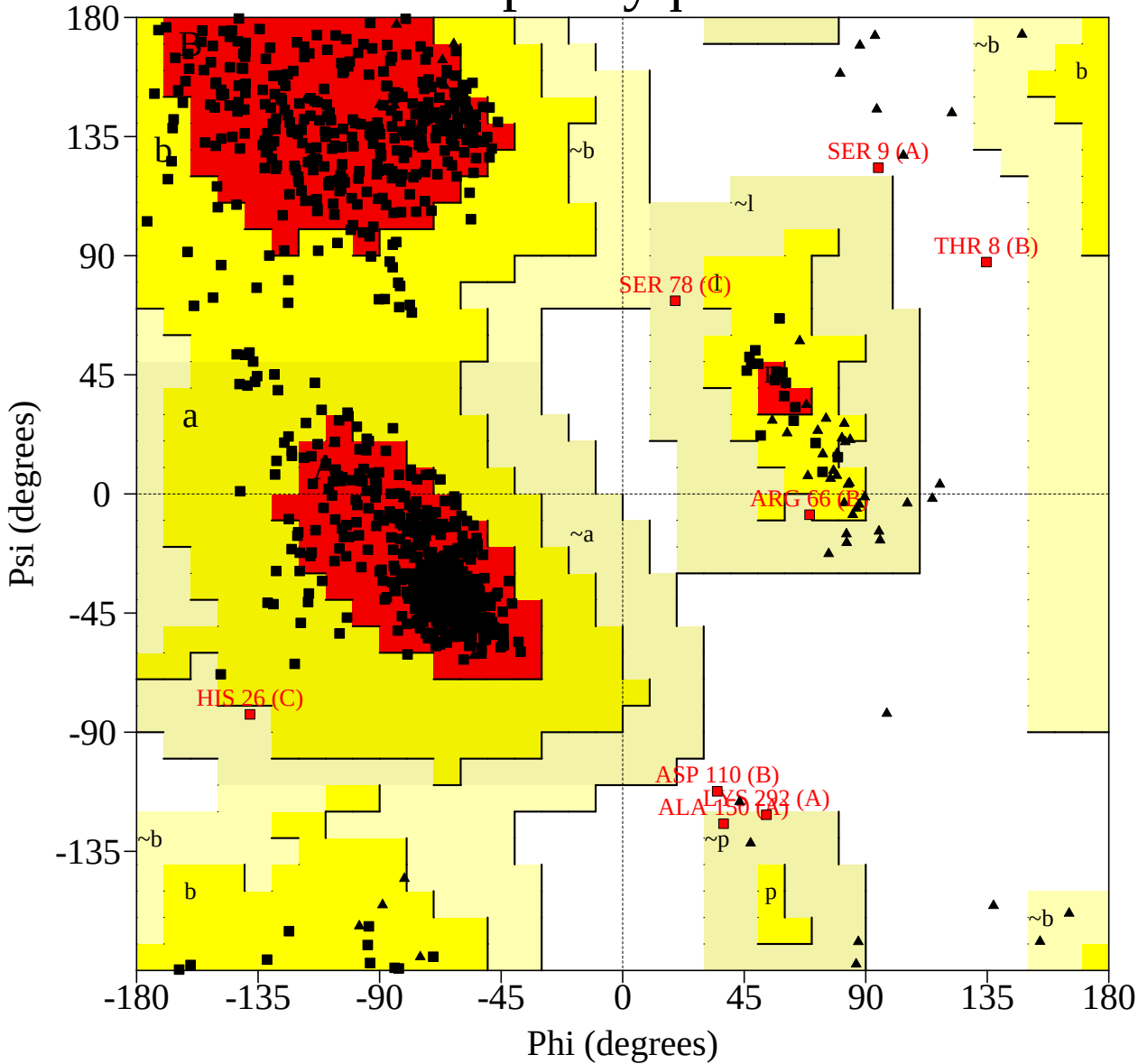


Ramachandran Plot

pdb1yq3



Plot statistics

Residues in most favoured regions [A,B,L]	842	88.6%
Residues in additional allowed regions [a,b,l,p]	100	10.5%
Residues in generously allowed regions [~a,~b,~l,~p]	5	0.5%
Residues in disallowed regions	3	0.3%

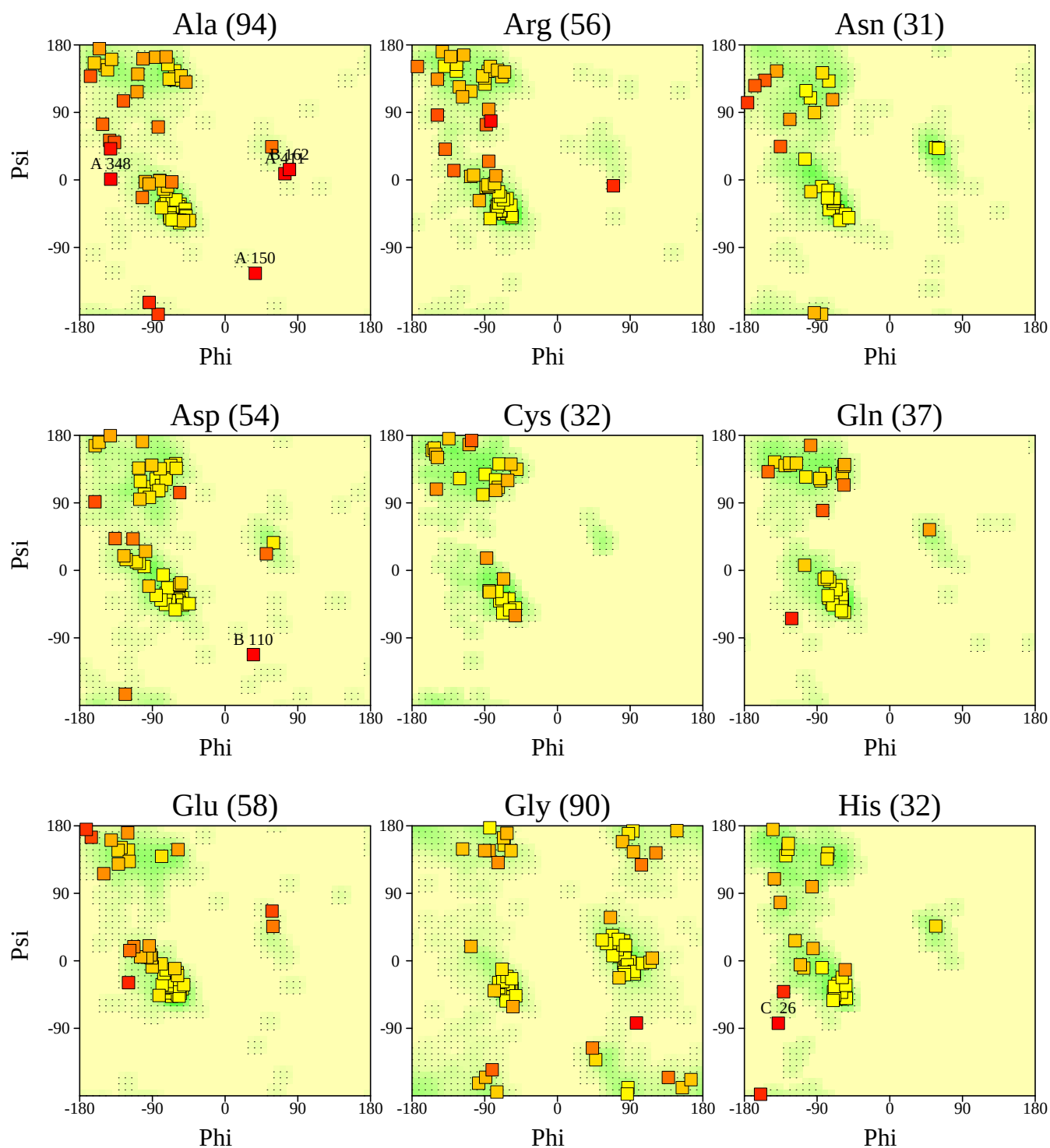
Number of non-glycine and non-proline residues	950	100.0%
Number of end-residues (excl. Gly and Pro)	8	
Number of glycine residues (shown as triangles)	90	
Number of proline residues	50	

Total number of residues	1098	

Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions.

Ramachandran plots for all residue types

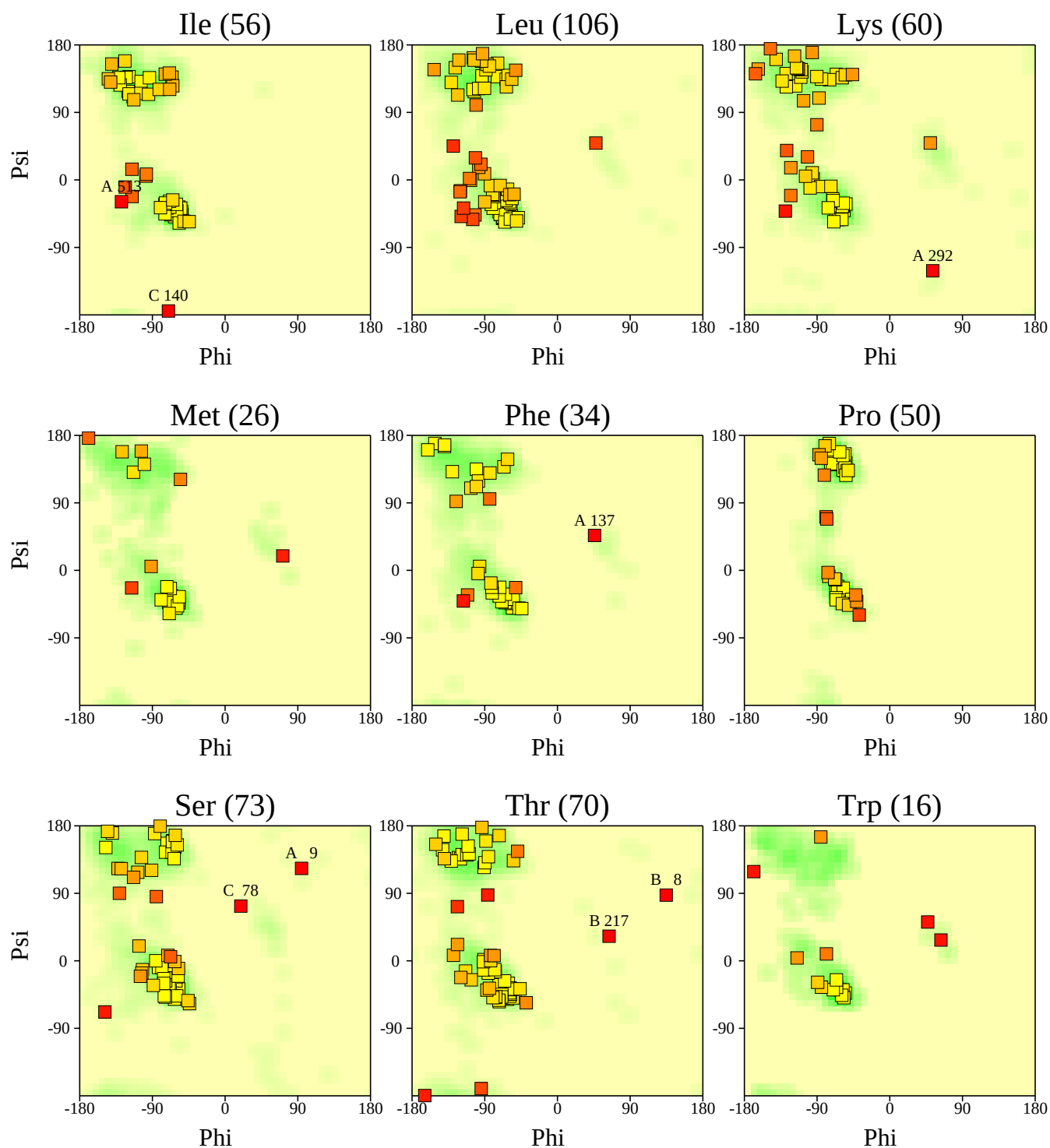
pdb1yq3



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

Ramachandran plots for all residue types

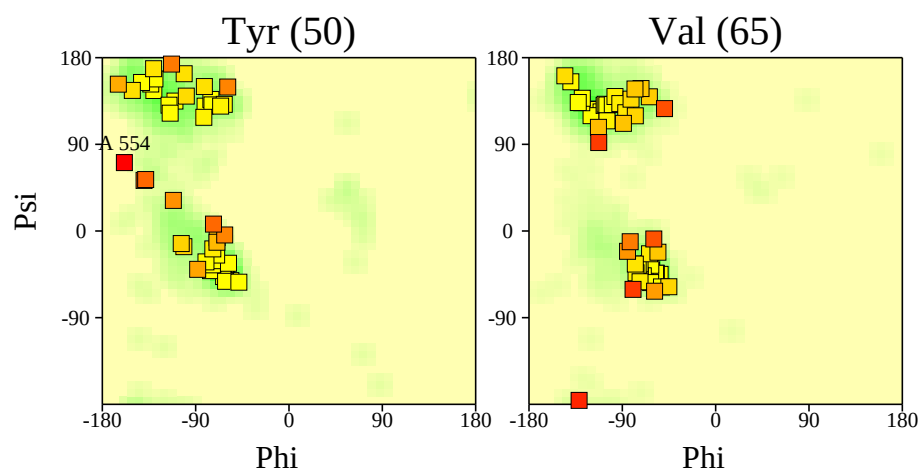
pdb1yq3



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

Ramachandran plots for all residue types

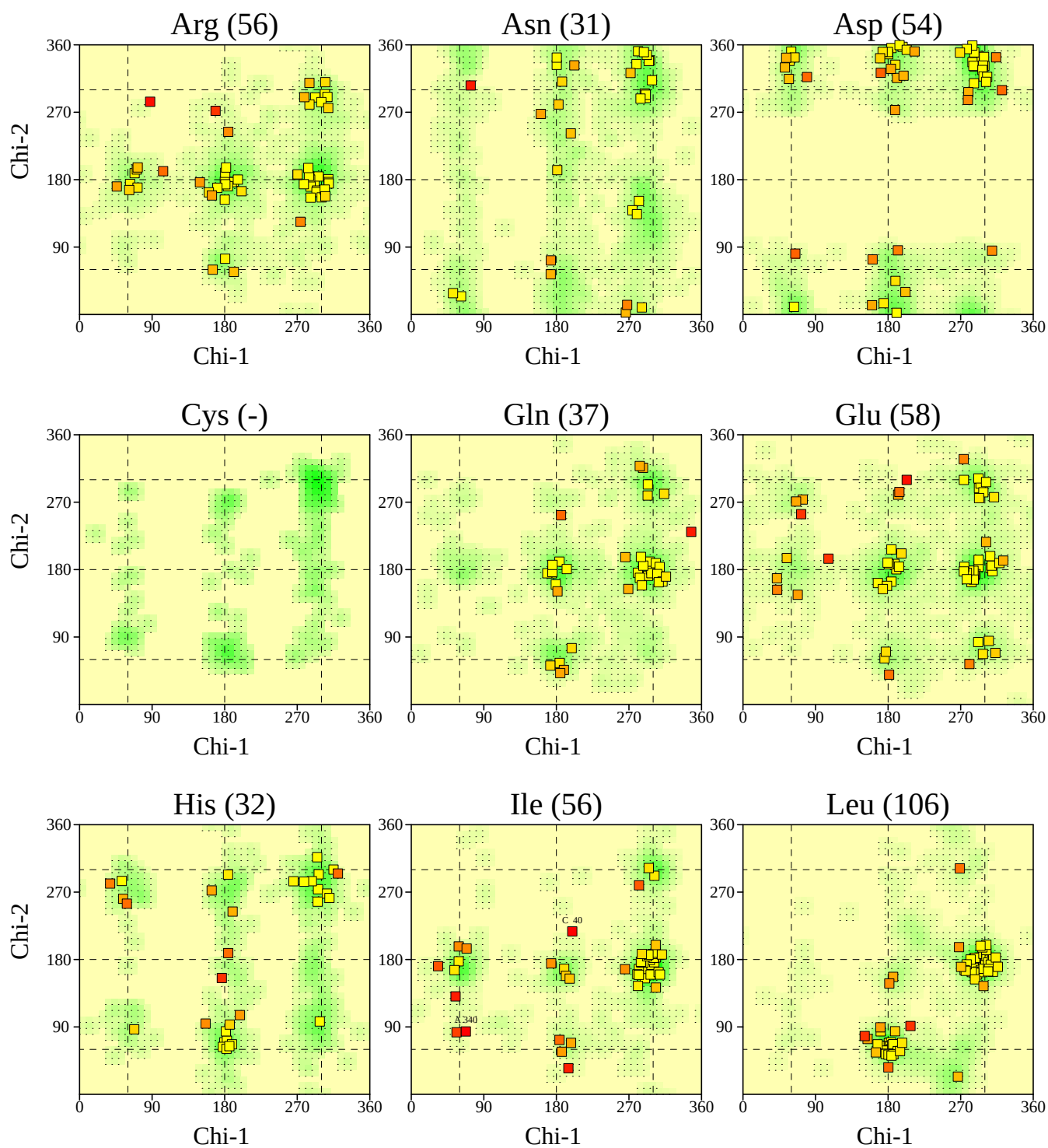
pdb1yq3



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

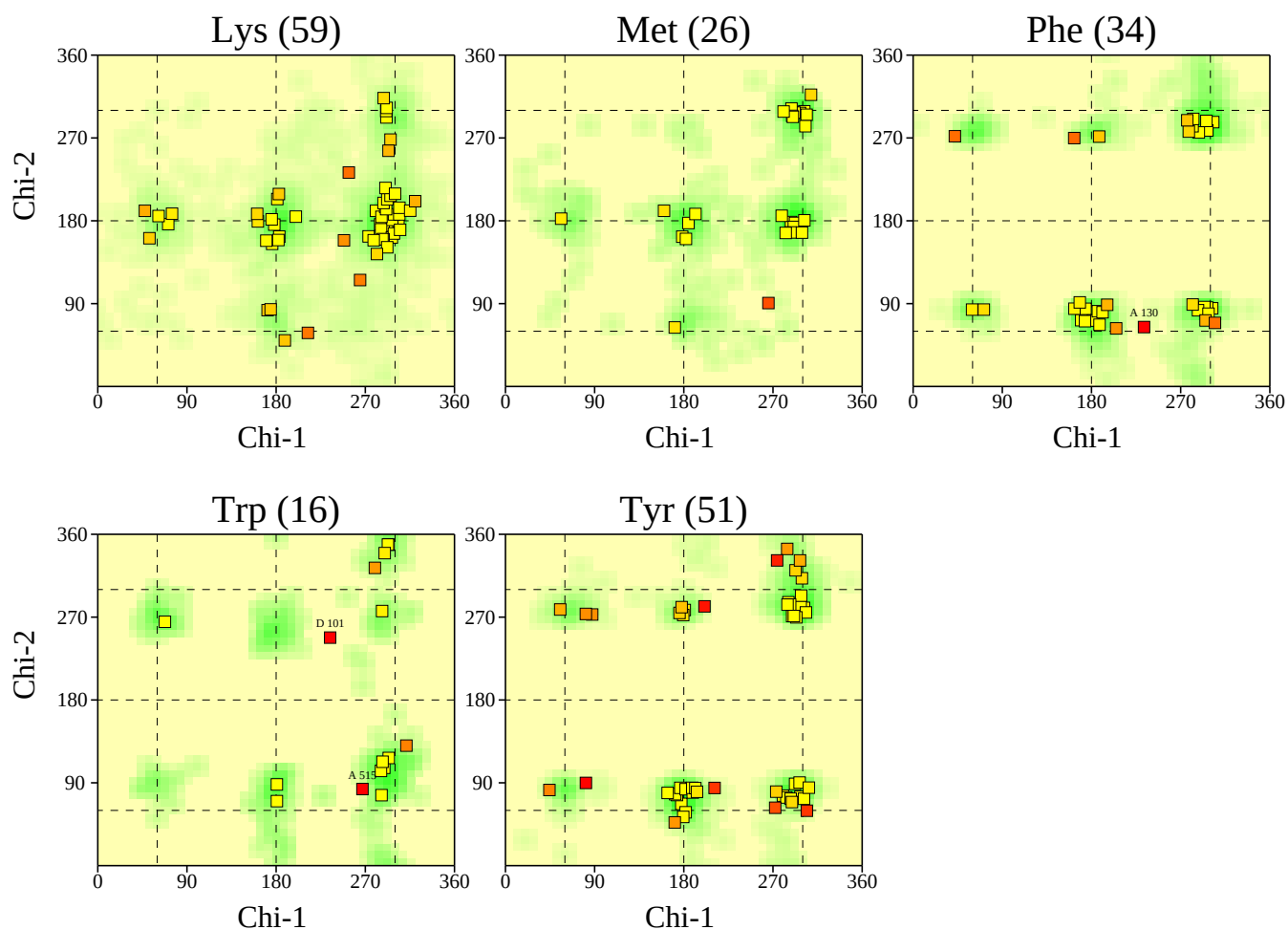
Chi1-Chi2 plots

pdb1yq3



Chi1-Chi2 plots

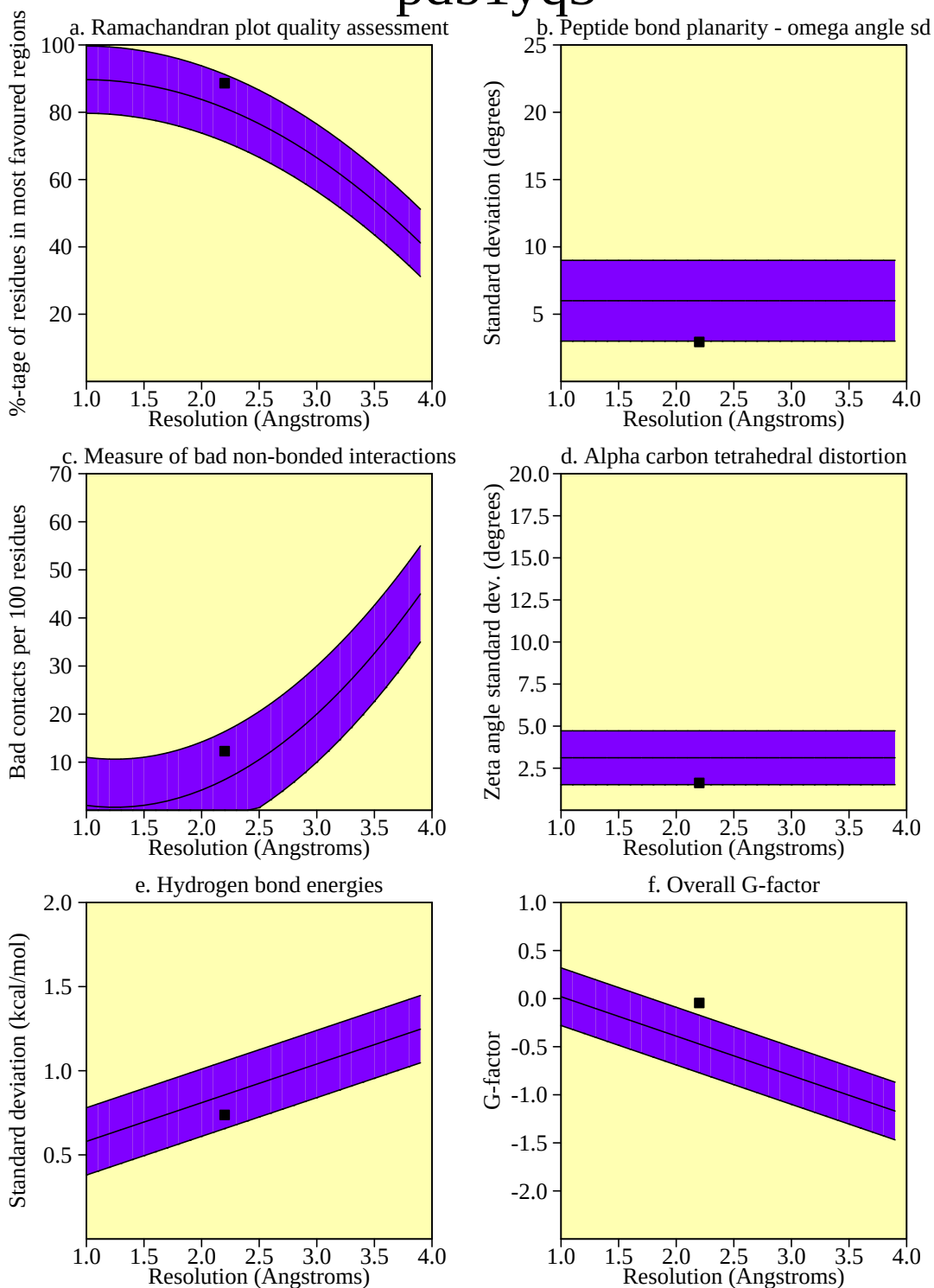
pdb1yq3



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

Main-chain parameters

pdb1yq3

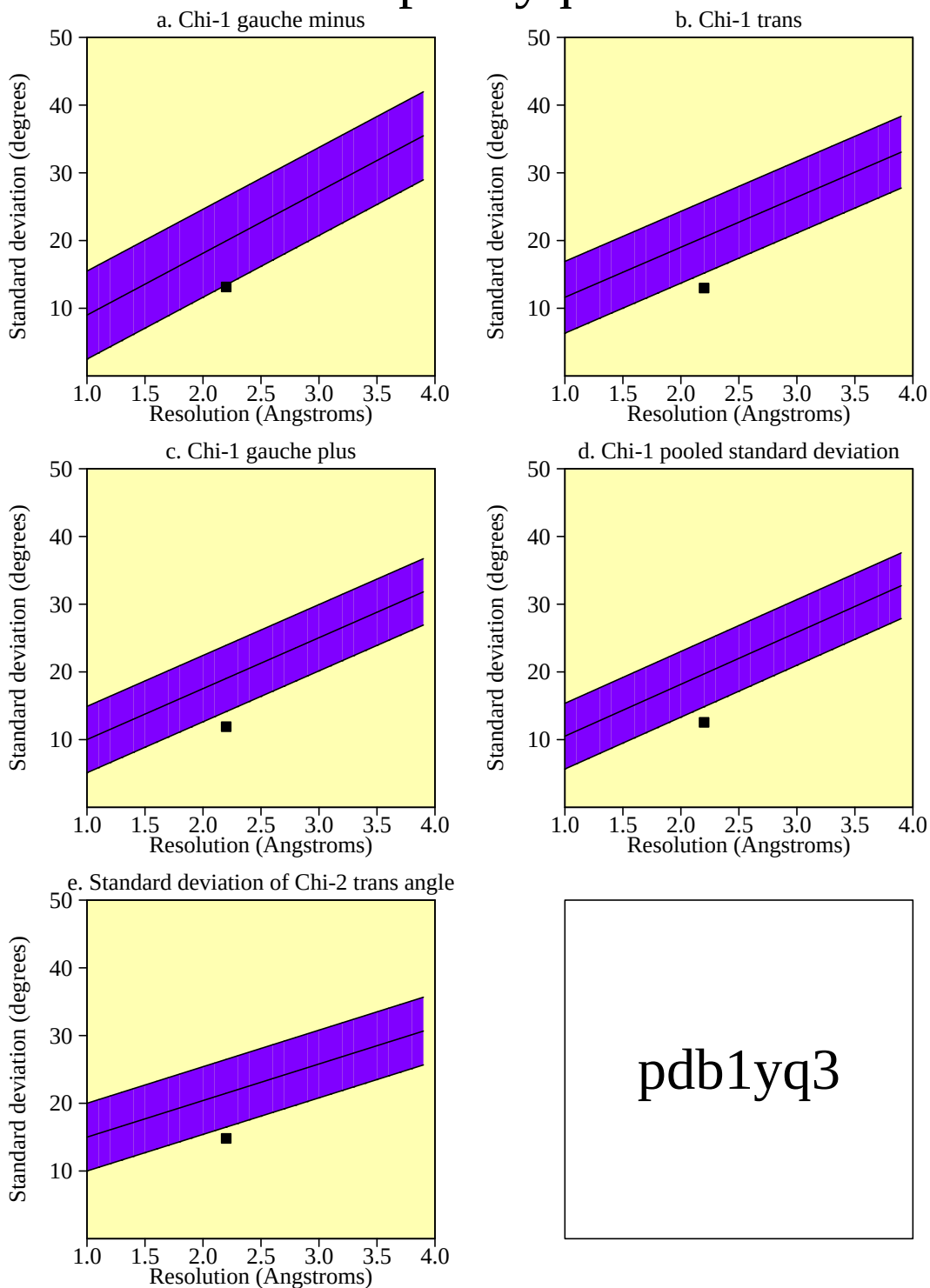


Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values Typical value	Band width	No. of band widths from mean	
a. %-tage residues in A, B, L	950	88.6	81.3	10.0	0.7	Inside
b. Omega angle st dev	1092	2.9	6.0	3.0	-1.0	BETTER
c. Bad contacts / 100 residues	135	12.3	6.4	10.0	0.6	Inside
d. Zeta angle st dev	1007	1.6	3.1	1.6	-0.9	Inside
e. H-bond energy st dev	717	0.7	0.9	0.2	-0.6	Inside
f. Overall G-factor	1098	0.0	-0.5	0.3	1.4	BETTER

Side-chain parameters

pdb1yq3



pdb1yq3

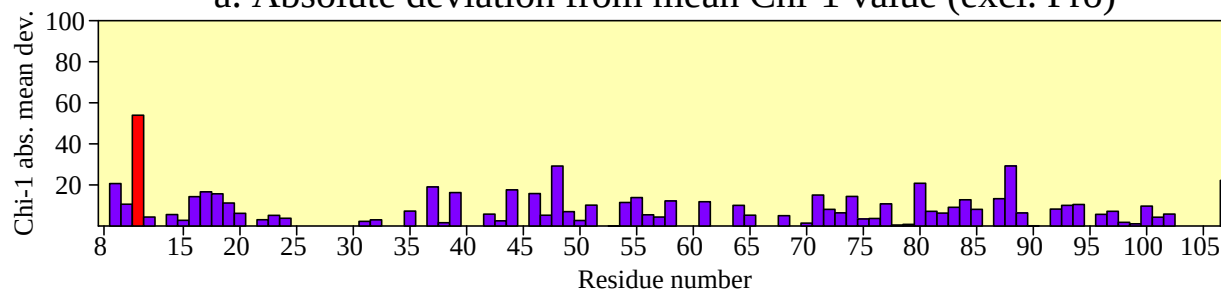
Plot statistics

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	129	13.1	19.9	6.5	-1.0	BETTER
b. Chi-1 trans st dev	274	13.0	20.5	5.3	-1.4	BETTER
c. Chi-1 gauche plus st dev	453	11.9	19.0	4.9	-1.5	BETTER
d. Chi-1 pooled st dev	856	12.5	19.7	4.8	-1.5	BETTER
e. Chi-2 trans st dev	287	14.8	21.5	5.0	-1.3	BETTER

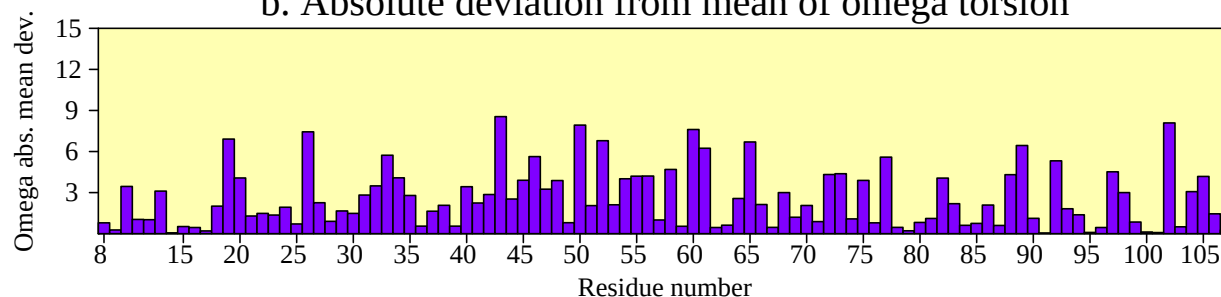
Residue properties

pdb1yq3

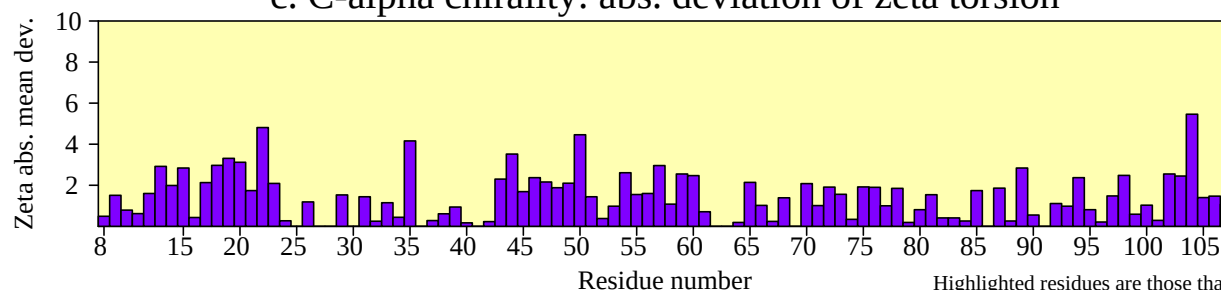
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

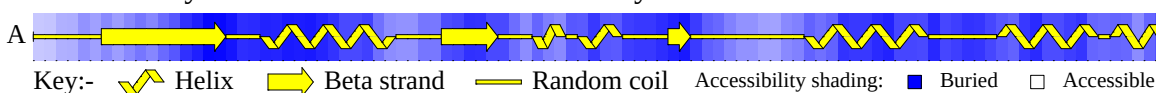


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



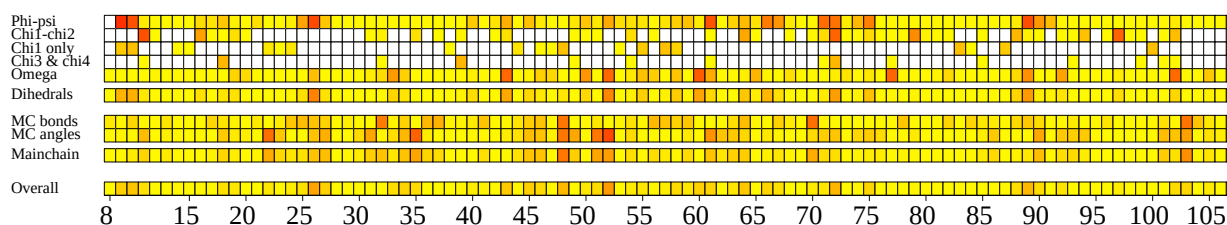
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



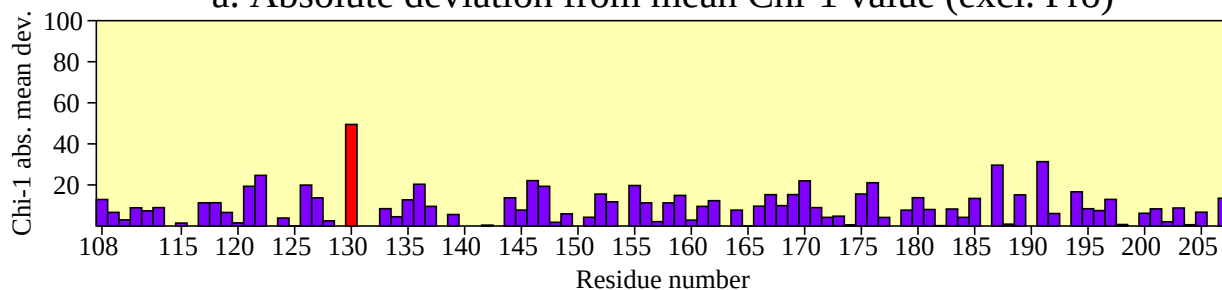
g. G-factors



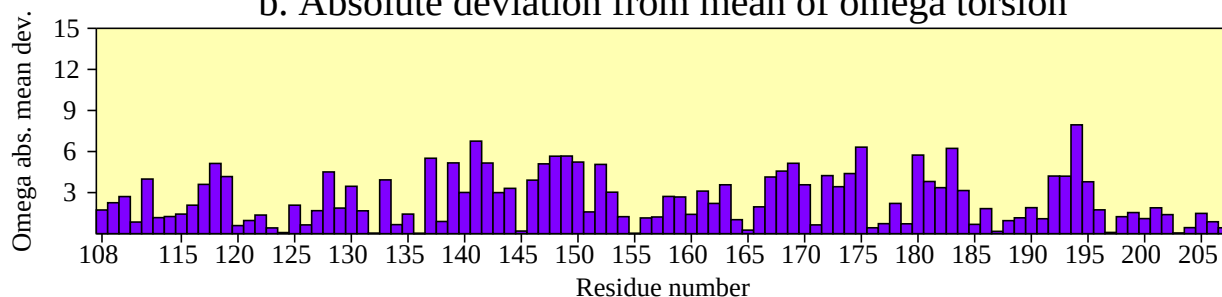
Residue properties

pdb1yq3

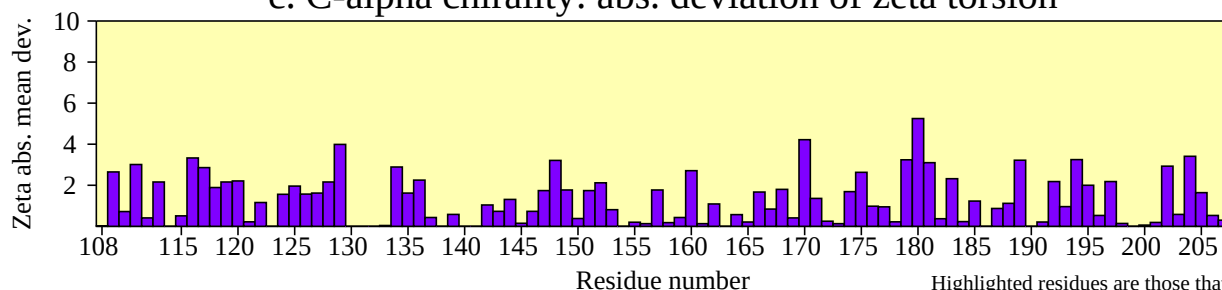
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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

d. Secondary structure & estimated accessibility

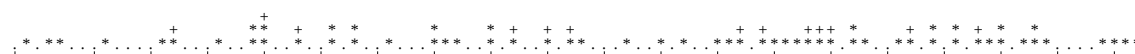


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

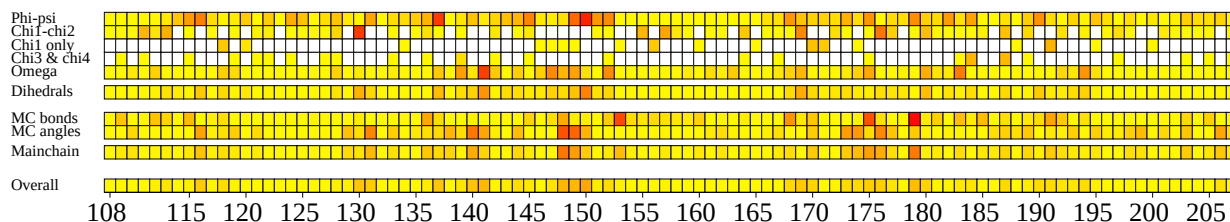
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



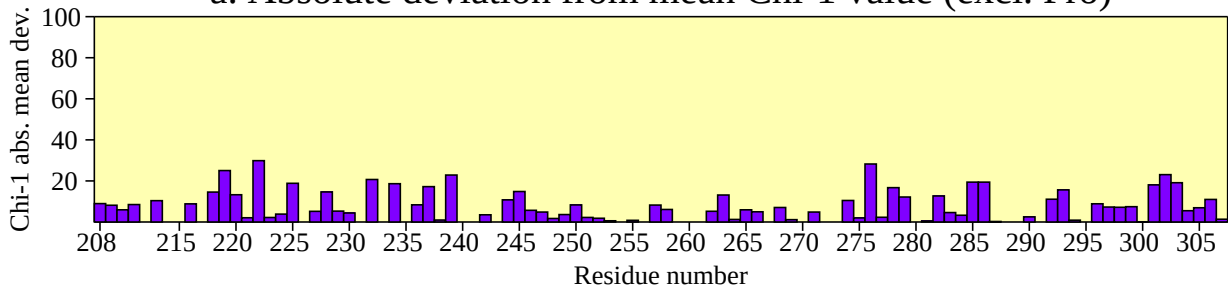
g. G-factors



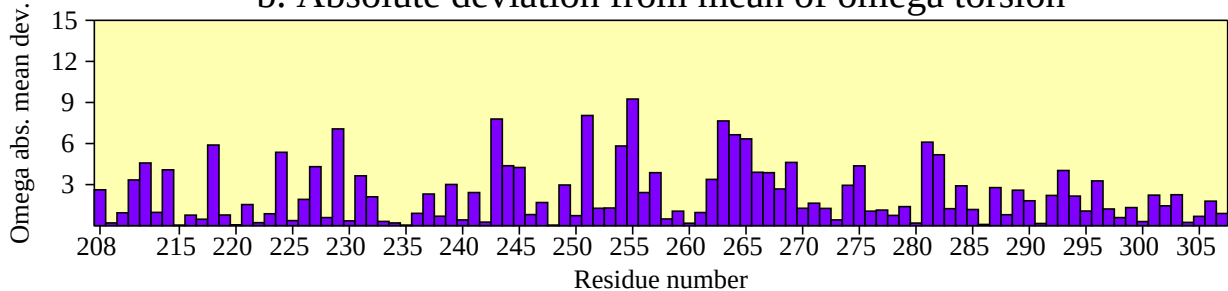
Residue properties

pdb1yq3

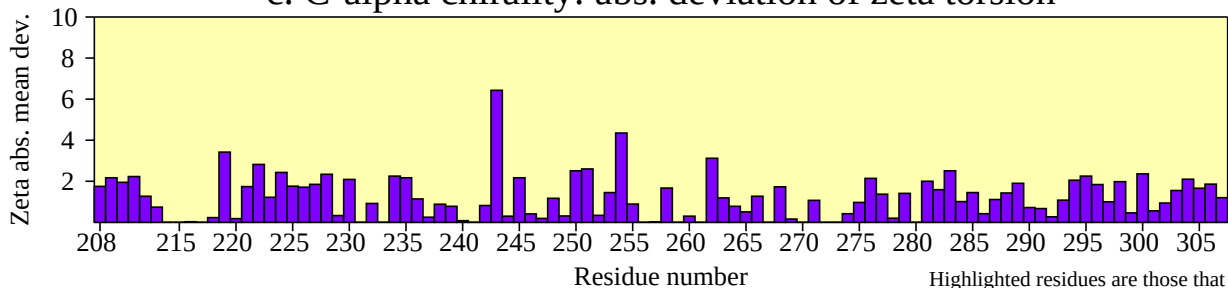
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

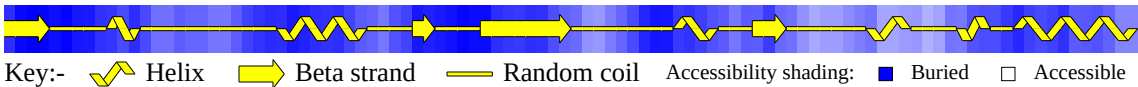


c. C-alpha chirality: abs. deviation of zeta torsion



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

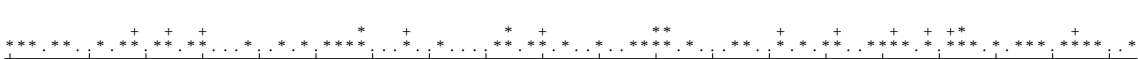
d. Secondary structure & estimated accessibility



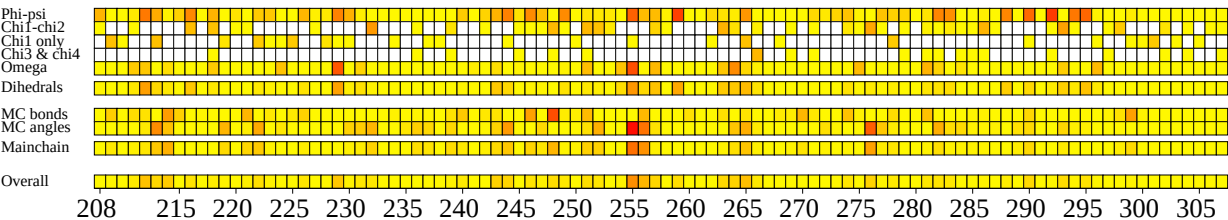
e. Sequence & Ramachandran regions



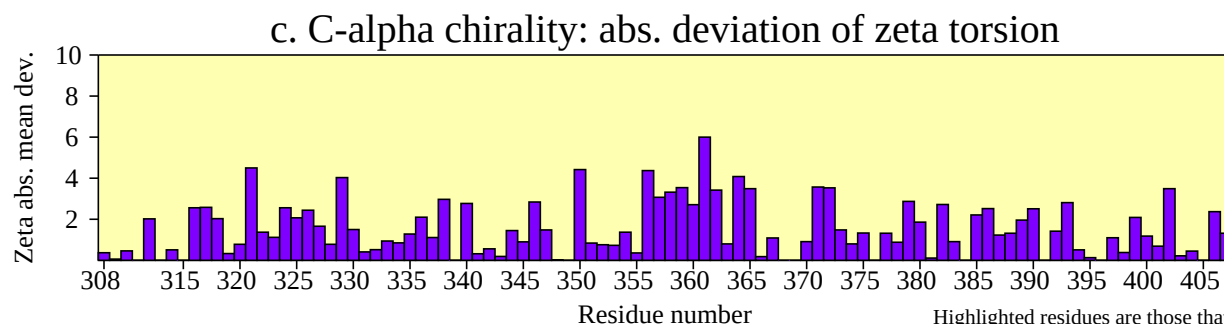
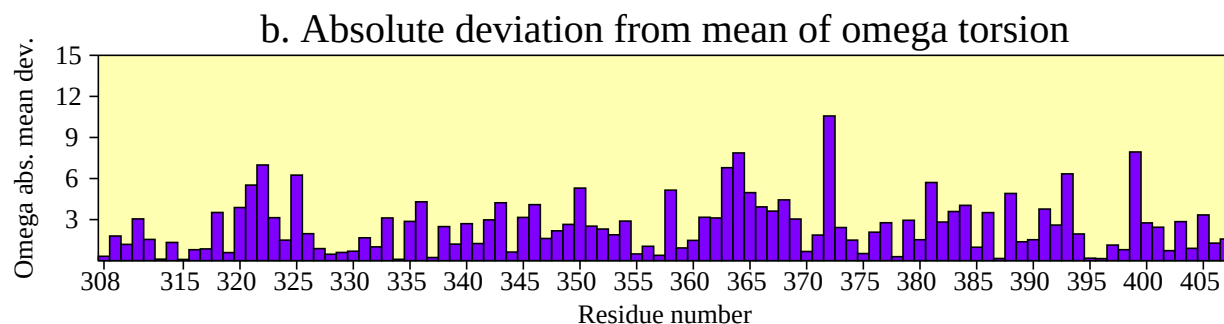
f. Max. deviation (see listing)



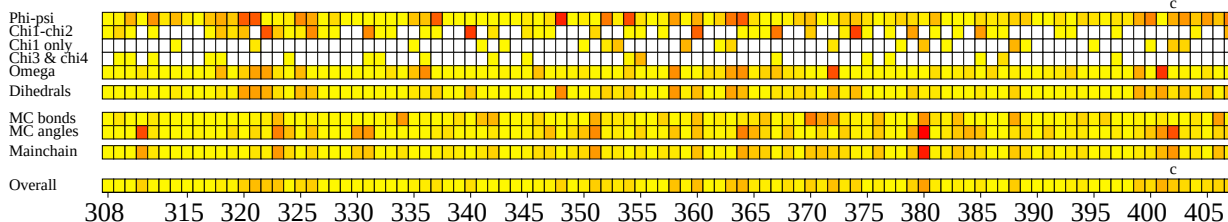
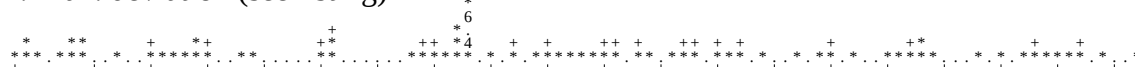
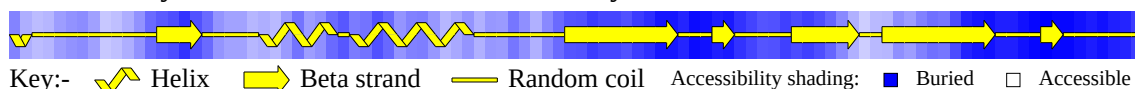
g. G-factors



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

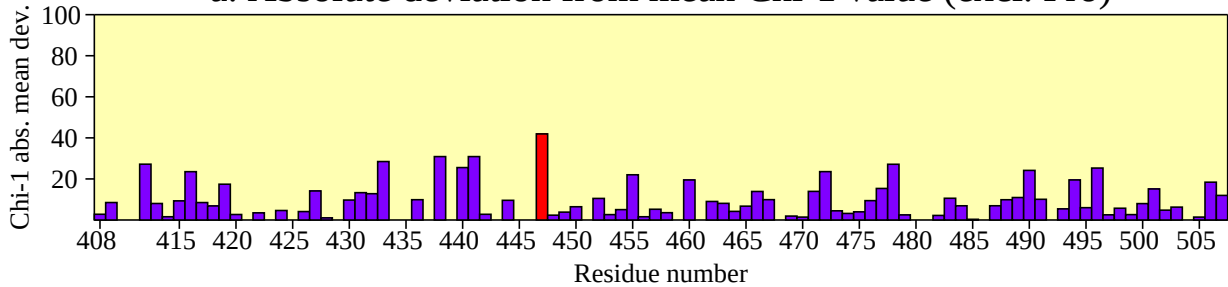


pdb1yq3_06.ps

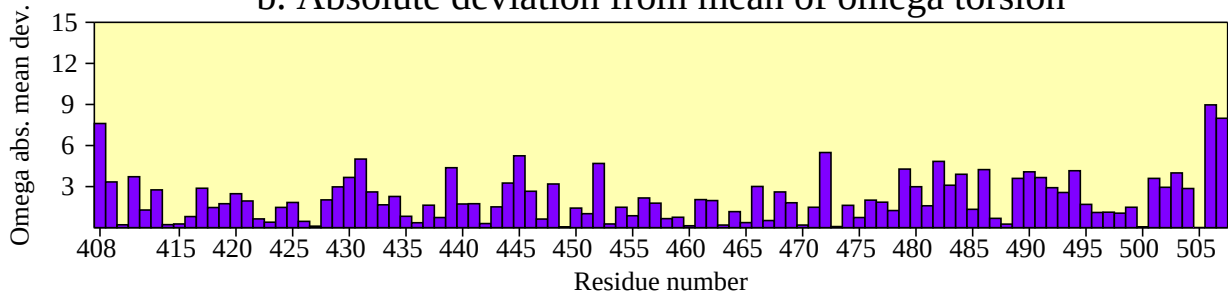
Residue properties

pdb1yq3

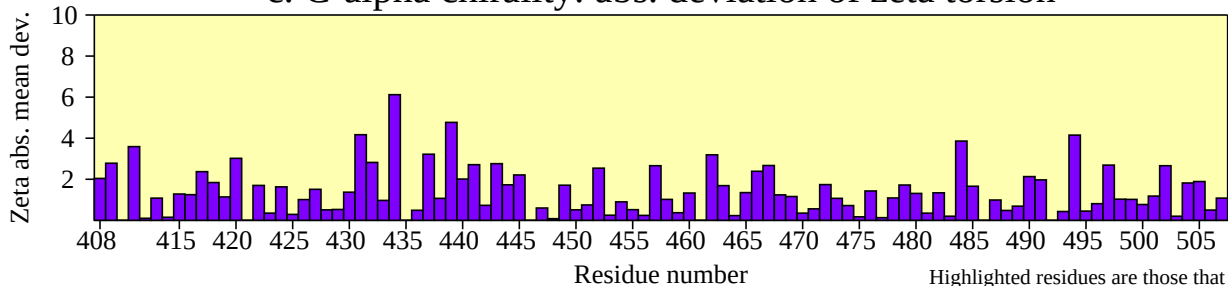
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

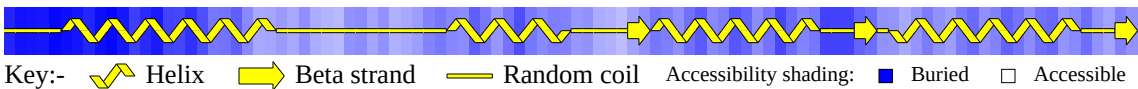


c. C-alpha chirality: abs. deviation of zeta torsion



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

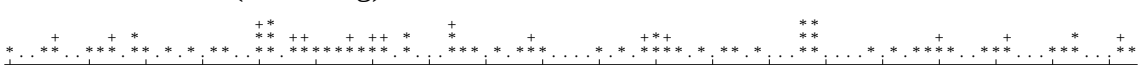
d. Secondary structure & estimated accessibility



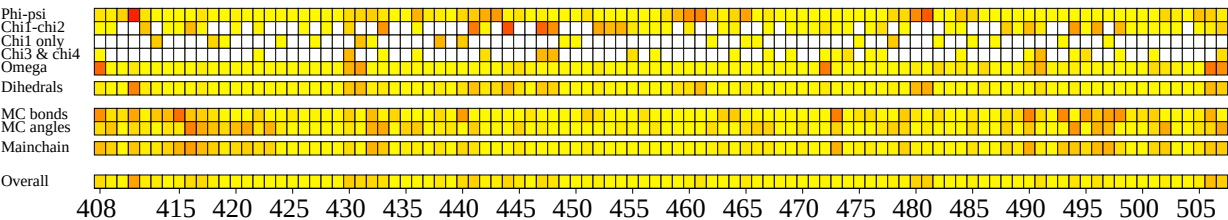
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



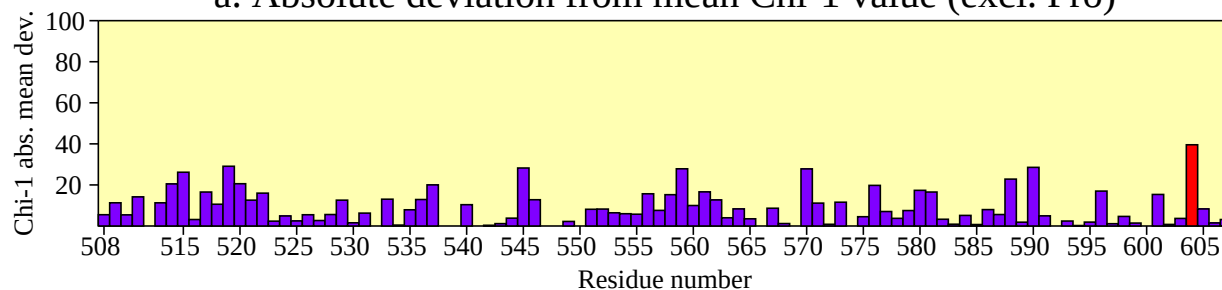
g. G-factors



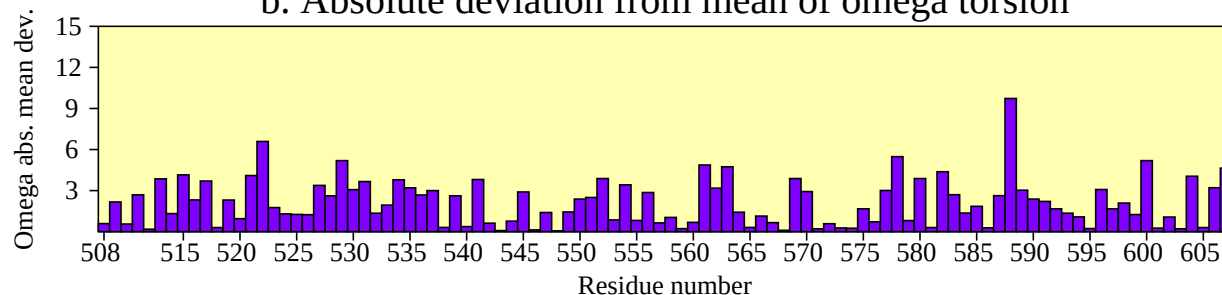
Residue properties

pdb1yq3

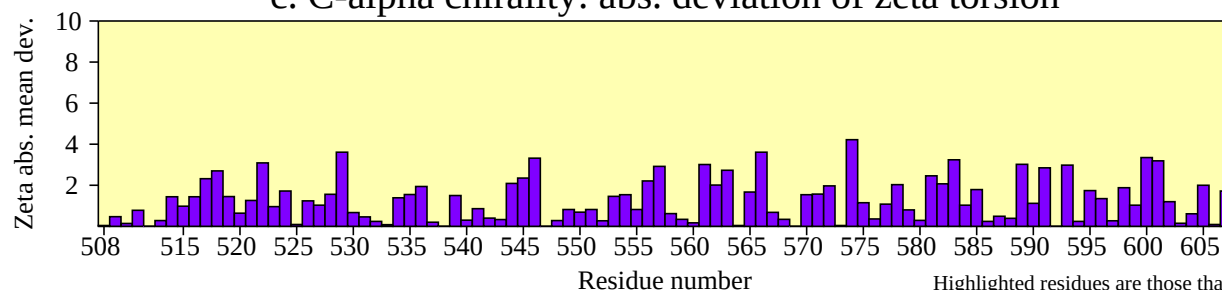
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

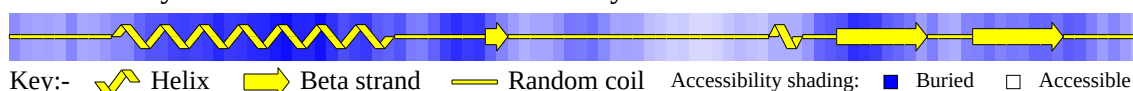


c. C-alpha chirality: abs. deviation of zeta torsion



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

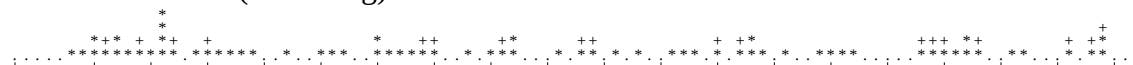
d. Secondary structure & estimated accessibility



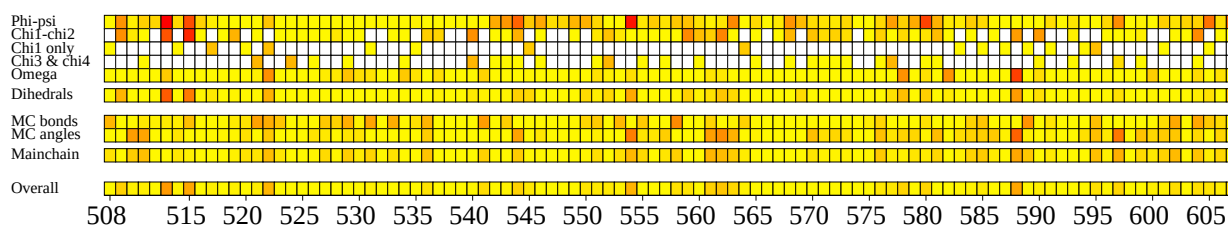
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed

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

f. Max. deviation (see listing)



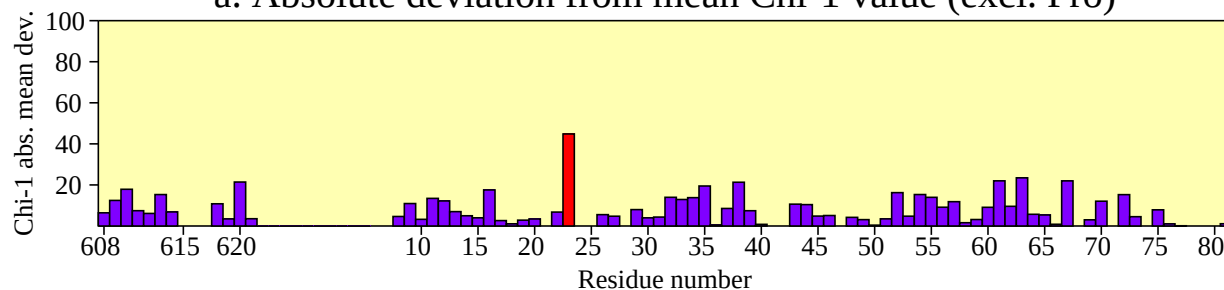
g. G-factors



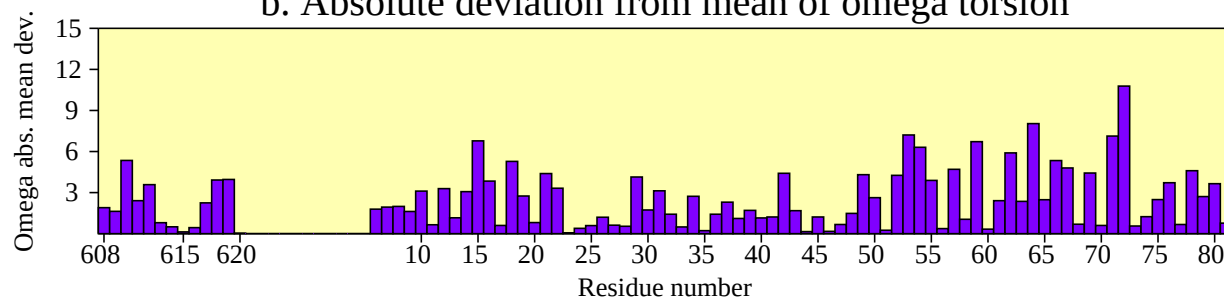
Residue properties

pdb1yq3

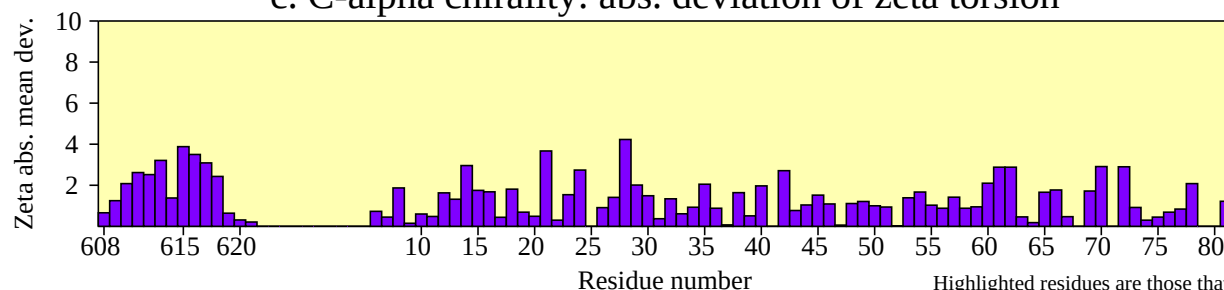
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

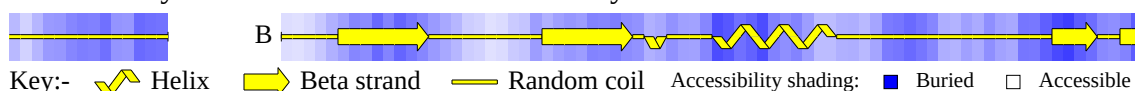


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



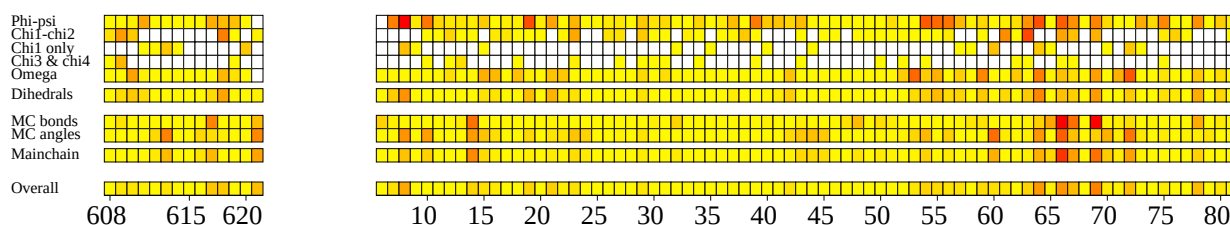
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



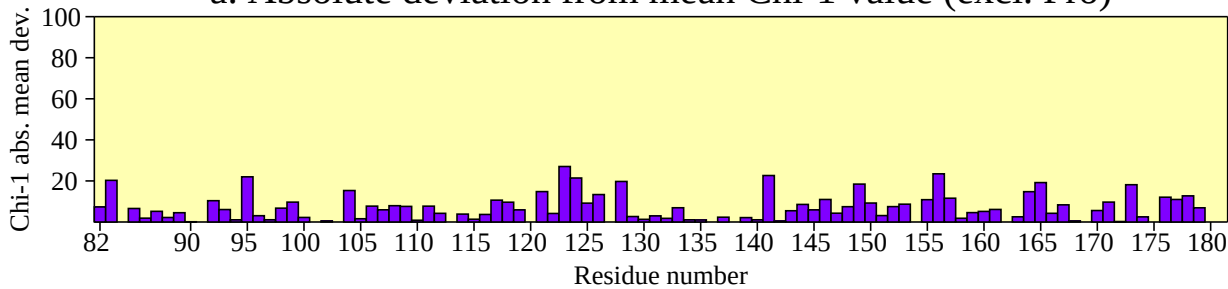
g. G-factors



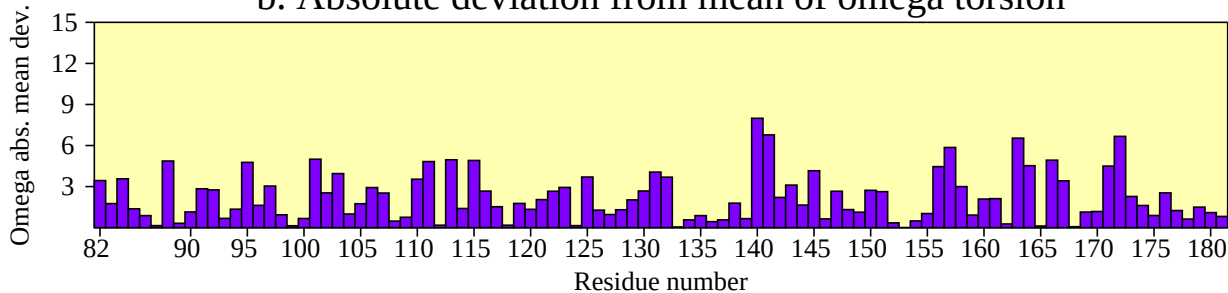
Residue properties

pdb1yq3

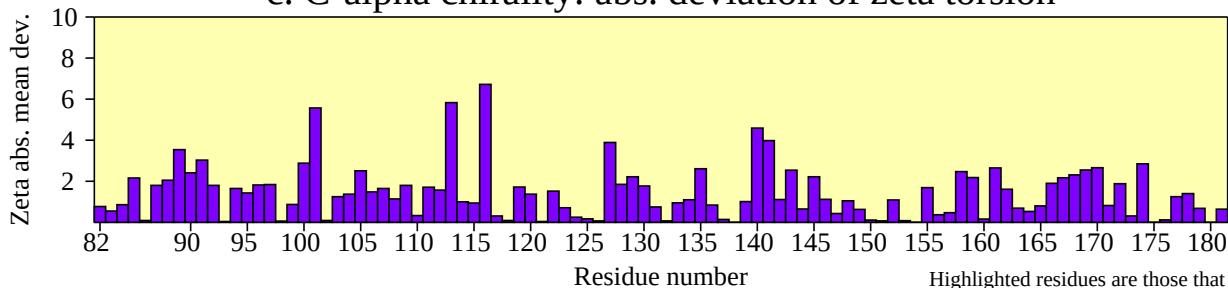
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

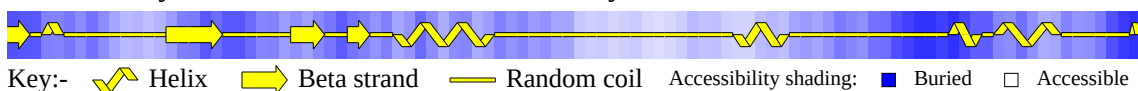


c. C-alpha chirality: abs. deviation of zeta torsion



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

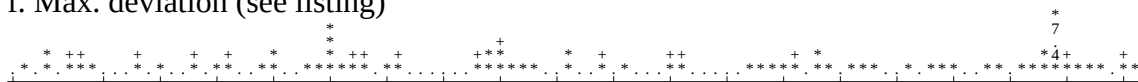
d. Secondary structure & estimated accessibility



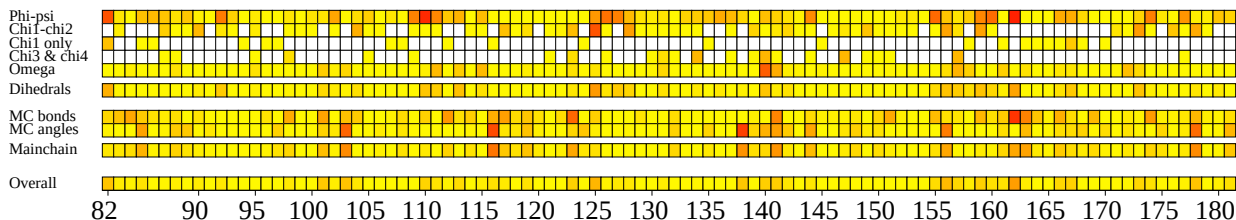
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



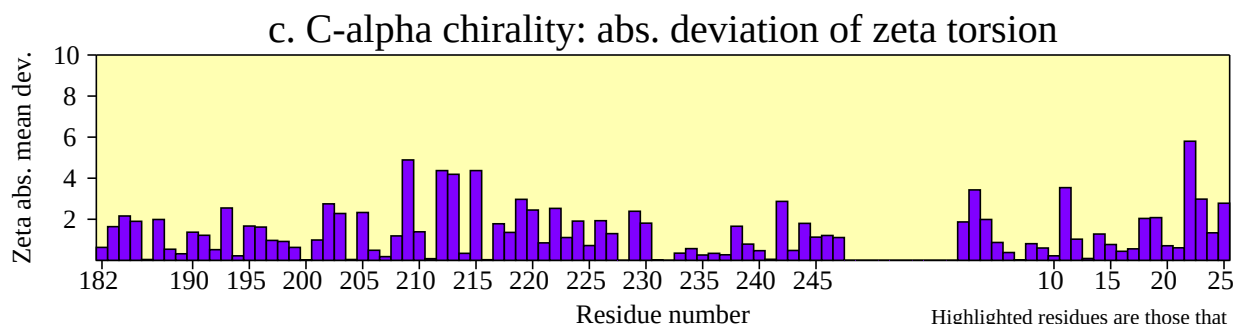
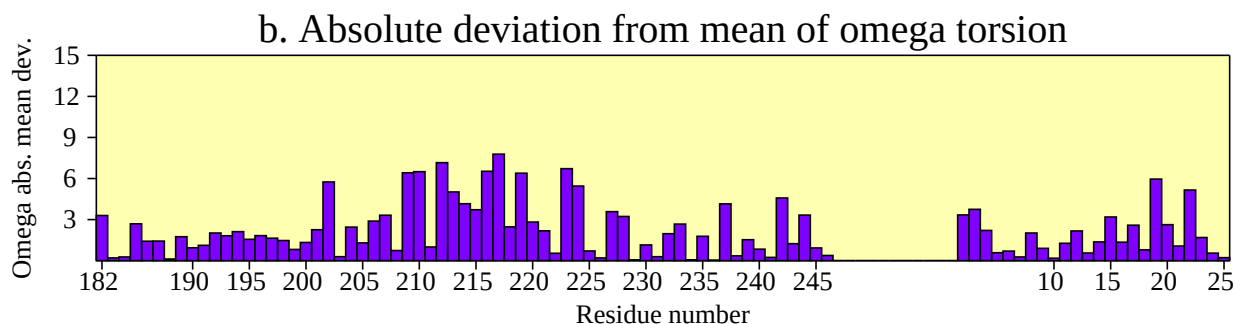
f. Max. deviation (see listing)



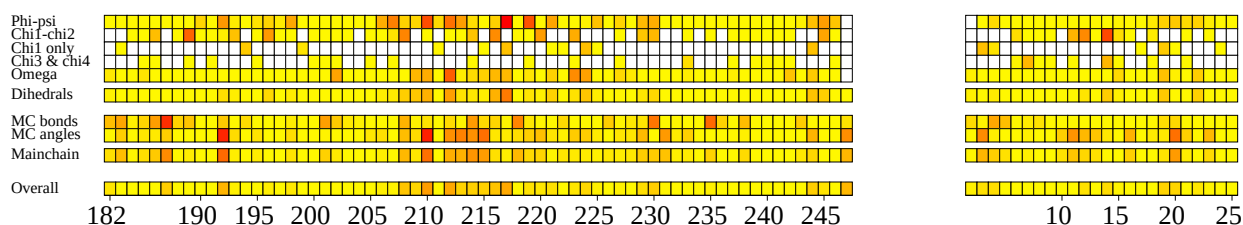
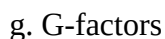
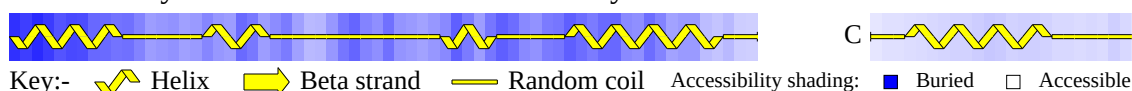
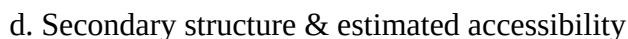
g. G-factors



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



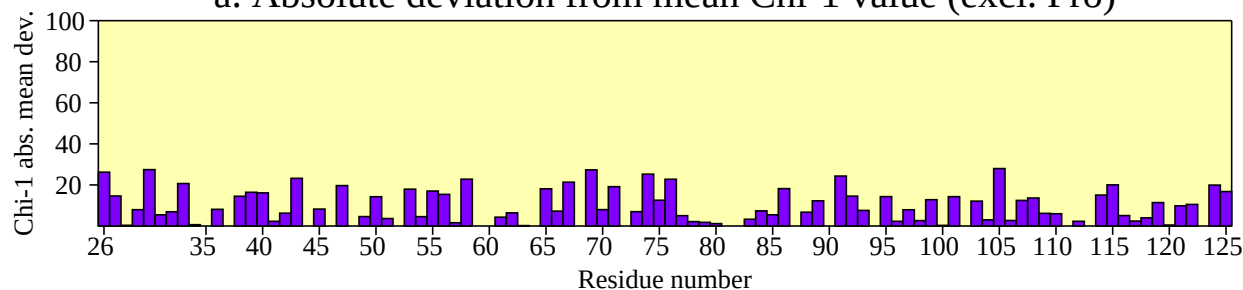
Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal



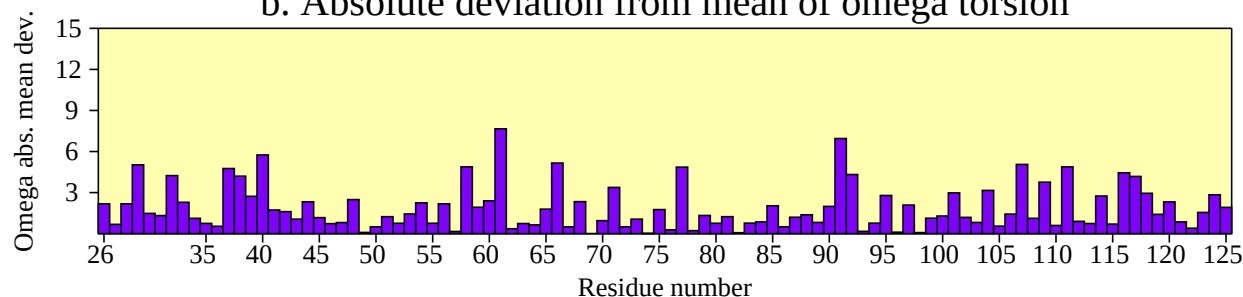
Residue properties

pdb1yq3

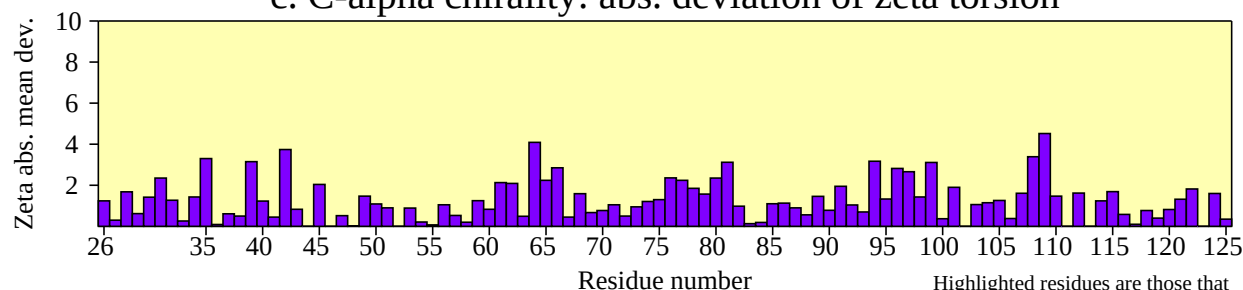
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

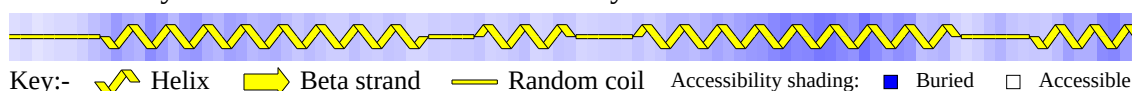


c. C-alpha chirality: abs. deviation of zeta torsion



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

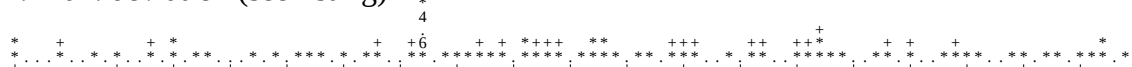
d. Secondary structure & estimated accessibility



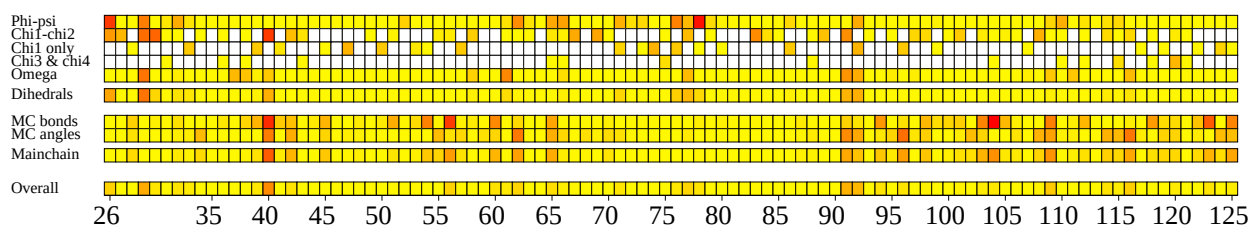
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



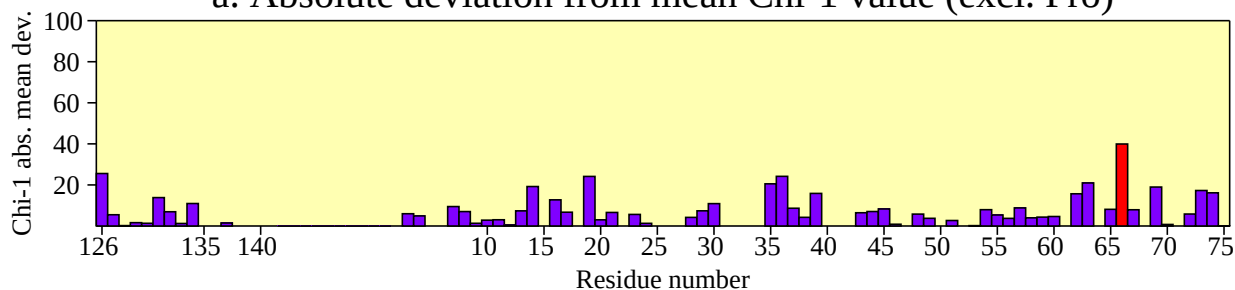
g. G-factors



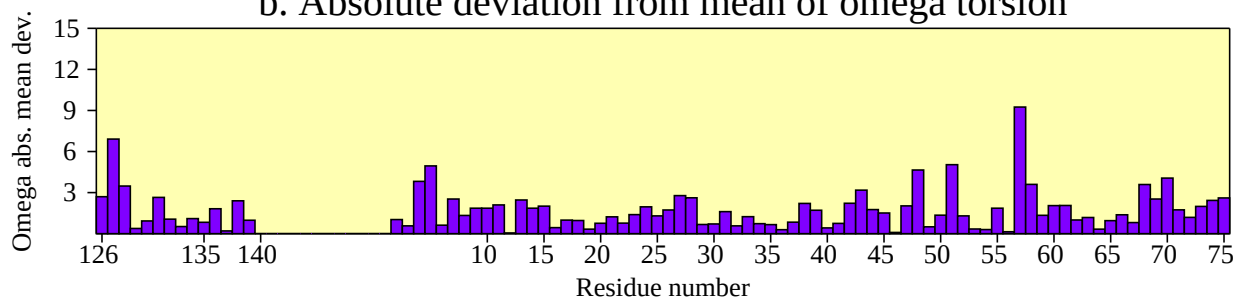
Residue properties

pdb1yq3

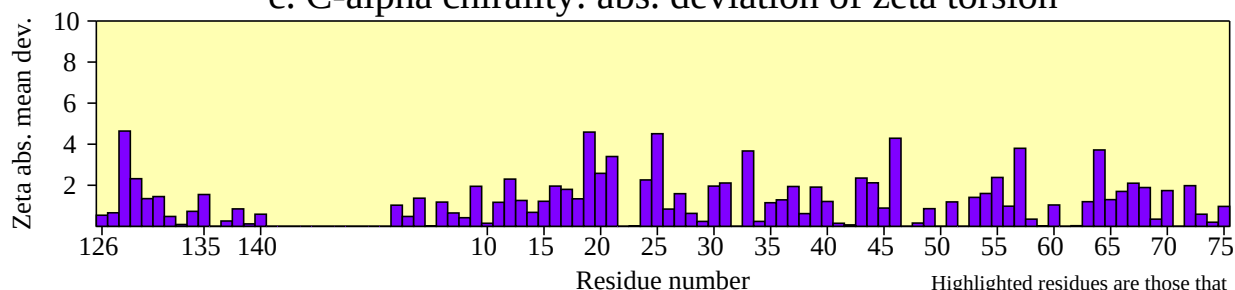
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

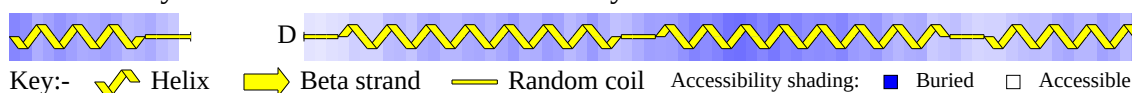


c. C-alpha chirality: abs. deviation of zeta torsion



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

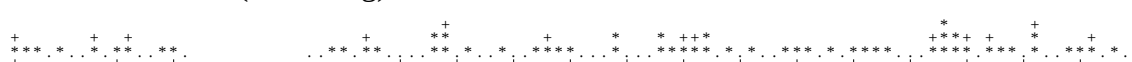
d. Secondary structure & estimated accessibility



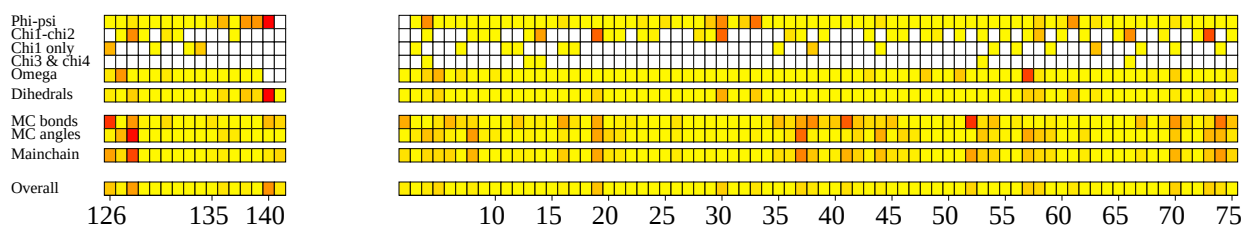
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



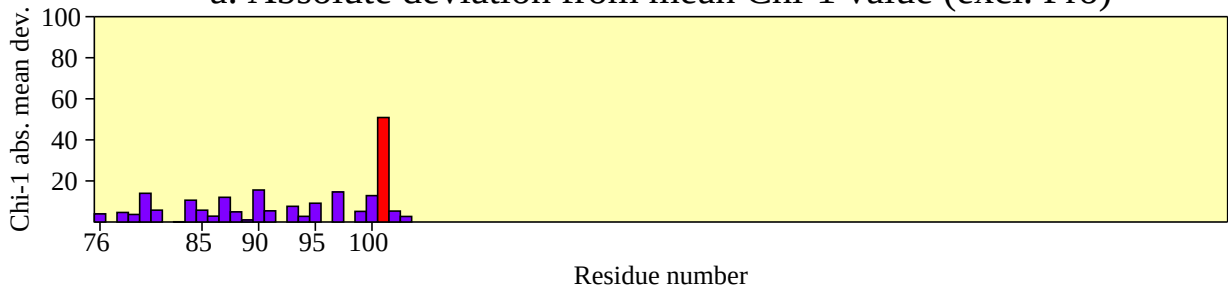
g. G-factors



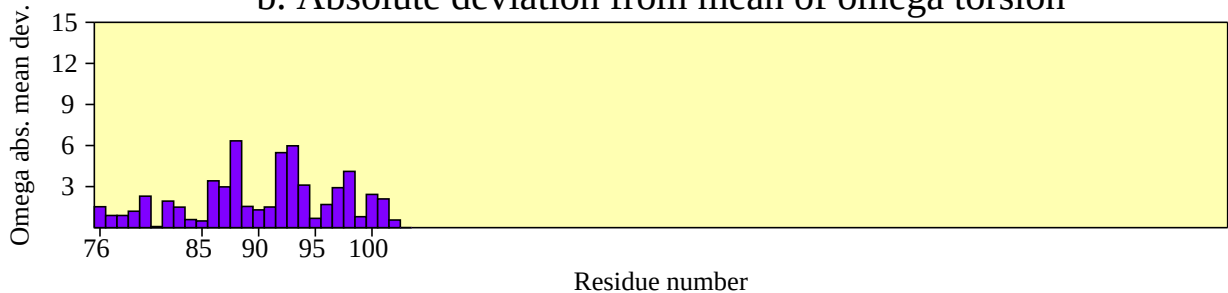
Residue properties

pdb1yq3

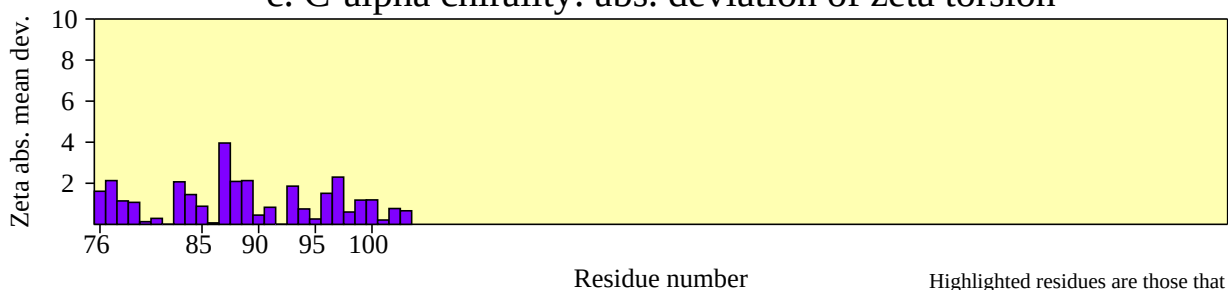
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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



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

d. Secondary structure & estimated accessibility

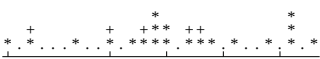


Key:- Helix Beta strand Random coil Accessibility shading: Buried Accessible

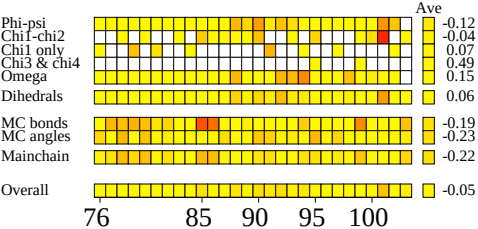
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

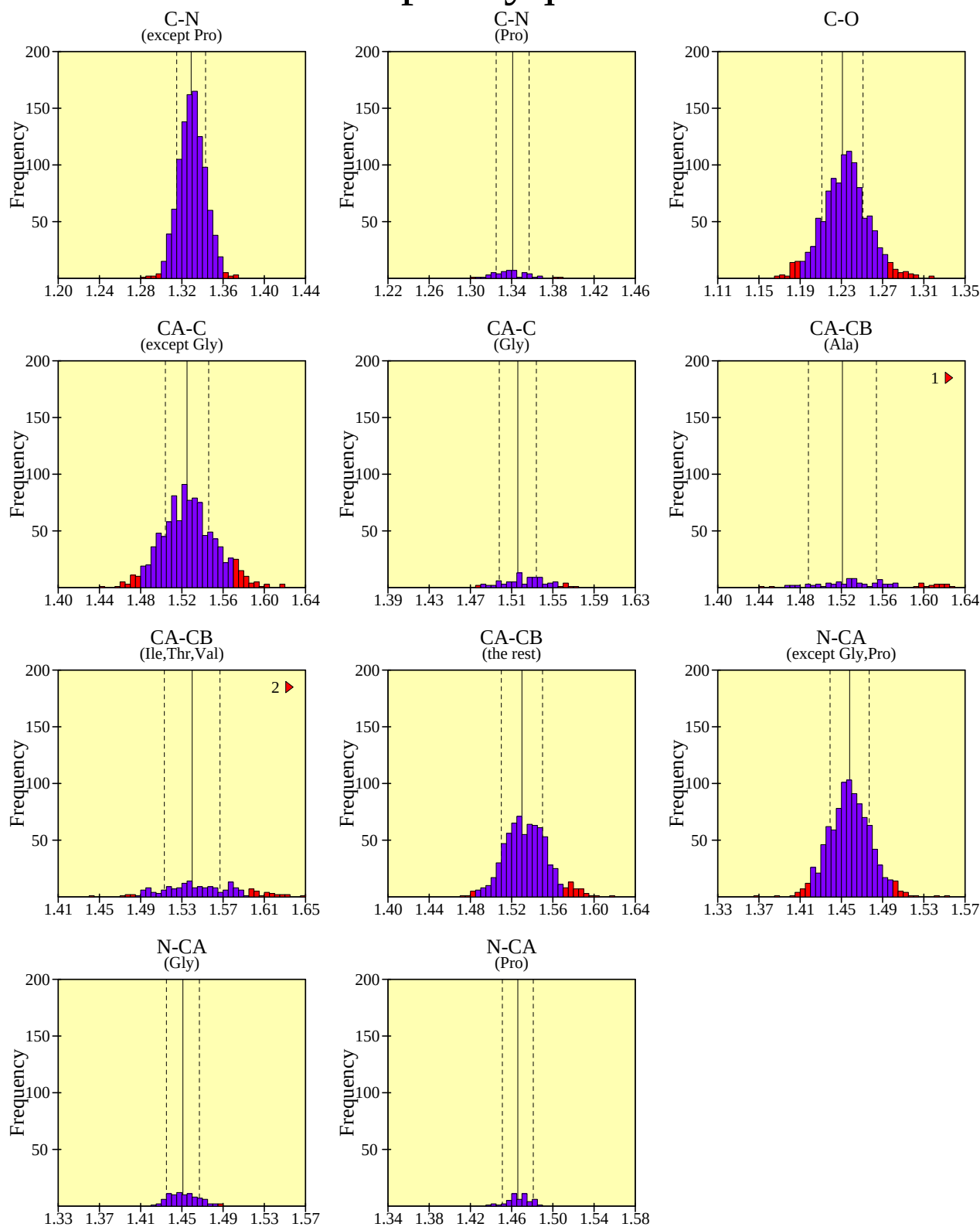


g. G-factors



Main-chain bond lengths

pdb1yq3



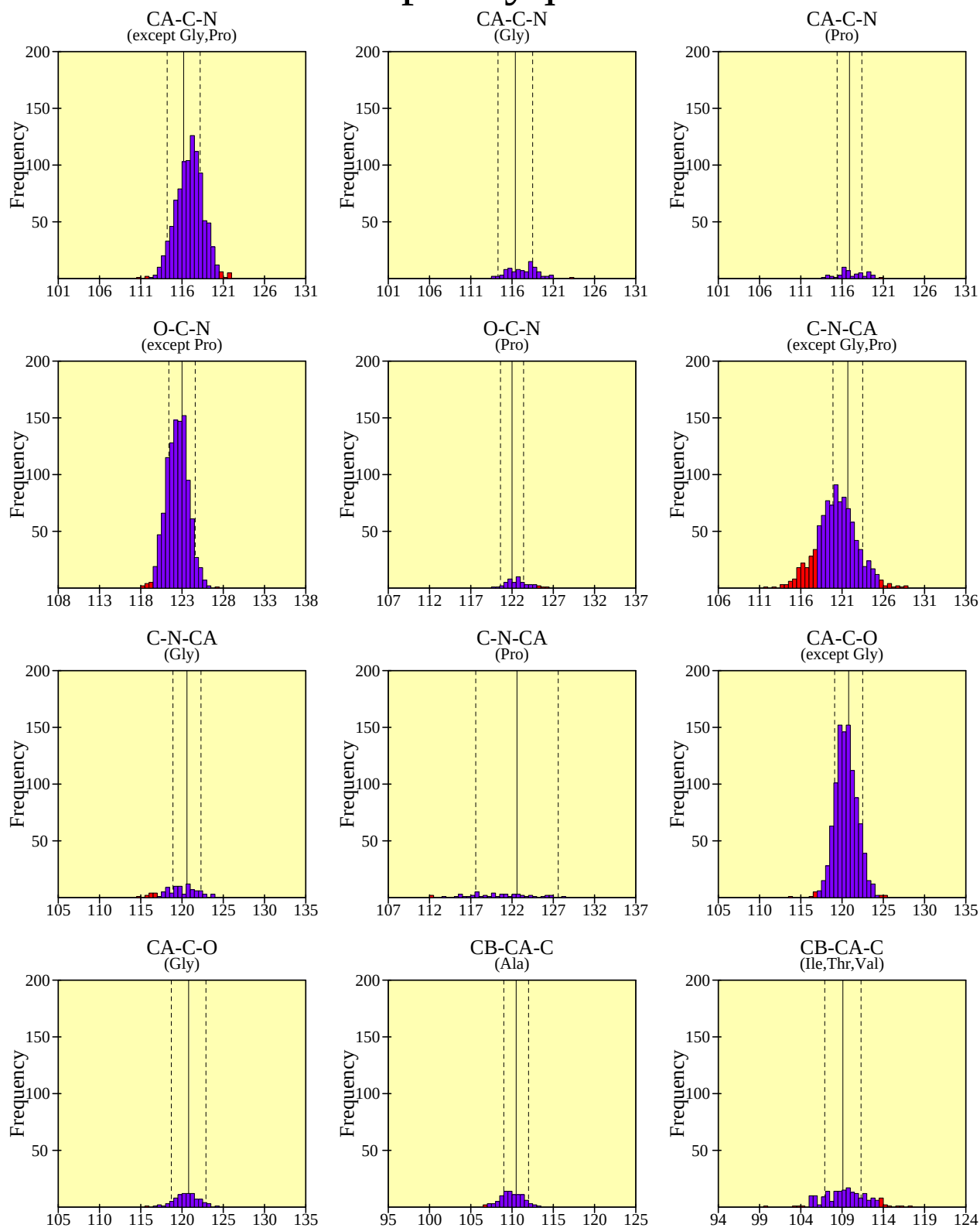
Black bars > 2.0 st. devs. from mean.

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

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

Main-chain bond angles

pdb1yq3

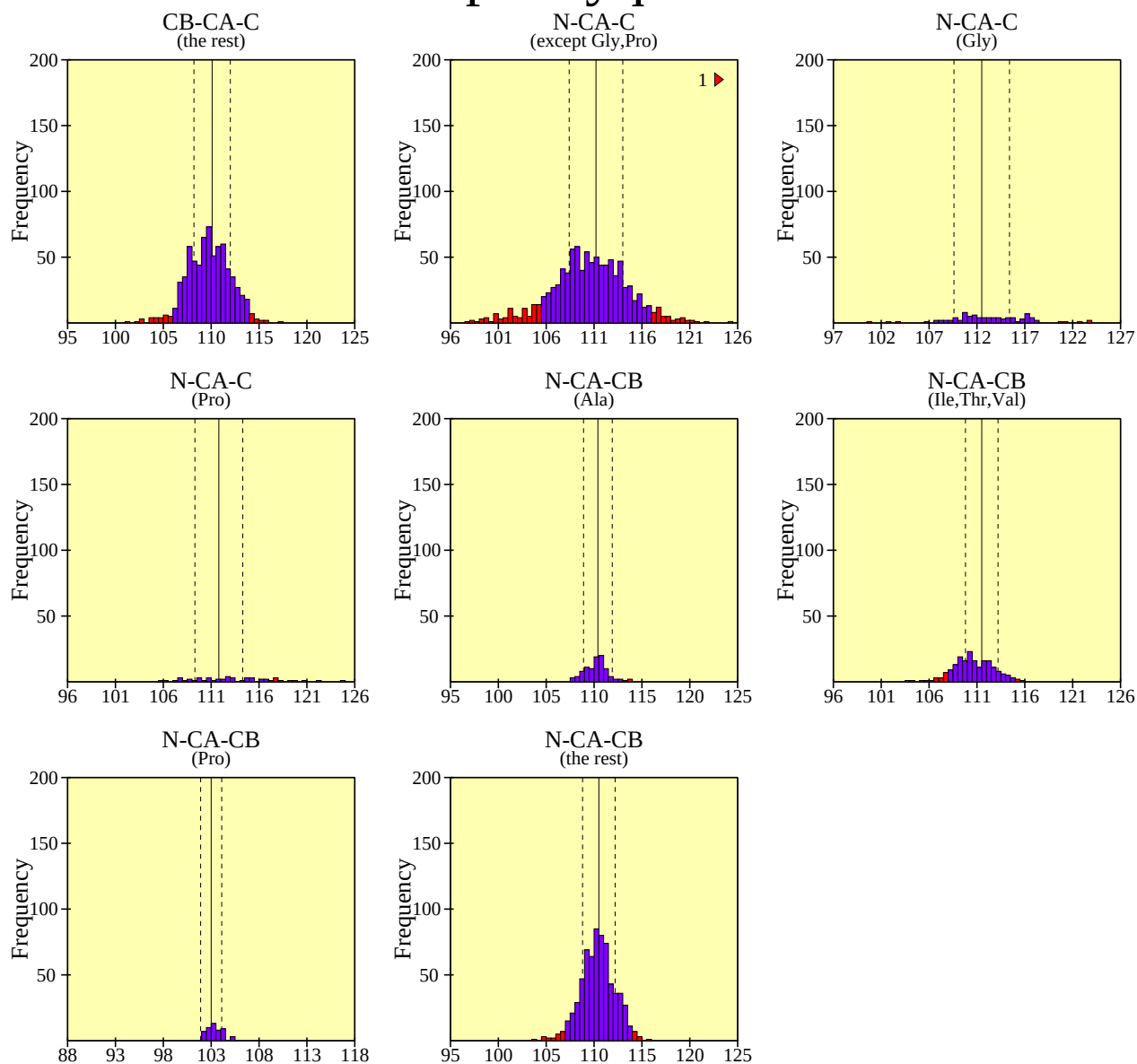


Black bars > 2.0 st. devs. from mean.

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

Main-chain bond angles

pdb1yq3



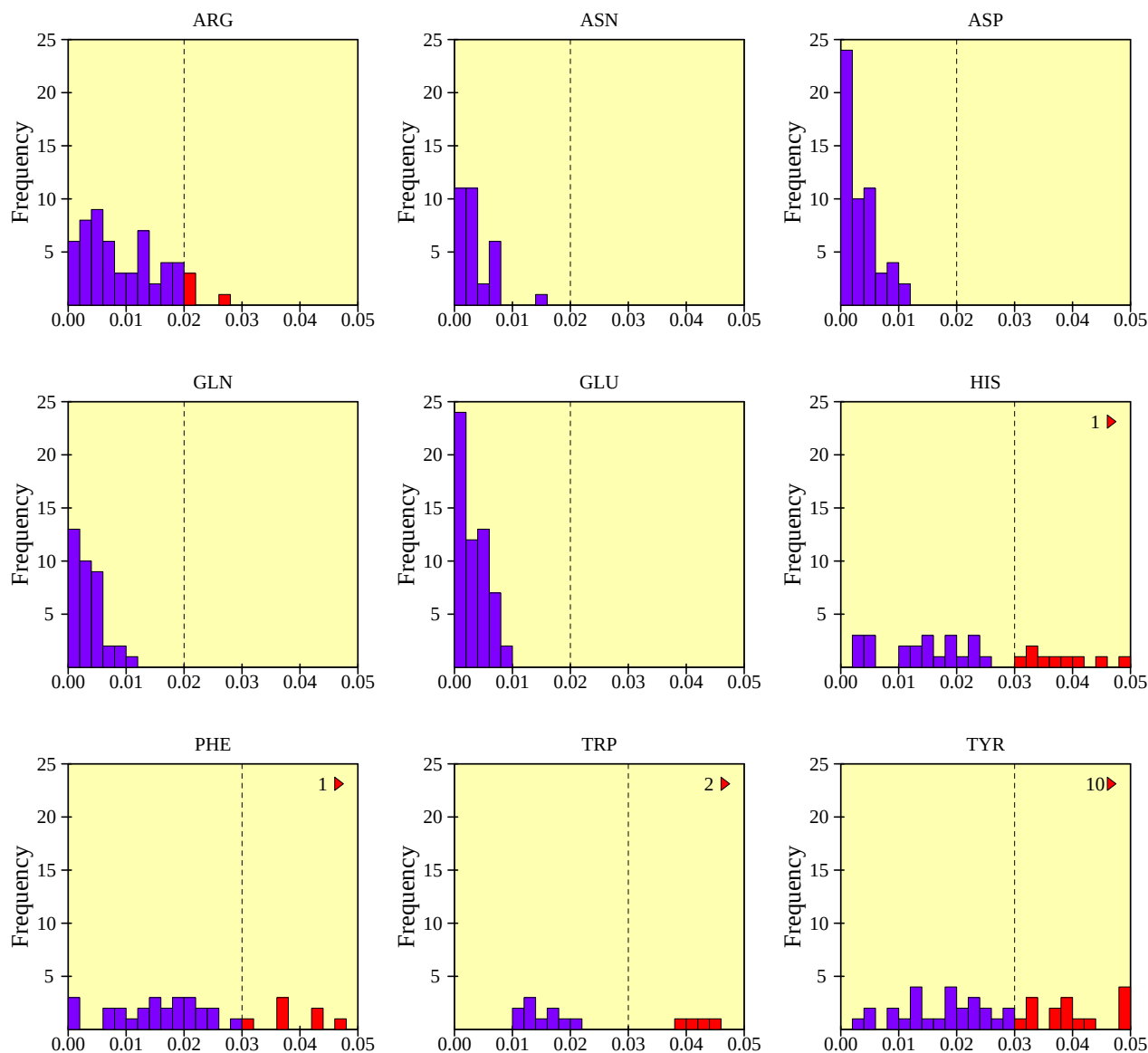
Black bars > 2.0 st. devs. from mean.

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

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

RMS distances from planarity

pdb1yq3



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

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

Distorted geometry

pdb1yq3

Main-chain bond lengths

CA 1.540 CB 0.056 1.596 A Thr 10	CA 1.540 CB 0.055 1.595 A Val 24	C 1.231 O 0.070 1.301 A Arg 32	CA 1.521 CB 0.076 1.597 A Ala 33	CA 1.525 C 0.051 1.576 A Ala 40	C 1.231 O 0.057 1.174 A Ala 45
CA 1.540 CB 0.116 1.656 A Thr 48	CA 1.530 CB 0.058 1.588 A His 56	CA 1.540 CB 0.063 1.603 A Ile 64	CA 1.525 C 0.066 1.591 A Asn 70	CA 1.525 C 0.056 1.469 A Asp 88	CA 1.521 CB 0.143 1.664 A Ala 103
CA 1.530 CB 0.057 1.587 A Pro 104	CA 1.521 CB 0.072 1.593 A Ala 105	C 1.231 O 0.051 1.281 A Glu 109	N 1.458 CA 0.052 1.510 A Gln 136	CA 1.530 CB 0.053 1.582 A Arg 145	C 1.231 O 0.050 1.281 A Cys 148
CA 1.525 C 0.052 1.577 A Ala 150	N 1.458 CA 0.051 1.509 A Arg 152	C 1.231 O 0.089 1.320 A Thr 153	C 1.231 O 0.056 1.175 A Tyr 168	CA 1.525 C 0.060 1.465 A Tyr 168	CA 1.540 CB 0.057 1.483 A Thr 170
CA 1.525 C 0.091 1.616 A Glu 175	N 1.458 CA 0.094 1.552 A Leu 179	CA 1.530 CB 0.056 1.586 A Asn 185	CA 1.540 CB 0.094 1.634 A Val 191	CA 1.540 CB 0.078 1.618 A Ile 192	CA 1.540 CB 0.063 1.603 A Thr 209
CA 1.521 CB 0.087 1.609 A Ala 212	CA 1.530 CB 0.063 1.593 A Asp 246	CA 1.530 CB 0.086 1.616 A Glu 248	C 1.231 O 0.061 1.292 A Gln 251	CA 1.516 C 0.056 1.572 A Gly 256	CA 1.540 CB 0.059 1.599 A Ile 274
CA 1.525 C 0.059 1.584 A Val 290	CA 1.540 CB 0.090 1.630 A Val 299	CA 1.521 CB 0.092 1.613 A Ala 334	C 1.231 O 0.061 1.292 A Ser 341	CA 1.525 C 0.058 1.583 A Glu 342	CA 1.525 C 0.052 1.577 A Ile 346
C 1.231 O 0.063 1.293 A Asp 351	CA 1.540 CB 0.056 1.596 A Val 352	CA 1.540 CB 0.075 1.615 A Ile 357	CA 1.525 C 0.063 1.588 A Leu 360	C 1.231 O 0.052 1.283 A Asn 366	C 1.231 O 0.068 1.299 A Pro 371
CA 1.540 CB 0.084 1.624 A Thr 372	CA 1.540 CB 0.074 1.614 A Thr 380	CA 1.525 C 0.055 1.580 A His 381	CA 1.540 CB 0.058 1.598 A Val 388	N 1.458 CA 0.053 1.405 A Val 388	CA 1.540 CB 0.061 1.479 A Val 389
CA 1.525 C 0.050 1.475 A Ala 406	CA 1.521 CB 0.098 1.619 A Ala 406	CA 1.525 C 0.069 1.456 A Ala 411	CA 1.521 CB 0.051 1.572 A Ala 411	CA 1.530 CB 0.058 1.472 A Leu 414	C 1.231 O 0.086 1.317 A Leu 415
C 1.231 O 0.052 1.179 A Asp 416	CA 1.525 C 0.050 1.475 A Leu 417	CA 1.525 C 0.062 1.463 A Cys 432	C 1.231 O 0.052 1.283 A Ser 440	CA 1.525 C 0.059 1.584 A Ser 440	CA 1.521 CB 0.078 1.599 A Ala 451

Distorted geometry

pdb1yq3

Main-chain bond lengths (contd)

CA 1.525 C 0.064 1.461 A Gln 473	CA 1.525 C 0.059 1.584 A Gln 490	C 1.231 O 0.066 1.297 A Cys 493	C 1.231 O 0.056 1.287 A Lys 495	C 1.231 O 0.069 1.300 A Ser 497	CA 1.530 CB 0.056 1.586 A Gln 498
CA 1.525 C 0.052 1.577 A Leu 506	CA 1.525 C 0.057 1.582 A Thr 508	CA 1.525 C 0.050 1.475 A Arg 511	CA 1.540 CB 0.085 1.625 A Thr 522	CA 1.525 C 0.057 1.582 A Asn 527	CA 1.530 CB 0.060 1.590 A Met 529
CA 1.530 CB 0.065 1.595 A Cys 531	CA 1.540 CB 0.066 1.606 A Thr 535	CA 1.521 CB 0.103 1.624 A Ala 541	CA 1.521 CB 0.051 1.572 A Ala 548	CA 1.525 C 0.058 1.583 A Ala 550	CA 1.525 C 0.066 1.591 A Asp 553
CA 1.525 C 0.054 1.579 A Ser 564	CA 1.525 C 0.054 1.579 A Leu 584	CA 1.525 C 0.051 1.576 A Ser 585	CA 1.540 CB 0.091 1.631 A Val 589	CA 1.540 CB 0.064 1.604 A Thr 595	CA 1.540 CB 0.057 1.483 A Val 601
C 1.231 O 0.059 1.172 A Ile 602	CA 1.530 CB 0.054 1.584 A Arg 604	CA 1.521 CB 0.107 1.628 A Ala 617	C 1.231 O 0.052 1.283 A Tyr 621	CA 1.521 CB 0.052 1.573 B Ala 7	CA 1.525 C 0.061 1.464 B Phe 14
CA 1.530 CB 0.056 1.586 B Cys 65	CA 1.525 C 0.094 1.619 B Arg 66	CA 1.530 CB 0.052 1.582 B Arg 66	CA 1.525 C 0.093 1.618 B Glu 67	CA 1.540 CB 0.108 1.648 B Ile 69	N 1.458 CA 0.071 1.387 B Ile 69
CA 1.521 CB 0.067 1.454 B Ala 74	CA 1.521 CB 0.099 1.620 B Ala 78	CA 1.540 CB 0.063 1.603 B Thr 82	CA 1.525 C 0.065 1.590 B Leu 83	C 1.231 O 0.057 1.288 B Ala 84	CA 1.540 CB 0.070 1.470 B Thr 96
C 1.231 O 0.060 1.291 B Lys 98	CA 1.525 C 0.050 1.575 B Pro 101	CA 1.525 C 0.051 1.474 B Pro 103	CA 1.540 CB 0.062 1.602 B Val 112	CA 1.525 C 0.062 1.587 B Asp 114	C 1.231 O 0.052 1.179 B Ser 116
CA 1.525 C 0.059 1.584 B Asn 117	CA 1.521 CB 0.076 1.597 B Ala 120	CA 1.530 CB 0.052 1.582 B Tyr 122	N 1.458 CA 0.082 1.540 B Lys 123	CA 1.525 C 0.050 1.475 B Lys 132	CA 1.525 C 0.053 1.578 B Gln 141
CA 1.530 CB 0.055 1.585 B Gln 141	CA 1.525 C 0.054 1.471 B Gln 144	N 1.458 CA 0.054 1.512 B Leu 155	C 1.231 O 0.056 1.287 B Ile 159	C 1.231 O 0.054 1.285 B Ala 162	CA 1.521 CB 0.091 1.612 B Ala 162
CA 1.530 CB 0.074 1.604 B Cys 163	CA 1.530 CB 0.054 1.584 B Cys 164	CA 1.525 C 0.051 1.474 B Asn 174	CA 1.525 C 0.052 1.577 B Tyr 178	CA 1.521 CB 0.090 1.611 B Ala 182	CA 1.525 C 0.057 1.582 B Val 183

Distorted geometry

pdb1yq3

Main-chain bond lengths (contd)

CA 1.530 CB 0.056 1.586 B Met 185	N 1.458 CA 0.062 1.520 B Gln 186	CA 1.525 C 0.069 1.594 B Ala 187	CA 1.521 CB 0.101 1.622 B Ala 187	CA 1.530 CB 0.052 1.582 B Arg 189	CA 1.525 C 0.055 1.470 B Ile 192
CA 1.525 C 0.076 1.601 B Arg 214	N 1.458 CA 0.054 1.512 B Cys 215	CA 1.525 C 0.073 1.598 B Ile 218	CA 1.525 C 0.053 1.472 B Pro 226	CA 1.525 C 0.054 1.579 B Asn 230	CA 1.540 CB 0.096 1.444 B Ile 235
CA 1.521 CB 0.098 1.619 B Ala 236	CA 1.525 C 0.058 1.583 C Thr 4	CA 1.521 CB 0.089 1.610 C Ala 5	CA 1.525 C 0.052 1.577 C Ser 28	CA 1.525 C 0.052 1.473 C Trp 32	N 1.458 CA 0.089 1.369 C Ile 40
CA 1.525 C 0.052 1.577 C Thr 41	CA 1.540 CB 0.058 1.598 C Thr 45	N 1.458 CA 0.056 1.402 C Leu 51	CA 1.525 C 0.054 1.471 C Ser 54	CA 1.530 CB 0.055 1.475 C Ser 54	C 1.231 O 0.065 1.166 C Phe 56
CA 1.525 C 0.080 1.605 C Ala 60	CA 1.521 CB 0.052 1.469 C Ala 87	CA 1.525 C 0.053 1.472 C Leu 91	CA 1.525 C 0.064 1.461 C Pro 94	CA 1.540 CB 0.080 1.620 C Ile 103	CA 1.525 C 0.060 1.585 C Arg 104
CA 1.530 CB 0.052 1.582 C Arg 104	N 1.458 CA 0.067 1.525 C Arg 104	C 1.231 O 0.063 1.294 C Gln 118	CA 1.530 CB 0.062 1.592 C Ser 122	C 1.231 O 0.073 1.304 C Gly 123	CA 1.525 C 0.066 1.591 C Val 125
CA 1.540 CB 0.140 1.680 C Val 126	CA 1.540 CB 0.076 1.616 C Ile 128	CA 1.521 CB 0.078 1.443 C Ala 135	C 1.231 O 0.051 1.282 C Ile 140	N 1.458 CA 0.056 1.514 D Ser 2	CA 1.521 CB 0.074 1.595 D Ala 6
CA 1.540 CB 0.076 1.616 D Val 16	CA 1.521 CB 0.053 1.468 D Ala 26	CA 1.540 CB 0.055 1.595 D Val 35	C 1.231 O 0.060 1.291 D Tyr 37	C 1.231 O 0.064 1.167 D Ser 38	CA 1.521 CB 0.079 1.600 D Ala 40
CA 1.525 C 0.080 1.605 D Ala 41	C 1.231 O 0.056 1.287 D Gly 52	C 1.231 O 0.054 1.285 D Val 54	CA 1.540 CB 0.051 1.488 D Thr 56	CA 1.540 CB 0.055 1.595 D Val 59	CA 1.525 C 0.062 1.463 D Thr 70
CA 1.540 CB 0.072 1.612 D Thr 70	CA 1.525 C 0.054 1.579 D Tyr 73	C 1.231 O 0.070 1.301 D Val 74	CA 1.521 CB 0.094 1.615 D Ala 77	CA 1.540 CB 0.072 1.612 D Ile 78	C 1.231 O 0.067 1.298 D Tyr 85
CA 1.525 C 0.068 1.593 D Tyr 85	N 1.458 CA 0.051 1.508 D Phe 86	CA 1.525 C 0.082 1.442 D Met 99	CA 1.540 CB 0.062 1.478 D Ile 103		

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

Distorted geometry

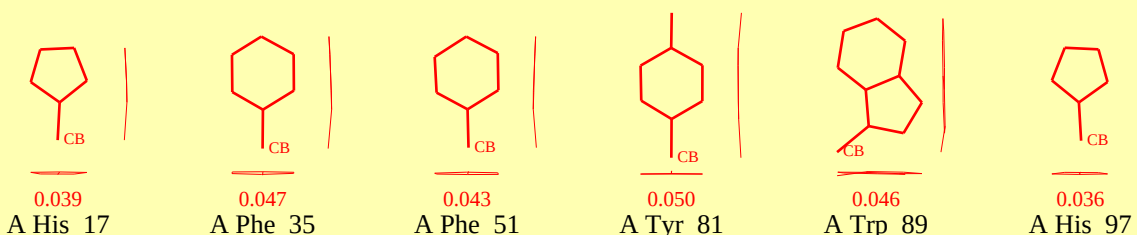
pdb1yq3

Main-chain bond angles



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

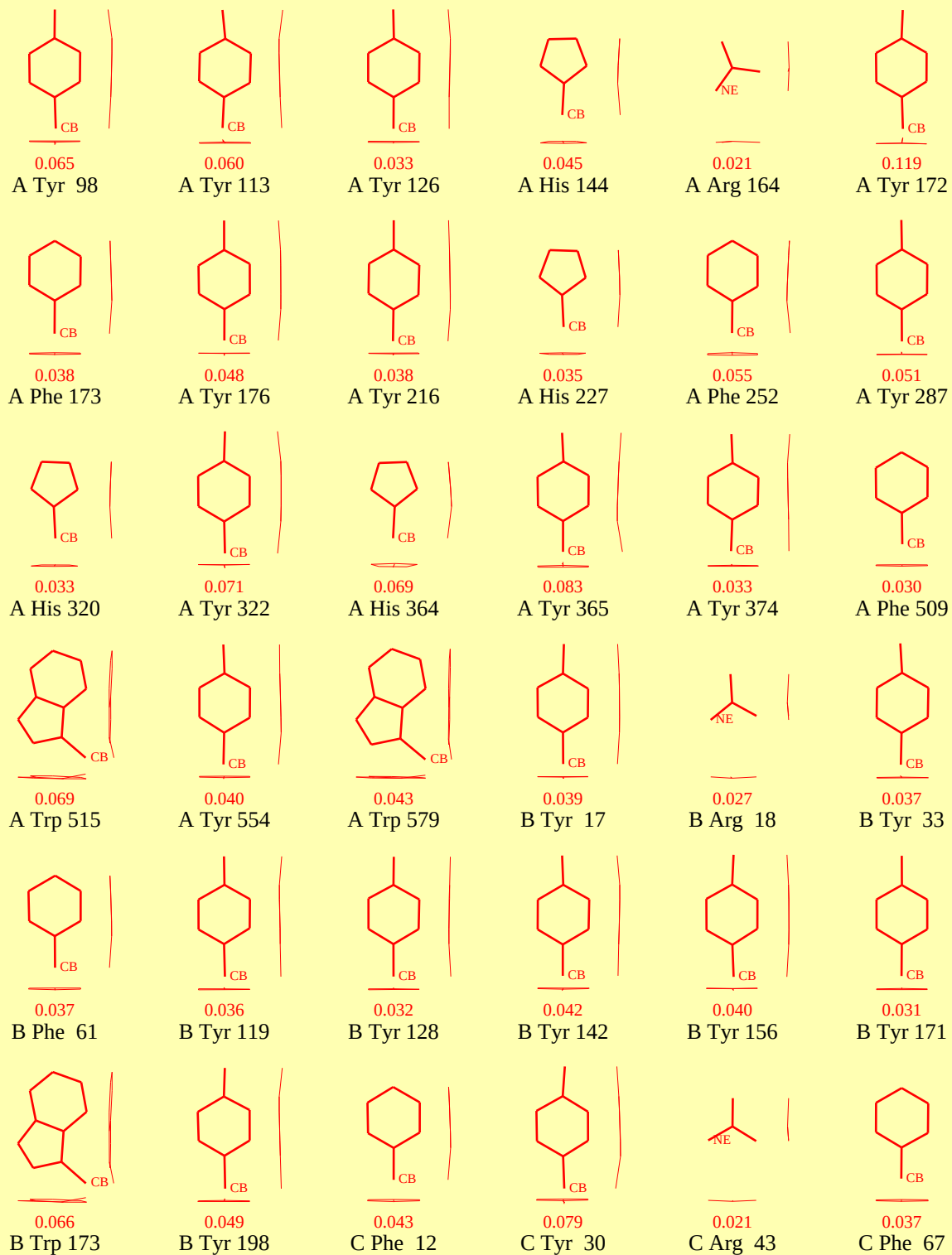
Planar groups



Distorted geometry

pdb1yq3

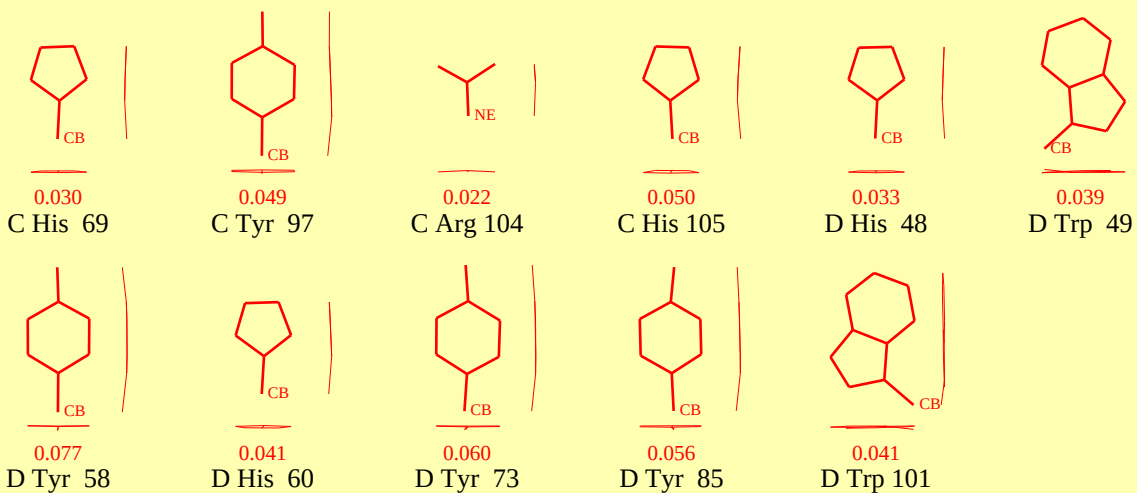
Planar groups (contd)



Distorted geometry

pdb1yq3

Planar groups (contd)



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