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

Aug 15, 2023 – 10:19 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 1XJQ |
| Title | : | ADP Complex OF HUMAN PAPS SYNTHETASE 1 |
| Authors | : | Harjes, S.; Bayer, P.; Scheidig, A.J. |
| Deposited on | : | 2004-09-24 |
| Resolution | : | 2.06 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

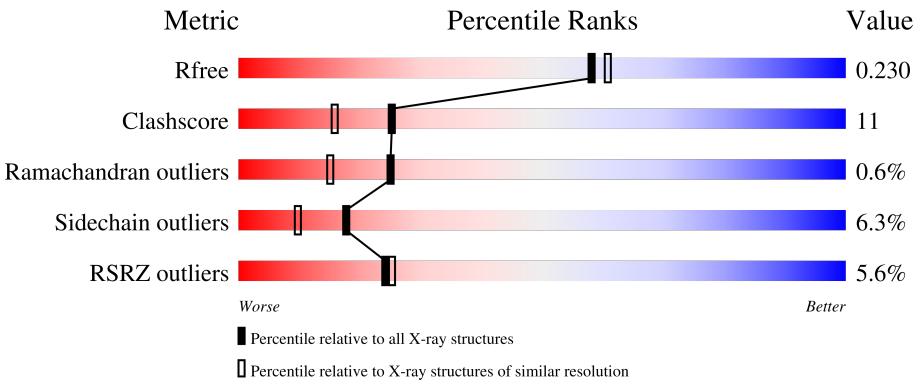
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 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) | : | 2.35 |

# 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 2.06 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)) |
|---|---|---|
| $R_{free}$ | 130704 | 2684 (2.08-2.04) |
| Clashscore | 141614 | 2801 (2.08-2.04) |
| Ramachandran outliers | 138981 | 2768 (2.08-2.04) |
| Sidechain outliers | 138945 | 2768 (2.08-2.04) |
| RSRZ outliers | 127900 | 2646 (2.08-2.04) |

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 of 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 | 630 | 5% 66% 20% • • 11% |
| 1 | B | 630 | 5% 66% 22% 5% • 6% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9997 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.

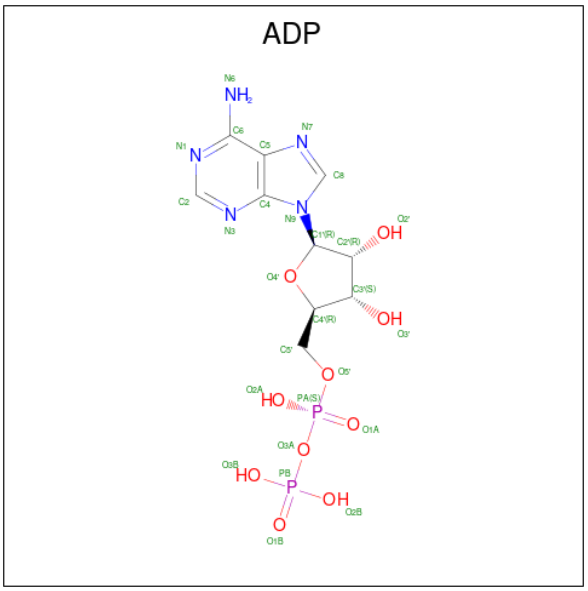
- Molecule 1 is a protein called Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | B | 590 | 4718 | 2990 | 830 | 867 | 31 | 0 | 5 | 0 |
| 1 | A | 563 | 4514 | 2864 | 790 | 828 | 32 | 0 | 8 | 0 |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 416 | SER | PHE | conflict | UNP O43252 |
| B | 625 | HIS | - | expression tag | UNP O43252 |
| B | 626 | HIS | - | expression tag | UNP O43252 |
| B | 627 | HIS | - | expression tag | UNP O43252 |
| B | 628 | HIS | - | expression tag | UNP O43252 |
| B | 629 | HIS | - | expression tag | UNP O43252 |
| B | 630 | HIS | - | expression tag | UNP O43252 |
| A | 416 | SER | PHE | conflict | UNP O43252 |
| A | 625 | HIS | - | expression tag | UNP O43252 |
| A | 626 | HIS | - | expression tag | UNP O43252 |
| A | 627 | HIS | - | expression tag | UNP O43252 |
| A | 628 | HIS | - | expression tag | UNP O43252 |
| A | 629 | HIS | - | expression tag | UNP O43252 |
| A | 630 | HIS | - | expression tag | UNP O43252 |

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




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

- Molecule 3 is water.

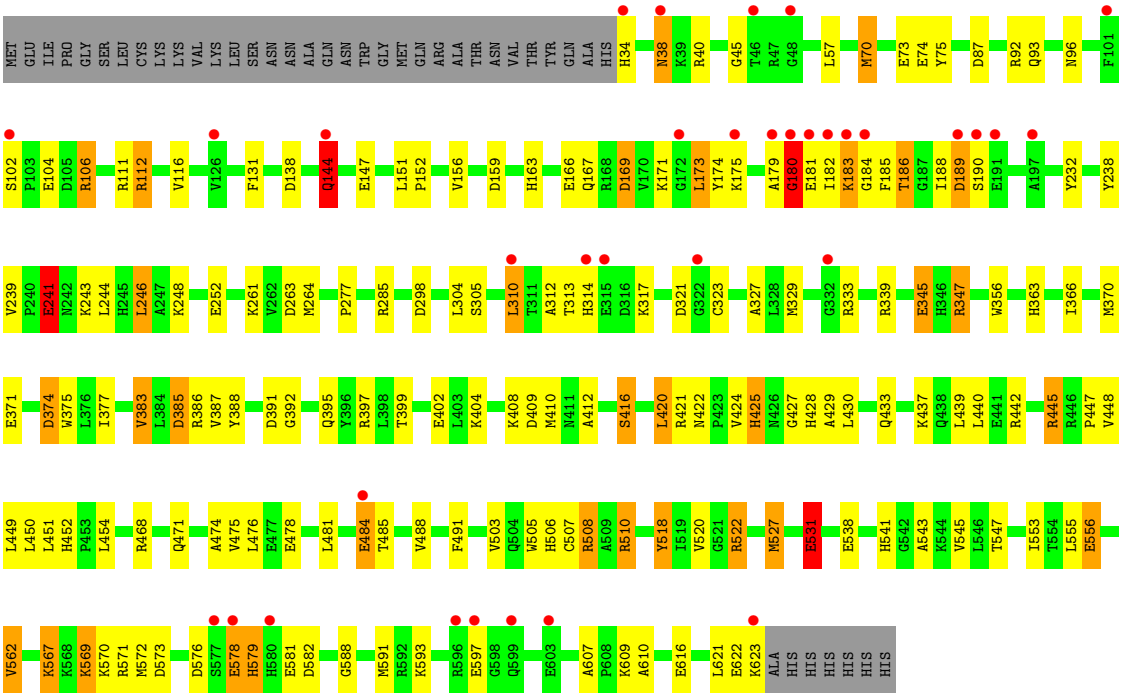
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | B | 323 | Total | O | 0 | 0 |
| | | | 323 | 323 | | |
| 3 | A | 361 | Total | O | 0 | 0 |
| | | | 361 | 361 | | |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

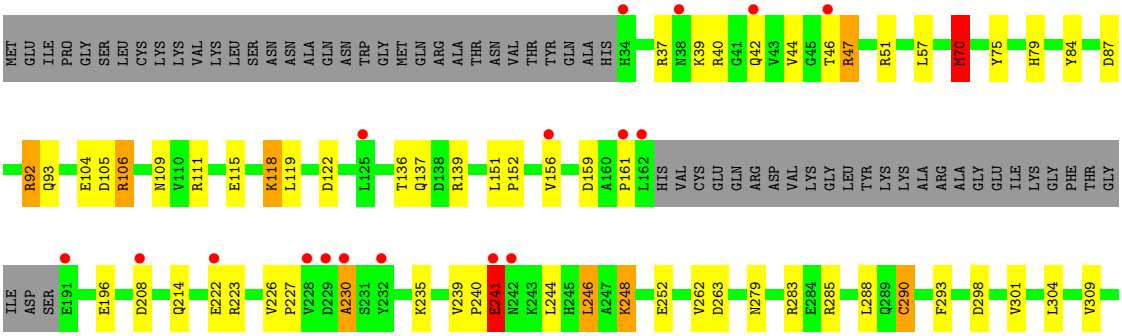
• Molecule 1: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1

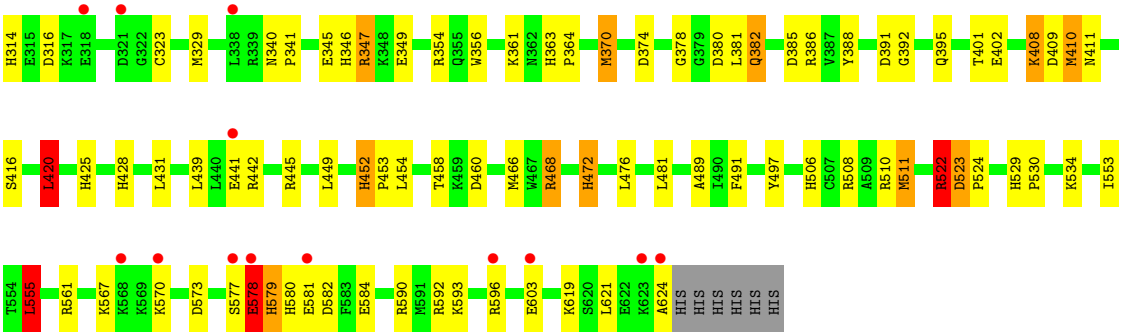
Chain B:




• Molecule 1: Bifunctional 3'-phosphoadenosine 5'-phosphosulfate synthetase 1

Chain A:




H314
E315
D316
K317
E318
D321
G322
C323
M329
L338
R339
N340
P341
E345
H346
R347
K348
E349
R354
Q355
W356
K361
N362
H363
P364
M370
D374
G378
G379
D380
L381
Q382
D385
R386
V387
Y388
D391
G392
Q395
T401
E402
K408
D409
M410
N411
S416
L420
H425
H428
L431
L439
L440
E441
R442
R445
L449
H452
P453
L454
T458
K459
D460
M466
W467
R468
H472
L476
L481
A489
I490
F491
Y497
H506
C507
R508
A509
R510
M511
R522
D523
P524
H529
P530
K534
I553
T554
L555
R561
K567
K568
K569
K570
D573
S577
E578
H579
H580
E581
D582
F583
E584
R590
M591
R592
K593
R596
E603
K619
S620
L621
E622
K623
A624
HIS
HIS
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HIS
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HIS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 78.50Å 82.50Å 133.00Å<br>90.00° 105.00° 90.00° | Depositor |
| Resolution (Å) | 129.10 – 2.06<br>19.65 – 2.06 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 96.6 (129.10-2.06)<br>96.7 (19.65-2.06) | Depositor<br>EDS |
| $R_{merge}$ | 0.10 | Depositor |
| $R_{sym}$ | 0.08 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.02 (at 2.06Å) | Xtriage |
| Refinement program | REFMAC 5.1.19 | Depositor |
| R, $R_{free}$ | 0.171 , 0.221<br>0.181 , 0.230 | Depositor<br>DCC |
| $R_{free}$ test set | 4869 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 33.8 | Xtriage |
| Anisotropy | 0.304 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 46.7 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.018 for h,-k,-h-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.96 | EDS |
| Total number of atoms | 9997 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 42.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[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)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 | $\#\|Z\|>5$ | RMSZ | $\#\|Z\|>5$ |
| 1 | A | 1.54 | 31/4657 (0.7%) | 1.32 | 56/6314 (0.9%) |
| 1 | B | 1.55 | 40/4854 (0.8%) | 1.31 | 42/6574 (0.6%) |
| All | All | 1.54 | 71/9511 (0.7%) | 1.31 | 98/12888 (0.8%) |

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 | 2 |
| 1 | B | 0 | 2 |
| All | All | 0 | 4 |

The worst 5 of 71 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 40 | ARG | CG-CD | 8.74 | 1.73 | 1.51 |
| 1 | B | 147 | GLU | CD-OE2 | 8.64 | 1.35 | 1.25 |
| 1 | A | 346 | HIS | C-O | 8.42 | 1.39 | 1.23 |
| 1 | B | 518 | TYR | CE2-CZ | -7.94 | 1.28 | 1.38 |
| 1 | A | 402 | GLU | CD-OE2 | 7.82 | 1.34 | 1.25 |

The worst 5 of 98 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 522 | ARG | NE-CZ-NH2 | 12.14 | 126.37 | 120.30 |
| 1 | B | 409 | ASP | CB-CG-OD2 | 11.11 | 128.30 | 118.30 |
| 1 | B | 347 | ARG | NE-CZ-NH2 | -10.41 | 115.10 | 120.30 |
| 1 | B | 576 | ASP | CB-CG-OD2 | 10.36 | 127.62 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 409 | ASP | CB-CG-OD2 | 10.02 | 127.32 | 118.30 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 161 | PRO | Peptide |
| 1 | A | 230 | ALA | Peptide |
| 1 | B | 102 | SER | Peptide |
| 1 | B | 180 | 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 | 4514 | 0 | 4448 | 89 | 0 |
| 1 | B | 4718 | 0 | 4650 | 107 | 0 |
| 2 | A | 27 | 0 | 12 | 0 | 0 |
| 2 | B | 54 | 0 | 23 | 6 | 0 |
| 3 | A | 361 | 0 | 0 | 24 | 1 |
| 3 | B | 323 | 0 | 0 | 38 | 1 |
| All | All | 9997 | 0 | 9133 | 197 | 1 |

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 11.

The worst 5 of 197 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:591:MET:SD | 1:B:591:MET:CE | 2.02 | 1.47 |
| 1:A:70:MET:CE | 1:A:70:MET:SD | 2.05 | 1.45 |
| 1:B:70:MET:CE | 1:B:70:MET:SD | 2.08 | 1.39 |
| 1:B:527:MET:CE | 1:B:527:MET:SD | 2.09 | 1.39 |
| 1:A:370:MET:CE | 1:A:370:MET:SD | 2.18 | 1.31 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:B:1218:HOH:O | 3:A:1007:HOH:O[1_455] | 2.00 | 0.20 |

## 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 | 566/630 (90%) | 551 (97%) | 14 (2%) | 1 (0%) | 47 39 |
| 1 | B | 592/630 (94%) | 567 (96%) | 19 (3%) | 6 (1%) | 15 6 |
| All | All | 1158/1260 (92%) | 1118 (96%) | 33 (3%) | 7 (1%) | 25 15 |

5 of 7 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 180 | GLY |
| 1 | B | 183 | LYS |
| 1 | B | 579 | HIS |
| 1 | A | 579 | HIS |
| 1 | B | 597 | GLU |

### 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 | 489/538 (91%) | 460 (94%) | 29 (6%) | 19 11 |
| 1 | B | 508/538 (94%) | 472 (93%) | 36 (7%) | 14 7 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| All | All | 997/1076 (93%) | 932 (94%) | 65 (6%) | 18 9 |

5 of 65 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 555[A] | LEU |
| 1 | A | 570 | LYS |
| 1 | B | 531 | GLU |
| 1 | B | 522 | ARG |
| 1 | A | 577 | SER |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 541 | HIS |
| 1 | B | 599 | GLN |
| 1 | A | 452 | HIS |
| 1 | A | 279 | ASN |
| 1 | A | 422 | ASN |

#### 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 monosaccharides 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 | $\#\|Z\| > 2$ |
| 2 | ADP | B | 800 | - | 24,29,29 | 1.77 | 6 (25%) | 29,45,45 | 1.42 | 3 (10%) |
| 2 | ADP | B | 900 | - | 24,29,29 | 1.95 | 7 (29%) | 29,45,45 | 3.07 | 11 (37%) |
| 2 | ADP | A | 900 | - | 24,29,29 | 1.51 | 5 (20%) | 29,45,45 | 1.92 | 9 (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 |
|---|---|---|---|---|---|---|---|
| 2 | ADP | B | 800 | - | - | 3/12/32/32 | 0/3/3/3 |
| 2 | ADP | B | 900 | - | - | 7/12/32/32 | 0/3/3/3 |
| 2 | ADP | A | 900 | - | - | 5/12/32/32 | 0/3/3/3 |

The worst 5 of 18 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 800 | ADP | C2-N3 | 5.38 | 1.40 | 1.32 |
| 2 | B | 900 | ADP | O5'-C5' | -4.42 | 1.27 | 1.44 |
| 2 | B | 900 | ADP | PB-O3B | -3.71 | 1.40 | 1.54 |
| 2 | A | 900 | ADP | O4'-C1' | 3.59 | 1.46 | 1.41 |
| 2 | B | 800 | ADP | C2'-C1' | -3.44 | 1.48 | 1.53 |

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

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 900 | ADP | O2A-PA-O5' | 8.11 | 145.42 | 107.75 |
| 2 | B | 900 | ADP | O4'-C4'-C5' | -6.92 | 86.60 | 109.37 |
| 2 | B | 900 | ADP | N3-C2-N1 | -5.49 | 120.10 | 128.68 |
| 2 | B | 900 | ADP | C5-C6-N6 | -5.38 | 112.18 | 120.35 |
| 2 | A | 900 | ADP | N3-C2-N1 | -4.93 | 120.97 | 128.68 |

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | B | 800 | ADP | PA-O3A-PB-O2B |
| 2 | B | 900 | ADP | PA-O3A-PB-O3B |
| 2 | B | 900 | ADP | C5'-O5'-PA-O2A |
| 2 | A | 900 | ADP | PA-O3A-PB-O3B |
| 2 | B | 900 | ADP | O4'-C4'-C5'-O5' |

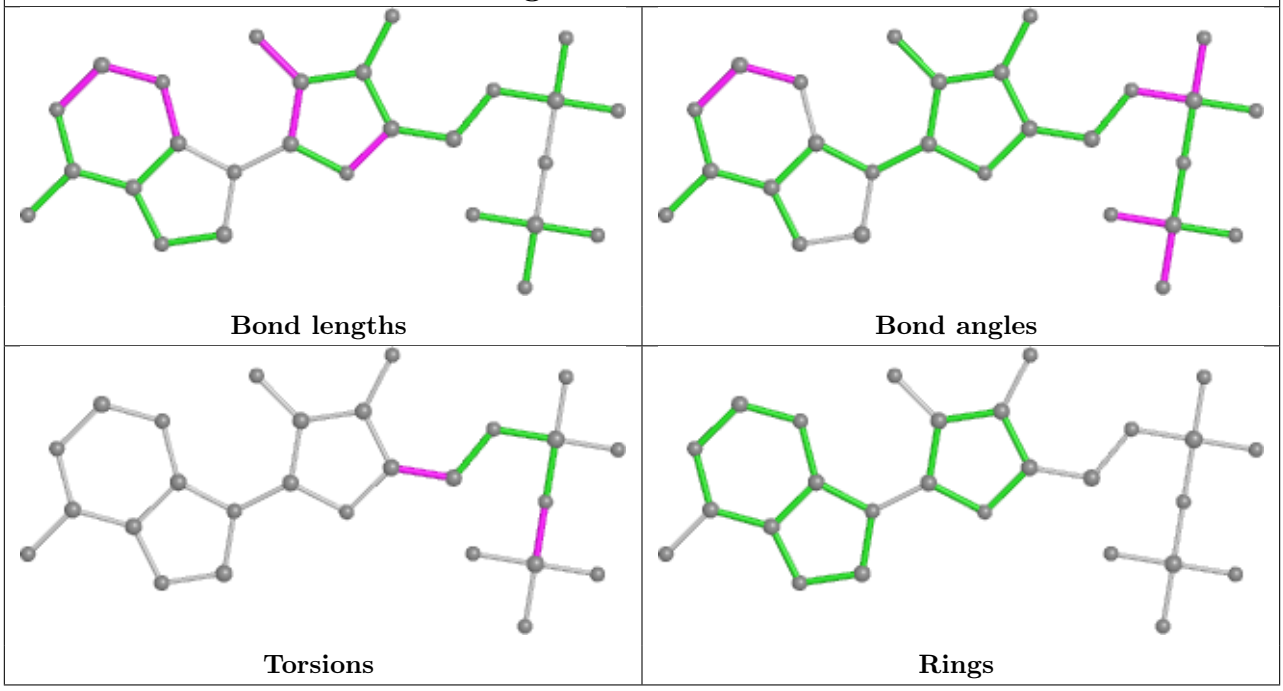
There are no ring outliers.

1 monomer is involved in 6 short contacts:

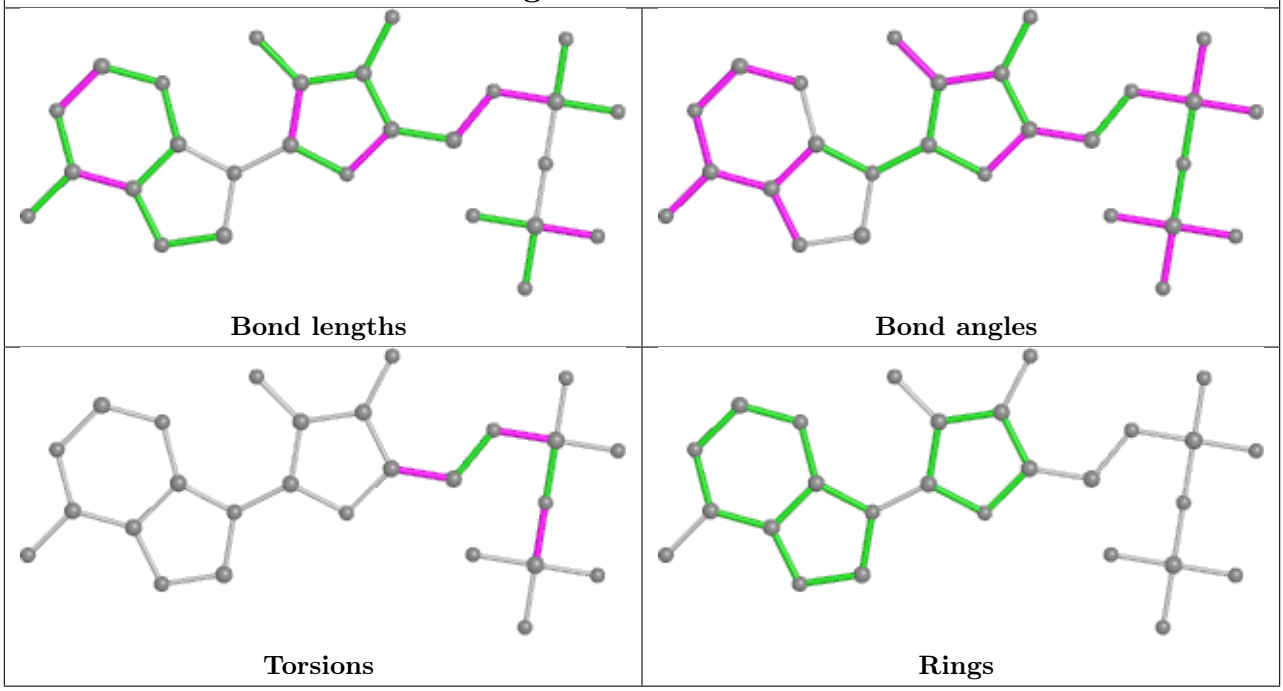
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 900 | ADP | 6 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

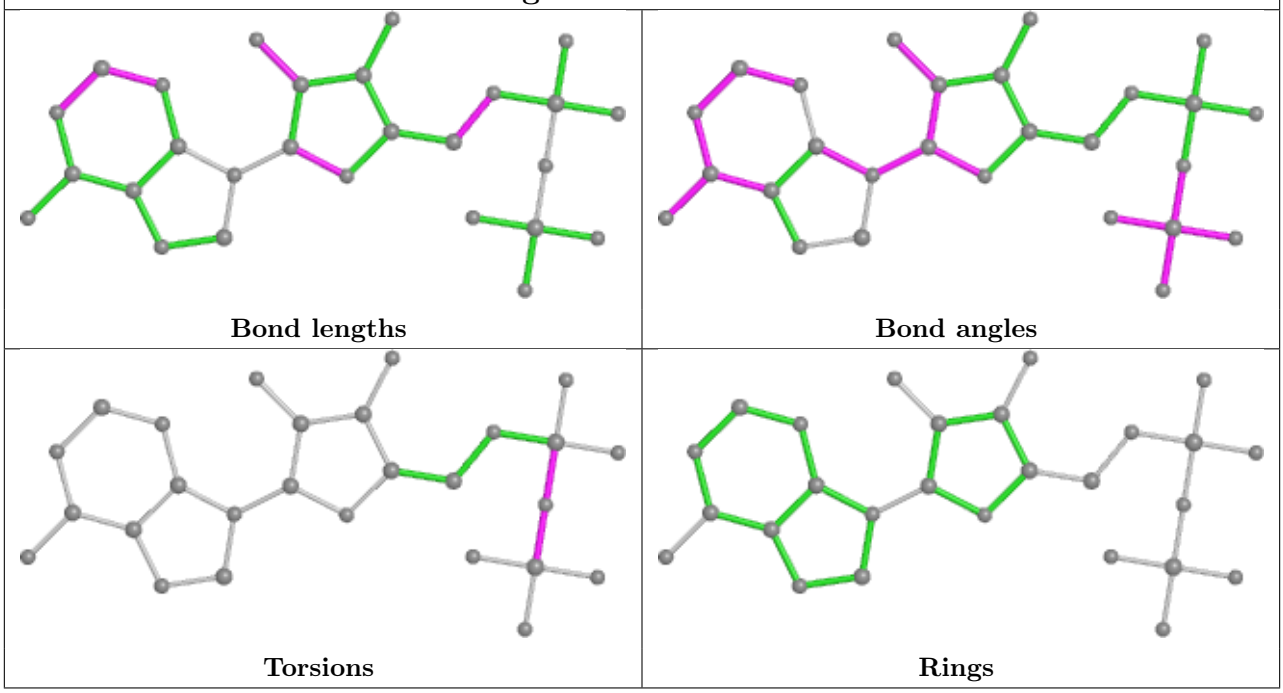
**Ligand ADP B 800**



**Ligand ADP B 900**




**Ligand ADP A 900**




## 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)

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(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 563/630 (89%) | 0.11 | 30 (5%) | 26 | 27 | 22, 37, 67, 90 | 3 (0%) |
| 1 | B | 590/630 (93%) | 0.20 | 34 (5%) | 23 | 24 | 23, 39, 72, 104 | 0 |
| All | All | 1153/1260 (91%) | 0.15 | 64 (5%) | 24 | 25 | 22, 38, 69, 104 | 3 (0%) |

The worst 5 of 64 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 181 | GLU | 6.8 |
| 1 | A | 624 | ALA | 6.0 |
| 1 | B | 184 | GLY | 5.2 |
| 1 | B | 180 | GLY | 4.6 |
| 1 | B | 179 | ALA | 4.4 |

## 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 monosaccharides in this entry.

## 6.4 Ligands (i)

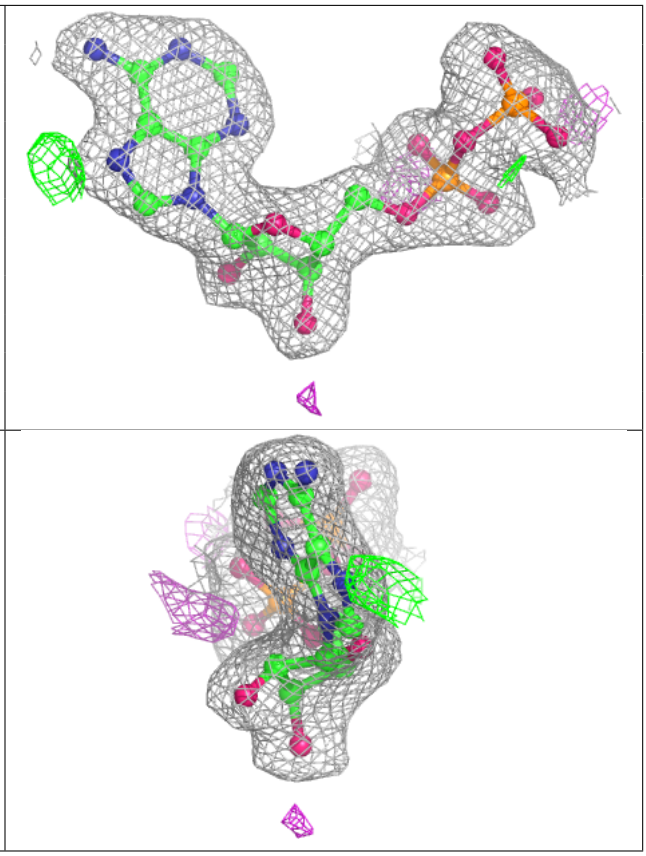
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | ADP | B | 800 | 27/27 | 0.98 | 0.07 | 37,41,43,49 | 0 |
| 2 | ADP | B | 900 | 27/27 | 0.98 | 0.07 | 33,38,46,48 | 0 |
| 2 | ADP | A | 900 | 27/27 | 0.99 | 0.07 | 30,33,39,41 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

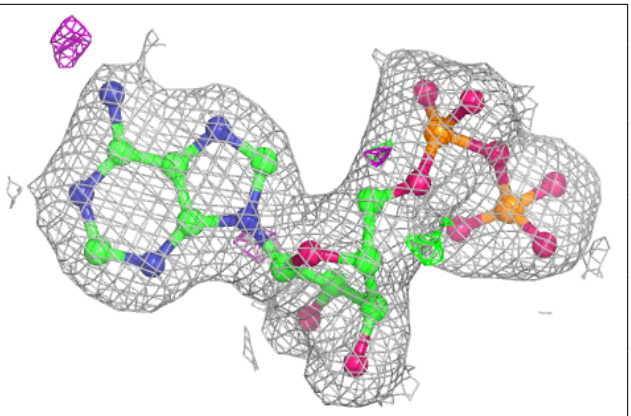
**Electron density around ADP B 800:**

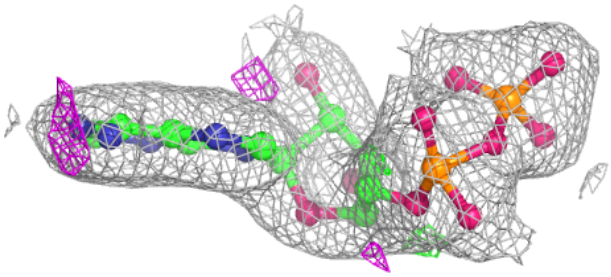
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

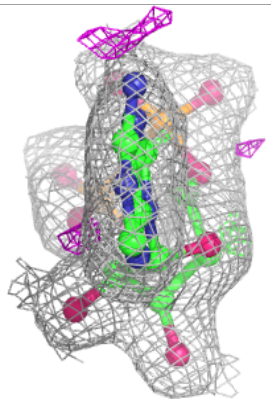


**Electron density around ADP B 900:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

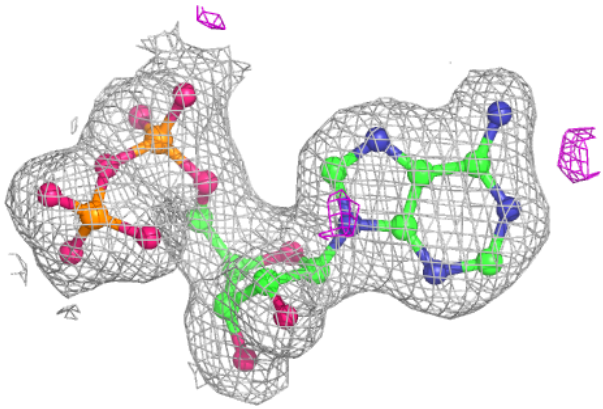


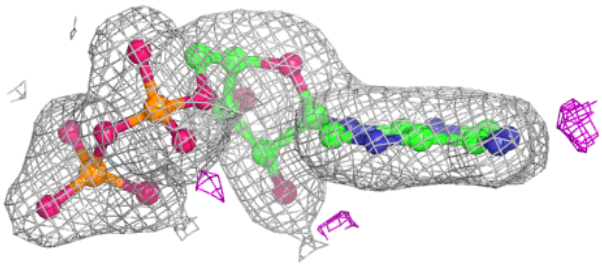


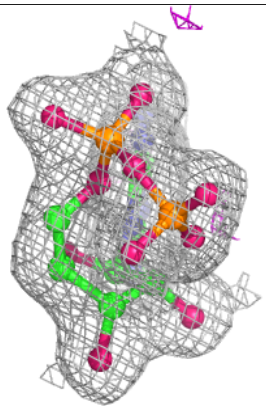


**Electron density around ADP A 900:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)







## 6.5 Other polymers (i)

There are no such residues in this entry.