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

Feb 1, 2016 – 02:11 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 2G1P |
| Title | : | Structure of E. coli DNA adenine methyltransferase (DAM) |
| Authors | : | Horton, J.R.; Liebert, K.; Bekes, M.; Jeltsch, A.; Cheng, X. |
| Deposited on | : | 2006-02-14 |
| Resolution | : | 1.89 Å(reported) |

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

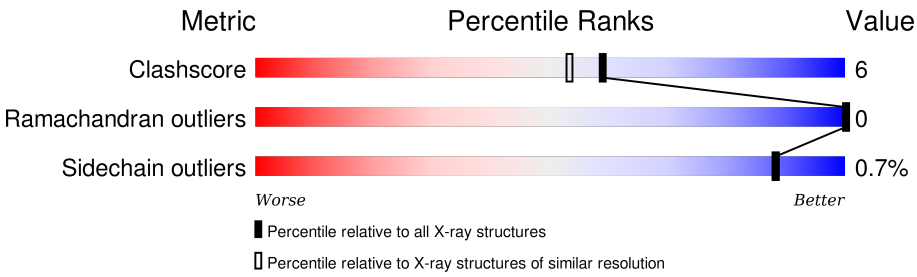
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.89 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) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 102246 | 5398 (1.90-1.90) |
| Ramachandran outliers | 100387 | 5338 (1.90-1.90) |
| Sidechain outliers | 100360 | 5339 (1.90-1.90) |

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. 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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 12 | 100% |
| 1 | G | 12 | 50% 50% |
| 2 | A | 278 | 79% 9% 12% |
| 2 | B | 278 | 79% 8% • 12% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 4 | GOL | B | 397 | - | X | - | - |

# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4865 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 DNA chain called 5'-D(*TP*CP*TP*AP*GP*AP*TP*CP*TP*AP*GP*A)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 1 | F | 12 | 243 | 118 | 44 | 70 | 11 | 0 | 0 | 0 |
| 1 | G | 12 | 243 | 118 | 44 | 70 | 11 | 0 | 0 | 0 |

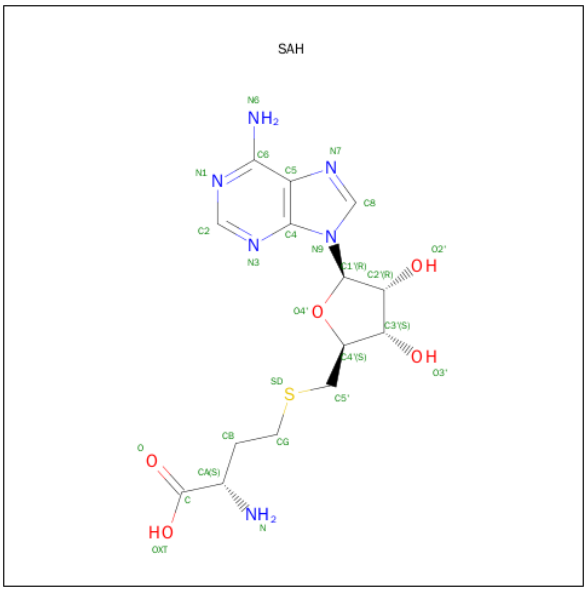
- Molecule 2 is a protein called DNA adenine methylase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | A | 244 | 1988 | 1287 | 335 | 359 | 7 | 0 | 0 | 0 |
| 2 | B | 246 | 2019 | 1304 | 341 | 367 | 7 | 0 | 1 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

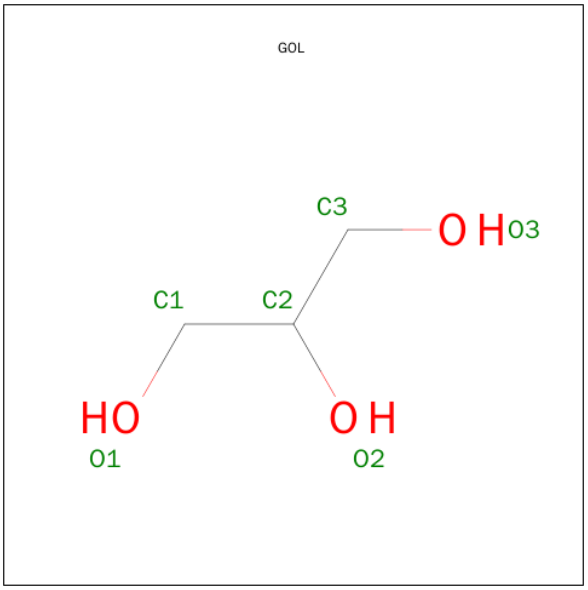
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 175 | SER | ALA | see remark 999 | UNP P0AEE8 |
| B | 175 | SER | ALA | see remark 999 | UNP P0AEE8 |

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | A | 1 | 26 | 14 | 6 | 5 | 1 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 3 | B | 1 | 26 | 14 | 6 | 5 | 1 | 0 | 0 |

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 4 | B | 1 | 6 | 3 | 3 | 0 | 0 |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 5 | A | 127 | 127 | 127 | 0 | 0 |
| | | | Total | O | | |
| 5 | B | 124 | 124 | 124 | 0 | 0 |
| | | | Total | O | | |
| 5 | F | 33 | 33 | 33 | 0 | 0 |
| | | | Total | O | | |
| 5 | G | 30 | 30 | 30 | 0 | 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 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.

Note EDS was not executed.

- Molecule 1: 5'-D(*TP*CP*TP*AP*GP*AP*TP*CP*TP*AP*GP*A)-3'

Chain F: 100%

There are no outlier residues recorded for this chain.

- Molecule 1: 5'-D(*TP*CP*TP*AP*GP*AP*TP*CP*TP*AP*GP*A)-3'

Chain G: 50% 50%

T1 C2 T3 A6 T7 C8 T9 A12

- Molecule 2: DNA adenine methylase

Chain A: 79% 9% 12%

MET LYS K3 A6 Y15 P16 L17 V36 V41 F42 L43 D54 E89 E96 K100 N120 N126 R137 Y179 I187 SER ALA THR ALA ASN PHE THR ALA TYR HIS THR N199 E214 R239 A240 K241 L242 H243 K246 VAL ARG ARG SER ILE

SER SER ASN GLY GLY THR ARG LYS K260 V261 D262 E263 L264 P270 GLY VAL VAL SER PRO ALA LYS LYS

- Molecule 2: DNA adenine methylase

Chain B: 79% 8% • 12%

MET LYS K3 A11 Y15 P16 L17 K27 G28 V41 D71 Q75 R78 L112 E145 Y179 L187 SER ALA THR ALA ASN PHE THR ALA TYR HIS T198 E214 R239 A240 K241 L242 V245 K246 V247 ARG ARG SER ILE SER SER ASN GLY GLY THR

ARG LYS K260 E263 L264 L267 Y268 K269 P270 GLY VAL VAL SER PRO ALA LYS LYS

# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 46.20Å 71.30Å 97.80Å<br>90.00° 90.03° 90.00° | Depositor |
| Resolution (Å) | 33.60 – 1.89 | Depositor |
| % Data completeness<br>(in resolution range) | 99.9 (33.60-1.89) | Depositor |
| $R_{merge}$ | 0.10 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.188 , 0.216 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 4865 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 29.0 | wwPDB-VP |

# 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: GOL, SAH

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 | F | 0.55 | 0/272 | 0.81 | 0/418 |
| 1 | G | 0.54 | 0/272 | 0.75 | 0/418 |
| 2 | A | 0.52 | 0/2043 | 0.66 | 0/2772 |
| 2 | B | 0.52 | 0/2074 | 0.66 | 0/2812 |
| All | All | 0.52 | 0/4661 | 0.68 | 0/6420 |

There are no bond length outliers.

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 | F | 243 | 0 | 138 | 0 | 0 |
| 1 | G | 243 | 0 | 138 | 13 | 0 |
| 2 | A | 1988 | 0 | 1891 | 19 | 0 |
| 2 | B | 2019 | 0 | 1931 | 21 | 0 |
| 3 | A | 26 | 0 | 19 | 0 | 0 |
| 3 | B | 26 | 0 | 19 | 0 | 0 |
| 4 | B | 6 | 0 | 5 | 1 | 0 |
| 5 | A | 127 | 0 | 0 | 0 | 0 |
| 5 | B | 124 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 5 | F | 33 | 0 | 0 | 0 | 0 |
| 5 | G | 30 | 0 | 0 | 0 | 0 |
| All | All | 4865 | 0 | 4141 | 50 | 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 6.

The worst 5 of 50 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:G:1:DT:H2" | 1:G:2:DC:C5' | 2.09 | 0.81 |
| 2:A:241:LYS:HE3 | 2:A:243:HIS:CE1 | 2.18 | 0.79 |
| 1:G:1:DT:H2" | 1:G:2:DC:H5' | 1.64 | 0.79 |
| 2:B:241:LYS:HD2 | 2:B:267:LEU:O | 1.84 | 0.76 |
| 1:G:1:DT:H1' | 1:G:2:DC:H5" | 1.68 | 0.74 |

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 | |
|---|---|---|---|---|---|---|---|
| 2 | A | 238/278 (86%) | 232 (98%) | 6 (2%) | 0 | 100 | 100 |
| 2 | B | 241/278 (87%) | 235 (98%) | 6 (2%) | 0 | 100 | 100 |
| All | All | 479/556 (86%) | 467 (98%) | 12 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | |
|---|---|---|---|---|---|---|
| 2 | A | 204/240 (85%) | 204 (100%) | 0 | 100 | 100 |
| 2 | B | 211/240 (88%) | 208 (99%) | 3 (1%) | 74 | 71 |
| All | All | 415/480 (86%) | 412 (99%) | 3 (1%) | 88 | 88 |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 27 | LYS |
| 2 | B | 112 | LEU |
| 2 | B | 241 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | A | 102 | GLN |
| 2 | A | 120 | ASN |
| 2 | B | 120 | ASN |
| 2 | B | 150 | 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)

3 ligands are 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 | $\#\|Z\| > 2$ |
| 3 | SAH | A | 401 | - | 20,28,28 | 1.65 | 4 (20%) | 19,40,40 | 2.28 | 7 (36%) |
| 4 | GOL | B | 397 | - | 5,5,5 | 4.65 | 4 (80%) | 5,5,5 | 5.67 | 3 (60%) |
| 3 | SAH | B | 402 | - | 20,28,28 | 1.49 | 4 (20%) | 19,40,40 | 2.26 | 6 (31%) |

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 | SAH | A | 401 | - | - | 0/7/31/31 | 0/3/3/3 |
| 4 | GOL | B | 397 | - | - | 0/4/4/4 | 0/0/0/0 |
| 3 | SAH | B | 402 | - | - | 0/7/31/31 | 0/3/3/3 |

The worst 5 of 12 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | B | 397 | GOL | C3-C2 | -8.23 | 1.20 | 1.52 |
| 4 | B | 397 | GOL | C1-C2 | -3.66 | 1.38 | 1.52 |
| 3 | A | 401 | SAH | C8-N7 | -2.16 | 1.30 | 1.34 |
| 3 | B | 402 | SAH | C8-N7 | -2.15 | 1.30 | 1.34 |
| 3 | B | 402 | SAH | C5'-C4' | 2.83 | 1.60 | 1.52 |

The worst 5 of 16 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | A | 401 | SAH | N3-C2-N1 | -6.93 | 123.59 | 128.89 |
| 3 | B | 402 | SAH | N3-C2-N1 | -6.90 | 123.61 | 128.89 |
| 3 | B | 402 | SAH | CB-CG-SD | -3.90 | 106.06 | 113.57 |
| 3 | A | 401 | SAH | CB-CG-SD | -3.67 | 106.49 | 113.57 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | A | 401 | SAH | C1'-N9-C4 | -2.95 | 122.50 | 126.94 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | B | 397 | GOL | 1 | 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.

# 6 Fit of model and data (i)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

## 6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

## 6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.