# wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Dec 5, 2016 – 12:05 PM EST

| | | |
|---|---|---|
| PDB ID | : | 5LJV |
| EMDB ID: | : | EMD-4062 |
| Title | : | MamK double helical filament |
| Authors | : | Lowe, J. |
| Deposited on | : | 2016-07-21 |
| Resolution | : | 3.65 Å(reported) |

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

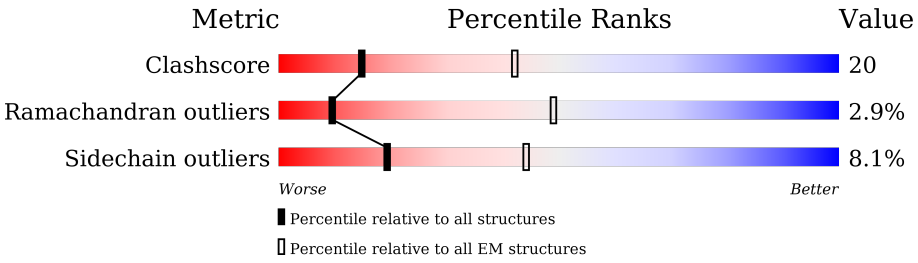
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20028442 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.65 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.




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 114402 | 924 |
| Ramachandran outliers | 111179 | 726 |
| Sidechain outliers | 111093 | 686 |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 347 | 49% 36% 8% • 6% |
| 1 | B | 347 | 50% 35% 8% • 6% |
| 1 | C | 347 | 49% 34% 10% • 6% |
| 1 | D | 347 | 51% 33% 9% • 6% |
| 1 | E | 347 | 50% 34% 9% • 6% |
| 1 | F | 347 | 48% 36% 9% • 6% |

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Actin-like ATPase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 325 | Total 2472 | C 1569 | N 425 | O 466 | S 12 | 0 | 0 |
| 1 | B | 325 | Total 2472 | C 1569 | N 425 | O 466 | S 12 | 0 | 0 |
| 1 | C | 325 | Total 2472 | C 1569 | N 425 | O 466 | S 12 | 0 | 0 |
| 1 | D | 325 | Total 2472 | C 1569 | N 425 | O 466 | S 12 | 0 | 0 |
| 1 | E | 325 | Total 2472 | C 1569 | N 425 | O 466 | S 12 | 0 | 0 |
| 1 | F | 325 | Total 2472 | C 1569 | N 425 | O 466 | S 12 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 16 | VAL | ILE | conflict | UNP Q2W8Q6 |
| B | 16 | VAL | ILE | conflict | UNP Q2W8Q6 |
| C | 16 | VAL | ILE | conflict | UNP Q2W8Q6 |
| D | 16 | VAL | ILE | conflict | UNP Q2W8Q6 |
| E | 16 | VAL | ILE | conflict | UNP Q2W8Q6 |
| F | 16 | VAL | ILE | conflict | UNP Q2W8Q6 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 2 | D | 1 | Total 1 | Mg 1 | 0 |
| 2 | E | 1 | Total 1 | Mg 1 | 0 |
| 2 | B | 1 | Total 1 | Mg 1 | 0 |
| 2 | C | 1 | Total 1 | Mg 1 | 0 |

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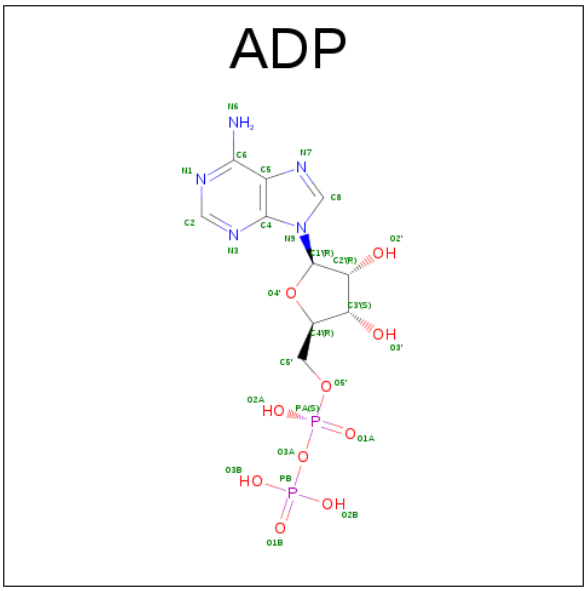
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 2 | A | 1 | Total Mg<br>1 1 | 0 |
| 2 | F | 1 | Total Mg<br>1 1 | 0 |

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



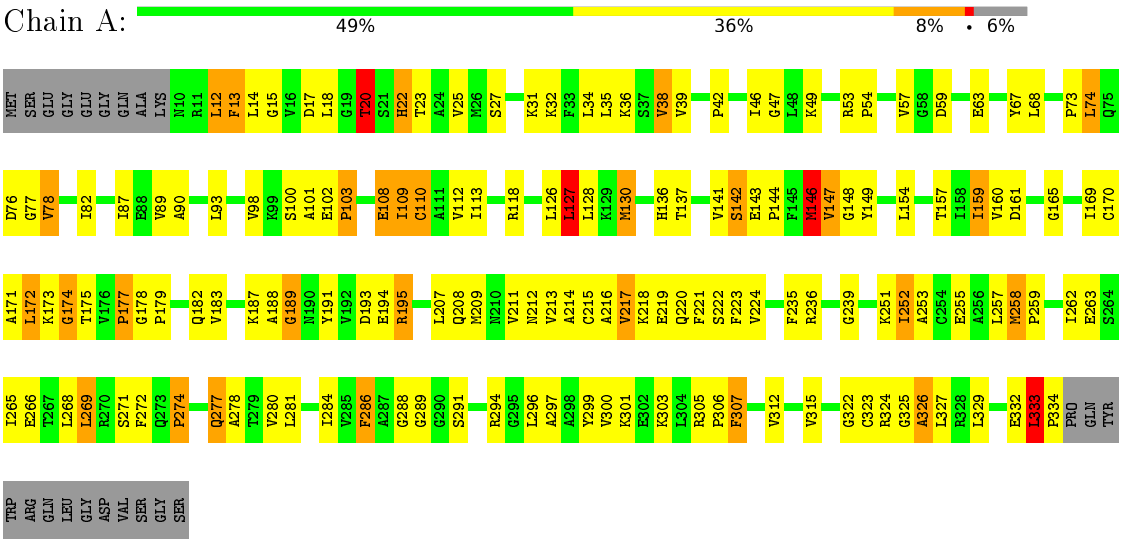

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 3 | A | 1 | Total C N O P<br>27 10 5 10 2 | 0 |
| 3 | B | 1 | Total C N O P<br>27 10 5 10 2 | 0 |
| 3 | C | 1 | Total C N O P<br>27 10 5 10 2 | 0 |
| 3 | D | 1 | Total C N O P<br>27 10 5 10 2 | 0 |
| 3 | E | 1 | Total C N O P<br>27 10 5 10 2 | 0 |
| 3 | F | 1 | Total C N O P<br>27 10 5 10 2 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

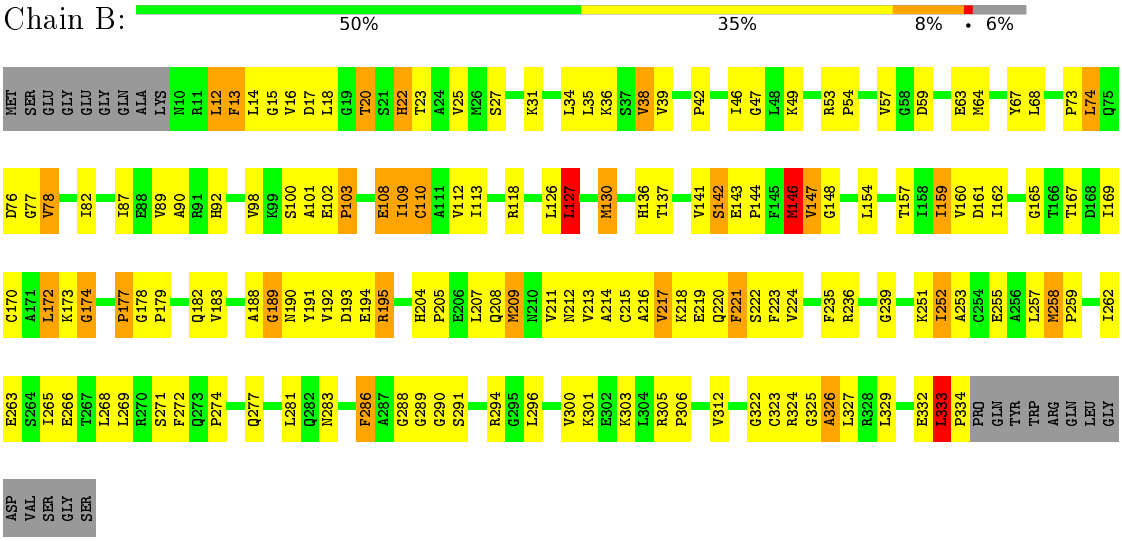
- Molecule 1: Actin-like ATPase

Chain A:



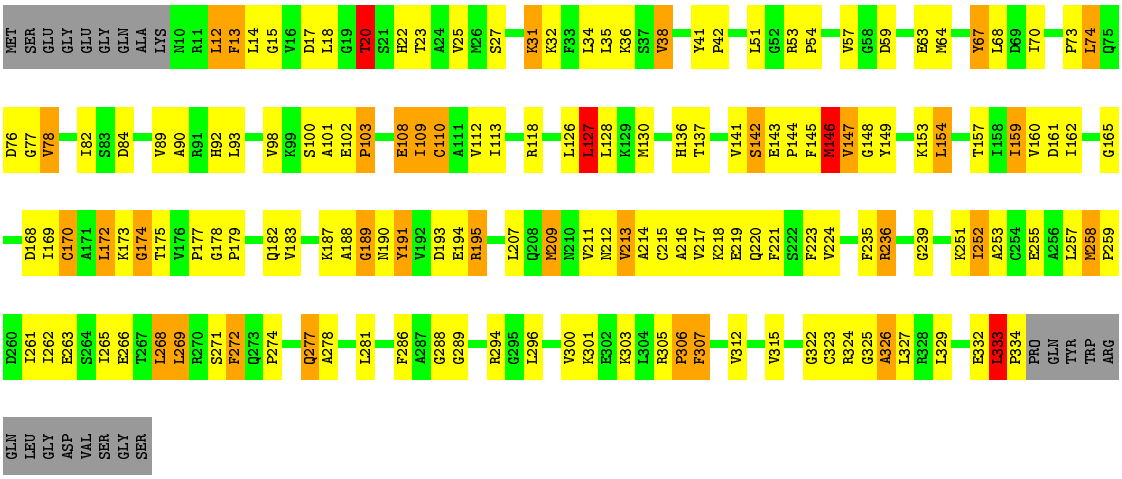

- Molecule 1: Actin-like ATPase

Chain B:



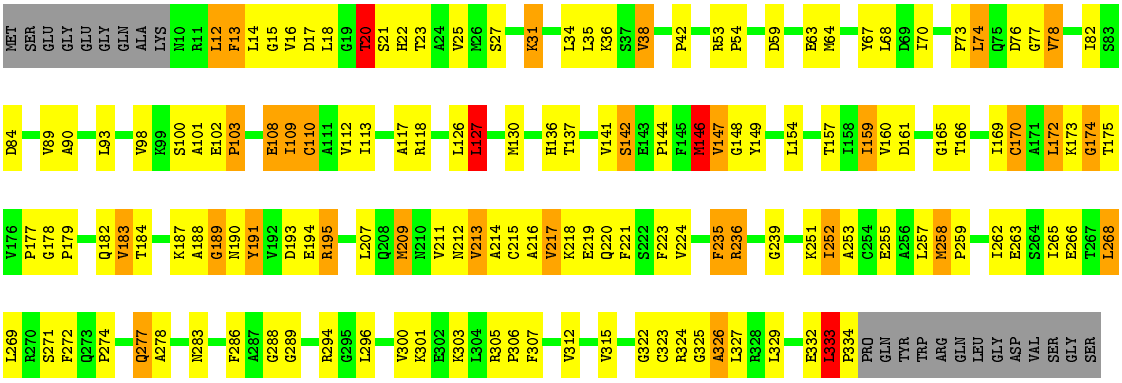

- Molecule 1: Actin-like ATPase

Chain C:



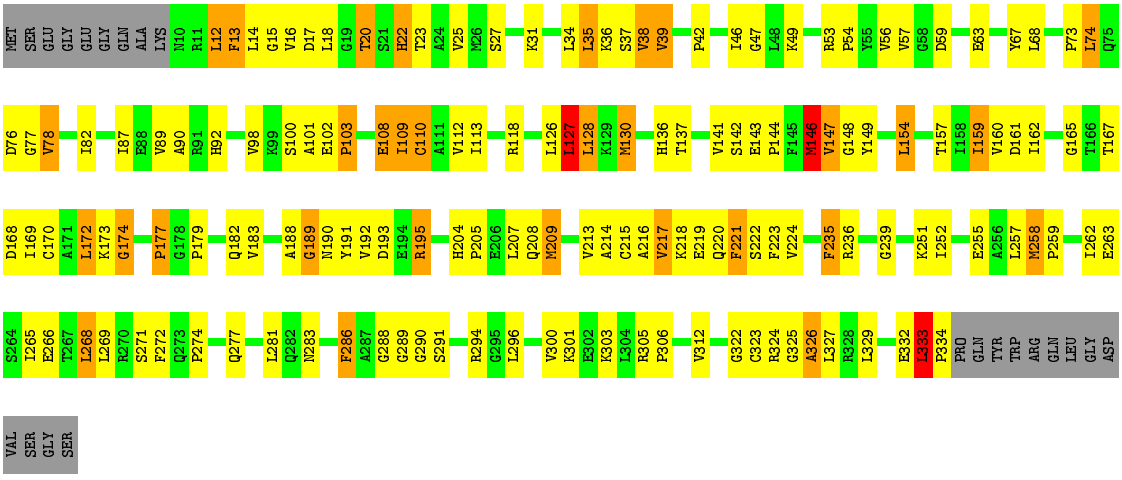
• Molecule 1: Actin-like ATPase

Chain D:

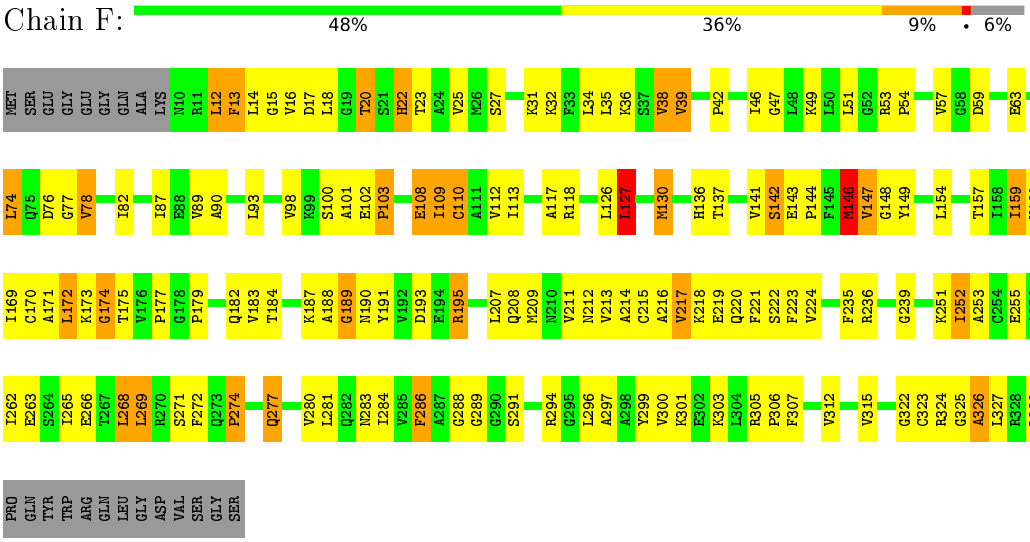
• Molecule 1: Actin-like ATPase

Chain E:

• Molecule 1: Actin-like ATPase

Chain F:


48%
36%
9%
6%
MET SER GLU GLY GLU GLY GLN ALA LYS N10 R11 L12 F13 L14 G15 V16 D17 L18 G19 T20 S21 H22 T23 A24 V25 M26 S27 K31 K32 F33 L34 L35 K36 S37 V38 V39 P42 I46 G47 L48 K49 L50 L51 G52 R53 P54 V57 G58 D59 E63 Y67 L68 P73
L74 Q75 D76 G77 V78 I82 I87 E88 V89 A90 L93 V98 K99 S100 A101 E102 P103 E108 I109 C110 A111 V112 I113 A117 R118 L126 L127 M130 H136 T137 V141 S142 E143 P144 F145 N146 V147 G148 Y149 L154 T157 I158 I159 V160 D161 G165
I169 C170 A171 L172 K173 G174 T175 V176 P177 G178 P179 Q182 V183 T184 K187 A188 G189 N190 Y191 V192 D193 E194 R195 L207 Q208 M209 N210 V211 N212 V213 A214 C215 A216 V217 K218 E219 Q220 F221 S222 F223 V224 F235 R236 G239 K251 I252 A253 C254 E255 A256 L257 M258 P259
I262 E263 S264 I265 E266 T267 L268 L269 R270 S271 F272 Q273 P274 Q277 V280 L281 Q282 N283 I284 V285 P286 A287 G288 G289 G290 S291 R294 G295 L296 A297 A298 Y299 V300 K301 E302 K303 L304 R305 P306 F307 V312 V315 G322 C323 R324 G325 A326 L327 R328 L329 E332 L333 P334
PRO GLN TYR TRP ARG GLN LEU GLY ASP VAL SER GLY SER

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | HELICAL | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of segments used | 596427 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI POLARA 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | Not provided | Depositor |
| Minimum defocus (nm) | Not provided | Depositor |
| Maximum defocus (nm) | Not provided | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | Not provided | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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 | #$\|Z\|>2$ | RMSZ | #$\|Z\|>2$ |
| 1 | A | 1.37 | 15/2514 (0.6%) | 1.39 | 18/3411 (0.5%) |
| 1 | B | 1.46 | 14/2514 (0.6%) | 1.38 | 21/3411 (0.6%) |
| 1 | C | 1.50 | 17/2514 (0.7%) | 1.39 | 20/3411 (0.6%) |
| 1 | D | 1.50 | 19/2514 (0.8%) | 1.40 | 20/3411 (0.6%) |
| 1 | E | 1.49 | 21/2514 (0.8%) | 1.39 | 22/3411 (0.6%) |
| 1 | F | 1.37 | 14/2514 (0.6%) | 1.39 | 21/3411 (0.6%) |
| All | All | 1.45 | 100/15084 (0.7%) | 1.39 | 122/20466 (0.6%) |

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 | 0 | 4 |
| 1 | B | 0 | 4 |
| 1 | C | 0 | 4 |
| 1 | D | 0 | 4 |
| 1 | E | 0 | 3 |
| 1 | F | 0 | 2 |
| All | All | 0 | 21 |

The worst 5 of 100 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | C | 286 | PHE | CB-CG | -9.62 | 1.34 | 1.51 |
| 1 | D | 286 | PHE | CB-CG | -9.31 | 1.35 | 1.51 |
| 1 | F | 67 | TYR | CB-CG | -7.99 | 1.39 | 1.51 |
| 1 | A | 67 | TYR | CB-CG | -7.66 | 1.40 | 1.51 |
| 1 | A | 286 | PHE | CB-CG | -7.24 | 1.39 | 1.51 |

The worst 5 of 122 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 269 | LEU | CB-CG-CD2 | -9.41 | 95.01 | 111.00 |
| 1 | F | 269 | LEU | CB-CG-CD2 | -9.35 | 95.11 | 111.00 |
| 1 | C | 269 | LEU | CB-CG-CD2 | -9.33 | 95.14 | 111.00 |
| 1 | A | 269 | LEU | CB-CG-CD2 | -9.30 | 95.18 | 111.00 |
| 1 | C | 172 | LEU | CA-CB-CG | -8.85 | 94.94 | 115.30 |

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 174 | GLY | Peptide |
| 1 | A | 177 | PRO | Peptide |
| 1 | A | 178 | GLY | Peptide |
| 1 | A | 333 | LEU | Peptide |
| 1 | B | 174 | GLY | Peptide |

## 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 | 2472 | 0 | 2524 | 110 | 0 |
| 1 | B | 2472 | 0 | 2524 | 101 | 0 |
| 1 | C | 2472 | 0 | 2524 | 110 | 0 |
| 1 | D | 2472 | 0 | 2524 | 101 | 0 |
| 1 | E | 2472 | 0 | 2524 | 97 | 0 |
| 1 | F | 2472 | 0 | 2524 | 114 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 1 | 0 | 0 | 0 | 0 |
| 2 | E | 1 | 0 | 0 | 0 | 0 |
| 2 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 27 | 0 | 12 | 2 | 0 |
| 3 | B | 27 | 0 | 12 | 1 | 0 |
| 3 | C | 27 | 0 | 12 | 2 | 0 |
| 3 | D | 27 | 0 | 12 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | E | 27 | 0 | 12 | 1 | 0 |
| 3 | F | 27 | 0 | 12 | 2 | 0 |
| All | All | 15000 | 0 | 15216 | 598 | 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 20.

The worst 5 of 598 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:49:LYS:NZ | 1:C:149:TYR:OH | 2.07 | 0.88 |
| 1:D:149:TYR:OH | 1:F:49:LYS:NZ | 2.07 | 0.87 |
| 1:A:149:TYR:OH | 1:B:49:LYS:NZ | 2.11 | 0.83 |
| 1:D:332:GLU:C | 1:D:333:LEU:HD12 | 1.99 | 0.83 |
| 1:C:332:GLU:C | 1:C:333:LEU:HD12 | 1.98 | 0.83 |

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 PDB entries followed by that with respect to all EM entries.

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 | 323/347 (93%) | 290 (90%) | 23 (7%) | 10 (3%) | 5 46 |
| 1 | B | 323/347 (93%) | 289 (90%) | 26 (8%) | 8 (2%) | 7 49 |
| 1 | C | 323/347 (93%) | 291 (90%) | 22 (7%) | 10 (3%) | 5 46 |
| 1 | D | 323/347 (93%) | 291 (90%) | 22 (7%) | 10 (3%) | 5 46 |
| 1 | E | 323/347 (93%) | 289 (90%) | 26 (8%) | 8 (2%) | 7 49 |
| 1 | F | 323/347 (93%) | 289 (90%) | 24 (7%) | 10 (3%) | 5 46 |
| All | All | 1938/2082 (93%) | 1739 (90%) | 143 (7%) | 56 (3%) | 9 47 |

5 of 56 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 103 | PRO |
| 1 | A | 179 | PRO |
| 1 | B | 103 | PRO |
| 1 | B | 179 | PRO |
| 1 | C | 103 | PRO |

### 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 PDB entries followed by that with respect to all EM entries.

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 | 268/285 (94%) | 248 (92%) | 20 (8%) | 17 | 58 |
| 1 | B | 268/285 (94%) | 246 (92%) | 22 (8%) | 14 | 54 |
| 1 | C | 268/285 (94%) | 244 (91%) | 24 (9%) | 12 | 50 |
| 1 | D | 268/285 (94%) | 245 (91%) | 23 (9%) | 13 | 53 |
| 1 | E | 268/285 (94%) | 247 (92%) | 21 (8%) | 16 | 56 |
| 1 | F | 268/285 (94%) | 247 (92%) | 21 (8%) | 16 | 56 |
| All | All | 1608/1710 (94%) | 1477 (92%) | 131 (8%) | 19 | 54 |

5 of 131 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 142 | SER |
| 1 | D | 74 | LEU |
| 1 | F | 118 | ARG |
| 1 | C | 146 | MET |
| 1 | D | 12 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 123 | ASN |
| 1 | D | 92 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 123 | ASN |
| 1 | C | 92 | HIS |
| 1 | E | 92 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | ADP | A | 402 | 2 | 24,29,29 | 1.26 | 2 (8%) | 23,45,45 | 3.24 | 6 (26%) |
| 3 | ADP | B | 402 | 2 | 24,29,29 | 1.36 | 5 (20%) | 23,45,45 | 3.73 | 10 (43%) |
| 3 | ADP | C | 402 | 2 | 24,29,29 | 1.43 | 3 (12%) | 23,45,45 | 3.17 | 8 (34%) |
| 3 | ADP | D | 402 | 2 | 24,29,29 | 1.43 | 5 (20%) | 23,45,45 | 3.07 | 9 (39%) |
| 3 | ADP | E | 402 | 2 | 24,29,29 | 1.42 | 5 (20%) | 23,45,45 | 3.87 | 10 (43%) |
| 3 | ADP | F | 402 | 2 | 24,29,29 | 1.32 | 3 (12%) | 23,45,45 | 3.29 | 7 (30%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | ADP | A | 402 | 2 | - | 0/12/32/32 | 0/3/3/3 |
| 3 | ADP | B | 402 | 2 | - | 0/12/32/32 | 0/3/3/3 |
| 3 | ADP | C | 402 | 2 | - | 0/12/32/32 | 0/3/3/3 |
| 3 | ADP | D | 402 | 2 | - | 0/12/32/32 | 0/3/3/3 |
| 3 | ADP | E | 402 | 2 | - | 0/12/32/32 | 0/3/3/3 |
| 3 | ADP | F | 402 | 2 | - | 0/12/32/32 | 0/3/3/3 |

The worst 5 of 23 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | E | 402 | ADP | O4'-C4' | -2.54 | 1.39 | 1.45 |
| 3 | C | 402 | ADP | C2'-C3' | -2.40 | 1.47 | 1.53 |
| 3 | D | 402 | ADP | C2'-C3' | -2.34 | 1.47 | 1.53 |
| 3 | B | 402 | ADP | O4'-C4' | -2.33 | 1.39 | 1.45 |
| 3 | D | 402 | ADP | O4'-C4' | -2.23 | 1.39 | 1.45 |

The worst 5 of 50 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | F | 402 | ADP | C1'-N9-C4 | -11.65 | 113.81 | 126.81 |
| 3 | A | 402 | ADP | C1'-N9-C4 | -11.64 | 113.81 | 126.81 |
| 3 | E | 402 | ADP | N3-C2-N1 | -10.70 | 120.46 | 128.87 |
| 3 | B | 402 | ADP | N3-C2-N1 | -9.83 | 121.15 | 128.87 |
| 3 | B | 402 | ADP | C1'-N9-C4 | -9.58 | 116.11 | 126.81 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 402 | ADP | 2 | 0 |
| 3 | B | 402 | ADP | 1 | 0 |
| 3 | C | 402 | ADP | 2 | 0 |
| 3 | D | 402 | ADP | 3 | 0 |
| 3 | E | 402 | ADP | 1 | 0 |
| 3 | F | 402 | ADP | 2 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.