Main-chain bond angles

23_128_72

CA-C-N
(except Gly,Pro)

O-C-N
(except Pro)

C-N-CA
(Gly)

C-N-CA
(Pro)

CA-C-O
(Gly)

CB-CA-C
(Gly)

CA-C-N
(Gly)

CA-C-N
(Pro)

O-C-N
(Pro)

C-N-CA
(except Gly,Pro)

CA-C-O
(except Gly)

CB-CA-C
(Ala)

CB-CA-C
(Ile, Thr, Val)

Frequency

10
20
30
40
50
60

101 106 111 116 121 126 131

108 113 118 123 128 133 138

105 110 115 120 125 130 135

107 112 117 122 127 132 137

95 100 105 110 115 120 125

94 99 104 109 114 119 124

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.
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

Model_12

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

Model_12

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 lengths

23_128_72

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 lengths

Model_12

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 parameters
23_128_72

a. Ramachandran plot quality assessment

b. Peptide bond planarity - omega angle sd

c. Measure of bad non-bonded interactions

d. Alpha carbon tetrahedral distortion

e. Hydrogen bond energies

f. Overall G-factor

Plot statistics

<table>
<thead>
<tr>
<th>Stereochemical parameter</th>
<th>No. of data pts</th>
<th>Parameter value</th>
<th>Comparison values</th>
<th>No. of band widths from mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>a. %-tage residues in A, B, L</td>
<td>209</td>
<td>84.7</td>
<td>83.8</td>
<td>10.0</td>
</tr>
<tr>
<td>b. Omega angle st dev</td>
<td>232</td>
<td>7.0</td>
<td>6.0</td>
<td>3.0</td>
</tr>
<tr>
<td>c. Bad contacts / 100 residues</td>
<td>24</td>
<td>10.3</td>
<td>4.2</td>
<td>10.0</td>
</tr>
<tr>
<td>d. Zeta angle st dev</td>
<td>231</td>
<td>1.5</td>
<td>3.1</td>
<td>1.6</td>
</tr>
<tr>
<td>e. H-bond energy st dev</td>
<td>89</td>
<td>0.9</td>
<td>0.8</td>
<td>0.2</td>
</tr>
<tr>
<td>f. Overall G-factor</td>
<td>233</td>
<td>-0.5</td>
<td>-0.4</td>
<td>0.3</td>
</tr>
</tbody>
</table>
**PROCHECK**

**Main-chain parameters**

**Model_12**

---

**a. Ramachandran plot quality assessment**

**Resolution (Angstroms)**

- %-tage of residues in most favoured regions
- Resolutions: 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0
- Plot shows percentage of residues in different regions.

**b. Peptide bond planarity - omega angle sd**

**Resolution (Angstroms)**

- Standard deviation (degrees)
- Resolutions: 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0
- Plot shows standard deviation of omega angles.

**c. Measure of bad non-bonded interactions**

**Bad contacts per 100 residues**

- Resolutions: 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0
- Plot shows number of bad contacts.

**d. Alpha carbon tetrahedral distortion**

**Resolution (Angstroms)**

- Zeta angle standard dev. (degrees)
- Resolutions: 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0
- Plot shows standard deviation of zeta angles.

**e. Hydrogen bond energies**

**Standard deviation (kcal/mol)**

- Resolutions: 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0
- Plot shows standard deviation of hydrogen bond energies.

**f. Overall G-factor**

**Resolution (Angstroms)**

- G-factor
- Resolutions: 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0
- Plot shows overall G-factor.

---

**Plot statistics**

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<th>Parameter value</th>
<th>Comparison values</th>
<th>No. of band widths from mean</th>
</tr>
</thead>
<tbody>
<tr>
<td>a. %-tage residues in A, B, L</td>
<td>164</td>
<td>84.8</td>
<td>83.8</td>
<td>10.0</td>
</tr>
<tr>
<td>b. Omega angle st dev</td>
<td>193</td>
<td>9.7</td>
<td>6.0</td>
<td>3.0</td>
</tr>
<tr>
<td>c. Bad contacts / 100 residues</td>
<td>8</td>
<td>4.1</td>
<td>4.2</td>
<td>10.0</td>
</tr>
<tr>
<td>d. Zeta angle st dev</td>
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<td>1.5</td>
<td>3.1</td>
<td>1.6</td>
</tr>
<tr>
<td>e. H-bond energy st dev</td>
<td>118</td>
<td>0.8</td>
<td>0.8</td>
<td>0.2</td>
</tr>
<tr>
<td>f. Overall G-factor</td>
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<td>-0.1</td>
<td>-0.4</td>
<td>0.3</td>
</tr>
</tbody>
</table>

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Model_12_04.ps