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Viewing spiderApoAK_UPDATED-5U8EFH-multi.table

When finished, you should

Hint: Use File | Save As... to save a copy of this page.

| | | | | |
|-------------------|-------------------------------------------------------------------------------|----------|--------------------------------------------------------|--------------------------------|
| All-Atom Contacts | Clashscore, all atoms: | 5 | 98 th percentile* (N=479, 2.180Å ± 0.25Å) | |
| | Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms. | | | |
| Protein Geometry | Poor rotamers | 0 | 0.00% | Goal: <0.3% |
| | Favored rotamers | 258 | 89.90% | Goal: >98% |
| | Ramachandran outliers | 1 | 0.29% | Goal: <0.05% |
| | Ramachandran favored | 331 | 97.35% | Goal: >98% |
| | MolProbity score [^] | 1.39 | 99 th percentile* (N=10453, 2.180Å ± 0.25Å) | |
| | Cβ deviations >0.25Å | 0 | 0.00% | Goal: 0 |
| | Bad bonds: | 0 / 2767 | 0.00% | Goal: 0% |
| Bad angles: | 0 / 3740 | 0.00% | Goal: <0.1% | |
| Peptide Omegas | Cis Prolines: | 1 / 15 | 6.67% | Expected: ≤1 per chain, or ≤5% |

In the two column results, the left column gives the raw count, right column gives the percentage.

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

[^] MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|-----|---------|------------------------|--------------|----------------------------------------------|------------------------------------------------------|--------------------|--------------------|--------------------|---------------------|
| | | Avg: Clashscore: 29.18 | 5 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 |
| A 1 | ALA | 40.25 | - | - | - | 0.03Å | - | - | - |
| A 2 | VAL | 34.77 | - | Favored (51.87%) Ile or Val / -98.7,124.4 | Favored (47.7%) chi angles: 169.1 | 0.03Å | - | - | - |
| A 3 | ASP | 37.23 | - | Favored (36.8%) General / -73.3,157.5 | Favored (17.2%) p0 chi angles: 58.4,36.1 | 0.06Å | - | - | - |
| A 4 | GLN | 33.95 | - | Favored (78.15%) General / -61.6,-35.5 | Favored (73.7%) tp40 chi angles: 183,66.5,38.5 | 0.02Å | - | - | - |

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|------|-----------|----------------------------------------|-------------------------------------------------|-------------------------------------------------------------------------|-------|---|---|---|
| A 5 | ALA 28.26 | - | Favored (81.75%) General / -59.4,-39.0 | - | 0.02Å | - | - | - |
| A 6 | THR 27.42 | 0.76Å HG21 with A 49 THR HG21 | Favored (76.84%) General / -69.6,-40.2 | Favored (33.7%) <i>m</i> chi angles: 306.2 | 0.04Å | - | - | - |
| A 7 | LEU 34.01 | - | Favored (90.36%) General / -61.9,-39.0 | Favored (95.5%) <i>mt</i> chi angles: 294.7,173.5 | 0.01Å | - | - | - |
| A 8 | ASP 39.26 | - | Favored (99.19%) General / -63.2,-42.4 | Favored (72.9%) <i>m-30</i> chi angles: 295.1,350.2 | 0.02Å | - | - | - |
| A 9 | LYS 38.44 | - | Favored (89.65%) General / -66.0,-38.9 | Favored (3.7%) <i>mttp</i> chi angles: 298.4,192.8,212.7,90.9 | 0.01Å | - | - | - |
| A 10 | LEU 22.64 | - | Favored (96.09%) General / -63.6,-43.7 | Favored (23%) <i>mt</i> chi angles: 281.9,161.4 | 0.03Å | - | - | - |
| A 11 | GLU 30.15 | 0.85Å OE1 with S 241 HOH O | Favored (97.99%) General / -63.7,-42.3 | Favored (44.6%) <i>mm-30</i> chi angles: 283.3,286.2,351.4 | 0.01Å | - | - | - |
| A 12 | ALA 32.11 | - | Favored (69.68%) General / -69.6,-31.5 | - | 0.01Å | - | - | - |
| A 13 | GLY 29.16 | - | Favored (87.25%) Glycine / -67.2,-44.1 | - | - | - | - | - |
| A 14 | PHE 36.26 | - | Favored (75.74%) General / -57.6,-49.6 | Favored (83.2%) <i>t80</i> chi angles: 177.6,72 | 0.03Å | - | - | - |
| A 15 | LYS 47.11 | - | Favored (91.21%) General / -64.8,-38.5 | Allowed (0.5%) <i>tttm</i> chi angles: 161.7,197.6,125.7,289.4 | 0.03Å | - | - | - |
| A 16 | LYS 34.29 | - | Favored (83.71%) General / -61.2,-37.6 | Favored (41.3%) <i>tttt</i> chi angles: 168.3,163,165.2,186.2 | 0.02Å | - | - | - |
| A 17 | LEU 36.4 | - | Favored (86.65%) General / -67.2,-40.6 | Favored (51.7%) <i>mt</i> chi angles: 284.5,167.8 | 0.02Å | - | - | - |

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|----------|----------------|-------------------|---------------------------------|-------------------------------------------------|-------------------------------------------------------------------------|-------------------------|-------------------------|------------------------|----------------------------|
| A 18 | GLN 46.73 | - | | Favored (81.78%) General / -60.6,-48.4 | Favored (13.2%) <i>mm110</i> chi angles: 308.6,319.1,122.3 | 0.01Å | - | - | - |
| A 19 | ASP 44.91 | - | | Favored (64.44%) General / -68.1,-17.6 | Favored (49.5%) <i>m-30</i> chi angles: 299,349.3 | 0.02Å | - | - | - |
| A 20 | ALA 39.88 | - | | Favored (6.18%) General / -81.4,90.2 | - | 0.02Å | - | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
| | | | Avg: Clashscore: 29.18 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non- Trans: 1 of 345 |
| A 21 | THR 47.52 | - | | Favored (67.99%) General / -66.5,-27.7 | Allowed (0.4%) <i>m</i> chi angles: 325.3 | 0.03Å | - | - | - |
| A 22 | ASP 51.88 | - | | - | Allowed (0.4%) <i>p0</i> chi angles: 38.8,56.3 | 0.05Å | - | - | - |
| A 23 | CSO 41.41 | - | 0.55Å OD with A 61 LEU O | - | - | 0.06Å | - | - | - |
| A 24 | LYS 52.53 | - | | - | Allowed (1.5%) <i>mmtp</i> chi angles: 321.1,279.3,201.5,103.9 | 0.03Å | - | - | - |
| A 25 | SER 22.87 | - | | Favored (41.18%) General / -72.8,153.2 | Favored (64.1%) <i>p</i> chi angles: 72.7 | 0.01Å | - | - | - |
| A 26 | LEU 22.74 | - | | Favored (76.84%) General / -60.9,-35.5 | Favored (70.6%) <i>mt</i> chi angles: 299.8,182.7 | 0.03Å | - | - | - |
| A 27 | LEU 22.7 | - | | Favored (54.64%) General / -55.2,-53.5 | Favored (48.1%) <i>tp</i> chi angles: 180,66.4 | 0.01Å | - | - | - |
| A 28 | LYS 38.45 | - | | Favored (77.85%) General / -58.1,-39.1 | Allowed (0.6%) <i>tmtm</i> chi angles: 203,244.7,176,303.2 | 0.02Å | - | - | - |
| A 29 | LYS 36.68 | - | 0.43Å NZ with S 259 HOH O | Favored (73.06%) General / -63.5,-31.8 | Favored (74.7%) <i>tttt</i> chi angles: 191,183.8,182.3,172.7 | 0.01Å | - | - | - |
| A 30 | TYR 22.74 | - | | Favored (9.24%) General / | Favored (67.7%) <i>m-80</i> chi angles: 295.5,292.9 | 0.02Å | - | - | - |

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| A 31 | LEU 26.48 | - | -119.1,-15.2 Favored (8.09%) General / -81.3,70.3 | Favored (19%) <i>tp</i> chi angles: 190.1,69.1 | 0.04Å | - | - | - |
| A 32 | ASN 32.42 | - | Favored (7.72%) General / -81.1,179.8 | Favored (33.3%) <i>p0</i> chi angles: 61.7,45.9 | 0.05Å | - | - | - |
| A 33 | ARG 35.82 | - | Favored (82.17%) General / -66.3,-36.1 | Favored (4.1%) <i>tpt170</i> chi angles: 187.1,75.8,214.7,181.9 | 0.04Å | - | - | - |
| A 34 | GLU 58.5 | - | Favored (71.26%) General / -63.5,-50.0 | Favored (3.3%) <i>mt-10</i> chi angles: 265,179.4,291.5 | 0.02Å | - | - | - |
| A 35 | VAL 29.1 | - | Favored (99.41%) Ile or Val / -61.8,-44.9 | Favored (75.8%) <i>t</i> chi angles: 172.7 | 0.06Å | - | - | - |
| A 36 | PHE 29.02 | - | Favored (70.11%) General / -53.6,-45.4 | Favored (80.8%) <i>t80</i> chi angles: 182.3,74 | 0.02Å | - | - | - |
| A 37 | ASP 34 | - | Favored (57.57%) General / -76.3,-30.3 | Favored (50.9%) <i>m-30</i> chi angles: 286.6,319.7 | 0.04Å | - | - | - |
| A 38 | GLN 35.45 | - | Favored (69.93%) General / -59.3,-32.4 | Favored (19%) <i>mt0</i> chi angles: 271.1,181.2,280.6 | 0.05Å | - | - | - |
| A 39 | CYS 24.02 | - | Favored (11.26%) General / -106.3,-27.0 | Favored (61.5%) <i>m</i> chi angles: 300.7 | 0.01Å | - | - | - |
| A 40 | LYS 31.47 | - | Favored (68.98%) General / -63.6,-27.1 | Favored (12.5%) <i>pttm</i> chi angles: 78.2,182.5,191.4,298.2 | 0.04Å | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|---|---------|--------|--------------|--------------|---------|--------------|--------------|-------------|--------------|
|---|---------|--------|--------------|--------------|---------|--------------|--------------|-------------|--------------|

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|------------------|----------------|---------------------|-----------|-----------|-----------|------------|
| Avg: Clashscore: | Outliers: 1 of | Poor rotamers: 0 of | Outliers: | Outliers: | Outliers: | Non-Trans: |
| 29.18 | 5 | 340 | 287 | 0 of 322 | 0 of 347 | 1 of 345 |

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|---------|-----------|---|-------------------------------------------------|---------------------------------------------------------|-------|---|---|---|
| A 41 | SER 33.67 | - | Favored (36.08%) General / -103.0,12.4 | Favored (88.3%) <i>p</i> chi angles: 69.4 | 0.04Å | - | - | - |
| A 42 | LEU 27.21 | - | Favored (16.8%) General / | Favored (46.5%) <i>mt</i> chi angles: 305.4,173.7 | 0.01Å | - | - | - |

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| A 43 | LYS 40.26 | - | -91.8,157.6 Favored (15.32%) General / -151.0,133.2 | Allowed (0.8%) <i>tttt</i> chi angles: 203.3,209.8,233.2,192.4 | 0.04Å | - | - | - |
| A 44 | THR 22.28 | - | Favored (22.04%) General / -79.5,166.4 | Favored (40.9%) <i>p</i> chi angles: 67.6 | 0.04Å | - | - | - |
| A 45 | ALA 23.89 | - | Favored (79.59%) General / -56.2,-44.3 | - | 0.01Å | - | - | - |
| A 46 | LEU 23.16 | - | Favored (26.85%) General / -72.1,-4.1 | Favored (90.4%) <i>mt</i> chi angles: 292.5,168.4 | 0.02Å | - | - | - |
| A 47 | GLY 23.13 | - | Favored (43.98%) Glycine / 103.7,6.3 | - | - | - | - | - |
| A 48 | ALA 20.07 | - | Favored (36%) General / -76.9,149.8 | - | 0.02Å | - | - | - |
| A 49 | THR 21.8 | 0.76Å HG21 with A 6 THR HG21 | Favored (20.1%) General / -120.3,162.1 | Allowed (0.4%) <i>m</i> chi angles: 278.8 | 0.15Å | - | - | - |
| A 50 | LEU 18.96 | - | Favored (70.04%) General / -56.1,-37.8 | Favored (59.3%) <i>tp</i> chi angles: 175.6,58.9 | 0.01Å | - | - | - |
| A 51 | LEU 17.87 | 0.73Å H with A 49 THR HG22 | Favored (73.96%) General / -59.3,-35.6 | Favored (46%) <i>tp</i> chi angles: 183.9,64 | 0.01Å | - | - | - |
| A 52 | ASP 18.44 | - | Favored (58.69%) General / -66.8,-12.4 | Favored (60%) <i>m-30</i> chi angles: 293.3,308.6 | 0.00Å | - | - | - |
| A 53 | CYS 13.78 | - | Favored (7.31%) General / -94.5,-45.7 | Favored (60.9%) <i>m</i> chi angles: 301.8 | 0.02Å | - | - | - |
| A 54 | ILE 20.55 | - | Favored (9.92%) Ile or Val / -105.6,-6.1 | Favored (8.4%) <i>pt</i> chi angles: 75.5,170.5 | 0.05Å | - | - | - |
| A 55 | GLN 21.44 | - | Favored (76.4%) General / -59.0,-37.2 | Favored (6.2%) <i>pt0</i> chi angles: 53,195.7,344.4 | 0.02Å | - | - | - |
| A 56 | SER 19.12 | - | Favored (71.88%) General / | Favored (46.5%) <i>t</i> chi angles: 179.9 | 0.02Å | - | - | - |

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|----------|----------------|--------------------------------|----------------------------------------------------------------|---------------------------------------------------------------------|-------------------------|---------------------|---------------------|--------------------|---------------------|
| A 57 | GLY 21.84 | - | -71.0,-35.1 Favored (75.86%) Glycine / -73.6,-23.9 | - | - | - | - | - | - |
| A 58 | VAL 27.41 | - | Favored (55.61%) Ile or Val / -72.0,-47.4 | Favored (8.8%) <i>t</i> chi angles: 161.3 | 0.07Å | - | - | - | - |
| A 59 | GLU 41.31 | - | Favored (77.94%) General / -69.0,-36.5 | Favored (55.3%) <i>mm-30</i> chi angles: 293.2,311.9,301.2 | 0.02Å | - | - | - | - |
| A 60 | ASN 24.27 | - | Favored (2.29%) General / -111.3,86.3 | Favored (57.4%) <i>m-40</i> chi angles: 298.1,277.7 | 0.03Å | - | - | - | - |
| # | Alt Res | High B | Clash ≥ 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
| | | | Avg: Clashscore: 29.18 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 |
| A 61 | LEU 24.92 | 0.55Å O with A 23 CSO OD | Favored (66.16%) General / -63.3,-21.3 | Favored (78.7%) <i>mt</i> chi angles: 300.4,180.3 | 0.01Å | - | - | - | - |
| A 62 | ASP 41.46 | - | Favored (19.2%) General / -81.0,4.5 | Favored (13.7%) <i>p0</i> chi angles: 51,348.4 | 0.03Å | - | - | - | - |
| A 63 | SER 24.4 | - | Favored (39.59%) General / -53.9,137.2 | Favored (54.9%) <i>m</i> chi angles: 300.1 | 0.06Å | - | - | - | - |
| A 64 | GLY 22.77 | - | Favored (41.68%) Glycine / -69.7,-48.6 | - | - | - | - | - | - |
| A 65 | VAL 20.86 | - | Allowed (0.76%) Ile or Val / -99.0,-69.4 | Favored (33.5%) <i>t</i> chi angles: 185.1 | 0.05Å | - | - | - | - |
| A 66 | GLY 17.72 | - | Favored (55.13%) Glycine / 89.5,17.4 | - | - | - | - | - | - |
| A 67 | ILE 15.56 | - | Favored (30.6%) Ile or Val / -136.4,145.4 | Favored (12.6%) <i>tt</i> chi angles: 199,171 | 0.04Å | - | - | - | - |
| A 68 | TYR 24.83 | - | Favored (31.97%) General / -134.9,162.6 | Favored (96.2%) <i>m-80</i> chi angles: 297.8,279.9 | 0.05Å | - | - | - | - |

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| A 69 | ALA 15.75 | - | Favored (42.37%) Pre-Pro / -102.1,123.8 | - | 0.02Å | - | - | - |
| A 70 | PRO 18.76 | - | Favored (5.25%) Trans-Pro / -84.0,-18.5 | Favored (54%) <i>Cg_endo</i> chi angles: 25.7,324.1,31 | 0.02Å | - | - | - |
| A 71 | ASP 18.85 | - | Favored (8.12%) General / -160.0,-179.8 | Favored (26.3%) <i>p0</i> chi angles: 61.2,29.7 | 0.06Å | - | - | - |
| A 72 | ALA 18.05 | - | Favored (82.53%) General / -67.7,-42.2 | - | 0.03Å | - | - | - |
| A 73 | GLU 23.69 | - | Favored (67.95%) General / -65.8,-27.0 | Favored (40.4%) <i>tt0</i> chi angles: 181.5,194,337.4 | 0.03Å | - | - | - |
| A 74 | ALA 14.04 | - | Favored (63.42%) General / -55.3,-33.5 | - | 0.02Å | - | - | - |
| A 75 | TYR 16.19 | - | Favored (93.03%) General / -60.7,-40.6 | Favored (11.9%) <i>m-80</i> chi angles: 273.5,298.7 | 0.03Å | - | - | - |
| A 76 | THR 19.86 | - | Favored (12.09%) General / -82.1,-47.8 | Favored (85.4%) <i>m</i> chi angles: 301.6 | 0.04Å | - | - | - |
| A 77 | LEU 17.94 | - | Favored (98.5%) General / -61.4,-43.6 | Favored (25.1%) <i>tp</i> chi angles: 188.9,59.1 | 0.02Å | - | - | - |
| A 78 | PHE 19.17 | - | Favored (6.55%) General / -98.8,25.5 | Favored (83.9%) <i>m-80</i> chi angles: 299.6,284.8 | 0.04Å | - | - | - |
| A 79 | ALA 15.76 | - | Favored (5.57%) Pre-Pro / -46.8,-35.6 | - | 0.03Å | - | - | - |
| A 80 | PRO 17.54 | - | Favored (76.6%) Trans-Pro / -58.2,-26.4 | Favored (49.1%) <i>Cg_exo</i> chi angles: 327.7,39.2,329.6 | 0.03Å | - | - | - |

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 29.18 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

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|---------|-----|-------|----------------------------------|----------------------------------------------------|---------------------------------------------------------------------|-------|---|---|---|
| A 81 | ILE | 16.22 | - | Favored (6.86%) Ile or Val / -99.7,-38.6 | Favored (6%) <i>tp</i> chi angles: 183.2,57.7 | 0.11Å | - | - | - |
| A 82 | PHE | 15.49 | - | Favored (97.85%) General / -63.7,-42.5 | Favored (25.8%) <i>m-80</i> chi angles: 278.3,291.4 | 0.01Å | - | - | - |
| A 83 | ASN | 15.39 | - | Favored (87.84%) Pre-Pro / -58.6,-50.5 | Favored (62.5%) <i>m-40</i> chi angles: 282.2,357.9 | 0.07Å | - | - | - |
| A 84 | PRO | 15.78 | - | Favored (26.85%) Trans-Pro / -67.3,-34.5 | Favored (51.2%) <i>Cg_endo</i> chi angles: 25.3,321.8,35.6 | 0.02Å | - | - | - |
| A 85 | ILE | 16.8 | - | Favored (96.75%) Ile or Val / -63.1,-46.2 | Favored (76.6%) <i>mt</i> chi angles: 291.9,174.5 | 0.07Å | - | - | - |
| A 86 | ILE | 17.63 | - | Favored (93.4%) Ile or Val / -60.0,-43.8 | Favored (37.1%) <i>mt</i> chi angles: 284.2,168.6 | 0.07Å | - | - | - |
| A 87 | GLU | 24.78 | - | Favored (91.45%) General / -61.2,-46.2 | Favored (21.4%) <i>tm-30</i> chi angles: 185.5,282.5,331.9 | 0.00Å | - | - | - |
| A 88 | ASP | 23.23 | - | Favored (36.72%) General / -63.7,-54.4 | Favored (30.1%) <i>t0</i> chi angles: 188.4,320.9 | 0.04Å | - | - | - |
| A 89 | TYR | 23.36 | - | Favored (89.46%) General / -59.0,-45.9 | Favored (88.7%) <i>t80</i> chi angles: 179.9,80.1 | 0.04Å | - | - | - |
| A 90 | HIS | 24.51 | - | Favored (6.88%) General / -88.1,15.9 | Favored (95.7%) <i>m-70</i> chi angles: 296.3,281 | 0.04Å | - | - | - |
| A 91 | GLU | 42.37 | - | Allowed (0.2%) General / 48.5,73.8 | Favored (68.9%) <i>mt-10</i> chi angles: 283.7,169.3,16.9 | 0.04Å | - | - | - |
| A 92 | GLY | 25.3 | - | Favored (44.89%) Glycine / 104.2,3.4 | - | - | - | - | - |
| A 93 | PHE | 22.73 | - | Favored (8.03%) General / -84.7,91.8 | Favored (41.5%) <i>t80</i> chi angles: 192.7,84.1 | 0.04Å | - | - | - |
| A 94 | LYS | 42.73 | 0.49Å HE2 with S 134 HOH O | Favored (58.07%) Pre-Pro / | Allowed (1.5%) <i>mttm</i> chi angles: | 0.03Å | - | - | - |

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|-----|---------|------------|----------------------------------|--------------------|---------------------------|----------------------|-------------------------------------|--------------------|---------------------|---|---|
| A | PRO | 20.05 | - | -77.4,164.5 | 325.2,222.9,174.2,278.8 | Favored (99%) | <i>Cg_exo</i> | 0.02Å | - | - | - |
| 95 | | | | (81.46%) | | Trans-Pro / | chi angles: | | | | |
| | | | | -55.7,-31.8 | | | 332.3,35.2,332 | | | | |
| A | THR | 25.16 | - | Favored (58.16%) | Favored (47.1%) <i>p</i> | General / -89.8,-2.1 | chi angles: 55.7 | 0.04Å | - | - | - |
| 96 | | | | | | | | | | | |
| A | ASP | 21.06 | 0.57Å OD1 with S 243 HOH O | Favored (32.04%) | Favored (66.4%) | General / | <i>m-30</i> | 0.01Å | - | - | - |
| 97 | | | | (37.72%) | | -74.6,159.5 | chi angles: 279.9,345 | | | | |
| A | LYS | 33.13 | - | Favored (37.72%) | Favored (70.9%) | General / | <i>tttt</i> | 0.04Å | - | - | - |
| 98 | | | | (45.26%) | | -136.8,135.2 | chi angles: 183.1,179.9,164.9,181.7 | | | | |
| A | HIS | 19.07 | - | Favored (45.26%) | Favored (83%) <i>t70</i> | Pre-Pro / | chi angles: 182.5,78.6 | 0.03Å | - | - | - |
| 99 | | | | (34.41%) | | -82.2,139.2 | | | | | |
| A | PRO | 19.52 | - | Favored (34.41%) | Favored (36.5%) | Trans-Pro / | <i>Cg_endo</i> | 0.04Å | - | - | - |
| 100 | | | | (34.41%) | | -68.5,164.1 | chi angles: 22.6,323.9,34.8 | | | | |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides | | |
| | | Avg: 29.18 | Clashscore: 5 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 | | |
| A | PRO | 23.66 | - | Favored (76.08%) | Favored (8.8%) | Trans-Pro / | <i>Cg_exo</i> | 0.03Å | - | - | - |
| 101 | | | | (35.63%) | | -65.1,153.9 | chi angles: 347.8,25.3,332.4 | | | | |
| A | THR | 22.28 | - | Favored (35.63%) | Favored (88.8%) <i>m</i> | General / | chi angles: 298.4 | 0.06Å | - | - | - |
| 102 | | | | (3.03%) | | -54.0,129.8 | | | | | |
| A | ASP | 27.09 | - | Favored (3.03%) | Favored (20.6%) <i>t0</i> | General / | chi angles: 177.7,30.1 | 0.01Å | - | - | - |
| 103 | | | | (56.83%) | | -152.7,106.0 | | | | | |
| A | PHE | 25.19 | - | Favored (56.83%) | Favored (71.3%) | General / -77.5,-7.8 | chi angles: 298.7,291.6 | 0.01Å | - | - | - |
| 104 | | | | (50.52%) | | | | | | | |
| A | GLY | 23.67 | - | Favored (50.52%) | - | Glycine / | - | - | - | - | - |
| 105 | | | | (13.43%) | | 71.9,-169.6 | | | | | |
| A | ASP | 37.86 | - | Favored (13.43%) | Favored (61.9%) <i>t0</i> | General / | chi angles: 182.5,2.7 | 0.04Å | - | - | - |
| 106 | | | | (13.43%) | | -90.2,100.6 | | | | | |

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|----------|-----------|----------------------------------------|-----------------------------------------------------|---------------------------------------------------------------------|-------|---|---|---|
| A 107 | ILE 40.65 | 0.43Å HG12 with A 244 GLN HB2 | Favored (19.12%) Ile or Val / -56.2,-25.1 | Favored (4.4%) <i>tp</i> chi angles: 188.3,52.8 | 0.08Å | - | - | - |
| A 108 | ASN 48.44 | - | Favored (59.22%) General / -72.5,-10.0 | Favored (78.9%) <i>m-40</i> chi angles: 283.4,330.1 | 0.01Å | - | - | - |
| A 109 | THR 27.18 | - | Favored (57.56%) General / -89.9,-4.3 | Favored (71.4%) <i>p</i> chi angles: 61.9 | 0.03Å | - | - | - |
| A 110 | ILE 23.84 | - | Favored (19.08%) Ile or Val / -90.6,138.6 | Favored (35.3%) <i>mm</i> chi angles: 306.7,296.6 | 0.05Å | - | - | - |
| A 111 | VAL 22.51 | - | Favored (19.59%) Ile or Val / -125.2,167.3 | Favored (11.4%) <i>m</i> chi angles: 306.4 | 0.02Å | - | - | - |
| A 112 | ASN 27.38 | - | Favored (10.17%) General / -69.8,116.4 | Favored (48.2%) <i>t0</i> chi angles: 188.3,318.3 | 0.07Å | - | - | - |
| A 113 | VAL 23.06 | - | Favored (17.99%) Ile or Val / -72.5,-16.1 | Favored (13.6%) <i>m</i> chi angles: 291.4 | 0.03Å | - | - | - |
| A 114 | ASP 24.46 | - | Favored (5.84%) Pre-Pro / -152.4,80.3 | Favored (38.2%) <i>t0</i> chi angles: 180,19.1 | 0.00Å | - | - | - |
| A 115 | PRO 28.58 | - | Favored (98.24%) Trans-Pro / -58.4,-33.9 | Favored (85.2%) <i>Cg_exo</i> chi angles: 334,33.4,333.1 | 0.02Å | - | - | - |
| A 116 | SER 33.17 | - | Favored (59.89%) General / -78.1,-11.1 | Favored (82.6%) <i>p</i> chi angles: 62.3 | 0.02Å | - | - | - |
| A 117 | GLY 26.79 | - | Favored (69.54%) Glycine / 64.3,25.0 | - | - | - | - | - |
| A 118 | LYS 29.1 | - | Favored (46.66%) General / -78.4,-28.2 | Favored (46%) <i>tttt</i> chi angles: 200.2,178.4,167.8,172.2 | 0.07Å | - | - | - |
| A 119 | TYR 29.11 | 0.46Å CE1 with A 353 GLU HG2 | Allowed (1.59%) General / -126.1,-48.6 | Favored (80%) <i>m-80</i> chi angles: 300.1,286.3 | 0.03Å | - | - | - |
| A 120 | VAL 21.88 | - | Favored (30.16%) | Favored (73%) <i>t</i> chi angles: 172.5 | 0.05Å | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ile or Val / -83.2,118.0 | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|-------|---------|------------|----------------------------------|-------------------------------------------------|----------------------------------------------------------------------------|--------------------|--------------------|--------------------|---------------------|--------------|
| | | Avg: 29.18 | Clashscore: 5 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 | |
| A 121 | VAL | 23.24 | - | Favored (45.43%) Ile or Val / -74.9,-43.8 | Favored (85.7%) <i>t</i> chi angles: 177.4 | 0.06Å | - | - | - | |
| A 122 | SER | 22.83 | - | Favored (26.15%) General / -161.1,157.5 | Favored (62.7%) <i>p</i> chi angles: 58.1 | 0.03Å | - | - | - | |
| A 123 | THR | 20.44 | - | Favored (50.95%) General / -126.8,144.4 | Favored (91.3%) <i>m</i> chi angles: 301.1 | 0.05Å | - | - | - | |
| A 124 | HIS | 29.22 | 0.56Å ND1 with S 166 HOH O | Favored (41.03%) General / -135.8,136.8 | Favored (22.9%) <i>m90</i> chi angles: 278.4,66.3 | 0.08Å | - | - | - | |
| A 125 | VAL | 20.3 | - | Favored (68.1%) Ile or Val / -128.4,128.2 | Favored (13.7%) <i>t</i> chi angles: 188.6 | 0.05Å | - | - | - | |
| A 126 | ARG | 46.29 | - | Favored (50.86%) General / -128.9,142.7 | Allowed (0.5%) <i>ttt180</i> chi angles: 154.9,182.5,126.7,197.6 | 0.02Å | - | - | - | |
| A 127 | CYS | 17.64 | - | Favored (9.66%) General / -138.3,175.3 | Favored (27.9%) <i>p</i> chi angles: 67.5 | 0.07Å | - | - | - | |
| A 128 | GLY | 14.89 | - | Favored (21.53%) Glycine / -138.2,151.7 | - | - | - | - | - | |
| A 129 | ARG | 15.9 | - | Favored (27.85%) General / -145.3,140.5 | Favored (81.1%) <i>mmt-90</i> chi angles: 293.1,295.4,190.8,264.2 | 0.04Å | - | - | - | |
| A 130 | SER | 17.38 | - | Favored (37.66%) General / -105.5,141.1 | Favored (58.9%) <i>m</i> chi angles: 299.3 | 0.03Å | - | - | - | |
| A 131 | LEU | 18.66 | - | Favored (32.06%) General / -84.6,125.0 | Favored (13.5%) <i>mt</i> chi angles: 307.4,190.7 | 0.04Å | - | - | - | |

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|----------|----------------|---------------|---------------------------------------|---------------------------------------------------|---------------------------------------------------------------------|---------------------|---------------------|--------------------|---------------------|
| A | LYS | 39.64 | - | Favored (50.66%) General / -55.7,136.3 | Favored (2.8%) <i>tttp</i> chi angles: 182.2,196.5,212.7,62.2 | 0.02Å | - | - | - |
| A | GLY | 21.9 | - | Favored (59.52%) Glycine / 97.8,-17.0 | - | - | - | - | - |
| A | TYR | 31.19 | - | Favored (32.14%) Pre-Pro / -104.0,146.2 | Favored (93.6%) <i>m-80</i> chi angles: 291.9,89.2 | 0.06Å | - | - | - |
| A | PRO | 17.54 | - | Favored (4.67%) Trans-Pro / -51.7,158.1 | Favored (13.5%) <i>Cg_exo</i> chi angles: 345.2,21.2,341.4 | 0.05Å | - | - | - |
| A | PHE | 17.83 | - | Favored (8.59%) General / -82.9,177.5 | Favored (5.6%) <i>m-10</i> chi angles: 296.2,359.6 | 0.04Å | - | - | - |
| A | ASN | 21.19 | 0.41Å HA with A 140 LEU HD12 | Favored (3.99%) Pre-Pro / -60.4,-28.1 | Favored (2.1%) <i>m-40</i> chi angles: 263,271.2 | 0.07Å | - | - | - |
| A | PRO | 17.9 | - | Favored (47.54%) Trans-Pro / -56.0,-24.2 | Favored (94.6%) <i>Cg_exo</i> chi angles: 331.4,35.8,331.4 | 0.04Å | - | - | - |
| A | CYS | 19.46 | - | Favored (4.68%) General / -131.2,8.1 | Favored (62.9%) <i>m</i> chi angles: 286 | 0.02Å | - | - | - |
| A | LEU | 20.42 | 0.41Å HD12 with A 137 ASN HA | Favored (58.22%) General / -66.0,139.1 | Favored (15.8%) <i>mt</i> chi angles: 280.7,159.3 | 0.01Å | - | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
| | | Avg: 29.18 | Clashscore: 5 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 |
| A | THR | 20.7 | 0.45Å H with A 144 ASN HD22 | Favored (16.64%) General / -86.9,164.3 | Favored (50.3%) <i>p</i> chi angles: 65.6 | 0.02Å | - | - | - |
| A | GLU | 36.54 | - | Favored (75.7%) General / -55.2,-45.8 | Favored (65.4%) <i>tt0</i> chi angles: 179.1,177.3,24.8 | 0.01Å | - | - | - |
| A | ALA | 19.72 | - | Favored (95.76%) General / -61.3,-40.9 | - | 0.02Å | - | - | - |

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|----------|-----------|------------------------------------|----------------------------------------------------|--------------------------------------------------------------------------|--------|---|---|---|
| A 144 | ASN 21.01 | 0.45 Å HD22 with A 141 THR H | Favored (72.15%) General / -54.8,-48.9 | Favored (84.2%) <i>m-40</i> chi angles: 283.3,338.4 | 0.02 Å | - | - | - |
| A 145 | TYR 19.41 | - | Favored (86.59%) General / -57.8,-45.2 | Favored (11.2%) <i>m-80</i> chi angles: 274.1,301.1 | 0.01 Å | - | - | - |
| A 146 | LYS 38.34 | - | Favored (76.88%) General / -66.0,-46.7 | Favored (85.4%) <i>mttt</i> chi angles: 299.3,179.6,176.3,168.8 | 0.02 Å | - | - | - |
| A 147 | GLU 39.51 | - | Favored (94.72%) General / -65.0,-40.3 | Favored (8.9%) <i>tt0</i> chi angles: 170.4,200,210.1 | 0.02 Å | - | - | - |
| A 148 | MET 22.43 | - | Favored (91.41%) General / -62.0,-45.9 | Favored (46.4%) <i>tmm</i> chi angles: 180.6,182.3,299.7 | 0.01 Å | - | - | - |
| A 149 | GLU 26.91 | 0.41 Å O with A 153 SER HB3 | Favored (85.65%) General / -58.5,-41.5 | Favored (39.1%) <i>tt0</i> chi angles: 193.3,180.6,26.5 | 0.02 Å | - | - | - |
| A 150 | ASP 40.34 | - | Favored (50.48%) General / -55.8,-54.0 | Favored (14.1%) <i>t0</i> chi angles: 205.5,9.9 | 0.03 Å | - | - | - |
| A 151 | LYS 42.96 | - | Favored (82.75%) General / -61.9,-47.9 | Allowed (2%) <i>mttt</i> chi angles: 257.5,149,182.2,162.7 | 0.01 Å | - | - | - |
| A 152 | VAL 22.85 | - | Favored (74.63%) Ile or Val / -69.9,-46.1 | Favored (16.4%) <i>t</i> chi angles: 163.8 | 0.09 Å | - | - | - |
| A 153 | SER 35.77 | 0.41 Å HB3 with A 149 GLU O | Favored (74.71%) General / -63.0,-33.1 | Allowed (0.3%) <i>t</i> chi angles: 147.8 | 0.03 Å | - | - | - |
| A 154 | ALA 29.19 | - | Favored (76.68%) General / -60.5,-49.7 | - | 0.03 Å | - | - | - |
| A 155 | ILE 37.41 | - | Favored (80.38%) Ile or Val / -56.0,-46.2 | Favored (4.2%) <i>mm</i> chi angles: 301.5,319 | 0.04 Å | - | - | - |
| A 156 | PHE 27.08 | - | Favored (73.12%) General / -57.2,-38.0 | Favored (14.7%) <i>m-10</i> chi angles: 286.5,350.8 | 0.02 Å | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|-----------------------------------|--------------|-----------------------------------------------|-----------------------------------------------------------------------|--------------|--------------|-------------|--------------|
| A 157 | GLY 34.34 | - | - | Favored (60.71%) Glycine / -66.4,-13.6 | - | - | - | - | - |
| A 158 | THR 35.24 | - | - | Favored (42.73%) General / -96.7,-3.4 | Favored (4.2%) <i>p</i> chi angles: 79.7 | 0.03Å | - | - | - |
| A 159 | PHE 30.93 | - | - | Favored (26.43%) General / -60.8,126.2 | Favored (3.8%) <i>m-10</i> chi angles: 280.3,340.4 | 0.04Å | - | - | - |
| A 160 | GLU 48.63 | 0.65Å O with S 222 HOH O | - | Favored (3.62%) General / -109.4,-178.7 | Favored (29.4%) <i>mt-10</i> chi angles: 301.9,172.1,251.7 | 0.01Å | - | - | - |
| <p>Avg: Clashscore: 29.18 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345</p> | | | | | | | | | |
| A 161 | GLY 33.18 | - | - | Favored (48.03%) Glycine / 60.6,-140.8 | - | - | - | - | - |
| A 162 | GLU 34.75 | - | - | Favored (65.92%) General / -63.3,-20.9 | Favored (17.1%) <i>pt0</i> chi angles: 68.7,173.6,346 | 0.02Å | - | - | - |
| A 163 | LEU 27.92 | - | - | Favored (56.62%) General / -87.5,-8.3 | Favored (50.8%) <i>mt</i> chi angles: 296.2,184.6 | 0.01Å | - | - | - |
| A 164 | LYS 45.76 | - | - | Favored (57.84%) General / -60.5,139.3 | Allowed (1.6%) <i>tttm</i> chi angles: 202.6,197,165.7,251.6 | 0.02Å | - | - | - |
| A 165 | GLY 22.88 | 0.42Å HA3 with A 213 ASN HA | - | Favored (3.98%) Glycine / -179.3,-140.3 | - | - | - | - | - |
| A 166 | LYS 41.5 | - | - | Favored (23.98%) General / -145.8,136.1 | Favored (14%) <i>tttt</i> chi angles: 185.5,166.5,155,154.3 | 0.02Å | - | - | - |
| A 167 | TYR 19.14 | - | - | Favored (33.64%) General / -88.4,135.1 | Favored (68.5%) <i>t80</i> chi angles: 181.2,67.8 | 0.02Å | - | - | - |
| A 168 | TYR 28.09 | - | - | Favored (43.98%) Pre-Pro / -119.1,106.0 | Favored (34.9%) <i>m-80</i> chi angles: 304.7,79.9 | 0.06Å | - | - | - |

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|----------|-----------|---|--------------------------------------------------|------------------------------------------------------------------------|-------|---|---|---|
| A 169 | PRO 18.45 | - | Favored (82.6%) Trans-Pro / -64.3,143.3 | Favored (2.7%) <i>Cg_exo</i> chi angles: 356.8,17,336.5 | 0.04Å | - | - | - |
| A 170 | LEU 17.67 | - | Favored (63.06%) General / -72.0,-28.0 | Favored (3.7%) <i>mp</i> chi angles: 262.3,54.4 | 0.02Å | - | - | - |
| A 171 | THR 18.21 | - | Favored (20.27%) General / -67.5,123.4 | Favored (84.9%) <i>m</i> chi angles: 301.7 | 0.03Å | - | - | - |
| A 172 | GLY 22.18 | - | Favored (75.78%) Glycine / 71.9,14.0 | - | - | - | - | - |
| A 173 | MET 18.79 | - | Favored (48.53%) General / -69.4,134.0 | Favored (62.6%) <i>tmm</i> chi angles: 185.7,181.4,287.6 | 0.02Å | - | - | - |
| A 174 | ASP 18.22 | - | Favored (14.22%) General / -92.3,162.6 | Favored (3.1%) <i>p0</i> chi angles: 65.8,63.2 | 0.03Å | - | - | - |
| A 175 | LYS 24.23 | - | Favored (72.93%) General / -65.0,-31.6 | Allowed (0.6%) <i>tttp</i> chi angles: 207.2,129.5,160.2,93.3 | 0.02Å | - | - | - |
| A 176 | ALA 18.4 | - | Favored (71.84%) General / -69.9,-43.3 | - | 0.02Å | - | - | - |
| A 177 | THR 19.48 | - | Favored (91.21%) General / -58.9,-43.7 | Favored (65.9%) <i>m</i> chi angles: 303.2 | 0.05Å | - | - | - |
| A 178 | GLN 31.69 | - | Favored (67.43%) General / -54.3,-50.4 | Allowed (0.4%) <i>tt0</i> chi angles: 231.4,158.8,13.8 | 0.03Å | - | - | - |
| A 179 | GLN 28.4 | - | Favored (95.06%) General / -62.7,-44.9 | Favored (66.6%) <i>tp40</i> chi angles: 194.7,55.4,56.5 | 0.02Å | - | - | - |
| A 180 | GLN 36.78 | - | Favored (74.25%) General / -62.9,-32.9 | Favored (4.8%) <i>pt0</i> chi angles: 67.1,174.8,251.5 | 0.03Å | - | - | - |

Alt Res High Clash > Ramachandran Rotamer Cβ Bond Bond Cis
B 0.4Å deviation lengths angles Peptides

Avg: Clashscore: 29.18 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

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|----------|-----------|----------------------------------|----------------------------------------------------|-------------------------------------------------------------------------|-------|---|---|---|
| A 181 | LEU 19.19 | - | Favored (60.14%) General / -74.2,-42.1 | Favored (79.8%) <i>mt</i> chi angles: 288.8,170.6 | 0.01Å | - | - | - |
| A 182 | ILE 23.19 | - | Favored (71.84%) Ile or Val / -54.5,-47.0 | Favored (68.8%) <i>mt</i> chi angles: 289.6,162.5 | 0.04Å | - | - | - |
| A 183 | ASP 30.5 | 0.78Å OD2 with S 191 HOH O | Favored (66.77%) General / -56.5,-34.3 | Favored (91.3%) <i>m-30</i> chi angles: 287.6,353.3 | 0.02Å | - | - | - |
| A 184 | ASP 32.16 | - | Favored (59.2%) General / -84.2,-5.1 | Favored (68.1%) <i>m-30</i> chi angles: 290.4,321.6 | 0.02Å | - | - | - |
| A 185 | HIS 35.6 | - | Favored (12.66%) General / 62.7,37.7 | Favored (55%) <i>m-70</i> chi angles: 307.4,268.9 | 0.06Å | - | - | - |
| A 186 | PHE 21.18 | - | Favored (15.48%) General / -107.2,-12.0 | Favored (17.2%) <i>m-10</i> chi angles: 288.8,351 | 0.03Å | - | - | - |
| A 187 | LEU 18.13 | - | Favored (27.04%) General / -86.2,145.4 | Favored (8.8%) <i>tp</i> chi angles: 193.4,77.1 | 0.03Å | - | - | - |
| A 188 | PHE 18.26 | - | Favored (34.42%) General / -120.5,155.0 | Favored (55.7%) <i>p90</i> chi angles: 65,94.1 | 0.05Å | - | - | - |
| A 189 | LYS 43.15 | - | Favored (2.35%) General / -112.9,-173.9 | Favored (4.5%) <i>pttm</i> chi angles: 51.2,205.6,177.9,309.2 | 0.04Å | - | - | - |
| A 190 | GLU 36.48 | - | Favored (41.79%) General / -58.1,143.9 | Allowed (0.3%) <i>mt-10</i> chi angles: 241,203.4,304 | 0.02Å | - | - | - |
| A 191 | GLY 22.13 | - | Favored (53.18%) Glycine / -69.8,159.8 | - | - | - | - | - |
| A 192 | ASP 26.76 | - | Favored (5.21%) General / -75.8,179.9 | Favored (47.3%) <i>p0</i> chi angles: 61.4,17.6 | 0.03Å | - | - | - |
| A 193 | ARG 24.3 | - | Favored (63.24%) General / -56.4,-30.8 | Favored (39.1%) <i>ptt90</i> chi angles: 59.7,187.5,166.6,87.8 | 0.02Å | - | - | - |
| A 194 | PHE 27.91 | - | Favored (82.78%) | Favored (93.3%) <i>m-80</i> | 0.02Å | - | - | - |

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|----------|----------------|---------------|------------------------|--------------------------|----------------------------------------|---------------------|---------------------|--------------------|---------------------|---------------------------|--|--|
| A | LEU | 24.28 | - | General / -66.5,-44.4 | chi angles: 298.9,280 | | | | | | | |
| 195 | | | | Favored (80.82%) | Favored (36.3%) <i>mt</i> | 0.01Å | - | - | - | | | |
| | | | | General / -68.7,-38.9 | chi angles: 293,184.9 | | | | | | | |
| A | GLN | 26.01 | - | Favored (81.47%) | Favored (47.9%) <i>mm-40</i> | 0.01Å | - | - | - | | | |
| 196 | | | | General / -59.8,-48.5 | chi angles: 299.8,280.5,335.4 | | | | | | | |
| A | ALA | 19.87 | - | Favored (64.34%) | - | 0.03Å | - | - | - | | | |
| 197 | | | | General / -68.7,-19.3 | | | | | | | | |
| A | ALA | 15.76 | - | Favored (36.38%) | - | 0.01Å | - | - | - | | | |
| 198 | | | | General / -83.7,2.7 | | | | | | | | |
| A | ASN | 24.14 | - | Favored (15.86%) | Favored (50.2%) <i>m-40</i> | 0.04Å | - | - | - | | | |
| 199 | | | | General / 63.0,27.3 | chi angles: 277.4,351.4 | | | | | | | |
| A | ALA | 19.31 | - | Favored (49.14%) | - | 0.02Å | - | - | - | | | |
| 200 | | | | General / -91.5,5.5 | | | | | | | | |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides | | | |
| | | | Avg: Clashscore: 29.18 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 | | | |
| A | CYS | 24.02 | - | Favored (9.42%) | Favored (55.5%) <i>m</i> | 0.04Å | - | - | - | | | |
| 201 | | | | General / -123.6,20.5 | chi angles: 302.4 | | | | | | | |
| A | ARG | 23.37 | - | Favored (43.46%) | Favored (24.3%) <i>mtm110</i> | 0.02Å | - | - | - | | | |
| 202 | | | | General / -72.0,151.2 | chi angles: 299.3,165.5,298.3,103.8 | | | | | | | |
| A | TYR | 32.19 | - | Favored (13.48%) | Favored (65.7%) <i>m-80</i> | 0.04Å | - | - | - | | | |
| 203 | | | | General / 62.8,22.6 | chi angles: 299.9,293.2 | | | | | | | |
| A | TRP | 23.94 | - | Favored (90.32%) | Favored (32.8%) <i>t-100</i> | 0.04Å | - | - | - | | | |
| 204 | | | | Pre-Pro / -60.3,132.4 | chi angles: 190.2,274.7 | | | | | | | |
| A | PRO | 16.9 | - | Favored (10.46%) | Favored (17.3%) <i>Cg_endo</i> | 0.04Å | - | - | - | Cis PRO omega= 4.29 | | |
| 205 | | | | Cis-Pro / -104.9,24.2 | chi angles: 37.3,328.9,12.6 | | | | | | | |
| A | THR | 22.08 | - | Favored (22.08%) | Favored (15.7%) <i>m</i> | 0.05Å | - | - | - | | | |
| 206 | | | | General / -53.8,126.4 | chi angles: 310 | | | | | | | |

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|----------|-----------|--------------------------------------|-----------------------------------------------------|--------------------------------------------------------------------------|-------|---|---|---|
| A 207 | GLY 14.53 | - | Favored (89.65%) Glycine / 80.5,2.6 | - | - | - | - | - |
| A 208 | ARG 16.94 | - | Favored (34.66%) General / -102.7,141.9 | Favored (2.2%) <i>mpt180</i> chi angles: 280.7,65.2,160.7,216.6 | 0.02Å | - | - | - |
| A 209 | GLY 12.59 | - | Favored (45.32%) Glycine / -173.5,172.6 | - | - | - | - | - |
| A 210 | ILE 18.01 | - | Favored (48.93%) Ile or Val / -136.2,131.3 | Favored (6.3%) <i>mt</i> chi angles: 292.8,147.8 | 0.04Å | - | - | - |
| A 211 | TYR 25.11 | - | Favored (50.45%) General / -120.3,141.0 | Favored (60.4%) <i>t80</i> chi angles: 180,272.1 | 0.02Å | - | - | - |
| A 212 | HIS 22.38 | - | Favored (42.13%) General / -148.1,156.0 | Favored (16.2%) <i>p90</i> chi angles: 73.3,74 | 0.09Å | - | - | - |
| A 213 | ASN 22.6 | 0.42Å HA with A 165 GLY HA3 | Favored (15.8%) General / -89.0,162.9 | Favored (41.9%) <i>p0</i> chi angles: 65.4,343.2 | 0.02Å | - | - | - |
| A 214 | ASP 38.46 | - | Favored (62.36%) General / -52.3,-40.8 | Favored (46.9%) <i>m-30</i> chi angles: 303.3,332.4 | 0.01Å | - | - | - |
| A 215 | ALA 24.85 | - | Favored (50.05%) General / -75.7,-6.3 | - | 0.02Å | - | - | - |
| A 216 | LYS 29.27 | - | Favored (29.23%) General / 56.3,41.3 | Favored (91.7%) <i>mttt</i> chi angles: 301.3,185,180.8,175.6 | 0.06Å | - | - | - |
| A 217 | THR 22.85 | - | Favored (15.27%) General / -116.8,14.4 | Favored (66.4%) <i>p</i> chi angles: 58.4 | 0.04Å | - | - | - |
| A 218 | PHE 21.4 | - | Favored (5.88%) General / -156.5,125.2 | Favored (68.9%) <i>t80</i> chi angles: 174,68.9 | 0.02Å | - | - | - |
| A 219 | LEU 16.76 | - | Favored (41.26%) General / -136.6,138.5 | Favored (12.7%) <i>tp</i> chi angles: 169.8,73.3 | 0.03Å | - | - | - |
| A 220 | VAL 15.33 | - | Favored (70.26%) | Favored (36.5%) <i>t</i> chi angles: 184.2 | 0.03Å | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ile or Val / -127.0,132.1 | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|-------|---------|------------------------|---------------------------------|-----------------------------------------------|----------------------------------------------------------------------|--------------------|--------------------|--------------------|---------------------|--------------|
| | | Avg: Clashscore: 29.18 | 5 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 | |
| A 221 | TRP | 18.28 | - | Favored (49.97%) General / -102.7,126.8 | Favored (42.9%) <i>m-10</i> chi angles: 286.3,354.2 | 0.02Å | - | - | - | |
| A 222 | VAL | 14.61 | - | Favored (45.61%) Ile or Val / -99.9,117.8 | Favored (34.6%) <i>t</i> chi angles: 184.7 | 0.04Å | - | - | - | |
| A 223 | ASN | 16.08 | - | Favored (18.01%) General / 61.9,31.9 | Favored (64.7%) <i>m-40</i> chi angles: 283.2,316.8 | 0.08Å | - | - | - | |
| A 224 | GLU | 24.92 | - | Favored (67.35%) General / -72.9,-36.4 | Favored (12.4%) <i>tm-30</i> chi angles: 182.8,266.5,335.9 | 0.02Å | - | - | - | |
| A 225 | GLU | 32.32 | 0.54Å HG3 with A 270 PHE CD2 | Allowed (0.11%) General / -154.8,-58.3 | Favored (2.9%) <i>tt0</i> chi angles: 156.7,163.4,341.4 | 0.02Å | - | - | - | |
| A 226 | ASP | 16.26 | - | Favored (17.59%) General / -87.0,162.5 | Favored (16.3%) <i>m-30</i> chi angles: 281.9,309.1 | 0.04Å | - | - | - | |
| A 227 | HIS | 13.93 | - | Favored (42.34%) General / -49.6,-50.4 | Favored (43.8%) <i>m170</i> chi angles: 296.8,152.6 | 0.01Å | - | - | - | |
| A 228 | LEU | 13.8 | - | Favored (44.98%) General / -129.3,129.6 | Favored (78.5%) <i>mt</i> chi angles: 301.7,176.2 | 0.03Å | - | - | - | |
| A 229 | ARG | 41.52 | 0.76Å NH1 with S 231 HOH O | Favored (26.55%) General / -113.2,114.3 | Favored (6.5%) <i>ttm-80</i> chi angles: 184.6,198.5,291.5,241 | 0.01Å | - | - | - | |
| A 230 | ILE | 19.74 | - | Favored (68.16%) Ile or Val / -111.6,124.2 | Favored (11.2%) <i>mt</i> chi angles: 308.5,157.1 | 0.06Å | - | - | - | |
| A 231 | ILE | 25.98 | - | Favored (50.8%) Ile or Val / -129.9,139.7 | Allowed (0.7%) <i>mt</i> chi angles: 312.4,138.4 | 0.01Å | - | - | - | |

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|----------|----------------|---------------|----------------------------------------|---------------------------------------------------|-------------------------------------------------------------------------|---------------------|---------------------|--------------------|---------------------|
| A 232 | SER | 19.29 | - | Favored (46.09%) General / -129.8,131.2 | Favored (46.5%) <i>t</i> chi angles: 179.8 | 0.03Å | - | - | - |
| A 233 | MET | 20.09 | - | Favored (41.32%) General / -154.5,162.1 | Allowed (0.4%) <i>pmt</i> chi angles: 68.7,296.4,187.8 | 0.01Å | - | - | - |
| A 234 | GLN | 22.11 | 0.59Å HG2 with A 242 ILE HD11 | Favored (7.32%) General / -171.1,163.9 | Favored (18.6%) <i>pt0</i> chi angles: 60.2,187.9,51.9 | 0.05Å | - | - | - |
| A 235 | LYS | 43.89 | - | Favored (38.62%) General / -60.0,147.6 | Favored (4.9%) <i>mmtm</i> chi angles: 300.5,291.4,214.9,318.3 | 0.04Å | - | - | - |
| A 236 | GLY | 19.41 | - | Favored (36.67%) Glycine / 84.2,-160.4 | - | - | - | - | - |
| A 237 | GLY | 19.55 | - | Favored (4.26%) Glycine / -130.2,25.9 | - | - | - | - | - |
| A 238 | ASP | 26.83 | - | Favored (3.97%) General / -77.4,75.5 | Favored (49.9%) <i>t0</i> chi angles: 187.8,2.5 | 0.05Å | - | - | - |
| A 239 | LEU | 22.63 | - | Favored (62.73%) General / -55.0,-33.8 | Favored (32.5%) <i>tp</i> chi angles: 186.7,58 | 0.02Å | - | - | - |
| A 240 | LYS | 38.93 | - | Favored (5.34%) General / -61.2,-59.4 | Favored (33.2%) <i>tttt</i> chi angles: 170.5,166.3,194,162.8 | 0.00Å | - | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
| | | Avg: 29.18 | Clashscore: 5 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 |
| A 241 | THR | 26.7 | - | Favored (74.76%) General / -57.1,-39.4 | Favored (81.6%) <i>m</i> chi angles: 296.5 | 0.05Å | - | - | - |
| A 242 | ILE | 21.78 | 0.59Å HD11 with A 234 GLN HG2 | Favored (75.1%) Ile or Val / -65.5,-49.9 | Favored (7.6%) <i>mt</i> chi angles: 283.9,153 | 0.07Å | - | - | - |
| A 243 | PHE | 21.66 | - | Favored (90.56%) General / -65.3,-43.6 | Favored (10.3%) <i>t80</i> chi angles: 184.3,38.5 | 0.03Å | - | - | - |

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|----------|-----------|----------------------------------------|----------------------------------------------------|--------------------------------------------------------------------------|-------|---|---|---|
| A 244 | GLN 40.16 | 0.43Å HB2 with A 107 ILE HG12 | Favored (93.31%) General / -60.3,-41.5 | Favored (25.9%) <i>tp40</i> chi angles: 179.3,70.7,86.1 | 0.02Å | - | - | - |
| A 245 | ARG 27.04 | - | Favored (79.48%) General / -60.6,-36.8 | Favored (12.9%) <i>ttm110</i> chi angles: 171.4,188.2,316,129.9 | 0.01Å | - | - | - |
| A 246 | LEU 21.8 | - | Favored (69.02%) General / -68.1,-47.1 | Favored (31.7%) <i>tp</i> chi angles: 181.3,69.7 | 0.02Å | - | - | - |
| A 247 | VAL 27.91 | - | Favored (75.19%) Ile or Val / -66.4,-35.6 | Allowed (1.8%) <i>p</i> chi angles: 53.4 | 0.11Å | - | - | - |
| A 248 | ASN 35.81 | - | Favored (89.46%) General / -58.5,-44.6 | Favored (80%) <i>m-40</i> chi angles: 289.7,352.2 | 0.02Å | - | - | - |
| A 249 | ALA 24.42 | - | Favored (73.6%) General / -64.6,-48.8 | - | 0.03Å | - | - | - |
| A 250 | VAL 22.8 | - | Favored (82.84%) Ile or Val / -57.0,-47.7 | Favored (60.1%) <i>t</i> chi angles: 170.8 | 0.06Å | - | - | - |
| A 251 | ASN 25.21 | - | Favored (91.76%) General / -61.1,-46.1 | Favored (99%) <i>m-40</i> chi angles: 287.6,337.9 | 0.01Å | - | - | - |
| A 252 | THR 27.64 | - | Favored (61.92%) General / -53.0,-51.3 | Favored (32%) <i>m</i> chi angles: 306.5 | 0.04Å | - | - | - |
| A 253 | ILE 22.89 | - | Favored (93.3%) Ile or Val / -60.9,-47.5 | Favored (71%) <i>mt</i> chi angles: 299.1,164.4 | 0.05Å | - | - | - |
| A 254 | GLU 27.27 | 0.50Å OE2 with S 21 HOH O | Favored (74.56%) General / -56.8,-39.6 | Favored (38.7%) <i>tt0</i> chi angles: 180.7,168.2,221.9 | 0.02Å | - | - | - |
| A 255 | SER 36.84 | - | Favored (24.26%) General / -52.9,-28.6 | Allowed (1.2%) <i>p</i> chi angles: 91.3 | 0.04Å | - | - | - |
| A 256 | LYS 41.6 | - | Favored (15.54%) General / -107.6,-10.9 | Favored (11%) <i>mmtp</i> chi angles: 305.6,279.7,168.8,80.1 | 0.01Å | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|-------|-----------|------------------|----------------|-----------------------------------------------|--------------------------------------------------------------------------|--------------|--------------|--------------|--------------|
| A 257 | LEU 35.32 | - | | Favored (2.3%) Pre-Pro / -154.9,104.6 | Allowed (0.9%) <i>tp</i> chi angles: 221.3,42 | 0.03Å | - | - | - |
| A 258 | PRO 27.87 | - | | Favored (59.9%) Trans-Pro / -70.5,148.4 | Favored (5.2%) <i>Cg_exo</i> chi angles: 350.8,25.1,329.5 | 0.04Å | - | - | - |
| A 259 | PHE 20.11 | - | | Favored (19.06%) General / -96.6,152.0 | Favored (23.2%) <i>m-10</i> chi angles: 301.4,321.6 | 0.02Å | - | - | - |
| A 260 | SER 25.25 | - | | Favored (20.57%) General / -81.2,115.3 | Favored (9.6%) <i>t</i> chi angles: 166 | 0.06Å | - | - | - |
| | | Avg: Clashscore: | Outliers: 1 of | Poor rotamers: 0 of | Outliers: | Outliers: | Outliers: | Non-Trans: 1 | |
| | | 29.18 | 5 | 340 | 287 | 0 of 322 | 0 of 347 | 0 of 347 | of 345 |
| A 261 | ARG 17.62 | - | | Favored (42.57%) General / -136.7,140.3 | Favored (43%) <i>ttt-90</i> chi angles: 196.5,187.3,191.2,279.5 | 0.04Å | - | - | - |
| A 262 | ASP 21.19 | - | | Favored (49.56%) General / -113.7,138.9 | Favored (30.1%) <i>t70</i> chi angles: 180.2,76.7 | 0.03Å | - | - | - |
| A 263 | ASP 33 | - | | Favored (82.88%) General / -57.2,-43.7 | Favored (88%) <i>m-30</i> chi angles: 285.5,341.5 | 0.01Å | - | - | - |
| A 264 | ARG 15.76 | - | | Favored (26.99%) General / -80.8,-39.2 | Favored (4.9%) <i>ttp80</i> chi angles: 187.1,176,103.5,76.7 | 0.01Å | - | - | - |
| A 265 | LEU 15.42 | - | | Favored (20.51%) General / -102.3,-9.3 | Favored (40.1%) <i>mt</i> chi angles: 296.2,186.1 | 0.02Å | - | - | - |
| A 266 | GLY 14.59 | - | | Favored (33.14%) Glycine / 79.0,-149.8 | - | - | - | - | - |
| A 267 | PHE 15.76 | - | | Favored (40.55%) General / -70.1,129.9 | Favored (79.2%) <i>m-80</i> chi angles: 290.4,281.4 | 0.02Å | - | - | - |
| A 268 | LEU 16.67 | - | | Favored (34.37%) General / -86.6,130.8 | Favored (56.6%) <i>mt</i> chi angles: 297.4,184.5 | 0.03Å | - | - | - |

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|----------|-----|-------|---------------------------------------|----------------------------------------------------|--------------------------------------------------------------------------|-------|---|---|---|
| A 269 | THR | 14.29 | - | Favored (28.06%) General / -127.0,161.6 | Favored (41.3%) <i>p</i> chi angles: 54.8 | 0.04Å | - | - | - |
| A 270 | PHE | 23.12 | 0.54Å CD2 with A 225 GLU HG3 | Favored (95.56%) General / -61.8,-45.0 | Favored (40.4%) <i>t80</i> chi angles: 164.4,76.4 | 0.08Å | - | - | - |
| A 271 | CYS | 26.06 | - | Favored (24.23%) Pre-Pro / -97.8,132.8 | Favored (18.1%) <i>t</i> chi angles: 191.8 | 0.05Å | - | - | - |
| A 272 | PRO | 16.46 | - | Favored (30.45%) Trans-Pro / -67.8,-10.9 | Favored (10.3%) <i>Cg_endo</i> chi angles: 15.4,335.5,23.2 | 0.04Å | - | - | - |
| A 273 | THR | 18.28 | - | Favored (62.03%) General / -70.2,-13.1 | Favored (66.5%) <i>p</i> chi angles: 62.9 | 0.03Å | - | - | - |
| A 274 | ASN | 22.14 | - | Favored (19.16%) General / -111.6,18.4 | Favored (43.1%) <i>m110</i> chi angles: 298.3,125.2 | 0.01Å | - | - | - |
| A 275 | LEU | 17.87 | - | Allowed (1.79%) General / -73.2,-175.3 | Favored (29.6%) <i>mt</i> chi angles: 292.4,159.8 | 0.02Å | - | - | - |
| A 276 | GLY | 16.54 | - | Favored (5.24%) Glycine / 77.7,-119.3 | - | - | - | - | - |
| A 277 | THR | 12.84 | - | Favored (66.02%) General / -68.7,-27.6 | Favored (70.2%) <i>p</i> chi angles: 62.2 | 0.06Å | - | - | - |
| A 278 | THR | 15.79 | - | Allowed (1.68%) General / 63.4,4.3 | Allowed (1.9%) <i>p</i> chi angles: 81.9 | 0.06Å | - | - | - |
| A 279 | ILE | 21.48 | - | Favored (38.08%) Ile or Val / -89.2,130.8 | Allowed (1.1%) <i>mt</i> chi angles: 275.4,182.8 | 0.05Å | - | - | - |
| A 280 | ARG | 43.96 | - | Favored (12.16%) General / -121.7,107.3 | Favored (57.3%) <i>ttt-90</i> chi angles: 189.6,182.7,179.8,264 | 0.04Å | - | - | - |

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 29.18 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

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|----------|-----------|---------------------------------------|-----------------------------------------------------|----------------------------------------------------------------------|-------|---|---|---|
| A 281 | ALA 23.3 | - | Favored (48.24%) General / -102.0,129.4 | - | 0.03Å | - | - | - |
| A 282 | SER 21.91 | - | Favored (44.59%) General / -144.0,157.0 | Favored (70.6%) <i>p</i> chi angles: 59 | 0.01Å | - | - | - |
| A 283 | VAL 23.44 | - | Favored (31.46%) Ile or Val / -126.7,148.3 | Favored (27.2%) <i>m</i> chi angles: 299.8 | 0.01Å | - | - | - |
| A 284 | HIS 58.48 | - | Favored (26.79%) General / -95.9,115.0 | Favored (3.4%) <i>m170</i> chi angles: 270.6,202.8 | 0.01Å | - | - | - |
| A 285 | ILE 25.22 | - | Favored (23.34%) Ile or Val / -141.5,146.4 | Favored (17.5%) <i>tt</i> chi angles: 185.1,171.8 | 0.05Å | - | - | - |
| A 286 | ALA 29.49 | - | Favored (40.24%) General / -109.3,119.7 | - | 0.01Å | - | - | - |
| A 287 | LEU 36.08 | - | Favored (57.78%) Pre-Pro / -124.3,72.7 | Allowed (0.6%) <i>mm</i> chi angles: 288.1,319 | 0.03Å | - | - | - |
| A 288 | PRO 40.26 | - | Favored (21.07%) Trans-Pro / -63.9,-42.0 | Favored (33.3%) <i>Cg_endo</i> chi angles: 21.9,326.4,31.2 | 0.04Å | - | - | - |
| A 289 | LYS 46.42 | 0.44Å HD3 with A 356 ALA HB3 | Favored (85.29%) General / -61.6,-47.5 | Favored (9.2%) <i>mttp</i> chi angles: 279,157.3,154.8,66.9 | 0.02Å | - | - | - |
| A 290 | LEU 41.23 | - | Favored (65.43%) General / -67.6,-21.6 | Favored (39.8%) <i>mt</i> chi angles: 298,186.6 | 0.03Å | - | - | - |
| A 291 | ALA 55.95 | - | Favored (61.18%) General / -72.4,-23.9 | - | 0.01Å | - | - | - |
| A 292 | ALA 66.57 | - | Favored (58.77%) General / -88.1,-4.4 | - | 0.02Å | - | - | - |
| A 293 | ALA 72.39 | 0.52Å O with A 295 ALA N | Favored (4.11%) General / -104.0,-47.7 | - | 0.02Å | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------|--------------------------|--------------|----------------------------------------------|---------------------------------------------------------------------|--------------|--------------|-------------|--------------|
| A 294 | ALA 66.69 | - | - | OUTLIER (0.02%) General / 56.9,-20.1 | - | 0.04Å | - | - | - |
| A 295 | ALA 71.56 | N with A 293 ALA O | 0.52Å | Favored (13.02%) General / -88.8,-40.6 | - | 0.00Å | - | - | - |
| A 296 | ALA 67.89 | O with A 300 ILE HG12 | 0.44Å | Favored (61.57%) General / -73.5,-27.9 | - | 0.03Å | - | - | - |
| A 297 | ALA 59.63 | - | - | Allowed (0.93%) General / -64.4,-64.2 | - | 0.01Å | - | - | - |
| A 298 | GLU 68.38 | - | - | Favored (63.58%) General / -59.0,-25.4 | Allowed (1.3%) <i>mp0</i> chi angles: 262.1,72.3,183 | 0.01Å | - | - | - |
| A 299 | ALA 54.02 | - | - | Favored (70.73%) General / -58.2,-34.7 | - | 0.01Å | - | - | - |
| A 300 | ILE 61.64 | HG12 with A 296 ALA O | 0.44Å | Favored (18.82%) Ile or Val / -83.2,-45.6 | Favored (6.1%) <i>mm</i> chi angles: 316.6,307.7 | 0.05Å | - | - | - |
| <p>Avg: Clashscore: 29.18 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345</p> | | | | | | | | | |
| A 301 | ALA 42.7 | - | - | Favored (18.63%) General / -52.2,-55.8 | - | 0.02Å | - | - | - |
| A 302 | ALA 48.39 | - | - | Favored (78.84%) General / -62.1,-35.5 | - | 0.01Å | - | - | - |
| A 303 | LYS 57.52 | HB2 with S 260 HOH O | 0.41Å | Favored (68.01%) General / -72.4,-34.5 | Allowed (0.4%) <i>ttm</i> chi angles: 151.7,152.3,202.3,253.3 | 0.00Å | - | - | - |
| A 304 | PHE 39.93 | - | - | Favored (38.67%) General / -100.9,11.9 | Favored (58.5%) <i>m-80</i> chi angles: 284.9,278.7 | 0.04Å | - | - | - |
| A 305 | ASN 32.46 | - | - | Favored (15.57%) General / 61.7,38.0 | Favored (68.5%) <i>m-40</i> chi angles: 305.1,302.6 | 0.03Å | - | - | - |

| | | | | | | | | |
|----------|-----------|----------------------------------------|-----------------------------------------------------|---------------------------------------------------------------------------|-------|---|---|---|
| A 306 | LEU 32.9 | 0.58Å HD11 with A 345 GLY HA3 | Favored (22.39%) General / -98.7,149.9 | Favored (72.7%) <i>mt</i> chi angles: 302.6,180.9 | 0.01Å | - | - | - |
| A 307 | GLN 54.84 | - | Favored (55.5%) General / -109.5,130.5 | Allowed (0.6%) <i>tt0</i> chi angles: 146.8,159.8,23.1 | 0.03Å | - | - | - |
| A 308 | VAL 42.27 | - | Favored (34.5%) Ile or Val / -107.9,111.1 | Favored (85.6%) <i>t</i> chi angles: 173.6 | 0.03Å | - | - | - |
| A 309 | ALA 46.93 | - | - | - | 0.02Å | - | - | - |
| A 320 | GLY 59.54 | - | - | - | - | - | - | - |
| A 321 | GLY 61.05 | - | Allowed (0.42%) Glycine / -141.6,-14.6 | - | - | - | - | - |
| A 322 | VAL 53.99 | - | Favored (42.35%) Ile or Val / -102.1,114.7 | Allowed (0.5%) <i>p</i> chi angles: 48.1 | 0.06Å | - | - | - |
| A 323 | TYR 56.8 | - | Favored (20.94%) General / -105.2,153.9 | Favored (77.9%) <i>m-80</i> chi angles: 300.1,287.4 | 0.05Å | - | - | - |
| A 324 | ASP 46.72 | - | Favored (36.03%) General / -103.0,118.1 | Favored (14.9%) <i>t70</i> chi angles: 174.8,264.8 | 0.02Å | - | - | - |
| A 325 | ILE 27.91 | - | Favored (75.09%) Ile or Val / -122.3,129.7 | Favored (27.4%) <i>mt</i> chi angles: 303.4,184.3 | 0.04Å | - | - | - |
| A 326 | SER 26.67 | - | Favored (43.7%) General / -142.9,158.3 | Favored (57.1%) <i>p</i> chi angles: 57.5 | 0.02Å | - | - | - |
| A 327 | ASN 26.1 | - | Favored (53.83%) General / -69.6,140.9 | Favored (15.3%) <i>p0</i> chi angles: 62.3,292.6 | 0.02Å | - | - | - |
| A 328 | LYS 43.34 | - | Favored (22.16%) General / -85.3,-33.0 | Favored (4.1%) <i>mtpt</i> chi angles: 290.2,163.5,94.8,144.4 | 0.04Å | - | - | - |
| A 329 | ARG 25.65 | - | Favored (31.84%) General / -88.2,138.0 | Favored (44.3%) <i>mtp180</i> chi angles: 301.6,157.7,68.8,200.7 | 0.02Å | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|----------|-----------|--------|---------------------------|-------------------------------------------------|---------------------------------------------------------------------------|-----------------------|-----------------------|-----------------------|------------------------|
| A 330 | ARG 29.18 | - | - | Favored (4.41%) General / -119.6,-32.1 | Favored (3.6%) <i>mmt-90</i> chi angles: 316.9,259.3,187.1,283.4 | 0.04Å | - | - | - |
| | | | Avg: Clashscore: 29.18 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 |
| A 331 | MET 18.5 | - | - | Favored (23.65%) General / -110.5,154.4 | Favored (23.3%) <i>mtp</i> chi angles: 312,190.9,64.3 | 0.02Å | - | - | - |
| A 332 | GLY 18 | - | - | Favored (88.43%) Glycine / 84.3,-1.8 | - | - | - | - | - |
| A 333 | LEU 19.44 | - | - | Favored (44.46%) General / -141.3,158.0 | Allowed (0.8%) <i>pt</i> chi angles: 76.7,183.4 | 0.02Å | - | - | - |
| A 334 | THR 16.91 | - | - | Favored (14.75%) General / -78.5,171.7 | Favored (30.3%) <i>p</i> chi angles: 69.3 | 0.02Å | - | - | - |
| A 335 | GLU 18.8 | - | - | Favored (96.04%) General / -60.3,-43.9 | Favored (54.9%) <i>mp0</i> chi angles: 289.4,77.8,0.5 | 0.01Å | - | - | - |
| A 336 | TYR 25.85 | - | - | Favored (76.47%) General / -58.2,-49.6 | Favored (92.4%) <i>t80</i> chi angles: 176.5,77.1 | 0.02Å | - | - | - |
| A 337 | GLN 24.55 | - | - | Favored (80.8%) General / -64.0,-35.5 | Favored (77.1%) <i>mt0</i> chi angles: 301.4,181.1,306 | 0.01Å | - | - | - |
| A 338 | ALA 19.92 | - | - | Favored (79.71%) General / -62.6,-48.4 | - | 0.02Å | - | - | - |
| A 339 | VAL 19.1 | - | - | Favored (86.53%) Ile or Val / -67.7,-43.5 | Favored (50.4%) <i>t</i> chi angles: 169.5 | 0.08Å | - | - | - |
| A 340 | LYS 31.26 | - | - | Favored (71.75%) General / -61.8,-31.6 | Allowed (1.7%) <i>tptp</i> chi angles: 184.4,74.5,167.8,21.1 | 0.02Å | - | - | - |
| A 341 | GLU 29.96 | - | - | Favored (71.52%) General / -68.7,-45.5 | Favored (21.9%) <i>tt0</i> chi angles: 194.6,171.1,54.9 | 0.04Å | - | - | - |

| | | | | | | | | | |
|----------|----------------|---------------|----------------------------------------|----------------------------------------------------|--------------------------------------------------------------------------|---------------------|---------------------|--------------------|---------------------|
| A 342 | MET | 33.72 | - | Favored (64.63%) General / -58.8,-52.7 | Favored (7.1%) <i>tmm</i> chi angles: 198.5,270.9,277.6 | 0.02Å | - | - | - |
| A 343 | GLN | 26.1 | - | Favored (30.55%) General / -49.8,-52.7 | Favored (21.9%) <i>tt0</i> chi angles: 163.6,178.2,298 | 0.01Å | - | - | - |
| A 344 | ASP | 30.84 | - | Favored (99.39%) General / -62.2,-42.6 | Favored (87.8%) <i>m-30</i> chi angles: 293.2,336 | 0.03Å | - | - | - |
| A 345 | GLY | 20.91 | 0.58Å HA3 with A 306 LEU HD11 | Favored (93.54%) Glycine / -61.6,-46.8 | - | - | - | - | - |
| A 346 | ILE | 21.13 | - | Favored (90.94%) Ile or Val / -64.3,-47.1 | Favored (3.5%) <i>mm</i> chi angles: 292.9,316.3 | 0.08Å | - | - | - |
| A 347 | LEU | 20.49 | - | Favored (54.77%) General / -50.4,-44.4 | Favored (26.6%) <i>mt</i> chi angles: 287,180.8 | 0.01Å | - | - | - |
| A 348 | GLU | 35.93 | - | Favored (79.49%) General / -67.4,-44.2 | Favored (2.8%) <i>tp30</i> chi angles: 210.3,49.6,45.1 | 0.03Å | - | - | - |
| A 349 | MET | 37.9 | - | Favored (98.51%) General / -63.5,-42.1 | Favored (68.5%) <i>mtt</i> chi angles: 294.2,178.6,186.5 | 0.02Å | - | - | - |
| A 350 | ILE | 22.8 | - | Favored (88.02%) Ile or Val / -63.0,-40.2 | Favored (25.9%) <i>mt</i> chi angles: 285.8,178.2 | 0.06Å | - | - | - |
| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
| | | | Avg: Clashscore: 29.18 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 |
| A 351 | LYS | 29.63 | - | Favored (78.47%) General / -55.9,-46.1 | Favored (22.1%) <i>ttmt</i> chi angles: 187.6,185.2,307.9,183.8 | 0.04Å | - | - | - |
| A 352 | MET | 58.16 | - | Favored (92.82%) General / -65.5,-42.0 | Favored (22.5%) <i>mmt</i> chi angles: 295.7,307.1,166.4 | 0.00Å | - | - | - |
| A 353 | GLU | 35.05 | 0.46Å HG2 with A 119 TYR | Favored (88.93%) General / | Favored (43.5%) <i>tp30</i> chi angles: | 0.03Å | - | - | - |

| | | | | | | | | | |
|-----|-----|-------|-------------|-------------|-------------------|-------|---|---|---|
| | | | CE1 | -59.1,-41.8 | 181.3,76.9,187.4 | | | | |
| A | | | | Favored | Favored (2.6%) | | | | |
| 354 | GLU | 47.38 | - | (69.34%) | <i>mm-30</i> | 0.02Å | - | - | - |
| | | | | General / | chi angles: | | | | |
| | | | | -68.6,-30.6 | 285.8,267.1,316.9 | | | | |
| A | | | | Favored | | | | | |
| 355 | ALA | 49.79 | - | (23.74%) | - | 0.00Å | - | - | - |
| | | | | General / | | | | | |
| | | | | -90.0,-20.1 | | | | | |
| A | | | | Favored | | | | | |
| 356 | ALA | 46.57 | 0.44Å | (32.7%) | - | 0.03Å | - | - | - |
| | | | HB3 with A | Pre-Pro / | | | | | |
| | | | 289 LYS HD3 | -57.0,151.7 | | | | | |
| A | | | | | Favored (83.5%) | | | | |
| 357 | PRO | 53.26 | - | - | <i>Cg_exo</i> | 0.04Å | - | - | - |
| | | | | | chi angles: | | | | |
| | | | | | 334.3,6.4,15.5 | | | | |
| B | NA | 41.35 | - | - | - | - | - | - | - |
| S | HOH | 8.5 | - | - | - | - | - | - | - |
| S | HOH | 8.22 | - | - | - | - | - | - | - |
| S | HOH | 12.77 | - | - | - | - | - | - | - |
| S | HOH | 11.56 | - | - | - | - | - | - | - |
| S | HOH | 22.16 | - | - | - | - | - | - | - |
| S | HOH | 17.16 | - | - | - | - | - | - | - |
| S | HOH | 13.22 | - | - | - | - | - | - | - |
| S | HOH | 14.72 | - | - | - | - | - | - | - |
| S | HOH | 13.6 | - | - | - | - | - | - | - |
| S | HOH | 11.71 | - | - | - | - | - | - | - |
| S | HOH | 12.98 | - | - | - | - | - | - | - |
| S | HOH | 24.37 | - | - | - | - | - | - | - |

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 29.18 Outliers: 5 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

| | | | | | | | | | |
|---|-----|-------|---|---|---|---|---|---|---|
| S | HOH | 19.48 | - | - | - | - | - | - | - |
| S | HOH | 21.09 | - | - | - | - | - | - | - |
| S | HOH | 18.89 | - | - | - | - | - | - | - |
| S | HOH | 21.11 | - | - | - | - | - | - | - |

| | | | | | | | | | |
|----|-----------|----------------------------------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 17 | HOH 12.05 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 18 | HOH 15.91 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 19 | HOH 11.64 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 20 | HOH 20.36 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 21 | HOH 23.35 | 0.50Å O with A 254 GLU OE2 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 22 | HOH 23.13 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 23 | HOH 16.32 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 24 | HOH 18.21 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 25 | HOH 20.62 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 26 | HOH 12.85 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 27 | HOH 19.37 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 28 | HOH 18.74 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 29 | HOH 13.82 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 30 | HOH 13.29 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 31 | HOH 23.6 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 32 | HOH 18.23 | - | - | - | - | - | - | - | - |

| # | Alt Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|---|---------|------------|---------------|--------------------|-------------------------|--------------------|--------------------|--------------------|---------------------|
| | | Avg: 29.18 | Clashscore: 5 | Outliers: 1 of 340 | Poor rotamers: 0 of 287 | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 |

| | | | | | | | | | |
|----|-----------|---|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 33 | HOH 36.42 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 34 | HOH 25.88 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 35 | HOH 23.74 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 36 | HOH 16.54 | - | - | - | - | - | - | - | - |

| | | | | | | | | | |
|----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 37 | HOH | 17.71 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 38 | HOH | 34.88 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 39 | HOH | 22.08 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 40 | HOH | 13.71 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 41 | HOH | 19.25 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 42 | HOH | 26.67 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 43 | HOH | 25.1 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 44 | HOH | 22.71 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 45 | HOH | 20.81 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 46 | HOH | 26.3 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 47 | HOH | 31.7 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 48 | HOH | 29.57 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 49 | HOH | 21.21 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 50 | HOH | 17.53 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 51 | HOH | 29.17 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 52 | HOH | 21.55 | - | - | - | - | - | - | - |

**Alt Res** **High B** **Clash > 0.4Å** **Ramachandran** **Rotamer** **Cβ deviation** **Bond lengths** **Bond angles** **Cis Peptides**

Avg: Clashscore: 29.18 Outliers: 5 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

| | | | | | | | | | |
|----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 53 | HOH | 30.63 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 54 | HOH | 25.19 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 55 | HOH | 27.07 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 56 | HOH | 32.53 | - | - | - | - | - | - | - |

| | | | | | | | | | |
|----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 57 | HOH | 24.2 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 58 | HOH | 39.84 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 59 | HOH | 18.87 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 60 | HOH | 31.08 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 61 | HOH | 24.09 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 62 | HOH | 20.53 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 63 | HOH | 22.4 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 64 | HOH | 20.86 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 65 | HOH | 30.99 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 66 | HOH | 16.89 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 67 | HOH | 32.59 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 68 | HOH | 19.48 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 69 | HOH | 34.3 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 70 | HOH | 21.36 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 71 | HOH | 22.38 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 72 | HOH | 26.88 | - | - | - | - | - | - | - |

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 29.18 Outliers: 5 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

| | | | | | | | | | |
|----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 73 | HOH | 19.81 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 74 | HOH | 26.75 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 75 | HOH | 30.57 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 76 | HOH | 20.86 | - | - | - | - | - | - | - |

| | | | | | | | | | |
|----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 77 | HOH | 24.54 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 78 | HOH | 24.53 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 79 | HOH | 24.72 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 80 | HOH | 24.4 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 81 | HOH | 37.9 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 82 | HOH | 20.98 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 83 | HOH | 25.13 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 84 | HOH | 25.11 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 85 | HOH | 27.93 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 86 | HOH | 27.15 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 87 | HOH | 27.74 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 88 | HOH | 23.92 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 89 | HOH | 42.57 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 90 | HOH | 29 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 91 | HOH | 32.31 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 92 | HOH | 34.2 | - | - | - | - | - | - | - |

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 29.18 Outliers: 5 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

| | | | | | | | | | |
|----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 93 | HOH | 25.65 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 94 | HOH | 29.25 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 95 | HOH | 22.56 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 96 | HOH | 15.03 | - | - | - | - | - | - | - |

| | | | | | | | | | |
|-----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 97 | HOH | 33.22 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 98 | HOH | 22.93 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 99 | HOH | 26.86 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 100 | HOH | 34.58 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 101 | HOH | 33.61 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 102 | HOH | 37.87 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 103 | HOH | 43.37 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 104 | HOH | 41.07 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 105 | HOH | 37.87 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 106 | HOH | 33.8 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 107 | HOH | 24.55 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 108 | HOH | 26.6 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 109 | HOH | 23.44 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 110 | HOH | 25.46 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 111 | HOH | 24.3 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 112 | HOH | 26.51 | - | - | - | - | - | - | - |

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 29.18 Outliers: 5 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

| | | | | | | | | | |
|-----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 113 | HOH | 24.51 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 114 | HOH | 40.77 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 115 | HOH | 28.66 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 116 | HOH | 20.3 | - | - | - | - | - | - | - |

| | | | | | | | | | |
|-----|-----------|---|---|---|---|---|---|---|---|
| S | HOH 29.92 | - | - | - | - | - | - | - | - |
| 117 | | | | | | | | | |
| S | HOH 22.84 | - | - | - | - | - | - | - | - |
| 118 | | | | | | | | | |
| S | HOH 36.15 | - | - | - | - | - | - | - | - |
| 119 | | | | | | | | | |
| S | HOH 39.73 | - | - | - | - | - | - | - | - |
| 120 | | | | | | | | | |
| S | HOH 43.31 | - | - | - | - | - | - | - | - |
| 121 | | | | | | | | | |
| S | HOH 34.83 | - | - | - | - | - | - | - | - |
| 122 | | | | | | | | | |
| S | HOH 28.56 | - | - | - | - | - | - | - | - |
| 123 | | | | | | | | | |
| S | HOH 32.17 | - | - | - | - | - | - | - | - |
| 124 | | | | | | | | | |
| S | HOH 30.3 | - | - | - | - | - | - | - | - |
| 125 | | | | | | | | | |
| S | HOH 35.47 | - | - | - | - | - | - | - | - |
| 126 | | | | | | | | | |
| S | HOH 34.3 | - | - | - | - | - | - | - | - |
| 127 | | | | | | | | | |
| S | HOH 29.61 | - | - | - | - | - | - | - | - |
| 128 | | | | | | | | | |
| S | HOH 28.27 | - | - | - | - | - | - | - | - |
| 129 | | | | | | | | | |
| S | HOH 31.79 | - | - | - | - | - | - | - | - |
| 130 | | | | | | | | | |
| S | HOH 33.54 | - | - | - | - | - | - | - | - |
| 131 | | | | | | | | | |
| S | HOH 32.27 | - | - | - | - | - | - | - | - |
| 132 | | | | | | | | | |

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 29.18 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

| | | | | | | | | | |
|-----|-----------|---------------------------------|---|---|---|---|---|---|---|
| S | HOH 41.57 | - | - | - | - | - | - | - | - |
| 133 | | | | | | | | | |
| S | HOH 43.23 | - | - | - | - | - | - | - | - |
| 134 | | 0.49Å O with A 94 LYS HE2 | | | | | | | |
| S | HOH 36.92 | - | - | - | - | - | - | - | - |
| 135 | | | | | | | | | |
| S | HOH 26.95 | - | - | - | - | - | - | - | - |
| 136 | | | | | | | | | |

| | | | | | | | | | |
|-----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 137 | HOH | 23.64 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 138 | HOH | 35.37 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 139 | HOH | 36.14 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 140 | HOH | 17.91 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 141 | HOH | 25.1 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 142 | HOH | 38.76 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 143 | HOH | 40.88 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 144 | HOH | 27.3 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 145 | HOH | 32.24 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 146 | HOH | 16.08 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 147 | HOH | 13.29 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 148 | HOH | 19.06 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 149 | HOH | 20.1 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 150 | HOH | 19.33 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 151 | HOH | 28.93 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 152 | HOH | 34.79 | - | - | - | - | - | - | - |

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 29.18 Outliers: 5 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

| | | | | | | | | | |
|-----|-----|-------|---|---|---|---|---|---|---|
| S | | | | | | | | | |
| 153 | HOH | 28.27 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 154 | HOH | 31.88 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 155 | HOH | 26.11 | - | - | - | - | - | - | - |
| S | | | | | | | | | |
| 156 | HOH | 28.02 | - | - | - | - | - | - | - |

| | | | | | | | | | |
|-----|-------------------------|-------|---|---|---|---|---|---|---|
| S | HOH 23.81 | - | - | - | - | - | - | - | - |
| 157 | | | | | | | | | |
| S | HOH 35.21 | - | - | - | - | - | - | - | - |
| 158 | | | | | | | | | |
| S | HOH 29.9 | - | - | - | - | - | - | - | - |
| 159 | | | | | | | | | |
| S | HOH 21.78 | - | - | - | - | - | - | - | - |
| 160 | | | | | | | | | |
| S | HOH 34.62 | - | - | - | - | - | - | - | - |
| 161 | | | | | | | | | |
| S | HOH 31.43 | - | - | - | - | - | - | - | - |
| 162 | | | | | | | | | |
| S | HOH 35.69 | - | - | - | - | - | - | - | - |
| 163 | | | | | | | | | |
| S | HOH 29.56 | - | - | - | - | - | - | - | - |
| 164 | | | | | | | | | |
| S | HOH 34.05 | - | - | - | - | - | - | - | - |
| 165 | | | | | | | | | |
| S | HOH 23.28 | - | - | - | - | - | - | - | - |
| 166 | O with A 124 HIS ND1 | 0.56Å | | | | | | | |
| S | HOH 39.56 | - | - | - | - | - | - | - | - |
| 167 | | | | | | | | | |
| S | HOH 30.32 | - | - | - | - | - | - | - | - |
| 168 | | | | | | | | | |
| S | HOH 29.31 | - | - | - | - | - | - | - | - |
| 169 | | | | | | | | | |
| S | HOH 35.63 | - | - | - | - | - | - | - | - |
| 170 | | | | | | | | | |
| S | HOH 21.31 | - | - | - | - | - | - | - | - |
| 171 | | | | | | | | | |
| S | HOH 34.39 | - | - | - | - | - | - | - | - |
| 172 | | | | | | | | | |

**Alt Res** **High B** **Clash > 0.4Å** **Ramachandran** **Rotamer** **Cβ deviation** **Bond lengths** **Bond angles** **Cis Peptides**

Avg: Clashscore: 29.18 Outliers: 5 Outliers: 1 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

| | | | | | | | | | |
|-----|-----------|---|---|---|---|---|---|---|---|
| S | HOH 40.07 | - | - | - | - | - | - | - | - |
| 173 | | | | | | | | | |
| S | HOH 30.24 | - | - | - | - | - | - | - | - |
| 174 | | | | | | | | | |
| S | HOH 32.7 | - | - | - | - | - | - | - | - |
| 175 | | | | | | | | | |
| S | HOH 35.4 | - | - | - | - | - | - | - | - |
| 176 | | | | | | | | | |

| | | | | | | | | | | |
|-----|-----|-------|----------------------------------|---|---|---|---|---|---|---|
| S | | | | | | | | | | |
| 177 | HOH | 34.96 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 178 | HOH | 40.25 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 179 | HOH | 32.44 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 180 | HOH | 31.92 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 181 | HOH | 38.23 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 182 | HOH | 32.41 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 183 | HOH | 29.56 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 184 | HOH | 32.4 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 185 | HOH | 44.17 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 186 | HOH | 39.6 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 187 | HOH | 35.14 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 188 | HOH | 48.83 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 189 | HOH | 37.33 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 190 | HOH | 28.2 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 191 | HOH | 30.39 | 0.78Å O with A 183 ASP OD2 | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 192 | HOH | 36.28 | - | - | - | - | - | - | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|---|-----|-----|------------------|-----------------|---------------------|-----------|-----------------|-----------------|---------------------|-----------------|
| | | | Avg: Clashscore: | Outliers: 1 of | Poor rotamers: 0 of | Outliers: | Outliers: | Outliers: | Non-Trans: 1 of 345 | |
| | | | 29.18 | 5 | 340 | 287 | 0 of 322 | 0 of 347 | 0 of 347 | |

| | | | | | | | | | | |
|-----|-----|-------|---|---|---|---|---|---|---|---|
| S | | | | | | | | | | |
| 193 | HOH | 29.36 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 194 | HOH | 43.25 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 195 | HOH | 36.14 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 196 | HOH | 26.42 | - | - | - | - | - | - | - | - |

| | | | | | | | | | | |
|-----|-----|-------|---|---|---|---|---|---|---|---|
| S | | | | | | | | | | |
| 197 | HOH | 35.9 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 198 | HOH | 27.85 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 199 | HOH | 27.44 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 200 | HOH | 35.37 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 201 | HOH | 26.18 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 202 | HOH | 26.31 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 203 | HOH | 44.17 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 204 | HOH | 47.73 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 205 | HOH | 44.75 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 206 | HOH | 48.32 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 207 | HOH | 24.08 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 208 | HOH | 40.9 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 209 | HOH | 17.74 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 210 | HOH | 30.58 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 211 | HOH | 35.73 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 212 | HOH | 31.4 | - | - | - | - | - | - | - | - |

Alt Res High B Clash > 0.4Å Ramachandran Rotamer Cβ deviation Bond lengths Bond angles Cis Peptides

Avg: Clashscore: 29.18 Outliers: 5 of 340 Poor rotamers: 0 of 287 Outliers: 0 of 322 Outliers: 0 of 347 Outliers: 0 of 347 Non-Trans: 1 of 345

| | | | | | | | | | | |
|-----|-----|-------|---|---|---|---|---|---|---|---|
| S | | | | | | | | | | |
| 213 | HOH | 25.82 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 214 | HOH | 38.71 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 215 | HOH | 42.61 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 216 | HOH | 48.63 | - | - | - | - | - | - | - | - |

| | | | | | | | | | |
|-----|-----------|----------------------------------|---|---|---|---|---|---|---|
| S | HOH 42.02 | - | - | - | - | - | - | - | - |
| 217 | | | | | | | | | |
| S | HOH 33.13 | - | - | - | - | - | - | - | - |
| 218 | | | | | | | | | |
| S | HOH 20.71 | - | - | - | - | - | - | - | - |
| 219 | | | | | | | | | |
| S | HOH 26.11 | - | - | - | - | - | - | - | - |
| 220 | | | | | | | | | |
| S | HOH 32.32 | - | - | - | - | - | - | - | - |
| 221 | | | | | | | | | |
| S | HOH 34.5 | 0.65Å O with A 160 GLU O | - | - | - | - | - | - | - |
| 222 | | | | | | | | | |
| S | HOH 39.5 | - | - | - | - | - | - | - | - |
| 223 | | | | | | | | | |
| S | HOH 44.67 | - | - | - | - | - | - | - | - |
| 224 | | | | | | | | | |
| S | HOH 38.45 | - | - | - | - | - | - | - | - |
| 225 | | | | | | | | | |
| S | HOH 40.91 | - | - | - | - | - | - | - | - |
| 226 | | | | | | | | | |
| S | HOH 40.59 | - | - | - | - | - | - | - | - |
| 227 | | | | | | | | | |
| S | HOH 45.19 | - | - | - | - | - | - | - | - |
| 228 | | | | | | | | | |
| S | HOH 32.02 | - | - | - | - | - | - | - | - |
| 229 | | | | | | | | | |
| S | HOH 23.79 | - | - | - | - | - | - | - | - |
| 230 | | | | | | | | | |
| S | HOH 35.68 | 0.76Å O with A 229 ARG NH1 | - | - | - | - | - | - | - |
| 231 | | | | | | | | | |
| S | HOH 36.51 | - | - | - | - | - | - | - | - |
| 232 | | | | | | | | | |

| # | <u>Alt Res</u> | <u>High B</u> | <u>Clash > 0.4Å</u> | <u>Ramachandran</u> | <u>Rotamer</u> | <u>Cβ deviation</u> | <u>Bond lengths</u> | <u>Bond angles</u> | <u>Cis Peptides</u> |
|---|----------------|---------------|------------------------|---------------------|----------------|---------------------|---------------------|--------------------|---------------------|
|---|----------------|---------------|------------------------|---------------------|----------------|---------------------|---------------------|--------------------|---------------------|

| | | | | | | | |
|--|------------------|----------------|---------------------|--------------------|--------------------|--------------------|---------------------|
| | Avg: Clashscore: | Outliers: 1 of | Poor rotamers: 0 of | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 |
| | 29.18 | 5 | 340 | 287 | | | |

| | | | | | | | | | |
|-----|-----------|---|---|---|---|---|---|---|---|
| S | HOH 40.59 | - | - | - | - | - | - | - | - |
| 233 | | | | | | | | | |
| S | HOH 38.23 | - | - | - | - | - | - | - | - |
| 234 | | | | | | | | | |
| S | HOH 44.76 | - | - | - | - | - | - | - | - |
| 235 | | | | | | | | | |

| | | | | | | | | | | |
|-----|-----|-------|---------------------------------|---|---|---|---|---|---|---|
| S | | | | | | | | | | |
| 236 | HOH | 33.8 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 237 | HOH | 48.35 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 238 | HOH | 42.89 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 239 | HOH | 44.32 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 240 | HOH | 26.71 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 241 | HOH | 34.87 | 0.85Å O with A 11 GLU OE1 | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 242 | HOH | 28.41 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 243 | HOH | 35.96 | 0.57Å O with A 97 ASP OD1 | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 244 | HOH | 33.34 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 245 | HOH | 50.32 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 246 | HOH | 31.1 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 247 | HOH | 36.32 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 248 | HOH | 20.6 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 249 | HOH | 26.22 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 250 | HOH | 32.22 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 251 | HOH | 30.16 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 252 | HOH | 36.21 | - | - | - | - | - | - | - | - |

| # | Alt | Res | High B | Clash > 0.4Å | Ramachandran | Rotamer | Cβ deviation | Bond lengths | Bond angles | Cis Peptides |
|---|-----|-----|-----------|-----------------|--------------|---------|-----------------|-----------------|----------------|-----------------|
|---|-----|-----|-----------|-----------------|--------------|---------|-----------------|-----------------|----------------|-----------------|

| | | | | | | | | | |
|--|--|--|------------------|----------------|---------------------|--------------------|--------------------|--------------------|---------------------|
| | | | Avg: Clashscore: | Outliers: 1 of | Poor rotamers: 0 of | Outliers: 0 of 322 | Outliers: 0 of 347 | Outliers: 0 of 347 | Non-Trans: 1 of 345 |
| | | | 29.18 | 5 | 340 | 287 | | | |

| | | | | | | | | | | |
|-----|-----|-------|---|---|---|---|---|---|---|---|
| S | | | | | | | | | | |
| 253 | HOH | 41.52 | - | - | - | - | - | - | - | - |
| S | | | | | | | | | | |
| 254 | HOH | 33.49 | - | - | - | - | - | - | - | - |

| | | | | | | | | |
|----------|-----------|-----------------------------------|---|---|---|---|---|---|
| S 255 | HOH 45.6 | - | - | - | - | - | - | - |
| S 256 | HOH 49.77 | - | - | - | - | - | - | - |
| S 257 | HOH 26.33 | - | - | - | - | - | - | - |
| S 258 | HOH 45.13 | - | - | - | - | - | - | - |
| S 259 | HOH 45.7 | 0.43 Å O with A 29 LYS NZ | - | - | - | - | - | - |
| S 260 | HOH 44.19 | 0.41 Å O with A 303 LYS HB2 | - | - | - | - | - | - |
| S 261 | HOH 47.53 | - | - | - | - | - | - | - |
| S 262 | HOH 35.38 | - | - | - | - | - | - | - |
| S 263 | HOH 45.76 | - | - | - | - | - | - | - |
| S 264 | HOH 39.55 | - | - | - | - | - | - | - |
| S 265 | HOH 42.7 | - | - | - | - | - | - | - |
| S 266 | HOH 35.81 | - | - | - | - | - | - | - |

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