# wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 10:44 pm BST

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|---|---|---|
| PDB ID | : | 2J69 |
| Title | : | Bacterial dynamin-like protein BDLP |
| Authors | : | Low, H.H.; Lowe, J. |
| Deposited on | : | 2006-09-26 |
| Resolution | : | 3.00 Å(reported) |

The following versions of software and data (see references (1)) were used in the production of this report:

| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.11 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Percentile relative to all X-ray structures
Percentile relative to X-ray structures of similar resolution
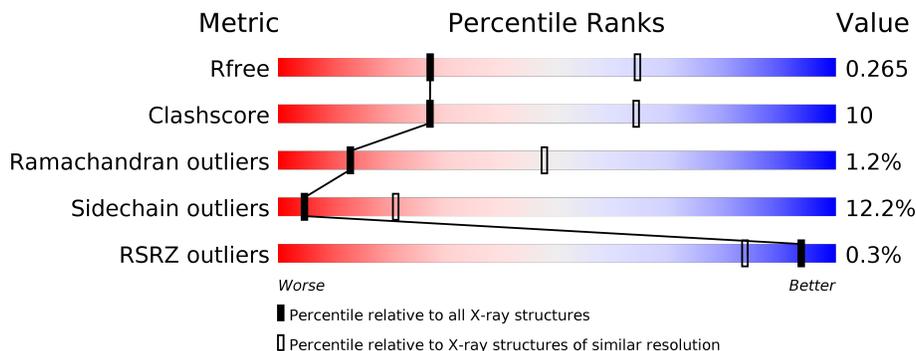
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 2092 (3.00-3.00) |
| Clashscore | 141614 | 2416 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 695 | 74% ... 18% .. . |
| 1 | B | 695 | 73% ... 20% .. . |
| 1 | C | 695 | 72% ... 20% .. . |
| 1 | D | 695 | 71% ... 21% .. . |

# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21500 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called BACTERIAL DYNAMIN-LIKE PROTEIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 671 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5375 | 3385 | 941 | 1037 | 12 | | | |
| 1 | B | 671 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5375 | 3385 | 941 | 1037 | 12 | | | |
| 1 | C | 671 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5375 | 3385 | 941 | 1037 | 12 | | | |
| 1 | D | 671 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5375 | 3385 | 941 | 1037 | 12 | | | |

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN



- Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN

S433 N441 A442 A443 L444 Q445 T462 A463 E464 K472 R476 T489 I492 K499 D500 V501 LYS HIS THR THR THR ALA E510 E511 S514 P515 A518 M522 L525 S526 LEU SER LYS GLY ASN LEU ALA GLY PHE ALA LEU ALA GLY A540 G541 W544

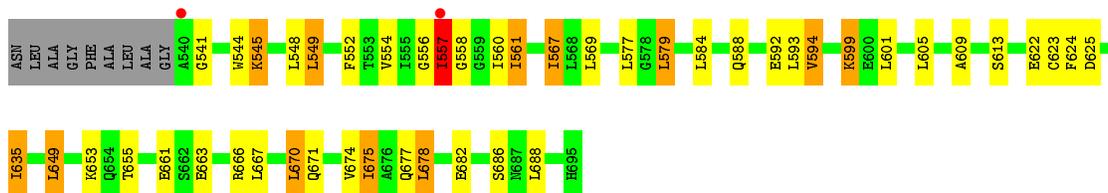K545 L548 L549 F552 T553 V554 I555 G556 I557 G558 G559 I560 I561 T562 I567 L568 L569 L577 G578 L579 G580 V581 L584 E592 L593 V594 K599 E600 L601 H604 E622 C623 F624 D625 I635 D638 R642 D647 N648 L649 T655 E661 S662 E663

R666 L667 L670 Q671 E672 D673 V674 I675 A676 Q677 L678 L689 H695

• Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN

Chain C:

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72%                    20%          •  •
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MET VAL ASN Q4 T7 F10 L14 V20 R21 S22 K37 A38 E39 S45 S46 G47 K48 V74 K79 R80 S83 T84 F85 L86 L89 I90 S97 D98 V99 N100 P101 C102 V105 R110 N122 D123 S126 P127 L130 N134 F135 I141

Q155 P158 E166 Y167 P168 L169 T170 L171 S181 P182 G183 L184 T187 E192 L193 N200 I204 S211 T215 L216 G217 R220 Y221 L222 I226 R229 V233 L236 V237 N238 D241 E245 R262 L263 Q265 V266 Q280 Y283

V287 L290 I293 Q294 R298 K314 F322 R325 E326 R327 A328 I329 A330 E331 R336 T337 L338 C343 T346 A349 R352 Q359 D360 V361 N362 E363 L364 R367 V371 E372 P373 R382 Q386 K387 N391 T392 R393 N410 N413 T414

L420 R421 Y422 Q423 P424 N427 L428 S433 R437 N441 A442 A443 L444 Q445 D454 W459 T462 A463 E464 S475 R476 S477 Y481 Y485 N486 T489 I492 K499 D500 V501 LYS VAL HIS THR THR THR ALA E510 E511 S514 P515 G516 S526 LEU

SER LYS GLY ASN LEU ALA GLY PHE ALA LEU ALA GLY A540 G541 W544 K545 L549 N550 Y551 F552 G556 I557 G558 G559 I560 I567 L568 L569 L577 G578 L579 E592 L593 V594 K599 E600 L601 H604 E622 C623 F624 D625 I635 N636 L649 K653 Q654 T655

E663 R666 L670 V674 I675 A676 Q677 L678 E682 S686 N687 L688 H695

• Molecule 1: BACTERIAL DYNAMIN-LIKE PROTEIN

Chain D:

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71%                    21%          •  •
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MET VAL ASN Q4 Q12 D13 L14 R21 K37 A38 E39 S45 S46 G47 K48 L65 G68 V74 R80 S83 L86 L89 I90 L95 P96 S97 D98 V99 N100 P101 C102 V108 L109 R110 K115 N122 D123 S126 P127 L130 D131 F132

F135 I141 D142 P143 K147 Q155 P158 V165 E166 Y167 P168 L169 T170 L171 I176 V179 P182 G183 L184 T187 E192 L193 N200 L205 R209 A210 S211 T215 L216 G217 E218 R219 R220 R229 V233 L236 V237 N238 D241 D249 P250

L263 Q280 S291 S292 I293 Q294 A295 L296 L300 K314 R325 I329 R336 T337 L338 C343 T346 A349 V350 A351 R352 R353 I354 Q359 D360 E363 L364 R367 V371 E372 P373 R382 Q386 I390 N391 T392 R393 V408 L409 N410

T414 L420 Q423 A426 N427 L428 F431 L432 S433 N441 A442 A443 L444 Q445 D454 W459 T462 A463 E464 T489 I492 K499 D500 V501 LYS VAL HIS THR THR THR ALA E510 E511 S514 P515 G516 W517 A518 M522 L525 S526 LEU SER LYS GLY

# 4  Data and refinement statistics  (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 214.29Å    218.60Å    151.20Å<br>90.00°    134.81°    90.00° | Depositor |
| Resolution (Å) | 50.00   –   3.00<br>34.50   –   3.00 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.5 (50.00-3.00)<br>97.0 (34.50-3.00) | Depositor<br>EDS |
| $R_{merge}$ | 0.06 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.05 (at 3.00Å) | Xtriage |
| Refinement program | REFMAC 5.2.0019 | Depositor |
| R, $R_{free}$ | 0.236   ,   0.281<br>0.226   ,   0.265 | Depositor<br>DCC |
| $R_{free}$ test set | 4869 reflections (5.02%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 74.0 | Xtriage |
| Anisotropy | 0.150 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.31 , 30.1 | EDS |
| L-test for twinning[2] | $< |L| > = 0.49$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.006 for -h,h+2*l,1/2*h+1/2*k<br>0.009 for -h,-h-2*l,1/2*h-1/2*k<br>0.004 for -k,-h,-1/2*h+1/2*k-l<br>0.009 for k,h,-1/2*h-1/2*k-l<br>0.417 for h+2*l,k,-h-l<br>0.005 for h+2*l,h,-1/2*h+1/2*k-l<br>0.007 for k,h+2*l,1/2*h-1/2*k<br>0.004 for k,-h-2*l,-1/2*h-1/2*k<br>0.006 for h+2*l,-h,-1/2*h-1/2*k-l<br>0.459 for -h-2*l,-k,l<br>0.418 for h,-k,-h-l | Xtriage |
| $F_o,F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 21500 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 61.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|------|--------|------|--------|
| | | RMSZ | #$|Z|$>5 | RMSZ | #$|Z|$>5 |
| 1 | A | 0.71 | 6/5459 (0.1%) | 0.71 | 8/7368 (0.1%) |
| 1 | B | 0.70 | 6/5459 (0.1%) | 0.71 | 9/7368 (0.1%) |
| 1 | C | 0.64 | 6/5459 (0.1%) | 0.67 | 5/7368 (0.1%) |
| 1 | D | 0.74 | 6/5459 (0.1%) | 0.68 | 8/7368 (0.1%) |
| All | All | 0.70 | 24/21836 (0.1%) | 0.69 | 30/29472 (0.1%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 1 | 0 |

The worst 5 of 24 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|---|-------------|----------|
| 1 | D | 557 | ILE | CB-CG1 | 32.69 | 2.45 | 1.54 |
| 1 | A | 557 | ILE | CB-CG1 | 29.34 | 2.36 | 1.54 |
| 1 | B | 557 | ILE | CB-CG1 | 27.52 | 2.31 | 1.54 |
| 1 | A | 567 | ILE | CB-CG1 | -22.89 | 0.90 | 1.54 |
| 1 | C | 557 | ILE | CB-CG1 | 22.48 | 2.17 | 1.54 |

The worst 5 of 30 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|-------|---|----------------|-------------|
| 1 | D | 557 | ILE | CG1-CB-CG2 | -20.40 | 66.53 | 111.40 |
| 1 | B | 557 | ILE | CG1-CB-CG2 | -18.37 | 70.98 | 111.40 |
| 1 | A | 557 | ILE | CG1-CB-CG2 | -18.25 | 71.25 | 111.40 |
| 1 | C | 557 | ILE | CG1-CB-CG2 | -17.13 | 73.71 | 111.40 |
| 1 | B | 567 | ILE | CG1-CB-CG2 | 15.15 | 144.74 | 111.40 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 1 | A | 567 | ILE | CB |

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 5375 | 0 | 5366 | 125 | 0 |
| 1 | B | 5375 | 0 | 5366 | 97 | 0 |
| 1 | C | 5375 | 0 | 5366 | 108 | 0 |
| 1 | D | 5375 | 0 | 5366 | 108 | 0 |
| All | All | 21500 | 0 | 21464 | 432 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 432 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|--------|--------|--------------------------|-------------------|
| 1:A:567:ILE:CB | 1:A:567:ILE:CG2 | 1.75 | 1.60 |
| 1:D:552:PHE:CD1 | 1:D:557:ILE:HD12 | 1.30 | 1.58 |
| 1:A:567:ILE:HB | 1:A:567:ILE:CD1 | 1.21 | 1.55 |
| 1:D:552:PHE:CD1 | 1:D:557:ILE:CD1 | 1.92 | 1.49 |
| 1:A:557:ILE:CG2 | 1:A:557:ILE:CB | 1.89 | 1.47 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|----------|----------|---------|----------|------|------|
| 1 | A | 665/695 (96%) | 610 (92%) | 48 (7%) | 7 (1%) | 14 | 50 |
| 1 | B | 665/695 (96%) | 612 (92%) | 45 (7%) | 8 (1%) | 13 | 48 |
| 1 | C | 665/695 (96%) | 602 (90%) | 54 (8%) | 9 (1%) | 11 | 43 |
| 1 | D | 665/695 (96%) | 600 (90%) | 56 (8%) | 9 (1%) | 11 | 43 |
| All | All | 2660/2780 (96%) | 2424 (91%) | 203 (8%) | 33 (1%) | 13 | 48 |

5 of 33 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 428 | LEU |
| 1 | A | 557 | ILE |
| 1 | B | 428 | LEU |
| 1 | B | 541 | GLY |
| 1 | B | 557 | ILE |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|------|------|
| 1 | A | 584/601 (97%) | 518 (89%) | 66 (11%) | 6 | 24 |
| 1 | B | 584/601 (97%) | 510 (87%) | 74 (13%) | 4 | 19 |
| 1 | C | 584/601 (97%) | 511 (88%) | 73 (12%) | 4 | 20 |
| 1 | D | 584/601 (97%) | 511 (88%) | 73 (12%) | 4 | 20 |
| All | All | 2336/2404 (97%) | 2050 (88%) | 286 (12%) | 5 | 21 |

5 of 286 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 601 | LEU |
| 1 | C | 200 | ASN |
| 1 | D | 511 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 649 | LEU |
| 1 | C | 46 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 659 | ASN |
| 1 | C | 294 | GLN |
| 1 | D | 486 | ASN |
| 1 | C | 100 | ASN |
| 1 | C | 155 | GLN |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å²) | Q<0.9 |
|-----|-------|----------|--------|---------|-----|-----|----------|-------|
| 1 | A | 671/695 (96%) | -0.09 | 1 (0%) | 95 | 89 | 35, 59, 84, 104 | 0 |
| 1 | B | 671/695 (96%) | -0.07 | 3 (0%) | 92 | 79 | 35, 59, 84, 104 | 0 |
| 1 | C | 671/695 (96%) | -0.08 | 0 | 100 | 100 | 35, 59, 84, 104 | 0 |
| 1 | D | 671/695 (96%) | -0.11 | 3 (0%) | 92 | 79 | 35, 59, 84, 104 | 0 |
| All | All | 2684/2780 (96%) | -0.09 | 7 (0%) | 94 | 84 | 35, 59, 84, 104 | 0 |

The worst 5 of 7 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 4 | GLN | 3.4 |
| 1 | B | 4 | GLN | 3.1 |
| 1 | D | 557 | ILE | 2.5 |
| 1 | D | 540 | ALA | 2.3 |
| 1 | B | 186 | ASP | 2.3 |

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.