



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:55 PM UTC

PDB ID : 4IVG / pdb\_00004ivg  
Title : Crystal structure of mitochondrial Hsp90 (TRAP1) NTD-Middle domain dimer with AMPPNP  
Authors : Partridge, J.R.; Lavery, L.A.; Agard, D.A.  
Deposited on : 2013-01-22  
Resolution : 1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

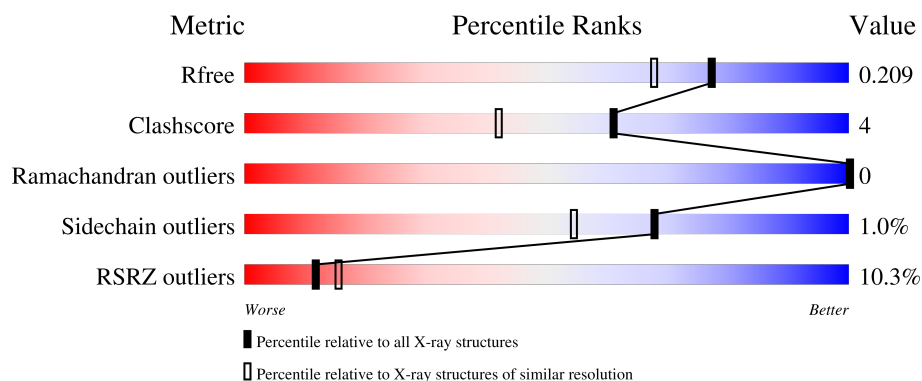
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1187 (1.74-1.74)                                      |
| Clashscore            | 190562                      | 1207 (1.74-1.74)                                      |
| Ramachandran outliers | 187476                      | 1200 (1.74-1.74)                                      |
| Sidechain outliers    | 187428                      | 1200 (1.74-1.74)                                      |
| RSRZ outliers         | 180081                      | 1188 (1.74-1.74)                                      |

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  $\geq 3$ , 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  $\leq 5\%$ . 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     | 647    | <div> <div>8%</div> <div>65%</div> <div>8%</div> <div>26%</div> </div> |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4257 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.

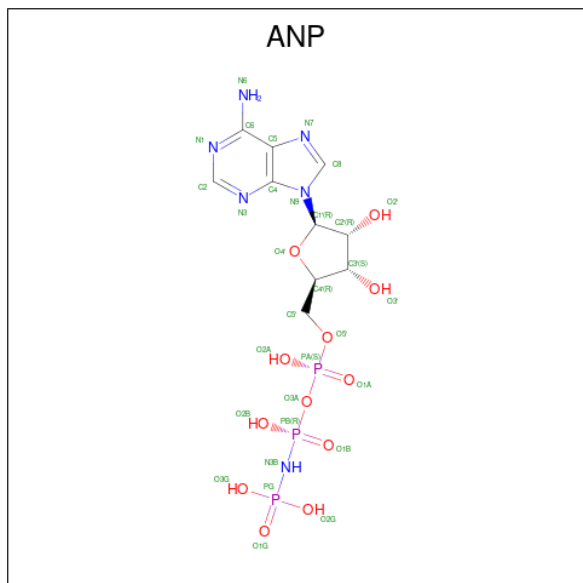
- Molecule 1 is a protein called TNF receptor-associated protein 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
|     |       |          | Total | C    | N   | O   | S  |         |         |       |
| 1   | A     | 477      | 3876  | 2459 | 662 | 737 | 18 | 0       | 4       | 0     |

There is a discrepancy between the modelled and reference sequences:

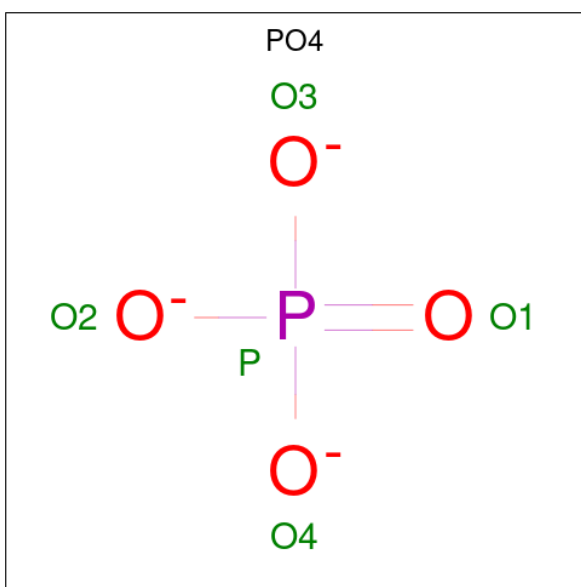
| Chain | Residue | Modelled | Actual | Comment             | Reference |
|-------|---------|----------|--------|---------------------|-----------|
| A     | 566     | ALA      | GLU    | engineered mutation | UNP A8WV1 |

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



| Mol | Chain | Residues | Atoms |    |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
|     |       |          | Total | C  | N | O  | P |         |         |
| 2   | A     | 1        | 31    | 10 | 6 | 12 | 3 | 0       | 0       |

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | P | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5   | A     | 344      | Total | O   | 0       | 0       |
|     |       |          | 344   | 344 |         |         |

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.

- Chain A:

8% 65% 8% 26%

SER THR GLN GLN HIS THR GLU PRO ALA GLU GLU THR T85 L86 H87 H88 T91 F100 V116 A117 H144 R145 H146 I147 T148 ALA GLY GLY ASP T153 K180 R192 S193 G194 G197 F198 L202 Q203 H204 S222 M225 V230 E231 V232 A237 E238 A239 T240  
 R454 Y244 K245 Y246 G250 Q264 L270 V296 S297 Y337 R341 L352 K367 F368 D369 S371 R372 GLU MET GLY S376 K384 Q388 K390 K391 T392 D393 T394 W398 L399 R400 T412 L413 H414 L419 L420 L425 V398 A399 T399 D399 T400 V401 A402 S403 T404 L405 L406 L407 L408 L409 L410 L411 L412 L413 L414 L415 L416 L417 L418 L419 L420 L421 L422 L423 L424 L425 L426 L427 L428 L429 L430 L431 L432 L433 L434 L435 L436 L437 L438 L439 L440 L441 L442 L443 L444 L445 L446 L447 L448 L449 L450 L451 L452 L453 L454 L455 L456 L457 L458 L459 L460 L461 L462 L463 L464 L465 L466 L467 L468 L469 L470 L471 L472 L473 L474 L475 L476 L477 L478 L479 L480 L481 L482 L483 L484 L485 L486 L487 L488 L489 L490 L491 L492 L493 L494 L495 L496 L497 L498 L499 L500 L501 L502 L503 L504 L505 L506 L507 L508 L509 L510 L511 L512 L513 L514 L515 L516 L517 L518 L519 L520 L521 L522 L523 L524 L525 L526 L527 L528 L529 L530 L531 L532 L533 L534 L535 L536 L537 L538 L539 L540 L541 L542 L543 L544 L545 L546 L547 L548 L549 L550 L551 L552 L553 L554 L555 L556 L557 L558 L559 L560 L561 L562 L563 L564 L565 L566 L567 L568 L569 L570 L571 L572 L573 L574 L575 L576 L577 L578 L579 L580 L581 L582 L583 L584 L585 L586 L587 L588 L589 L590 L591 L592 L593 L594 L595 L596 L597 L598 L599 L600 L601 L602 L603 L604 L605 L606 L607 L608 L609 L610 L611 L612 L613 L614 L615 L616 L617 L618 L619 L620 L621 L622 L623 L624 L625 L626 L627 L628 L629 L630 L631 L632 L633 L634 L635 L636 L637 L638 L639 L640 L641 L642 L643 L644 L645 L646 L647 L648 L649 L650 L651 L652 L653 L654 L655 L656 L657 L658 L659 L660 L661 L662 L663 L664 L665 L666 L667 L668 L669 L670 L671 L672 L673 L674 L675 L676 L677 L678 L679 L680 L681 L682 L683 L684 L685 L686 L687 L688 L689 L690 L691 L692 L693 L694 L695 L696 L697 L698 L699 L700 L701 L702 L703 L704 L705 L706 L707 L708 L709 L710 L711 L712 L713 L714 L715 L716 L717 L718 L719 L720 L721 L722 L723 L724 L725 L726 L727 L728 L729 L730 L731 L732 L733 L734 L735 L736 L737 L738 L739 L740 L741 L742 L743 L744 L745 L746 L747 L748 L749 L750 L751 L752 L753 L754 L755 L756 L757 L758 L759 L760 L761 L762 L763 L764 L765 L766 L767 L768 L769 L770 L771 L772 L773 L774 L775 L776 L777 L778 L779 L780 L781 L782 L783 L784 L785 L786 L787 L788 L789 L790 L791 L792 L793 L794 L795 L796 L797 L798 L799 L800 L801 L802 L803 L804 L805 L806 L807 L808 L809 L810 L811 L812 L813 L814 L815 L816 L817 L818 L819 L820 L821 L822 L823 L824 L825 L826 L827 L828 L829 L830 L831 L832 L833 L834 L835 L836 L837 L838 L839 L840 L841 L842 L843 L844 L845 L846 L847 L848 L849 L850 L851 L852 L853 L854 L855 L856 L857 L858 L859 L860 L861 L862 L863 L864 L865 L866 L867 L868 L869 L870 L871 L872 L873 L874 L875 L876 L877 L878 L879 L880 L881 L882 L883 L884 L885 L886 L887 L888 L889 L890 L891 L892 L893 L894 L895 L896 L897 L898 L899 L900 L901 L902 L903 L904 L905 L906 L907 L908 L909 L910 L911 L912 L913 L914 L915 L916 L917 L918 L919 L920 L921 L922 L923 L924 L925 L926 L927 L928 L929 L930 L931 L932 L933 L934 L935 L936 L937 L938 L939 L940 L941 L942 L943 L944 L945 L946 L947 L948 L949 L950 L951 L952 L953 L954 L955 L956 L957 L958 L959 L960 L961 L962 L963 L964 L965 L966 L967 L968 L969 L970 L971 L972 L973 L974 L975 L976 L977 L978 L979 L980 L981 L982 L983 L984 L985 L986 L987 L988 L989 L990 L991 L992 L993 L994 L995 L996 L997 L998 L999

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | I 2 2 2                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 85.15Å 94.51Å 155.46Å<br>90.00° 90.00° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 29.55 – 1.75<br>29.55 – 1.75                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.2 (29.55-1.75)<br>90.6 (29.55-1.75)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.60 (at 1.75Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: dev_1214)                            | Depositor        |
| R, $R_{free}$                                                           | 0.189 , 0.203<br>0.194 , 0.209                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2000 reflections (3.17%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 27.6                                                        | Xtriage          |
| Anisotropy                                                              | 0.486                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 44.7                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.97                                                        | EDS              |
| Total number of atoms                                                   | 4257                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, PO4, MG

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     | 0.46         | 0/3950      | 0.76        | 0/5318      |

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

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     | 3876  | 0        | 3841     | 33      | 0            |
| 2   | A     | 31    | 0        | 13       | 0       | 0            |
| 3   | A     | 5     | 0        | 0        | 0       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 344   | 0        | 0        | 6       | 0            |
| All | All   | 4257  | 0        | 3854     | 33      | 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 4.

All (33) 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:A:372:ARG:HG3  | 1:A:400:ARG:HD2    | 1.75                     | 0.68              |
| 1:A:412:PRO:HG2  | 5:A:1231:HOH:O     | 1.95                     | 0.66              |
| 1:A:198:PHE:CZ   | 1:A:202:LEU:HD11   | 2.36                     | 0.59              |
| 1:A:391:ALA:HB1  | 1:A:394:ILE:H      | 1.68                     | 0.58              |
| 1:A:414:ASN:ND2  | 5:A:1204:HOH:O     | 2.37                     | 0.56              |
| 1:A:491:PRO:HG2  | 1:A:494:GLN:HE21   | 1.70                     | 0.56              |
| 1:A:147:ILE:N    | 1:A:148:THR:HA     | 2.21                     | 0.56              |
| 1:A:297:SER:HB3  | 1:A:384:LYS:NZ     | 2.22                     | 0.55              |
| 1:A:414:ASN:HB3  | 1:A:420:LEU:HD13   | 1.89                     | 0.54              |
| 1:A:117:ALA:O    | 1:A:225:MET:HG2    | 2.09                     | 0.51              |
| 1:A:116:VAL:HG12 | 5:A:1196:HOH:O     | 2.12                     | 0.49              |
| 1:A:180:LYS:HB2  | 1:A:244:TYR:CZ     | 2.48                     | 0.49              |
| 1:A:297:SER:HB3  | 1:A:384:LYS:HZ2    | 1.79                     | 0.48              |
| 1:A:237:ALA:HB2  | 1:A:264:GLN:NE2    | 2.28                     | 0.48              |
| 1:A:222:SER:HA   | 5:A:1196:HOH:O     | 2.13                     | 0.47              |
| 1:A:398:TRP:HZ3  | 1:A:463[B]:MET:HE2 | 1.79                     | 0.47              |
| 1:A:519:ASN:HD21 | 1:A:522:LEU:HD13   | 1.80                     | 0.46              |
| 1:A:391:ALA:C    | 1:A:393:ASP:HA     | 2.42                     | 0.45              |
| 1:A:352:LEU:HD11 | 1:A:429:LEU:HD13   | 1.98                     | 0.45              |
| 1:A:192:ARG:NH2  | 5:A:1068:HOH:O     | 2.50                     | 0.45              |
| 1:A:392:THR:N    | 1:A:393:ASP:HA     | 2.32                     | 0.45              |
| 1:A:555:ARG:NH2  | 1:A:556:GLU:OE2    | 2.50                     | 0.45              |
| 1:A:230:VAL:HG22 | 1:A:270:LEU:HD22   | 2.01                     | 0.43              |
| 1:A:341:ARG:HG2  | 1:A:451:LYS:HE2    | 2.01                     | 0.42              |
| 1:A:419:LEU:HD22 | 5:A:1231:HOH:O     | 2.19                     | 0.42              |
| 1:A:502:SER:HA   | 1:A:505:MET:SD     | 2.60                     | 0.42              |
| 1:A:450:GLU:HG2  | 1:A:454:ARG:NH1    | 2.35                     | 0.42              |
| 1:A:367:MET:O    | 1:A:371:SER:HB2    | 2.20                     | 0.41              |
| 1:A:554:LEU:HD23 | 1:A:562:LEU:HD11   | 2.03                     | 0.41              |
| 1:A:239:ALA:O    | 1:A:240:ASP:OD1    | 2.39                     | 0.41              |
| 1:A:492:ALA:HB2  | 1:A:520:ARG:HD3    | 2.03                     | 0.40              |
| 1:A:232:VAL:HB   | 1:A:246:TRP:HB3    | 2.03                     | 0.40              |
| 1:A:546:PHE:N    | 1:A:546:PHE:CD1    | 2.90                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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     | 475/647 (73%) | 460 (97%) | 15 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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     | 425/568 (75%) | 420 (99%) | 5 (1%)   | 63          | 47 |

All (5) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 296    | VAL  |
| 1   | A     | 390    | LYS  |
| 1   | A     | 463[A] | MET  |
| 1   | A     | 463[B] | MET  |
| 1   | A     | 494    | GLN  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 205 | GLN  |
| 1   | A     | 271 | HIS  |
| 1   | A     | 494 | GLN  |
| 1   | A     | 521 | HIS  |

### 5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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 | $\# Z  > 2$ |
| 3   | PO4  | A     | 802 | -    | 4,4,4        | 0.78 | 0           | 6,6,6       | 0.59 | 0           |
| 2   | ANP  | A     | 801 | 4    | 33,33,33     | 1.27 | 5 (15%)     | 45,52,52    | 1.14 | 2 (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   | ANP  | A     | 801 | 4    | -       | 2/18/38/38 | 0/3/3/3 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | A     | 801 | ANP  | PA-O3A | 3.49 | 1.63        | 1.59     |
| 2   | A     | 801 | ANP  | PB-O1B | 3.26 | 1.51        | 1.46     |
| 2   | A     | 801 | ANP  | PG-N3B | 3.25 | 1.71        | 1.63     |
| 2   | A     | 801 | ANP  | PG-O1G | 2.62 | 1.50        | 1.46     |
| 2   | A     | 801 | ANP  | PB-N3B | 2.34 | 1.69        | 1.63     |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2   | A     | 801 | ANP  | O1B-PB-N3B | -4.77 | 104.74      | 111.77   |
| 2   | A     | 801 | ANP  | O2B-PB-O3A | 3.93  | 117.77      | 104.64   |

There are no chirality outliers.

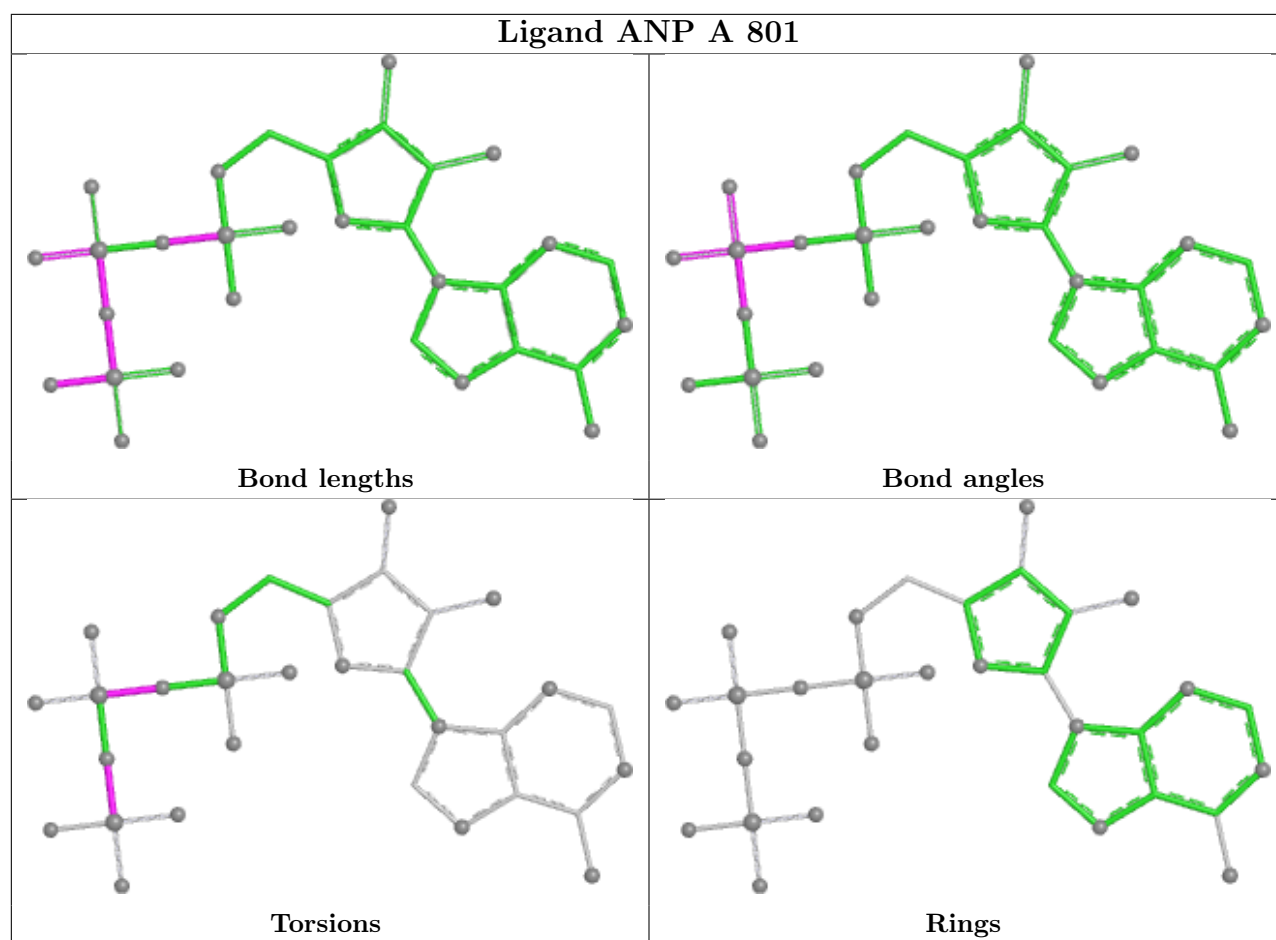
All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 2   | A     | 801 | ANP  | PB-N3B-PG-O1G |
| 2   | A     | 801 | ANP  | PA-O3A-PB-O2B |

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9  |
|-----|-------|---------------|--------|------------------------------|-----------------------|--------|
| 1   | A     | 477/647 (73%) | 0.61   | 49 (10%) <b>12</b> <b>15</b> | 15, 44, 84, 100       | 9 (1%) |

All (49) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 369 | ASP  | 5.7  |
| 1   | A     | 391 | ALA  | 5.6  |
| 1   | A     | 392 | THR  | 5.3  |
| 1   | A     | 88  | ASN  | 5.0  |
| 1   | A     | 389 | THR  | 4.9  |
| 1   | A     | 368 | PHE  | 4.7  |
| 1   | A     | 147 | ILE  | 4.5  |
| 1   | A     | 388 | GLN  | 4.4  |
| 1   | A     | 372 | ARG  | 4.2  |
| 1   | A     | 337 | TYR  | 4.1  |
| 1   | A     | 393 | ASP  | 3.7  |
| 1   | A     | 148 | THR  | 3.7  |
| 1   | A     | 239 | ALA  | 3.6  |
| 1   | A     | 499 | MET  | 3.6  |
| 1   | A     | 237 | ALA  | 3.5  |
| 1   | A     | 202 | LEU  | 3.4  |
| 1   | A     | 516 | CYS  | 3.3  |
| 1   | A     | 546 | PHE  | 3.2  |
| 1   | A     | 370 | VAL  | 3.2  |
| 1   | A     | 390 | LYS  | 3.1  |
| 1   | A     | 371 | SER  | 3.0  |
| 1   | A     | 545 | GLN  | 3.0  |
| 1   | A     | 367 | MET  | 2.9  |
| 1   | A     | 568 | ASP  | 2.9  |
| 1   | A     | 567 | THR  | 2.9  |
| 1   | A     | 508 | GLY  | 2.9  |
| 1   | A     | 86  | LEU  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 297 | SER  | 2.7  |
| 1   | A     | 559 | ARG  | 2.6  |
| 1   | A     | 153 | THR  | 2.6  |
| 1   | A     | 250 | GLY  | 2.6  |
| 1   | A     | 204 | ASN  | 2.6  |
| 1   | A     | 240 | ASP  | 2.6  |
| 1   | A     | 85  | THR  | 2.6  |
| 1   | A     | 194 | GLY  | 2.5  |
| 1   | A     | 241 | ALA  | 2.5  |
| 1   | A     | 376 | SER  | 2.4  |
| 1   | A     | 145 | ARG  | 2.4  |
| 1   | A     | 197 | ALA  | 2.4  |
| 1   | A     | 91  | THR  | 2.3  |
| 1   | A     | 100 | PHE  | 2.3  |
| 1   | A     | 566 | ALA  | 2.3  |
| 1   | A     | 144 | HIS  | 2.2  |
| 1   | A     | 524 | GLU  | 2.2  |
| 1   | A     | 146 | MET  | 2.1  |
| 1   | A     | 420 | LEU  | 2.1  |
| 1   | A     | 502 | SER  | 2.1  |
| 1   | A     | 394 | ILE  | 2.1  |
| 1   | A     | 425 | LEU  | 2.1  |

## 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 oligosaccharides 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<sup>th</sup> 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.

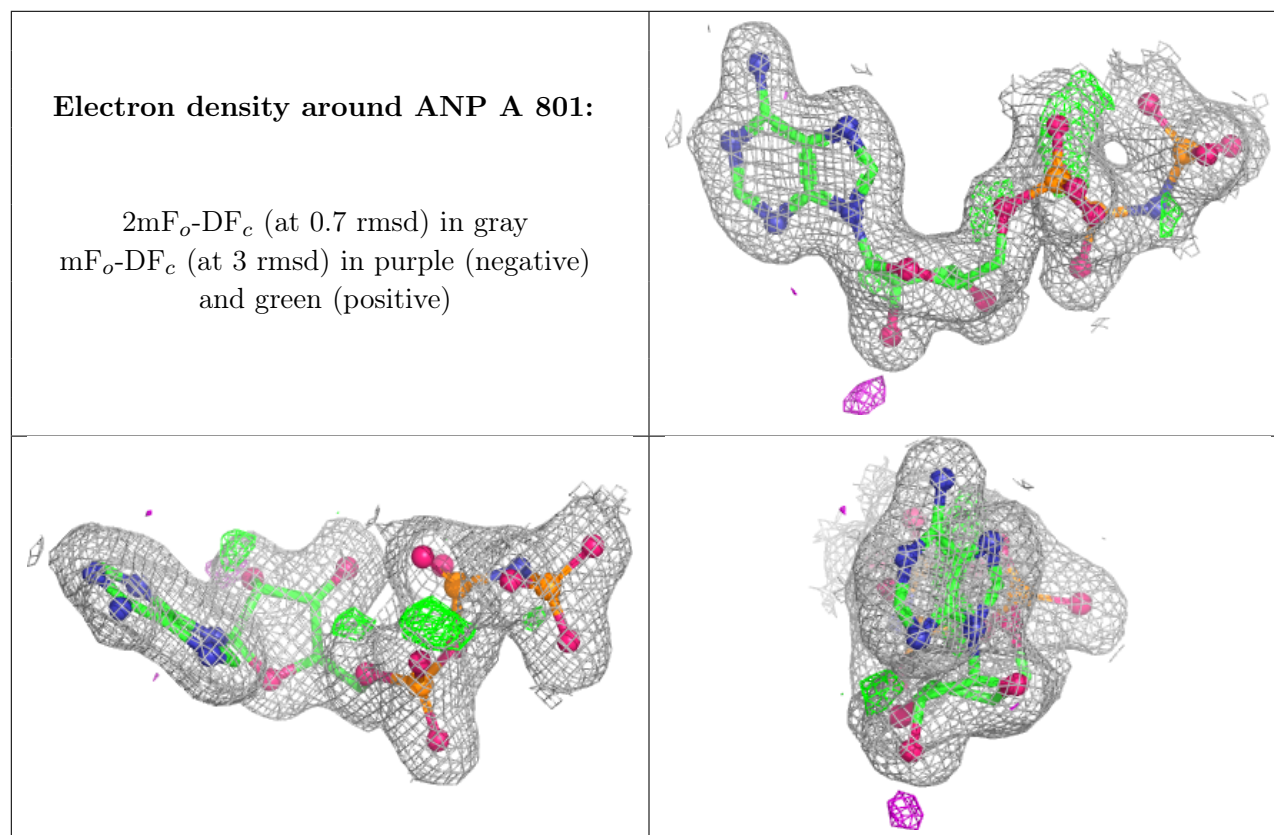
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | PO4  | A     | 802 | 5/5   | 0.87 | 0.10 | 47,55,64,66                | 5     |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | ANP  | A     | 801 | 31/31 | 0.98 | 0.05 | 22,27,32,35                 | 0     |
| 4   | MG   | A     | 803 | 1/1   | 0.98 | 0.05 | 26,26,26,26                 | 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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.