# wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:40 PM BST

| | | |
|---|---|---|
| PDB ID | : | 3BBV |
| EMDB ID: | : | EMD-1455 |
| Title | : | The tRNA(phe) fitted into the low resolution Cryo-EM map of the 50S.nc-tRNA.Hsp15 complex |
| Authors | : | Jiang, L.; Abrahams, J.P. |
| Deposited on | : | 2007-11-11 |
| Resolution | : | 10.00 Å(reported) |

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

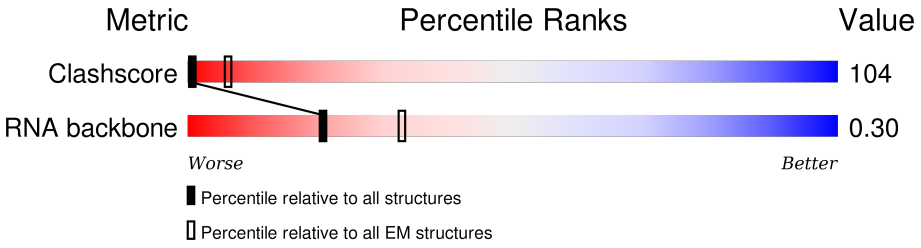
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk27241 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.00 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 (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 114402 | 924 |
| RNA backbone | 3027 | 244 |

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 >=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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | z | 76 | 17% 61% 22% |

## 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1628 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 RNA chain called tRNA(Phe).

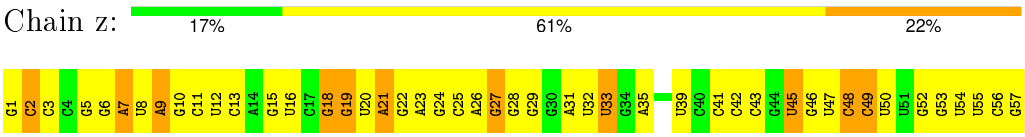
| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | | |
| 1 | z | 76 | 1628 | 731 | 290 | 530 | 75 | 2 | 0 | 0 |

# 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 errors 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: tRNA(Phe)

Chain z:







# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| Reconstruction method | Not provided | Depositor |
| Imposed symmetry | POINT, Not provided | Depositor |
| Number of images | Not provided | Depositor |
| Resolution determination method | Not provided | Depositor |
| CTF correction method | CTF correction of each particle | Depositor |
| Microscope | FEI Tecnai F20 | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | Not provided | Depositor |
| Minimum defocus (nm) | 1.5 | Depositor |
| Maximum defocus (nm) | 3.5 | Depositor |
| Magnification | 50000 | Depositor |
| Image detector | Kodak SO-163 film | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, MIA, 4SU, 7MG, PSU

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 | #$\|Z\|>2$ | RMSZ | #$\|Z\|>2$ |
| 1 | z | 2.66 | 94/1602 (5.9%) | 2.11 | 76/2493 (3.0%) |

All (94) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | z | 47 | U | O3'-P | 12.52 | 1.76 | 1.61 |
| 1 | z | 26 | A | C5-C6 | 9.54 | 1.49 | 1.41 |
| 1 | z | 26 | A | N7-C5 | 7.99 | 1.44 | 1.39 |
| 1 | z | 26 | A | N9-C4 | 7.94 | 1.42 | 1.37 |
| 1 | z | 12 | U | C2-N3 | 7.84 | 1.43 | 1.37 |
| 1 | z | 10 | G | N9-C8 | 7.38 | 1.43 | 1.37 |
| 1 | z | 65 | G | N7-C5 | -7.30 | 1.34 | 1.39 |
| 1 | z | 33 | U | C4'-C3' | -7.23 | 1.45 | 1.53 |
| 1 | z | 50 | U | C2-N3 | -7.15 | 1.32 | 1.37 |
| 1 | z | 53 | G | N3-C4 | -7.09 | 1.30 | 1.35 |
| 1 | z | 24 | G | N9-C8 | 7.06 | 1.42 | 1.37 |
| 1 | z | 52 | G | N7-C5 | -6.96 | 1.35 | 1.39 |
| 1 | z | 5 | G | N7-C5 | -6.93 | 1.35 | 1.39 |
| 1 | z | 28 | G | N3-C4 | 6.92 | 1.40 | 1.35 |
| 1 | z | 64 | A | N7-C5 | -6.78 | 1.35 | 1.39 |
| 1 | z | 57 | G | N7-C5 | 6.73 | 1.43 | 1.39 |
| 1 | z | 75 | C | P-O5' | -6.73 | 1.53 | 1.59 |
| 1 | z | 59 | U | P-O5' | 6.68 | 1.66 | 1.59 |
| 1 | z | 21 | A | N7-C5 | 6.67 | 1.43 | 1.39 |
| 1 | z | 53 | G | N9-C8 | -6.60 | 1.33 | 1.37 |
| 1 | z | 28 | G | C6-N1 | 6.58 | 1.44 | 1.39 |
| 1 | z | 28 | G | N7-C5 | 6.57 | 1.43 | 1.39 |
| 1 | z | 5 | G | N9-C4 | -6.56 | 1.32 | 1.38 |
| 1 | z | 19 | G | C5-C4 | -6.54 | 1.33 | 1.38 |
| 1 | z | 57 | G | C8-N7 | -6.52 | 1.27 | 1.30 |
| 1 | z | 10 | G | N3-C4 | 6.42 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | z | 76 | A | C5-C6 | 6.29 | 1.46 | 1.41 |
| 1 | z | 73 | A | N7-C5 | 6.25 | 1.43 | 1.39 |
| 1 | z | 56 | C | N1-C6 | -6.20 | 1.33 | 1.37 |
| 1 | z | 25 | C | C2-N3 | 6.19 | 1.40 | 1.35 |
| 1 | z | 13 | C | N1-C2 | 6.18 | 1.46 | 1.40 |
| 1 | z | 15 | G | N3-C4 | 6.18 | 1.39 | 1.35 |
| 1 | z | 57 | G | P-O5' | 6.18 | 1.66 | 1.59 |
| 1 | z | 33 | U | C2-N3 | 6.15 | 1.42 | 1.37 |
| 1 | z | 76 | A | N9-C4 | 6.13 | 1.41 | 1.37 |
| 1 | z | 24 | G | C5-C4 | 6.10 | 1.42 | 1.38 |
| 1 | z | 1 | G | C2'-C1' | -6.06 | 1.46 | 1.53 |
| 1 | z | 28 | G | N9-C8 | 6.05 | 1.42 | 1.37 |
| 1 | z | 69 | G | N7-C5 | -6.03 | 1.35 | 1.39 |
| 1 | z | 52 | G | N3-C4 | -6.03 | 1.31 | 1.35 |
| 1 | z | 53 | G | C6-N1 | -6.03 | 1.35 | 1.39 |
| 1 | z | 52 | G | C6-N1 | -5.98 | 1.35 | 1.39 |
| 1 | z | 71 | G | N9-C8 | -5.97 | 1.33 | 1.37 |
| 1 | z | 50 | U | C4-O4 | -5.94 | 1.18 | 1.23 |
| 1 | z | 58 | A | N9-C4 | -5.94 | 1.34 | 1.37 |
| 1 | z | 70 | G | N9-C8 | -5.90 | 1.33 | 1.37 |
| 1 | z | 18 | G | N9-C8 | -5.88 | 1.33 | 1.37 |
| 1 | z | 12 | U | C4-O4 | 5.85 | 1.28 | 1.23 |
| 1 | z | 26 | A | C2-N3 | 5.85 | 1.38 | 1.33 |
| 1 | z | 50 | U | C5-C6 | -5.84 | 1.28 | 1.34 |
| 1 | z | 11 | C | N3-C4 | 5.79 | 1.38 | 1.33 |
| 1 | z | 75 | C | N1-C6 | -5.78 | 1.33 | 1.37 |
| 1 | z | 71 | G | C5-C4 | -5.72 | 1.34 | 1.38 |
| 1 | z | 31 | A | C3'-C2' | -5.72 | 1.46 | 1.52 |
| 1 | z | 6 | G | N7-C5 | -5.71 | 1.35 | 1.39 |
| 1 | z | 76 | A | N9-C8 | -5.70 | 1.33 | 1.37 |
| 1 | z | 23 | A | N9-C4 | 5.67 | 1.41 | 1.37 |
| 1 | z | 67 | C | C2-N3 | -5.64 | 1.31 | 1.35 |
| 1 | z | 61 | C | C5-C6 | -5.63 | 1.29 | 1.34 |
| 1 | z | 67 | C | C5-C6 | -5.60 | 1.29 | 1.34 |
| 1 | z | 1 | G | N3-C4 | -5.53 | 1.31 | 1.35 |
| 1 | z | 24 | G | C6-N1 | 5.52 | 1.43 | 1.39 |
| 1 | z | 10 | G | C6-N1 | 5.49 | 1.43 | 1.39 |
| 1 | z | 27 | G | N7-C5 | 5.49 | 1.42 | 1.39 |
| 1 | z | 65 | G | C6-N1 | -5.48 | 1.35 | 1.39 |
| 1 | z | 74 | C | N1-C6 | -5.47 | 1.33 | 1.37 |
| 1 | z | 28 | G | C2-N2 | 5.47 | 1.40 | 1.34 |
| 1 | z | 65 | G | N3-C4 | -5.45 | 1.31 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | z | 61 | C | C2-N3 | -5.43 | 1.31 | 1.35 |
| 1 | z | 53 | G | C3'-O3' | 5.42 | 1.49 | 1.42 |
| 1 | z | 12 | U | C5-C6 | 5.41 | 1.39 | 1.34 |
| 1 | z | 24 | G | N3-C4 | 5.40 | 1.39 | 1.35 |
| 1 | z | 66 | U | C2-N3 | -5.31 | 1.34 | 1.37 |
| 1 | z | 62 | C | N1-C6 | 5.28 | 1.40 | 1.37 |
| 1 | z | 70 | G | N7-C5 | -5.28 | 1.36 | 1.39 |
| 1 | z | 61 | C | C4-N4 | -5.27 | 1.29 | 1.33 |
| 1 | z | 43 | C | C3'-O3' | 5.27 | 1.49 | 1.42 |
| 1 | z | 15 | G | N7-C5 | 5.27 | 1.42 | 1.39 |
| 1 | z | 58 | A | C5'-C4' | 5.26 | 1.57 | 1.51 |
| 1 | z | 58 | A | C3'-O3' | 5.24 | 1.49 | 1.42 |
| 1 | z | 57 | G | C5-C4 | -5.24 | 1.34 | 1.38 |
| 1 | z | 57 | G | N1-C2 | -5.23 | 1.33 | 1.37 |
| 1 | z | 15 | G | P-O5' | 5.22 | 1.65 | 1.59 |
| 1 | z | 25 | C | C5-C6 | 5.21 | 1.38 | 1.34 |
| 1 | z | 57 | G | N3-C4 | 5.20 | 1.39 | 1.35 |
| 1 | z | 2 | C | C3'-O3' | 5.18 | 1.49 | 1.42 |
| 1 | z | 15 | G | C6-N1 | 5.17 | 1.43 | 1.39 |
| 1 | z | 70 | G | N3-C4 | -5.11 | 1.31 | 1.35 |
| 1 | z | 10 | G | N7-C5 | 5.10 | 1.42 | 1.39 |
| 1 | z | 10 | G | C5-C4 | 5.09 | 1.42 | 1.38 |
| 1 | z | 65 | G | N9-C8 | -5.09 | 1.34 | 1.37 |
| 1 | z | 3 | C | C5-C6 | -5.08 | 1.30 | 1.34 |
| 1 | z | 22 | G | N9-C4 | 5.06 | 1.42 | 1.38 |
| 1 | z | 26 | A | C8-N7 | 5.04 | 1.35 | 1.31 |

All (76) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | z | 31 | A | C3'-C2'-C1' | -8.56 | 94.65 | 101.50 |
| 1 | z | 57 | G | C8-N9-C4 | 7.77 | 109.51 | 106.40 |
| 1 | z | 74 | C | N3-C4-C5 | -7.64 | 118.84 | 121.90 |
| 1 | z | 1 | G | N9-C4-C5 | 7.52 | 108.41 | 105.40 |
| 1 | z | 61 | C | C6-N1-C2 | 7.51 | 123.31 | 120.30 |
| 1 | z | 74 | C | C6-N1-C2 | -7.39 | 117.34 | 120.30 |
| 1 | z | 76 | A | N9-C4-C5 | 7.30 | 108.72 | 105.80 |
| 1 | z | 67 | C | C6-N1-C2 | 7.29 | 123.22 | 120.30 |
| 1 | z | 41 | C | C3'-C2'-C1' | -7.15 | 95.78 | 101.50 |
| 1 | z | 7 | A | C2'-C3'-O3' | 7.10 | 125.12 | 109.50 |
| 1 | z | 57 | G | C5-C6-N1 | 7.05 | 115.02 | 111.50 |
| 1 | z | 76 | A | C4-C5-N7 | -6.95 | 107.22 | 110.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | z | 53 | G | C4-C5-N7 | -6.91 | 108.04 | 110.80 |
| 1 | z | 52 | G | N9-C4-C5 | 6.83 | 108.13 | 105.40 |
| 1 | z | 71 | G | C4-C5-N7 | -6.74 | 108.10 | 110.80 |
| 1 | z | 61 | C | N3-C4-C5 | 6.67 | 124.57 | 121.90 |
| 1 | z | 53 | G | N9-C4-C5 | 6.55 | 108.02 | 105.40 |
| 1 | z | 57 | G | N9-C4-C5 | -6.54 | 102.78 | 105.40 |
| 1 | z | 57 | G | C2-N3-C4 | 6.46 | 115.13 | 111.90 |
| 1 | z | 52 | G | C8-N9-C4 | -6.30 | 103.88 | 106.40 |
| 1 | z | 49 | C | N1-C2-O2 | 6.28 | 122.67 | 118.90 |
| 1 | z | 75 | C | C4-C5-C6 | 6.21 | 120.51 | 117.40 |
| 1 | z | 1 | G | C4-C5-N7 | -6.19 | 108.33 | 110.80 |
| 1 | z | 70 | G | N9-C4-C5 | 6.17 | 107.87 | 105.40 |
| 1 | z | 48 | C | C3'-C2'-C1' | 6.12 | 106.40 | 101.50 |
| 1 | z | 69 | G | C8-N9-C4 | -6.07 | 103.97 | 106.40 |
| 1 | z | 15 | G | N9-C4-C5 | -5.81 | 103.08 | 105.40 |
| 1 | z | 76 | A | N1-C6-N6 | -5.79 | 115.13 | 118.60 |
| 1 | z | 71 | G | C5-N7-C8 | 5.75 | 107.17 | 104.30 |
| 1 | z | 18 | G | C4-C5-N7 | -5.73 | 108.51 | 110.80 |
| 1 | z | 5 | G | C2-N3-C4 | -5.71 | 109.05 | 111.90 |
| 1 | z | 45 | U | C3'-C2'-C1' | -5.70 | 96.94 | 101.50 |
| 1 | z | 70 | G | C4-C5-N7 | -5.67 | 108.53 | 110.80 |
| 1 | z | 69 | G | N7-C8-N9 | 5.67 | 115.93 | 113.10 |
| 1 | z | 5 | G | N1-C6-O6 | 5.66 | 123.29 | 119.90 |
| 1 | z | 73 | A | N9-C4-C5 | -5.62 | 103.55 | 105.80 |
| 1 | z | 76 | A | O4'-C1'-N9 | 5.58 | 112.66 | 108.20 |
| 1 | z | 3 | C | N3-C4-C5 | 5.57 | 124.13 | 121.90 |
| 1 | z | 19 | G | C2-N3-C4 | 5.57 | 114.68 | 111.90 |
| 1 | z | 57 | G | N3-C4-N9 | 5.56 | 129.34 | 126.00 |
| 1 | z | 47 | U | OP2-P-O3' | -5.55 | 93.00 | 105.20 |
| 1 | z | 5 | G | C5-N7-C8 | -5.52 | 101.54 | 104.30 |
| 1 | z | 59 | U | C5-C6-N1 | 5.49 | 125.44 | 122.70 |
| 1 | z | 31 | A | C4'-C3'-C2' | 5.48 | 108.08 | 102.60 |
| 1 | z | 35 | A | C8-N9-C4 | 5.45 | 107.98 | 105.80 |
| 1 | z | 74 | C | N1-C2-O2 | -5.45 | 115.63 | 118.90 |
| 1 | z | 10 | G | N9-C1'-C2' | 5.44 | 121.07 | 114.00 |
| 1 | z | 1 | G | C8-N9-C4 | -5.40 | 104.24 | 106.40 |
| 1 | z | 6 | G | N9-C4-C5 | 5.39 | 107.56 | 105.40 |
| 1 | z | 9 | A | C8-N9-C4 | 5.39 | 107.95 | 105.80 |
| 1 | z | 3 | C | C6-N1-C2 | 5.37 | 122.45 | 120.30 |
| 1 | z | 19 | G | C8-N9-C4 | 5.35 | 108.54 | 106.40 |
| 1 | z | 72 | C | C6-N1-C2 | 5.35 | 122.44 | 120.30 |
| 1 | z | 28 | G | N9-C4-C5 | -5.34 | 103.26 | 105.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | z | 67 | C | N3-C4-C5 | 5.33 | 124.03 | 121.90 |
| 1 | z | 58 | A | N9-C4-C5 | -5.29 | 103.68 | 105.80 |
| 1 | z | 9 | A | C4-C5-C6 | -5.28 | 114.36 | 117.00 |
| 1 | z | 21 | A | C2-N3-C4 | 5.25 | 113.23 | 110.60 |
| 1 | z | 69 | G | C2-N3-C4 | -5.25 | 109.28 | 111.90 |
| 1 | z | 71 | G | C2-N3-C4 | 5.23 | 114.52 | 111.90 |
| 1 | z | 67 | C | N1-C2-O2 | 5.22 | 122.03 | 118.90 |
| 1 | z | 29 | G | C4-C5-N7 | 5.20 | 112.88 | 110.80 |
| 1 | z | 75 | C | N3-C4-C5 | -5.18 | 119.83 | 121.90 |
| 1 | z | 76 | A | C5-N7-C8 | 5.14 | 106.47 | 103.90 |
| 1 | z | 15 | G | C4-C5-N7 | 5.14 | 112.86 | 110.80 |
| 1 | z | 50 | U | N1-C2-O2 | 5.09 | 126.37 | 122.80 |
| 1 | z | 19 | G | C5-C6-N1 | 5.08 | 114.04 | 111.50 |
| 1 | z | 71 | G | O4'-C1'-N9 | 5.07 | 112.25 | 108.20 |
| 1 | z | 28 | G | C4-C5-N7 | 5.06 | 112.82 | 110.80 |
| 1 | z | 19 | G | N7-C8-N9 | -5.05 | 110.57 | 113.10 |
| 1 | z | 73 | A | C4-C5-C6 | -5.04 | 114.48 | 117.00 |
| 1 | z | 18 | G | C5-N7-C8 | 5.03 | 106.82 | 104.30 |
| 1 | z | 10 | G | C4-C5-N7 | 5.03 | 112.81 | 110.80 |
| 1 | z | 58 | A | C4-C5-N7 | 5.02 | 113.21 | 110.70 |
| 1 | z | 76 | A | C8-N9-C4 | -5.01 | 103.80 | 105.80 |
| 1 | z | 73 | A | C8-N9-C4 | 5.01 | 107.80 | 105.80 |

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 | z | 1628 | 0 | 833 | 0 | 0 |
| All | All | 1628 | 0 | 833 | 0 | 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 104.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains

There are no protein molecules in this entry.

### 5.3.3 RNA

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | z | 73/76 (96%) | 27 (36%) | 0 |

All (27) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | z | 2 | C |
| 1 | z | 7 | A |
| 1 | z | 8 | 4SU |
| 1 | z | 9 | A |
| 1 | z | 16 | H2U |
| 1 | z | 18 | G |
| 1 | z | 19 | G |
| 1 | z | 20 | H2U |
| 1 | z | 21 | A |
| 1 | z | 27 | G |
| 1 | z | 32 | PSU |
| 1 | z | 33 | U |
| 1 | z | 39 | PSU |
| 1 | z | 42 | C |
| 1 | z | 45 | U |
| 1 | z | 46 | 7MG |
| 1 | z | 48 | C |
| 1 | z | 49 | C |
| 1 | z | 54 | 5MU |
| 1 | z | 55 | PSU |
| 1 | z | 59 | U |
| 1 | z | 61 | C |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | z | 63 | G |
| 1 | z | 65 | G |
| 1 | z | 67 | C |
| 1 | z | 72 | C |
| 1 | z | 76 | A |

There are no RNA pucker outliers to report.

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

9 non-standard protein/DNA/RNA residues are modelled in this entry.

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 | $\#\|Z\| > 2$ |
| 1 | H2U | z | 16 | 1 | 17,21,22 | 1.48 | 2 (11%) | 23,30,33 | 1.36 | 5 (21%) |
| 1 | H2U | z | 20 | 1 | 17,21,22 | 1.23 | 3 (17%) | 23,30,33 | 1.37 | 3 (13%) |
| 1 | PSU | z | 32 | 1 | 15,21,22 | 1.30 | 3 (20%) | 16,30,33 | 2.44 | 8 (50%) |
| 1 | MIA | z | 37 | 1 | 22,31,32 | 1.95 | 5 (22%) | 26,44,47 | 2.36 | 9 (34%) |
| 1 | PSU | z | 39 | 1 | 15,21,22 | 2.49 | 3 (20%) | 16,30,33 | 2.60 | 5 (31%) |
| 1 | 7MG | z | 46 | 1 | 20,26,27 | 2.99 | 9 (45%) | 23,39,42 | 2.60 | 7 (30%) |
| 1 | 5MU | z | 54 | 1 | 13,22,23 | 2.04 | 5 (38%) | 16,32,35 | 3.14 | 4 (25%) |
| 1 | PSU | z | 55 | 1 | 15,21,22 | 2.71 | 2 (13%) | 16,30,33 | 3.03 | 5 (31%) |
| 1 | 4SU | z | 8 | 1 | 12,21,22 | 2.28 | 4 (33%) | 15,30,33 | 1.92 | 4 (26%) |

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 | H2U | z | 16 | 1 | - | 0/7/38/39 | 0/2/2/2 |
| 1 | H2U | z | 20 | 1 | - | 0/7/38/39 | 0/2/2/2 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 1 | PSU | z | 32 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | MIA | z | 37 | 1 | - | 0/11/33/34 | 0/3/3/3 |
| 1 | PSU | z | 39 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 7MG | z | 46 | 1 | - | 0/7/37/38 | 0/3/3/3 |
| 1 | 5MU | z | 54 | 1 | - | 0/3/25/26 | 0/2/2/2 |
| 1 | PSU | z | 55 | 1 | - | 0/7/25/26 | 0/2/2/2 |
| 1 | 4SU | z | 8 | 1 | - | 0/3/25/26 | 0/2/2/2 |

All (36) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | z | 55 | PSU | C5-C1' | -9.28 | 1.44 | 1.52 |
| 1 | z | 39 | PSU | C5-C1' | -7.62 | 1.45 | 1.52 |
| 1 | z | 39 | PSU | O4'-C4' | -4.05 | 1.35 | 1.45 |
| 1 | z | 37 | MIA | C2-S10 | -3.62 | 1.72 | 1.75 |
| 1 | z | 37 | MIA | C2'-C1' | -3.58 | 1.47 | 1.53 |
| 1 | z | 46 | 7MG | C8-N9 | -3.58 | 1.40 | 1.45 |
| 1 | z | 54 | 5MU | C6-C5 | -3.02 | 1.32 | 1.40 |
| 1 | z | 46 | 7MG | C8-N7 | -2.84 | 1.30 | 1.43 |
| 1 | z | 54 | 5MU | C2-N3 | -2.79 | 1.32 | 1.38 |
| 1 | z | 20 | H2U | C2-N3 | -2.73 | 1.32 | 1.38 |
| 1 | z | 20 | H2U | C6-C5 | -2.50 | 1.48 | 1.52 |
| 1 | z | 8 | 4SU | C2'-C1' | -2.27 | 1.50 | 1.53 |
| 1 | z | 46 | 7MG | C2-N3 | -2.12 | 1.31 | 1.35 |
| 1 | z | 20 | H2U | O4'-C1' | 2.02 | 1.47 | 1.42 |
| 1 | z | 54 | 5MU | C4-N3 | 2.07 | 1.36 | 1.33 |
| 1 | z | 32 | PSU | C2-N1 | 2.19 | 1.42 | 1.38 |
| 1 | z | 46 | 7MG | C2-N2 | 2.35 | 1.39 | 1.34 |
| 1 | z | 39 | PSU | C2-N1 | 2.44 | 1.43 | 1.38 |
| 1 | z | 32 | PSU | C2'-C1' | 2.47 | 1.56 | 1.53 |
| 1 | z | 32 | PSU | C4-N3 | 2.55 | 1.37 | 1.33 |
| 1 | z | 55 | PSU | C2-N1 | 2.59 | 1.43 | 1.38 |
| 1 | z | 37 | MIA | C16-C14 | 2.69 | 1.67 | 1.51 |
| 1 | z | 16 | H2U | O4-C4 | 2.89 | 1.29 | 1.23 |
| 1 | z | 46 | 7MG | CM7-N7 | 2.95 | 1.51 | 1.46 |
| 1 | z | 54 | 5MU | O4-C4 | 3.11 | 1.32 | 1.24 |
| 1 | z | 37 | MIA | C2-N1 | 3.16 | 1.39 | 1.34 |
| 1 | z | 16 | H2U | C1'-N1 | 3.43 | 1.53 | 1.45 |
| 1 | z | 8 | 4SU | C6-C5 | 3.44 | 1.45 | 1.38 |
| 1 | z | 54 | 5MU | O4'-C1' | 3.45 | 1.46 | 1.41 |
| 1 | z | 8 | 4SU | C6-N1 | 3.58 | 1.40 | 1.35 |
| 1 | z | 46 | 7MG | C4-N3 | 4.16 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | z | 46 | 7MG | C6-C5 | 4.53 | 1.47 | 1.41 |
| 1 | z | 37 | MIA | C6-N1 | 4.59 | 1.39 | 1.33 |
| 1 | z | 46 | 7MG | C2-N1 | 4.60 | 1.44 | 1.35 |
| 1 | z | 8 | 4SU | O4'-C1' | 4.63 | 1.47 | 1.41 |
| 1 | z | 46 | 7MG | C6-N1 | 8.28 | 1.48 | 1.33 |

All (50) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | z | 46 | 7MG | C5-C6-N1 | -7.67 | 111.97 | 123.39 |
| 1 | z | 54 | 5MU | C5-C4-N3 | -7.34 | 119.19 | 125.35 |
| 1 | z | 39 | PSU | C4'-O4'-C1' | -6.91 | 102.42 | 109.54 |
| 1 | z | 55 | PSU | C5-C1'-C2' | -6.88 | 103.75 | 115.44 |
| 1 | z | 37 | MIA | C12-N6-C6 | -5.97 | 116.55 | 123.46 |
| 1 | z | 55 | PSU | C4'-O4'-C1' | -5.48 | 103.90 | 109.54 |
| 1 | z | 55 | PSU | C5-C6-N1 | -5.10 | 117.26 | 124.38 |
| 1 | z | 8 | 4SU | C5-C4-N3 | -4.60 | 118.68 | 123.56 |
| 1 | z | 37 | MIA | C5-C6-N1 | -3.88 | 116.64 | 120.58 |
| 1 | z | 8 | 4SU | C5'-C4'-C3' | -3.48 | 101.74 | 115.20 |
| 1 | z | 37 | MIA | C2'-C1'-N9 | -3.22 | 104.84 | 113.47 |
| 1 | z | 39 | PSU | C5-C6-N1 | -3.14 | 120.00 | 124.38 |
| 1 | z | 32 | PSU | C5-C6-N1 | -3.00 | 120.20 | 124.38 |
| 1 | z | 37 | MIA | C1'-N9-C4 | -2.85 | 123.63 | 126.81 |
| 1 | z | 46 | 7MG | N1-C2-N3 | -2.67 | 121.14 | 125.51 |
| 1 | z | 54 | 5MU | O3'-C3'-C4' | -2.63 | 103.17 | 111.01 |
| 1 | z | 20 | H2U | C4-N3-C2 | -2.59 | 123.42 | 125.77 |
| 1 | z | 20 | H2U | C5-C6-N1 | -2.56 | 107.96 | 110.76 |
| 1 | z | 46 | 7MG | C5'-C4'-C3' | -2.37 | 106.03 | 115.20 |
| 1 | z | 32 | PSU | C5'-C4'-C3' | -2.24 | 106.55 | 115.20 |
| 1 | z | 37 | MIA | O4'-C4'-C3' | -2.07 | 100.95 | 105.16 |
| 1 | z | 39 | PSU | O4'-C1'-C2' | 2.08 | 106.94 | 104.69 |
| 1 | z | 32 | PSU | O4'-C4'-C3' | 2.09 | 109.41 | 105.16 |
| 1 | z | 16 | H2U | C3'-C2'-C1' | 2.12 | 105.70 | 101.44 |
| 1 | z | 46 | 7MG | C3'-C2'-C1' | 2.13 | 105.72 | 101.44 |
| 1 | z | 46 | 7MG | C8-N9-C1' | 2.14 | 128.84 | 122.43 |
| 1 | z | 8 | 4SU | O4'-C4'-C5' | 2.17 | 117.06 | 109.29 |
| 1 | z | 32 | PSU | O3'-C3'-C4' | 2.25 | 117.72 | 111.01 |
| 1 | z | 20 | H2U | C1'-N1-C2 | 2.29 | 121.39 | 118.19 |
| 1 | z | 16 | H2U | O4-C4-N3 | 2.30 | 124.05 | 120.46 |
| 1 | z | 8 | 4SU | C2'-C3'-C4' | 2.30 | 107.34 | 102.64 |
| 1 | z | 16 | H2U | C4-N3-C2 | 2.30 | 127.86 | 125.77 |
| 1 | z | 32 | PSU | O5'-C5'-C4' | 2.36 | 117.57 | 109.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | z | 32 | PSU | O4'-C1'-C2' | 2.39 | 107.27 | 104.69 |
| 1 | z | 39 | PSU | C4-C5-C1' | 2.46 | 125.36 | 121.22 |
| 1 | z | 37 | MIA | C13-C12-N6 | 2.61 | 117.14 | 112.25 |
| 1 | z | 16 | H2U | C5-C6-N1 | 2.69 | 113.71 | 110.76 |
| 1 | z | 16 | H2U | O4'-C4'-C3' | 2.76 | 110.75 | 105.16 |
| 1 | z | 37 | MIA | C2-N1-C6 | 2.89 | 121.07 | 113.13 |
| 1 | z | 54 | 5MU | C5M-C5-C4 | 3.02 | 123.31 | 119.97 |
| 1 | z | 37 | MIA | C4'-O4'-C1' | 3.03 | 112.85 | 109.64 |
| 1 | z | 55 | PSU | C4-N3-C2 | 3.19 | 117.82 | 115.16 |
| 1 | z | 46 | 7MG | O4'-C4'-C3' | 3.25 | 111.75 | 105.16 |
| 1 | z | 32 | PSU | C3'-C2'-C1' | 3.44 | 105.79 | 101.71 |
| 1 | z | 55 | PSU | C3'-C2'-C1' | 4.94 | 107.57 | 101.71 |
| 1 | z | 37 | MIA | C11-S10-C2 | 5.39 | 106.11 | 102.31 |
| 1 | z | 39 | PSU | C4-N3-C2 | 5.42 | 119.68 | 115.16 |
| 1 | z | 32 | PSU | C4-N3-C2 | 6.23 | 120.35 | 115.16 |
| 1 | z | 46 | 7MG | C6-N1-C2 | 6.92 | 123.99 | 115.88 |
| 1 | z | 54 | 5MU | C4-N3-C2 | 8.41 | 122.18 | 115.16 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.