



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

Jul 24, 2017 – 04:57 AM EDT

PDB ID : 5FWP  
EMDB ID: : EMD-3340  
Title : Atomic cryoEM structure of Hsp90-Cdc37-Cdk4 complex  
Authors : Verba, K.A.; Wang, R.Y.R.; Arakawa, A.; Liu, Y.; Yokoyama, S.; Agard, D.A.  
Deposited on : unknown  
Resolution : 7.20 Å(reported)  
Based on PDB ID : ?

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

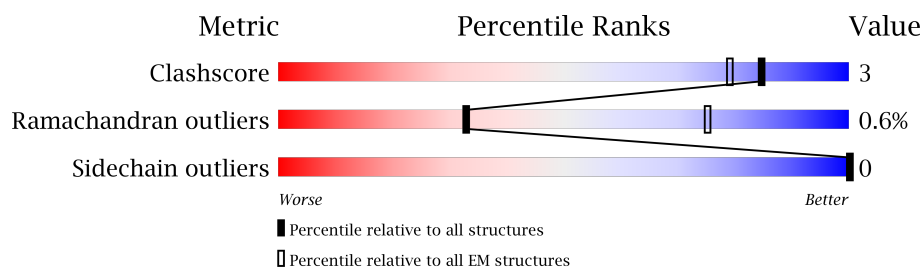
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.20 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<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 125131                      | 1336                        |
| Ramachandran outliers | 121729                      | 1120                        |
| Sidechain outliers    | 121581                      | 1026                        |

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  $\geq 3$ , 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  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 727    |                  |
| 1   | B     | 727    |                  |
| 2   | E     | 378    |                  |
| 3   | K     | 310    |                  |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28355 atoms, of which 14168 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 HEAT SHOCK PROTEIN HSP 90 BETA.

| Mol | Chain | Residues | Atoms |      |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|------|----|---------|-------|
| 1   | A     | 638      | Total | C    | H    | N   | O    | S  | 0       | 0     |
|     |       |          | 10399 | 3280 | 5226 | 870 | 1000 | 23 |         |       |
| 1   | B     | 630      | Total | C    | H    | N   | O    | S  | 0       | 0     |
|     |       |          | 10242 | 3235 | 5139 | 856 | 989  | 23 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -2      | GLY      | -      | expression tag | UNP P08238 |
| A     | -1      | GLY      | -      | expression tag | UNP P08238 |
| A     | 0       | PHE      | -      | expression tag | UNP P08238 |
| B     | -2      | GLY      | -      | expression tag | UNP P08238 |
| B     | -1      | GLY      | -      | expression tag | UNP P08238 |
| B     | 0       | PHE      | -      | expression tag | UNP P08238 |

- Molecule 2 is a protein called HSP90 CO-CHAPERONE CDC37.

| Mol | Chain | Residues | Atoms |      |      |     |     |   |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|----|---------|-------|
| 2   | E     | 259      | Total | C    | H    | N   | O   | P | S  | 0       | 0     |
|     |       |          | 4307  | 1358 | 2125 | 383 | 425 | 1 | 15 |         |       |

- Molecule 3 is a protein called CYCLIN-DEPENDENT KINASE 4.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|-------|
| 3   | K     | 209      | Total | C    | H    | N   | O   | S | 0       | 0     |
|     |       |          | 3343  | 1077 | 1678 | 284 | 295 | 9 |         |       |

There are 7 discrepancies between the modelled and reference sequences:

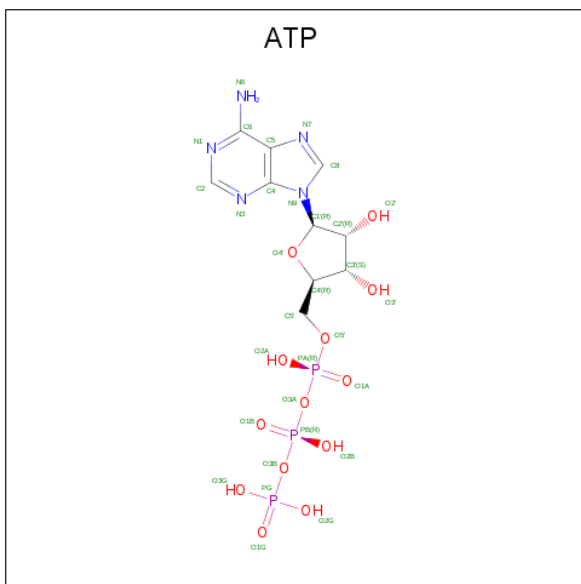
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | -6      | GLY      | -      | expression tag | UNP P11802 |
| K     | -5      | ALA      | -      | expression tag | UNP P11802 |
| K     | -4      | MET      | -      | expression tag | UNP P11802 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | -3      | ASP      | -      | expression tag | UNP P11802 |
| K     | -2      | PRO      | -      | expression tag | UNP P11802 |
| K     | -1      | GLU      | -      | expression tag | UNP P11802 |
| K     | 0       | PHE      | -      | expression tag | UNP P11802 |

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 4   | A     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |
| 4   | B     | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 31    | 10 | 5 | 13 | 3 |         |

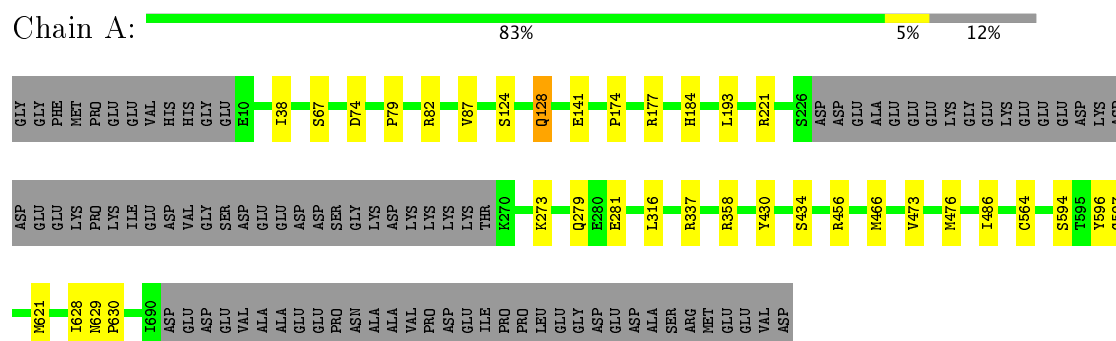
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 5   | B     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 5   | A     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

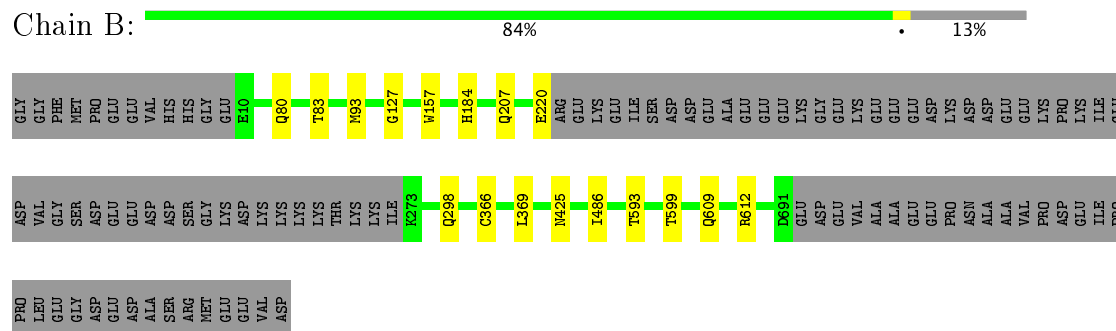
### 3 Residue-property plots

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. 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.

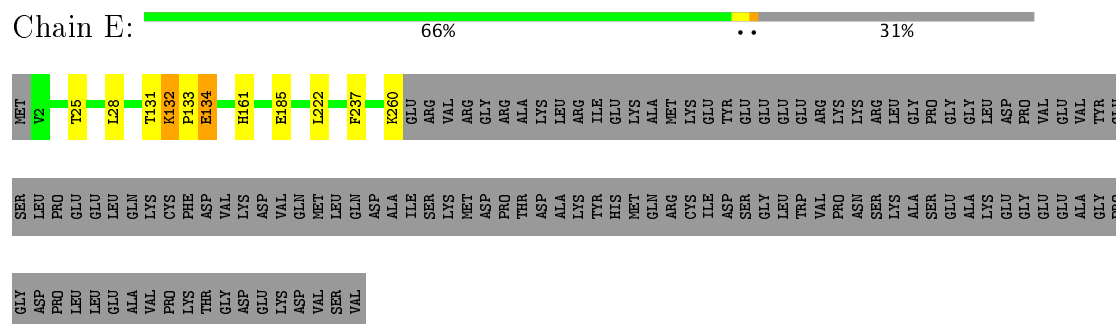
- Molecule 1: HEAT SHOCK PROTEIN HSP 90 BETA



- Molecule 1: HEAT SHOCK PROTEIN HSP 90 BETA

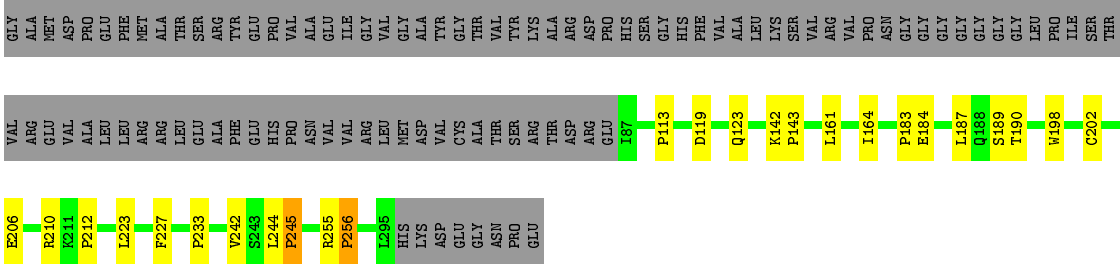


- Molecule 2: HSP90 CO-CHAPERONE CDC37



- Molecule 3: CYCLIN-DEPENDENT KINASE 4





## 4 Experimental information

| Property                             | Value                     | Source    |
|--------------------------------------|---------------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE           | Depositor |
| Imposed symmetry                     | POINT, C1                 | Depositor |
| Number of particles used             | 114683                    | Depositor |
| Resolution determination method      | Not provided              | Depositor |
| CTF correction method                | Not provided              | Depositor |
| Microscope                           | FEI TITAN KRIOS           | Depositor |
| Voltage (kV)                         | 300                       | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 44                        | Depositor |
| Minimum defocus (nm)                 | 1400                      | Depositor |
| Maximum defocus (nm)                 | 3800                      | Depositor |
| Magnification                        | 22500                     | Depositor |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k) | Depositor |

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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     | 0.92         | 0/5257         | 0.56        | 0/7062  |
| 1   | B     | 0.91         | 0/5187         | 0.56        | 0/6972  |
| 2   | E     | 0.98         | 1/2209 (0.0%)  | 0.50        | 0/2955  |
| 3   | K     | 0.81         | 1/1711 (0.1%)  | 0.60        | 0/2330  |
| All | All   | 0.92         | 2/14364 (0.0%) | 0.55        | 0/19319 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 2   | E     | 134 | GLU  | CD-OE2 | -5.07 | 1.20        | 1.25     |
| 3   | K     | 184 | GLU  | CD-OE2 | -5.06 | 1.20        | 1.25     |

There are no bond angle outliers.

There are no chirality outliers.

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     | 5173  | 5226     | 5224     | 20      | 0            |
| 1   | B     | 5103  | 5139     | 5137     | 22      | 0            |
| 2   | E     | 2182  | 2125     | 2124     | 13      | 0            |
| 3   | K     | 1665  | 1678     | 1677     | 14      | 0            |
| 4   | A     | 31    | 0        | 12       | 3       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4   | B     | 31    | 0        | 12       | 2       | 0            |
| 5   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | B     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 14187 | 14168    | 14186    | 72      | 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 3.

The worst 5 of 72 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:B:609:GLN:HB3 | 1:B:612:ARG:CG  | 1.78                     | 1.14              |
| 1:B:609:GLN:HB3 | 1:B:612:ARG:HG2 | 1.47                     | 0.94              |
| 1:B:609:GLN:CG  | 1:B:612:ARG:HG2 | 1.96                     | 0.94              |
| 1:B:609:GLN:CB  | 1:B:612:ARG:HG2 | 1.99                     | 0.92              |
| 1:B:609:GLN:HB3 | 1:B:612:ARG:HG3 | 1.51                     | 0.89              |

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     | 634/727 (87%)   | 607 (96%)  | 24 (4%) | 3 (0%)   | 32          | 74 |
| 1   | B     | 626/727 (86%)   | 612 (98%)  | 13 (2%) | 1 (0%)   | 51          | 84 |
| 2   | E     | 256/378 (68%)   | 242 (94%)  | 13 (5%) | 1 (0%)   | 38          | 77 |
| 3   | K     | 207/310 (67%)   | 185 (89%)  | 17 (8%) | 5 (2%)   | 7           | 42 |
| All | All   | 1723/2142 (80%) | 1646 (96%) | 67 (4%) | 10 (1%)  | 33          | 71 |

5 of 10 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | E     | 132 | LYS  |
| 3   | K     | 256 | PRO  |
| 1   | A     | 174 | PRO  |
| 1   | A     | 281 | GLU  |
| 3   | K     | 113 | 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     | 577/653 (88%)   | 577 (100%)  | 0        | 100         | 100 |
| 1   | B     | 569/653 (87%)   | 569 (100%)  | 0        | 100         | 100 |
| 2   | E     | 238/340 (70%)   | 238 (100%)  | 0        | 100         | 100 |
| 3   | K     | 183/262 (70%)   | 183 (100%)  | 0        | 100         | 100 |
| All | All   | 1567/1908 (82%) | 1567 (100%) | 0        | 100         | 100 |

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 425 | ASN  |
| 2   | E     | 161 | HIS  |
| 3   | K     | 98  | 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](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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   | SEP  | E     | 13  | 2    | 9,9,10       | 1.44 | 2 (22%)     | 9,12,14     | 1.26 | 1 (11%)     |

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   | SEP  | E     | 13  | 2    | -       | 0/5/8/10 | 0/0/0/0 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | E     | 13  | SEP  | CA-C  | 2.15 | 1.53        | 1.50     |
| 2   | E     | 13  | SEP  | P-O1P | 2.96 | 1.60        | 1.50     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2   | E     | 13  | SEP  | OG-CB-CA | 2.82 | 110.95      | 108.17   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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 | $\# Z  > 2$ |
| 4   | ATP  | A     | 1691 | 5    | 27,33,33     | 1.14 | 2 (7%)      | 25,52,52    | 1.70 | 2 (8%)      |
| 4   | ATP  | B     | 1692 | 5    | 27,33,33     | 1.05 | 2 (7%)      | 25,52,52    | 1.68 | 2 (8%)      |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 4   | ATP  | A     | 1691 | 5    | -       | 0/18/38/38 | 0/3/3/3 |
| 4   | ATP  | B     | 1692 | 5    | -       | 0/18/38/38 | 0/3/3/3 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 4   | B     | 1692 | ATP  | C2'-C1' | -2.02 | 1.50        | 1.53     |
| 4   | A     | 1691 | ATP  | O4'-C1' | 2.18  | 1.44        | 1.41     |
| 4   | A     | 1691 | ATP  | C5-C4   | 3.11  | 1.47        | 1.40     |
| 4   | B     | 1692 | ATP  | C5-C4   | 3.23  | 1.47        | 1.40     |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 4   | A     | 1691 | ATP  | N3-C2-N1 | -6.08 | 123.56      | 128.86   |
| 4   | B     | 1692 | ATP  | N3-C2-N1 | -6.06 | 123.58      | 128.86   |
| 4   | B     | 1692 | ATP  | C4-C5-N7 | -2.55 | 106.94      | 109.41   |
| 4   | A     | 1691 | ATP  | C4-C5-N7 | -2.43 | 107.06      | 109.41   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4   | A     | 1691 | ATP  | 3       | 0            |
| 4   | B     | 1692 | ATP  | 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.