# wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:51 PM BST

| | | |
|---|---|---|
| PDB ID | : | 3J8I |
| EMDB ID: | : | EMD-6179 |
| Title | : | Near-Atomic Resolution for One State of F-Actin |
| Authors | : | Galkin, V.E. |
| Deposited on | : | 2014-11-06 |
| Resolution | : | 4.70 Å(reported) |

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

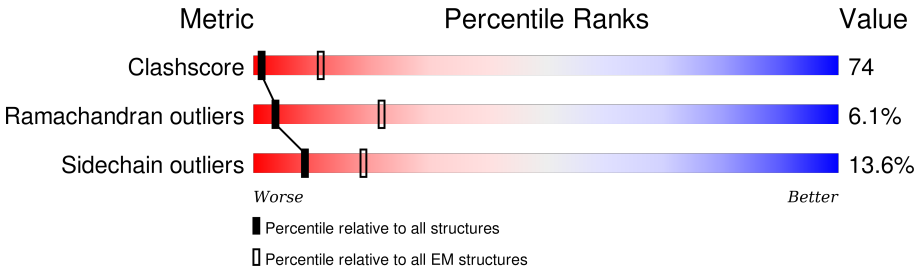
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk27241 |

# 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 4.70 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 | D | 377 | 22% 62% 14% |
| 1 | E | 377 | 23% 62% 14% |
| 1 | F | 377 | 21% 64% 14% |
| 1 | G | 377 | 23% 62% 14% |
| 1 | H | 377 | 21% 64% 14% |

## 2 Entry composition

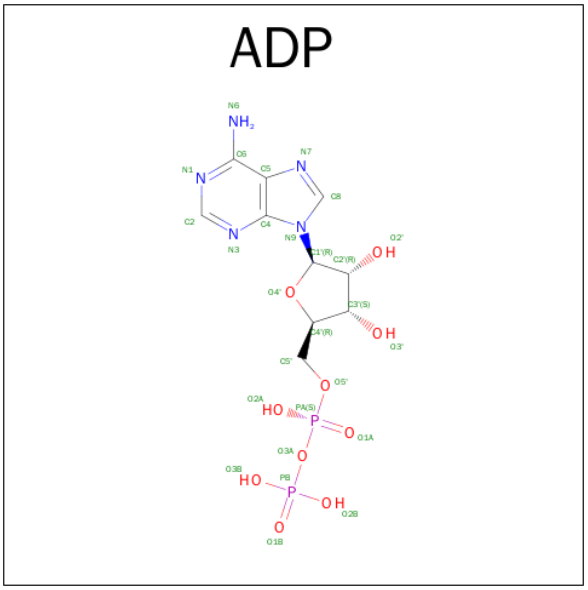
There are 3 unique types of molecules in this entry. The entry contains 14800 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, alpha skeletal muscle.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | D | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |
| 1 | E | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |
| 1 | F | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |
| 1 | G | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |
| 1 | H | 375 | Total | C | N | O | S | 0 | 0 |
| | | | 2932 | 1854 | 493 | 564 | 21 | | |

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | D | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 2 | E | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | F | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | G | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |
| 2 | H | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | |

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

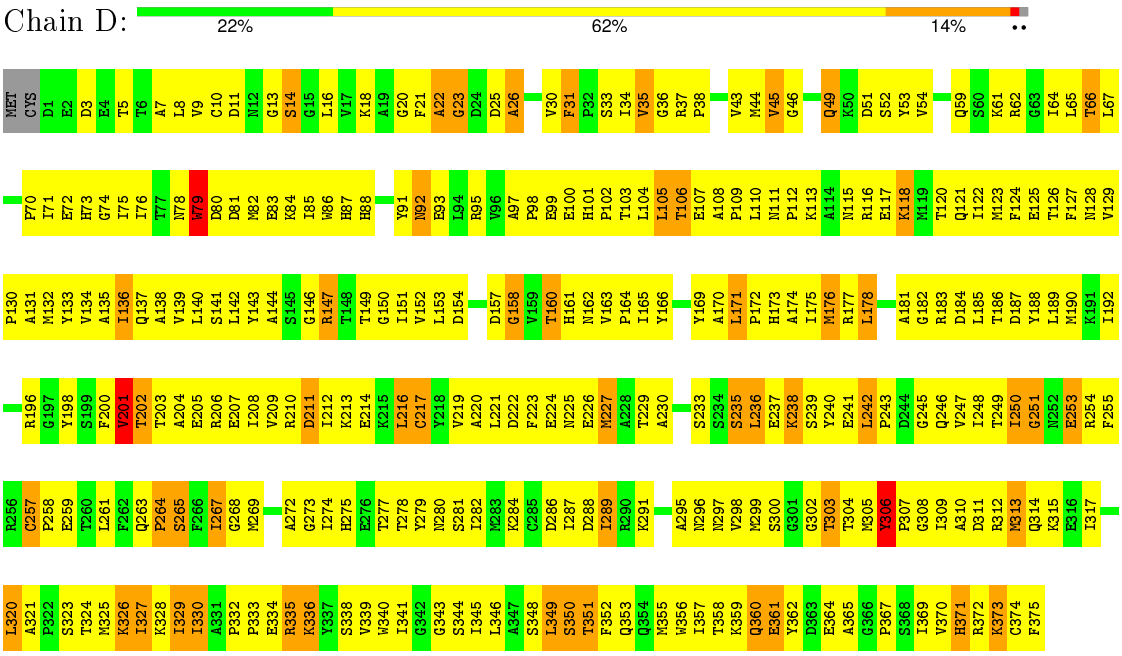
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 3 | H | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 3 | G | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 3 | D | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 3 | F | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 3 | E | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

# 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.

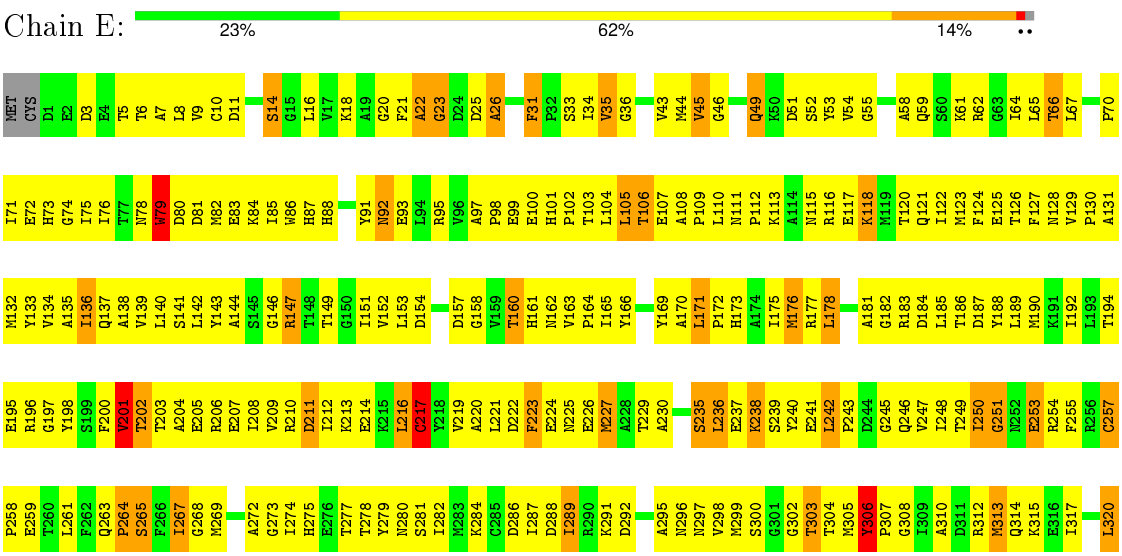
- Molecule 1: Actin, alpha skeletal muscle

Chain D:



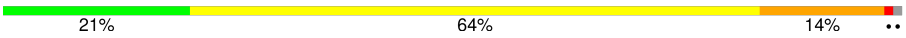

- Molecule 1: Actin, alpha skeletal muscle

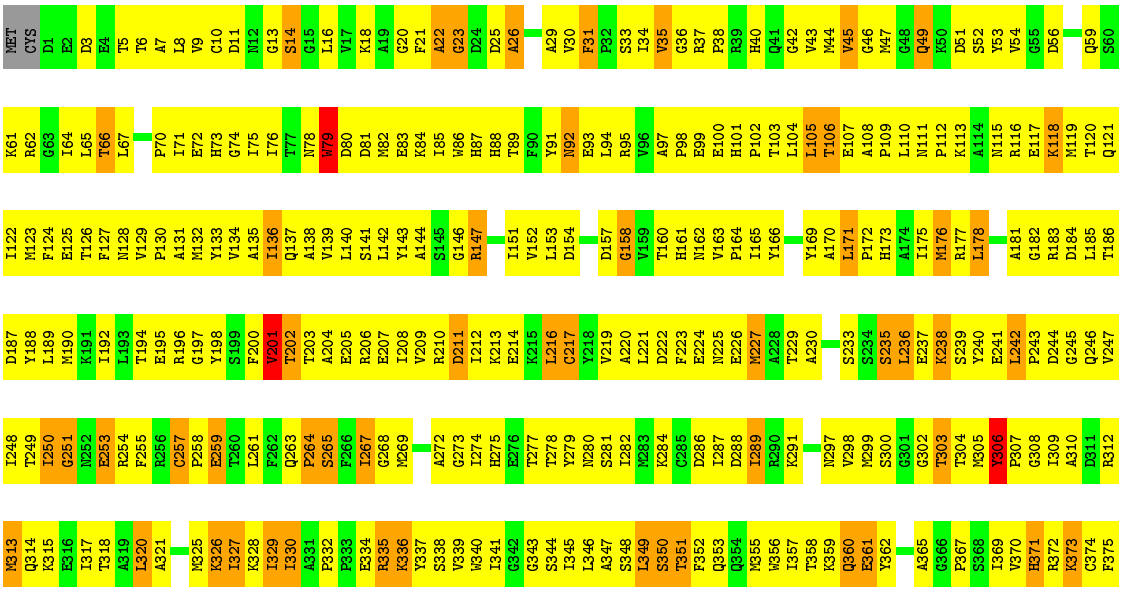
Chain E:



- Molecule 1: Actin, alpha skeletal muscle

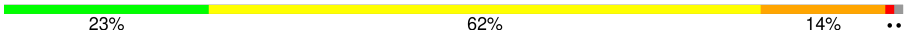
Chain F:

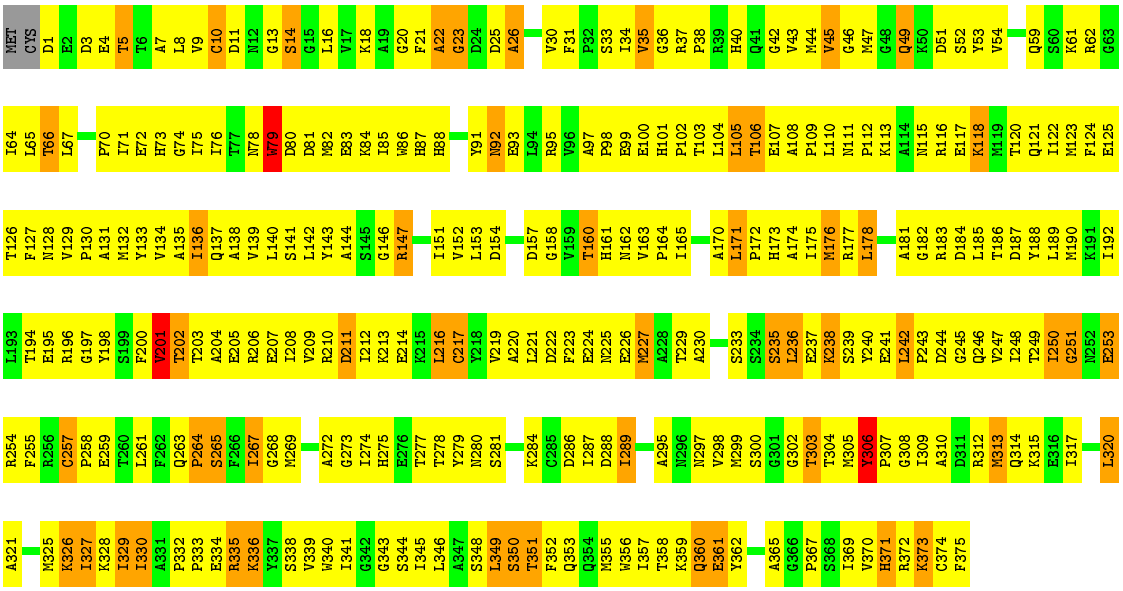


- Molecule 1: Actin, alpha skeletal muscle

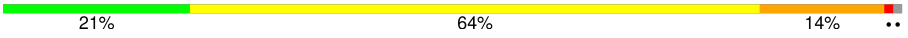
Chain G:

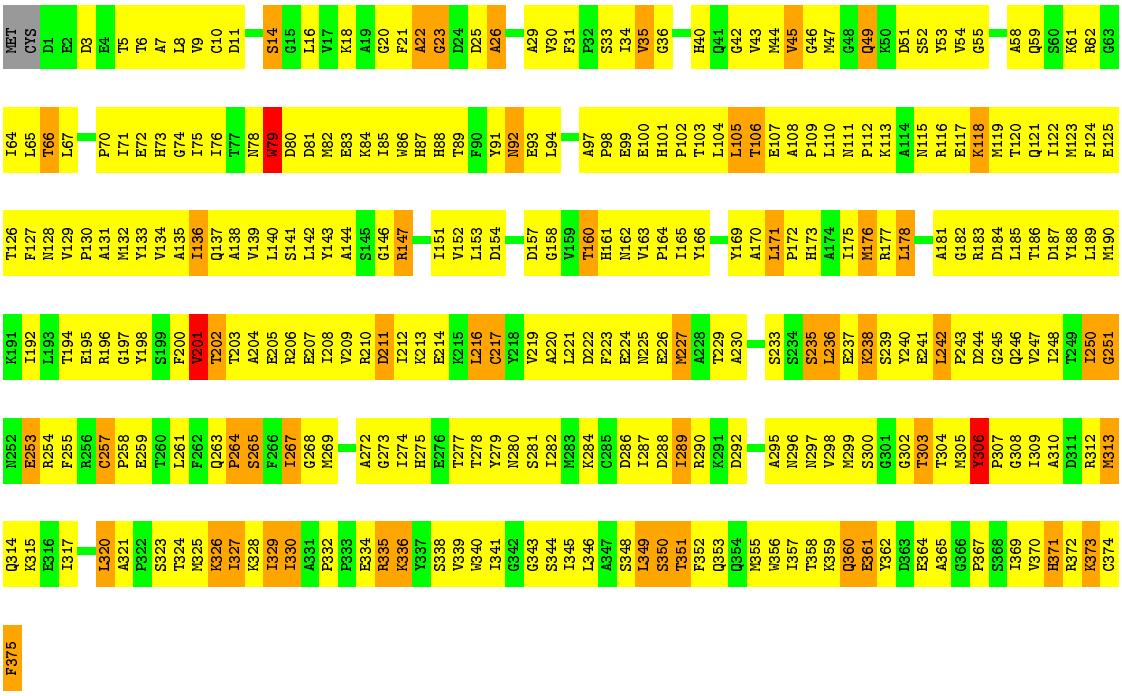


- Molecule 1: Actin, alpha skeletal muscle

Chain H:




MET CYS D1 E2 D3 E4 T5 T6 A7 L8 V9 C10 D11 S14 G15 L16 V17 K18 A19 G20 F21 A22 G23 D24 D25 A26 A29 V30 F31 P32 S33 I34 V35 G36 H40 Q41 G42 V43 M44 V45 G46 M47 G48 Q49 K50 D51 S52 Y53 V54 G55 A58 Q59 S60 K61 R62 G63
I64 L65 T66 L67 P70 I71 E72 H73 G74 I75 I76 T77 N78 W79 D80 D81 M82 E83 K84 I85 W86 H87 H88 T89 F90 Y91 N92 E93 L94 A97 P98 E99 E100 H101 P102 T103 L104 L105 T106 E107 A108 P109 L110 N111 P112 K113 A114 N115 R116 E117 K118 M119 T120 Q121 I122 M123 F124 E125
T126 F127 N128 V129 P130 A131 M132 Y133 V134 A135 I136 Q137 A138 V139 L140 S141 L142 Y143 A144 S145 G146 R147 I151 V152 L153 D154 D157 G158 V159 T160 H161 N162 V163 P164 I165 Y166 Y169 A170 L171 P172 H173 A174 I175 M176 R177 L178 A181 G182 R183 D184 L185 T186 D187 Y188 L189 M190
K191 I192 L193 T194 E195 R196 G197 Y198 S199 F200 V201 T202 T203 A204 E205 R206 E207 I208 V209 R210 D211 I212 K213 E214 K215 L216 C217 Y218 V219 A220 L221 D222 F223 E224 N225 E226 N227 A228 T229 A230 S233 S234 S235 L236 E237 K238 S239 Y240 E241 L242 P243 D244 G245 Q246 V247 I248 T249 I250 G251
N252 E253 R254 F255 R256 C257 P258 E259 T260 L261 F262 Q263 P264 S265 F266 I267 G268 M269 A272 G273 I274 H275 E276 T277 T278 Y279 N280 S281 I282 M283 K284 C285 D286 I287 D288 I289 R290 K291 D292 A295 N296 N297 V298 M299 S300 G301 G302 T303 T304 M305 Y306 P307 G308 I309 A310 D311 R312 M313
Q314 K315 E316 I317 L320 A321 P322 S323 T324 M325 K326 I327 K328 I329 I330 A331 P332 P333 E334 R335 K336 Y337 S338 V339 W340 I341 G342 G343 S344 I345 L346 A347 S348 L349 S350 T351 F352 Q353 Q354 M355 W356 I357 T358 K359 Q360 E361 Y362 D363 E364 A365 G366 P367 S368 I369 V370 H371 R372 K373 C374
F375

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | HELICAL | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | Not provided | Depositor |
| Resolution determination method | FSC and comparison with atomic model | Depositor |
| CTF correction method | Not provided | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | Not provided | Depositor |
| Image detector | FEI Falcon II (4k x 4k) | 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 | D | 0.81 | 0/2995 | 0.73 | 0/4058 |
| 1 | E | 0.81 | 0/2995 | 0.72 | 0/4058 |
| 1 | F | 0.80 | 0/2995 | 0.72 | 0/4058 |
| 1 | G | 0.82 | 1/2995 (0.0%) | 0.72 | 0/4058 |
| 1 | H | 0.82 | 1/2995 (0.0%) | 0.72 | 0/4058 |
| All | All | 0.81 | 2/14975 (0.0%) | 0.72 | 0/20290 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | G | 10 | CYS | CB-SG | 5.58 | 1.91 | 1.82 |
| 1 | H | 375 | PHE | CE1-CZ | 5.04 | 1.47 | 1.37 |

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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 | D | 2932 | 0 | 2894 | 445 | 0 |
| 1 | E | 2932 | 0 | 2894 | 438 | 0 |
| 1 | F | 2932 | 0 | 2894 | 475 | 0 |
| 1 | G | 2932 | 0 | 2894 | 439 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | H | 2932 | 0 | 2894 | 450 | 0 |
| 2 | D | 27 | 0 | 12 | 2 | 0 |
| 2 | E | 27 | 0 | 12 | 2 | 0 |
| 2 | F | 27 | 0 | 12 | 2 | 0 |
| 2 | G | 27 | 0 | 12 | 2 | 0 |
| 2 | H | 27 | 0 | 12 | 2 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | G | 1 | 0 | 0 | 0 | 0 |
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| All | All | 14800 | 0 | 14530 | 2165 | 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 74.

The worst 5 of 2165 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:H:259:GLU:HB3 | 1:H:263:GLN:HE22 | 1.06 | 1.18 |
| 1:E:259:GLU:HB3 | 1:E:263:GLN:HE22 | 1.06 | 1.13 |
| 1:G:259:GLU:HB3 | 1:G:263:GLN:HE22 | 1.06 | 1.12 |
| 1:F:259:GLU:HB3 | 1:F:263:GLN:HE22 | 1.08 | 1.11 |
| 1:D:259:GLU:HB3 | 1:D:263:GLN:HE22 | 1.08 | 1.08 |

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 | D | 373/377 (99%) | 326 (87%) | 24 (6%) | 23 (6%) | 2 26 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | E | 373/377 (99%) | 326 (87%) | 24 (6%) | 23 (6%) | 2 26 |
| 1 | F | 373/377 (99%) | 326 (87%) | 24 (6%) | 23 (6%) | 2 26 |
| 1 | G | 373/377 (99%) | 327 (88%) | 24 (6%) | 22 (6%) | 2 27 |
| 1 | H | 373/377 (99%) | 327 (88%) | 24 (6%) | 22 (6%) | 2 27 |
| All | All | 1865/1885 (99%) | 1632 (88%) | 120 (6%) | 113 (6%) | 4 26 |

5 of 113 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 92 | ASN |
| 1 | D | 144 | ALA |
| 1 | D | 223 | PHE |
| 1 | D | 235 | SER |
| 1 | D | 351 | THR |

### 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 | D | 318/320 (99%) | 275 (86%) | 43 (14%) | 5 29 |
| 1 | E | 318/320 (99%) | 275 (86%) | 43 (14%) | 5 29 |
| 1 | F | 318/320 (99%) | 274 (86%) | 44 (14%) | 4 28 |
| 1 | G | 318/320 (99%) | 274 (86%) | 44 (14%) | 4 28 |
| 1 | H | 318/320 (99%) | 275 (86%) | 43 (14%) | 5 29 |
| All | All | 1590/1600 (99%) | 1373 (86%) | 217 (14%) | 9 29 |

5 of 217 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 147 | ARG |
| 1 | F | 326 | LYS |
| 1 | H | 253 | GLU |
| 1 | F | 176 | MET |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 242 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 92 | ASN |
| 1 | F | 296 | ASN |
| 1 | H | 162 | ASN |
| 1 | F | 162 | ASN |
| 1 | F | 354 | GLN |

#### 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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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 | $\#\|Z\| > 2$ |
| 2 | ADP | D | 401 | 3 | 24,29,29 | 1.36 | 3 (12%) | 23,45,45 | 3.11 | 1 (4%) |
| 2 | ADP | E | 401 | 3 | 24,29,29 | 1.45 | 4 (16%) | 23,45,45 | 2.99 | 1 (4%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | ADP | F | 401 | 3 | 24,29,29 | 1.40 | 6 (25%) | 23,45,45 | 3.17 | 1 (4%) |
| 2 | ADP | G | 401 | 3 | 24,29,29 | 1.53 | 4 (16%) | 23,45,45 | 2.77 | 1 (4%) |
| 2 | ADP | H | 401 | 3 | 24,29,29 | 1.39 | 4 (16%) | 23,45,45 | 3.12 | 1 (4%) |

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 |
|---|---|---|---|---|---|---|---|
| 2 | ADP | D | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | E | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | F | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | G | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |
| 2 | ADP | H | 401 | 3 | - | 0/12/32/32 | 0/3/3/3 |

The worst 5 of 21 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | F | 401 | ADP | C5-N7 | -2.24 | 1.31 | 1.39 |
| 2 | D | 401 | ADP | C5-N7 | -2.20 | 1.31 | 1.39 |
| 2 | H | 401 | ADP | C5-N7 | -2.19 | 1.31 | 1.39 |
| 2 | F | 401 | ADP | PB-O2B | 2.00 | 1.61 | 1.54 |
| 2 | G | 401 | ADP | C5'-C4' | 2.07 | 1.58 | 1.51 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | F | 401 | ADP | N3-C2-N1 | -14.64 | 117.37 | 128.87 |
| 2 | D | 401 | ADP | N3-C2-N1 | -14.42 | 117.55 | 128.87 |
| 2 | H | 401 | ADP | N3-C2-N1 | -14.39 | 117.57 | 128.87 |
| 2 | E | 401 | ADP | N3-C2-N1 | -13.78 | 118.05 | 128.87 |
| 2 | G | 401 | ADP | N3-C2-N1 | -12.56 | 119.01 | 128.87 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | D | 401 | ADP | 2 | 0 |
| 2 | E | 401 | ADP | 2 | 0 |
| 2 | F | 401 | ADP | 2 | 0 |
| 2 | G | 401 | ADP | 2 | 0 |
| 2 | H | 401 | 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.