



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2LEJ
Title : human prion protein mutant HuPrP(90-231, M129, V210I)
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This is a wwPDB NMR 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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

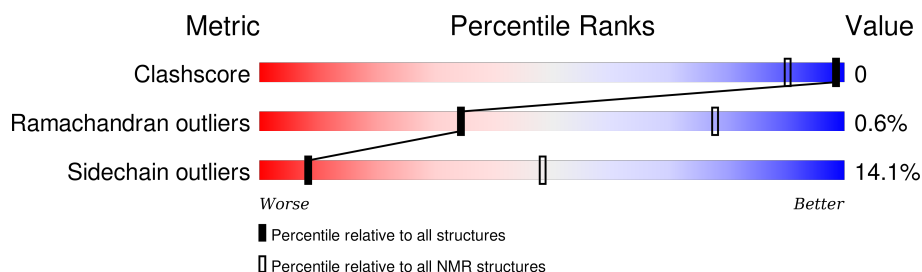
1 Overall quality at a glance

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 | Whole archive (#Entries) | NMR archive (#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore | 114402 | 11133 |
| Ramachandran outliers | 111179 | 9975 |
| Sidechain outliers | 111093 | 9958 |

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 $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 147 | |

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|--------------------------------------|----------------------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:117-A:165, A:172-A:220 (98) | 0.24 | 15 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 5 single-model clusters were found.

| Cluster number | Models |
|-----------------------|--------------------|
| 1 | 2, 4, 5, 7, 10, 19 |
| 2 | 9, 12, 13, 15, 18 |
| 3 | 16, 17 |
| 4 | 8, 11 |
| Single-model clusters | 1; 3; 6; 14; 20 |

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2254 atoms, of which 1091 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|-------|
| 1 | A | 147 | Total | C | H | N | O | S | 0 |
| | | | 2254 | 715 | 1091 | 209 | 227 | 12 | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | 85 | GLY | - | EXPRESSION TAG | UNP P04156 |
| A | 86 | ALA | - | EXPRESSION TAG | UNP P04156 |
| A | 87 | MET | - | EXPRESSION TAG | UNP P04156 |
| A | 88 | ASP | - | EXPRESSION TAG | UNP P04156 |
| A | 89 | PRO | - | EXPRESSION TAG | UNP P04156 |
| A | 210 | ILE | VAL | ENGINEERED MUTATION | UNP P04156 |

5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| CYANA | structure solution | 3.0 |
| YASARA | refinement | 11.5.22 |

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

| | |
|--|-------------|
| Chemical shift file(s) | 2lej_cs.str |
| Number of chemical shift lists | 1 |
| Total number of shifts | 1536 |
| Number of shifts mapped to atoms | 0 |
| Number of unparsed shifts | 1536 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 0% |

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|--------------------|-------------|---------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 0.69±0.01 | 0±0/813 (0.0±0.0%) | 0.74±0.02 | 3±1/1099 (0.3±0.1%) |
| All | All | 0.69 | 0/16260 (0.0%) | 0.74 | 60/21980 (0.3%) |

There are no bond-length outliers.

5 of 7 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 151 | ARG | NE-CZ-NH1 | 6.79 | 123.70 | 120.30 | 9 | 3 |
| 1 | A | 208 | ARG | NE-CZ-NH1 | 6.29 | 123.45 | 120.30 | 9 | 13 |
| 1 | A | 164 | ARG | NE-CZ-NH1 | 6.07 | 123.34 | 120.30 | 1 | 9 |
| 1 | A | 148 | ARG | NE-CZ-NH1 | 6.04 | 123.32 | 120.30 | 9 | 13 |
| 1 | A | 156 | ARG | NE-CZ-NH1 | 5.65 | 123.12 | 120.30 | 2 | 16 |

There are no chirality outliers.

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.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 795 | 756 | 756 | 0±1 |
| All | All | 15900 | 15120 | 15120 | 10 |

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 0.

All unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:130:LEU:HD13 | 1:A:162:TYR:CE2 | 0.52 | 2.38 | 14 | 9 |
| 1:A:180:VAL:HG11 | 1:A:211:GLU:HA | 0.42 | 1.92 | 14 | 1 |

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 | A | 98/147 (67%) | 91±1 (92±1%) | 7±1 (7±1%) | 1±0 (1±1%) | 34 | 78 |
| All | All | 1960/2940 (67%) | 1813 (92%) | 136 (7%) | 11 (1%) | 34 | 78 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 121 | VAL | 11 |

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 | A | 86/123 (70%) | 74±2 (86±2%) | 12±2 (14±2%) | 8 | 48 |
| All | All | 1720/2460 (70%) | 1478 (86%) | 242 (14%) | 8 | 48 |

5 of 29 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 159 | ASN | 20 |
| 1 | A | 204 | LYS | 20 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 214 | CYS | 20 |
| 1 | A | 175 | PHE | 20 |
| 1 | A | 163 | TYR | 20 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: 2lej_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

| | |
|---|------|
| Total number of shifts | 1536 |
| Number of shifts mapped to atoms | 0 |
| Number of unparsed shifts | 1536 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following errors were found when reading this chemical shift list.

- Entity instance (chain) must be specified. First 5 (of 1536) occurrences are reported below.

| Shift ID | Chain | Res | Type | Atom | Shift Data | | |
|----------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | . | 86 | ALA | H | 8.614 | 0.02 | 1 |
| 2 | . | 86 | ALA | HA | 4.295 | 0.02 | 1 |
| 3 | . | 86 | ALA | HB | 1.380 | 0.02 | 1 |
| 4 | . | 86 | ALA | HB | 1.380 | 0.02 | 1 |
| 5 | . | 86 | ALA | HB | 1.380 | 0.02 | 1 |

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical

shift out of a possible 1224. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹H | ¹³C | ¹⁵N |
|-----------|--------------|----------------------|-----------------------|-----------------------|
| Backbone | 0/484 (0%) | 0/193 (0%) | 0/196 (0%) | 0/95 (0%) |
| Sidechain | 0/621 (0%) | 0/365 (0%) | 0/221 (0%) | 0/35 (0%) |
| Aromatic | 0/119 (0%) | 0/63 (0%) | 0/52 (0%) | 0/4 (0%) |
| Overall | 0/1224 (0%) | 0/621 (0%) | 0/469 (0%) | 0/134 (0%) |

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.