



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 30, 2019 – 08:01 PM EDT

PDB ID : 2CSE  
Title : Features of Reovirus Outer-Capsid Protein  $\mu$ 1 Revealed by Electron and Image Reconstruction of the virion at 7.0-Å Resolution  
Authors : Zhang, X.; Ji, Y.; Zhang, L.; Harrison, S.C.; Marinescu, D.C.; Nibert, M.L.; Baker, T.S.  
Deposited on : 2005-05-21  
Resolution : 7.00 Å (reported)  
Based on PDB ID : 1EJ6, 1JMU, 1N35

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

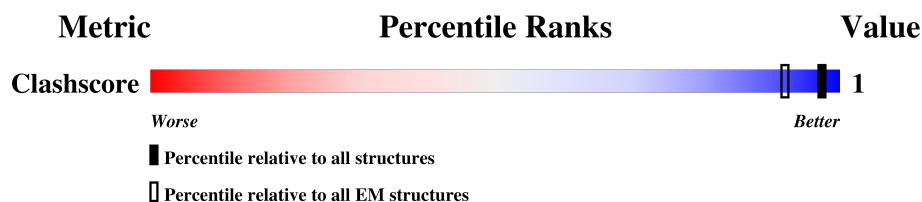
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

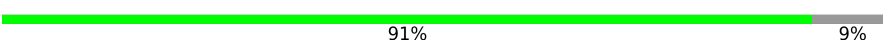
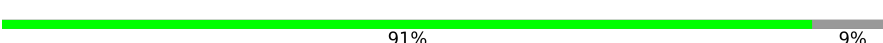




The reported resolution of this entry is 7.00 Å.

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.













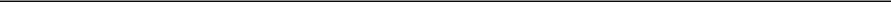

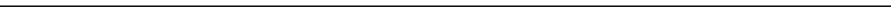


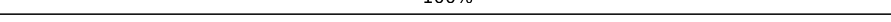
| Metric     | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|------------|-----------------------------|-----------------------------|
| Clashscore | 136327                      | 1886                        |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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     | 708    |  90% 9% |
| 1   | B     | 708    |  91% 9% |
| 1   | C     | 708    |  90% 9% |
| 1   | J     | 708    |  91% 9% |
| 1   | K     | 708    |  90% 9% |
| 1   | L     | 708    |  91% 9% |
| 1   | P     | 708    |  91% 9% |
| 1   | Q     | 708    |  91% 9% |
| 1   | R     | 708    |  91% 9% |
| 1   | T     | 708    |  91% 9% |
| 2   | D     | 365    |  100%   |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | E     | 365    |  100%    |
| 2   | F     | 365    |  100%    |
| 2   | G     | 365    |  100%    |
| 2   | H     | 365    |  100%    |
| 2   | I     | 365    |  100%    |
| 2   | M     | 365    |  100%    |
| 2   | N     | 365    |  100%    |
| 2   | O     | 365    |  100%    |
| 2   | S     | 365    |  100%    |
| 3   | U     | 1289   |  99%     |
| 4   | V     | 1275   |  81% 19% |
| 4   | W     | 1275   |  96% .   |
| 5   | X     | 418    |  100%  |
| 5   | Y     | 418    |  100%  |
| 5   | Z     | 418    |  100%  |
| 6   | 1     | 1267   |  100%  |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16111 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 major outer-capsid protein mu1.

| Mol | Chain | Residues | Atoms              | AltConf | Trace |
|-----|-------|----------|--------------------|---------|-------|
| 1   | A     | 641      | Total C<br>641 641 | 0       | 641   |
| 1   | B     | 641      | Total C<br>641 641 | 0       | 641   |
| 1   | C     | 641      | Total C<br>641 641 | 0       | 641   |
| 1   | P     | 641      | Total C<br>641 641 | 0       | 641   |
| 1   | Q     | 641      | Total C<br>641 641 | 0       | 641   |
| 1   | R     | 641      | Total C<br>641 641 | 0       | 641   |
| 1   | J     | 641      | Total C<br>641 641 | 0       | 641   |
| 1   | K     | 641      | Total C<br>641 641 | 0       | 641   |
| 1   | L     | 641      | Total C<br>641 641 | 0       | 641   |
| 1   | T     | 641      | Total C<br>641 641 | 0       | 641   |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| A     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| A     | 359     | PHE      | LEU    | conflict | UNP P11077 |
| B     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| B     | 359     | PHE      | LEU    | conflict | UNP P11077 |
| C     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| C     | 359     | PHE      | LEU    | conflict | UNP P11077 |
| J     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| J     | 359     | PHE      | LEU    | conflict | UNP P11077 |
| K     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| K     | 359     | PHE      | LEU    | conflict | UNP P11077 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| L     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| L     | 359     | PHE      | LEU    | conflict | UNP P11077 |
| P     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| P     | 359     | PHE      | LEU    | conflict | UNP P11077 |
| Q     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| Q     | 359     | PHE      | LEU    | conflict | UNP P11077 |
| R     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| R     | 359     | PHE      | LEU    | conflict | UNP P11077 |
| T     | 344     | LEU      | PRO    | conflict | UNP P11077 |
| T     | 359     | PHE      | LEU    | conflict | UNP P11077 |

- Molecule 2 is a protein called major capsid surface protein sigma-3.

| Mol | Chain | Residues | Atoms              | AltConf | Trace |
|-----|-------|----------|--------------------|---------|-------|
| 2   | S     | 365      | Total C<br>365 365 | 0       | 365   |
| 2   | D     | 365      | Total C<br>365 365 | 0       | 365   |
| 2   | E     | 365      | Total C<br>365 365 | 0       | 365   |
| 2   | F     | 365      | Total C<br>365 365 | 0       | 365   |
| 2   | M     | 365      | Total C<br>365 365 | 0       | 365   |
| 2   | N     | 365      | Total C<br>365 365 | 0       | 365   |
| 2   | O     | 365      | Total C<br>365 365 | 0       | 365   |
| 2   | G     | 365      | Total C<br>365 365 | 0       | 365   |
| 2   | H     | 365      | Total C<br>365 365 | 0       | 365   |
| 2   | I     | 365      | Total C<br>365 365 | 0       | 365   |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| D     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| D     | 325     | ASN      | ASP    | conflict | UNP P07939 |
| E     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| E     | 325     | ASN      | ASP    | conflict | UNP P07939 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| F     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| F     | 325     | ASN      | ASP    | conflict | UNP P07939 |
| G     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| G     | 325     | ASN      | ASP    | conflict | UNP P07939 |
| H     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| H     | 325     | ASN      | ASP    | conflict | UNP P07939 |
| I     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| I     | 325     | ASN      | ASP    | conflict | UNP P07939 |
| M     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| M     | 325     | ASN      | ASP    | conflict | UNP P07939 |
| N     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| N     | 325     | ASN      | ASP    | conflict | UNP P07939 |
| O     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| O     | 325     | ASN      | ASP    | conflict | UNP P07939 |
| S     | 104     | CYS      | ALA    | conflict | UNP P07939 |
| S     | 325     | ASN      | ASP    | conflict | UNP P07939 |

- Molecule 3 is a protein called guanylyltransferase.

| Mol | Chain | Residues | Atoms                | AltConf | Trace |
|-----|-------|----------|----------------------|---------|-------|
| 3   | U     | 1284     | Total C<br>1284 1284 | 0       | 1284  |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| U     | 609     | GLY      | PHE    | conflict | UNP P11079 |

- Molecule 4 is a protein called major core protein lambda 1.

| Mol | Chain | Residues | Atoms                | AltConf | Trace |
|-----|-------|----------|----------------------|---------|-------|
| 4   | V     | 1031     | Total C<br>1031 1031 | 0       | 1031  |
| 4   | W     | 1221     | Total C<br>1221 1221 | 0       | 1221  |

- Molecule 5 is a protein called Sigma 2 protein.

| Mol | Chain | Residues | Atoms              | AltConf | Trace |
|-----|-------|----------|--------------------|---------|-------|
| 5   | X     | 417      | Total C<br>417 417 | 0       | 417   |

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| Mol | Chain | Residues | Atoms              | AltConf | Trace |
|-----|-------|----------|--------------------|---------|-------|
| 5   | Y     | 417      | Total C<br>417 417 | 0       | 417   |
| 5   | Z     | 417      | Total C<br>417 417 | 0       | 417   |

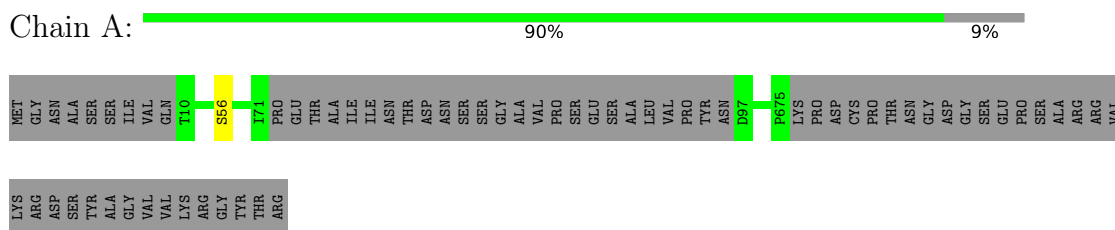
- Molecule 6 is a protein called Minor core protein lambda 3.

| Mol | Chain | Residues | Atoms                | AltConf | Trace |
|-----|-------|----------|----------------------|---------|-------|
| 6   | 1     | 1264     | Total C<br>1264 1264 | 0       | 1264  |

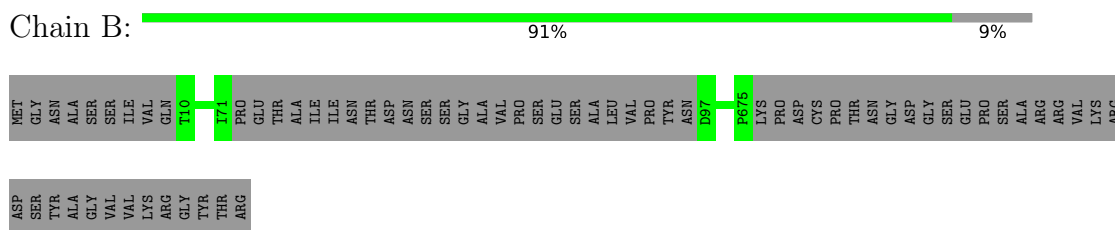
### 3 Residue-property plots [i](#)

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.

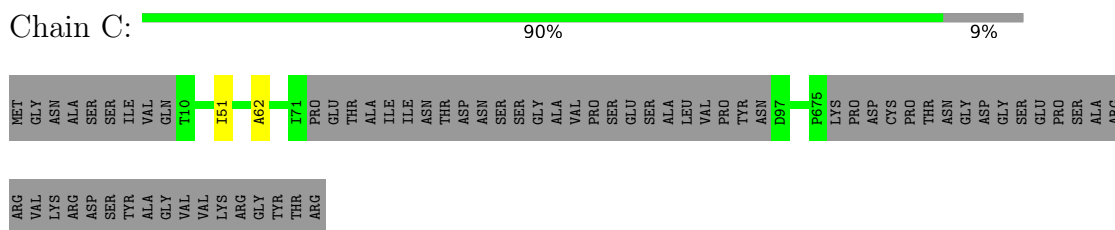
- Molecule 1: major outer-capsid protein mu1



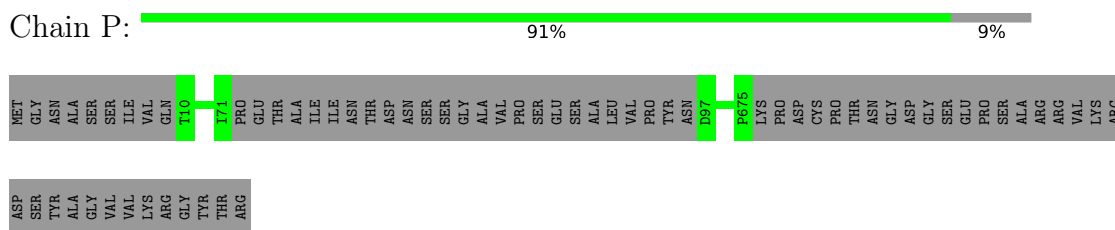
- Molecule 1: major outer-capsid protein mu1



- Molecule 1: major outer-capsid protein mu1



- Molecule 1: major outer-capsid protein mu1



- Molecule 1: major outer-capsid protein mu1



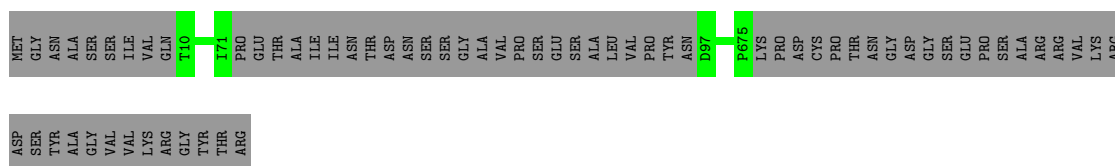
- Molecule 1: major outer-capsid protein mu1

- Molecule 1: major outer-capsid protein mu1

- Molecule 1: major outer-capsid protein mu1

- Molecule 1: major outer-capsid protein mu1

- Molecule 1: major outer-capsid protein mu1



- Molecule 2: major capsid surface protein sigma-3

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain G:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: major capsid surface protein sigma-3

Chain I:  100%


There are no outlier residues recorded for this chain.

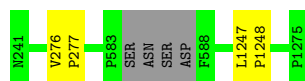
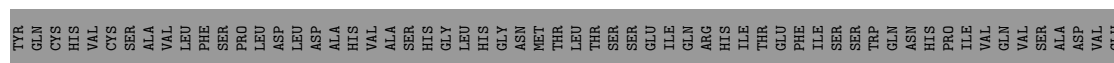
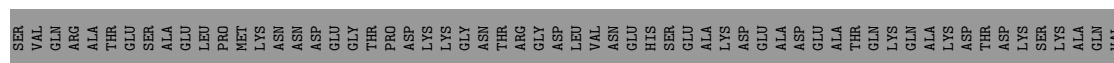
- Molecule 3: guanylyltransferase

Chain U:  99%



- Molecule 4: major core protein lambda 1

Chain V:  81% 19%



- Molecule 4: major core protein lambda 1

Chain W:  96%



- Molecule 5: Sigma 2 protein

Chain X:  100%



- Molecule 5: Sigma 2 protein

Chain Y:  100%



- Molecule 5: Sigma 2 protein

Chain Z:  100%



- Molecule 6: Minor core protein lambda 3

Chain 1:  100%



## 4 Experimental information

| Property                             | Value  | Source    |
|--------------------------------------|--|-----------|
| Reconstruction method                | SINGLE PARTICLE                              | Depositor |
| Imposed symmetry                     | POINT, I                                     | Depositor |
| Number of particles used             | 7939   | Depositor |
| Resolution determination method      | Not provided                                 | Depositor |
| CTF correction method                | CTF correction of each particle              | Depositor |
| Microscope                           | FEI/PHILIPS CM200FEG, FEI/PHILIPS CM300FEG/T | Depositor |
| Voltage (kV)                         | 200, 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 20   | Depositor |
| Minimum defocus (nm)                 | 1300, Not provided                           | Depositor |
| Maximum defocus (nm)                 | 3200, Not provided                           | Depositor |
| Magnification                        | 45000, 47440                                 | Depositor |
| Image detector                       | KODAK SO-163 FILM                            | Depositor |

## 5 Model quality [i](#)

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

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 [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     | 641   | 0        | 0        | 1       | 0            |
| 1   | B     | 641   | 0        | 0        | 0       | 0            |
| 1   | C     | 641   | 0        | 0        | 1       | 0            |
| 1   | J     | 641   | 0        | 0        | 0       | 0            |
| 1   | K     | 641   | 0        | 0        | 1       | 0            |
| 1   | L     | 641   | 0        | 0        | 0       | 0            |
| 1   | P     | 641   | 0        | 0        | 0       | 0            |
| 1   | Q     | 641   | 0        | 0        | 0       | 0            |
| 1   | R     | 641   | 0        | 0        | 0       | 0            |
| 1   | T     | 641   | 0        | 0        | 0       | 0            |
| 2   | D     | 365   | 0        | 0        | 0       | 0            |
| 2   | E     | 365   | 0        | 0        | 0       | 0            |
| 2   | F     | 365   | 0        | 0        | 0       | 0            |
| 2   | G     | 365   | 0        | 0        | 0       | 0            |
| 2   | H     | 365   | 0        | 0        | 0       | 0            |
| 2   | I     | 365   | 0        | 0        | 0       | 0            |
| 2   | M     | 365   | 0        | 0        | 0       | 0            |
| 2   | N     | 365   | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | O     | 365   | 0        | 0        | 0       | 0            |
| 2   | S     | 365   | 0        | 0        | 0       | 0            |
| 3   | U     | 1284  | 0        | 0        | 2       | 0            |
| 4   | V     | 1031  | 0        | 0        | 2       | 0            |
| 4   | W     | 1221  | 0        | 0        | 1       | 0            |
| 5   | X     | 417   | 0        | 0        | 0       | 0            |
| 5   | Y     | 417   | 0        | 0        | 1       | 0            |
| 5   | Z     | 417   | 0        | 0        | 0       | 0            |
| 6   | 1     | 1264  | 0        | 0        | 1       | 0            |
| All | All   | 16111 | 0        | 0        | 9       | 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 1.

All (9) 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:56:SER:CA   | 5:Y:15:GLY:CA   | 2.13                     | 1.25              |
| 1:C:51:ILE:CA   | 1:C:62:ALA:CA   | 2.63                     | 0.77              |
| 3:U:245:PRO:CA  | 3:U:246:PRO:CA  | 2.83                     | 0.56              |
| 4:V:1247:LEU:CA | 4:V:1248:PRO:CA | 2.84                     | 0.56              |
| 1:K:51:ILE:CA   | 1:K:62:ALA:CA   | 2.85                     | 0.55              |
| 4:W:1247:LEU:CA | 4:W:1248:PRO:CA | 2.86                     | 0.53              |
| 6:1:301:GLU:CA  | 6:1:302:PRO:CA  | 2.89                     | 0.51              |
| 3:U:420:LEU:CA  | 3:U:421:PRO:CA  | 2.90                     | 0.49              |
| 4:V:276:VAL:CA  | 4:V:277:PRO:CA  | 2.95                     | 0.44              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

There are no ligands in this entry.

### 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.