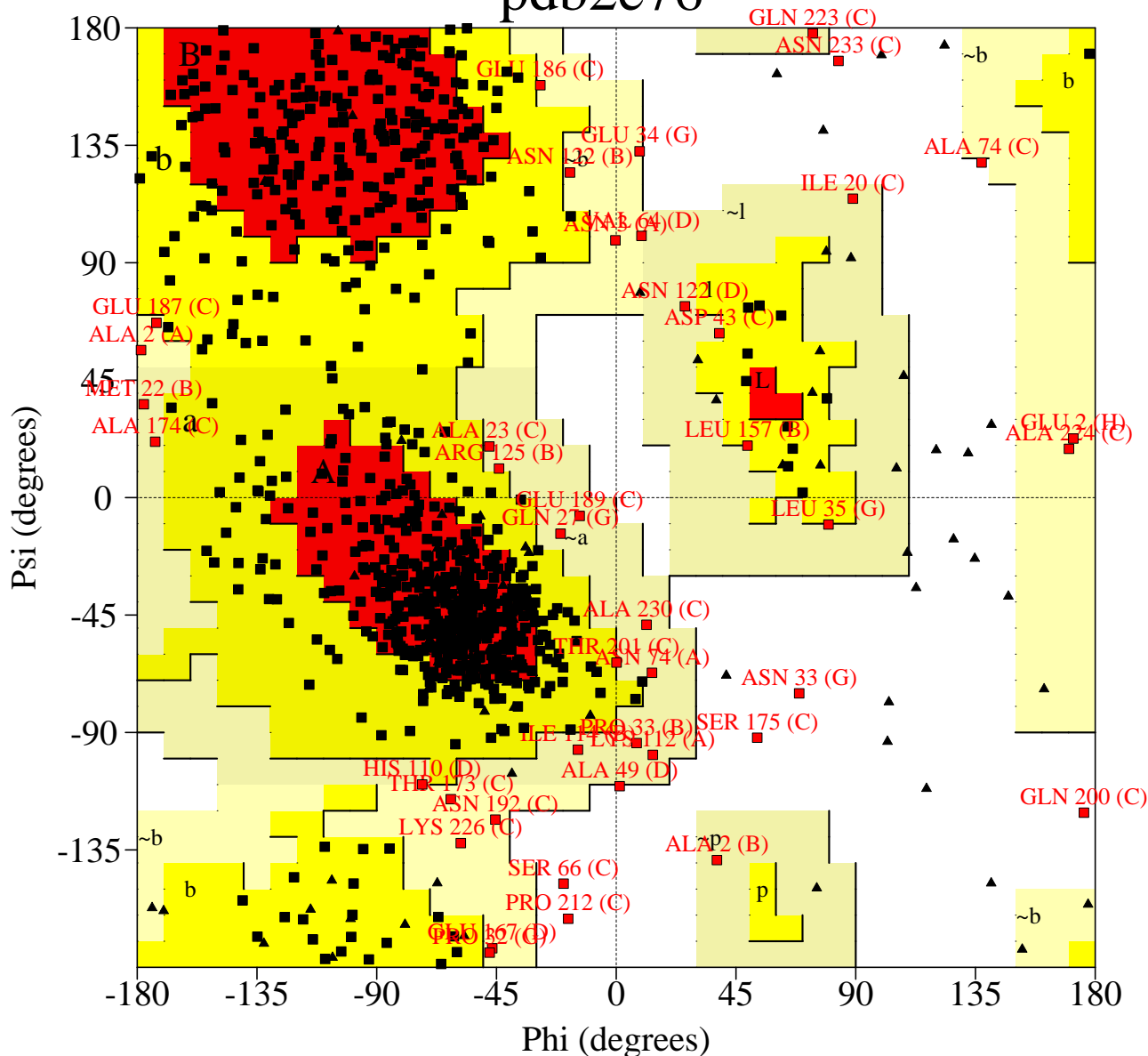


# Ramachandran Plot

pdb2e76



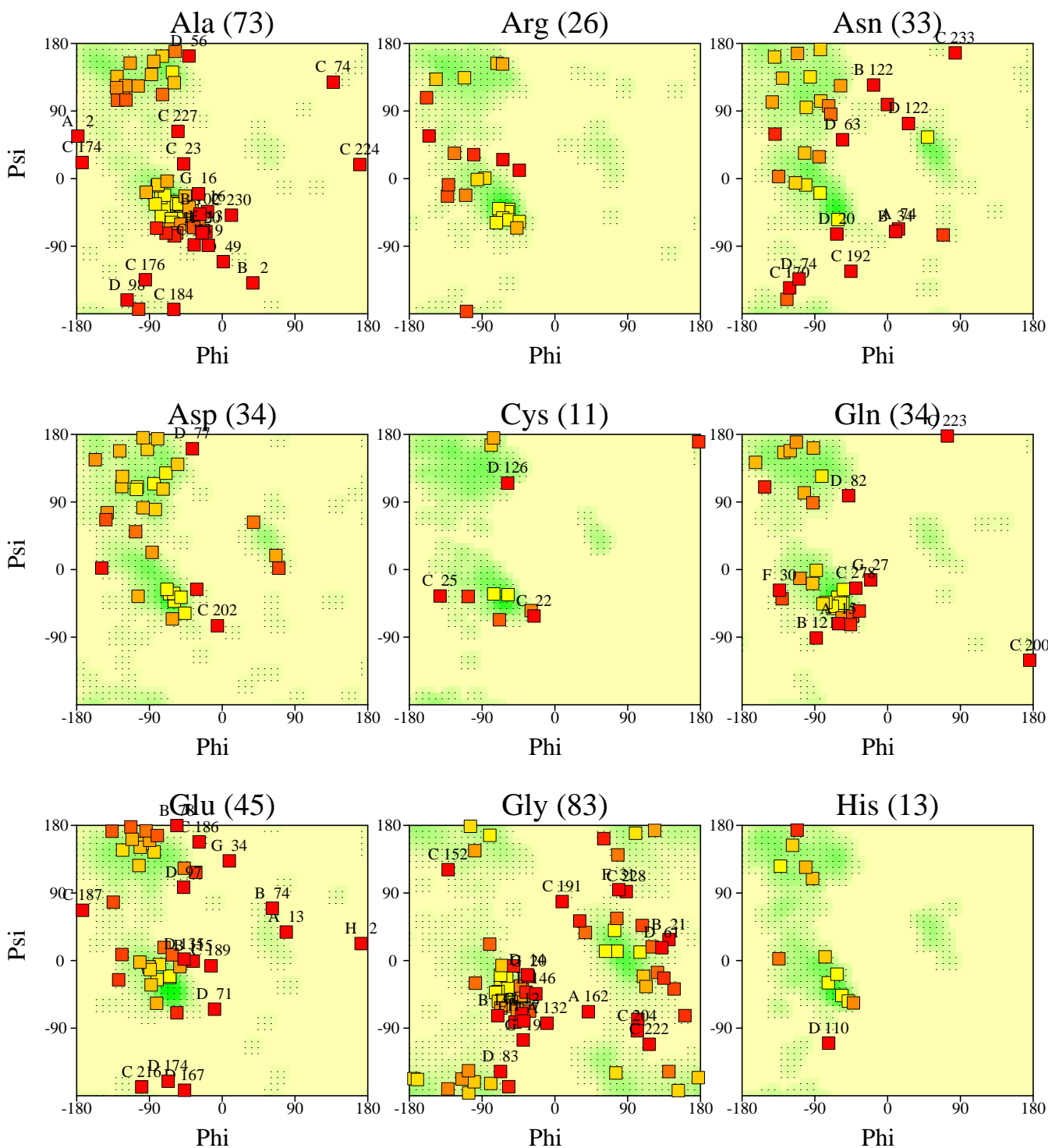
### Plot statistics

Residues in most favoured regions [A,B,L]	550	68.9%
Residues in additional allowed regions [a,b,l,p]	209	26.2%
Residues in generously allowed regions [-a,-b,-l,-p]	32	4.0%
Residues in disallowed regions	7	0.9%
Number of non-glycine and non-proline residues	798	100.0%
Number of end-residues (excl. Gly and Pro)	17	
Number of glycine residues (shown as triangles)	84	
Number of proline residues	62	
Total number of residues	961	

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

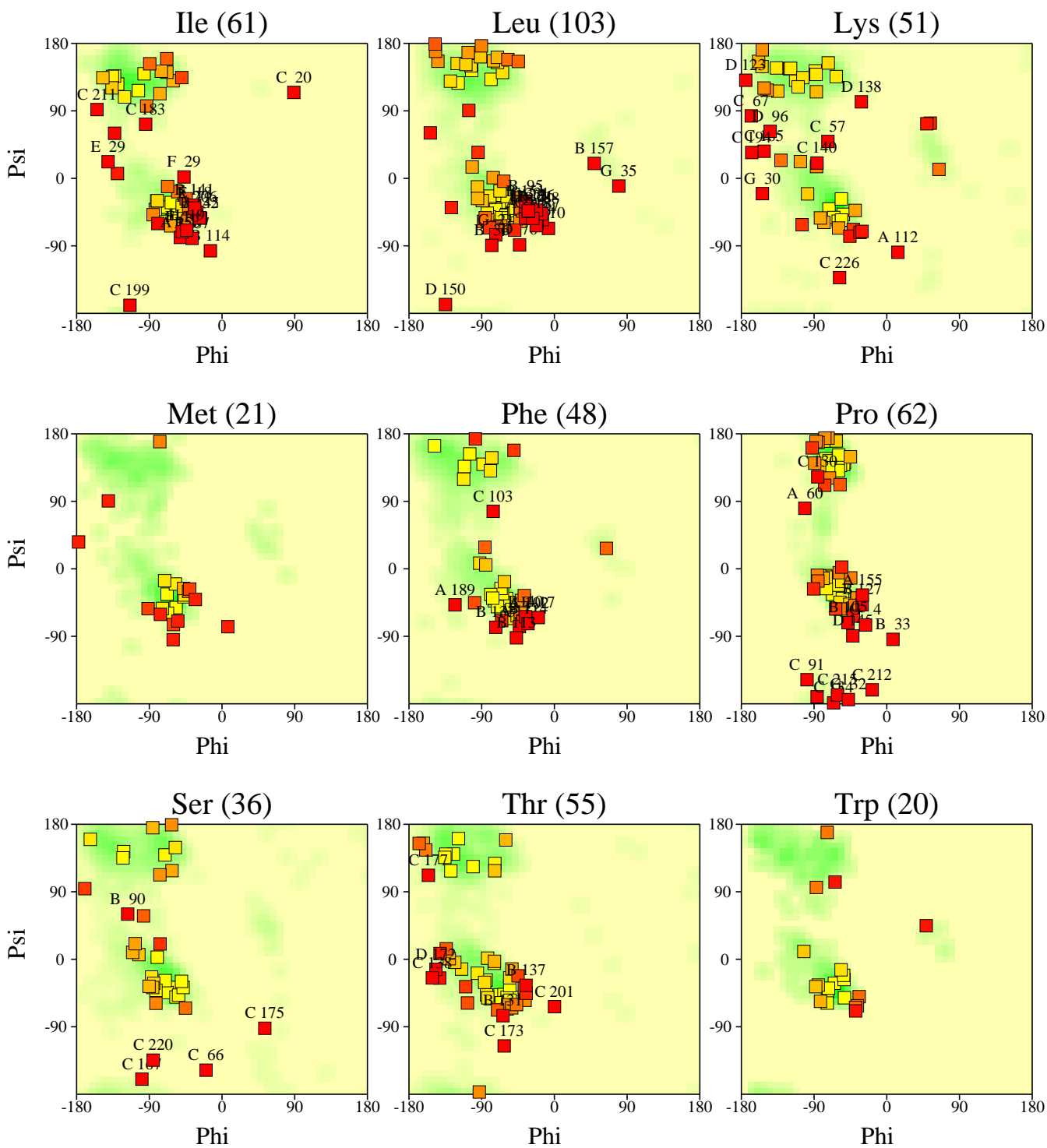
## pdb2e76



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

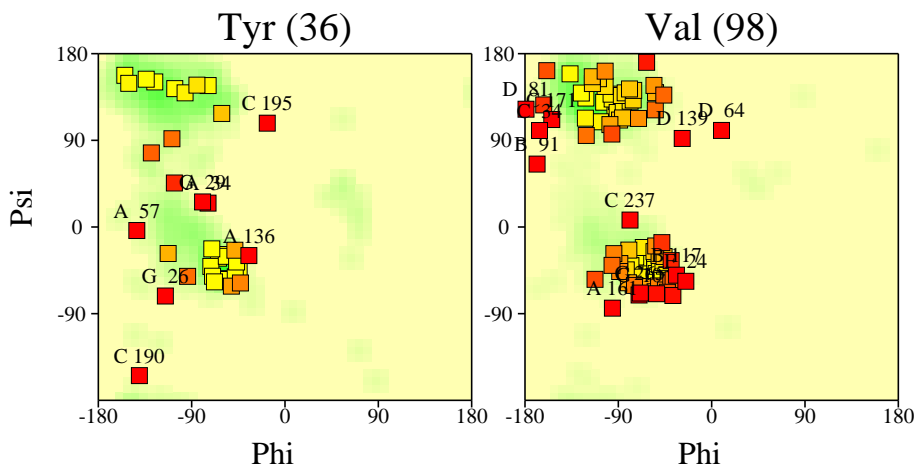
## pdb2e76



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

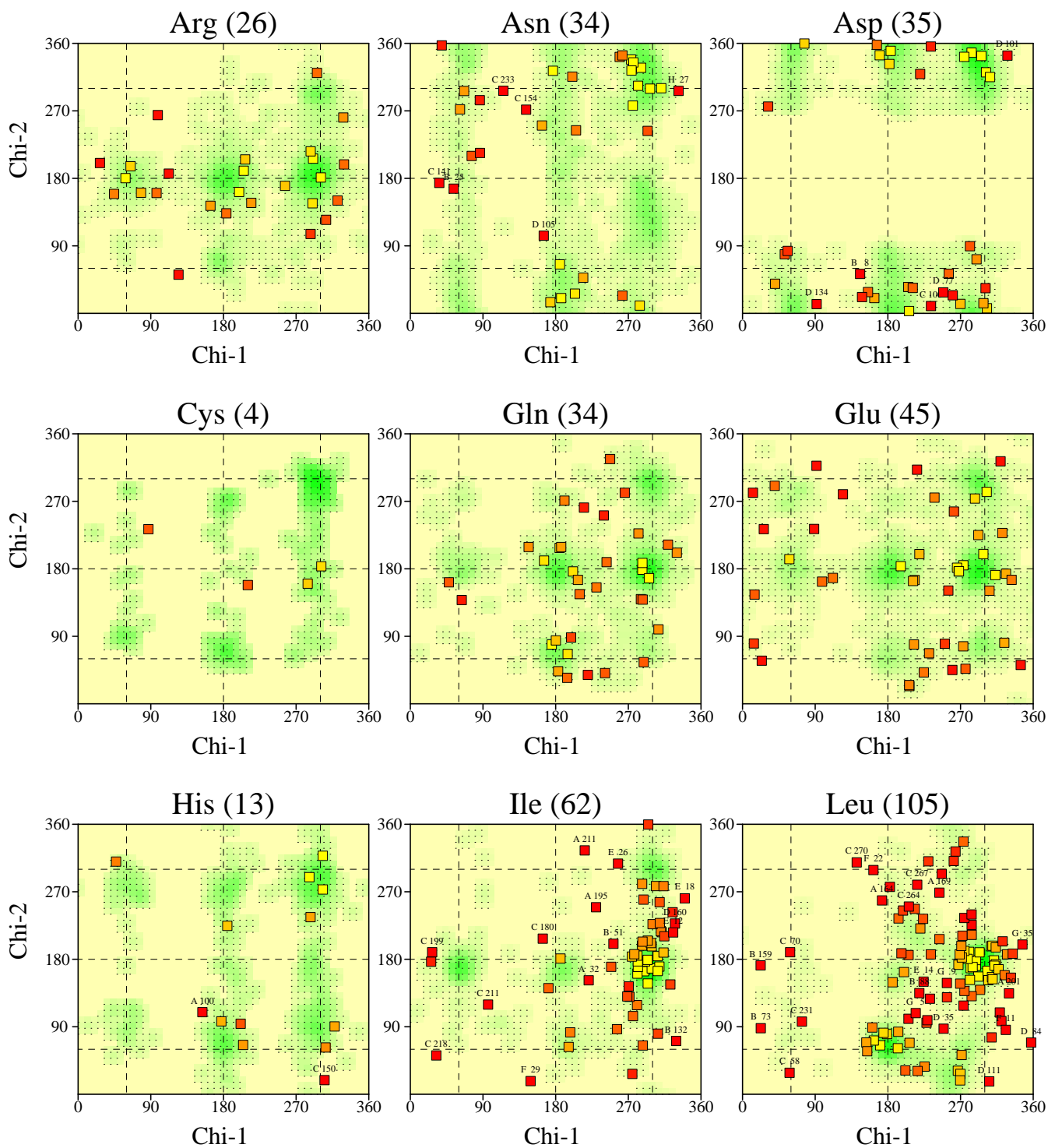
## pdb2e76



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

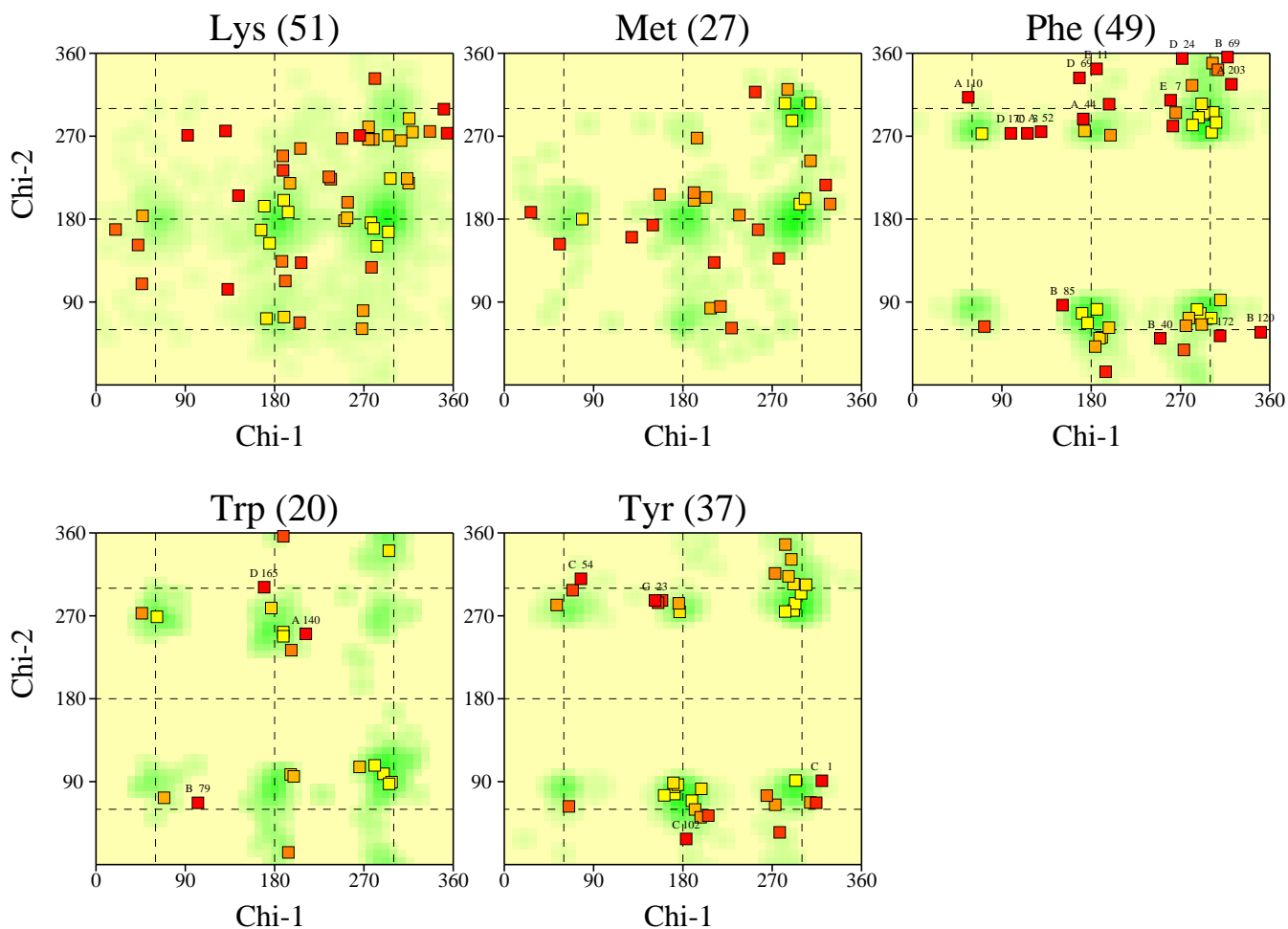
## pdb2e76



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

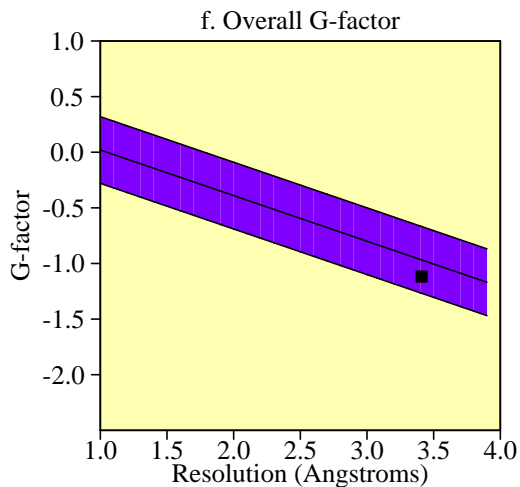
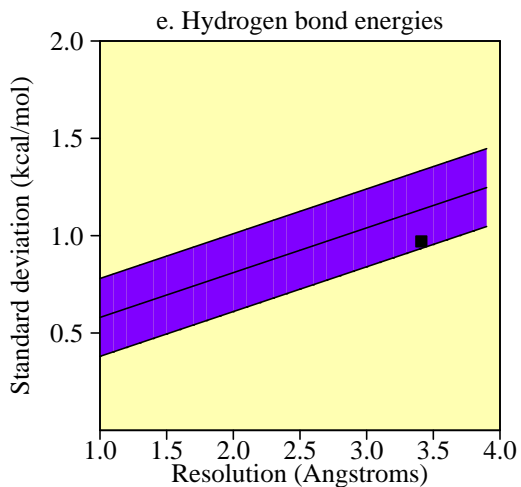
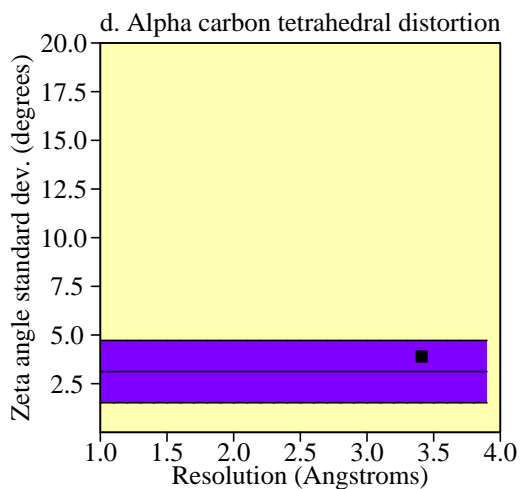
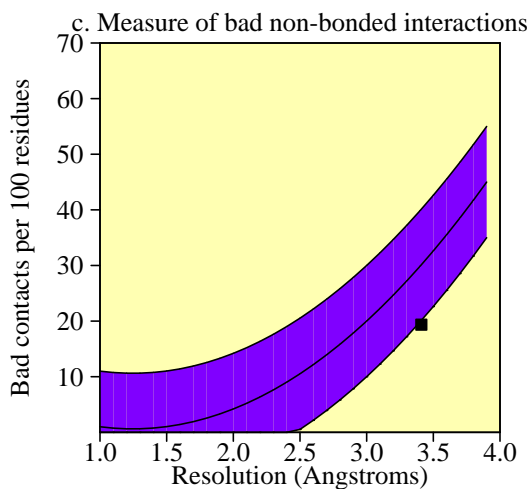
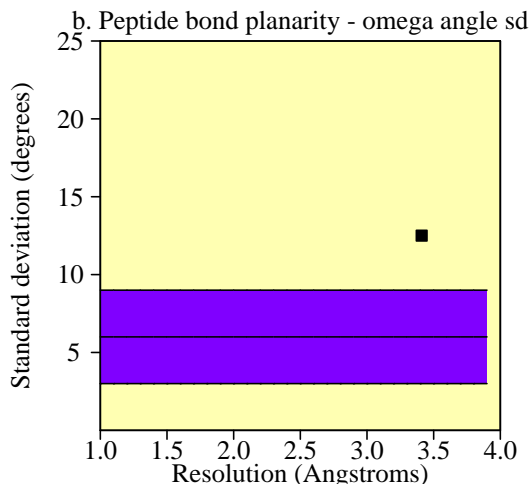
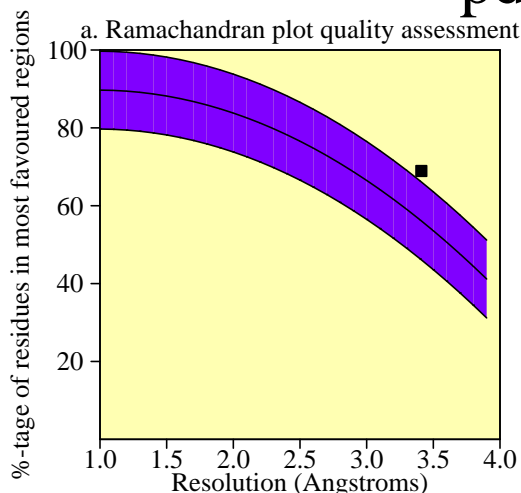
## pdb2e76



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

# Main-chain parameters

## pdb2e76

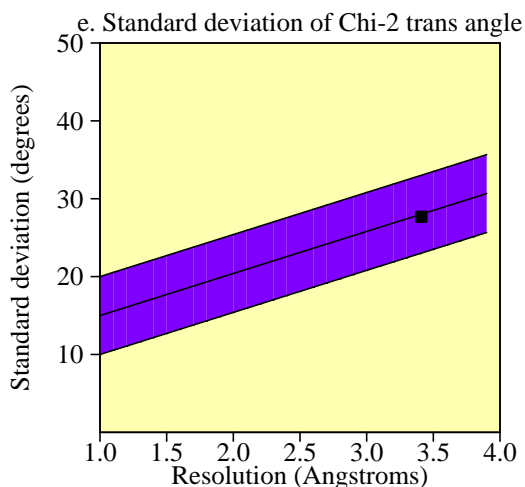
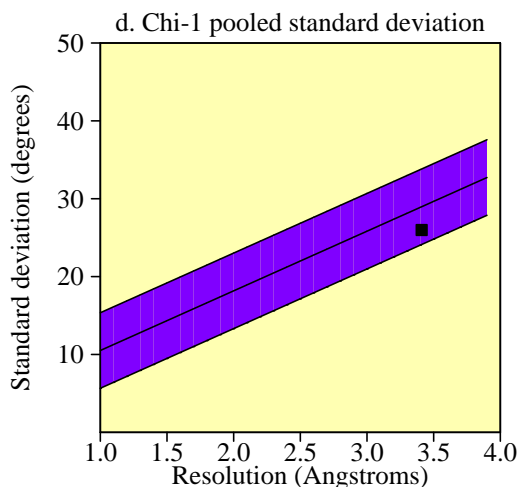
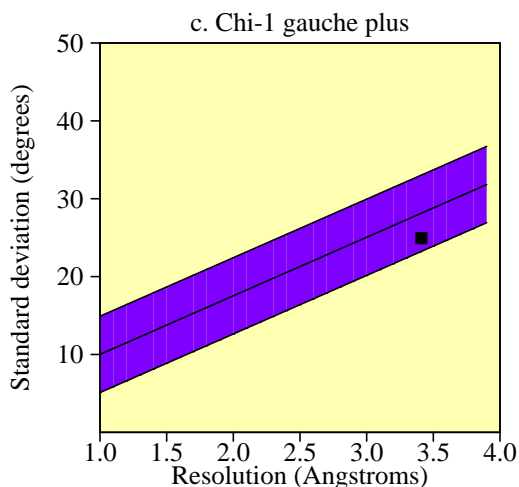
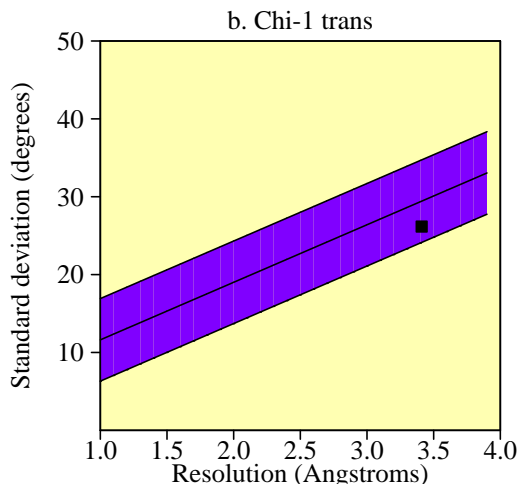
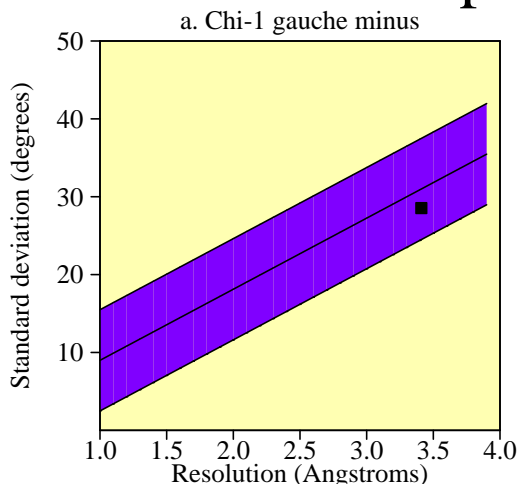


### Plot statistics

Stereochemical parameter	No. of data pts	Parameter value	Comparison values		No. of band widths from mean	
			Typical value	Band width		
a. %-tage residues in A, B, L	798	68.9	56.1	10.0	1.3	BETTER
b. Omega angle st dev	950	12.5	6.0	3.0	2.2	WORSE
c. Bad contacts / 100 residues	186	19.4	30.1	10.0	-1.1	BETTER
d. Zeta angle st dev	877	3.9	3.1	1.6	0.5	Inside
e. H-bond energy st dev	584	1.0	1.1	0.2	-0.8	Inside
f. Overall G-factor	961	-1.1	-1.0	0.3	-0.5	Inside

# Side-chain parameters

## pdb2e76



pdb2e76

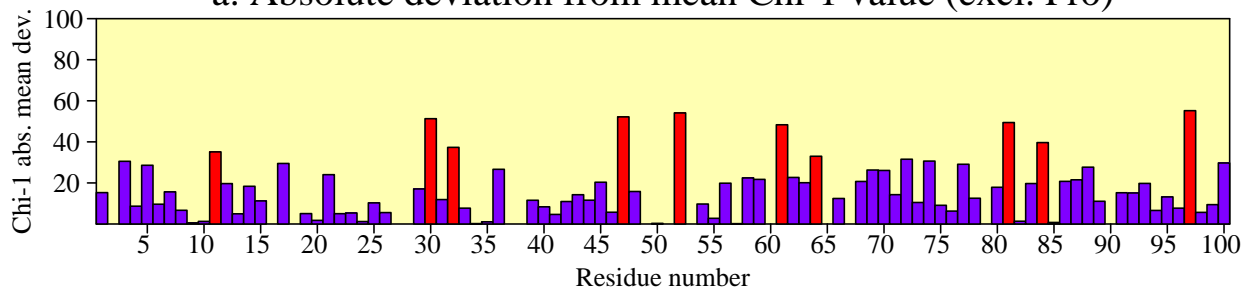
### Plot statistics

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	113	28.5	31.0	6.5	-0.4	Inside
b. Chi-1 trans st dev	277	26.2	29.4	5.3	-0.6	Inside
c. Chi-1 gauche plus st dev	351	24.9	28.1	4.9	-0.7	Inside
d. Chi-1 pooled st dev	741	26.0	29.0	4.8	-0.6	Inside
e. Chi-2 trans st dev	207	27.7	28.0	5.0	-0.1	Inside

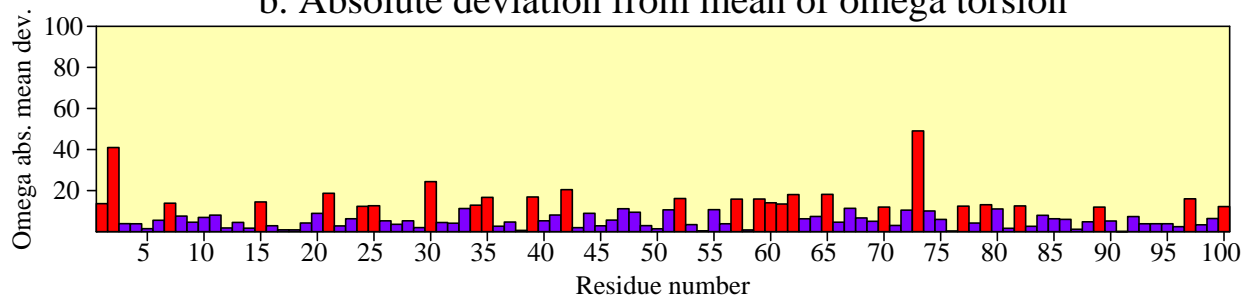


# Residue properties pdb2e76

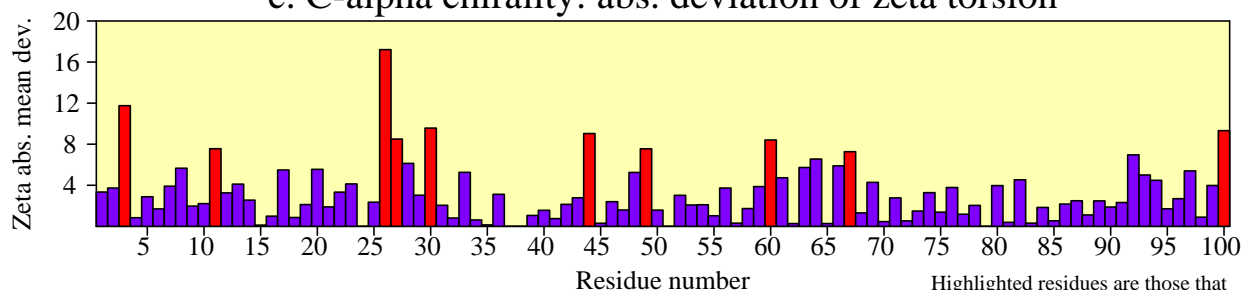
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



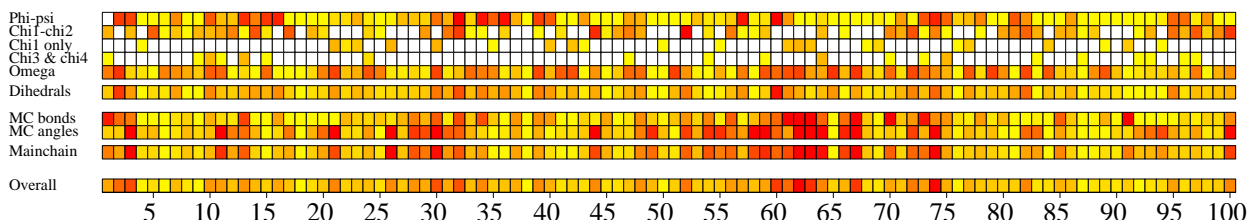
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

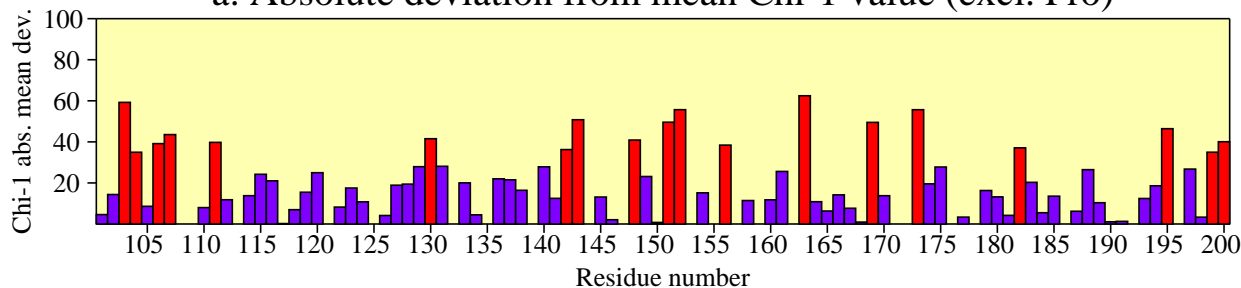


g. G-factors

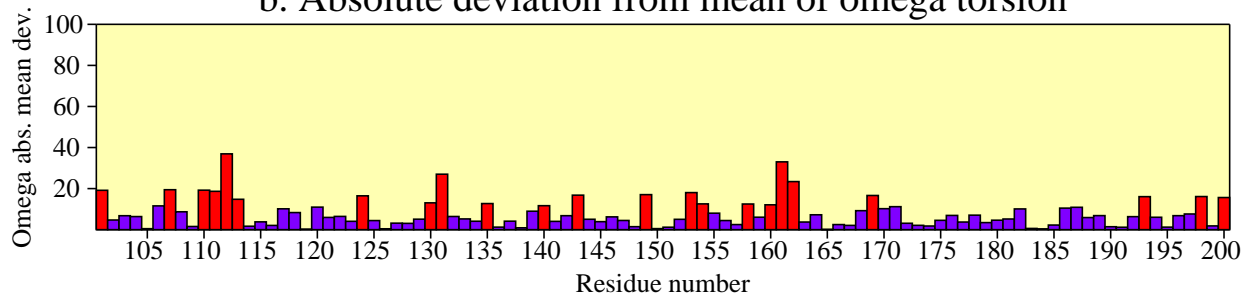


# Residue properties pdb2e76

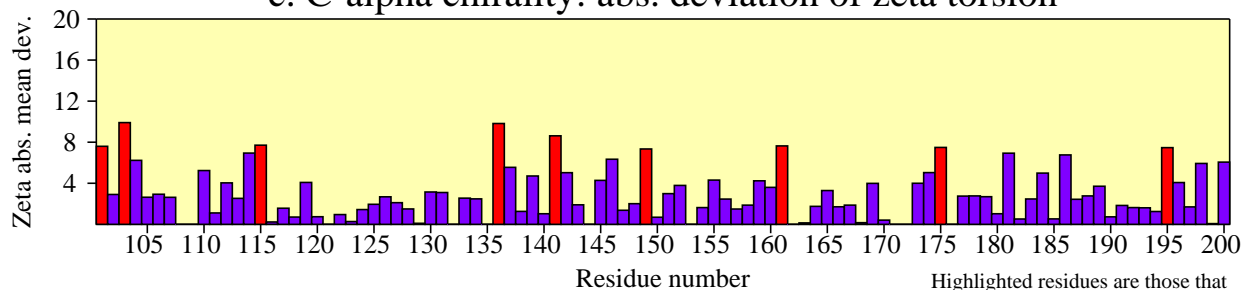
a. Absolute deviation from mean Chi-1 value (excl. Pro)



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



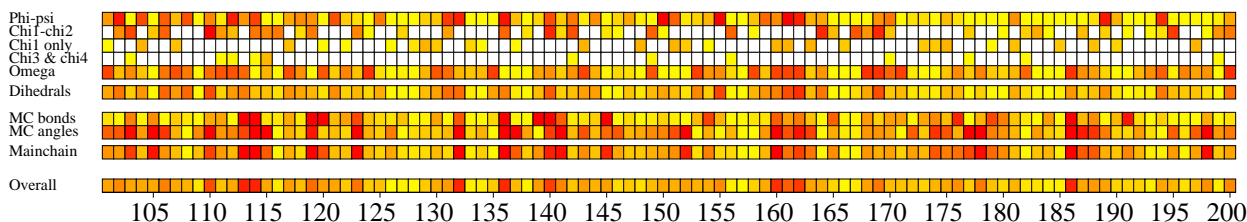
e. Sequence & Ramachandran regions Most favoured Allowed Generous Disallowed



f. Max. deviation (see listing)



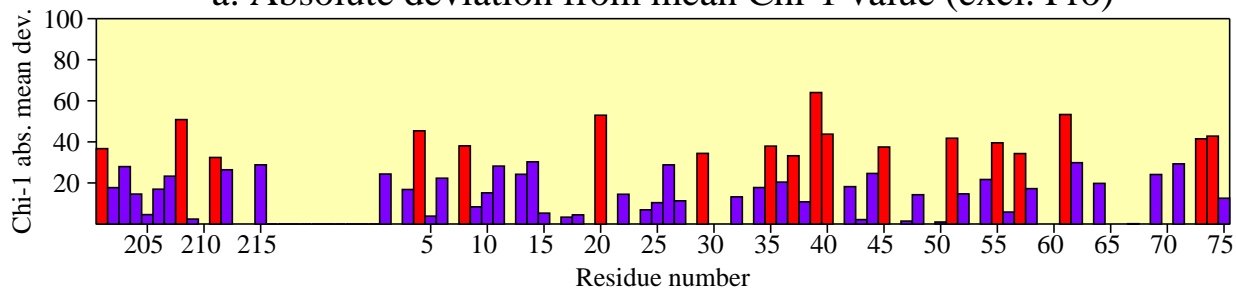
g. G-factors



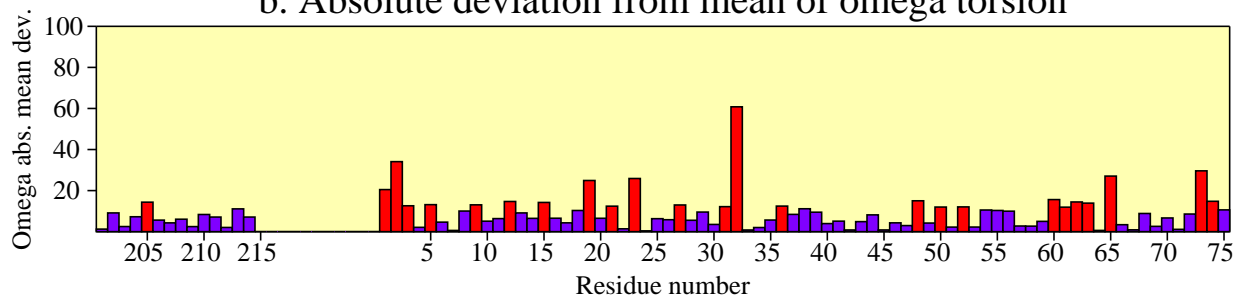
# Residue properties

## pdb2e76

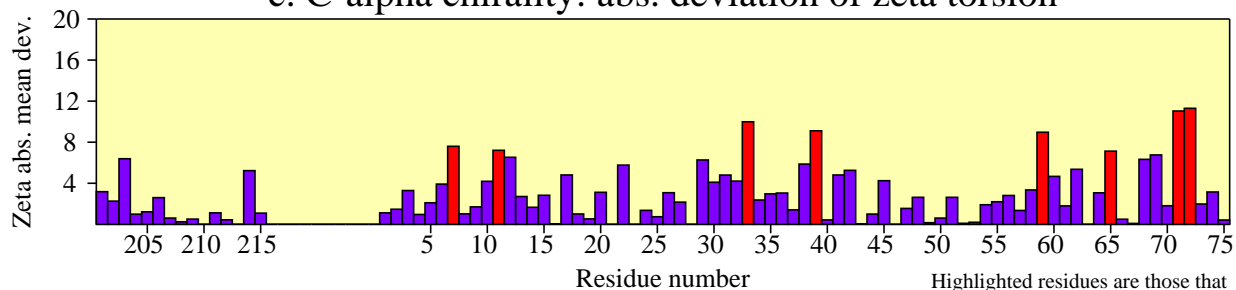
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

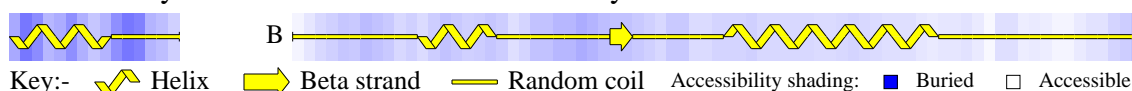


c. C-alpha chirality: abs. deviation of zeta torsion



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

d. Secondary structure & estimated accessibility



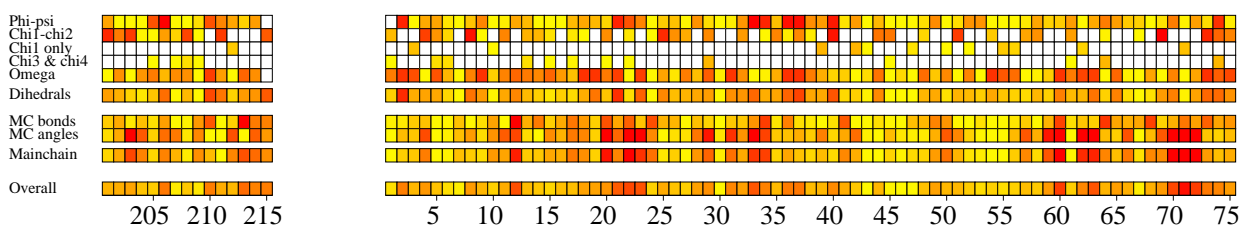
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

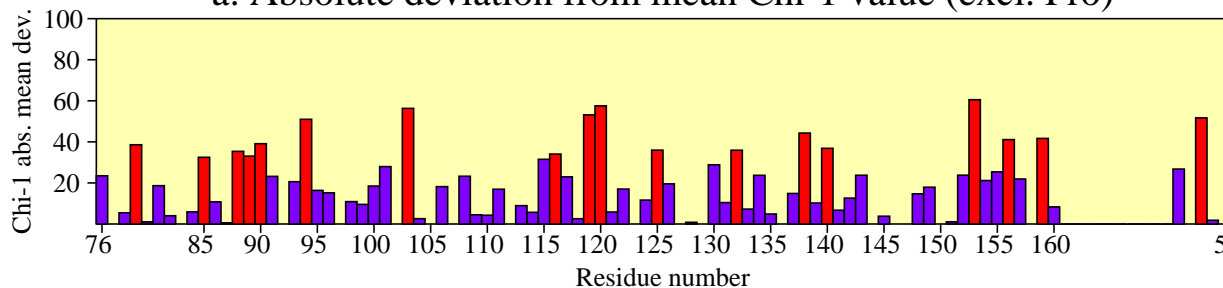


g. G-factors

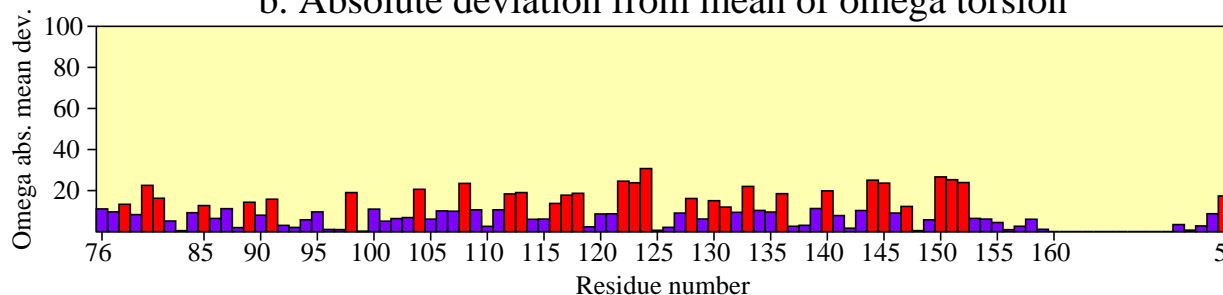


# Residue properties pdb2e76

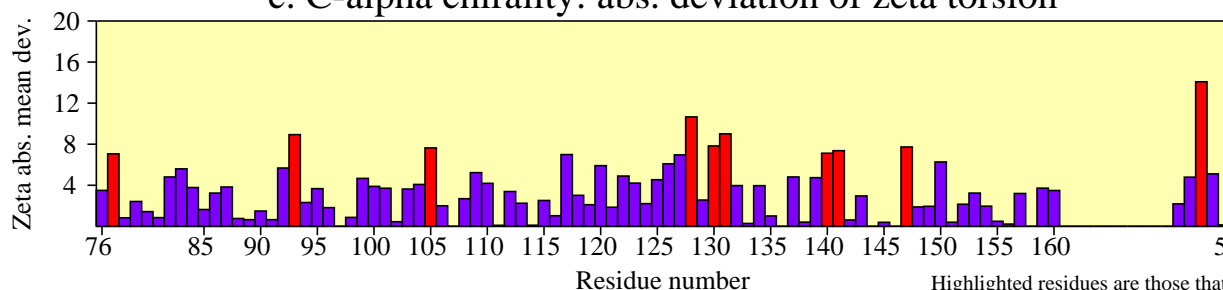
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

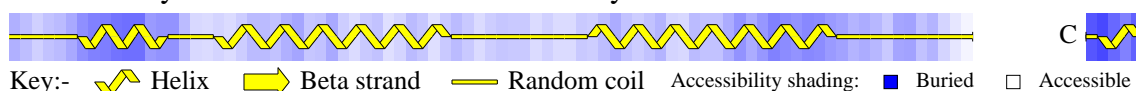


c. C-alpha chirality: abs. deviation of zeta torsion



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

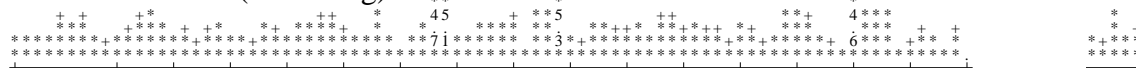
d. Secondary structure & estimated accessibility



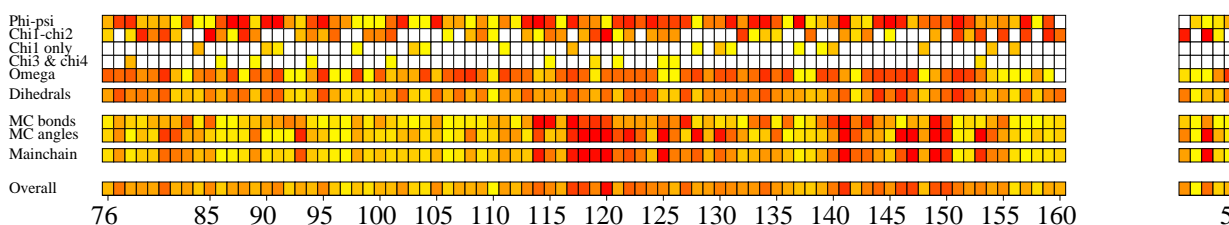
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

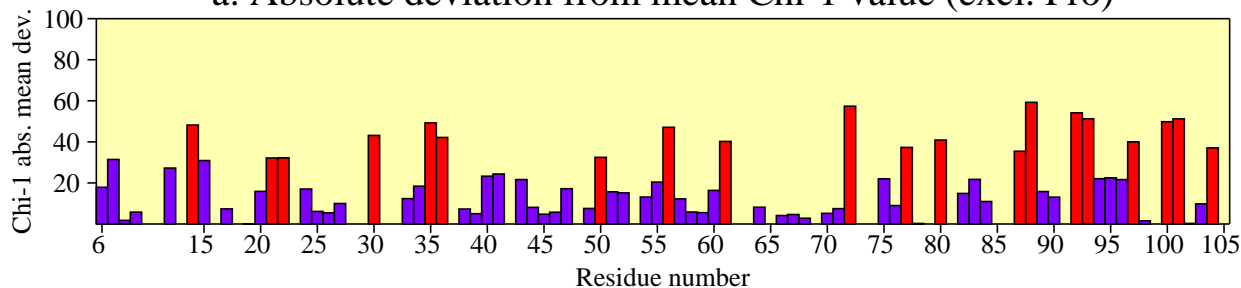


g. G-factors

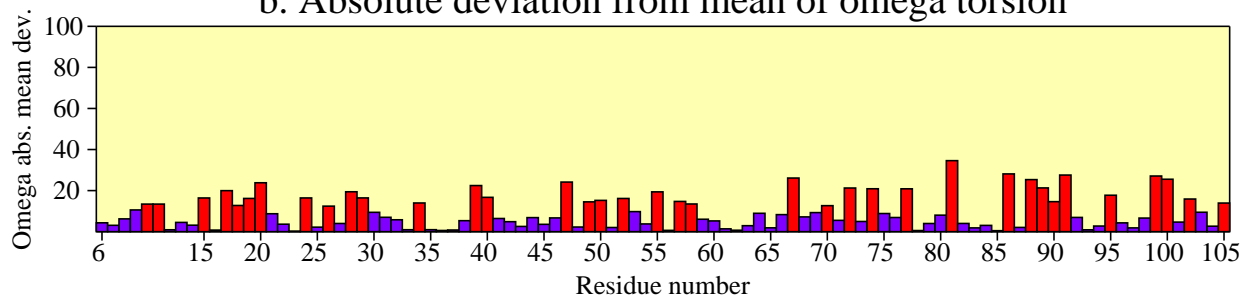


# Residue properties pdb2e76

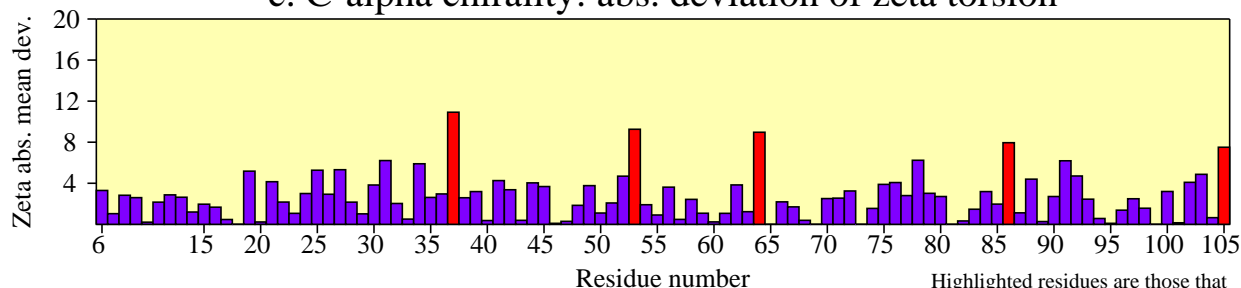
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

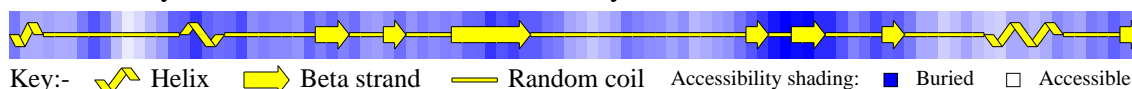


### c. C-alpha chirality: abs. deviation of zeta torsion



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

### d. Secondary structure & estimated accessibility



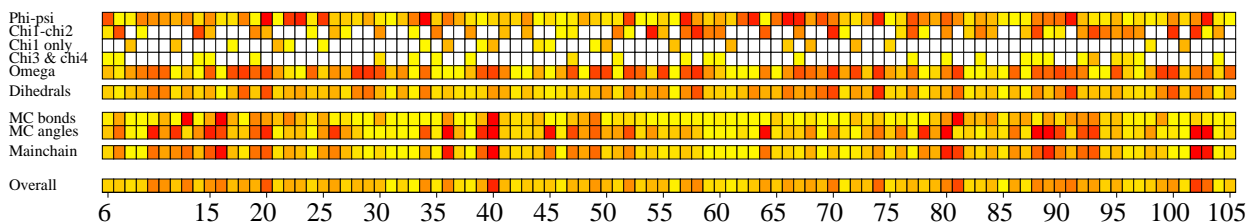
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

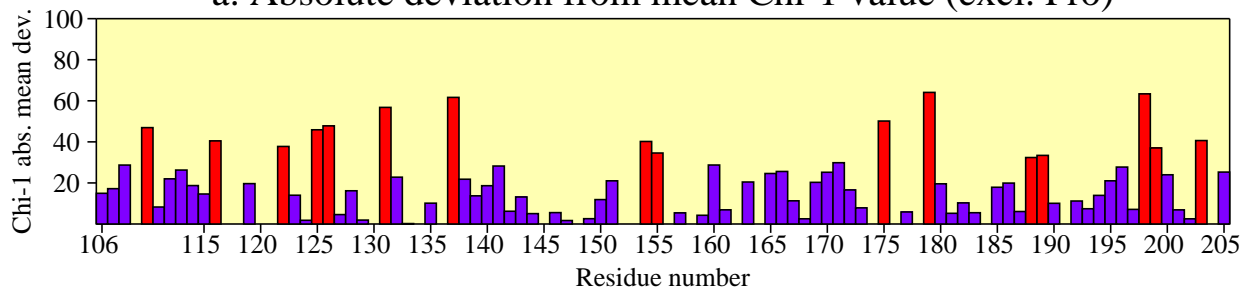


### g. G-factors

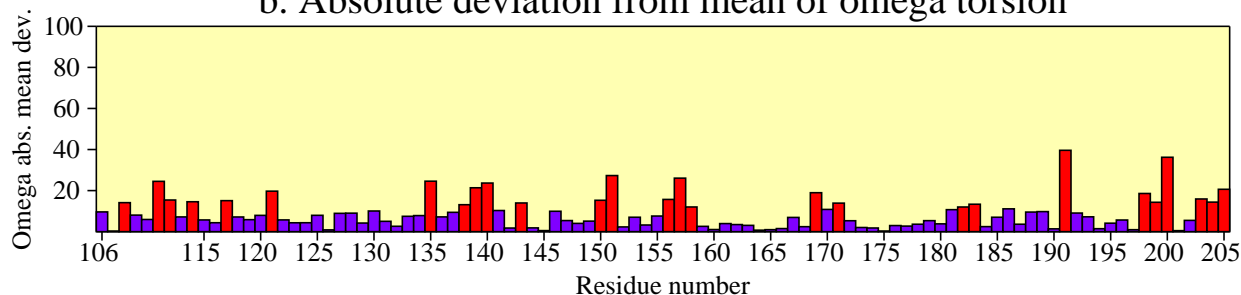


# Residue properties pdb2e76

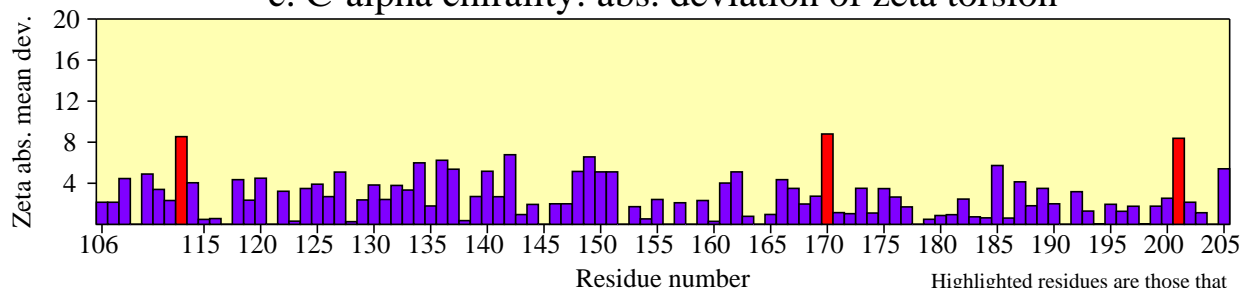
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

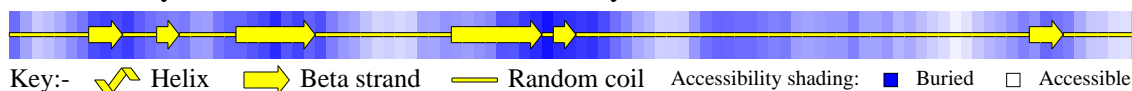


c. C-alpha chirality: abs. deviation of zeta torsion



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

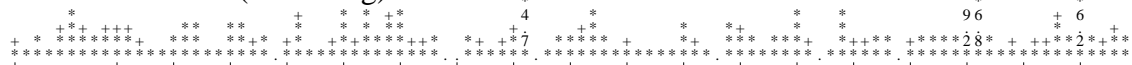
d. Secondary structure & estimated accessibility



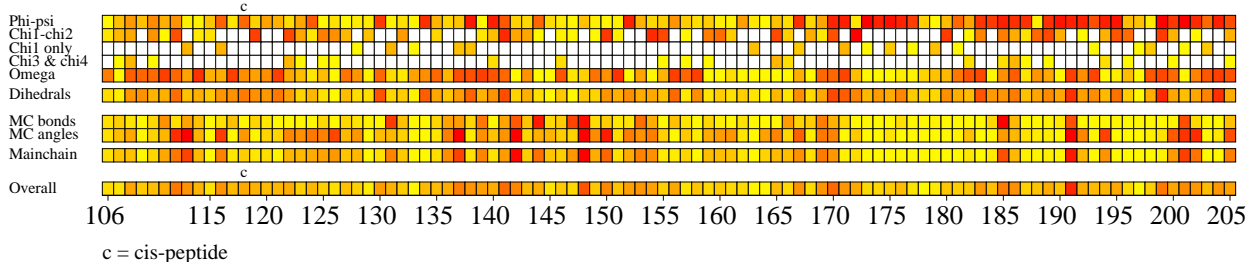
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

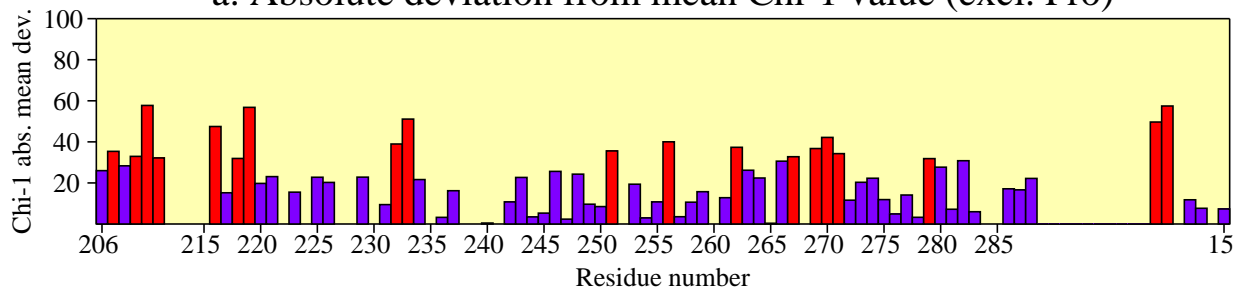


g. G-factors

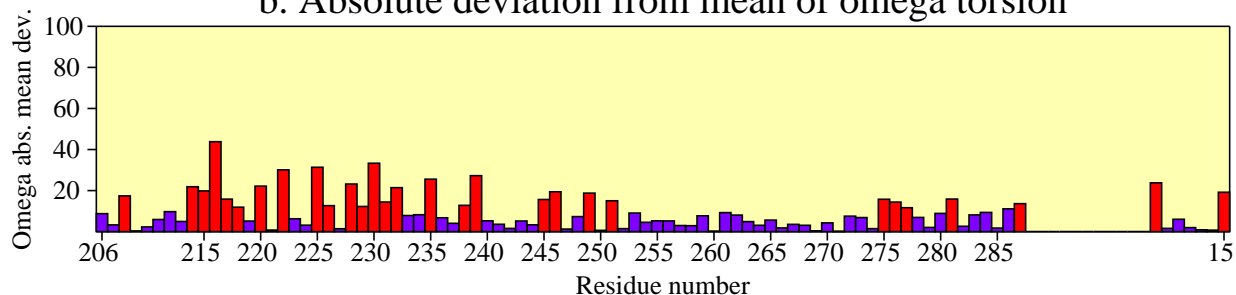


# Residue properties pdb2e76

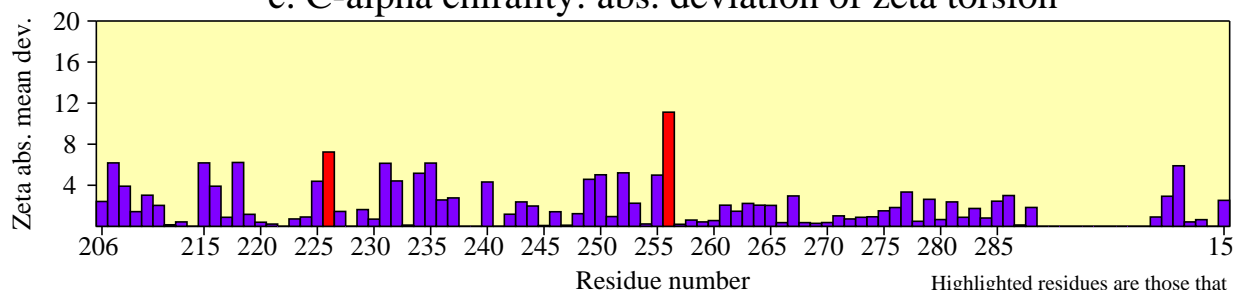
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

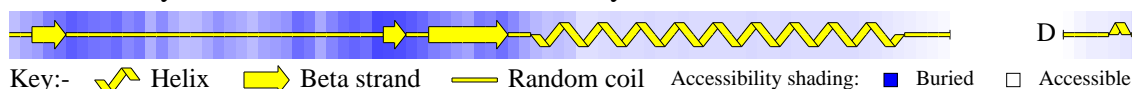


c. C-alpha chirality: abs. deviation of zeta torsion



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

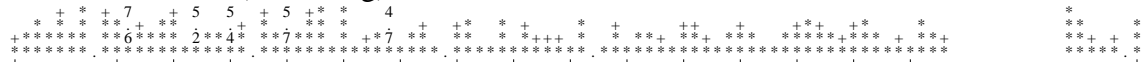
d. Secondary structure & estimated accessibility



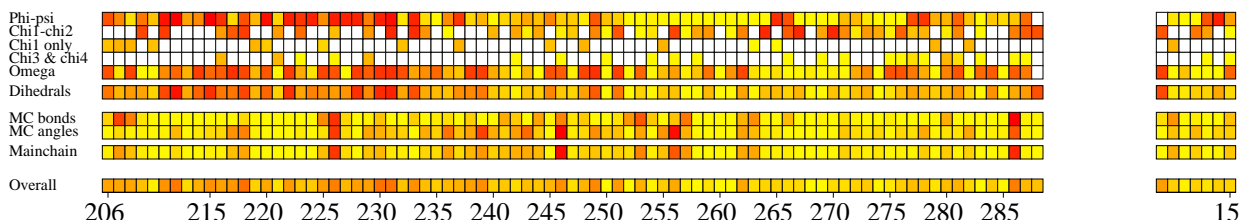
e. Sequence & Ramachandran regions



f. Max. deviation\* (see listing)

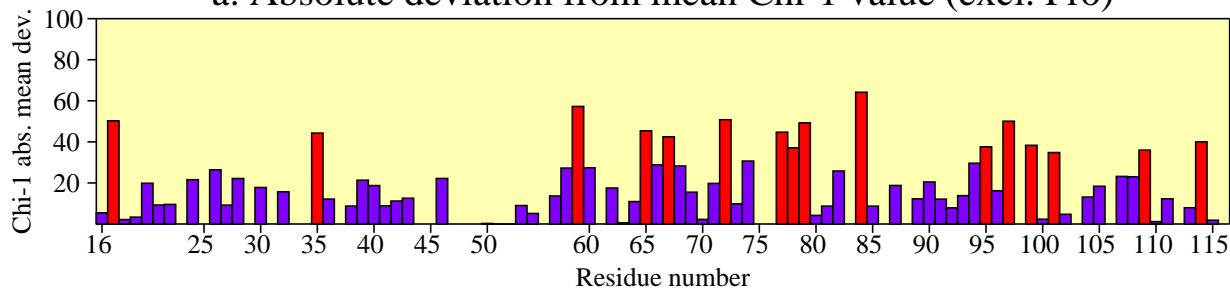


g. G-factors

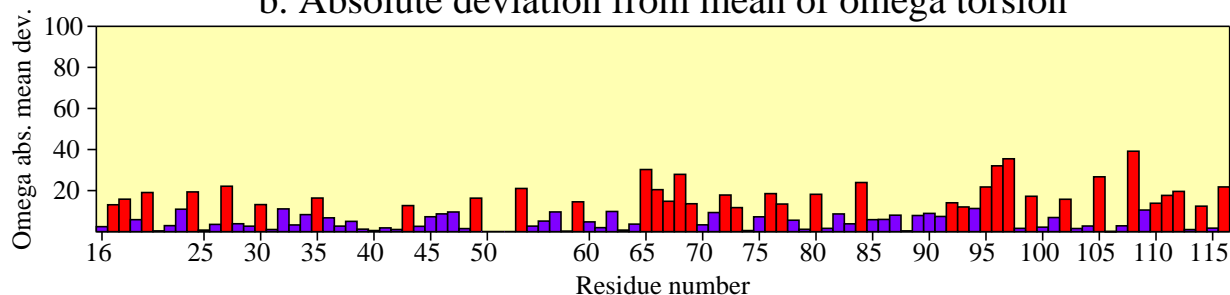


# Residue properties pdb2e76

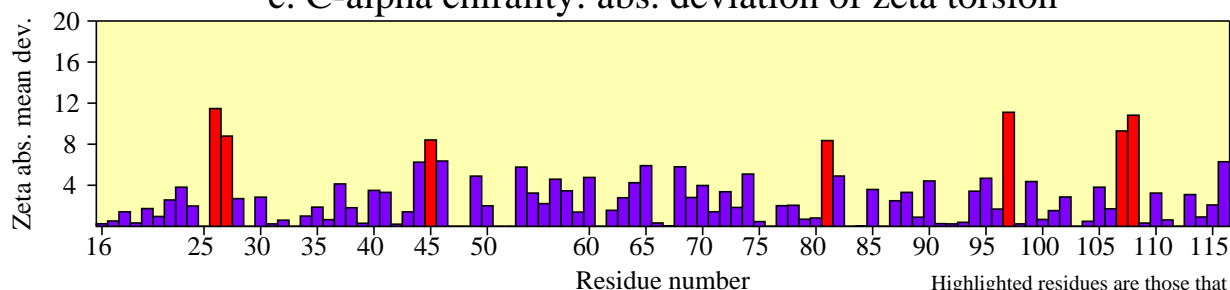
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion

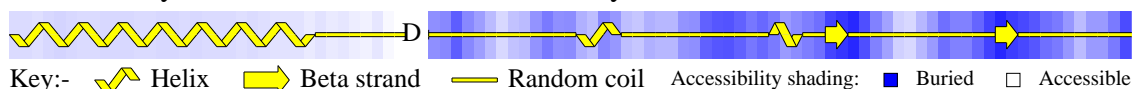


c. C-alpha chirality: abs. deviation of zeta torsion



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

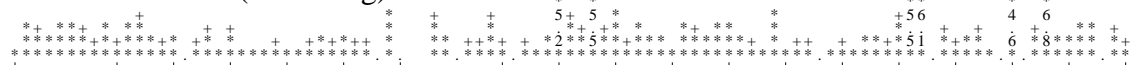
d. Secondary structure & estimated accessibility



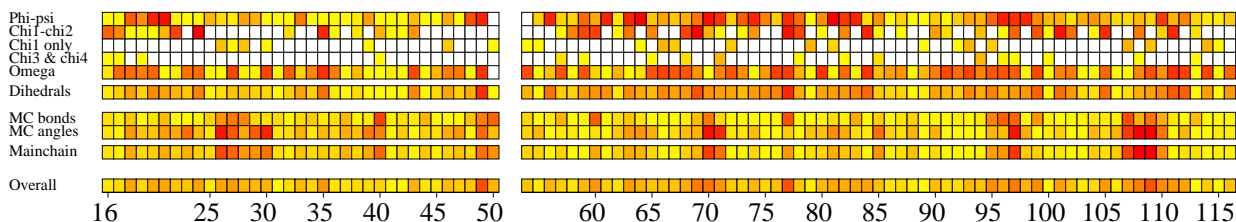
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)



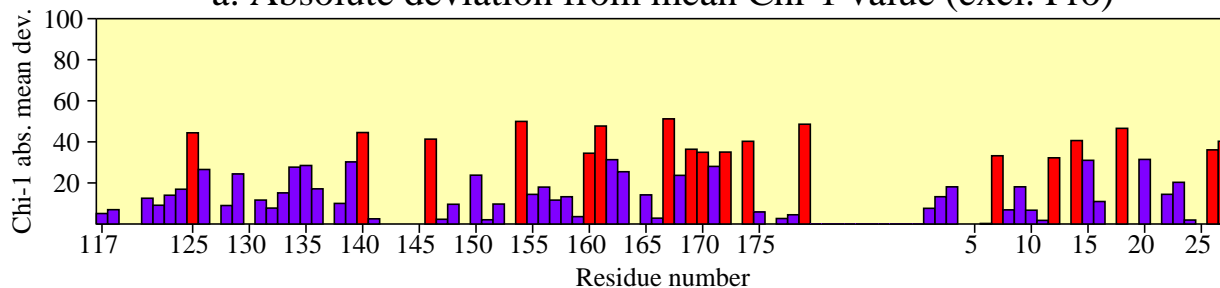
g. G-factors



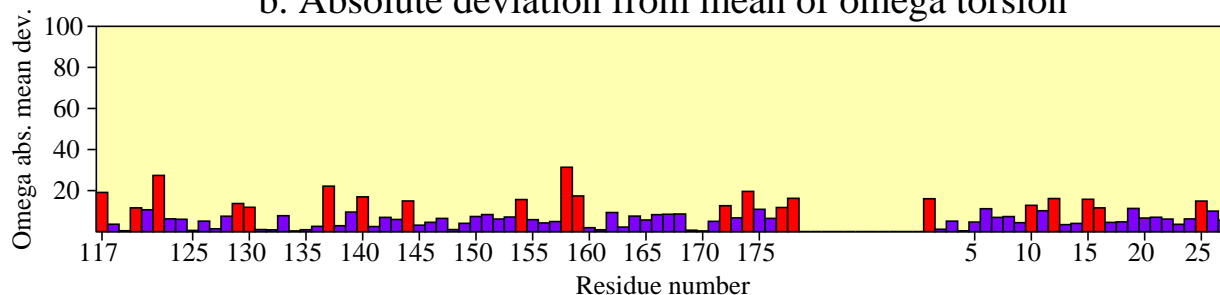


# Residue properties pdb2e76

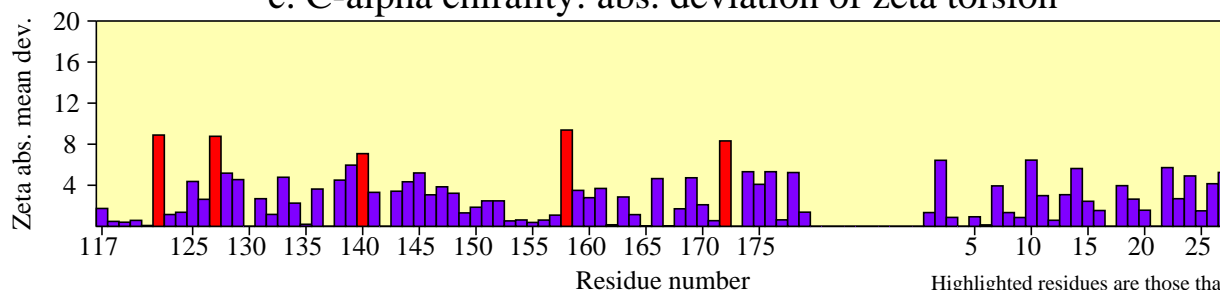
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

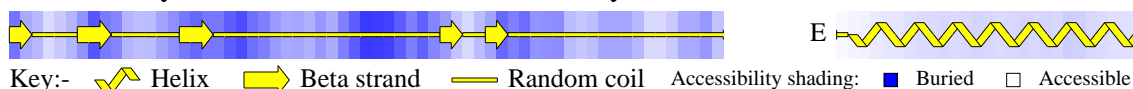


### c. C-alpha chirality: abs. deviation of zeta torsion

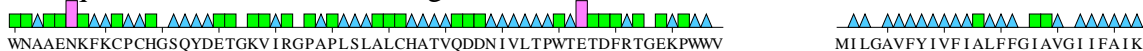


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

### d. Secondary structure & estimated accessibility



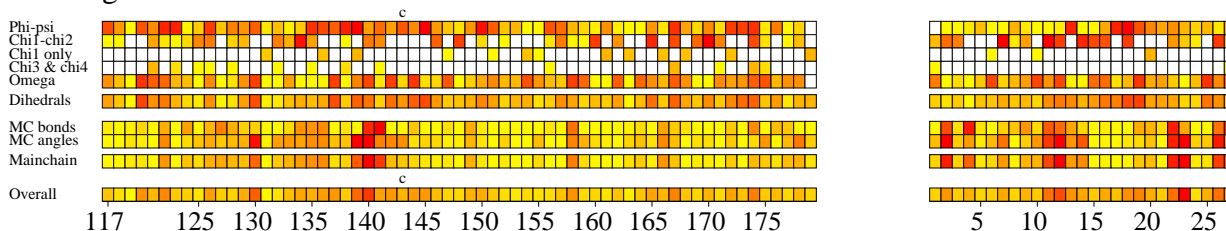
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)



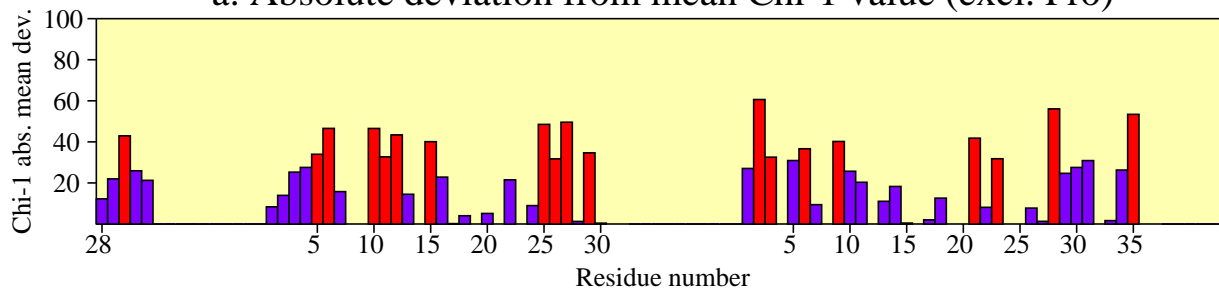
### g. G-factors



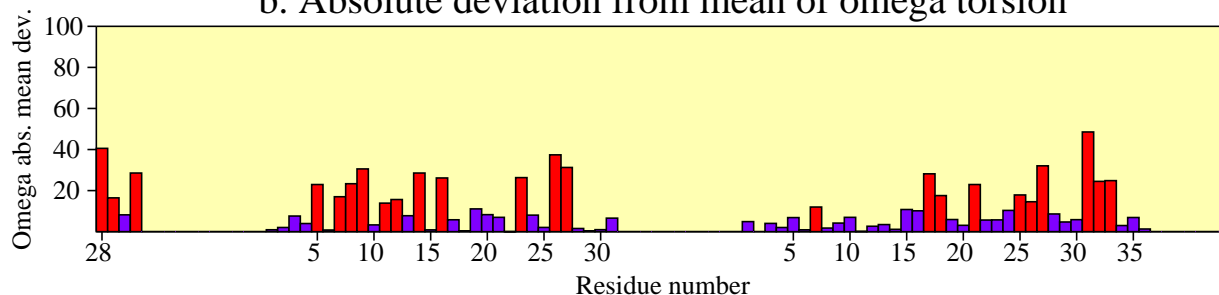
c = cis-peptide

# Residue properties pdb2e76

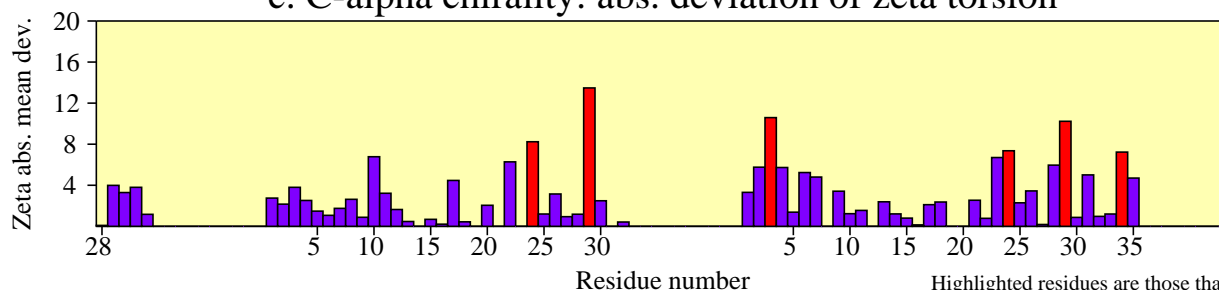
### a. Absolute deviation from mean Chi-1 value (excl. Pro)



### b. Absolute deviation from mean of omega torsion

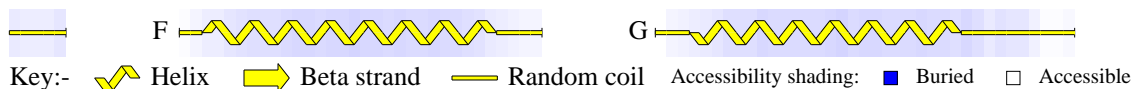


### c. C-alpha chirality: abs. deviation of zeta torsion



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

### d. Secondary structure & estimated accessibility



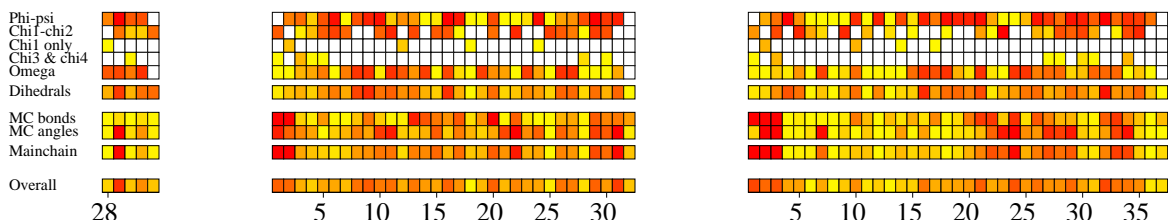
### e. Sequence & Ramachandran regions



### f. Max. deviation (see listing)

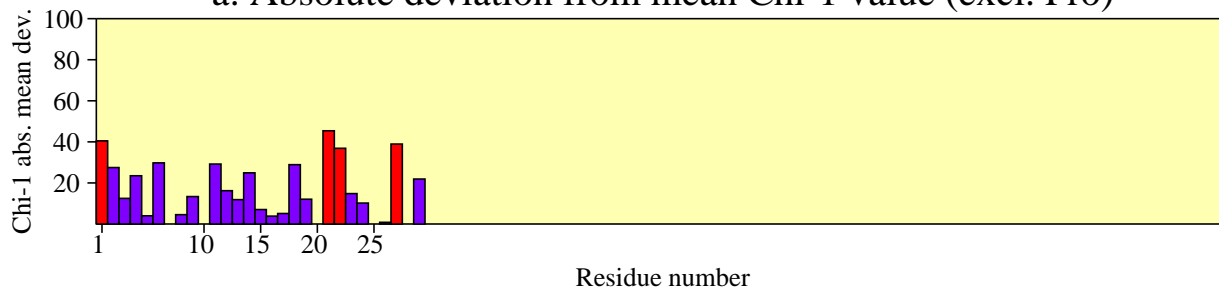


### g. G-factors

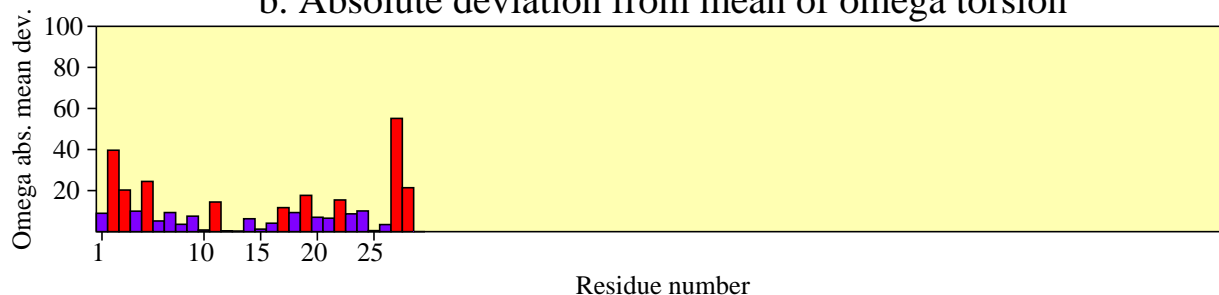


# Residue properties pdb2e76

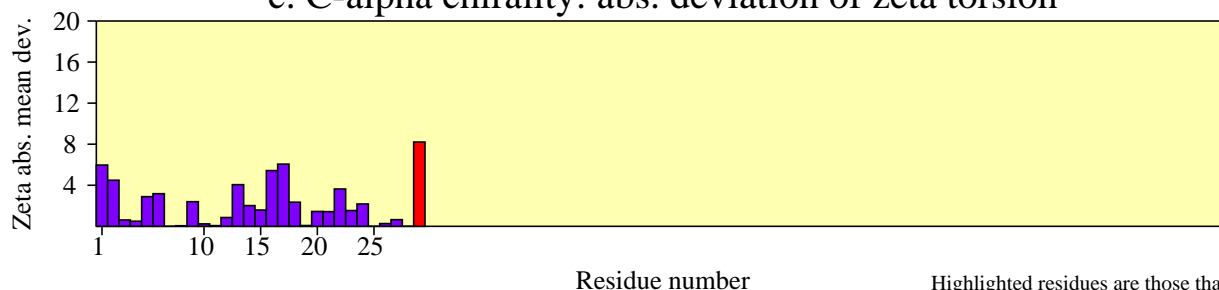
a. Absolute deviation from mean Chi-1 value (excl. Pro)



b. Absolute deviation from mean of omega torsion



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

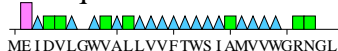


Highlighted residues are those that deviate by more than 2.0 st. devs. from ideal

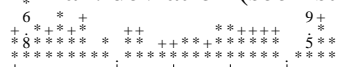
d. Secondary structure & estimated accessibility



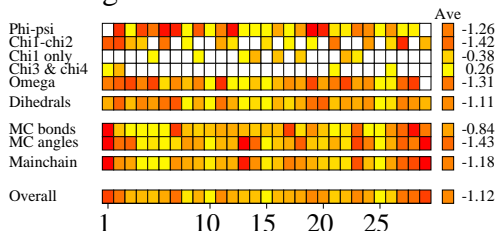
e. Sequence & Ramachandran regions



f. Max. deviation (see listing)

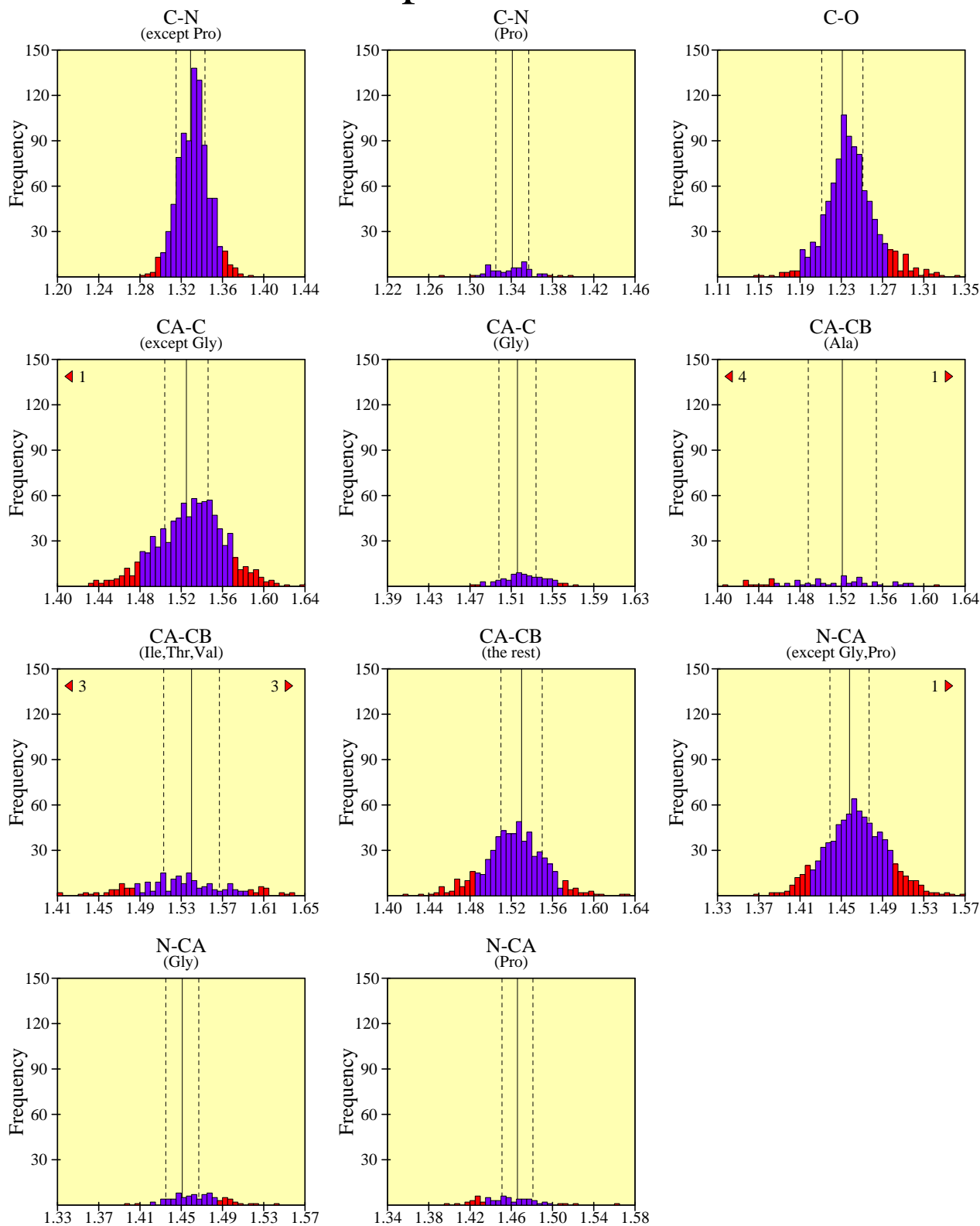


g. G-factors



# Main-chain bond lengths

## pdb2e76



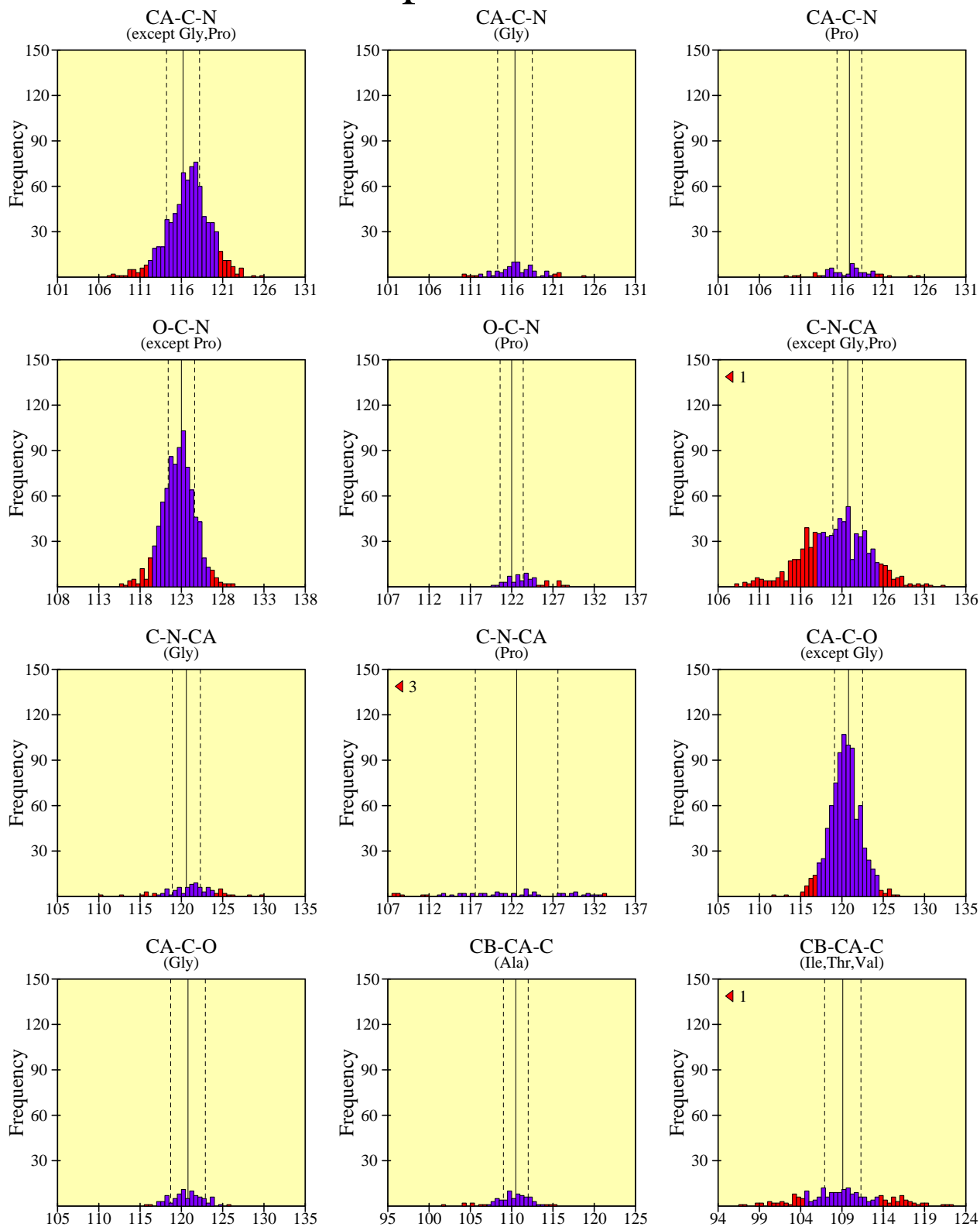
Black bars > 2.0 st. devs. from mean.

◀ 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

## pdb2e76



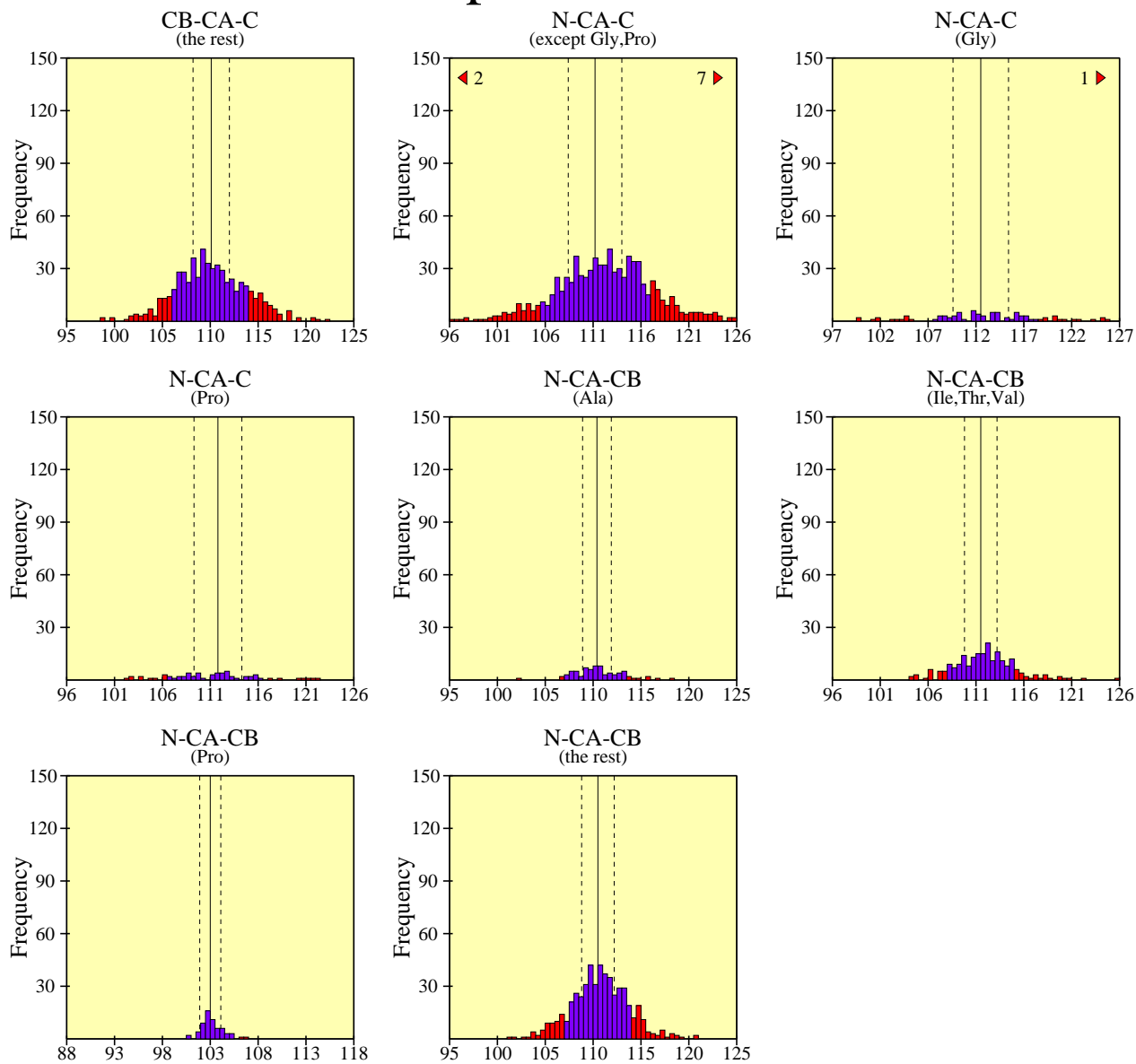
Black bars > 2.0 st. devs. from mean.

◀ 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

## pdb2e76



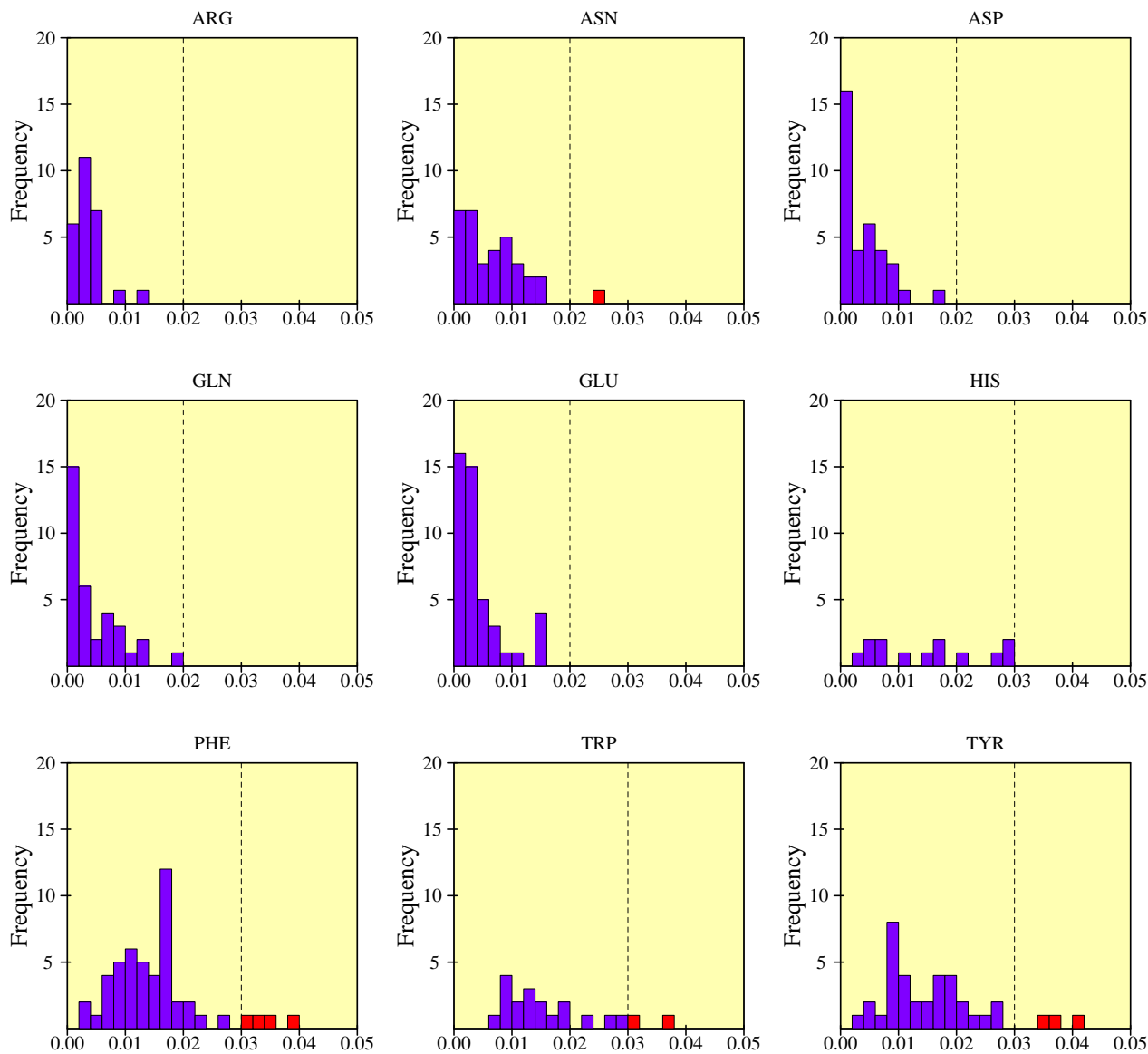
Black bars > 2.0 st. devs. from mean.

◀ 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

## pdb2e76



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

## pdb2e76

### Main-chain bond lengths

CA 1.525 C 0.084 1.609 A Met 1	CA 1.521 CB 0.050 1.571 A Ala 2	N 1.458 CA 0.069 1.526 A Ala 2	N 1.458 CA 0.067 1.525 A Asn 3	CA 1.530 CB 0.050 1.480 A Phe 8	C 1.231 O 0.053 1.284 A Glu 10
CA 1.530 CB 0.067 1.597 A Glu 13	N 1.458 CA 0.071 1.529 A Glu 13	CA 1.521 CB 0.091 1.430 A Ala 16	C 1.231 O 0.051 1.282 A Lys 24	C 1.231 O 0.061 1.292 A Tyr 25	C 1.231 O 0.073 1.304 A Val 30
CA 1.540 CB 0.073 1.613 A Val 30	CA 1.525 C 0.052 1.577 A Ile 32	N 1.458 CA 0.076 1.534 A Ile 32	CA 1.530 CB 0.055 1.475 A Phe 33	CA 1.525 C 0.087 1.612 A Tyr 34	C 1.231 O 0.062 1.293 A Gly 37
CA 1.540 CB 0.051 1.489 A Ile 39	C 1.231 O 0.067 1.298 A Thr 40	CA 1.525 C 0.051 1.474 A Cys 43	CA 1.525 C 0.071 1.596 A Leu 45	CA 1.530 CB 0.080 1.450 A Phe 48	C 1.231 O 0.055 1.286 A Gly 51
N 1.458 CA 0.050 1.408 A Phe 52	CA 1.530 CB 0.055 1.475 A Met 54	CA 1.540 CB 0.063 1.477 A Thr 55	CA 1.525 C 0.081 1.606 A Phe 56	C 1.231 O 0.068 1.163 A Lys 59	CA 1.525 C 0.083 1.442 A Pro 60
CA 1.525 C 0.079 1.446 A Thr 61	CA 1.540 CB 0.075 1.465 A Thr 61	N 1.458 CA 0.067 1.391 A Thr 61	CA 1.525 C 0.127 1.398 A Val 62	CA 1.540 CB 0.127 1.413 A Val 62	CA 1.540 CB 0.225 1.315 A Thr 63
CA 1.530 CB 0.084 1.446 A Glu 64	CA 1.530 CB 0.073 1.457 A Tyr 66	CA 1.521 CB 0.210 1.311 A Ala 67	N 1.458 CA 0.059 1.399 A Ser 68	C 1.231 O 0.068 1.299 A Gln 70	CA 1.530 CB 0.084 1.446 A Gln 70
CA 1.530 CB 0.063 1.467 A Tyr 71	CA 1.540 CB 0.092 1.448 A Ile 72	C 1.231 O 0.083 1.314 A Met 73	CA 1.525 C 0.069 1.594 A Met 73	CA 1.530 CB 0.079 1.451 A Asn 74	N 1.458 CA 0.072 1.530 A Glu 75
N 1.458 CA 0.062 1.520 A Phe 78	CA 1.530 CB 0.061 1.469 A Trp 80	CA 1.540 CB 0.104 1.436 A Ile 85	N 1.458 CA 0.053 1.511 A His 86	CA 1.530 CB 0.054 1.476 A Ser 89	CA 1.525 C 0.064 1.461 A Ser 91
CA 1.530 CB 0.075 1.455 A Ser 91	N 1.458 CA 0.057 1.401 A Ser 91	N 1.458 CA 0.064 1.522 A Arg 103	C 1.231 O 0.060 1.171 A Tyr 105	CA 1.530 CB 0.050 1.480 A Phe 110	C 1.231 O 0.066 1.296 A Lys 111
CA 1.525 C 0.054 1.579 A Pro 113	N 1.466 CA 0.097 1.563 A Pro 113	C 1.231 O 0.051 1.282 A Arg 114	CA 1.525 C 0.097 1.622 A Arg 114	N 1.458 CA 0.074 1.532 A Arg 114	C 1.231 O 0.064 1.295 A Ile 119



# Distorted geometry

## pdb2e76

### Main-chain bond lengths (contd)

CA 1.525 C 0.076 1.601 A Ile 119	CA 1.540 CB 0.079 1.461 A Ile 119	C 1.231 O 0.087 1.318 A Ser 120	CA 1.525 C 0.081 1.606 A Ser 120	N 1.458 CA 0.051 1.407 A Val 122	C 1.231 O 0.081 1.312 A Ile 123
CA 1.530 CB 0.051 1.479 A Leu 124	CA 1.521 CB 0.072 1.449 A Ala 125	CA 1.540 CB 0.068 1.472 A Ile 127	CA 1.516 C 0.059 1.575 A Gly 132	C 1.231 O 0.053 1.178 A Tyr 136	CA 1.525 C 0.084 1.441 A Tyr 136
CA 1.530 CB 0.060 1.470 A Tyr 136	C 1.231 O 0.054 1.177 A Pro 139	CA 1.525 C 0.058 1.467 A Pro 139	CA 1.530 CB 0.079 1.451 A Pro 139	CA 1.530 CB 0.112 1.418 A Trp 140	N 1.458 CA 0.076 1.382 A Asp 141
C 1.231 O 0.050 1.181 A Tyr 145	CA 1.530 CB 0.089 1.441 A Tyr 145	N 1.458 CA 0.058 1.400 A Tyr 145	CA 1.521 CB 0.051 1.470 A Ala 147	CA 1.540 CB 0.051 1.489 A Val 154	N 1.458 CA 0.074 1.384 A Val 154
CA 1.540 CB 0.052 1.488 A Ile 158	CA 1.540 CB 0.098 1.638 A Val 160	CA 1.525 C 0.052 1.577 A Val 163	CA 1.540 CB 0.061 1.479 A Val 163	CA 1.540 CB 0.109 1.431 A Ile 165	C 1.231 O 0.064 1.295 A Leu 168
CA 1.530 CB 0.055 1.585 A Arg 170	CA 1.530 CB 0.062 1.468 A Ser 173	CA 1.525 C 0.067 1.592 A Ser 174	CA 1.540 CB 0.080 1.460 A Val 175	N 1.451 CA 0.052 1.503 A Gly 176	CA 1.521 CB 0.111 1.410 A Ala 178
C 1.231 O 0.070 1.301 A Thr 179	CA 1.540 CB 0.078 1.462 A Thr 179	C 1.231 O 0.061 1.292 A Tyr 184	CA 1.525 C 0.074 1.451 A Ala 186	CA 1.521 CB 0.163 1.358 A Ala 186	CA 1.530 CB 0.051 1.581 A His 187
CA 1.525 C 0.059 1.465 A Thr 188	N 1.458 CA 0.056 1.513 A Thr 188	CA 1.540 CB 0.073 1.467 A Val 190	C 1.341 N 0.066 1.275 A Leu 191 - A Pro 192	CA 1.530 CB 0.068 1.462 A Phe 198	CA 1.540 CB 0.073 1.467 A Ile 206
N 1.458 CA 0.051 1.407 A Ile 206	CA 1.530 CB 0.068 1.462 A Gln 209	C 1.231 O 0.082 1.313 A Gly 213	C 1.341 N 0.057 1.398 A Gly 213 - A Pro 214	CA 1.525 C 0.068 1.593 A Leu 215	CA 1.521 CB 0.064 1.585 B Ala 2
N 1.458 CA 0.060 1.518 B Leu 4	CA 1.525 C 0.057 1.582 B Ser 10	CA 1.525 C 0.090 1.435 B Pro 12	CA 1.530 CB 0.058 1.472 B Pro 12	C 1.231 O 0.063 1.294 B Lys 13	C 1.231 O 0.063 1.294 B Leu 14
CA 1.521 CB 0.092 1.429 B Ala 16	CA 1.521 CB 0.069 1.452 B Ala 19	C 1.231 O 0.091 1.322 B Lys 20	N 1.458 CA 0.056 1.402 B Met 22	CA 1.530 CB 0.079 1.451 B His 24	CA 1.530 CB 0.052 1.478 B Tyr 26

# Distorted geometry

## pdb2e76

### Main-chain bond lengths (contd)

C 1.231 O 0.059 1.290 B Glu 29	CA 1.530 CB 0.060 1.470 B Asn 34	N 1.458 CA 0.072 1.386 B Asn 34	CA 1.525 C 0.051 1.576 B Leu 37	N 1.466 CA 0.058 1.408 B Pro 41	CA 1.540 CB 0.051 1.489 B Thr 47
CA 1.530 CB 0.065 1.465 B Phe 48	CA 1.521 CB 0.135 1.386 B Ala 49	C 1.231 O 0.059 1.290 B Cys 50	CA 1.525 C 0.059 1.466 B Ala 60	N 1.458 CA 0.063 1.521 B Ala 60	C 1.231 O 0.083 1.148 B Glu 64
CA 1.525 C 0.053 1.472 B Ala 66	N 1.458 CA 0.051 1.407 B Asp 67	N 1.466 CA 0.067 1.399 B Pro 68	CA 1.521 CB 0.092 1.429 B Ala 70	CA 1.525 C 0.068 1.593 B Thr 71	CA 1.525 C 0.066 1.459 B Pro 72
N 1.458 CA 0.079 1.537 B Leu 73	C 1.231 O 0.060 1.291 B Glu 74	C 1.231 O 0.055 1.176 B Ile 75	CA 1.540 CB 0.055 1.485 B Ile 75	CA 1.525 C 0.057 1.582 B Leu 81	CA 1.525 C 0.087 1.438 B Pro 83
C 1.231 O 0.071 1.302 B Phe 85	CA 1.525 C 0.056 1.581 B Arg 89	CA 1.540 CB 0.062 1.478 B Val 91	CA 1.525 C 0.064 1.461 B Pro 92	CA 1.525 C 0.064 1.589 B Asn 93	CA 1.540 CB 0.072 1.467 B Val 98
CA 1.530 CB 0.063 1.467 B Leu 100	C 1.231 O 0.060 1.171 B Val 111	CA 1.525 C 0.063 1.588 B Phe 113	C 1.231 O 0.076 1.155 B Ile 114	CA 1.525 C 0.071 1.596 B Ile 114	CA 1.540 CB 0.068 1.472 B Ile 114
C 1.231 O 0.050 1.281 B Glu 115	CA 1.525 C 0.062 1.587 B Glu 115	CA 1.530 CB 0.060 1.590 B Glu 115	N 1.458 CA 0.057 1.515 B Asn 116	CA 1.540 CB 0.123 1.663 B Val 117	N 1.458 CA 0.057 1.515 B Val 117
CA 1.525 C 0.063 1.462 B Asn 118	CA 1.530 CB 0.058 1.472 B Asn 118	N 1.458 CA 0.089 1.369 B Lys 119	CA 1.525 C 0.093 1.432 B Phe 120	N 1.458 CA 0.051 1.407 B Gln 121	CA 1.530 CB 0.063 1.467 B Asn 122
CA 1.525 C 0.051 1.576 B Phe 124	N 1.458 CA 0.057 1.515 B Arg 125	CA 1.525 C 0.077 1.448 B Pro 127	CA 1.530 CB 0.061 1.469 B Pro 127	CA 1.540 CB 0.051 1.489 B Val 128	C 1.231 O 0.063 1.294 B Ala 129
CA 1.540 CB 0.066 1.606 B Thr 131	CA 1.530 CB 0.075 1.455 B Phe 133	N 1.458 CA 0.089 1.547 B Leu 134	N 1.451 CA 0.056 1.507 B Gly 136	CA 1.540 CB 0.066 1.474 B Val 139	N 1.458 CA 0.055 1.403 B Val 139
C 1.231 O 0.058 1.289 B Thr 140	CA 1.540 CB 0.098 1.638 B Thr 140	CA 1.540 CB 0.149 1.391 B Ile 141	N 1.458 CA 0.073 1.385 B Trp 142	C 1.231 O 0.087 1.318 B Leu 143	C 1.231 O 0.061 1.292 B Gly 144

# Distorted geometry

## pdb2e76

### Main-chain bond lengths (contd)

CA 1.540 CB 0.069 1.470 B Ile 145	C 1.231 O 0.050 1.281 B Ala 147	N 1.458 CA 0.083 1.541 B Phe 149	CA 1.525 C 0.086 1.439 B Pro 150	CA 1.525 C 0.061 1.464 B Leu 155	N 1.458 CA 0.057 1.515 B Leu 155
CA 1.525 C 0.059 1.584 C Phe 3	CA 1.530 CB 0.055 1.585 C Phe 3	CA 1.530 CB 0.052 1.582 C Pro 11	C 1.231 O 0.053 1.284 C Pro 13	CA 1.525 C 0.077 1.602 C Pro 13	N 1.458 CA 0.062 1.520 C Glu 15
C 1.231 O 0.113 1.344 C Pro 16	CA 1.540 CB 0.081 1.459 C Thr 17	CA 1.525 C 0.058 1.467 C Val 21	CA 1.525 C 0.085 1.610 C Cys 22	CA 1.525 C 0.065 1.590 C Ala 23	CA 1.525 C 0.071 1.454 C Cys 25
CA 1.521 CB 0.054 1.467 C Ala 29	C 1.231 O 0.059 1.172 C Val 36	CA 1.525 C 0.053 1.578 C Ser 39	CA 1.525 C 0.088 1.437 C Val 40	CA 1.540 CB 0.137 1.403 C Val 40	N 1.458 CA 0.063 1.395 C Val 40
CA 1.521 CB 0.086 1.435 C Ala 48	CA 1.540 CB 0.102 1.438 C Val 49	CA 1.540 CB 0.054 1.486 C Ile 52	CA 1.540 CB 0.057 1.483 C Val 72	CA 1.525 C 0.066 1.591 C Glu 80	N 1.451 CA 0.092 1.543 C Gly 81
C 1.231 O 0.054 1.285 C Lys 83	CA 1.540 CB 0.091 1.449 C Ile 84	CA 1.521 CB 0.051 1.572 C Ala 85	CA 1.525 C 0.058 1.467 C Pro 86	CA 1.525 C 0.056 1.469 C Glu 87	N 1.466 CA 0.050 1.416 C Pro 91
N 1.458 CA 0.056 1.402 C Glu 92	CA 1.525 C 0.054 1.471 C Glu 93	N 1.451 CA 0.052 1.399 C Gly 99	CA 1.530 CB 0.058 1.472 C Tyr 102	CA 1.525 C 0.056 1.469 C Asp 111	CA 1.540 CB 0.065 1.475 C Val 113
CA 1.525 C 0.051 1.474 C Leu 114	C 1.231 O 0.052 1.283 C Gly 117	CA 1.530 CB 0.052 1.478 C Leu 119	CA 1.525 C 0.086 1.439 C Val 131	CA 1.540 CB 0.071 1.610 C Val 131	CA 1.540 CB 0.072 1.612 C Thr 137
CA 1.530 CB 0.052 1.478 C Asp 139	N 1.458 CA 0.057 1.515 C Asn 141	C 1.231 O 0.070 1.301 C Ile 142	CA 1.540 CB 0.066 1.474 C Ile 142	CA 1.525 C 0.068 1.457 C His 143	CA 1.530 CB 0.097 1.433 C Phe 144
C 1.231 O 0.092 1.323 C Tyr 147	CA 1.521 CB 0.141 1.380 C Ala 148	N 1.458 CA 0.063 1.521 C Ala 148	CA 1.540 CB 0.058 1.482 C Ile 149	CA 1.525 C 0.059 1.466 C His 150	CA 1.525 C 0.062 1.463 C Ala 153
N 1.458 CA 0.059 1.517 C Ala 153	CA 1.525 C 0.070 1.455 C Asn 154	N 1.458 CA 0.061 1.519 C Lys 166	CA 1.525 C 0.053 1.472 C Ser 167	CA 1.525 C 0.064 1.461 C Asn 169	N 1.458 CA 0.054 1.512 C Asn 170

# Distorted geometry

## pdb2e76

### Main-chain bond lengths (contd)

CA 1.540 CB 0.059 1.599 C Val 171	CA 1.540 CB 0.053 1.593 C Thr 179	CA 1.540 CB 0.052 1.592 C Ile 183	CA 1.525 C 0.051 1.576 C Ala 184	CA 1.525 C 0.062 1.587 C Lys 185	CA 1.530 CB 0.067 1.597 C Lys 185
N 1.458 CA 0.069 1.527 C Lys 185	N 1.458 CA 0.064 1.521 C Glu 186	N 1.451 CA 0.070 1.521 C Gly 191	CA 1.540 CB 0.055 1.595 C Thr 201	N 1.458 CA 0.078 1.536 C Thr 201	CA 1.525 C 0.053 1.578 C Val 207
CA 1.540 CB 0.090 1.630 C Val 207	CA 1.525 C 0.060 1.585 C Val 208	CA 1.540 CB 0.062 1.602 C Val 208	CA 1.540 CB 0.056 1.596 C Ile 218	CA 1.540 CB 0.065 1.605 C Val 225	CA 1.525 C 0.066 1.591 C Lys 226
N 1.458 CA 0.068 1.526 C Lys 226	CA 1.521 CB 0.067 1.588 C Ala 227	CA 1.521 CB 0.090 1.611 C Ala 230	CA 1.530 CB 0.052 1.478 C Gln 242	N 1.458 CA 0.061 1.397 C Asp 244	CA 1.540 CB 0.059 1.481 C Thr 245
CA 1.530 CB 0.065 1.595 C Glu 246	CA 1.540 CB 0.075 1.465 C Val 248	CA 1.525 C 0.055 1.470 C Asn 253	CA 1.530 CB 0.062 1.468 C Asn 253	CA 1.525 C 0.052 1.473 C Trp 257	CA 1.521 CB 0.068 1.453 C Ala 260
CA 1.540 CB 0.069 1.471 C Ile 262	CA 1.525 C 0.078 1.447 C Cys 263	CA 1.525 C 0.057 1.582 C Met 266	C 1.231 O 0.053 1.284 C Glu 280	CA 1.525 C 0.052 1.577 C Glu 286	N 1.458 CA 0.094 1.552 C Glu 286
CA 1.540 CB 0.087 1.627 D Val 10	CA 1.525 C 0.063 1.462 D Arg 15	CA 1.525 C 0.056 1.581 D Phe 18	C 1.231 O 0.051 1.180 D Leu 21	CA 1.540 CB 0.059 1.599 D Thr 26	N 1.458 CA 0.056 1.514 D Thr 26
CA 1.540 CB 0.097 1.443 D Val 27	CA 1.525 C 0.060 1.585 D Thr 28	CA 1.521 CB 0.068 1.453 D Ala 31	CA 1.521 CB 0.071 1.450 D Ala 34	C 1.231 O 0.063 1.294 D Pro 37	C 1.231 O 0.061 1.292 D Lys 40
N 1.458 CA 0.066 1.392 D Lys 40	CA 1.525 C 0.072 1.453 D Pro 44	CA 1.521 CB 0.056 1.577 D Ala 49	N 1.458 CA 0.059 1.517 D Ala 49	CA 1.540 CB 0.066 1.606 D Val 50	N 1.458 CA 0.071 1.529 D Val 50
CA 1.525 C 0.085 1.610 D Leu 60	CA 1.530 CB 0.064 1.594 D Leu 70	N 1.458 CA 0.050 1.508 D Glu 71	CA 1.530 CB 0.076 1.606 D Asp 77	N 1.458 CA 0.051 1.509 D Asp 77	CA 1.540 CB 0.064 1.476 D Val 81
N 1.451 CA 0.051 1.502 D Gly 83	C 1.231 O 0.052 1.283 D Lys 85	CA 1.525 C 0.058 1.583 D Ser 95	N 1.458 CA 0.054 1.512 D Ser 95	CA 1.525 C 0.060 1.585 D Lys 96	N 1.458 CA 0.073 1.531 D Glu 97

# Distorted geometry

## pdb2e76

### Main-chain bond lengths (contd)

CA 1.540 CB 0.072 1.612 D Ile 99	CA 1.540 CB 0.128 1.412 D Val 107	CA 1.525 C 0.069 1.456 D Thr 109	N 1.458 CA 0.052 1.406 D Thr 109	CA 1.525 C 0.056 1.469 D Cys 113	CA 1.525 C 0.057 1.468 D Ala 120
N 1.458 CA 0.056 1.514 D Asn 122	CA 1.525 C 0.059 1.584 D Cys 126	CA 1.525 C 0.076 1.449 D Pro 127	CA 1.525 C 0.063 1.588 D Cys 128	CA 1.525 C 0.059 1.466 D His 129	N 1.458 CA 0.067 1.525 D Asp 134
CA 1.525 C 0.067 1.592 D Glu 135	CA 1.525 C 0.059 1.584 D Thr 136	N 1.458 CA 0.054 1.512 D Thr 136	CA 1.525 C 0.074 1.599 D Ile 140	N 1.458 CA 0.108 1.566 D Arg 141	CA 1.521 CB 0.050 1.571 D Ala 144
CA 1.521 CB 0.062 1.459 D Ala 149	N 1.458 CA 0.052 1.510 D Ala 149	CA 1.525 C 0.073 1.598 D Asp 158	CA 1.540 CB 0.072 1.612 D Thr 166	N 1.458 CA 0.053 1.511 D Glu 167	CA 1.540 CB 0.068 1.608 D Thr 172
CA 1.525 C 0.073 1.598 D Glu 174	N 1.458 CA 0.059 1.517 D Trp 177	C 1.231 O 0.080 1.311 E Ile 2	CA 1.540 CB 0.065 1.605 E Ile 2	C 1.231 O 0.091 1.322 E Gly 4	CA 1.521 CB 0.066 1.455 E Ala 5
C 1.231 O 0.053 1.284 E Phe 7	C 1.231 O 0.051 1.282 E Ile 9	CA 1.540 CB 0.068 1.472 E Ile 9	C 1.231 O 0.054 1.285 E Phe 11	C 1.231 O 0.072 1.303 E Ile 12	CA 1.521 CB 0.096 1.425 E Ala 13
CA 1.521 CB 0.088 1.433 E Ala 19	CA 1.540 CB 0.056 1.596 E Ile 22	C 1.329 N 0.058 1.387 E Ile 22 - E Ile 23	N 1.458 CA 0.063 1.521 E Ile 23	CA 1.540 CB 0.088 1.628 E Ile 26	CA 1.530 CB 0.074 1.604 E Lys 27
N 1.458 CA 0.060 1.518 E Lys 27	CA 1.540 CB 0.066 1.606 E Ile 29	CA 1.525 C 0.056 1.469 E Leu 31	CA 1.525 C 0.111 1.636 F Met 1	N 1.458 CA 0.064 1.522 F Met 1	CA 1.540 CB 0.141 1.681 F Thr 2
N 1.458 CA 0.093 1.551 F Thr 2	CA 1.530 CB 0.057 1.587 F Glu 3	CA 1.530 CB 0.073 1.457 F Met 5	CA 1.521 CB 0.067 1.454 F Ala 8	CA 1.525 C 0.065 1.590 F Ala 9	CA 1.525 C 0.066 1.591 F Phe 13
CA 1.530 CB 0.064 1.466 F Phe 13	C 1.231 O 0.078 1.309 F Gly 14	C 1.231 O 0.063 1.294 F Ile 16	CA 1.530 CB 0.066 1.464 F Phe 17	C 1.231 O 0.061 1.292 F Gly 19	C 1.231 O 0.096 1.327 F Trp 20
CA 1.525 C 0.068 1.593 F Leu 22	CA 1.525 C 0.066 1.459 F Leu 27	CA 1.540 CB 0.123 1.663 F Ile 29	CA 1.525 C 0.071 1.454 F Gln 30	CA 1.521 CB 0.062 1.583 F Ala 32	N 1.458 CA 0.051 1.509 F Ala 32

# Distorted geometry

## pdb2e76

### Main-chain bond lengths (contd)

CA 1.530 CB 0.103 1.633 G Met 1	N 1.458 CA 0.120 1.578 G Met 1	CA 1.525 C 0.070 1.595 G Val 2	N 1.458 CA 0.083 1.541 G Val 2	CA 1.525 C 0.055 1.580 G Glu 3	CA 1.530 CB 0.098 1.628 G Glu 3
CA 1.540 CB 0.069 1.471 G Val 10	N 1.458 CA 0.052 1.406 G Val 10	CA 1.540 CB 0.060 1.480 G Val 14	CA 1.530 CB 0.057 1.473 G Phe 15	CA 1.525 C 0.053 1.578 G Ala 16	CA 1.540 CB 0.068 1.608 G Thr 17
C 1.231 O 0.072 1.303 G Leu 21	CA 1.530 CB 0.060 1.470 G Phe 22	N 1.458 CA 0.071 1.529 G Phe 22	CA 1.521 CB 0.129 1.650 G Ala 24	N 1.458 CA 0.053 1.511 G Ala 24	CA 1.521 CB 0.061 1.582 G Ala 25
N 1.458 CA 0.057 1.401 G Tyr 26	CA 1.525 C 0.079 1.604 G Gln 27	N 1.458 CA 0.051 1.407 G Tyr 29	N 1.466 CA 0.054 1.520 G Pro 32	C 1.231 O 0.051 1.282 G Asn 33	CA 1.525 C 0.056 1.581 G Asn 33
N 1.458 CA 0.058 1.516 G Glu 34	CA 1.530 CB 0.051 1.581 H Met 1	N 1.458 CA 0.101 1.559 H Met 1	CA 1.525 C 0.056 1.581 H Glu 2	C 1.231 O 0.065 1.296 H Gly 7	CA 1.530 CB 0.054 1.476 H Trp 8
CA 1.540 CB 0.058 1.482 H Val 9	N 1.458 CA 0.054 1.404 H Val 13	N 1.458 CA 0.055 1.513 H Val 14	C 1.231 O 0.083 1.314 H Trp 17	C 1.231 O 0.050 1.281 H Ile 19	CA 1.540 CB 0.054 1.486 H Ile 19
CA 1.521 CB 0.081 1.440 H Ala 20	CA 1.525 C 0.072 1.597 H Val 23	CA 1.540 CB 0.081 1.459 H Val 23	CA 1.525 C 0.055 1.580 H Arg 26	N 1.451 CA 0.069 1.520 H Gly 28	CA 1.525 C 0.054 1.579 H Leu 29
CA 1.530 CB 0.052 1.582 H Leu 29					

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

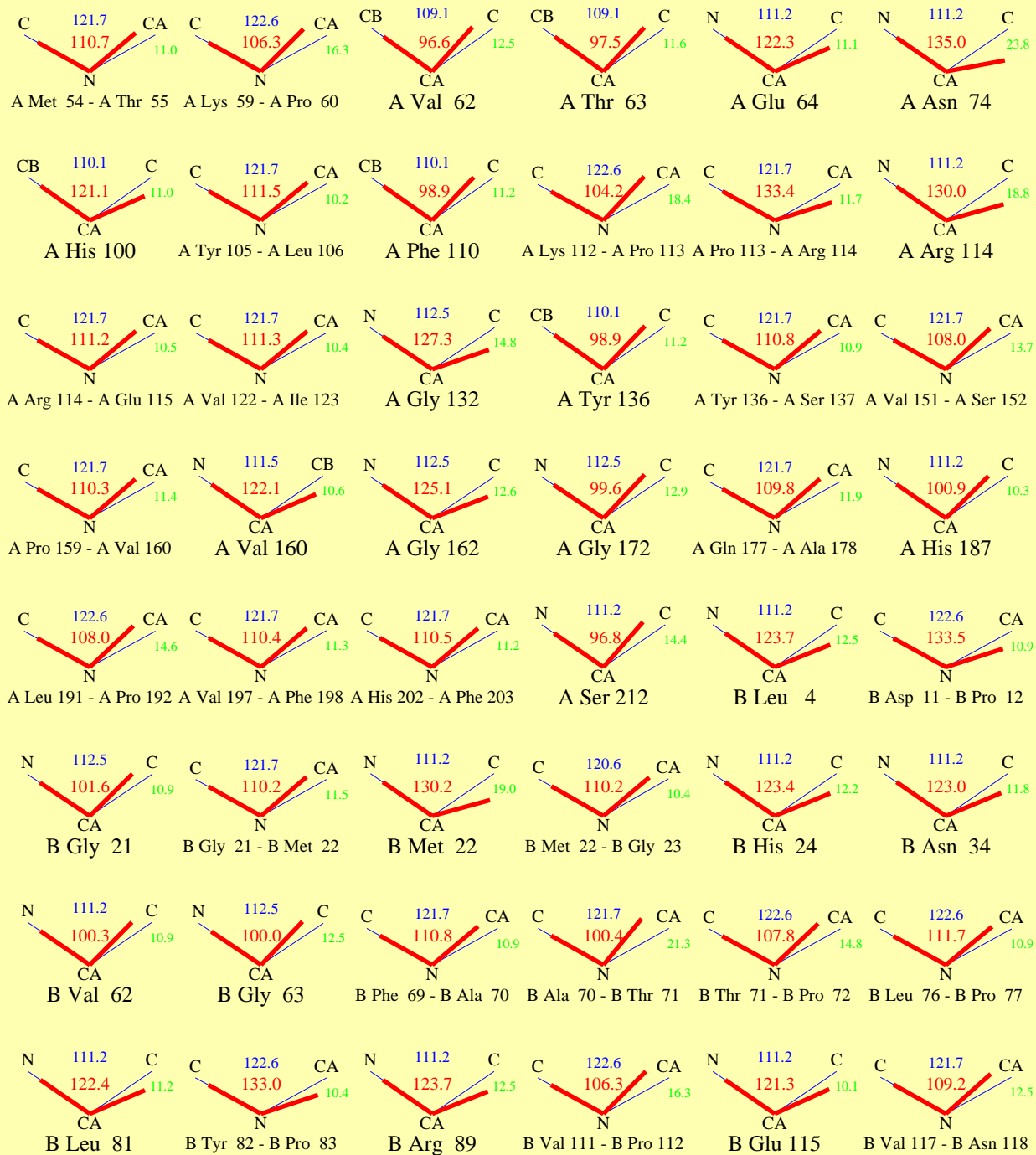
### Main-chain bond angles

N 111.2 C 130.8 19.6 CA A Asn 3	C 121.7 CA 131.8 10.1 N A Glu 10 - A Arg 11	C 121.7 CA 110.2 11.5 N A Tyr 25 - A Val 26	N 111.2 C 122.9 11.7 CA A Val 26	N 111.2 C 123.6 12.4 CA A Ile 32	C 121.7 CA 111.6 10.1 N A Cys 43 - A Phe 44
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# Distorted geometry

## pdb2e76

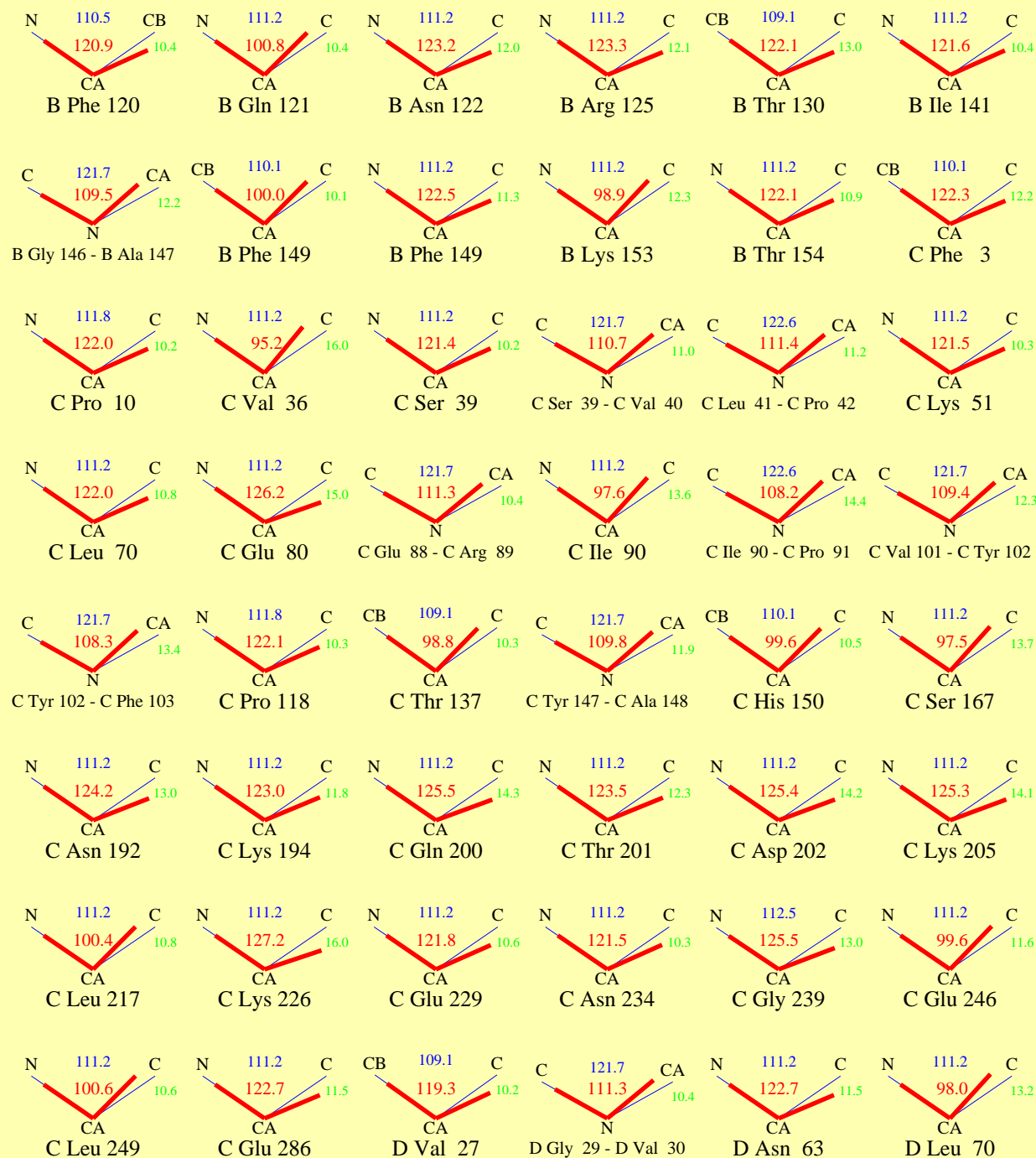
### Main-chain bond angles (contd)



# Distorted geometry

## pdb2e76

### Main-chain bond angles (contd)

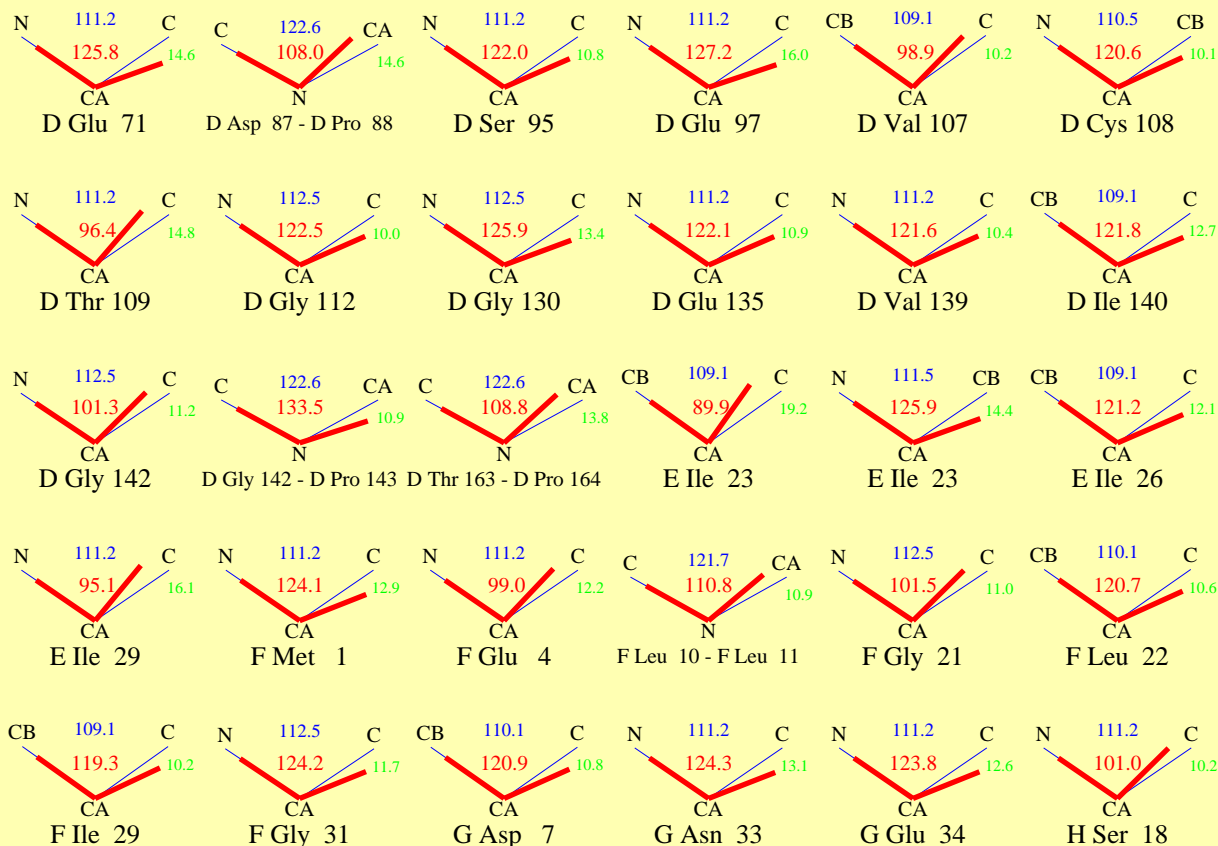




# Distorted geometry

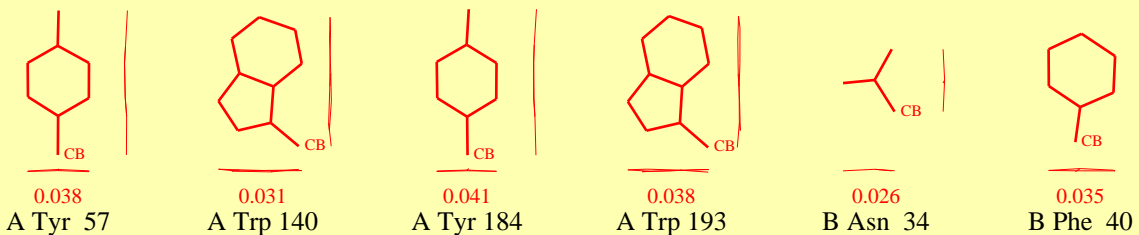
## pdb2e76

### Main-chain bond angles (contd)



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

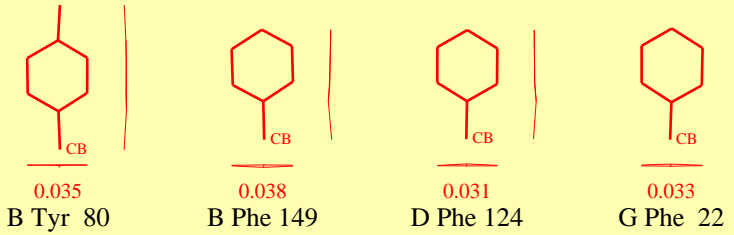
### Planar groups



# Distorted geometry

## pdb2e76

### 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.