

Full wwPDB NMR Structure Validation Report (i)

Oct 17, 2021 – 09:26 AM EDT

| PDB ID | : | 1JC8 |
|--------------|---|--|
| Title | : | Solution structure of lactam analogue (DDap) of gp41 600-612 loop of HIV |
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| Deposited on | : | 2001-06-08 |

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

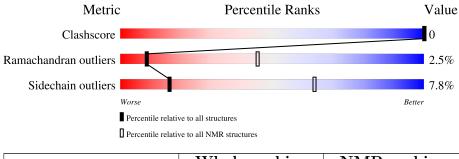
| MolProbity | : | 4.02b-467 |
|--------------------------------|---|--|
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.23.2 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.23.2 |

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION\ NMR$

The overall completeness of chemical shifts assignment was not calculated.

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 | $egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$ | ${f NMR} { m archive} \ (\#{ m Entries})$ |
|-----------------------|--|--|
| Clashscore | 158937 | 12864 |
| Ramachandran outliers | 154571 | 11451 |
| Sidechain outliers | 154315 | 11428 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

| Mol | Chain | Length | Quality of chain | |
|-----|-------|--------|------------------|-----|
| | | | | |
| 1 | А | 14 | 79% | 21% |

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

| Mol | Chain | hain Compound | | Total models with violations | | |
|-----|-------|---------------|-----|------------------------------|----------|--|
| | Unam | Compound | nes | Chirality | Geometry | |
| 1 | А | SET | 11 | 20 | - | |



2 Ensemble composition and analysis (i)

This entry contains 20 models.

Cyrange was unable to find well-defined residues.

Error message: Only domains with < 8 residues could be identified.

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 196 atoms, of which 99 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41.

| Mol | Chain | Residues | | At | oms | | | Trace |
|-----|-------|----------|-------|----|-----|----|----|-------|
| 1 | ٨ | 1.4 | Total | С | Η | Ν | 0 | 0 |
| 1 | А | 14 | 196 | 62 | 99 | 16 | 19 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| А | 1 | ACE | - | acetylation | UNP P12488 |
| А | 5 | ASP | CYS | engineered mutation | UNP P12488 |
| А | 11 | SET | CYS | engineered mutation | UNP P12488 |

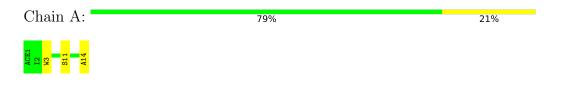


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

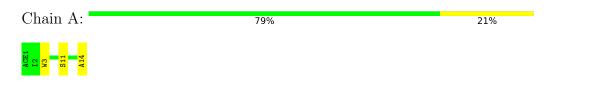


4.2 Scores per residue for each member of the ensemble

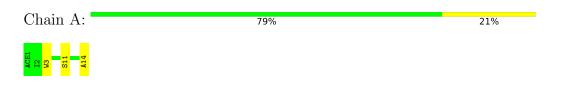
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41



4.2.2 Score per residue for model 2





4.2.3 Score per residue for model 3

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41



4.2.4 Score per residue for model 4

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 79% | 21% |
|---------------------------------|-----|-----|
| AGE1 12 811 811 A14 | | |

4.2.5 Score per residue for model 5

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

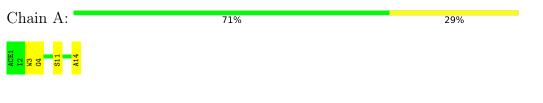
| Chain A: | 79% | 21% |
|-----------------------------------|-----|-----|
| ACB1 12 81 81 1 81 | | |

4.2.6 Score per residue for model 6

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 79% | 21% |
|---------------------------------|-----|-----|
| ACE1 13 811 A14 A14 | | |

4.2.7 Score per residue for model 7





4.2.8 Score per residue for model 8

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41



4.2.9 Score per residue for model 9

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 71% | 29% | |
|--|-----|-----|--|
| AGE1 12 11 11 11 11 11 11 | | | |

4.2.10 Score per residue for model 10

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

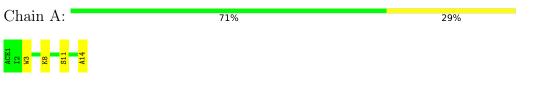
| Chain A: | 79% | 21% |
|------------------------------------|-----|-----|
| ACE1 12 13 11 14 14 | | |

4.2.11 Score per residue for model 11

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 79% | 21% |
|---------------------------------|-----|-----|
| ACE1 12 811 A14 A14 | | |

4.2.12 Score per residue for model 12





4.2.13 Score per residue for model 13

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 71% | 29% |
|--------------------------------|-----|-----|
| ACE1 12 81 A14 A14 | | |

4.2.14 Score per residue for model 14

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 64% | 36% |
|--|-----|-----|
| ACE1 12 13 13 110 110 14 14 | | |

4.2.15 Score per residue for model 15

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 71% | 29% | |
|---------------------------------------|-----|-----|--|
| AGE1 12 W3 110 811 A14 | | | |

4.2.16 Score per residue for model 16

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 71% | 29% |
|----------------------------------|-----|-----|
| AGE1 110 110 114 114 | | |

4.2.17 Score per residue for model 17

| Chain A: | 57% | 43% |
|--|-----|-----|
| 0551 13 110 110 114 114 | | |



4.2.18 Score per residue for model 18

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 57% | 43% |
|---|-----|-----|
| ACE1 112 113 110 110 110 114 114 | | |

4.2.19 Score per residue for model 19

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

| Chain A: | 57% | 43% |
|---|-----|-----|
| ACE1 12 W3 G4 G4 S11 A14 A14 | | |

4.2.20 Score per residue for model 20

• Molecule 1: DDap: (ACE)IWGDSGKLI(DNP)TTA ANALOGUE OF HIV GP41

Chain A: 64% 36%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: torsion angles dynamics, molecular dynamics, energy minimization..

Of the 50 calculated structures, 20 were deposited, based on the following criterion: target function.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|----------------|---------|
| DYANA | refinement | 1.5 |
| Discover | refinement | 3 |

No chemical shift data was provided.



6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, SET

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol Ch | Chain B | | ond lengths | Bond angles | |
|--------|---------|-------------------|-------------------------------------|-------------------|---------------------------------|
| | Chain | RMSZ | $\#Z{>}5$ | RMSZ | #Z>5 |
| 1 | А | $1.45 {\pm} 0.01$ | $1{\pm}0/89$ ($1.1{\pm}$ 0.0%) | $1.30 {\pm} 0.07$ | $1{\pm}0/117~(~0.9{\pm}~0.0\%)$ |
| All | All | 1.45 | 20/1780~(~1.1%) | 1.30 | 20/2340~(~0.9%) |

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 | Planarity |
|-----|-------|---------------|---------------|
| 1 | А | $1.0{\pm}0.0$ | $0.0{\pm}0.0$ |
| All | All | 20 | 0 |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) | Moo Worst | |
|-----|-------|-----|------|-------|------|-------------|----------|--------------|-------|
| | | | • - | | | · · · | · · · | Worst | Total |
| 1 | А | 14 | ALA | C-OXT | 7.71 | 1.38 | 1.23 | 5 | 20 |

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $\operatorname{Ideal}(^{o})$ | Moo Worst | dels Total |
|-----|-------|-----|------|-------------|-------|------------------|------------------------------|--------------|----------------------|
| 1 | А | 3 | TRP | CD1-NE1-CE2 | -5.76 | 103.81 | 109.00 | 6 | 20 |

All unique chiral outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Models (Total) |
|-----|-------|-----|------|-------|----------------|
| 1 | А | 11 | SET | CA | 20 |

There are no planarity outliers.



6.2 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 each 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 averaged over the ensemble.

| M | ol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|----|-------|-------|----------|----------|---------|
| A | 1 | All | 1940 | 1980 | 1860 | - |

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 -.

There are no clashes.

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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 | А | 10/14~(71%) | $5\pm1 (52\pm12\%)$ | $5\pm1 (46\pm14\%)$ | $0\pm1~(2\pm5\%)$ | Ģ | 45 |
| All | All | 200/280 (71%) | 103 (52%) | 92 (46%) | 5(2%) | Ģ | 45 |

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | А | 4 | GLY | 3 |
| 1 | А | 2 | ILE | 2 |

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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 | А | 9/9~(100%) | 8 ± 1 (92 $\pm11\%$) | $1\pm1 (8\pm11\%)$ | 16 | 64 |
| All | All | 180/180~(100%) | 166 (92%) | 14 (8%) | 16 | 64 |

All 4 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | А | 10 | ILE | 7 |
| 1 | А | 2 | ILE | 4 |
| 1 | А | 8 | LYS | 2 |
| 1 | А | 9 | LEU | 1 |

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Γ | Mal | Туре | Type | Type | Type | Chain | Dec | Tiple | | Bond len | gths |
|---|-------|------|------|------|-------|--------|-----------------|-------------|--|----------|------|
| | IVIOI | туре | Unam | nes | LIIIK | Counts | RMSZ | #Z>2 | | | |
| | 1 | SET | А | 11 | 1 | 4,5,6 | 2.61 ± 0.04 | 2±0 (50±0%) | | | |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with |Z| > 2 is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.



| Mol | Type | Chain | Res | Link | Counts | Bond ang RMSZ | gles #Z>2 | |
|-----|------|-------|-----|------|-------------|------------------|--------------|--|
| | | | | | Bond angles | | | |
| Mal | Type | Chain | Bos | Link | | Bond ang | gles | |
| Mol | Type | Chain | Res | Link | Counts | Bond ang RMSZ | gles #Z>2 | |

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 |
|-----|------|-------|-----|------|---------------|----------------|-------|
| 1 | SET | А | 11 | 1 | $1\pm0,1,1,2$ | $0\pm 0,4,4,6$ | - |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mal | Chain | Dec | Trune | Atoma | 7 | Observed(Å) | Ideal(Å) | Mod | |
|-----|-------|-----|-------|-------|------|-------------|----------|-------|-------|
| | Chain | nes | Type | Atoms | | Observed(A) | Ideal(A) | Worst | Total |
| 1 | А | 11 | SET | OG-CB | 4.45 | 1.23 | 1.42 | 18 | 20 |
| 1 | А | 11 | SET | CB-CA | 3.03 | 1.57 | 1.52 | 4 | 20 |

There are no bond-angle outliers.

All unique chiral outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Models (Total) |
|-----|-------|-----|------|-------|----------------|
| 1 | А | 11 | SET | CA | 20 |

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

