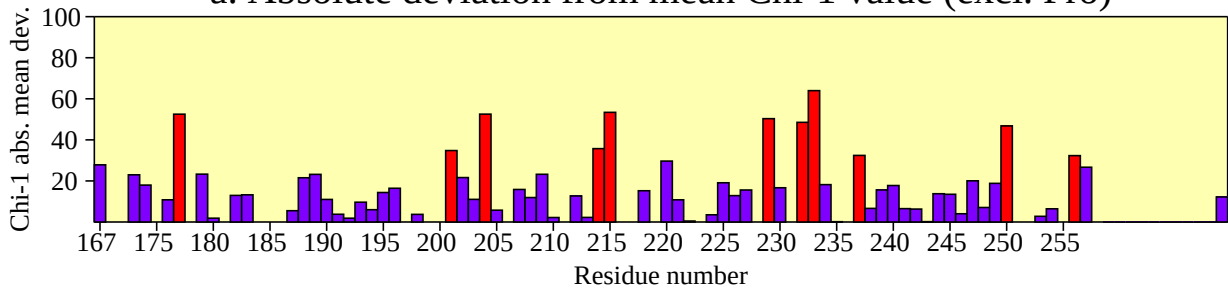
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal



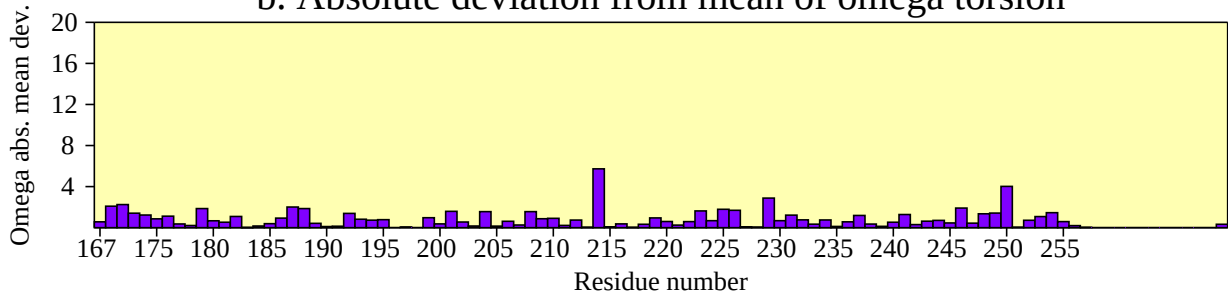
Residue properties

pdb1zrt

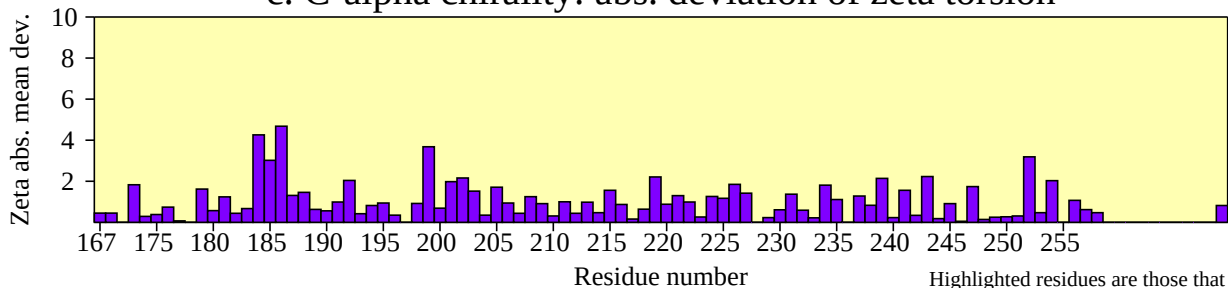
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



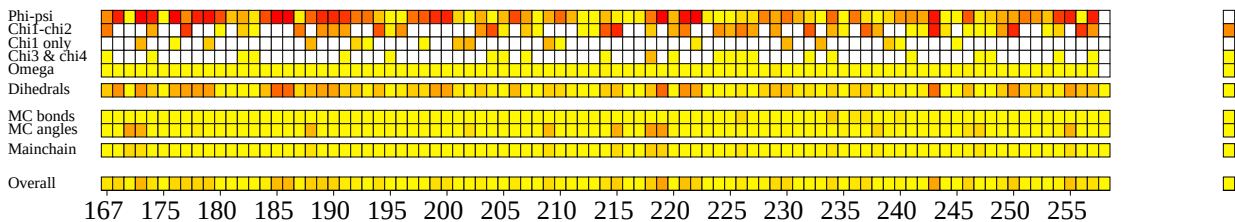
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



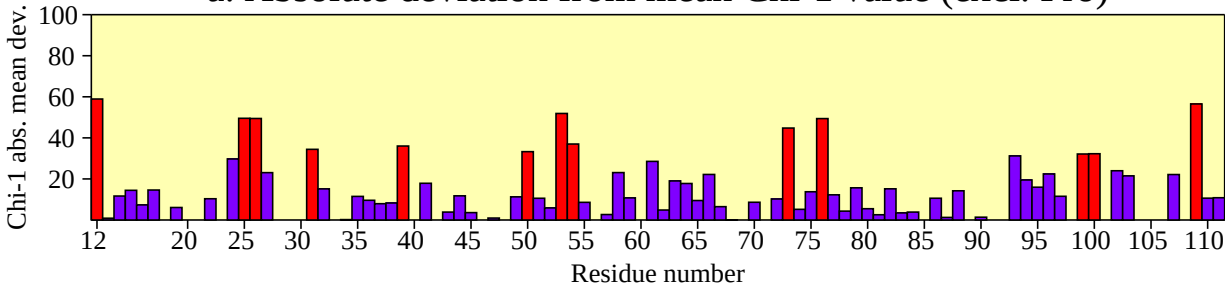
g. G-factors



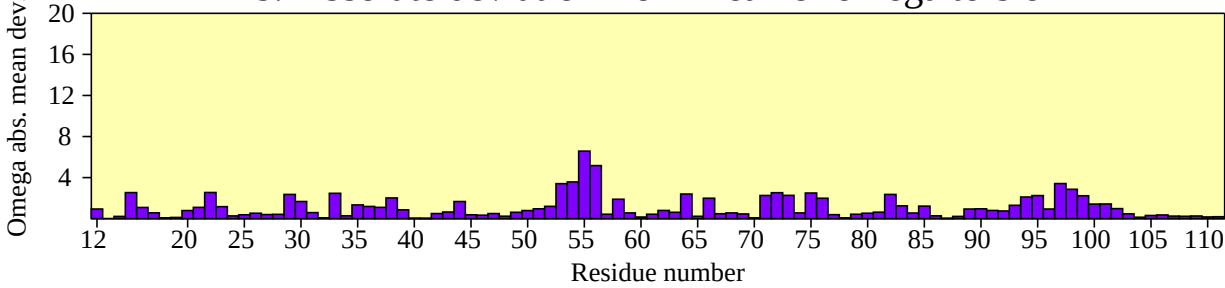
Residue properties

pdb1zrt

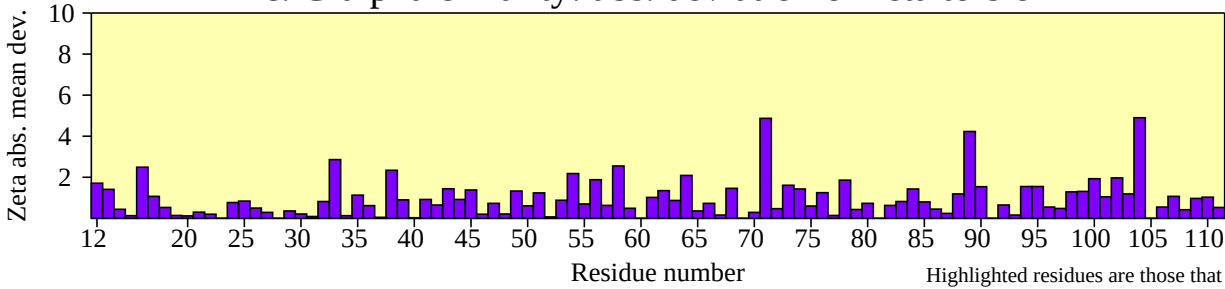
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

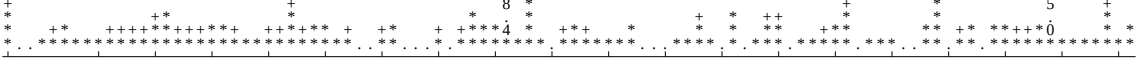
d. Secondary structure & estimated accessibility



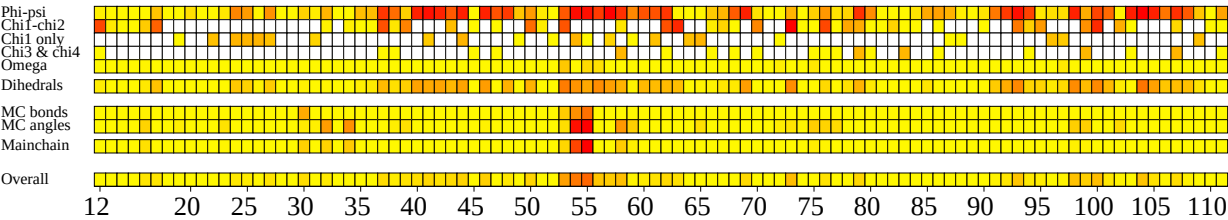
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



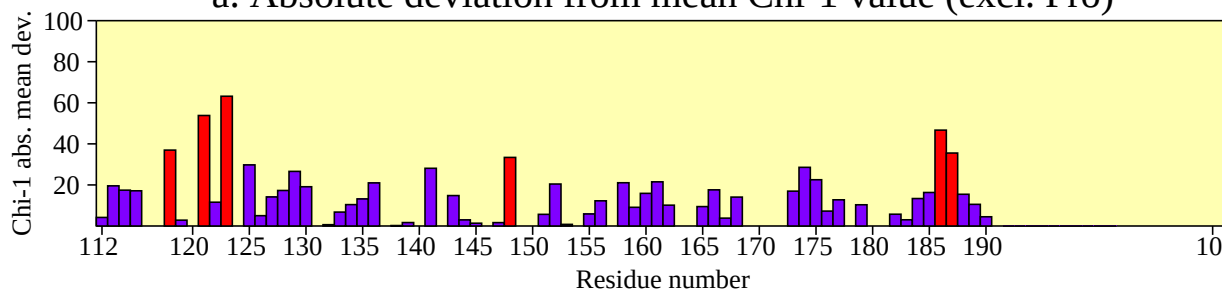
g. G-factors



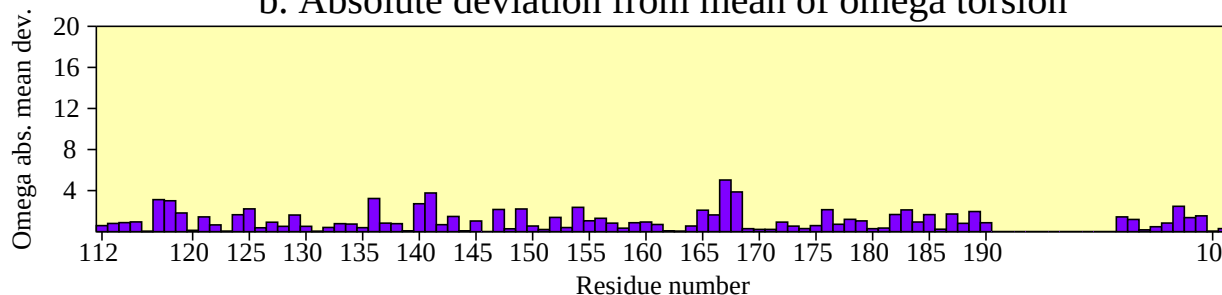
Residue properties

pdb1zrt

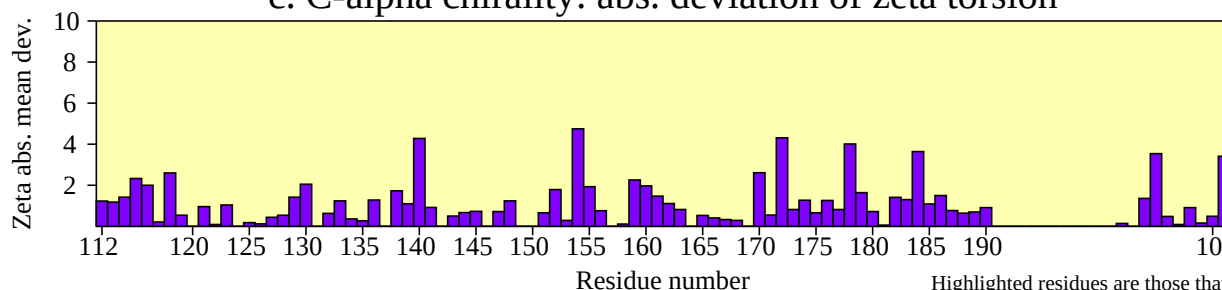
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

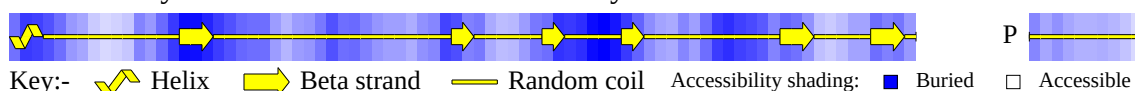


c. C-alpha chirality: abs. deviation of zeta torsion

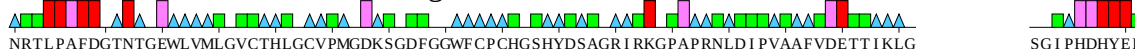


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

d. Secondary structure & estimated accessibility



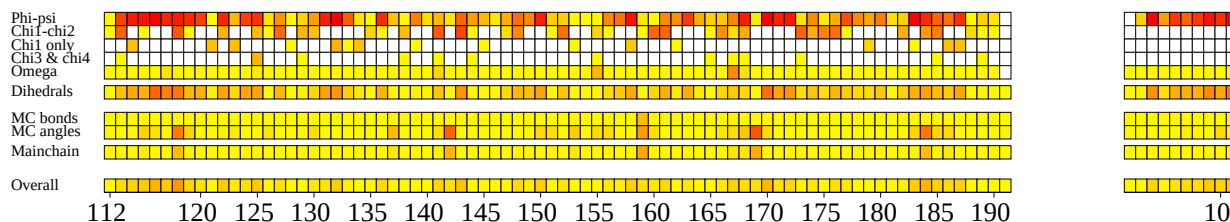
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



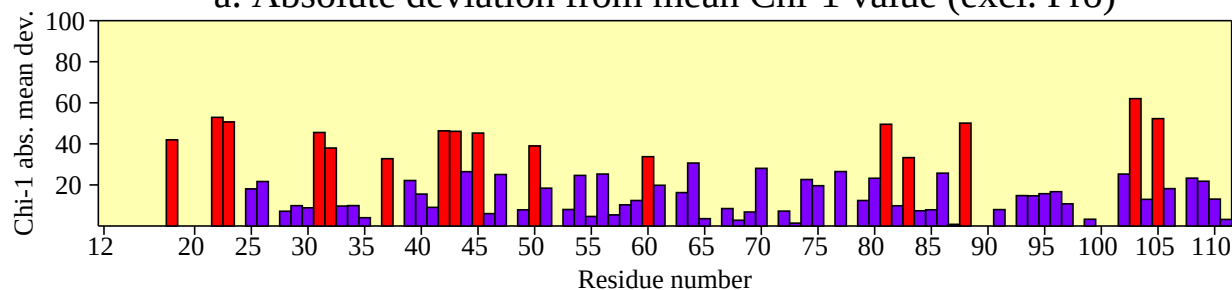
g. G-factors



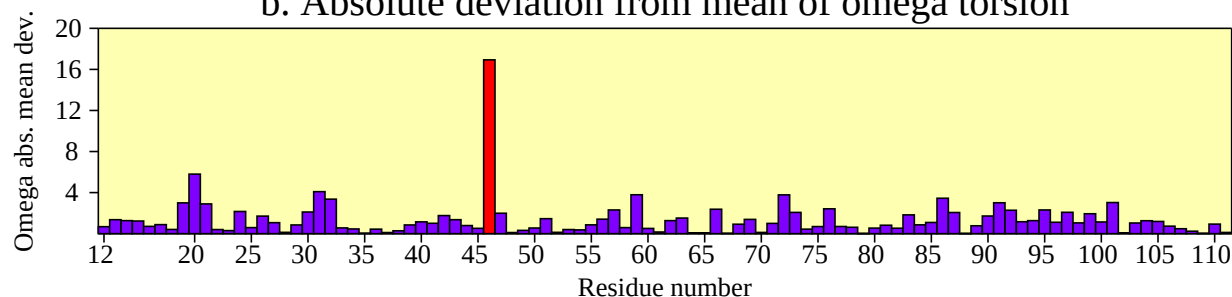
Residue properties

pdb1zrt

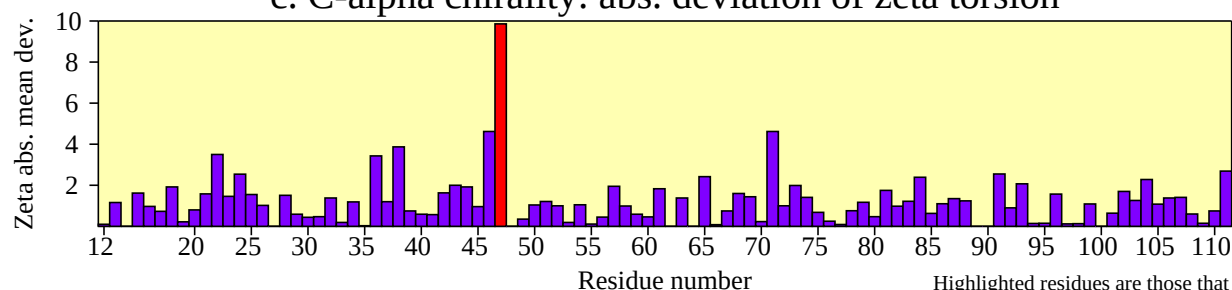
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

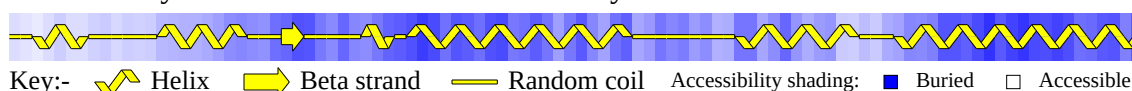


c. C-alpha chirality: abs. deviation of zeta torsion



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

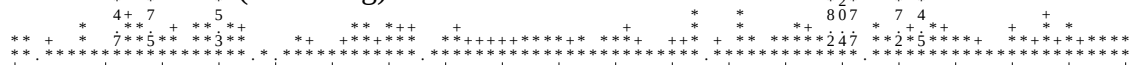
d. Secondary structure & estimated accessibility



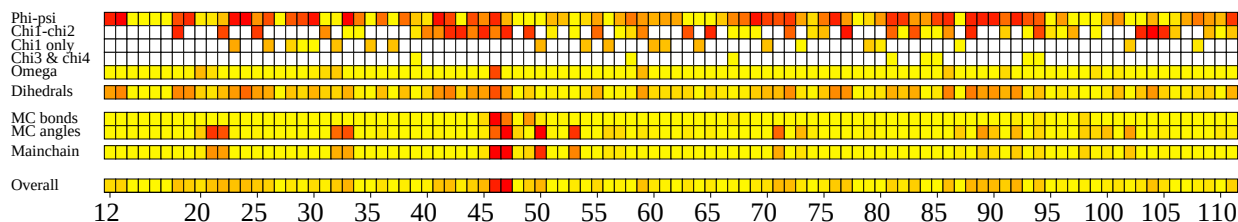
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



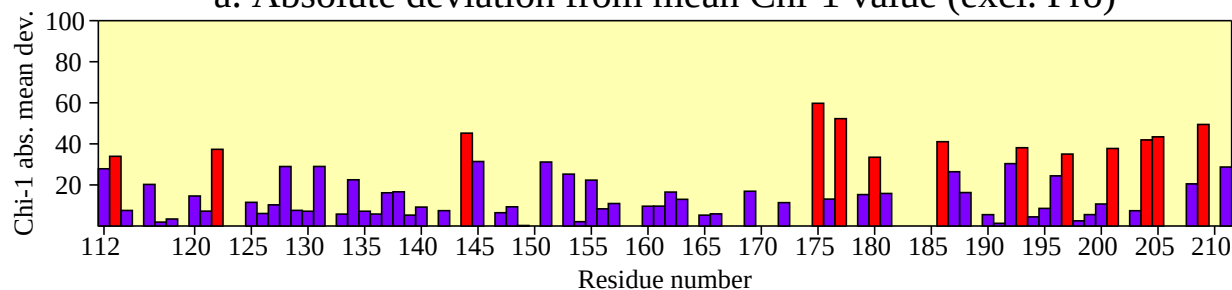
g. G-factors



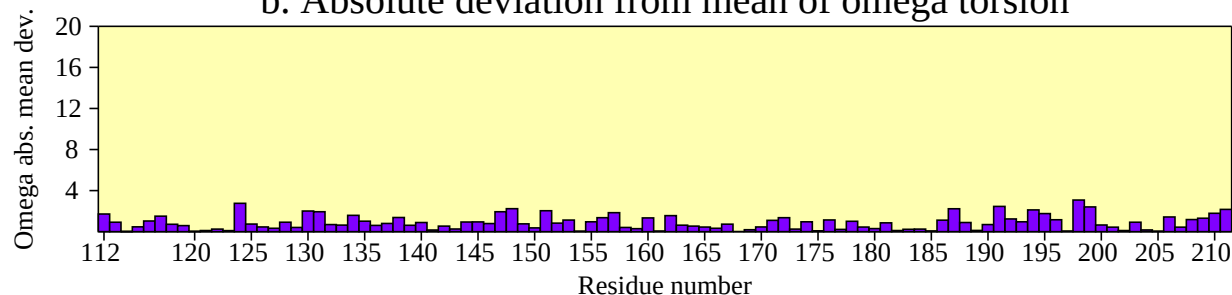
Residue properties

pdb1zrt

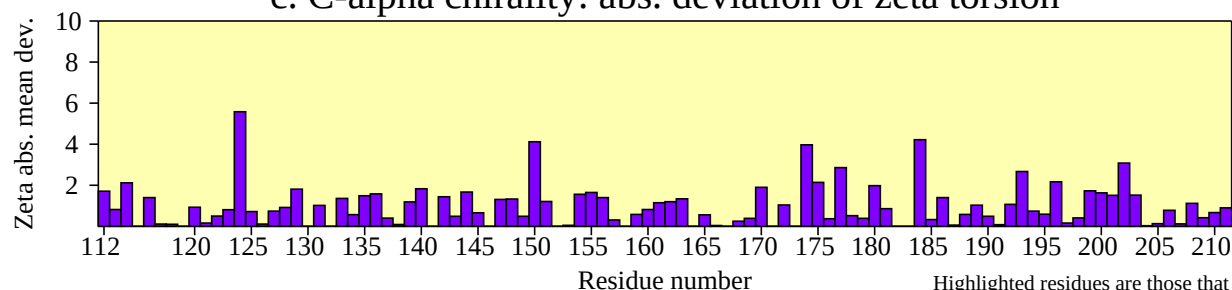
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

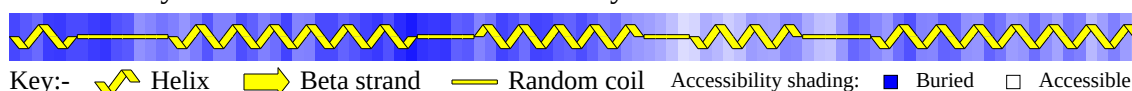


c. C-alpha chirality: abs. deviation of zeta torsion



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

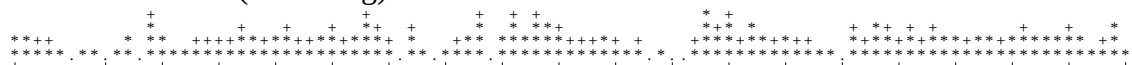
d. Secondary structure & estimated accessibility



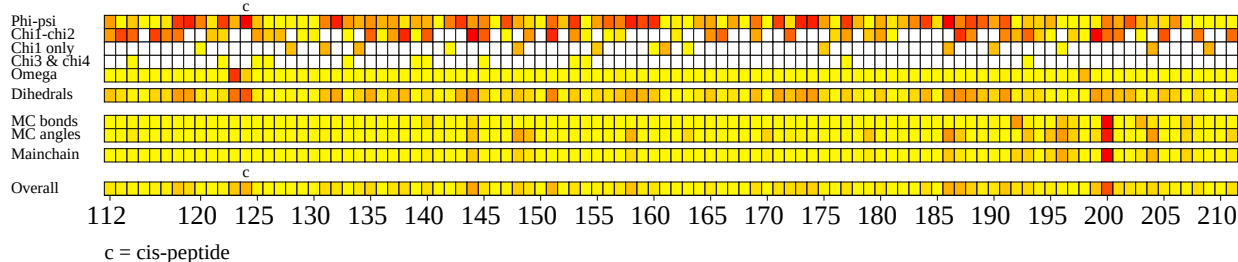
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



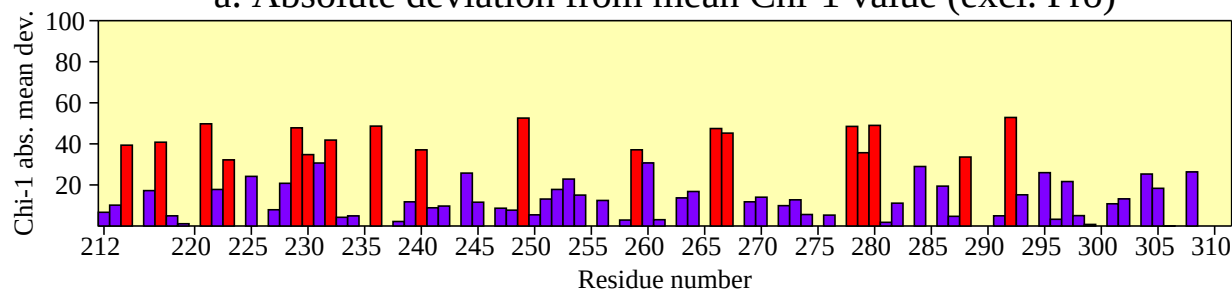
g. G-factors



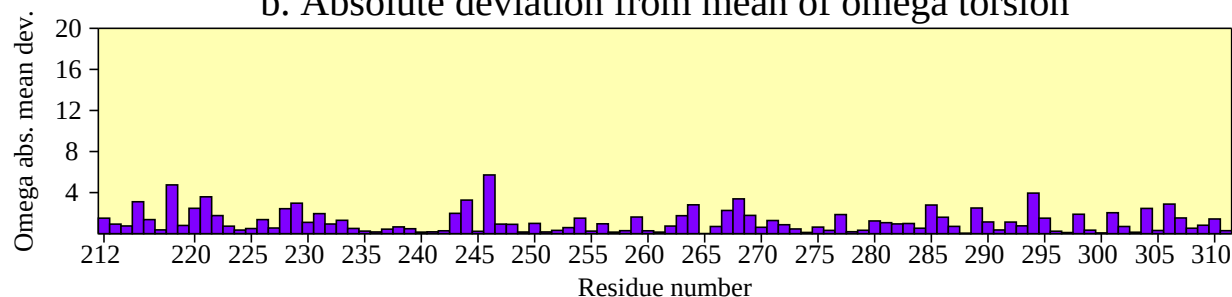
Residue properties

pdb1zrt

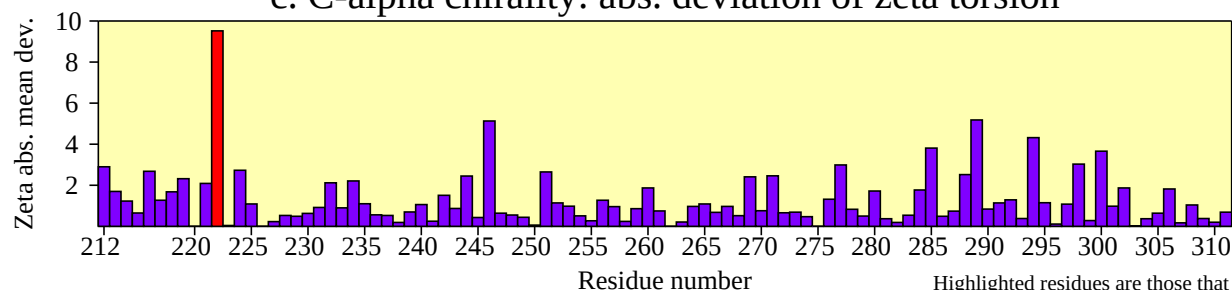
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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

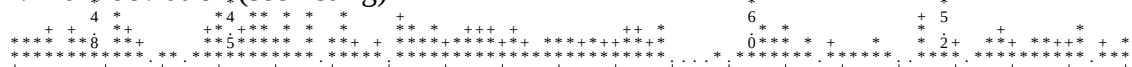


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

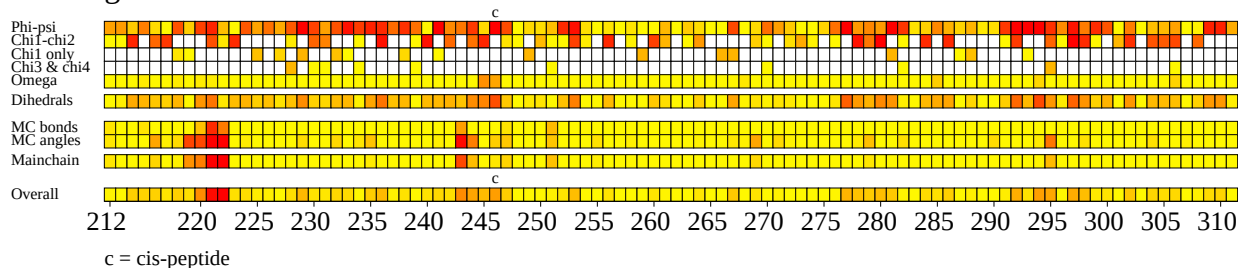
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



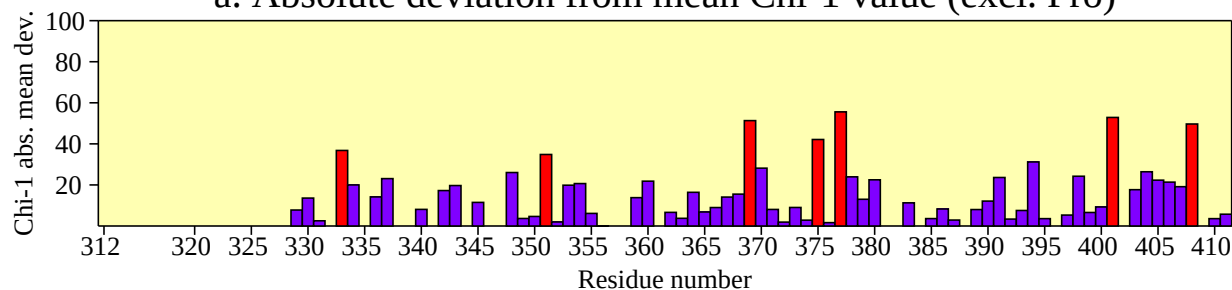
g. G-factors



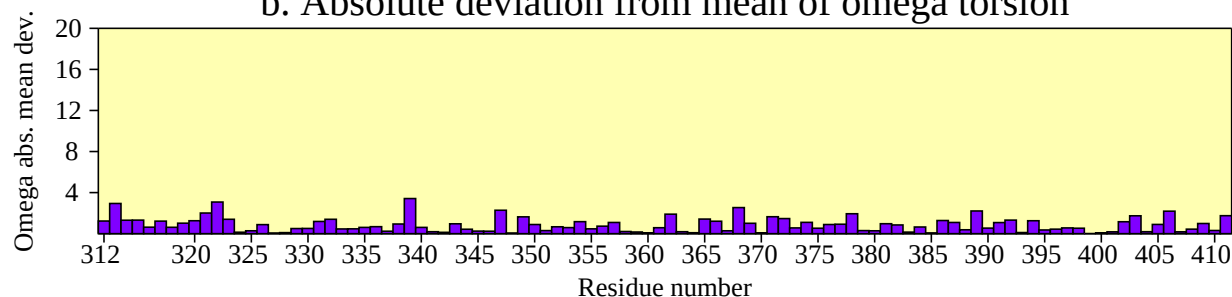
Residue properties

pdb1zrt

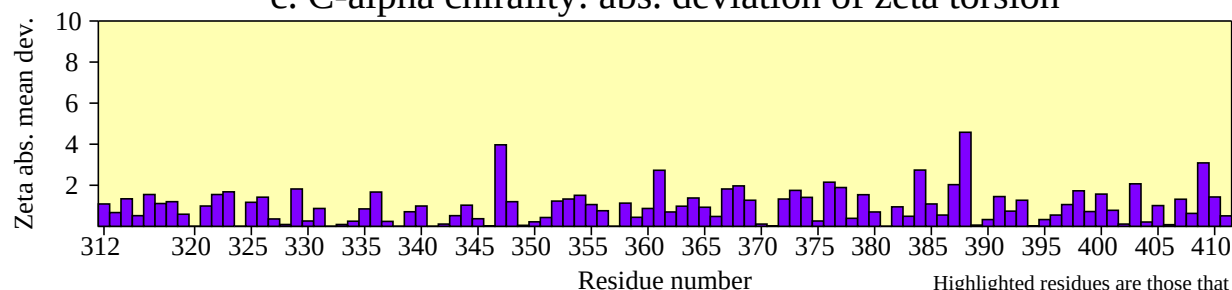
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

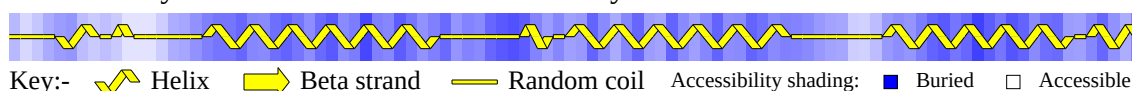


c. C-alpha chirality: abs. deviation of zeta torsion



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

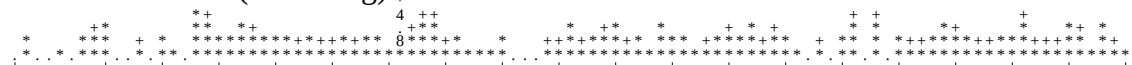
d. Secondary structure & estimated accessibility



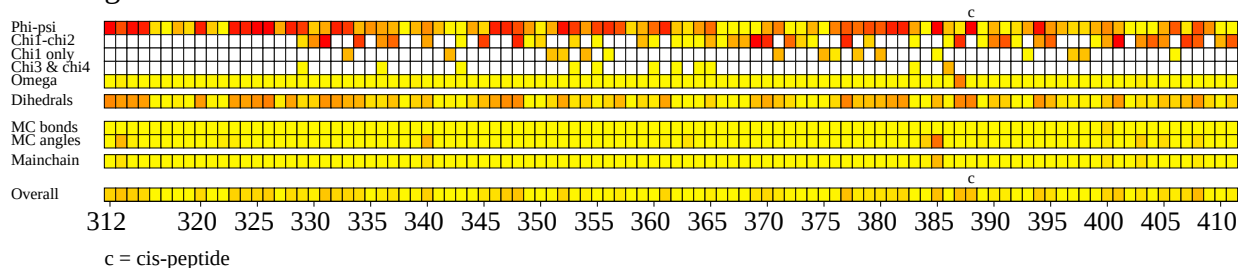
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



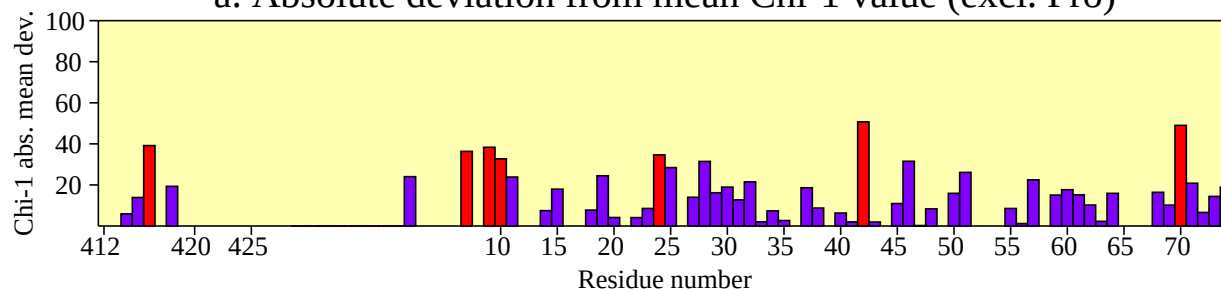
g. G-factors



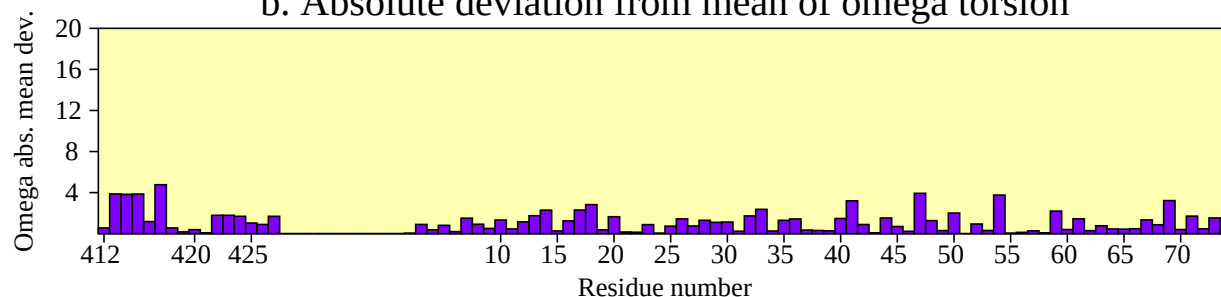
Residue properties

pdb1zrt

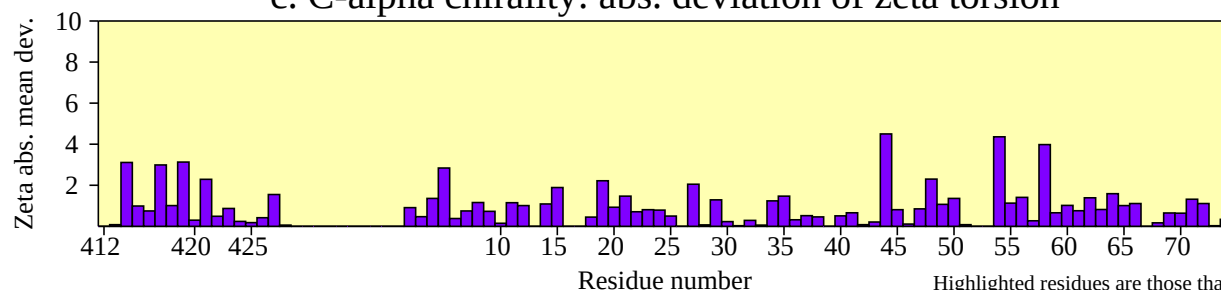
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

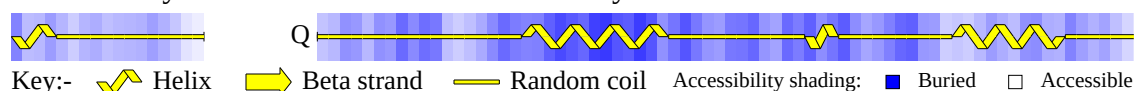


c. C-alpha chirality: abs. deviation of zeta torsion



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

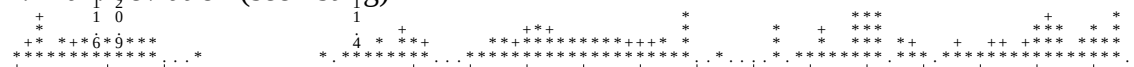
d. Secondary structure & estimated accessibility



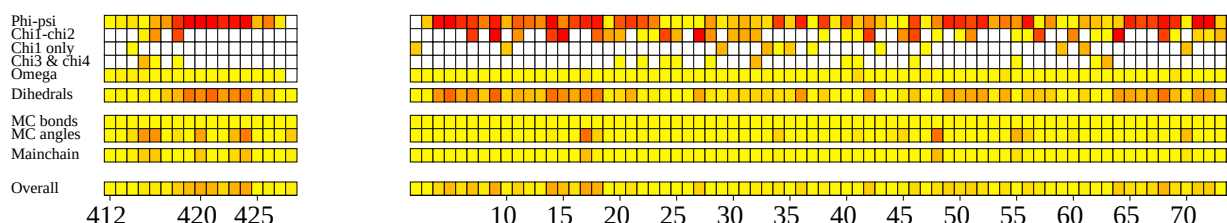
e. Sequence & Ramachandran regions



f. Max* deviation (see listing)



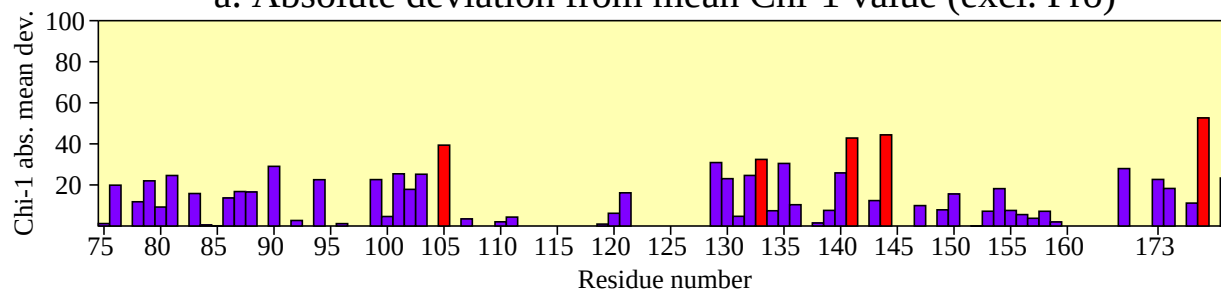
g. G-factors



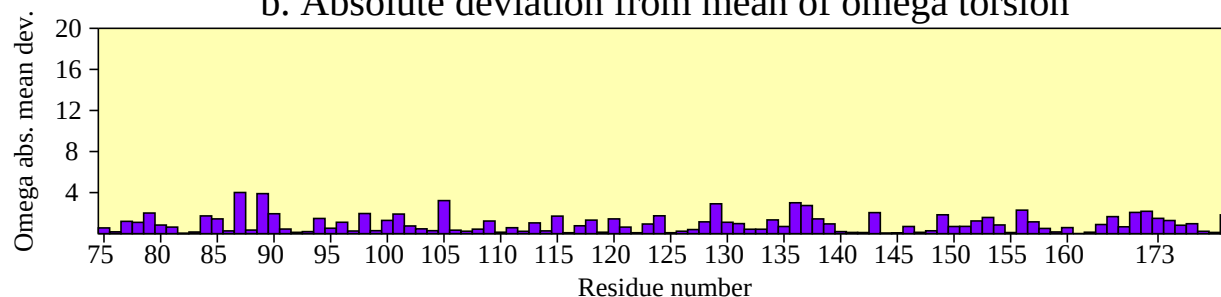
Residue properties

pdb1zrt

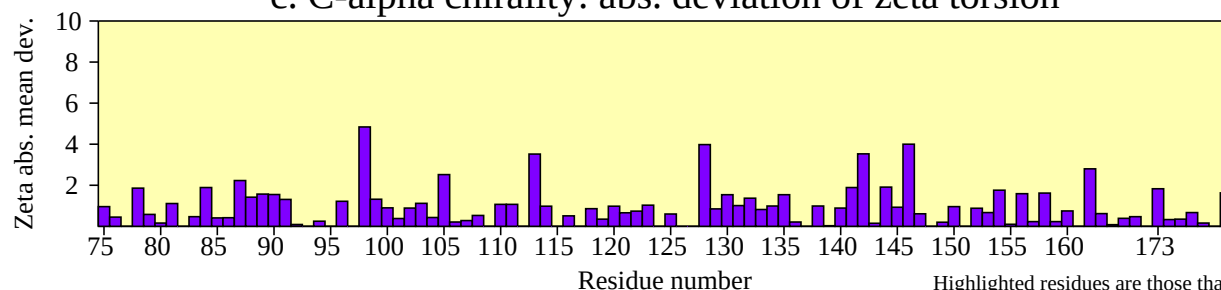
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

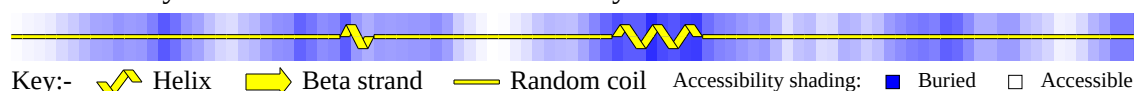


c. C-alpha chirality: abs. deviation of zeta torsion



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

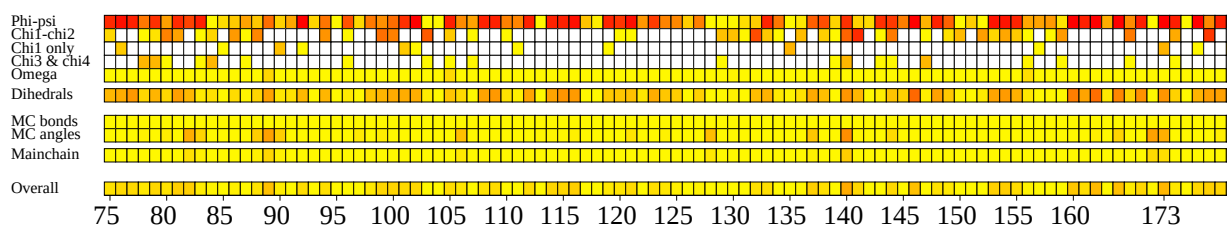
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



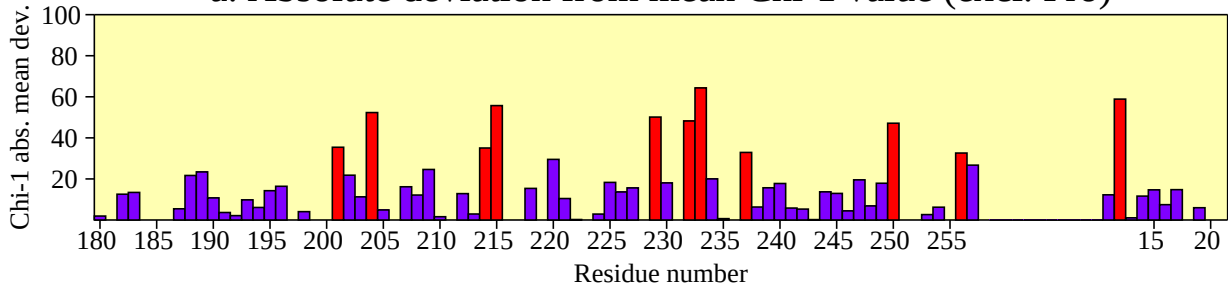
g. G-factors



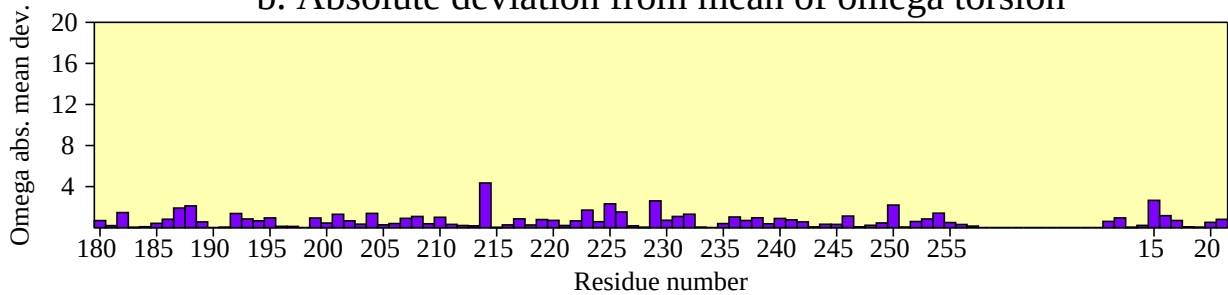
Residue properties

pdb1zrt

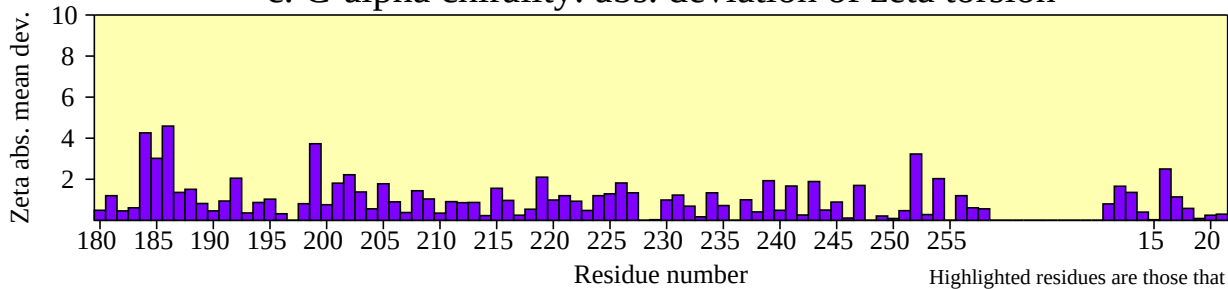
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

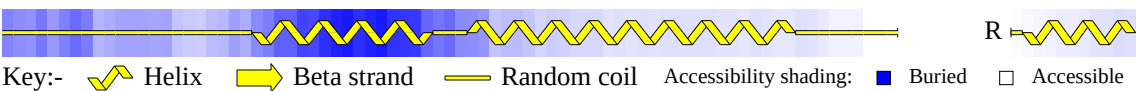


c. C-alpha chirality: abs. deviation of zeta torsion



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

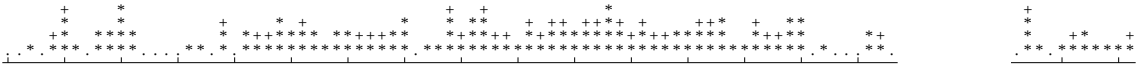
d. Secondary structure & estimated accessibility



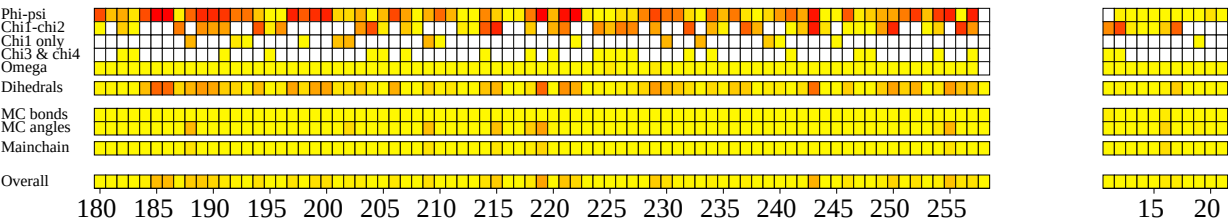
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



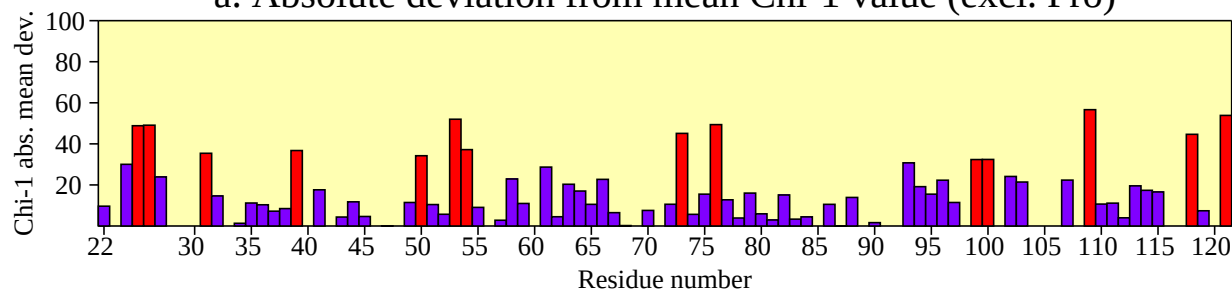
g. G-factors



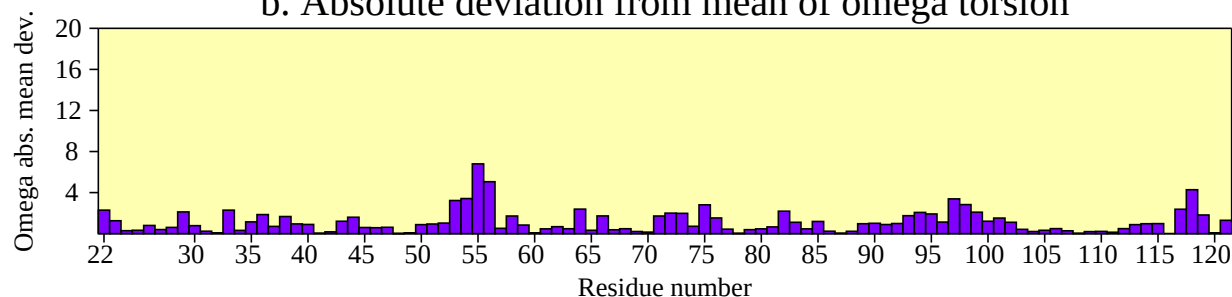
Residue properties

pdb1zrt

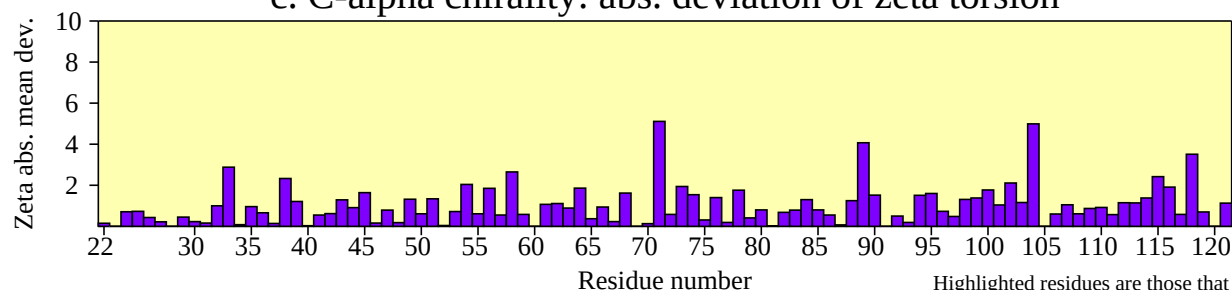
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

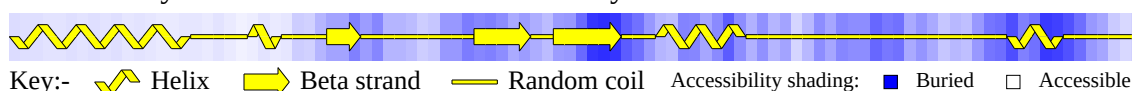


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

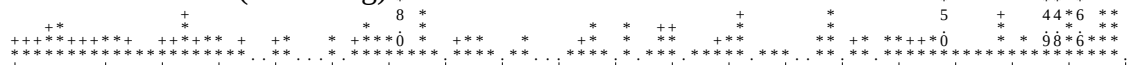


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

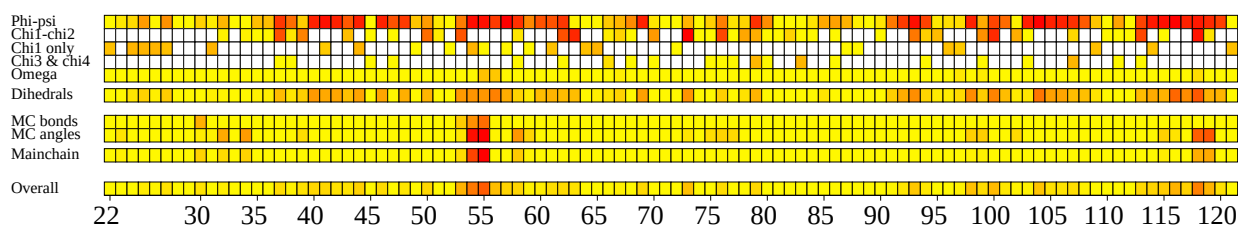
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



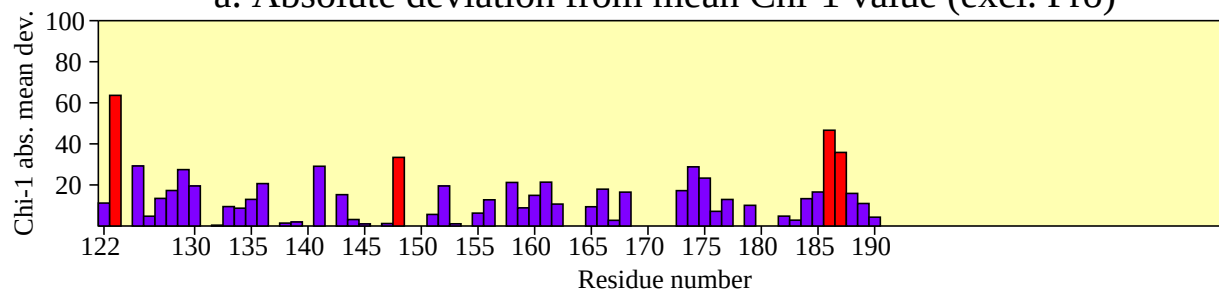
g. G-factors



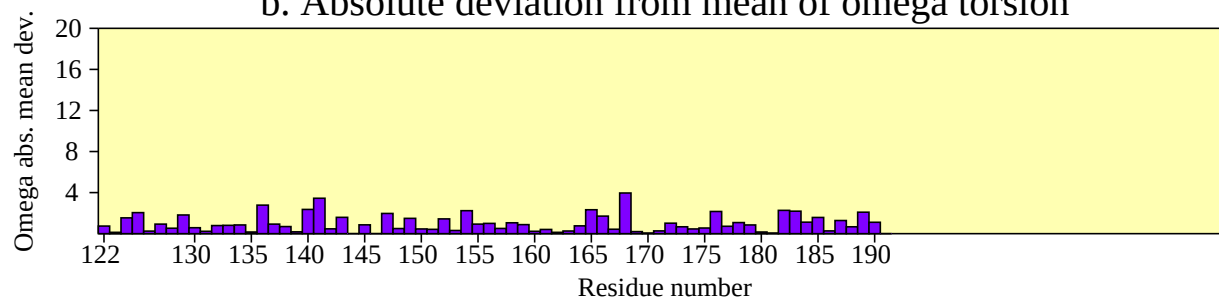
Residue properties

pdb1zrt

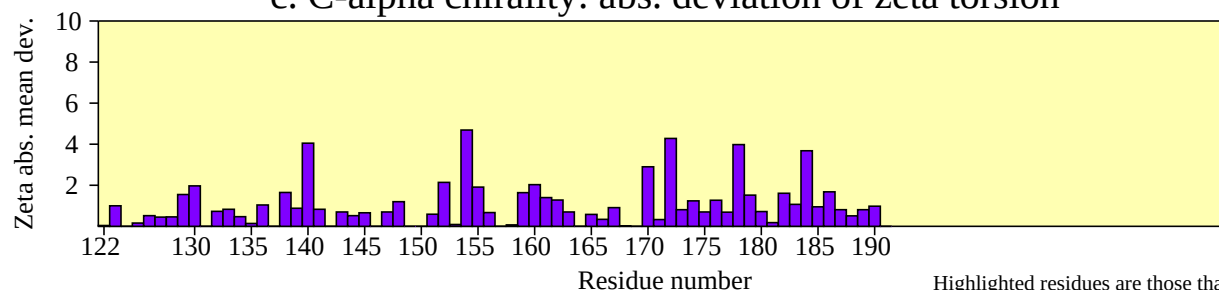
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

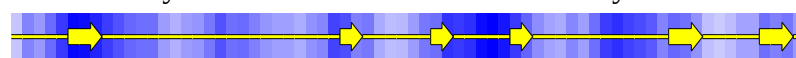


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility

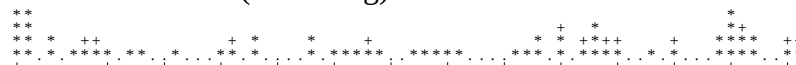


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

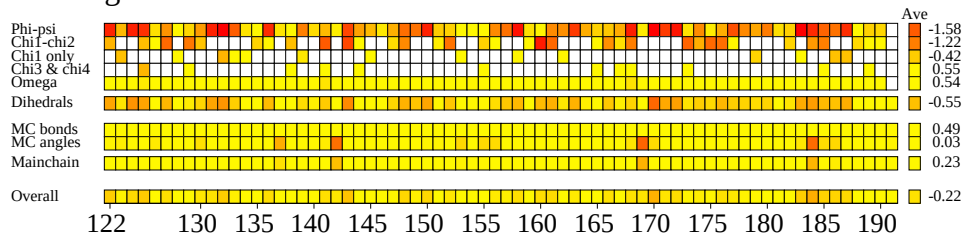
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

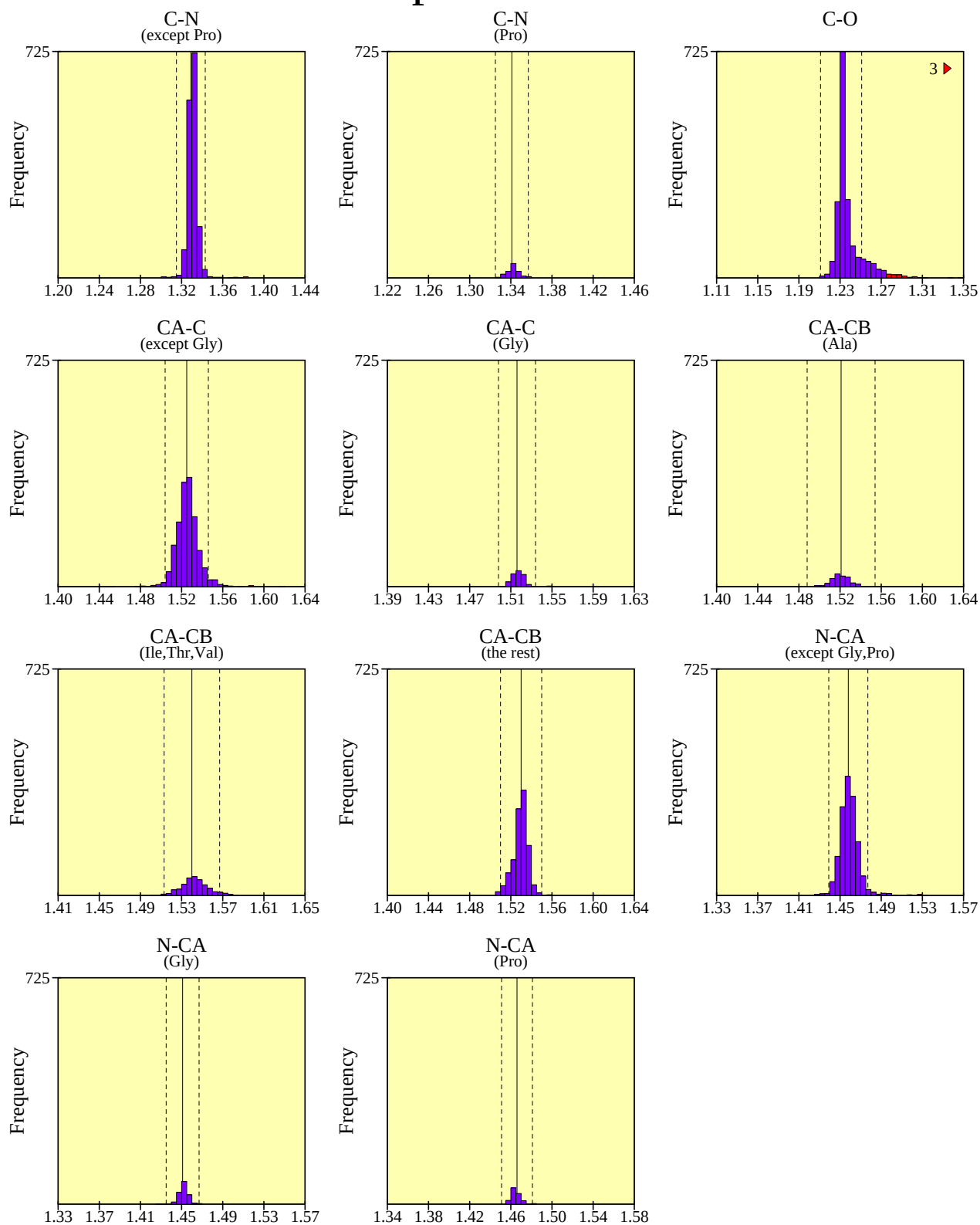


g. G-factors



Main-chain bond lengths

pdb1zrt



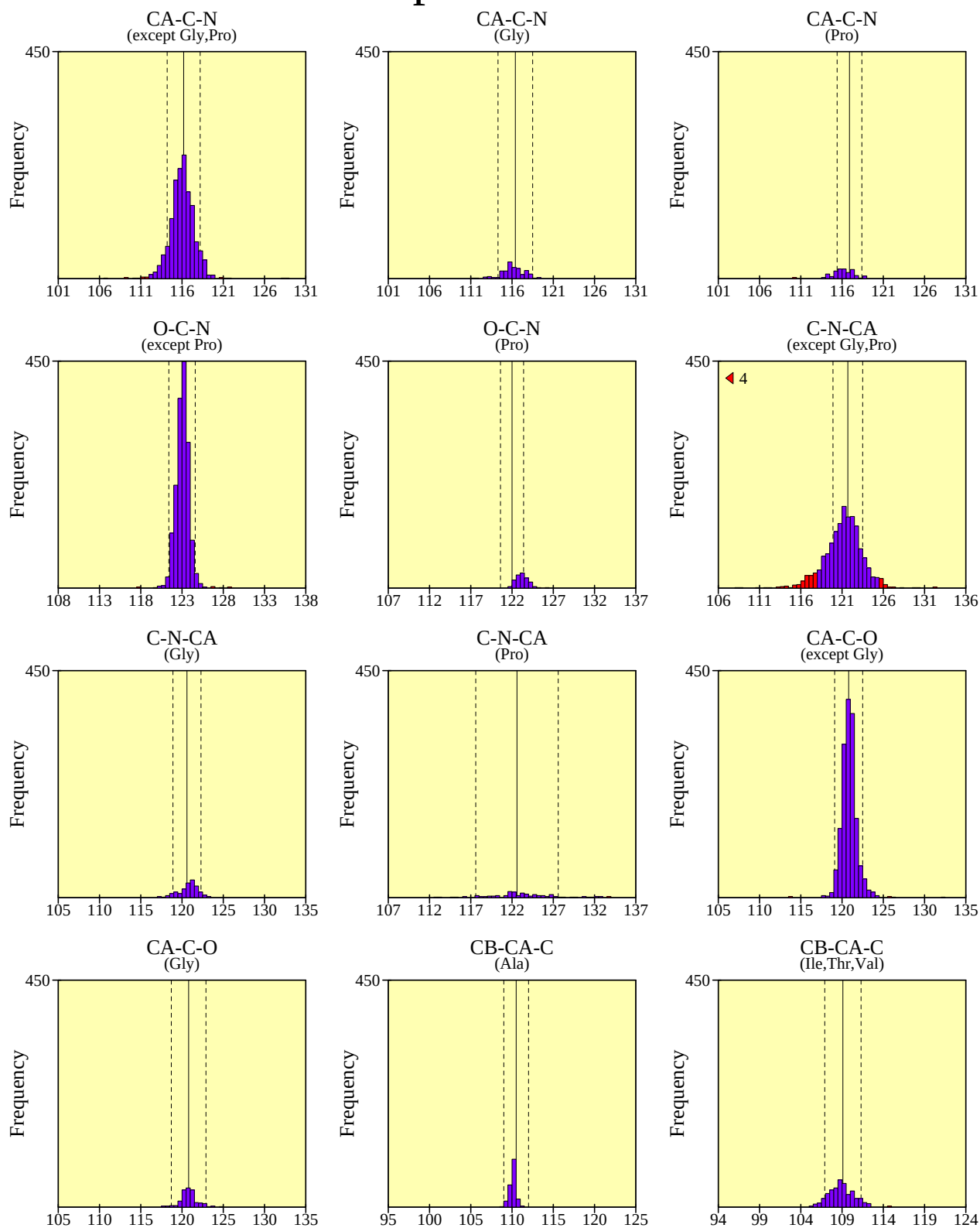
Black bars > 2.0 st. devs. from mean.

◀ 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

pdb1zrt



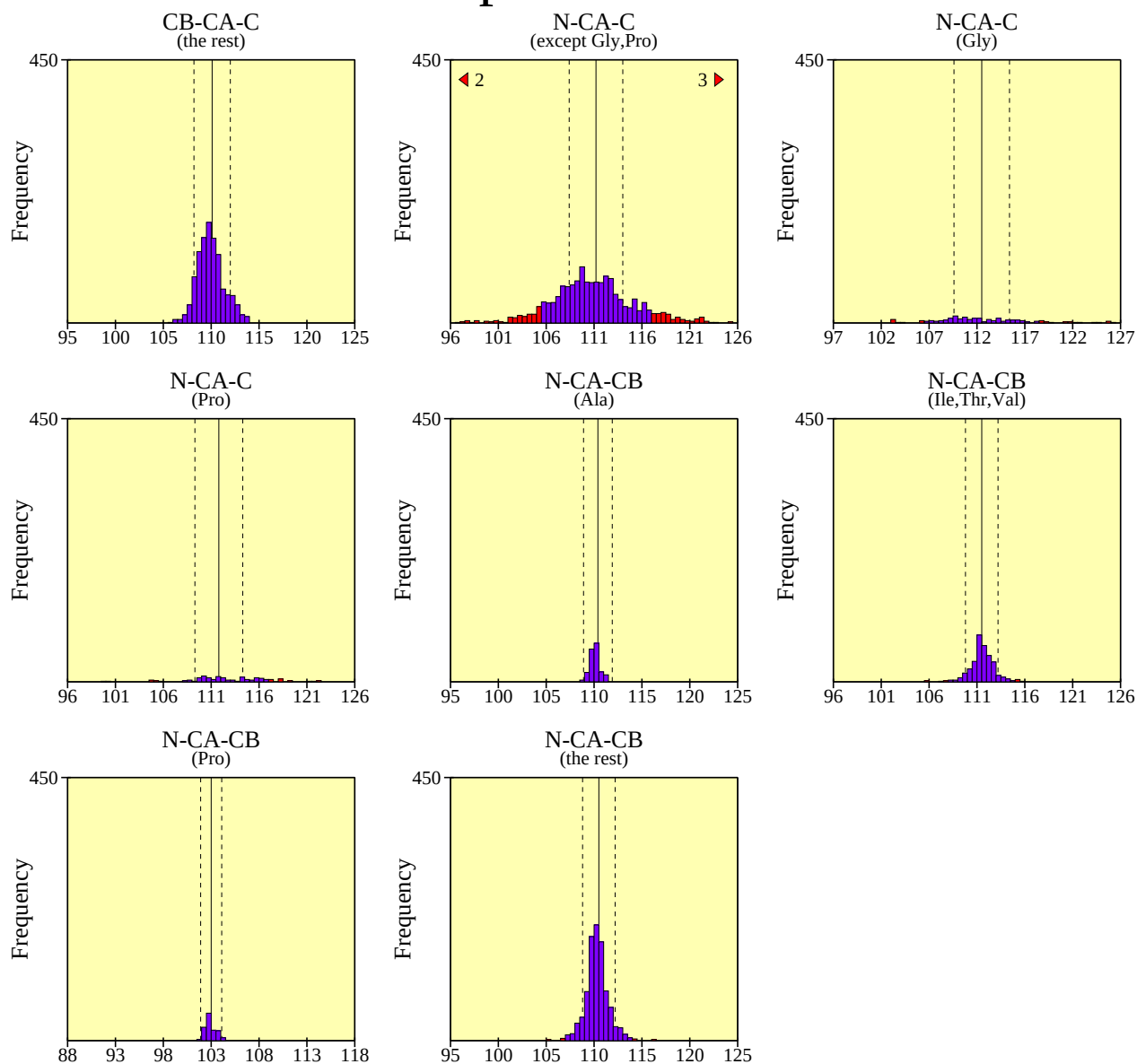
Black bars > 2.0 st. devs. from mean.

◀ 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

pdb1zrt



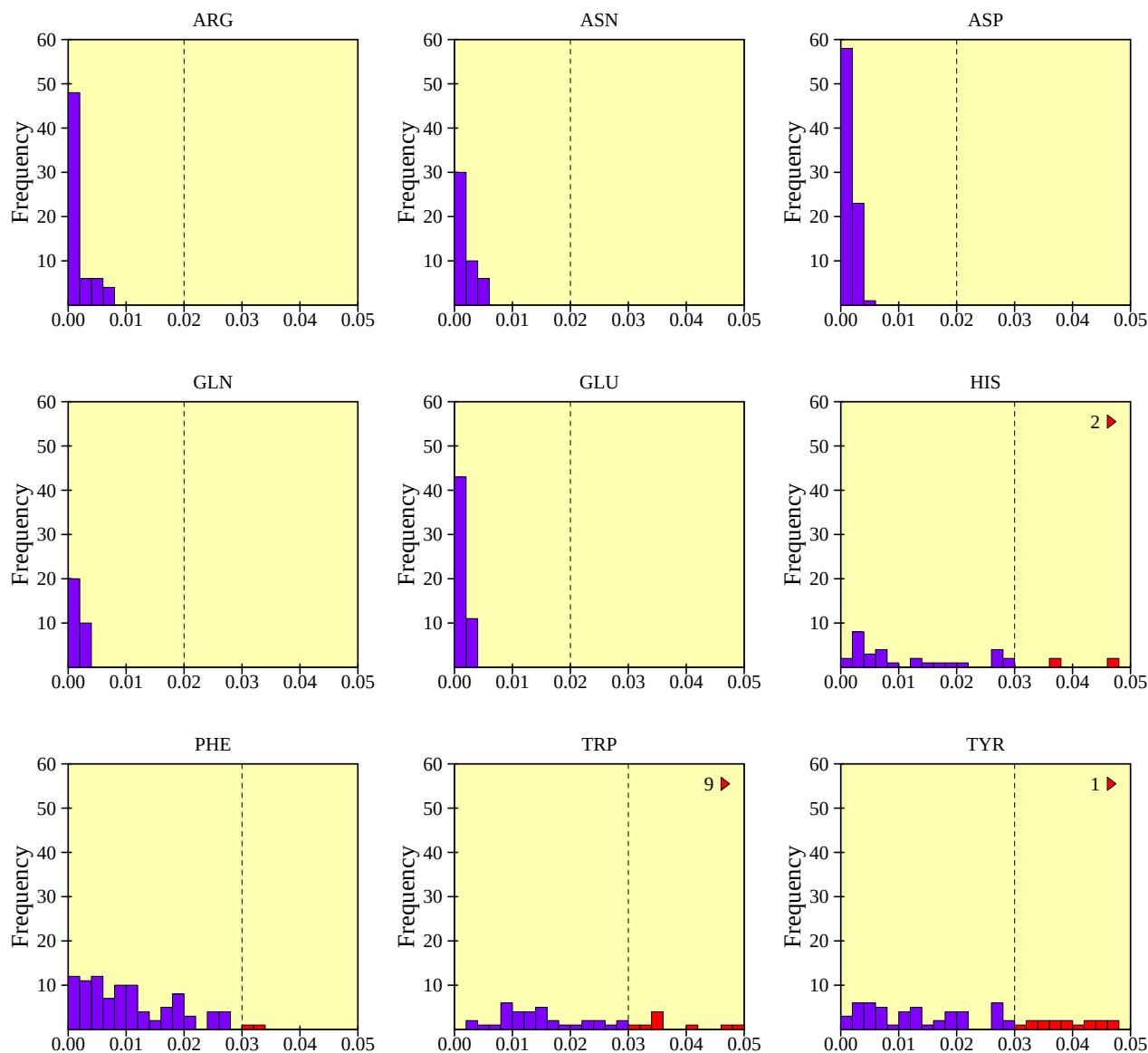
Black bars > 2.0 st. devs. from mean.

◀ 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

pdb1zrt



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

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

Distorted geometry

pdb1zrt

Main-chain bond lengths

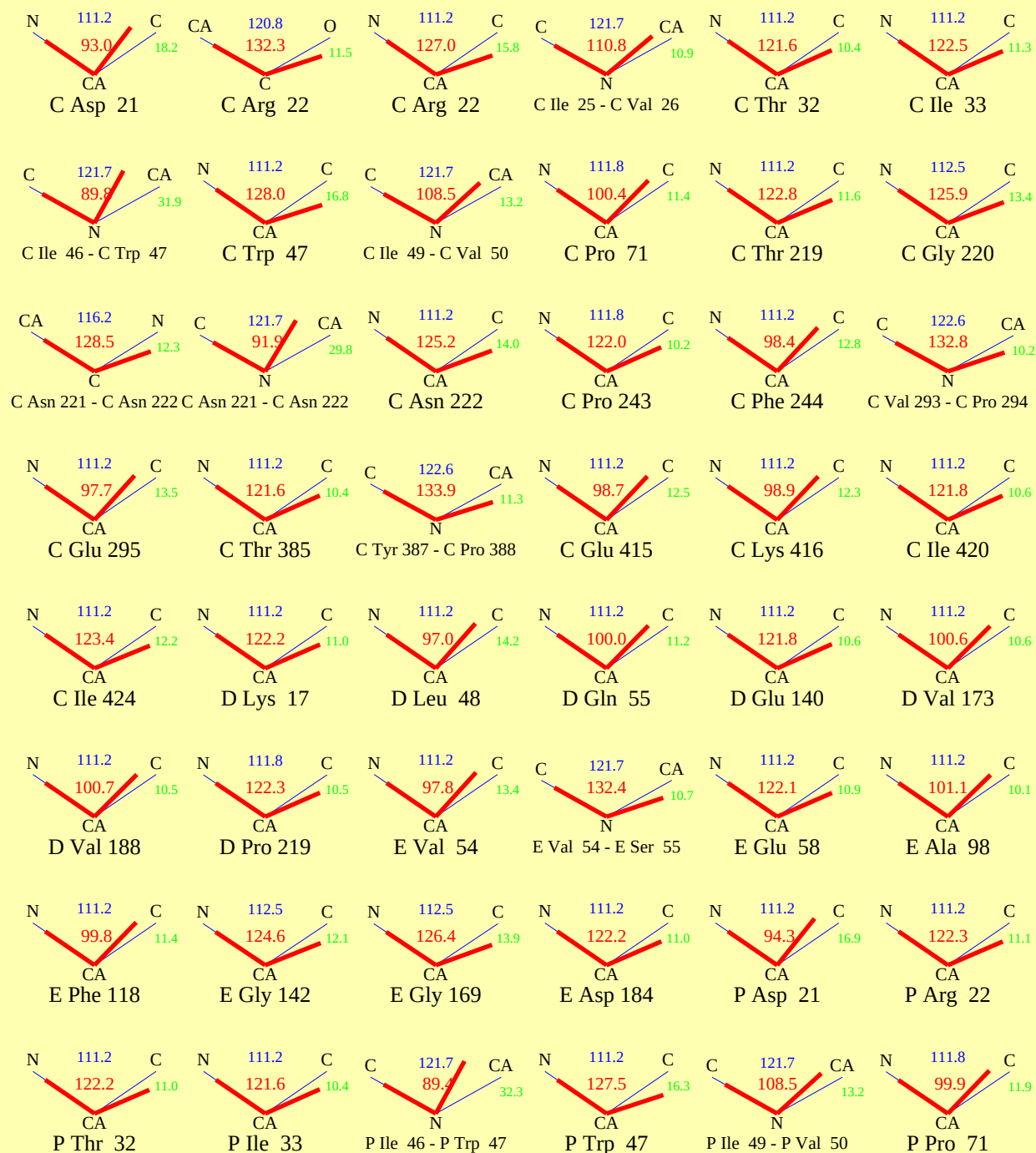
C 1.231 O 0.138 1.369 C Arg 22	CA 1.525 C 0.094 1.619 C Arg 22	C 1.231 O 0.077 1.308 C Ile 25	C 1.231 O 0.055 1.286 C Val 26	CA 1.525 C 0.063 1.588 C Val 26	C 1.231 O 0.124 1.355 C Ile 46
C 1.329 N 0.052 1.381 C Ile 46 - C Trp 47	C 1.231 O 0.055 1.286 C Trp 47	N 1.458 CA 0.060 1.518 C Trp 47	C 1.231 O 0.071 1.302 C Ile 49	CA 1.525 C 0.052 1.577 C Met 67	C 1.231 O 0.051 1.282 C Arg 94
C 1.231 O 0.059 1.290 C Ala 98	C 1.231 O 0.063 1.294 C Asn 192	C 1.231 O 0.106 1.337 C Leu 200	CA 1.525 C 0.060 1.585 C Leu 200	C 1.231 O 0.068 1.299 C Phe 203	C 1.231 O 0.056 1.287 C Ala 215
N 1.458 CA 0.069 1.527 C Asn 221	N 1.458 CA 0.072 1.530 C Asn 222	C 1.231 O 0.080 1.311 C Pro 243	C 1.231 O 0.051 1.282 C Tyr 247	C 1.231 O 0.057 1.288 C Lys 251	C 1.231 O 0.056 1.287 C Trp 400
C 1.231 O 0.053 1.284 D Gln 226	C 1.231 O 0.062 1.293 D Met 234	C 1.231 O 0.052 1.283 D Leu 237	C 1.231 O 0.057 1.288 E Ala 30	C 1.231 O 0.062 1.293 E Asp 53	CA 1.525 C 0.074 1.451 E Ser 55
C 1.231 O 0.056 1.287 E His 159	C 1.231 O 0.121 1.352 P Ile 46	C 1.329 N 0.052 1.381 P Ile 46 - P Trp 47	C 1.231 O 0.055 1.286 P Trp 47	N 1.458 CA 0.058 1.516 P Trp 47	C 1.231 O 0.072 1.303 P Ile 49
C 1.231 O 0.053 1.284 P Ala 98	C 1.231 O 0.052 1.283 P Met 140	C 1.231 O 0.071 1.302 P Asn 192	C 1.231 O 0.050 1.281 P Ser 196	C 1.231 O 0.119 1.350 P Leu 200	CA 1.525 C 0.065 1.590 P Leu 200
C 1.231 O 0.068 1.299 P Phe 203	C 1.231 O 0.051 1.282 P Ala 207	C 1.231 O 0.053 1.284 P Ala 215	N 1.458 CA 0.069 1.527 P Asn 221	C 1.329 N 0.052 1.381 P Asn 221 - P Asn 222	N 1.458 CA 0.075 1.533 P Asn 222
C 1.231 O 0.072 1.303 P Pro 243	C 1.231 O 0.051 1.282 P Tyr 247	C 1.231 O 0.055 1.286 P Lys 251	C 1.231 O 0.055 1.286 P Trp 400	C 1.231 O 0.060 1.291 R Ala 30	C 1.231 O 0.062 1.293 R Asp 53
CA 1.525 C 0.076 1.449 R Ser 55					

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

Distorted geometry

pdb1zrt

Main-chain bond angles



Distorted geometry

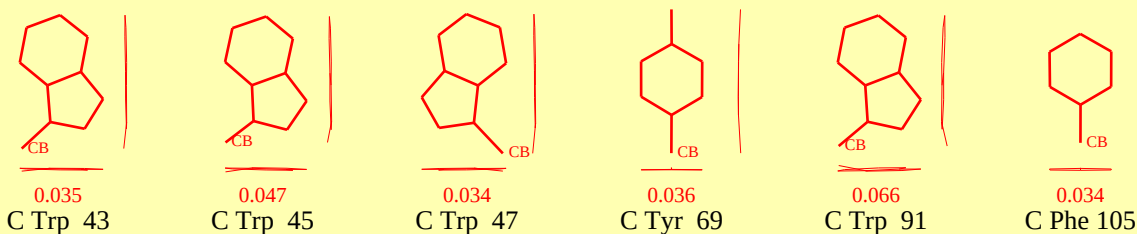
pdb1zrt

Main-chain bond angles (contd)



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

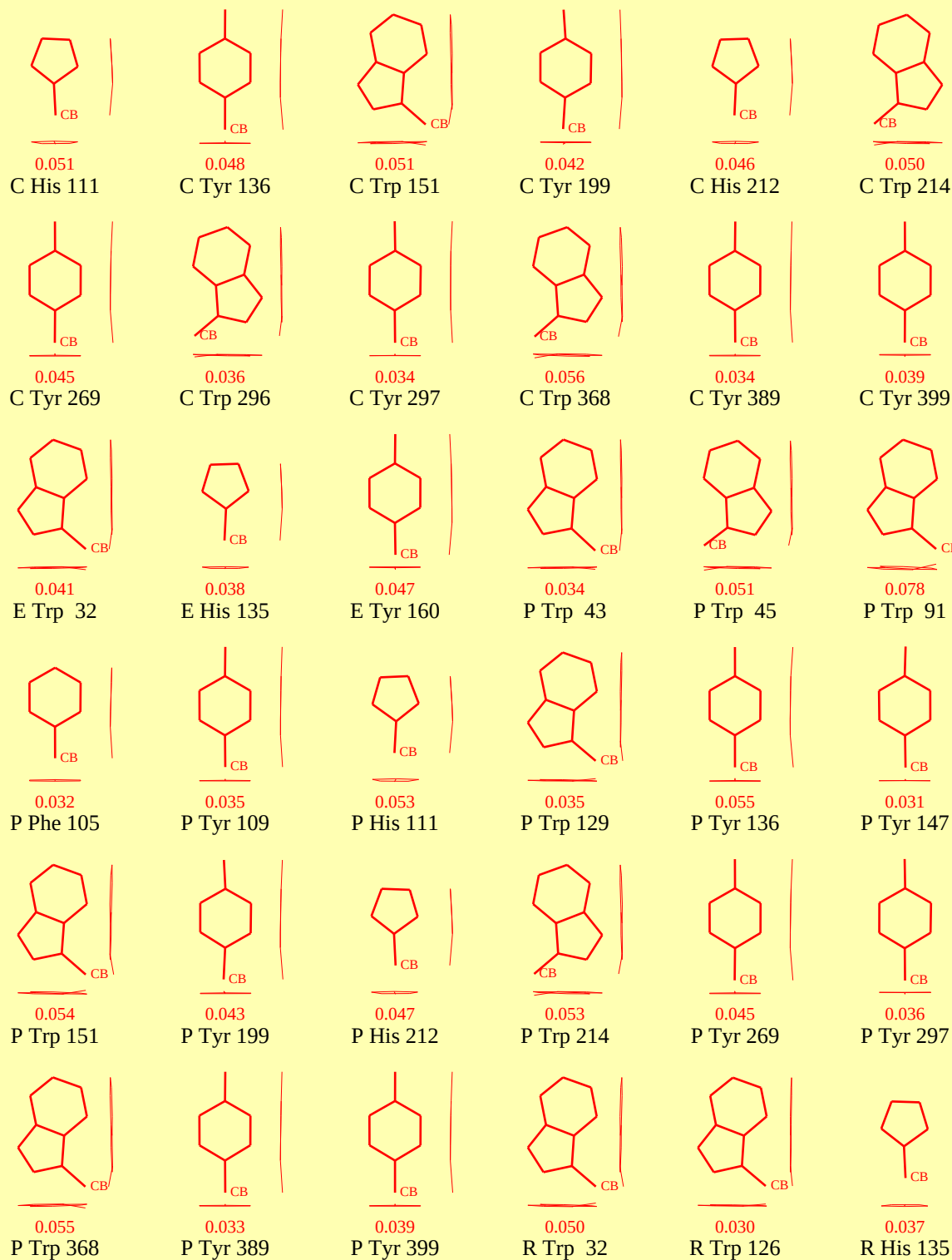
Planar groups



Distorted geometry

pdb1zrt

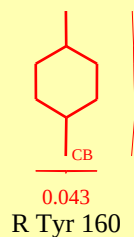
Planar groups (contd)



Distorted geometry

pdb1zrt

Planar groups (contd)



Sidechains with RMS dist. from planarity $> 0.03\text{\AA}$ for rings, or $> 0.02\text{\AA}$ otherwise. Value shown is RMS dist.