# Full wwPDB EM Validation Report (i)

Apr 29, 2024 – 09:05 am BST

| | | |
|---|---|---|
| PDB ID | : | 4BKK |
| EMDB ID | : | EMD-2369 |
| Title | : | The Respiratory Syncytial Virus nucleoprotein-RNA complex forms a left-handed helical nucleocapsid. |
| Authors | : | Bakker, S.E.; Duquerroy, S.; Galloux, M.; Loney, C.; Conner, E.; Eleouet, J.F.; Rey, F.A.; Bhella, D. |
| Deposited on | : | 2013-04-26 |
| Resolution | : | Not provided |
| Based on initial model | : | 2WJ8 |

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

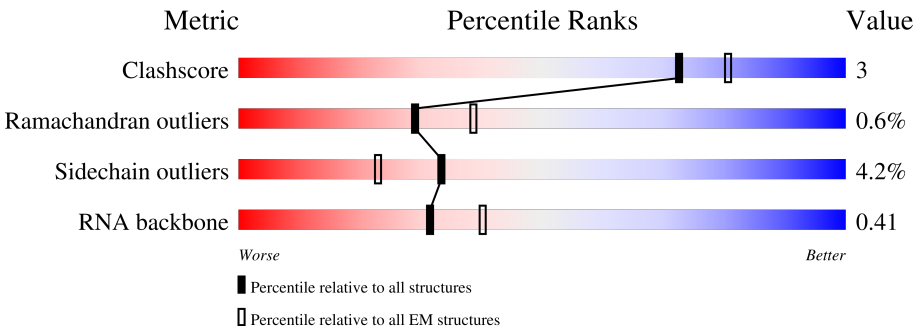
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev92 |
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | FAILED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 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 unknown.

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 | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 161 | 86% 14% |
| 2 | B | 391 | 86% 8% • 5% |
| 2 | C | 391 | 85% 9% 5% |
| 2 | D | 391 | 85% 9% • 5% |
| 2 | E | 391 | 85% 9% • 5% |
| 2 | F | 391 | 85% 9% • 5% |
| 2 | G | 391 | 85% 9% • 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | H | 391 | 85% 9% • 5% |
| 2 | I | 391 | 85% 9% • 5% |
| 2 | J | 391 | 85% 9% • 5% |
| 2 | K | 391 | 85% 9% • 5% |
| 2 | L | 391 | 83% 10% • 5% |
| 2 | M | 391 | 83% 10% • 5% |
| 2 | N | 391 | 83% 10% • 5% |
| 2 | O | 391 | 84% 9% • 5% |
| 2 | P | 391 | 84% 9% • 5% |
| 2 | Q | 391 | 84% 9% • 5% |
| 2 | R | 391 | 84% 9% • 5% |
| 2 | S | 391 | 85% 9% • 5% |
| 2 | T | 391 | 84% 9% • 5% |
| 2 | U | 391 | 84% 9% • 5% |
| 2 | V | 391 | 85% 8% • 5% |
| 2 | W | 391 | 85% 9% • 5% |
| 2 | X | 391 | 85% 9% • 5% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 69483 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 RNA (161-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | |
| 1 | A | 161 | 3220 | 1449 | 483 | 1127 | 161 | 0 | 0 |

- Molecule 2 is a protein called NUCLEOPROTEIN.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | C | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | D | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | E | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | F | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | G | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | H | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | I | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | J | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | K | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | L | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | M | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | N | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | O | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |

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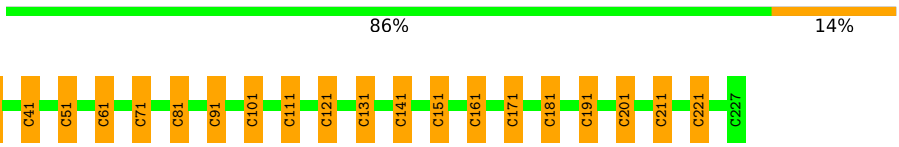
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | P | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | Q | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | R | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | S | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | T | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | U | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | V | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | W | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |
| 2 | X | 370 | 2881 | 1824 | 501 | 540 | 16 | 0 | 0 |

# 3 Residue-property plots (i)

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. 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.

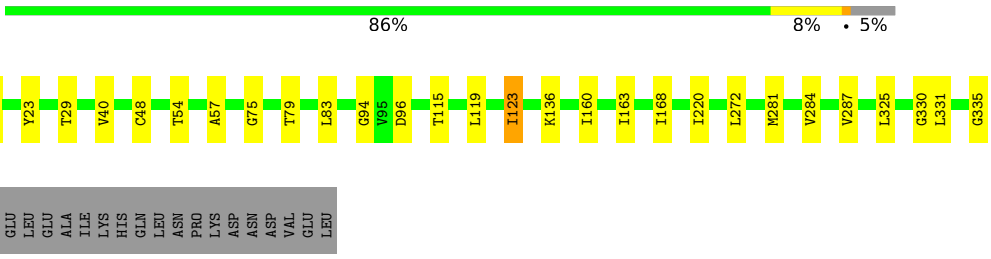
• Molecule 1: RNA (161-MER)

Chain A:



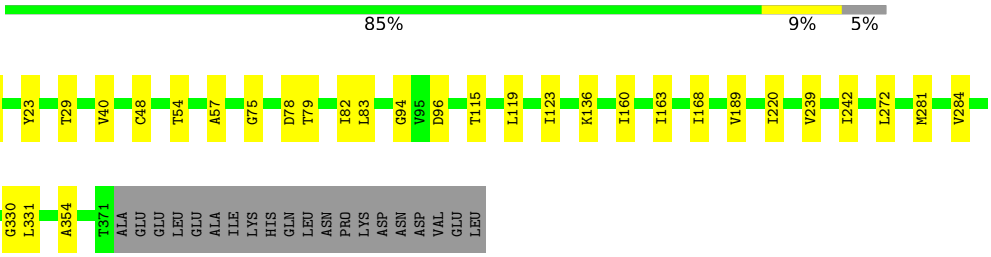

• Molecule 2: NUCLEOPROTEIN

Chain B:



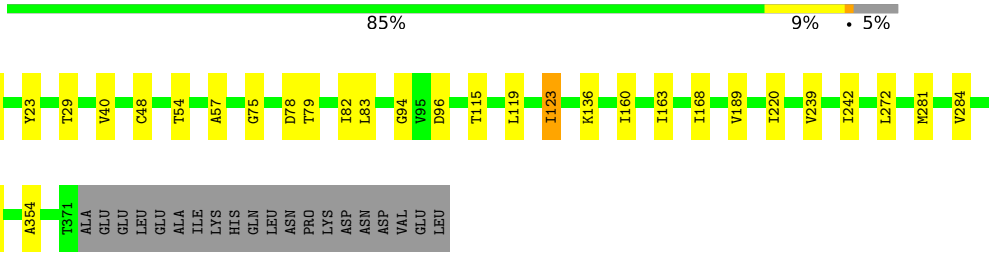

• Molecule 2: NUCLEOPROTEIN

Chain C:



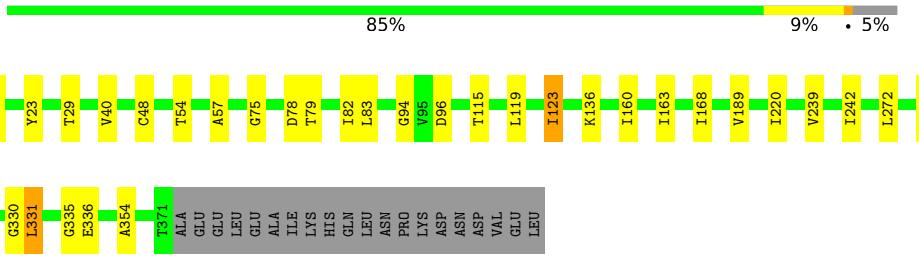

• Molecule 2: NUCLEOPROTEIN

Chain D:



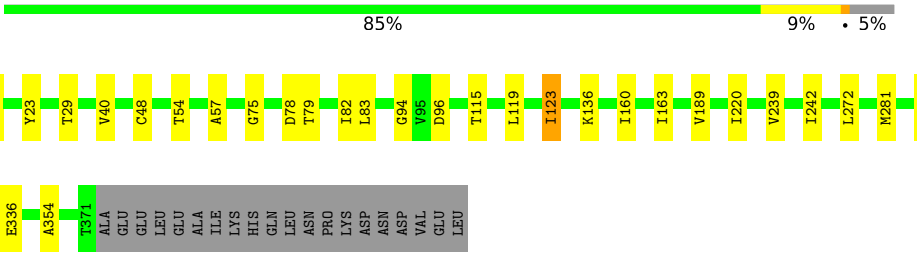

• Molecule 2: NUCLEOPROTEIN

Chain E:



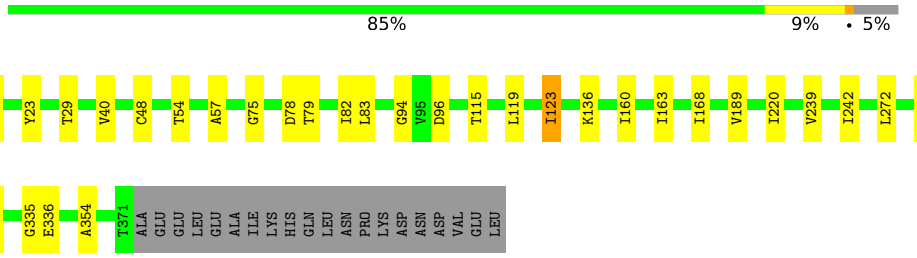

• Molecule 2: NUCLEOPROTEIN

Chain F:



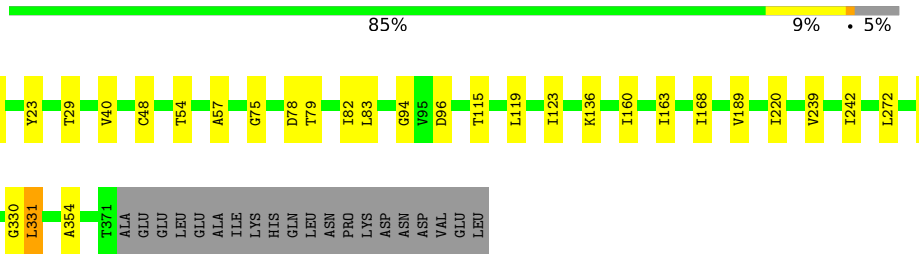

• Molecule 2: NUCLEOPROTEIN

Chain G:



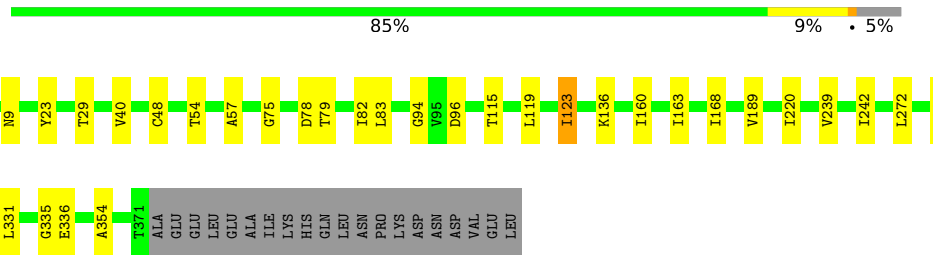

• Molecule 2: NUCLEOPROTEIN

Chain H:




• Molecule 2: NUCLEOPROTEIN

Chain I:




• Molecule 2: NUCLEOPROTEIN

Chain J: 85% 9% • 5%

MET A2 L3 V6 N9 Y23 T29 V40 C48 T54 A57 G75 D78 T79 I82 L83 G94 V95 D96 T115 L119 I123 K136 I160 I163 I168 V189 I220 V239 I242 L272 M281 V284

V287 Y288 Y301 L325 G330 L331 A354 T371 ALA GLU GLU LEU GLU ALA ILE LYS HIS GLN LEU ASN PRO LYS ASP ASN ASP VAL GLU LEU

• Molecule 2: NUCLEOPROTEIN

Chain K: 85% 9% • 5%

MET A2 L3 V6 N9 Y23 T29 V40 C48 T54 A57 G75 D78 T79 I82 L83 G94 V95 D96 T115 L119 I123 K136 I160 I163 V189 I220 V239 I242 L272 A275 M281 V284

V287 Y288 L325 G330 L331 A354 T371 ALA GLU GLU LEU GLU ALA ILE LYS HIS GLN LEU ASN PRO LYS ASP ASN ASP VAL GLU LEU

• Molecule 2: NUCLEOPROTEIN

Chain L: 83% 10% • 5%

MET A2 L3 V6 N9 Y23 T29 V40 C48 T54 A57 G75 D78 T79 I82 L83 G94 V95 D96 T115 L119 I123 K136 I160 I163 V189 I220 V239 I242 I270 M271 L272 A275 M281

V284 V287 Y288 L325 G330 L331 G335 E336 A354 E359 N360 G361 V362 I363 T371 ALA GLU GLU LEU GLU ALA ILE LYS HIS GLN LEU ASN PRO LYS ASP ASN ASP VAL GLU LEU

• Molecule 2: NUCLEOPROTEIN

Chain M: 83% 10% • 5%

MET A2 L3 V6 N9 Y23 T29 V40 C48 T54 A57 G75 D78 T79 I82 L83 G94 V95 D96 T115 L119 I123 K136 I160 I163 I168 V189 I220 V239 I242 I270 M271 L272 A275

M281 V284 V287 Y288 Y301 L325 G330 L331 A354 E359 N360 G361 V362 I363 T371 ALA GLU GLU LEU GLU ALA ILE LYS HIS GLN LEU ASN PRO LYS ASP ASN ASP VAL GLU LEU

• Molecule 2: NUCLEOPROTEIN

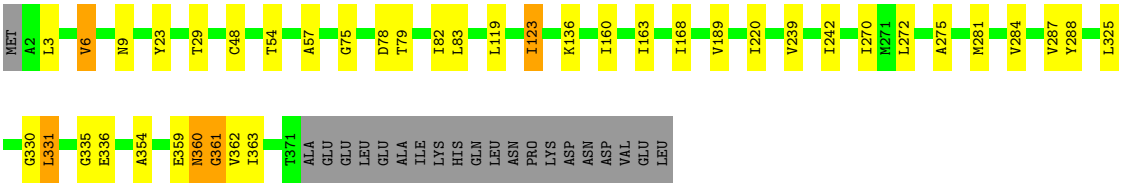
Chain N: 83% 10% • 5%

MET A2 L3 V6 N9 Y23 T29 V40 C48 T54 A57 G75 D78 T79 I82 L83 G94 V95 D96 T115 L119 I123 K136 I160 I163 I168 V189 I220 V239 I242 I270 M271 L272 A275

M281 V284 V287 Y288 L325 G330 L331 G335 E336 A354 E359 N360 G361 V362 I363 T371 ALA GLU GLU LEU GLU ALA ILE LYS HIS GLN LEU ASN PRO LYS ASP ASN ASP VAL GLU LEU

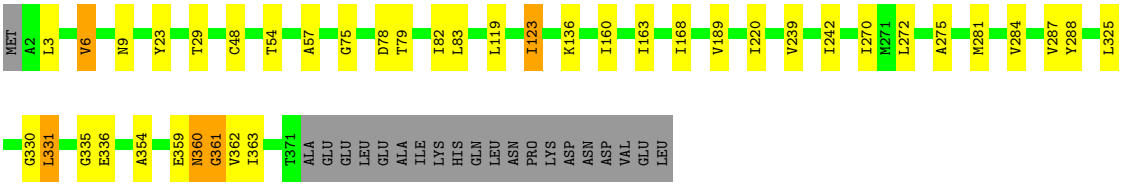
• Molecule 2: NUCLEOPROTEIN

Chain O:



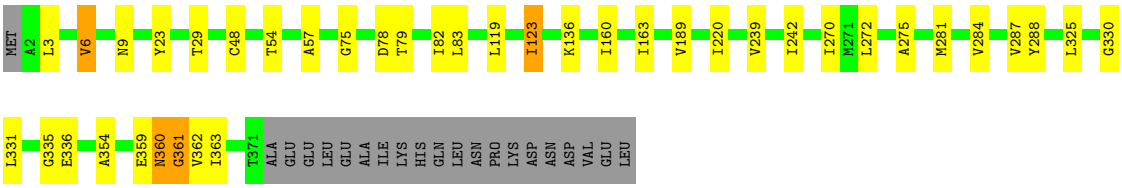

• Molecule 2: NUCLEOPROTEIN

Chain P:



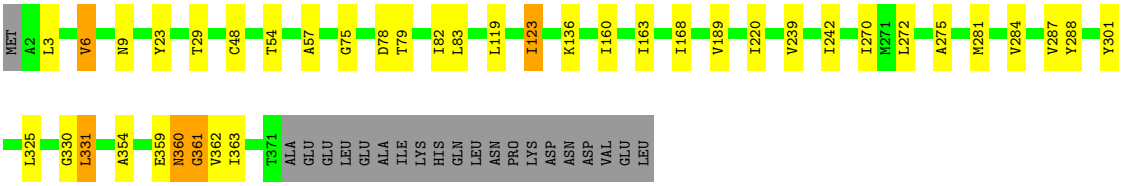

• Molecule 2: NUCLEOPROTEIN

Chain Q:



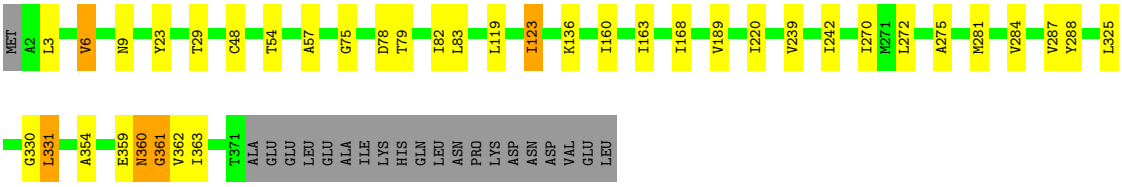

• Molecule 2: NUCLEOPROTEIN

Chain R:



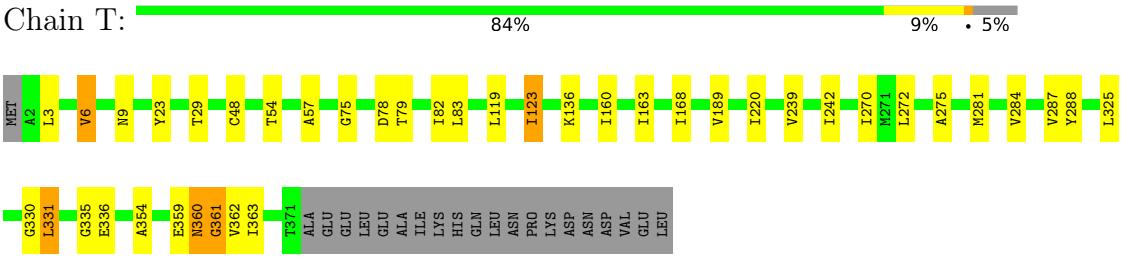

• Molecule 2: NUCLEOPROTEIN

Chain S:



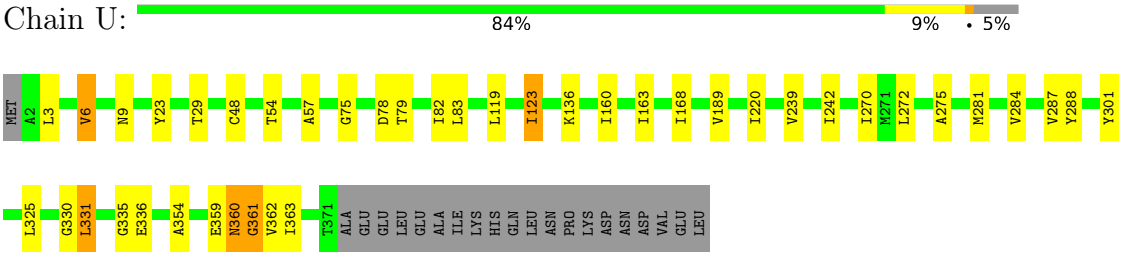

• Molecule 2: NUCLEOPROTEIN

Chain T:



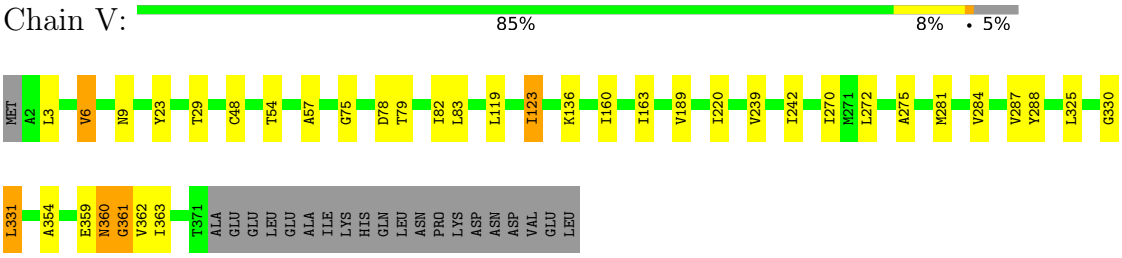

• Molecule 2: NUCLEOPROTEIN

Chain U:



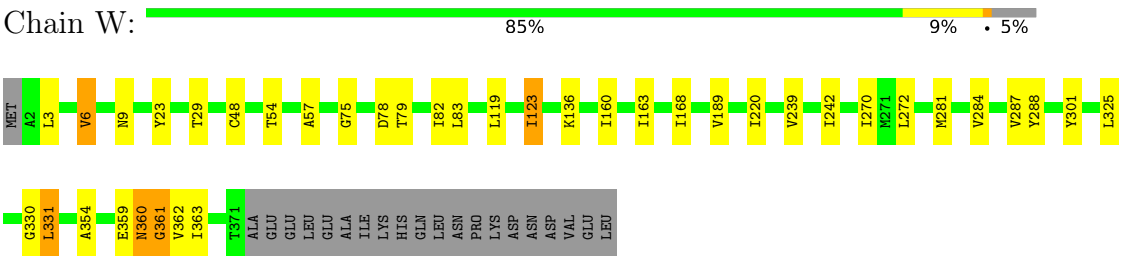

• Molecule 2: NUCLEOPROTEIN

Chain V:



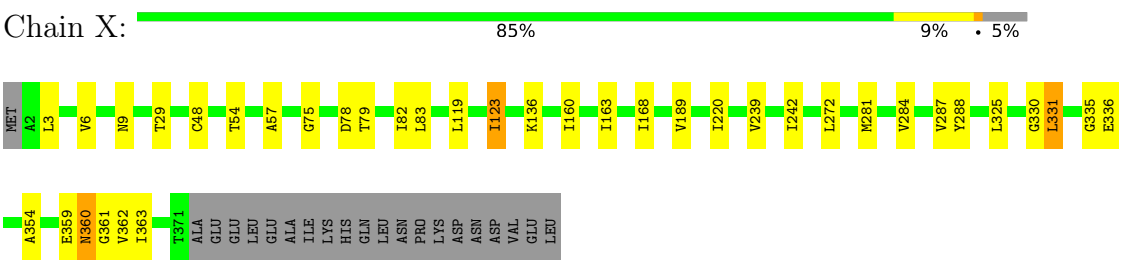

• Molecule 2: NUCLEOPROTEIN

Chain W:




• Molecule 2: NUCLEOPROTEIN

Chain X:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | TOMOGRAPHY | Depositor |
| Imposed symmetry | HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided | Depositor |
| Number of tilted images used | 911 | Depositor |
| Resolution determination method | Not provided | |
| CTF correction method | Not provided | |
| Microscope | JEOL 2200FSC | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/Å^2$) | 131 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 40000 | Depositor |
| Image detector | GATAN ULTRASCAN 4000 (4k x 4k) | 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).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| >5$ | RMSZ | $\#\|Z\| >5$ |
| 1 | A | 0.22 | 0/3541 | 0.73 | 0/5470 |
| 2 | B | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | C | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | D | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | E | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | F | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | G | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | H | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | I | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | J | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | K | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | L | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | M | 0.27 | 0/2929 | 0.43 | 0/3946 |
| 2 | N | 0.27 | 0/2929 | 0.43 | 0/3946 |
| 2 | O | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | P | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | Q | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | R | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | S | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | T | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | U | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | V | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | W | 0.27 | 0/2929 | 0.42 | 0/3946 |
| 2 | X | 0.27 | 0/2929 | 0.42 | 0/3946 |
| All | All | 0.27 | 0/70908 | 0.45 | 0/96228 |

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 | 3220 | 0 | 1772 | 76 | 0 |
| 2 | B | 2881 | 0 | 2915 | 17 | 0 |
| 2 | C | 2881 | 0 | 2915 | 24 | 0 |
| 2 | D | 2881 | 0 | 2915 | 22 | 0 |
| 2 | E | 2881 | 0 | 2915 | 24 | 0 |
| 2 | F | 2881 | 0 | 2915 | 26 | 0 |
| 2 | G | 2881 | 0 | 2915 | 23 | 0 |
| 2 | H | 2881 | 0 | 2915 | 25 | 0 |
| 2 | I | 2881 | 0 | 2915 | 23 | 0 |
| 2 | J | 2881 | 0 | 2915 | 23 | 0 |
| 2 | K | 2881 | 0 | 2915 | 25 | 0 |
| 2 | L | 2881 | 0 | 2915 | 36 | 0 |
| 2 | M | 2881 | 0 | 2915 | 36 | 0 |
| 2 | N | 2881 | 0 | 2915 | 37 | 0 |
| 2 | O | 2881 | 0 | 2915 | 28 | 0 |
| 2 | P | 2881 | 0 | 2915 | 30 | 0 |
| 2 | Q | 2881 | 0 | 2915 | 28 | 0 |
| 2 | R | 2881 | 0 | 2915 | 28 | 0 |
| 2 | S | 2881 | 0 | 2915 | 29 | 0 |
| 2 | T | 2881 | 0 | 2915 | 27 | 0 |
| 2 | U | 2881 | 0 | 2915 | 30 | 0 |
| 2 | V | 2881 | 0 | 2915 | 28 | 0 |
| 2 | W | 2881 | 0 | 2915 | 26 | 0 |
| 2 | X | 2881 | 0 | 2915 | 25 | 0 |
| All | All | 69483 | 0 | 68817 | 472 | 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 3.

All (472) 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:221:C:H5” | 2:C:189:VAL:HG22 | 1.77 | 0.66 |
| 1:A:211:C:H5” | 2:D:189:VAL:HG22 | 1.77 | 0.66 |
| 1:A:101:C:H5” | 2:O:189:VAL:HG22 | 1.78 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:11:C:H5” | 2:X:189:VAL:HG22 | 1.78 | 0.66 |
| 1:A:91:C:H5” | 2:P:189:VAL:HG22 | 1.78 | 0.66 |
| 1:A:121:C:H5” | 2:M:189:VAL:HG22 | 1.78 | 0.65 |
| 1:A:81:C:H5” | 2:Q:189:VAL:HG22 | 1.78 | 0.65 |
| 1:A:161:C:H5” | 2:I:189:VAL:HG22 | 1.77 | 0.65 |
| 1:A:131:C:H5” | 2:L:189:VAL:HG22 | 1.78 | 0.65 |
| 1:A:181:C:H5” | 2:G:189:VAL:HG22 | 1.78 | 0.65 |
| 1:A:191:C:H5” | 2:F:189:VAL:HG22 | 1.78 | 0.65 |
| 1:A:141:C:H5” | 2:K:189:VAL:HG22 | 1.78 | 0.65 |
| 1:A:21:C:H5” | 2:W:189:VAL:HG22 | 1.78 | 0.65 |
| 1:A:61:C:H5” | 2:S:189:VAL:HG22 | 1.78 | 0.65 |
| 1:A:71:C:H5” | 2:R:189:VAL:HG22 | 1.78 | 0.64 |
| 1:A:111:C:H5” | 2:N:189:VAL:HG22 | 1.78 | 0.64 |
| 1:A:151:C:H5” | 2:J:189:VAL:HG22 | 1.78 | 0.64 |
| 1:A:171:C:H5” | 2:H:189:VAL:HG22 | 1.77 | 0.64 |
| 1:A:201:C:H5” | 2:E:189:VAL:HG22 | 1.78 | 0.64 |
| 1:A:31:C:H5” | 2:V:189:VAL:HG22 | 1.78 | 0.64 |
| 1:A:51:C:H5” | 2:T:189:VAL:HG22 | 1.78 | 0.64 |
| 1:A:41:C:H5” | 2:U:189:VAL:HG22 | 1.78 | 0.63 |
| 1:A:161:C:C5’ | 2:I:189:VAL:HG22 | 2.30 | 0.61 |
| 1:A:31:C:C5’ | 2:V:189:VAL:HG22 | 2.31 | 0.61 |
| 1:A:151:C:C5’ | 2:J:189:VAL:HG22 | 2.31 | 0.61 |
| 1:A:81:C:C5’ | 2:Q:189:VAL:HG22 | 2.31 | 0.61 |
| 1:A:101:C:C5’ | 2:O:189:VAL:HG22 | 2.31 | 0.61 |
| 1:A:131:C:C5’ | 2:L:189:VAL:HG22 | 2.31 | 0.61 |
| 1:A:201:C:C5’ | 2:E:189:VAL:HG22 | 2.31 | 0.61 |
| 1:A:181:C:C5’ | 2:G:189:VAL:HG22 | 2.31 | 0.61 |
| 1:A:211:C:C5’ | 2:D:189:VAL:HG22 | 2.30 | 0.61 |
| 1:A:91:C:C5’ | 2:P:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:191:C:C5’ | 2:F:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:51:C:C5’ | 2:T:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:171:C:C5’ | 2:H:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:141:C:C5’ | 2:K:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:21:C:C5’ | 2:W:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:221:C:C5’ | 2:C:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:61:C:C5’ | 2:S:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:11:C:C5’ | 2:X:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:41:C:C5’ | 2:U:189:VAL:HG22 | 2.31 | 0.60 |
| 1:A:71:C:C5’ | 2:R:189:VAL:HG22 | 2.31 | 0.59 |
| 1:A:121:C:C5’ | 2:M:189:VAL:HG22 | 2.31 | 0.59 |
| 1:A:111:C:C5’ | 2:N:189:VAL:HG22 | 2.31 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:X:119:LEU:HD11 | 2:X:123:ILE:HD11 | 1.86 | 0.57 |
| 2:D:40:VAL:CG2 | 2:D:96:ASP:HA | 2.34 | 0.57 |
| 2:G:40:VAL:CG2 | 2:G:96:ASP:HA | 2.34 | 0.57 |
| 2:L:40:VAL:CG2 | 2:L:96:ASP:HA | 2.34 | 0.57 |
| 2:S:119:LEU:HD11 | 2:S:123:ILE:HD11 | 1.87 | 0.57 |
| 2:C:119:LEU:HD11 | 2:C:123:ILE:HD11 | 1.87 | 0.57 |
| 2:N:40:VAL:CG2 | 2:N:96:ASP:HA | 2.35 | 0.57 |
| 2:I:40:VAL:CG2 | 2:I:96:ASP:HA | 2.35 | 0.56 |
| 2:B:40:VAL:CG2 | 2:B:96:ASP:HA | 2.35 | 0.56 |
| 2:J:40:VAL:CG2 | 2:J:96:ASP:HA | 2.36 | 0.56 |
| 2:H:119:LEU:HD11 | 2:H:123:ILE:HD11 | 1.87 | 0.56 |
| 2:C:40:VAL:CG2 | 2:C:96:ASP:HA | 2.36 | 0.56 |
| 2:F:40:VAL:CG2 | 2:F:96:ASP:HA | 2.35 | 0.56 |
| 2:H:40:VAL:CG2 | 2:H:96:ASP:HA | 2.36 | 0.56 |
| 2:P:119:LEU:HD11 | 2:P:123:ILE:HD11 | 1.88 | 0.56 |
| 2:K:40:VAL:CG2 | 2:K:96:ASP:HA | 2.35 | 0.55 |
| 2:K:119:LEU:HD11 | 2:K:123:ILE:HD11 | 1.88 | 0.55 |
| 2:L:239:VAL:HA | 2:L:242:ILE:HD12 | 1.88 | 0.55 |
| 2:M:40:VAL:CG2 | 2:M:96:ASP:HA | 2.36 | 0.55 |
| 2:V:239:VAL:HA | 2:V:242:ILE:HD12 | 1.88 | 0.55 |
| 2:E:40:VAL:CG2 | 2:E:96:ASP:HA | 2.36 | 0.55 |
| 2:G:239:VAL:HA | 2:G:242:ILE:HD12 | 1.88 | 0.55 |
| 2:F:119:LEU:HD11 | 2:F:123:ILE:HD11 | 1.89 | 0.55 |
| 2:N:119:LEU:HD11 | 2:N:123:ILE:HD11 | 1.89 | 0.55 |
| 2:Q:239:VAL:HA | 2:Q:242:ILE:HD12 | 1.88 | 0.55 |
| 2:C:115:THR:OG1 | 2:M:360:ASN:OD1 | 2.25 | 0.55 |
| 2:I:239:VAL:HA | 2:I:242:ILE:HD12 | 1.89 | 0.55 |
| 2:H:115:THR:OG1 | 2:R:360:ASN:OD1 | 2.25 | 0.55 |
| 2:W:239:VAL:HA | 2:W:242:ILE:HD12 | 1.89 | 0.54 |
| 2:M:119:LEU:HD11 | 2:M:123:ILE:HD11 | 1.89 | 0.54 |
| 2:T:239:VAL:HA | 2:T:242:ILE:HD12 | 1.88 | 0.54 |
| 2:U:119:LEU:HD11 | 2:U:123:ILE:HD11 | 1.89 | 0.54 |
| 2:H:239:VAL:HA | 2:H:242:ILE:HD12 | 1.89 | 0.54 |
| 2:J:239:VAL:HA | 2:J:242:ILE:HD12 | 1.89 | 0.54 |
| 2:M:239:VAL:HA | 2:M:242:ILE:HD12 | 1.89 | 0.54 |
| 2:R:239:VAL:HA | 2:R:242:ILE:HD12 | 1.89 | 0.54 |
| 2:O:239:VAL:HA | 2:O:242:ILE:HD12 | 1.88 | 0.54 |
| 2:K:115:THR:OG1 | 2:U:360:ASN:OD1 | 2.26 | 0.54 |
| 2:I:119:LEU:HD11 | 2:I:123:ILE:HD11 | 1.90 | 0.54 |
| 2:K:96:ASP:OD2 | 2:U:360:ASN:HB3 | 2.09 | 0.53 |
| 2:Q:119:LEU:HD11 | 2:Q:123:ILE:HD11 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R:119:LEU:HD11 | 2:R:123:ILE:HD11 | 1.91 | 0.53 |
| 2:D:239:VAL:HA | 2:D:242:ILE:HD12 | 1.88 | 0.53 |
| 2:N:239:VAL:HA | 2:N:242:ILE:HD12 | 1.89 | 0.53 |
| 2:V:119:LEU:HD11 | 2:V:123:ILE:HD11 | 1.90 | 0.53 |
| 2:S:239:VAL:HA | 2:S:242:ILE:HD12 | 1.90 | 0.53 |
| 2:E:239:VAL:HA | 2:E:242:ILE:HD12 | 1.89 | 0.53 |
| 2:X:239:VAL:HA | 2:X:242:ILE:HD12 | 1.90 | 0.53 |
| 2:K:239:VAL:HA | 2:K:242:ILE:HD12 | 1.90 | 0.53 |
| 2:D:119:LEU:HD11 | 2:D:123:ILE:HD11 | 1.91 | 0.53 |
| 2:F:239:VAL:HA | 2:F:242:ILE:HD12 | 1.89 | 0.53 |
| 2:U:239:VAL:HA | 2:U:242:ILE:HD12 | 1.91 | 0.52 |
| 2:C:96:ASP:OD2 | 2:M:360:ASN:HB3 | 2.09 | 0.52 |
| 2:P:239:VAL:HA | 2:P:242:ILE:HD12 | 1.90 | 0.52 |
| 2:H:96:ASP:OD2 | 2:R:360:ASN:HB3 | 2.10 | 0.52 |
| 2:C:239:VAL:HA | 2:C:242:ILE:HD12 | 1.90 | 0.52 |
| 2:X:48:CYS:HB3 | 2:X:160:ILE:HD12 | 1.92 | 0.52 |
| 2:F:96:ASP:OD2 | 2:P:360:ASN:HB3 | 2.10 | 0.52 |
| 2:D:48:CYS:HB3 | 2:D:160:ILE:HD12 | 1.92 | 0.51 |
| 2:M:96:ASP:OD2 | 2:W:360:ASN:HB3 | 2.10 | 0.51 |
| 2:P:48:CYS:HB3 | 2:P:160:ILE:HD12 | 1.92 | 0.51 |
| 2:W:119:LEU:HD11 | 2:W:123:ILE:HD11 | 1.92 | 0.51 |
| 2:I:48:CYS:HB3 | 2:I:160:ILE:HD12 | 1.92 | 0.51 |
| 2:N:48:CYS:HB3 | 2:N:160:ILE:HD12 | 1.92 | 0.51 |
| 2:F:48:CYS:HB3 | 2:F:160:ILE:HD12 | 1.92 | 0.51 |
| 2:E:48:CYS:HB3 | 2:E:160:ILE:HD12 | 1.93 | 0.51 |
| 2:O:48:CYS:HB3 | 2:O:160:ILE:HD12 | 1.93 | 0.51 |
| 2:B:48:CYS:HB3 | 2:B:160:ILE:HD12 | 1.92 | 0.51 |
| 2:M:48:CYS:HB3 | 2:M:160:ILE:HD12 | 1.93 | 0.51 |
| 2:C:48:CYS:HB3 | 2:C:160:ILE:HD12 | 1.93 | 0.51 |
| 2:N:96:ASP:OD2 | 2:X:360:ASN:HB3 | 2.11 | 0.51 |
| 2:L:48:CYS:HB3 | 2:L:160:ILE:HD12 | 1.92 | 0.51 |
| 2:Q:78:ASP:O | 2:Q:82:ILE:HG23 | 2.11 | 0.51 |
| 2:S:48:CYS:HB3 | 2:S:160:ILE:HD12 | 1.92 | 0.51 |
| 2:W:48:CYS:HB3 | 2:W:160:ILE:HD12 | 1.92 | 0.51 |
| 2:J:78:ASP:O | 2:J:82:ILE:HG23 | 2.11 | 0.50 |
| 2:L:96:ASP:OD2 | 2:V:360:ASN:HB3 | 2.11 | 0.50 |
| 2:N:96:ASP:HB2 | 2:X:360:ASN:HB3 | 1.93 | 0.50 |
| 2:J:48:CYS:HB3 | 2:J:160:ILE:HD12 | 1.93 | 0.50 |
| 2:D:78:ASP:O | 2:D:82:ILE:HG23 | 2.11 | 0.50 |
| 2:I:78:ASP:O | 2:I:82:ILE:HG23 | 2.12 | 0.50 |
| 2:K:48:CYS:HB3 | 2:K:160:ILE:HD12 | 1.92 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Q:48:CYS:HB3 | 2:Q:160:ILE:HD12 | 1.92 | 0.50 |
| 2:V:48:CYS:HB3 | 2:V:160:ILE:HD12 | 1.92 | 0.50 |
| 2:V:78:ASP:O | 2:V:82:ILE:HG23 | 2.12 | 0.50 |
| 2:E:78:ASP:O | 2:E:82:ILE:HG23 | 2.12 | 0.50 |
| 2:G:78:ASP:O | 2:G:82:ILE:HG23 | 2.11 | 0.50 |
| 2:J:96:ASP:OD2 | 2:T:360:ASN:HB3 | 2.12 | 0.50 |
| 2:F:78:ASP:O | 2:F:82:ILE:HG23 | 2.12 | 0.50 |
| 2:G:48:CYS:HB3 | 2:G:160:ILE:HD12 | 1.92 | 0.50 |
| 2:T:48:CYS:HB3 | 2:T:160:ILE:HD12 | 1.92 | 0.50 |
| 2:U:78:ASP:O | 2:U:82:ILE:HG23 | 2.12 | 0.50 |
| 2:C:78:ASP:O | 2:C:82:ILE:HG23 | 2.12 | 0.50 |
| 2:T:78:ASP:O | 2:T:82:ILE:HG23 | 2.12 | 0.50 |
| 2:D:96:ASP:HB2 | 2:N:360:ASN:HB3 | 1.94 | 0.50 |
| 2:G:96:ASP:OD2 | 2:Q:360:ASN:HB3 | 2.12 | 0.50 |
| 2:G:119:LEU:HD11 | 2:G:123:ILE:HD11 | 1.94 | 0.50 |
| 2:O:78:ASP:O | 2:O:82:ILE:HG23 | 2.12 | 0.50 |
| 2:R:48:CYS:HB3 | 2:R:160:ILE:HD12 | 1.93 | 0.50 |
| 2:R:78:ASP:O | 2:R:82:ILE:HG23 | 2.12 | 0.50 |
| 2:D:96:ASP:OD2 | 2:N:360:ASN:HB3 | 2.12 | 0.49 |
| 2:W:78:ASP:O | 2:W:82:ILE:HG23 | 2.12 | 0.49 |
| 2:H:48:CYS:HB3 | 2:H:160:ILE:HD12 | 1.93 | 0.49 |
| 2:I:96:ASP:OD2 | 2:S:360:ASN:HB3 | 2.12 | 0.49 |
| 2:K:78:ASP:O | 2:K:82:ILE:HG23 | 2.12 | 0.49 |
| 2:M:330:GLY:HA3 | 2:M:354:ALA:HB3 | 1.94 | 0.49 |
| 2:N:78:ASP:O | 2:N:82:ILE:HG23 | 2.12 | 0.49 |
| 2:P:78:ASP:O | 2:P:82:ILE:HG23 | 2.12 | 0.49 |
| 2:P:281:MET:HA | 2:P:284:VAL:HG22 | 1.93 | 0.49 |
| 2:E:96:ASP:OD2 | 2:O:360:ASN:HB3 | 2.12 | 0.49 |
| 2:L:78:ASP:O | 2:L:82:ILE:HG23 | 2.11 | 0.49 |
| 2:L:119:LEU:HD11 | 2:L:123:ILE:HD11 | 1.93 | 0.49 |
| 2:U:48:CYS:HB3 | 2:U:160:ILE:HD12 | 1.92 | 0.49 |
| 2:U:281:MET:HA | 2:U:284:VAL:HG22 | 1.93 | 0.49 |
| 2:R:75:GLY:O | 2:R:79:THR:HG22 | 2.13 | 0.49 |
| 2:E:75:GLY:O | 2:E:79:THR:HG22 | 2.13 | 0.49 |
| 2:E:281:MET:HA | 2:E:284:VAL:HG22 | 1.93 | 0.49 |
| 2:L:96:ASP:HB2 | 2:V:360:ASN:HB3 | 1.95 | 0.49 |
| 2:M:78:ASP:O | 2:M:82:ILE:HG23 | 2.12 | 0.49 |
| 2:W:75:GLY:O | 2:W:79:THR:HG22 | 2.13 | 0.49 |
| 2:W:330:GLY:HA3 | 2:W:354:ALA:HB3 | 1.94 | 0.49 |
| 2:E:115:THR:OG1 | 2:O:360:ASN:OD1 | 2.28 | 0.49 |
| 2:J:75:GLY:O | 2:J:79:THR:HG22 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:96:ASP:OD2 | 2:L:360:ASN:HB3 | 2.12 | 0.49 |
| 2:E:119:LEU:HD11 | 2:E:123:ILE:HD11 | 1.95 | 0.49 |
| 2:H:78:ASP:O | 2:H:82:ILE:HG23 | 2.12 | 0.49 |
| 2:J:281:MET:HA | 2:J:284:VAL:HG22 | 1.94 | 0.49 |
| 2:O:330:GLY:HA3 | 2:O:354:ALA:HB3 | 1.95 | 0.49 |
| 2:T:281:MET:HA | 2:T:284:VAL:HG22 | 1.94 | 0.49 |
| 2:F:281:MET:HA | 2:F:284:VAL:HG22 | 1.94 | 0.49 |
| 2:I:96:ASP:HB2 | 2:S:360:ASN:HB3 | 1.94 | 0.49 |
| 2:O:281:MET:HA | 2:O:284:VAL:HG22 | 1.94 | 0.49 |
| 2:R:330:GLY:HA3 | 2:R:354:ALA:HB3 | 1.94 | 0.49 |
| 2:B:119:LEU:HD11 | 2:B:123:ILE:HD11 | 1.94 | 0.48 |
| 2:S:78:ASP:O | 2:S:82:ILE:HG23 | 2.12 | 0.48 |
| 2:X:78:ASP:O | 2:X:82:ILE:HG23 | 2.12 | 0.48 |
| 2:C:96:ASP:HB2 | 2:M:360:ASN:HB3 | 1.95 | 0.48 |
| 2:M:75:GLY:O | 2:M:79:THR:HG22 | 2.13 | 0.48 |
| 2:M:115:THR:OG1 | 2:W:360:ASN:OD1 | 2.25 | 0.48 |
| 2:J:115:THR:OG1 | 2:T:360:ASN:OD1 | 2.29 | 0.48 |
| 2:O:75:GLY:O | 2:O:79:THR:HG22 | 2.14 | 0.48 |
| 2:O:119:LEU:HD11 | 2:O:123:ILE:HD11 | 1.95 | 0.48 |
| 2:T:119:LEU:HD11 | 2:T:123:ILE:HD11 | 1.95 | 0.48 |
| 2:H:75:GLY:O | 2:H:79:THR:HG22 | 2.14 | 0.48 |
| 2:K:96:ASP:HB2 | 2:U:360:ASN:HB3 | 1.95 | 0.48 |
| 2:K:281:MET:HA | 2:K:284:VAL:HG22 | 1.93 | 0.48 |
| 2:F:96:ASP:HB2 | 2:P:360:ASN:HB3 | 1.95 | 0.48 |
| 2:P:330:GLY:HA3 | 2:P:354:ALA:HB3 | 1.96 | 0.48 |
| 2:M:115:THR:OG1 | 2:W:359:GLU:HG3 | 2.14 | 0.48 |
| 2:V:281:MET:HA | 2:V:284:VAL:HG22 | 1.96 | 0.48 |
| 2:E:96:ASP:HB2 | 2:O:360:ASN:HB3 | 1.96 | 0.48 |
| 2:M:96:ASP:HB2 | 2:W:360:ASN:HB3 | 1.96 | 0.48 |
| 2:D:281:MET:HA | 2:D:284:VAL:HG22 | 1.95 | 0.47 |
| 2:K:115:THR:OG1 | 2:U:359:GLU:HG3 | 2.14 | 0.47 |
| 2:X:281:MET:HA | 2:X:284:VAL:HG22 | 1.96 | 0.47 |
| 2:G:96:ASP:HB2 | 2:Q:360:ASN:HB3 | 1.95 | 0.47 |
| 2:J:96:ASP:HB2 | 2:T:360:ASN:HB3 | 1.96 | 0.47 |
| 2:T:75:GLY:O | 2:T:79:THR:HG22 | 2.14 | 0.47 |
| 2:E:115:THR:OG1 | 2:O:359:GLU:HG3 | 2.14 | 0.47 |
| 2:H:115:THR:OG1 | 2:R:359:GLU:HG3 | 2.14 | 0.47 |
| 2:T:330:GLY:HA3 | 2:T:354:ALA:HB3 | 1.96 | 0.47 |
| 2:J:119:LEU:HD11 | 2:J:123:ILE:HD11 | 1.96 | 0.47 |
| 2:L:115:THR:OG1 | 2:V:360:ASN:OD1 | 2.31 | 0.47 |
| 2:U:75:GLY:O | 2:U:79:THR:HG22 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:115:THR:OG1 | 2:P:360:ASN:OD1 | 2.27 | 0.47 |
| 2:B:96:ASP:HB2 | 2:L:360:ASN:HB3 | 1.97 | 0.47 |
| 2:C:75:GLY:O | 2:C:79:THR:HG22 | 2.15 | 0.47 |
| 2:C:115:THR:OG1 | 2:M:359:GLU:HG3 | 2.15 | 0.47 |
| 2:J:115:THR:OG1 | 2:T:359:GLU:HG3 | 2.14 | 0.47 |
| 2:L:75:GLY:O | 2:L:79:THR:HG22 | 2.15 | 0.47 |
| 2:B:115:THR:OG1 | 2:L:360:ASN:OD1 | 2.31 | 0.47 |
| 2:G:75:GLY:O | 2:G:79:THR:HG22 | 2.14 | 0.47 |
| 2:I:281:MET:HA | 2:I:284:VAL:HG22 | 1.96 | 0.47 |
| 2:N:281:MET:HA | 2:N:284:VAL:HG22 | 1.96 | 0.47 |
| 2:B:96:ASP:CG | 2:L:361:GLY:H | 2.19 | 0.46 |
| 2:B:281:MET:HA | 2:B:284:VAL:HG22 | 1.97 | 0.46 |
| 2:N:115:THR:OG1 | 2:X:360:ASN:OD1 | 2.30 | 0.46 |
| 2:Q:281:MET:HA | 2:Q:284:VAL:HG22 | 1.96 | 0.46 |
| 2:U:330:GLY:HA3 | 2:U:354:ALA:HB3 | 1.95 | 0.46 |
| 2:W:281:MET:HA | 2:W:284:VAL:HG22 | 1.98 | 0.46 |
| 2:B:75:GLY:O | 2:B:79:THR:HG22 | 2.16 | 0.46 |
| 2:C:281:MET:HA | 2:C:284:VAL:HG22 | 1.97 | 0.46 |
| 2:H:96:ASP:HB2 | 2:R:360:ASN:HB3 | 1.96 | 0.46 |
| 2:P:75:GLY:O | 2:P:79:THR:HG22 | 2.16 | 0.46 |
| 2:D:23:TYR:CD1 | 2:E:82:ILE:HG22 | 2.51 | 0.46 |
| 2:D:75:GLY:O | 2:D:79:THR:HG22 | 2.16 | 0.46 |
| 2:E:23:TYR:CD1 | 2:F:82:ILE:HG22 | 2.51 | 0.46 |
| 2:M:23:TYR:CD1 | 2:N:82:ILE:HG22 | 2.51 | 0.46 |
| 2:B:23:TYR:CD1 | 2:C:82:ILE:HG22 | 2.51 | 0.46 |
| 2:G:23:TYR:CD1 | 2:H:82:ILE:HG22 | 2.51 | 0.46 |
| 2:J:23:TYR:CD1 | 2:K:82:ILE:HG22 | 2.51 | 0.46 |
| 2:L:23:TYR:CD1 | 2:M:82:ILE:HG22 | 2.51 | 0.46 |
| 2:L:330:GLY:HA3 | 2:L:354:ALA:HB3 | 1.97 | 0.46 |
| 2:S:330:GLY:HA3 | 2:S:354:ALA:HB3 | 1.98 | 0.46 |
| 2:G:94:GLY:O | 2:Q:360:ASN:ND2 | 2.49 | 0.46 |
| 2:I:23:TYR:CD1 | 2:J:82:ILE:HG22 | 2.51 | 0.46 |
| 2:C:23:TYR:CD1 | 2:D:82:ILE:HG22 | 2.51 | 0.46 |
| 2:H:23:TYR:CD1 | 2:I:82:ILE:HG22 | 2.51 | 0.46 |
| 2:Q:330:GLY:HA3 | 2:Q:354:ALA:HB3 | 1.98 | 0.46 |
| 2:S:281:MET:HA | 2:S:284:VAL:HG22 | 1.97 | 0.46 |
| 2:X:75:GLY:O | 2:X:79:THR:HG22 | 2.16 | 0.46 |
| 2:D:94:GLY:O | 2:N:360:ASN:ND2 | 2.49 | 0.45 |
| 2:E:330:GLY:HA3 | 2:E:354:ALA:HB3 | 1.98 | 0.45 |
| 2:D:115:THR:OG1 | 2:N:360:ASN:OD1 | 2.32 | 0.45 |
| 2:G:115:THR:OG1 | 2:Q:359:GLU:HG3 | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:23:TYR:CD1 | 2:L:82:ILE:HG22 | 2.51 | 0.45 |
| 2:L:281:MET:HA | 2:L:284:VAL:HG22 | 1.97 | 0.45 |
| 2:Q:75:GLY:O | 2:Q:79:THR:HG22 | 2.16 | 0.45 |
| 2:X:330:GLY:HA3 | 2:X:354:ALA:HB3 | 1.97 | 0.45 |
| 2:F:23:TYR:CD1 | 2:G:82:ILE:HG22 | 2.52 | 0.45 |
| 2:K:75:GLY:O | 2:K:79:THR:HG22 | 2.16 | 0.45 |
| 2:J:330:GLY:HA3 | 2:J:354:ALA:HB3 | 1.99 | 0.45 |
| 2:N:23:TYR:CD1 | 2:O:82:ILE:HG22 | 2.52 | 0.45 |
| 2:N:75:GLY:O | 2:N:79:THR:HG22 | 2.17 | 0.45 |
| 2:O:23:TYR:CD1 | 2:P:82:ILE:HG22 | 2.51 | 0.45 |
| 2:F:335:GLY:HA2 | 2:F:336:GLU:HA | 1.82 | 0.45 |
| 2:M:281:MET:HA | 2:M:284:VAL:HG22 | 1.98 | 0.45 |
| 2:Q:23:TYR:CD1 | 2:R:82:ILE:HG22 | 2.52 | 0.45 |
| 2:R:23:TYR:CD1 | 2:S:82:ILE:HG22 | 2.51 | 0.45 |
| 2:R:281:MET:HA | 2:R:284:VAL:HG22 | 1.98 | 0.45 |
| 2:G:281:MET:HA | 2:G:284:VAL:HG22 | 1.97 | 0.45 |
| 2:H:281:MET:HA | 2:H:284:VAL:HG22 | 1.98 | 0.45 |
| 2:P:23:TYR:CD1 | 2:Q:82:ILE:HG22 | 2.52 | 0.45 |
| 2:S:75:GLY:O | 2:S:79:THR:HG22 | 2.17 | 0.45 |
| 2:V:75:GLY:O | 2:V:79:THR:HG22 | 2.17 | 0.45 |
| 2:B:115:THR:OG1 | 2:L:359:GLU:HG3 | 2.16 | 0.45 |
| 2:F:75:GLY:O | 2:F:79:THR:HG22 | 2.17 | 0.45 |
| 2:L:94:GLY:O | 2:V:360:ASN:ND2 | 2.49 | 0.45 |
| 2:M:94:GLY:O | 2:W:360:ASN:ND2 | 2.50 | 0.45 |
| 2:N:115:THR:OG1 | 2:X:359:GLU:HG3 | 2.17 | 0.45 |
| 2:B:94:GLY:O | 2:L:360:ASN:ND2 | 2.50 | 0.45 |
| 2:F:115:THR:OG1 | 2:P:359:GLU:HG3 | 2.16 | 0.45 |
| 2:G:115:THR:OG1 | 2:Q:360:ASN:OD1 | 2.30 | 0.45 |
| 2:I:75:GLY:O | 2:I:79:THR:HG22 | 2.17 | 0.45 |
| 2:S:23:TYR:CD1 | 2:T:82:ILE:HG22 | 2.52 | 0.45 |
| 2:C:330:GLY:HA3 | 2:C:354:ALA:HB3 | 1.99 | 0.45 |
| 2:E:94:GLY:O | 2:O:360:ASN:ND2 | 2.50 | 0.45 |
| 2:H:330:GLY:HA3 | 2:H:354:ALA:HB3 | 1.98 | 0.45 |
| 2:I:94:GLY:O | 2:S:360:ASN:ND2 | 2.50 | 0.45 |
| 2:N:94:GLY:O | 2:X:360:ASN:ND2 | 2.50 | 0.45 |
| 2:B:330:GLY:HA3 | 2:B:354:ALA:HB3 | 2.00 | 0.44 |
| 2:D:115:THR:OG1 | 2:N:359:GLU:HG3 | 2.17 | 0.44 |
| 2:N:335:GLY:HA2 | 2:N:336:GLU:HA | 1.82 | 0.44 |
| 2:T:23:TYR:CD1 | 2:U:82:ILE:HG22 | 2.51 | 0.44 |
| 2:H:94:GLY:O | 2:R:360:ASN:ND2 | 2.50 | 0.44 |
| 2:W:23:TYR:CD1 | 2:X:82:ILE:HG22 | 2.51 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:94:GLY:O | 2:T:360:ASN:ND2 | 2.50 | 0.44 |
| 2:N:362:VAL:HG12 | 2:N:363:ILE:N | 2.33 | 0.44 |
| 2:H:96:ASP:N | 2:R:360:ASN:OD1 | 2.49 | 0.44 |
| 2:V:23:TYR:CD1 | 2:W:82:ILE:HG22 | 2.52 | 0.44 |
| 2:V:330:GLY:HA3 | 2:V:354:ALA:HB3 | 1.98 | 0.44 |
| 2:X:335:GLY:HA2 | 2:X:336:GLU:HA | 1.82 | 0.44 |
| 1:A:21:C:C4 | 2:W:242:ILE:HG12 | 2.53 | 0.44 |
| 2:F:94:GLY:O | 2:P:360:ASN:ND2 | 2.51 | 0.44 |
| 2:I:115:THR:OG1 | 2:S:359:GLU:HG3 | 2.17 | 0.44 |
| 2:N:330:GLY:HA3 | 2:N:354:ALA:HB3 | 1.98 | 0.44 |
| 1:A:181:C:C4 | 2:G:242:ILE:HG12 | 2.53 | 0.44 |
| 2:U:23:TYR:CD1 | 2:V:82:ILE:HG22 | 2.52 | 0.44 |
| 2:X:119:LEU:CD1 | 2:X:123:ILE:HD11 | 2.48 | 0.44 |
| 2:L:115:THR:OG1 | 2:V:359:GLU:HG3 | 2.17 | 0.44 |
| 1:A:71:C:C4 | 2:R:242:ILE:HG12 | 2.53 | 0.43 |
| 1:A:91:C:C4 | 2:P:242:ILE:HG12 | 2.53 | 0.43 |
| 1:A:131:C:C4 | 2:L:242:ILE:HG12 | 2.53 | 0.43 |
| 2:C:94:GLY:O | 2:M:360:ASN:ND2 | 2.51 | 0.43 |
| 2:K:94:GLY:O | 2:U:360:ASN:ND2 | 2.51 | 0.43 |
| 2:M:331:LEU:HD13 | 2:M:354:ALA:HB1 | 2.00 | 0.43 |
| 2:C:119:LEU:CD1 | 2:C:123:ILE:HD11 | 2.48 | 0.43 |
| 1:A:41:C:C4 | 2:U:242:ILE:HG12 | 2.53 | 0.43 |
| 2:Q:275:ALA:HB3 | 2:R:361:GLY:HA2 | 1.99 | 0.43 |
| 2:V:362:VAL:HG12 | 2:V:363:ILE:N | 2.34 | 0.43 |
| 1:A:221:C:C4 | 2:C:242:ILE:HG12 | 2.54 | 0.43 |
| 2:L:335:GLY:HA2 | 2:L:336:GLU:HA | 1.82 | 0.43 |
| 2:W:331:LEU:HD13 | 2:W:354:ALA:HB1 | 2.00 | 0.43 |
| 1:A:121:C:C4 | 2:M:242:ILE:HG12 | 2.53 | 0.43 |
| 1:A:101:C:C4 | 2:O:242:ILE:HG12 | 2.54 | 0.43 |
| 1:A:201:C:C4 | 2:E:242:ILE:HG12 | 2.54 | 0.43 |
| 2:G:335:GLY:HA2 | 2:G:336:GLU:HA | 1.82 | 0.43 |
| 2:S:119:LEU:CD1 | 2:S:123:ILE:HD11 | 2.49 | 0.43 |
| 2:X:362:VAL:HG12 | 2:X:363:ILE:N | 2.34 | 0.43 |
| 1:A:191:C:C4 | 2:F:242:ILE:HG12 | 2.53 | 0.43 |
| 2:L:275:ALA:HB3 | 2:M:361:GLY:HA2 | 2.00 | 0.43 |
| 2:T:362:VAL:HG12 | 2:T:363:ILE:N | 2.34 | 0.43 |
| 2:V:275:ALA:HB3 | 2:W:361:GLY:HA2 | 2.00 | 0.43 |
| 1:A:11:C:C4 | 2:X:242:ILE:HG12 | 2.54 | 0.42 |
| 1:A:31:C:C4 | 2:V:242:ILE:HG12 | 2.53 | 0.42 |
| 1:A:151:C:C4 | 2:J:242:ILE:HG12 | 2.54 | 0.42 |
| 2:T:275:ALA:HB3 | 2:U:361:GLY:HA2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:U:335:GLY:HA2 | 2:U:336:GLU:HA | 1.82 | 0.42 |
| 1:A:61:C:C4 | 2:S:242:ILE:HG12 | 2.54 | 0.42 |
| 1:A:141:C:C4 | 2:K:242:ILE:HG12 | 2.53 | 0.42 |
| 1:A:171:C:C4 | 2:H:242:ILE:HG12 | 2.54 | 0.42 |
| 1:A:211:C:C4 | 2:D:242:ILE:HG12 | 2.55 | 0.42 |
| 1:A:51:C:C4 | 2:T:242:ILE:HG12 | 2.54 | 0.42 |
| 1:A:161:C:C4 | 2:I:242:ILE:HG12 | 2.55 | 0.42 |
| 2:I:335:GLY:HA2 | 2:I:336:GLU:HA | 1.82 | 0.42 |
| 2:M:96:ASP:N | 2:W:360:ASN:OD1 | 2.49 | 0.42 |
| 2:R:331:LEU:HD13 | 2:R:354:ALA:HB1 | 2.01 | 0.42 |
| 2:S:6:VAL:HG23 | 2:T:288:TYR:CE2 | 2.55 | 0.42 |
| 2:S:275:ALA:HB3 | 2:T:361:GLY:HA2 | 2.01 | 0.42 |
| 2:L:270:ILE:HG23 | 2:M:363:ILE:HG21 | 2.02 | 0.42 |
| 2:O:335:GLY:HA2 | 2:O:336:GLU:HA | 1.82 | 0.42 |
| 2:S:362:VAL:HG12 | 2:S:363:ILE:N | 2.34 | 0.42 |
| 1:A:81:C:C4 | 2:Q:242:ILE:HG12 | 2.53 | 0.42 |
| 1:A:111:C:C4 | 2:N:242:ILE:HG12 | 2.55 | 0.42 |
| 2:K:330:GLY:HA3 | 2:K:354:ALA:HB3 | 2.01 | 0.42 |
| 2:N:275:ALA:HB3 | 2:O:361:GLY:HA2 | 2.01 | 0.42 |
| 2:O:331:LEU:HD13 | 2:O:354:ALA:HB1 | 2.02 | 0.42 |
| 2:O:362:VAL:HG12 | 2:O:363:ILE:N | 2.34 | 0.42 |
| 2:Q:335:GLY:HA2 | 2:Q:336:GLU:HA | 1.82 | 0.42 |
| 2:C:6:VAL:HG23 | 2:D:288:TYR:CE2 | 2.55 | 0.42 |
| 2:N:6:VAL:HG23 | 2:O:288:TYR:CE2 | 2.55 | 0.42 |
| 2:O:275:ALA:HB3 | 2:P:361:GLY:HA2 | 2.02 | 0.42 |
| 2:H:119:LEU:CD1 | 2:H:123:ILE:HD11 | 2.49 | 0.42 |
| 2:I:6:VAL:HG23 | 2:J:288:TYR:CE2 | 2.55 | 0.42 |
| 2:K:275:ALA:HB3 | 2:L:361:GLY:HA2 | 2.02 | 0.42 |
| 2:L:362:VAL:HG12 | 2:L:363:ILE:N | 2.35 | 0.42 |
| 2:S:270:ILE:HG23 | 2:T:363:ILE:HG21 | 2.02 | 0.42 |
| 2:H:54:THR:HB | 2:H:57:ALA:HB2 | 2.02 | 0.42 |
| 2:O:270:ILE:HG23 | 2:P:363:ILE:HG21 | 2.02 | 0.42 |
| 2:Q:270:ILE:HG23 | 2:R:363:ILE:HG21 | 2.02 | 0.42 |
| 2:F:330:GLY:HA3 | 2:F:354:ALA:HB3 | 2.02 | 0.42 |
| 2:G:330:GLY:HA3 | 2:G:354:ALA:HB3 | 2.01 | 0.42 |
| 2:H:6:VAL:HG23 | 2:I:288:TYR:CE2 | 2.55 | 0.42 |
| 2:I:330:GLY:HA3 | 2:I:354:ALA:HB3 | 2.02 | 0.42 |
| 2:K:119:LEU:CD1 | 2:K:123:ILE:HD11 | 2.50 | 0.42 |
| 2:X:331:LEU:HD13 | 2:X:354:ALA:HB1 | 2.02 | 0.42 |
| 2:D:96:ASP:CB | 2:N:360:ASN:HB3 | 2.50 | 0.41 |
| 2:F:6:VAL:HG23 | 2:G:288:TYR:CE2 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:N:96:ASP:CB | 2:X:360:ASN:HB3 | 2.50 | 0.41 |
| 2:R:54:THR:HB | 2:R:57:ALA:HB2 | 2.02 | 0.41 |
| 2:I:96:ASP:CB | 2:S:360:ASN:HB3 | 2.50 | 0.41 |
| 2:P:6:VAL:HG23 | 2:Q:288:TYR:CE2 | 2.55 | 0.41 |
| 2:U:270:ILE:HD13 | 2:U:270:ILE:HA | 1.97 | 0.41 |
| 2:V:270:ILE:HG23 | 2:W:363:ILE:HG21 | 2.02 | 0.41 |
| 2:M:54:THR:HB | 2:M:57:ALA:HB2 | 2.02 | 0.41 |
| 2:P:54:THR:HB | 2:P:57:ALA:HB2 | 2.03 | 0.41 |
| 2:S:54:THR:HB | 2:S:57:ALA:HB2 | 2.03 | 0.41 |
| 2:U:331:LEU:HD13 | 2:U:354:ALA:HB1 | 2.01 | 0.41 |
| 2:I:115:THR:OG1 | 2:S:360:ASN:OD1 | 2.31 | 0.41 |
| 2:P:331:LEU:HD13 | 2:P:354:ALA:HB1 | 2.02 | 0.41 |
| 2:T:335:GLY:HA2 | 2:T:336:GLU:HA | 1.82 | 0.41 |
| 2:W:362:VAL:HG12 | 2:W:363:ILE:N | 2.35 | 0.41 |
| 2:X:54:THR:HB | 2:X:57:ALA:HB2 | 2.02 | 0.41 |
| 2:C:54:THR:HB | 2:C:57:ALA:HB2 | 2.02 | 0.41 |
| 2:F:54:THR:HB | 2:F:57:ALA:HB2 | 2.03 | 0.41 |
| 2:K:54:THR:HB | 2:K:57:ALA:HB2 | 2.03 | 0.41 |
| 2:M:119:LEU:CD1 | 2:M:123:ILE:HD11 | 2.51 | 0.41 |
| 2:M:362:VAL:HG12 | 2:M:363:ILE:N | 2.36 | 0.41 |
| 2:P:335:GLY:HA2 | 2:P:336:GLU:HA | 1.82 | 0.41 |
| 2:Q:6:VAL:HG23 | 2:R:288:TYR:CE2 | 2.56 | 0.41 |
| 2:U:54:THR:HB | 2:U:57:ALA:HB2 | 2.03 | 0.41 |
| 2:U:275:ALA:HB3 | 2:V:361:GLY:HA2 | 2.02 | 0.41 |
| 2:B:335:GLY:HA2 | 2:B:336:GLU:HA | 1.82 | 0.41 |
| 2:C:96:ASP:N | 2:M:360:ASN:OD1 | 2.49 | 0.41 |
| 2:L:331:LEU:HD13 | 2:L:354:ALA:HB1 | 2.02 | 0.41 |
| 2:N:119:LEU:CD1 | 2:N:123:ILE:HD11 | 2.50 | 0.41 |
| 2:N:331:LEU:HD13 | 2:N:354:ALA:HB1 | 2.03 | 0.41 |
| 2:S:270:ILE:HD13 | 2:S:270:ILE:HA | 1.97 | 0.41 |
| 2:T:270:ILE:HG23 | 2:U:363:ILE:HG21 | 2.03 | 0.41 |
| 2:U:362:VAL:HG12 | 2:U:363:ILE:N | 2.35 | 0.41 |
| 2:B:96:ASP:OD2 | 2:L:361:GLY:N | 2.41 | 0.41 |
| 2:E:23:TYR:CG | 2:F:82:ILE:HG22 | 2.56 | 0.41 |
| 2:J:23:TYR:CG | 2:K:82:ILE:HG22 | 2.56 | 0.41 |
| 2:N:270:ILE:HG23 | 2:O:363:ILE:HG21 | 2.03 | 0.41 |
| 2:R:362:VAL:HG12 | 2:R:363:ILE:N | 2.36 | 0.41 |
| 2:T:6:VAL:HG23 | 2:U:288:TYR:CE2 | 2.56 | 0.41 |
| 2:V:6:VAL:HG23 | 2:W:288:TYR:CE2 | 2.55 | 0.41 |
| 2:D:6:VAL:HG23 | 2:E:288:TYR:CE2 | 2.55 | 0.41 |
| 2:M:275:ALA:HB3 | 2:N:361:GLY:HA2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P:362:VAL:HG12 | 2:P:363:ILE:N | 2.35 | 0.41 |
| 2:Q:54:THR:HB | 2:Q:57:ALA:HB2 | 2.03 | 0.41 |
| 2:Q:270:ILE:HD13 | 2:Q:270:ILE:HA | 1.96 | 0.41 |
| 2:R:6:VAL:HG23 | 2:S:288:TYR:CE2 | 2.56 | 0.41 |
| 2:E:54:THR:HB | 2:E:57:ALA:HB2 | 2.03 | 0.41 |
| 2:E:335:GLY:HA2 | 2:E:336:GLU:HA | 1.82 | 0.41 |
| 2:G:6:VAL:HG23 | 2:H:288:TYR:CE2 | 2.56 | 0.41 |
| 2:J:6:VAL:HG23 | 2:K:288:TYR:CE2 | 2.56 | 0.41 |
| 2:K:6:VAL:HG23 | 2:L:288:TYR:CE2 | 2.55 | 0.41 |
| 2:L:96:ASP:CB | 2:V:360:ASN:HB3 | 2.51 | 0.41 |
| 2:M:6:VAL:HG23 | 2:N:288:TYR:CE2 | 2.55 | 0.41 |
| 2:P:119:LEU:CD1 | 2:P:123:ILE:HD11 | 2.50 | 0.41 |
| 2:T:331:LEU:HD13 | 2:T:354:ALA:HB1 | 2.02 | 0.41 |
| 2:W:54:THR:HB | 2:W:57:ALA:HB2 | 2.03 | 0.41 |
| 2:D:330:GLY:HA3 | 2:D:354:ALA:HB3 | 2.02 | 0.41 |
| 2:E:6:VAL:HG23 | 2:F:288:TYR:CE2 | 2.56 | 0.41 |
| 2:G:54:THR:HB | 2:G:57:ALA:HB2 | 2.03 | 0.41 |
| 2:H:331:LEU:HD13 | 2:H:354:ALA:HB1 | 2.03 | 0.41 |
| 2:I:54:THR:HB | 2:I:57:ALA:HB2 | 2.03 | 0.41 |
| 2:S:331:LEU:HD13 | 2:S:354:ALA:HB1 | 2.02 | 0.41 |
| 2:T:54:THR:HB | 2:T:57:ALA:HB2 | 2.03 | 0.41 |
| 2:U:6:VAL:HG23 | 2:V:288:TYR:CE2 | 2.56 | 0.41 |
| 2:U:119:LEU:CD1 | 2:U:123:ILE:HD11 | 2.51 | 0.41 |
| 2:W:6:VAL:HG23 | 2:X:288:TYR:CE2 | 2.56 | 0.41 |
| 1:A:221:C:C2 | 2:C:242:ILE:HA | 2.56 | 0.40 |
| 2:J:54:THR:HB | 2:J:57:ALA:HB2 | 2.03 | 0.40 |
| 2:U:270:ILE:HG23 | 2:V:363:ILE:HG21 | 2.03 | 0.40 |
| 1:A:11:C:C2 | 2:X:242:ILE:HA | 2.57 | 0.40 |
| 1:A:191:C:C2 | 2:F:242:ILE:HA | 2.57 | 0.40 |
| 2:B:54:THR:HB | 2:B:57:ALA:HB2 | 2.03 | 0.40 |
| 2:F:96:ASP:CB | 2:P:360:ASN:HB3 | 2.50 | 0.40 |
| 2:F:119:LEU:CD1 | 2:F:123:ILE:HD11 | 2.50 | 0.40 |
| 2:G:96:ASP:CB | 2:Q:360:ASN:HB3 | 2.52 | 0.40 |
| 2:L:54:THR:HB | 2:L:57:ALA:HB2 | 2.03 | 0.40 |
| 2:M:23:TYR:CG | 2:N:82:ILE:HG22 | 2.56 | 0.40 |
| 2:N:54:THR:HB | 2:N:57:ALA:HB2 | 2.03 | 0.40 |
| 2:P:270:ILE:HG23 | 2:Q:363:ILE:HG21 | 2.03 | 0.40 |
| 2:P:275:ALA:HB3 | 2:Q:361:GLY:HA2 | 2.02 | 0.40 |
| 2:R:275:ALA:HB3 | 2:S:361:GLY:HA2 | 2.02 | 0.40 |
| 2:V:331:LEU:HD13 | 2:V:354:ALA:HB1 | 2.03 | 0.40 |
| 2:W:270:ILE:HG23 | 2:X:363:ILE:HG21 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:91:C:C2 | 2:P:242:ILE:HA | 2.57 | 0.40 |
| 1:A:171:C:C2 | 2:H:242:ILE:HA | 2.57 | 0.40 |
| 2:B:6:VAL:HG23 | 2:C:288:TYR:CE2 | 2.56 | 0.40 |
| 2:O:6:VAL:HG23 | 2:P:288:TYR:CE2 | 2.56 | 0.40 |
| 2:V:54:THR:HB | 2:V:57:ALA:HB2 | 2.03 | 0.40 |
| 1:A:71:C:C2 | 2:R:242:ILE:HA | 2.57 | 0.40 |
| 1:A:101:C:C2 | 2:O:242:ILE:HA | 2.57 | 0.40 |
| 1:A:131:C:C2 | 2:L:242:ILE:HA | 2.57 | 0.40 |
| 2:D:54:THR:HB | 2:D:57:ALA:HB2 | 2.03 | 0.40 |
| 2:E:331:LEU:HD13 | 2:E:354:ALA:HB1 | 2.03 | 0.40 |
| 2:K:96:ASP:CB | 2:U:360:ASN:HB3 | 2.51 | 0.40 |
| 2:M:270:ILE:HG23 | 2:N:363:ILE:HG21 | 2.03 | 0.40 |
| 2:O:54:THR:HB | 2:O:57:ALA:HB2 | 2.03 | 0.40 |
| 2:R:270:ILE:HG23 | 2:S:363:ILE:HG21 | 2.03 | 0.40 |
| 1:A:31:C:C2 | 2:V:242:ILE:HA | 2.57 | 0.40 |
| 1:A:151:C:C2 | 2:J:242:ILE:HA | 2.57 | 0.40 |
| 2:L:6:VAL:HG23 | 2:M:288:TYR:CE2 | 2.56 | 0.40 |
| 2:Q:362:VAL:HG12 | 2:Q:363:ILE:N | 2.35 | 0.40 |

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 PDB entries followed by that with respect to all EM 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 | |
|---|---|---|---|---|---|---|---|
| 2 | B | 368/391 (94%) | 354 (96%) | 13 (4%) | 1 (0%) | 41 | 41 |
| 2 | C | 368/391 (94%) | 352 (96%) | 15 (4%) | 1 (0%) | 41 | 41 |
| 2 | D | 368/391 (94%) | 352 (96%) | 15 (4%) | 1 (0%) | 41 | 41 |
| 2 | E | 368/391 (94%) | 353 (96%) | 14 (4%) | 1 (0%) | 41 | 41 |
| 2 | F | 368/391 (94%) | 352 (96%) | 15 (4%) | 1 (0%) | 41 | 41 |
| 2 | G | 368/391 (94%) | 353 (96%) | 14 (4%) | 1 (0%) | 41 | 41 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | H | 368/391 (94%) | 353 (96%) | 14 (4%) | 1 (0%) | 41 | 41 |
| 2 | I | 368/391 (94%) | 352 (96%) | 15 (4%) | 1 (0%) | 41 | 41 |
| 2 | J | 368/391 (94%) | 353 (96%) | 14 (4%) | 1 (0%) | 41 | 41 |
| 2 | K | 368/391 (94%) | 352 (96%) | 15 (4%) | 1 (0%) | 41 | 41 |
| 2 | L | 368/391 (94%) | 353 (96%) | 13 (4%) | 2 (0%) | 29 | 29 |
| 2 | M | 368/391 (94%) | 353 (96%) | 12 (3%) | 3 (1%) | 19 | 19 |
| 2 | N | 368/391 (94%) | 352 (96%) | 13 (4%) | 3 (1%) | 19 | 19 |
| 2 | O | 368/391 (94%) | 353 (96%) | 12 (3%) | 3 (1%) | 19 | 19 |
| 2 | P | 368/391 (94%) | 352 (96%) | 13 (4%) | 3 (1%) | 19 | 19 |
| 2 | Q | 368/391 (94%) | 352 (96%) | 13 (4%) | 3 (1%) | 19 | 19 |
| 2 | R | 368/391 (94%) | 353 (96%) | 12 (3%) | 3 (1%) | 19 | 19 |
| 2 | S | 368/391 (94%) | 352 (96%) | 13 (4%) | 3 (1%) | 19 | 19 |
| 2 | T | 368/391 (94%) | 353 (96%) | 12 (3%) | 3 (1%) | 19 | 19 |
| 2 | U | 368/391 (94%) | 353 (96%) | 12 (3%) | 3 (1%) | 19 | 19 |
| 2 | V | 368/391 (94%) | 352 (96%) | 13 (4%) | 3 (1%) | 19 | 19 |
| 2 | W | 368/391 (94%) | 353 (96%) | 12 (3%) | 3 (1%) | 19 | 19 |
| 2 | X | 368/391 (94%) | 352 (96%) | 13 (4%) | 3 (1%) | 19 | 19 |
| All | All | 8464/8993 (94%) | 8109 (96%) | 307 (4%) | 48 (1%) | 29 | 25 |

All (48) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | M | 360 | ASN |
| 2 | O | 360 | ASN |
| 2 | P | 360 | ASN |
| 2 | R | 360 | ASN |
| 2 | U | 360 | ASN |
| 2 | W | 360 | ASN |
| 2 | X | 360 | ASN |
| 2 | M | 361 | GLY |
| 2 | O | 361 | GLY |
| 2 | P | 361 | GLY |
| 2 | R | 361 | GLY |
| 2 | S | 360 | ASN |
| 2 | S | 361 | GLY |
| 2 | T | 360 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | W | 361 | GLY |
| 2 | X | 361 | GLY |
| 2 | N | 360 | ASN |
| 2 | N | 361 | GLY |
| 2 | Q | 360 | ASN |
| 2 | Q | 361 | GLY |
| 2 | T | 361 | GLY |
| 2 | U | 361 | GLY |
| 2 | V | 360 | ASN |
| 2 | V | 361 | GLY |
| 2 | L | 361 | GLY |
| 2 | C | 6 | VAL |
| 2 | D | 6 | VAL |
| 2 | E | 6 | VAL |
| 2 | H | 6 | VAL |
| 2 | I | 6 | VAL |
| 2 | J | 6 | VAL |
| 2 | M | 6 | VAL |
| 2 | N | 6 | VAL |
| 2 | O | 6 | VAL |
| 2 | S | 6 | VAL |
| 2 | T | 6 | VAL |
| 2 | W | 6 | VAL |
| 2 | X | 6 | VAL |
| 2 | B | 6 | VAL |
| 2 | F | 6 | VAL |
| 2 | G | 6 | VAL |
| 2 | K | 6 | VAL |
| 2 | L | 6 | VAL |
| 2 | P | 6 | VAL |
| 2 | Q | 6 | VAL |
| 2 | R | 6 | VAL |
| 2 | U | 6 | VAL |
| 2 | V | 6 | VAL |

### 5.3.2 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 EM 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 | |
|---|---|---|---|---|---|---|
| 2 | B | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | C | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | D | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | E | 309/328 (94%) | 295 (96%) | 14 (4%) | 27 | 27 |
| 2 | F | 309/328 (94%) | 297 (96%) | 12 (4%) | 32 | 32 |
| 2 | G | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | H | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | I | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | J | 309/328 (94%) | 295 (96%) | 14 (4%) | 27 | 27 |
| 2 | K | 309/328 (94%) | 297 (96%) | 12 (4%) | 32 | 32 |
| 2 | L | 309/328 (94%) | 297 (96%) | 12 (4%) | 32 | 32 |
| 2 | M | 309/328 (94%) | 295 (96%) | 14 (4%) | 27 | 27 |
| 2 | N | 309/328 (94%) | 297 (96%) | 12 (4%) | 32 | 32 |
| 2 | O | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | P | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | Q | 309/328 (94%) | 297 (96%) | 12 (4%) | 32 | 32 |
| 2 | R | 309/328 (94%) | 295 (96%) | 14 (4%) | 27 | 27 |
| 2 | S | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | T | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| 2 | U | 309/328 (94%) | 295 (96%) | 14 (4%) | 27 | 27 |
| 2 | V | 309/328 (94%) | 297 (96%) | 12 (4%) | 32 | 32 |
| 2 | W | 309/328 (94%) | 295 (96%) | 14 (4%) | 27 | 27 |
| 2 | X | 309/328 (94%) | 296 (96%) | 13 (4%) | 30 | 30 |
| All | All | 7107/7544 (94%) | 6808 (96%) | 299 (4%) | 33 | 30 |

All (299) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 3 | LEU |
| 2 | B | 9 | ASN |
| 2 | B | 29 | THR |
| 2 | B | 83 | LEU |
| 2 | B | 123 | ILE |
| 2 | B | 136 | LYS |
| 2 | B | 163 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 168 | ILE |
| 2 | B | 220 | ILE |
| 2 | B | 272 | LEU |
| 2 | B | 287 | VAL |
| 2 | B | 325 | LEU |
| 2 | B | 331 | LEU |
| 2 | C | 3 | LEU |
| 2 | C | 9 | ASN |
| 2 | C | 29 | THR |
| 2 | C | 83 | LEU |
| 2 | C | 136 | LYS |
| 2 | C | 163 | ILE |
| 2 | C | 168 | ILE |
| 2 | C | 220 | ILE |
| 2 | C | 272 | LEU |
| 2 | C | 287 | VAL |
| 2 | C | 301 | TYR |
| 2 | C | 325 | LEU |
| 2 | C | 331 | LEU |
| 2 | D | 3 | LEU |
| 2 | D | 9 | ASN |
| 2 | D | 29 | THR |
| 2 | D | 83 | LEU |
| 2 | D | 123 | ILE |
| 2 | D | 136 | LYS |
| 2 | D | 163 | ILE |
| 2 | D | 168 | ILE |
| 2 | D | 220 | ILE |
| 2 | D | 272 | LEU |
| 2 | D | 287 | VAL |
| 2 | D | 325 | LEU |
| 2 | D | 331 | LEU |
| 2 | E | 3 | LEU |
| 2 | E | 9 | ASN |
| 2 | E | 29 | THR |
| 2 | E | 83 | LEU |
| 2 | E | 123 | ILE |
| 2 | E | 136 | LYS |
| 2 | E | 163 | ILE |
| 2 | E | 168 | ILE |
| 2 | E | 220 | ILE |
| 2 | E | 272 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | E | 287 | VAL |
| 2 | E | 301 | TYR |
| 2 | E | 325 | LEU |
| 2 | E | 331 | LEU |
| 2 | F | 3 | LEU |
| 2 | F | 9 | ASN |
| 2 | F | 29 | THR |
| 2 | F | 83 | LEU |
| 2 | F | 123 | ILE |
| 2 | F | 136 | LYS |
| 2 | F | 163 | ILE |
| 2 | F | 220 | ILE |
| 2 | F | 272 | LEU |
| 2 | F | 287 | VAL |
| 2 | F | 325 | LEU |
| 2 | F | 331 | LEU |
| 2 | G | 3 | LEU |
| 2 | G | 9 | ASN |
| 2 | G | 29 | THR |
| 2 | G | 83 | LEU |
| 2 | G | 123 | ILE |
| 2 | G | 136 | LYS |
| 2 | G | 163 | ILE |
| 2 | G | 168 | ILE |
| 2 | G | 220 | ILE |
| 2 | G | 272 | LEU |
| 2 | G | 287 | VAL |
| 2 | G | 325 | LEU |
| 2 | G | 331 | LEU |
| 2 | H | 3 | LEU |
| 2 | H | 9 | ASN |
| 2 | H | 29 | THR |
| 2 | H | 83 | LEU |
| 2 | H | 136 | LYS |
| 2 | H | 163 | ILE |
| 2 | H | 168 | ILE |
| 2 | H | 220 | ILE |
| 2 | H | 272 | LEU |
| 2 | H | 287 | VAL |
| 2 | H | 301 | TYR |
| 2 | H | 325 | LEU |
| 2 | H | 331 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | I | 3 | LEU |
| 2 | I | 9 | ASN |
| 2 | I | 29 | THR |
| 2 | I | 83 | LEU |
| 2 | I | 123 | ILE |
| 2 | I | 136 | LYS |
| 2 | I | 163 | ILE |
| 2 | I | 168 | ILE |
| 2 | I | 220 | ILE |
| 2 | I | 272 | LEU |
| 2 | I | 287 | VAL |
| 2 | I | 325 | LEU |
| 2 | I | 331 | LEU |
| 2 | J | 3 | LEU |
| 2 | J | 9 | ASN |
| 2 | J | 29 | THR |
| 2 | J | 83 | LEU |
| 2 | J | 123 | ILE |
| 2 | J | 136 | LYS |
| 2 | J | 163 | ILE |
| 2 | J | 168 | ILE |
| 2 | J | 220 | ILE |
| 2 | J | 272 | LEU |
| 2 | J | 287 | VAL |
| 2 | J | 301 | TYR |
| 2 | J | 325 | LEU |
| 2 | J | 331 | LEU |
| 2 | K | 3 | LEU |
| 2 | K | 9 | ASN |
| 2 | K | 29 | THR |
| 2 | K | 83 | LEU |
| 2 | K | 123 | ILE |
| 2 | K | 136 | LYS |
| 2 | K | 163 | ILE |
| 2 | K | 220 | ILE |
| 2 | K | 272 | LEU |
| 2 | K | 287 | VAL |
| 2 | K | 325 | LEU |
| 2 | K | 331 | LEU |
| 2 | L | 3 | LEU |
| 2 | L | 9 | ASN |
| 2 | L | 29 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | L | 83 | LEU |
| 2 | L | 123 | ILE |
| 2 | L | 136 | LYS |
| 2 | L | 163 | ILE |
| 2 | L | 220 | ILE |
| 2 | L | 272 | LEU |
| 2 | L | 287 | VAL |
| 2 | L | 325 | LEU |
| 2 | L | 331 | LEU |
| 2 | M | 3 | LEU |
| 2 | M | 9 | ASN |
| 2 | M | 29 | THR |
| 2 | M | 83 | LEU |
| 2 | M | 123 | ILE |
| 2 | M | 136 | LYS |
| 2 | M | 163 | ILE |
| 2 | M | 168 | ILE |
| 2 | M | 220 | ILE |
| 2 | M | 272 | LEU |
| 2 | M | 287 | VAL |
| 2 | M | 301 | TYR |
| 2 | M | 325 | LEU |
| 2 | M | 331 | LEU |
| 2 | N | 3 | LEU |
| 2 | N | 9 | ASN |
| 2 | N | 29 | THR |
| 2 | N | 83 | LEU |
| 2 | N | 136 | LYS |
| 2 | N | 163 | ILE |
| 2 | N | 168 | ILE |
| 2 | N | 220 | ILE |
| 2 | N | 272 | LEU |
| 2 | N | 287 | VAL |
| 2 | N | 325 | LEU |
| 2 | N | 331 | LEU |
| 2 | O | 3 | LEU |
| 2 | O | 9 | ASN |
| 2 | O | 29 | THR |
| 2 | O | 83 | LEU |
| 2 | O | 123 | ILE |
| 2 | O | 136 | LYS |
| 2 | O | 163 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | O | 168 | ILE |
| 2 | O | 220 | ILE |
| 2 | O | 272 | LEU |
| 2 | O | 287 | VAL |
| 2 | O | 325 | LEU |
| 2 | O | 331 | LEU |
| 2 | P | 3 | LEU |
| 2 | P | 9 | ASN |
| 2 | P | 29 | THR |
| 2 | P | 83 | LEU |
| 2 | P | 123 | ILE |
| 2 | P | 136 | LYS |
| 2 | P | 163 | ILE |
| 2 | P | 168 | ILE |
| 2 | P | 220 | ILE |
| 2 | P | 272 | LEU |
| 2 | P | 287 | VAL |
| 2 | P | 325 | LEU |
| 2 | P | 331 | LEU |
| 2 | Q | 3 | LEU |
| 2 | Q | 9 | ASN |
| 2 | Q | 29 | THR |
| 2 | Q | 83 | LEU |
| 2 | Q | 123 | ILE |
| 2 | Q | 136 | LYS |
| 2 | Q | 163 | ILE |
| 2 | Q | 220 | ILE |
| 2 | Q | 272 | LEU |
| 2 | Q | 287 | VAL |
| 2 | Q | 325 | LEU |
| 2 | Q | 331 | LEU |
| 2 | R | 3 | LEU |
| 2 | R | 9 | ASN |
| 2 | R | 29 | THR |
| 2 | R | 83 | LEU |
| 2 | R | 123 | ILE |
| 2 | R | 136 | LYS |
| 2 | R | 163 | ILE |
| 2 | R | 168 | ILE |
| 2 | R | 220 | ILE |
| 2 | R | 272 | LEU |
| 2 | R | 287 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | R | 301 | TYR |
| 2 | R | 325 | LEU |
| 2 | R | 331 | LEU |
| 2 | S | 3 | LEU |
| 2 | S | 9 | ASN |
| 2 | S | 29 | THR |
| 2 | S | 83 | LEU |
| 2 | S | 123 | ILE |
| 2 | S | 136 | LYS |
| 2 | S | 163 | ILE |
| 2 | S | 168 | ILE |
| 2 | S | 220 | ILE |
| 2 | S | 272 | LEU |
| 2 | S | 287 | VAL |
| 2 | S | 325 | LEU |
| 2 | S | 331 | LEU |
| 2 | T | 3 | LEU |
| 2 | T | 9 | ASN |
| 2 | T | 29 | THR |
| 2 | T | 83 | LEU |
| 2 | T | 123 | ILE |
| 2 | T | 136 | LYS |
| 2 | T | 163 | ILE |
| 2 | T | 168 | ILE |
| 2 | T | 220 | ILE |
| 2 | T | 272 | LEU |
| 2 | T | 287 | VAL |
| 2 | T | 325 | LEU |
| 2 | T | 331 | LEU |
| 2 | U | 3 | LEU |
| 2 | U | 9 | ASN |
| 2 | U | 29 | THR |
| 2 | U | 83 | LEU |
| 2 | U | 123 | ILE |
| 2 | U | 136 | LYS |
| 2 | U | 163 | ILE |
| 2 | U | 168 | ILE |
| 2 | U | 220 | ILE |
| 2 | U | 272 | LEU |
| 2 | U | 287 | VAL |
| 2 | U | 301 | TYR |
| 2 | U | 325 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | U | 331 | LEU |
| 2 | V | 3 | LEU |
| 2 | V | 9 | ASN |
| 2 | V | 29 | THR |
| 2 | V | 83 | LEU |
| 2 | V | 123 | ILE |
| 2 | V | 136 | LYS |
| 2 | V | 163 | ILE |
| 2 | V | 220 | ILE |
| 2 | V | 272 | LEU |
| 2 | V | 287 | VAL |
| 2 | V | 325 | LEU |
| 2 | V | 331 | LEU |
| 2 | W | 3 | LEU |
| 2 | W | 9 | ASN |
| 2 | W | 29 | THR |
| 2 | W | 83 | LEU |
| 2 | W | 123 | ILE |
| 2 | W | 136 | LYS |
| 2 | W | 163 | ILE |
| 2 | W | 168 | ILE |
| 2 | W | 220 | ILE |
| 2 | W | 272 | LEU |
| 2 | W | 287 | VAL |
| 2 | W | 301 | TYR |
| 2 | W | 325 | LEU |
| 2 | W | 331 | LEU |
| 2 | X | 3 | LEU |
| 2 | X | 9 | ASN |
| 2 | X | 29 | THR |
| 2 | X | 83 | LEU |
| 2 | X | 123 | ILE |
| 2 | X | 136 | LYS |
| 2 | X | 163 | ILE |
| 2 | X | 168 | ILE |
| 2 | X | 220 | ILE |
| 2 | X | 272 | LEU |
| 2 | X | 287 | VAL |
| 2 | X | 325 | LEU |
| 2 | X | 331 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 26 | GLN |
| 2 | B | 59 | HIS |
| 2 | B | 187 | ASN |
| 2 | B | 274 | HIS |
| 2 | B | 327 | ASN |
| 2 | C | 26 | GLN |
| 2 | C | 59 | HIS |
| 2 | C | 274 | HIS |
| 2 | C | 327 | ASN |
| 2 | D | 26 | GLN |
| 2 | D | 59 | HIS |
| 2 | D | 274 | HIS |
| 2 | D | 327 | ASN |
| 2 | E | 26 | GLN |
| 2 | E | 59 | HIS |
| 2 | E | 274 | HIS |
| 2 | E | 327 | ASN |
| 2 | F | 26 | GLN |
| 2 | F | 59 | HIS |
| 2 | F | 274 | HIS |
| 2 | F | 327 | ASN |
| 2 | G | 26 | GLN |
| 2 | G | 59 | HIS |
| 2 | G | 274 | HIS |
| 2 | G | 327 | ASN |
| 2 | H | 26 | GLN |
| 2 | H | 59 | HIS |
| 2 | H | 274 | HIS |
| 2 | H | 327 | ASN |
| 2 | I | 26 | GLN |
| 2 | I | 59 | HIS |
| 2 | I | 274 | HIS |
| 2 | I | 327 | ASN |
| 2 | J | 26 | GLN |
| 2 | J | 59 | HIS |
| 2 | J | 274 | HIS |
| 2 | J | 327 | ASN |
| 2 | K | 26 | GLN |
| 2 | K | 59 | HIS |
| 2 | K | 274 | HIS |
| 2 | K | 327 | ASN |
| 2 | L | 26 | GLN |
| 2 | L | 59 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | L | 274 | HIS |
| 2 | L | 327 | ASN |
| 2 | M | 26 | GLN |
| 2 | M | 59 | HIS |
| 2 | M | 274 | HIS |
| 2 | M | 327 | ASN |
| 2 | N | 26 | GLN |
| 2 | N | 59 | HIS |
| 2 | N | 274 | HIS |
| 2 | N | 327 | ASN |
| 2 | O | 26 | GLN |
| 2 | O | 59 | HIS |
| 2 | O | 274 | HIS |
| 2 | O | 327 | ASN |
| 2 | P | 26 | GLN |
| 2 | P | 59 | HIS |
| 2 | P | 274 | HIS |
| 2 | P | 327 | ASN |
| 2 | Q | 26 | GLN |
| 2 | Q | 59 | HIS |
| 2 | Q | 274 | HIS |
| 2 | Q | 327 | ASN |
| 2 | R | 26 | GLN |
| 2 | R | 59 | HIS |
| 2 | R | 274 | HIS |
| 2 | R | 327 | ASN |
| 2 | S | 26 | GLN |
| 2 | S | 59 | HIS |
| 2 | S | 274 | HIS |
| 2 | S | 327 | ASN |
| 2 | T | 26 | GLN |
| 2 | T | 59 | HIS |
| 2 | T | 274 | HIS |
| 2 | T | 327 | ASN |
| 2 | U | 26 | GLN |
| 2 | U | 59 | HIS |
| 2 | U | 274 | HIS |
| 2 | U | 327 | ASN |
| 2 | V | 26 | GLN |
| 2 | V | 59 | HIS |
| 2 | V | 274 | HIS |
| 2 | V | 327 | ASN |

*Continued on next page...*

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | W | 26 | GLN |
| 2 | W | 59 | HIS |
| 2 | W | 274 | HIS |
| 2 | W | 327 | ASN |
| 2 | X | 59 | HIS |
| 2 | X | 274 | HIS |
| 2 | X | 327 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 1 | A | 160/161 (99%) | 22 (13%) | 0 |

All (22) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 11 | C |
| 1 | A | 21 | C |
| 1 | A | 31 | C |
| 1 | A | 41 | C |
| 1 | A | 51 | C |
| 1 | A | 61 | C |
| 1 | A | 71 | C |
| 1 | A | 81 | C |
| 1 | A | 91 | C |
| 1 | A | 101 | C |
| 1 | A | 111 | C |
| 1 | A | 121 | C |
| 1 | A | 131 | C |
| 1 | A | 141 | C |
| 1 | A | 151 | C |
| 1 | A | 161 | C |
| 1 | A | 171 | C |
| 1 | A | 181 | C |
| 1 | A | 191 | C |
| 1 | A | 201 | C |
| 1 | A | 211 | C |
| 1 | A | 221 | C |

There are no RNA pucker outliers to report.

## 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 monosaccharides 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.

# 6 Tomogram visualisation (i)

This section contains visualisations of the EMDB entry EMD-2369. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

## 6.1 Orthogonal projections (i)

This section was not generated.

## 6.2 Central slices (i)

This section was not generated.

## 6.3 Largest variance slices (i)

This section was not generated.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

## 6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Tomogram analysis (i)

This section contains the results of statistical analysis of the tomogram.

## 7.1 Map-value distribution (i)

This section was not generated.

# 8 Map-model fit (i)

This section was not generated.