



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 11:48 pm BST

PDB ID : 3PJR
Title : HELICASE SUBSTRATE COMPLEX
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Deposited on : 1999-03-12
Resolution : 3.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

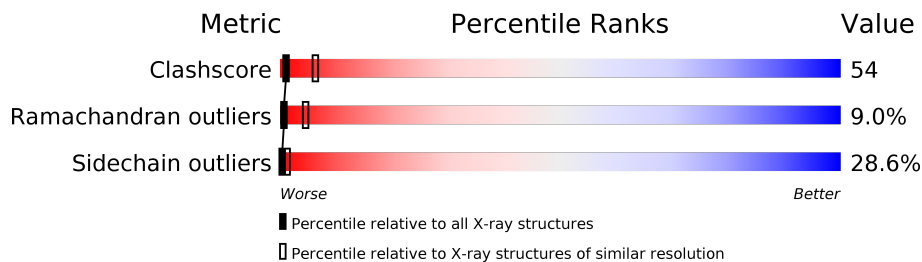
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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 | 141614 | 1205 (3.34-3.26) |
| Ramachandran outliers | 138981 | 1183 (3.34-3.26) |
| Sidechain outliers | 138945 | 1182 (3.34-3.26) |

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 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 $\leq 5\%$

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------|
| 1 | Y | 15 | 20% 80% |
| 2 | Z | 10 | 100% |
| 3 | A | 724 | 23% 40% 21% 6% 11% |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5765 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(*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*TP*TP*T)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 1 | Y | 15 | 303 | 147 | 48 | 94 | 14 | 0 | 0 | 0 |

- Molecule 2 is a DNA chain called 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*C)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| | | | Total | C | N | O | P | | | |
| 2 | Z | 10 | 201 | 96 | 39 | 57 | 9 | 0 | 0 | 0 |

- Molecule 3 is a protein called HELICASE PCRA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 3 | A | 646 | 5230 | 3304 | 916 | 991 | 19 | 0 | 0 | 0 |

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

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 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.

Note EDS was not executed.

- Molecule 1: 5'-D(*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*TP*TP*T)-3'

Chain Y: 

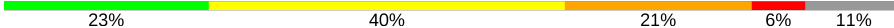
G1 C2 A3 G4 T5 G6 C7 T8 C9 G10 T11 T12 T13 T14 T15

- Molecule 2: 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*C)-3'

Chain Z: 

C25 G26 A27 G28 C29 A30 C31 T32 G33 C34

- Molecule 3: HELICASE PCRA

Chain A: 

NET ASM PHE L4 S5 E6 Q7 L8 L9 A10 H11 L12 N13 K14 E15 Q16 G22 Q17 E18 A19 T23 E24 G25 P26 L27 L28 L29 M30 A31 G32 A33 G34 S35 G36 R37 T38 R39 V40 L41 A46 Y47 L48 M49 A50 B51 F52 H53 V54 A55 P56 Q57 N58 L59 L60 A61 L62 T63 F64 T65

M66 R67 A68 A69 S70 E71 M72 R73 V76 F77 S78 L80 G81 G82 A83 Q17 A84 E85 S86 R87 M88 R89 S90 T91 F92 M95 L100 R101 G102 D103 K104 D105 R106 L107 G108 I109 M110 N111 M112 M113 S114 L115 H116 D117 V54 P118 T119 D120 Q121 L122 I123 L124 M125 K126 T127 I128

L129 K130 E131 K132 N133 L134 D135 P136 K137 F138 R139 D140 Q141 P142 A143 T144 L145 G146 T147 I148 S149 A150 D151 K152 N153 E154 L155 M156 P157 P158 E159 Q160 K163 R164 A165 S166 T167 Y168 E169 Q170 K171 M172 V173 S174 Y177 Q178 E179 Y180 Q181 Q182 R183 L184 L185 G261 A262 M187 H188 D191

F192 D193 L194 D195 M196 L197 L202 F203 D204 R205 V206 L210 Y213 Q214 L220 R221 I222 D223 R224 A225 Y226 R227 M228 N229 R230 R231 L232 R233 T234 L235 R236 R237 K238 R242 F243 Q244 M245 I246 V249 G250 D251 A252 D253 Q254 S255 I256 R260 G261 A262 D263 A264 Q265 R266

L267 L268 S269 F270 E271 R272 D273 P274 Y275 R276 A277 K278 L279 L280 L281 E283 R287 S288 T289 R290 R291 L292 L293 Q294 A295 N296 R297 E300 R301 R302 R303 V304 R305 R306 R309 R310 L311 R312 R313 E314 M315 F316 Y317 Y318 G318 R319 F320 L321 L322 L323 Y324 Y325 Y326 Y327 Y328 Y329 Y330 Y331 Y332 Y333 Y334 Y335 Y336 Y337 Y338 Y339 Y340 Y341 Y342 Y343 Y344 Y345 Y346 Y347 Y348 Y349 Y350 Y351 Y352 Y353 Y354 Y355 Y356 Y357 Y358 R359 R360 N361 A362 Q363 S364 S425 T426 L427 D428 K429 L430 V431 R432 Y433 A434 A435 D436 H437 E438 L439 S440 L441 F442 E443 A444 L445 G446 F447 M450 L451 G452

A330 D331 K332 A333 Q334 L335 V336 G337 G338 R339 L340 R341 Y344 E345 G347 G348 R349 R350 R351 R352 R353 F354 A355 G356 L357 Y358 R359 R420 G421 L422 G423 A424 S425 T426 L427 D428 K429 L430 V431 R432 Y433 A434 A435 D436 H437 E438 L439 S440 L441 F442 E443 A444 L445 G446 F447 M450 L451 G452

E391 L392 K393 D394 L395 L396 A397 L398 L399 R400 V401 I402 P405 D406 D407 D408 L409 L410 L411 L412 R413 R414 L415 I416 V417 F418 K419 R420 G421 L422 G423 A424 S425 T426 L427 D428 K429 L430 V431 R432 Y433 A434 A435 D436 H437 E438 L439 S440 L441 F442 E443 A444 L445 G446 F447 M450 L451 G452

| | | | | |
|-----|------|------|------|------|
| PRO | T648 | M587 | E523 | L483 |
| ILE | A649 | M588 | M524 | G484 |
| GLY | S650 | R589 | D627 | A485 |
| ILE | R651 | S590 | D628 | G459 |
| LYS | R652 | L591 | K529 | A460 |
| ARG | ALA | D593 | L461 | L461 |
| LEU | ALA | D594 | A462 | A462 |
| LEU | GLY | D595 | L531 | A463 |
| LEU | ALA | D596 | L532 | F464 |
| ALA | ALA | E596 | A533 | R465 |
| ALA | SER | M597 | F534 | S466 |
| PRO | ARG | E598 | L535 | Q467 |
| PRO | PRO | E599 | T636 | L468 |
| ILE | ALA | E600 | L469 | E469 |
| ILE | VAL | R601 | I540 | T472 |
| GLU | SER | R602 | S542 | Q473 |
| LYS | ARG | L603 | D543 | Q475 |
| LYS | ARG | A604 | L544 | E476 |
| VAL | GLN | Y605 | D545 | Y477 |
| VAL | ALA | V606 | E546 | V478 |
| VAL | SER | G607 | LEU | E482 |
| GLY | GLY | I608 | ASP | L483 |
| SER | GLY | T609 | ASP | V484 |
| TRP | SER | R610 | GLY | E486 |
| LYS | TRP | A611 | T550 | V487 |
| VAL | LYS | E612 | E551 | K490 |
| VAL | VAL | E613 | Q552 | Y493 |
| GLY | VAL | E614 | A553 | M496 |
| ASP | ASP | L615 | A554 | L497 |
| ARG | ARG | V616 | D557 | E500 |
| ALA | ALA | S619 | A558 | R501 |
| ASN | ASN | A620 | V559 | I503 |
| HIS | HIS | Q621 | M560 | E504 |
| ARG | ARG | M622 | L561 | A505 |
| LYS | LYS | R623 | M562 | R508 |
| TRP | TRP | T624 | T563 | L509 |
| GLY | GLY | I625 | L564 | E510 |
| ILE | ILE | F626 | H565 | M511 |
| PRO | GLY | G627 | A566 | L512 |
| ILE | THR | M628 | A567 | B513 |
| VAL | VAL | I629 | K568 | E514 |
| VAL | VAL | Q630 | G569 | F515 |
| SER | SER | M631 | L570 | L516 |
| VAL | VAL | D632 | E571 | S517 |
| ARG | ARG | P633 | F572 | T518 |
| GLY | GLY | F634 | P573 | E519 |
| GLY | GLY | S635 | V574 | F519 |
| GLY | GLY | R636 | V575 | L519 |
| ASP | ASP | F637 | F576 | L520 |
| ASP | ASP | L638 | L577 | T519 |
| GLN | GLN | M639 | L578 | V518 |
| GLU | GLU | E640 | G579 | T519 |
| LEU | LEU | I641 | M580 | F521 |
| ASP | ASP | P642 | E581 | H522 |
| ILE | ILE | A643 | E582 | |
| ALA | ALA | H644 | G583 | |
| PHE | PHE | L645 | I584 | |
| PRO | PRO | L646 | F585 | |
| SER | SER | E647 | P586 | |

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|--|-----------|
| Space group | P 61 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 105.12Å 105.12Å 380.80Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 10.00 – 3.30 | Depositor |
| % Data completeness (in resolution range) | 92.0 (10.00-3.30) | Depositor |
| R_{merge} | 0.06 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | REFMAC | Depositor |
| R, R_{free} | 0.236 , 0.315 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtrriage |
| Total number of atoms | 5765 | wwPDB-VP |
| Average B, all atoms (Å ²) | 55.0 | 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: ATP

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 | Y | 1.56 | 4/337 (1.2%) | 3.06 | 50/519 (9.6%) |
| 2 | Z | 2.27 | 6/225 (2.7%) | 3.84 | 39/345 (11.3%) |
| 3 | A | 0.68 | 7/5319 (0.1%) | 1.60 | 69/7184 (1.0%) |
| All | All | 0.87 | 17/5881 (0.3%) | 1.88 | 158/8048 (2.0%) |

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 |
|-----|-------|---------------------|---------------------|
| 2 | Z | 1 | 0 |
| 3 | A | 0 | 63 |
| All | All | 1 | 63 |

The worst 5 of 17 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 2 | Z | 28 | DG | N9-C8 | 12.27 | 1.46 | 1.37 |
| 2 | Z | 28 | DG | C2'-C1' | 11.86 | 1.64 | 1.52 |
| 2 | Z | 28 | DG | C8-N7 | -11.06 | 1.24 | 1.30 |
| 1 | Y | 11 | DT | C3'-O3' | -7.58 | 1.34 | 1.44 |
| 2 | Z | 27 | DA | C2'-C1' | 7.16 | 1.59 | 1.52 |

The worst 5 of 158 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 3 | A | 652 | ARG | CD-NE-CZ | 38.94 | 178.12 | 123.60 |
| 3 | A | 310 | ARG | CD-NE-CZ | 36.72 | 175.00 | 123.60 |
| 2 | Z | 28 | DG | C4-N9-C1' | 21.13 | 153.97 | 126.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 2 | Z | 28 | DG | C8-N9-C1' | -20.87 | 99.87 | 127.00 |
| 2 | Z | 28 | DG | N3-C4-C5 | -20.27 | 118.47 | 128.60 |

All (1) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 2 | Z | 33 | DG | C3' |

5 of 63 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 3 | A | 16 | GLN | Mainchain |
| 3 | A | 24 | GLU | Mainchain |
| 3 | A | 27 | LEU | Mainchain |
| 3 | A | 31 | ALA | Mainchain |
| 3 | A | 9 | LEU | Mainchain |

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 | Y | 303 | 0 | 174 | 56 | 0 |
| 2 | Z | 201 | 0 | 113 | 36 | 0 |
| 3 | A | 5230 | 0 | 5230 | 530 | 0 |
| 4 | A | 31 | 0 | 12 | 7 | 0 |
| All | All | 5765 | 0 | 5529 | 607 | 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 54.

The worst 5 of 607 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:Y:12:DT:H5'' | 1:Y:12:DT:C6 | 1.65 | 1.31 |
| 1:Y:12:DT:C5' | 1:Y:12:DT:H6 | 1.47 | 1.27 |
| 1:Y:5:DT:H2' | 1:Y:6:DG:C8 | 1.77 | 1.19 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------|--------------------------|-------------------|
| 3:A:31:ALA:HB3 | 3:A:251:ASP:HB2 | 1.36 | 1.08 |
| 1:Y:12:DT:C6 | 1:Y:12:DT:C5' | 2.31 | 1.00 |

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 |
|-----|-------|---------------|-----------|-----------|----------|-------------------|
| 3 | A | 642/724 (89%) | 471 (73%) | 113 (18%) | 58 (9%) | 1 4 |

5 of 58 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 33 | ALA |
| 3 | A | 35 | SER |
| 3 | A | 83 | ALA |
| 3 | A | 84 | ALA |
| 3 | A | 113 | PHE |

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 |
|-----|-------|---------------|-----------|-----------|-------------------|
| 3 | A | 560/618 (91%) | 400 (71%) | 160 (29%) | 0 1 |

5 of 160 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 329 | GLU |
| 3 | A | 375 | ASN |
| 3 | A | 599 | GLU |
| 3 | A | 339 | ARG |
| 3 | A | 352 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | A | 187 | ASN |
| 3 | A | 245 | ASN |
| 3 | A | 511 | ASN |
| 3 | A | 214 | GLN |
| 3 | A | 232 | 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](#)

1 ligand 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 |
| 4 | ATP | A | 725 | - | 26,33,33 | 1.54 | 6 (23%) | 31,52,52 | 1.60 | 6 (19%) |

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 | 725 | - | - | 11/18/38/38 | 0/3/3/3 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | A | 725 | ATP | C8-N7 | -3.51 | 1.28 | 1.34 |
| 4 | A | 725 | ATP | C2-N1 | 2.31 | 1.38 | 1.33 |
| 4 | A | 725 | ATP | PG-O2G | -2.28 | 1.46 | 1.54 |
| 4 | A | 725 | ATP | O4'-C1' | -2.27 | 1.37 | 1.41 |
| 4 | A | 725 | ATP | C5-N7 | -2.21 | 1.31 | 1.39 |

The worst 5 of 6 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | A | 725 | ATP | PB-O3B-PG | -4.26 | 118.21 | 132.83 |
| 4 | A | 725 | ATP | C4-C5-N7 | 3.76 | 113.31 | 109.40 |
| 4 | A | 725 | ATP | PA-O3A-PB | -3.12 | 122.12 | 132.83 |
| 4 | A | 725 | ATP | C5-C6-N1 | -2.40 | 114.92 | 120.35 |
| 4 | A | 725 | ATP | O2'-C2'-C3' | -2.25 | 104.54 | 111.82 |

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

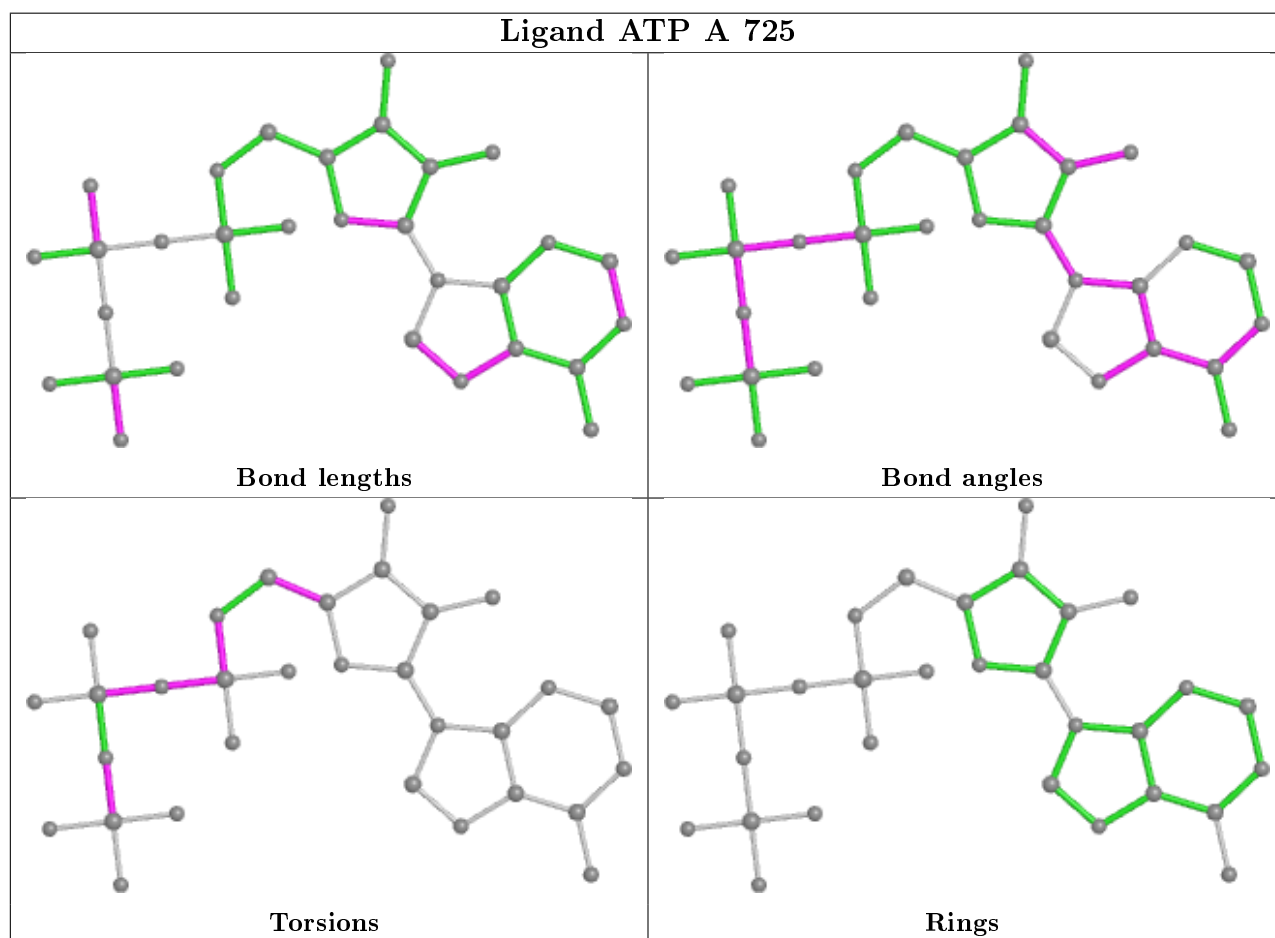
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 4 | A | 725 | ATP | PB-O3B-PG-O3G |
| 4 | A | 725 | ATP | C5'-O5'-PA-O1A |
| 4 | A | 725 | ATP | C5'-O5'-PA-O2A |
| 4 | A | 725 | ATP | C5'-O5'-PA-O3A |
| 4 | A | 725 | ATP | O4'-C4'-C5'-O5' |

There are no ring outliers.

1 monomer is involved in 7 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | A | 725 | ATP | 7 | 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 than 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.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.