



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:40 PM UTC

PDB ID : 7K7T / pdb\_00007k7t  
Title : Crystal structure of human MORC4 ATPase-CW in complex with AMPPNP  
Authors : Klein, B.J.; Tencer, A.H.; Kutateladze, T.G.  
Deposited on : 2020-09-24  
Resolution : 2.94 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](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

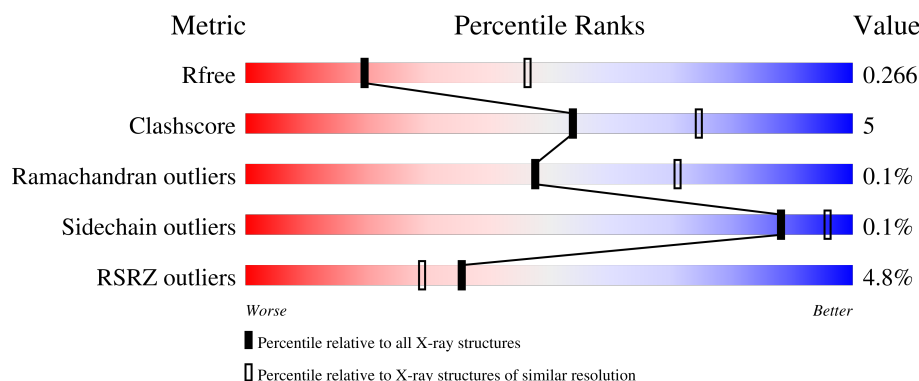
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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                      | 1159 (2.96-2.92)                                      |
| Clashscore            | 190562                      | 1184 (2.96-2.92)                                      |
| Ramachandran outliers | 187476                      | 1131 (2.96-2.92)                                      |
| Sidechain outliers    | 187428                      | 1131 (2.96-2.92)                                      |
| RSRZ outliers         | 180081                      | 1159 (2.96-2.92)                                      |

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     | 458    | <br>5% 74% 11% 15% |
| 1   | B     | 458    | <br>3% 73% 12% 16% |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6338 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 Isoform 3 of MORC family CW-type zinc finger protein 4.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 390      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3135  | 2004 | 536 | 572 | 23 |         |         |       |
| 1   | B     | 386      | Total | C    | N   | O   | S  | 0       | 1       | 0     |
|     |       |          | 3107  | 1990 | 525 | 570 | 22 |         |         |       |

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2   | A     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 2   | B     | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | B     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



| Mol | Chain | Residues | Atoms       |         |        |         |        | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|---------|
| 4   | A     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |
| 4   | B     | 1        | Total<br>31 | C<br>10 | N<br>6 | O<br>12 | P<br>3 | 0       | 0       |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5   | A     | 15       | Total O<br>15 15 | 0       | 0       |
| 5   | B     | 15       | Total O<br>15 15 | 0       | 0       |

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:
- 
- 5% 74% 11% 15%
- 329  
I179  
I332  
N456  
S457  
H458  
PRO  
LYS  
Y461  
E471  
LEU  
THR  
THR  
ASP  
GLU  
ASP  
LEU  
CYS  
SER  
SER  
LYS  
ALA  
LYS  
LYS  
LYS  
GLN  
GLU
- Y39  
N43  
L58  
A61  
P64  
D65  
V66  
R69  
I73  
D74  
V75  
C91  
G92  
M93  
T94  
P95  
H96  
K97  
S103  
F104  
T107  
D108  
K109  
VAL  
ILE  
LYS  
LYS  
SER  
SER  
GLN  
C116  
P117  
M123  
K126  
K141  
L146  
T147  
V169  
P170  
F171  
ASN  
GLN  
GLN  
W172
- I179  
ILE  
THR  
GLU  
D183  
M201  
D202  
L203  
L204  
A205  
G212  
D234  
F235  
D236  
Q239  
Y240  
D241  
L242  
L243  
V244  
S245  
D246  
PHE  
ASP  
THR  
GLU  
GLU  
LYS  
MET  
THR  
THR  
GLY  
GLY  
VAL  
VAL  
THR  
THR  
ILE  
ILE  
E260  
R269  
R280  
K288  
K308  
P309  
T310  
F311  
T312  
Q315  
N326  
SER  
SER  
ASN  
D330  
V330
- I332  
R339  
L340  
I341  
V351  
LYS  
PRO  
THR  
ARG  
GLY  
G358  
Y374  
E384  
A391  
L392  
K395  
T404  
SER  
GLN  
ASP  
ASN  
PHE  
GLU  
THR  
SER  
THR  
VAL  
ALA  
ARG  
PRO  
ILE  
PRO  
K420  
V421  
P422  
C429  
D430  
E431  
C432  
L433  
I442  
ASP  
PRO  
SER  
M446  
L447  
V454  
Y455

- Chain B:
- 
- 73% 12% 16%
- 3%
- Y455  
R462  
C464  
S465  
E469  
GLN  
GLU  
LEU  
THR  
ASP  
GLU  
ASP  
LEU  
CYS  
LEU  
SER  
LYS  
ALA  
LYS  
GLN  
GLU
- SER  
ASN  
GLN  
F330  
M334  
R339  
K342  
E345  
V351  
LYS  
PRO  
THR  
ARG  
GLY  
GLU  
G358  
I365  
E364  
A391  
L392  
K395  
W400  
T404  
SER  
GLN  
ASP  
ASN  
PHE  
GLU  
THR  
SER  
THR  
VAL  
ALA  
ARG  
PRO  
ILE  
PRO  
K420  
V421  
Q428  
L433  
G440  
LYS  
I442
- I210  
P211  
R225  
LYS  
ASN  
GLY  
LYS  
S231  
D234  
D241  
I242  
L243  
V244  
S245  
D246  
PHE  
ASP  
THR  
GLU  
GLU  
LYS  
MET  
THR  
GLY  
GLY  
VAL  
THR  
SER  
E260  
E263  
Y266  
I274  
K282  
I295  
L299  
A300  
T306  
Y307  
K308  
N313  
K314  
Q315  
G321  
C324  
LYS  
ASN
- G29  
N43  
S46  
L58  
V62  
D65  
I73  
D74  
V75  
D89  
P95  
G105  
K109  
VAL  
ILE  
LYS  
LYS  
SER  
GLN  
CYS  
P117  
I118  
G119  
N123  
K141  
G144  
T146  
T147  
Y155  
L156  
E157  
C158  
V159  
F171  
I180  
THR  
GLU  
D163  
I191  
S195

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 52.42Å 109.93Å 70.39Å<br>90.00° 95.95° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 47.11 – 2.94<br>47.11 – 2.94                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 89.2 (47.11-2.94)<br>88.8 (47.11-2.94)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.31 (at 2.96Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.18_3845                                            | Depositor        |
| R, $R_{free}$                                                           | 0.237 , 0.264<br>0.237 , 0.266                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1599 reflections (10.01%)                                   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 41.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.346                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 36.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.87                                                        | EDS              |
| Total number of atoms                                                   | 6338                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 39.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: ANP, ZN, 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     | 0.23         | 1/3195 (0.0%) | 0.39        | 3/4297 (0.1%) |
| 1   | B     | 0.13         | 0/3169        | 0.34        | 0/4268        |
| All | All   | 0.19         | 1/6364 (0.0%) | 0.37        | 3/8565 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 58  | LEU  | C-O   | -6.19 | 1.16        | 1.24     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 61  | ALA  | N-CA-C | -5.79 | 106.05      | 113.23   |
| 1   | A     | 61  | ALA  | CA-C-N | -5.42 | 113.97      | 121.77   |
| 1   | A     | 61  | ALA  | C-N-CA | -5.42 | 113.97      | 121.77   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3135  | 0        | 3139     | 33      | 0            |
| 1   | B     | 3107  | 0        | 3101     | 32      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | A     | 1     | 0        | 0        | 0       | 0            |
| 2   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | A     | 31    | 0        | 13       | 2       | 0            |
| 4   | B     | 31    | 0        | 13       | 0       | 0            |
| 5   | A     | 15    | 0        | 0        | 0       | 0            |
| 5   | B     | 15    | 0        | 0        | 0       | 0            |
| All | All   | 6338  | 0        | 6266     | 62      | 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 5.

The worst 5 of 62 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:146:LEU:HB2 | 1:A:171:PHE:HB2  | 1.63                     | 0.80              |
| 1:A:308:LYS:HB2 | 1:A:315:GLN:OE1  | 1.93                     | 0.68              |
| 1:A:93:MET:HG2  | 1:A:97:LYS:HE3   | 1.76                     | 0.66              |
| 1:B:391:ALA:O   | 1:B:395:LYS:HG2  | 1.97                     | 0.65              |
| 1:A:351:VAL:HB  | 1:B:351:VAL:HG12 | 1.82                     | 0.62              |

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 |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 370/458 (81%) | 353 (95%) | 17 (5%) | 0        | 100         | 100 |
| 1   | B     | 367/458 (80%) | 354 (96%) | 12 (3%) | 1 (0%)   | 36          | 59  |
| All | All   | 737/916 (80%) | 707 (96%) | 29 (4%) | 1 (0%)   | 48          | 71  |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 144 | GLY  |

### 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     | 349/412 (85%) | 349 (100%) | 0        | 100         | 100 |
| 1   | B     | 347/412 (84%) | 346 (100%) | 1 (0%)   | 86          | 93  |
| All | All   | 696/824 (84%) | 695 (100%) | 1 (0%)   | 88          | 96  |

All (1) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 421 | VAL  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 377 | GLN  |
| 1   | B     | 428 | GLN  |
| 1   | A     | 377 | GLN  |
| 1   | B     | 43  | ASN  |
| 1   | B     | 123 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | ANP  | A     | 503 | 3    | 33,33,33     | 0.93 | 4 (12%)     | 45,52,52    | 0.58 | 0           |
| 4   | ANP  | B     | 503 | 3    | 33,33,33     | 0.93 | 4 (12%)     | 45,52,52    | 0.57 | 0           |

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   | ANP  | A     | 503 | 3    | -       | 8/18/38/38 | 0/3/3/3 |
| 4   | ANP  | B     | 503 | 3    | -       | 7/18/38/38 | 0/3/3/3 |

The worst 5 of 8 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 4   | A     | 503 | ANP  | PG-O1G | 2.56 | 1.50        | 1.46     |
| 4   | B     | 503 | ANP  | PG-O1G | 2.55 | 1.50        | 1.46     |
| 4   | A     | 503 | ANP  | PG-N3B | 2.44 | 1.69        | 1.63     |
| 4   | A     | 503 | ANP  | PB-O1B | 2.42 | 1.49        | 1.46     |
| 4   | B     | 503 | ANP  | PG-N3B | 2.42 | 1.69        | 1.63     |

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

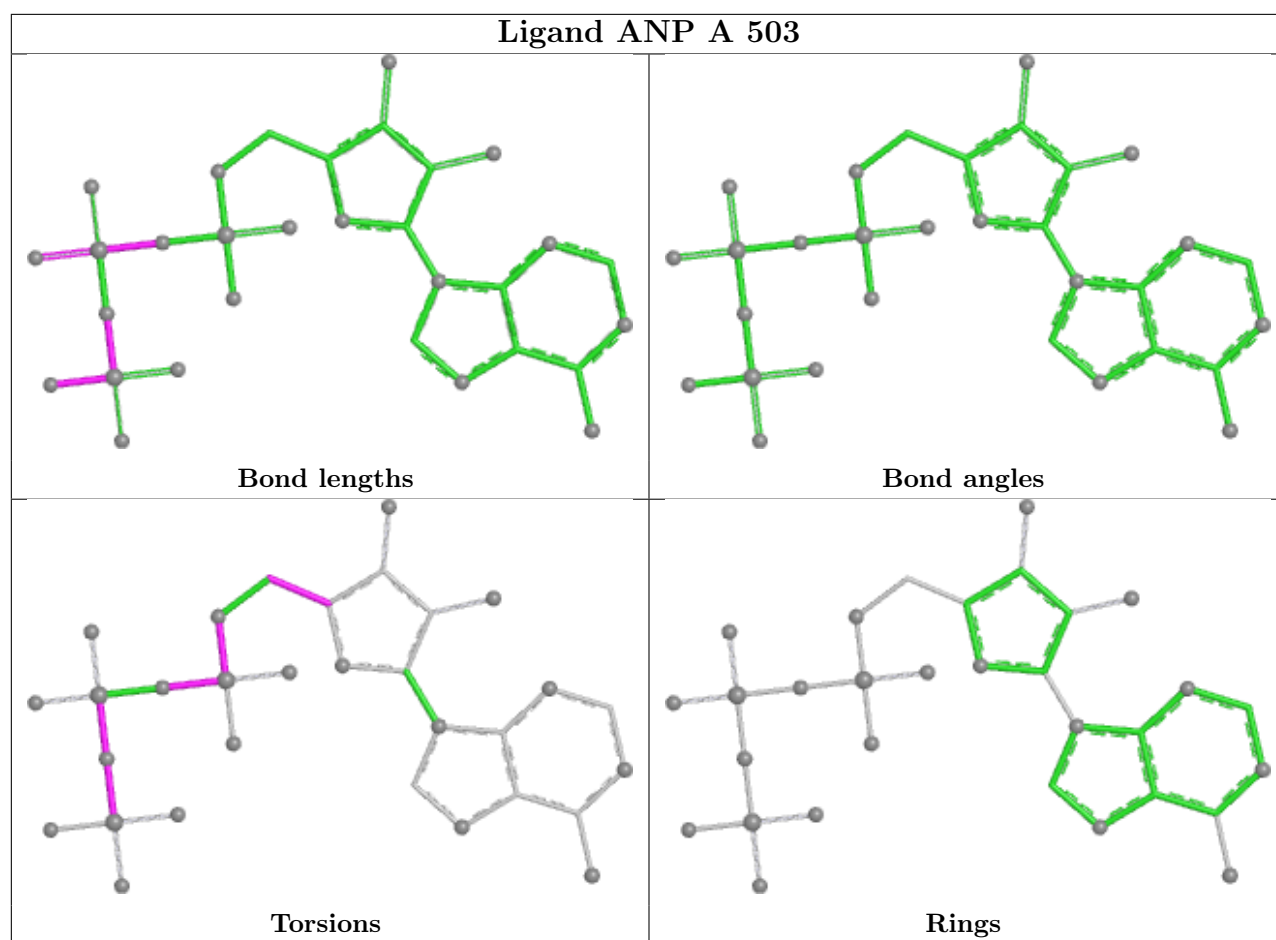
| Mol | Chain | Res | Type | Atoms          |
|-----|-------|-----|------|----------------|
| 4   | A     | 503 | ANP  | PB-N3B-PG-O1G  |
| 4   | A     | 503 | ANP  | PG-N3B-PB-O1B  |
| 4   | A     | 503 | ANP  | PG-N3B-PB-O3A  |
| 4   | A     | 503 | ANP  | C5'-O5'-PA-O3A |
| 4   | B     | 503 | ANP  | PB-N3B-PG-O1G  |

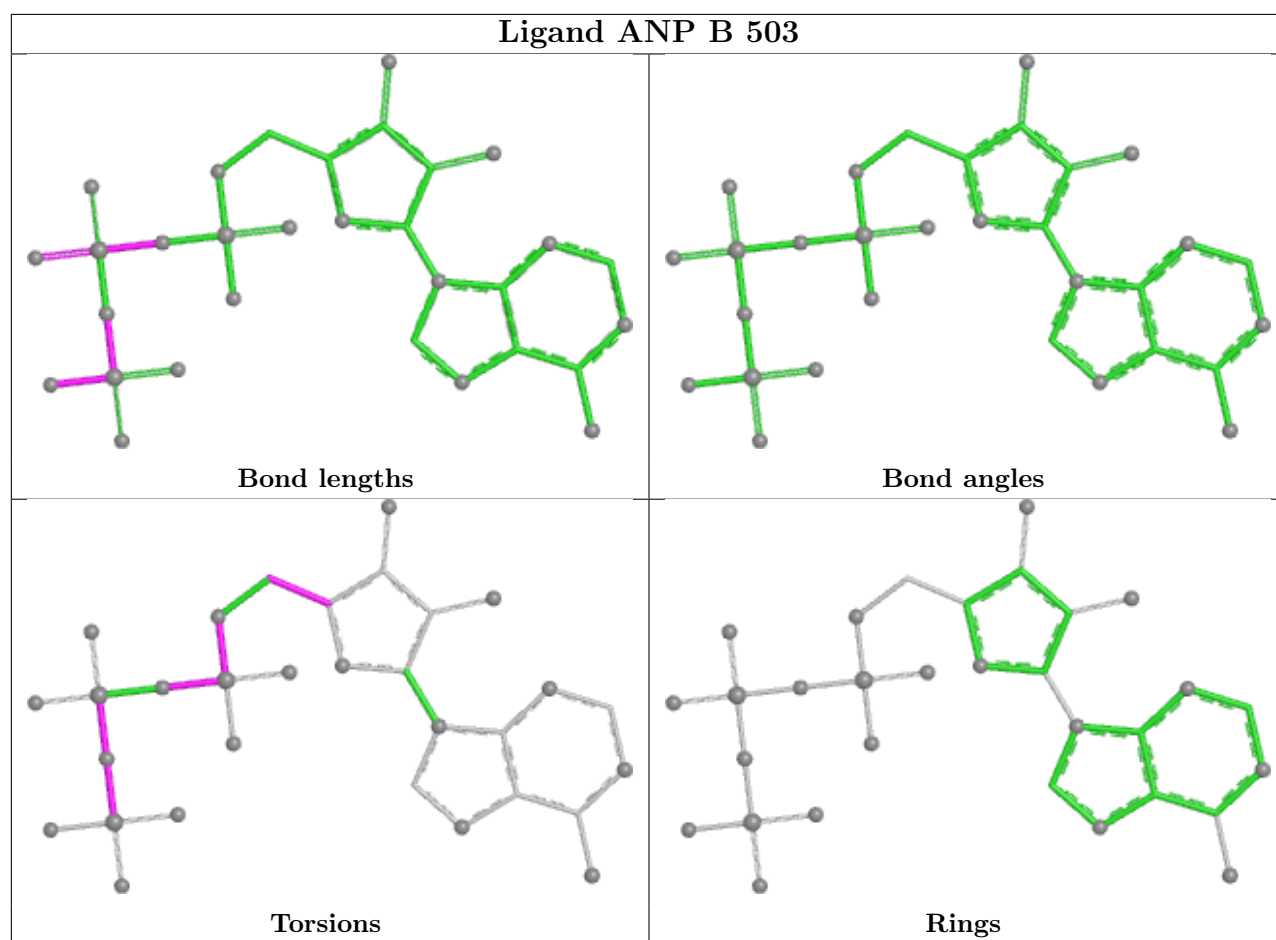
There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | A     | 503 | ANP  | 2       | 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 [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<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     | 390/458 (85%) | 0.63   | 23 (5%) | 28 23 | 20, 38, 66, 90        | 0      |
| 1   | B     | 386/458 (84%) | 0.54   | 14 (3%) | 46 38 | 16, 35, 66, 117       | 1 (0%) |
| All | All   | 776/916 (84%) | 0.58   | 37 (4%) | 35 29 | 16, 36, 67, 117       | 1 (0%) |

The worst 5 of 37 RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | B     | 384[A] | GLU  | 5.8  |
| 1   | B     | 420    | LYS  | 4.0  |
| 1   | A     | 91     | CYS  | 3.5  |
| 1   | B     | 300    | ALA  | 3.5  |
| 1   | A     | 65     | ASP  | 3.5  |

### 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](#)

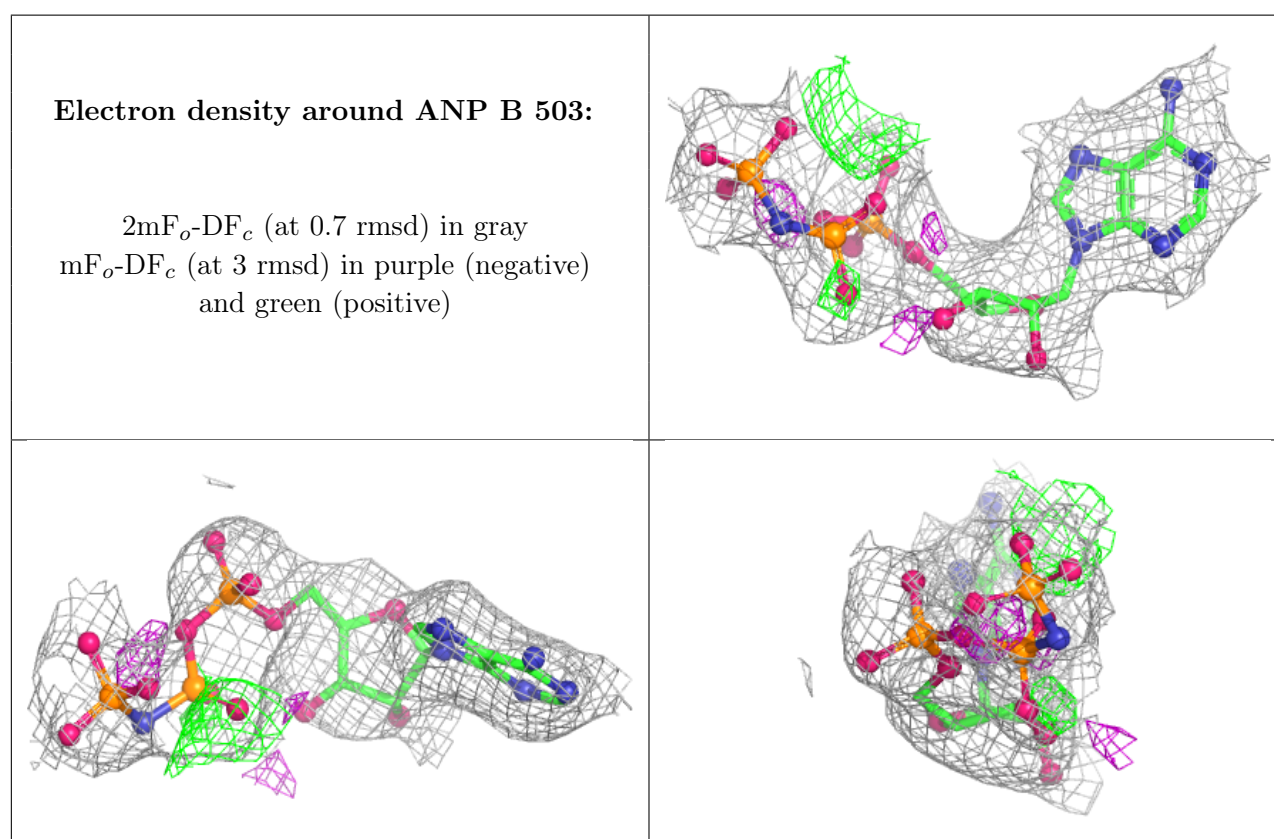
There are no oligosaccharides in this entry.

### 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.

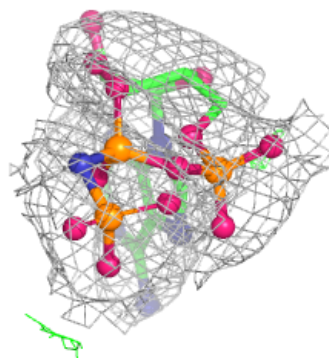
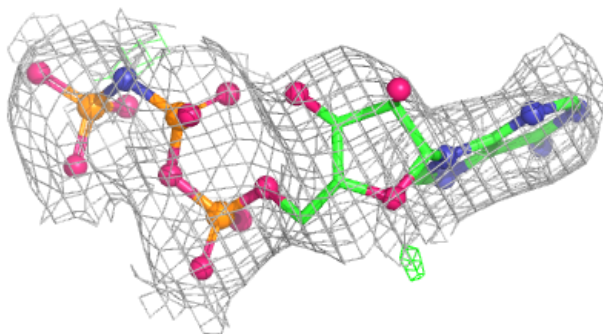
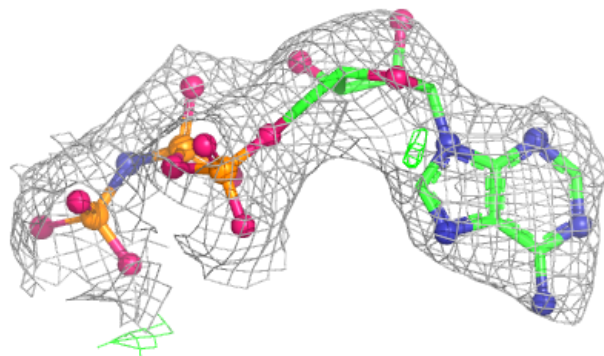
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | MG   | B     | 502 | 1/1   | 0.90 | 0.12 | 26,26,26,26                 | 0     |
| 4   | ANP  | B     | 503 | 31/31 | 0.91 | 0.10 | 22,28,31,35                 | 0     |
| 4   | ANP  | A     | 503 | 31/31 | 0.93 | 0.10 | 27,33,39,44                 | 0     |
| 3   | MG   | A     | 502 | 1/1   | 0.94 | 0.06 | 30,30,30,30                 | 0     |
| 2   | ZN   | A     | 501 | 1/1   | 0.97 | 0.03 | 41,41,41,41                 | 0     |
| 2   | ZN   | B     | 501 | 1/1   | 0.97 | 0.04 | 67,67,67,67                 | 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 ANP A 503:**

$2mF_o-DF_c$  (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.