



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:28 AM UTC

PDB ID : 5UK4 / pdb\_00005uk4  
Title : VESICULAR STOMATITIS VIRUS N PROTEIN IN COMPLEX WITH INHIBITORY NANOBODY 1307  
Authors : Hanke, L.; Knockenhauer, K.E.; Ploegh, H.L.; Schwartz, T.U.  
Deposited on : 2017-01-19  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

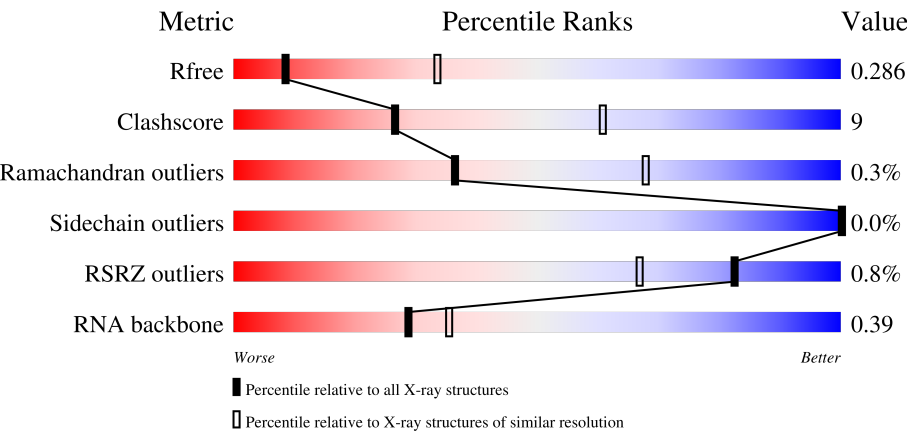
|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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.



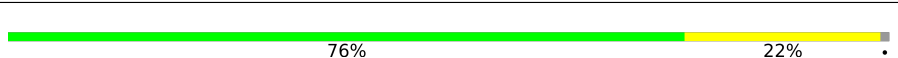
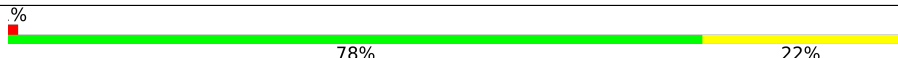
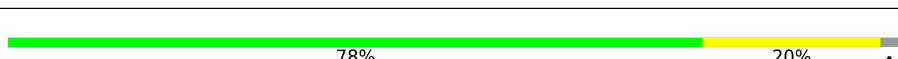
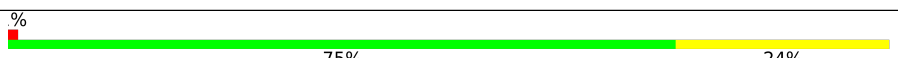
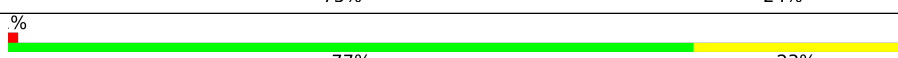
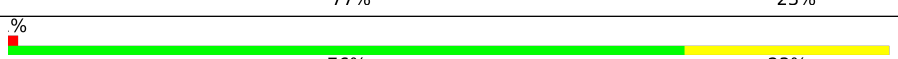
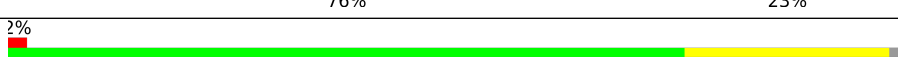
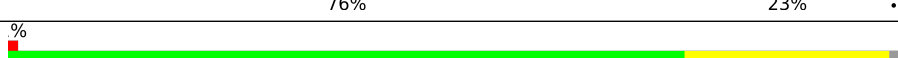
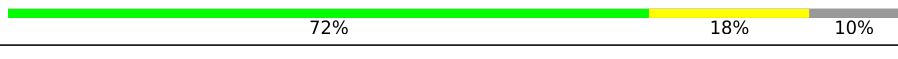
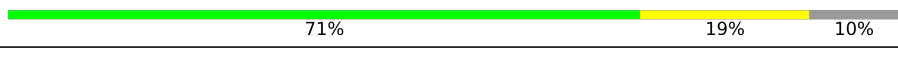
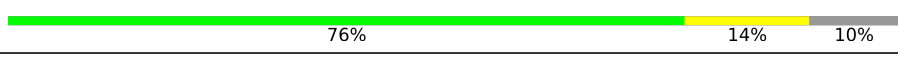
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |
| RNA backbone          | 3983                        | 1222 (3.50-2.90)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                           |
|-----|-------|--------|--------------------------------------------|
| 1   | A     | 422    | <div><div></div><div>75%24%.</div></div>   |
| 1   | B     | 422    | <div><div>%</div><div>75%22%.</div></div>  |
| 1   | C     | 422    | <div><div>%</div><div>75%24%.</div></div>  |
| 1   | D     | 422    | <div><div>%</div><div>78%20%..</div></div> |

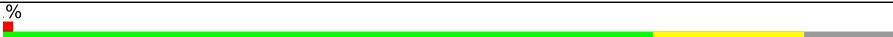
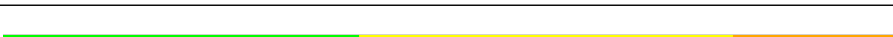
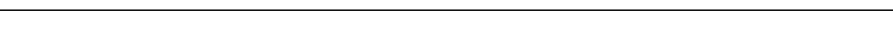
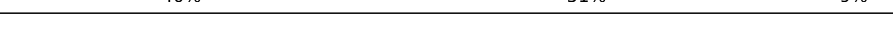
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| Mol | Chain | Length | Quality of chain                                                                     |   |
|-----|-------|--------|--------------------------------------------------------------------------------------|---|
| 1   | E     | 422    |    | • |
| 1   | F     | 422    |    |   |
| 1   | G     | 422    |    | • |
| 1   | H     | 422    |    |   |
| 1   | I     | 422    |    | • |
| 1   | J     | 422    |    |   |
| 1   | K     | 422    |    |   |
| 1   | L     | 422    |    |   |
| 1   | M     | 422    |    | • |
| 1   | N     | 422    |    | • |
| 1   | O     | 422    |    |   |
| 1   | P     | 422    |    | • |
| 1   | Q     | 422    |   | • |
| 1   | R     | 422    |  | • |
| 1   | S     | 422    |  |   |
| 1   | T     | 422    |  |   |
| 2   | a     | 139    |  |   |
| 2   | b     | 139    |  |   |
| 2   | c     | 139    |  |   |
| 2   | d     | 139    |  | • |
| 2   | e     | 139    |  |   |
| 2   | f     | 139    |  |   |
| 2   | g     | 139    |  |   |
| 2   | h     | 139    |  |   |
| 2   | i     | 139    |  |   |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | j     | 139    |    |
| 2   | k     | 139    |    |
| 2   | l     | 139    |    |
| 2   | m     | 139    |    |
| 2   | n     | 139    |    |
| 2   | o     | 139    |    |
| 2   | p     | 139    |    |
| 2   | q     | 139    |    |
| 2   | r     | 139    |    |
| 2   | s     | 139    |    |
| 2   | t     | 139    |    |
| 3   | u     | 45     |    |
| 3   | v     | 45     |  |
| 3   | w     | 45     |  |
| 3   | x     | 45     |  |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 89086 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Nucleoprotein.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | P     | 414      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3281  | 2090 | 551 | 622 | 18 |         |         |       |
| 1   | B     | 412      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3270  | 2083 | 548 | 621 | 18 |         |         |       |
| 1   | Q     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3316  | 2111 | 556 | 631 | 18 |         |         |       |
| 1   | C     | 417      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3299  | 2102 | 554 | 625 | 18 |         |         |       |
| 1   | R     | 419      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3315  | 2112 | 556 | 629 | 18 |         |         |       |
| 1   | D     | 418      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3305  | 2106 | 552 | 629 | 18 |         |         |       |
| 1   | S     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3327  | 2118 | 558 | 633 | 18 |         |         |       |
| 1   | E     | 413      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3273  | 2084 | 550 | 621 | 18 |         |         |       |
| 1   | T     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3327  | 2118 | 558 | 633 | 18 |         |         |       |
| 1   | K     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3327  | 2118 | 558 | 633 | 18 |         |         |       |
| 1   | L     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3327  | 2118 | 558 | 633 | 18 |         |         |       |
| 1   | N     | 418      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3305  | 2106 | 552 | 629 | 18 |         |         |       |
| 1   | M     | 416      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3291  | 2099 | 550 | 624 | 18 |         |         |       |
| 1   | F     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3327  | 2118 | 558 | 633 | 18 |         |         |       |
| 1   | G     | 416      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3295  | 2099 | 553 | 625 | 18 |         |         |       |
| 1   | H     | 420      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3316  | 2112 | 554 | 632 | 18 |         |         |       |

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| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | I     | 415      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3289  | 2094 | 552 | 625 | 18 |         |         |       |
| 1   | O     | 420      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3323  | 2116 | 557 | 632 | 18 |         |         |       |
| 1   | J     | 420      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3323  | 2116 | 557 | 632 | 18 |         |         |       |
| 1   | A     | 416      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3290  | 2097 | 550 | 625 | 18 |         |         |       |

- Molecule 2 is a protein called Anti-vesicular stomatitis virus N VHH.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | p     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | b     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | q     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | c     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | r     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | d     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | s     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | e     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | t     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | k     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | l     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | n     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | m     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | f     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |
| 2   | g     | 125      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 605 | 171 | 187 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms        |          |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|---------|-------|
| 2   | h     | 125      | Total<br>968 | C<br>605 | N<br>171 | O<br>187 | S<br>5 | 0       | 0       | 0     |
| 2   | i     | 125      | Total<br>968 | C<br>605 | N<br>171 | O<br>187 | S<br>5 | 0       | 0       | 0     |
| 2   | o     | 125      | Total<br>968 | C<br>605 | N<br>171 | O<br>187 | S<br>5 | 0       | 0       | 0     |
| 2   | j     | 125      | Total<br>968 | C<br>605 | N<br>171 | O<br>187 | S<br>5 | 0       | 0       | 0     |
| 2   | a     | 125      | Total<br>968 | C<br>605 | N<br>171 | O<br>187 | S<br>5 | 0       | 0       | 0     |

There are 280 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| p     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| p     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| p     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| p     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| p     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| p     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| p     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| p     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| p     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| p     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| p     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| p     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| p     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| p     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| b     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| b     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| b     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| b     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| b     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| b     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| b     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| b     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| b     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| b     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| b     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| b     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| b     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| b     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| q     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| q     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| q     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| q     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| q     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| q     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| q     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| q     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| q     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| q     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| q     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| q     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| q     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| q     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| c     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| c     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| c     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| c     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| c     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| c     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| c     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| c     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| c     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| c     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| c     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| c     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| c     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| c     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| r     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| r     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| r     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| r     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| r     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| r     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| r     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| r     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| r     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| r     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| r     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| r     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| r     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| r     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| d     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| d     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| d     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| d     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| d     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| d     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| d     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| d     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| d     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| d     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| d     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| d     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| d     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| d     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| s     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| s     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| s     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| s     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| s     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| s     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| s     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| s     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| s     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| s     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| s     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| s     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| s     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| s     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| e     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| e     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| e     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| e     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| e     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| e     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| e     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| e     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| e     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| e     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| e     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| e     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| e     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| e     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| t     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| t     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| t     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| t     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| t     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| t     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| t     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| t     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| t     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| t     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| t     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| t     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| t     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| t     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| k     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| k     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| k     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| k     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| k     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| k     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| k     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| k     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| k     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| k     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| k     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| k     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| k     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| k     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| l     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| l     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| l     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| l     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| l     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| l     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| l     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| l     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| l     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| l     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| l     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| l     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| l     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| l     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| n     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |

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*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| n     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| n     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| n     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| n     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| n     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| n     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| n     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| n     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| n     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| n     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| n     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| n     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| n     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| m     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| m     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| m     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| m     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| m     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| m     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| m     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| m     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| m     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| m     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| m     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| m     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| m     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| m     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| f     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| f     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| f     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| f     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| f     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| f     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| f     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| f     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| f     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| f     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| f     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| f     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| f     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| f     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| g     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| g     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| g     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| g     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| g     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| g     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| g     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| g     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| g     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| g     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| g     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| g     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| g     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| g     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| h     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| h     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| h     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| h     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| h     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| h     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| h     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| h     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| h     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| h     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| h     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| h     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| h     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| h     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| i     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| i     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| i     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| i     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| i     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| i     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| i     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| i     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| i     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| i     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| i     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| i     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| i     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| i     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| o     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| o     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| o     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| o     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| o     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| o     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| o     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| o     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| o     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| o     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| o     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| o     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| o     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| o     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| j     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| j     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| j     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| j     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| j     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| j     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| j     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| j     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| j     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| j     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| j     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| j     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| j     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| j     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| a     | 126     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| a     | 127     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| a     | 128     | LEU      | -      | expression tag | UNP A0A192B6J6 |
| a     | 129     | PRO      | -      | expression tag | UNP A0A192B6J6 |
| a     | 130     | GLU      | -      | expression tag | UNP A0A192B6J6 |
| a     | 131     | THR      | -      | expression tag | UNP A0A192B6J6 |
| a     | 132     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| a     | 133     | GLY      | -      | expression tag | UNP A0A192B6J6 |
| a     | 134     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| a     | 135     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| a     | 136     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| a     | 137     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| a     | 138     | HIS      | -      | expression tag | UNP A0A192B6J6 |
| a     | 139     | HIS      | -      | expression tag | UNP A0A192B6J6 |

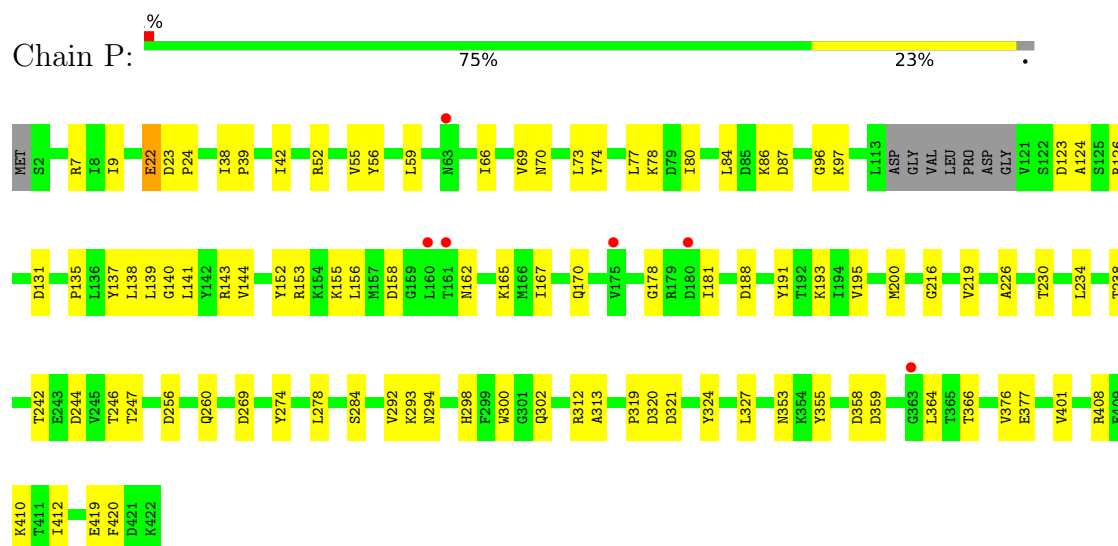
- Molecule 3 is a RNA chain called RNA (45-MER).

| Mol | Chain | Residues | Atoms        |          |         |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|---------|-------|
| 3   | u     | 45       | Total<br>900 | C<br>405 | N<br>90 | O<br>360 | P<br>45 | 0       | 0       | 0     |
| 3   | v     | 45       | Total<br>900 | C<br>405 | N<br>90 | O<br>360 | P<br>45 | 0       | 0       | 0     |
| 3   | w     | 45       | Total<br>900 | C<br>405 | N<br>90 | O<br>360 | P<br>45 | 0       | 0       | 0     |
| 3   | x     | 45       | Total<br>900 | C<br>405 | N<br>90 | O<br>360 | P<br>45 | 0       | 0       | 0     |

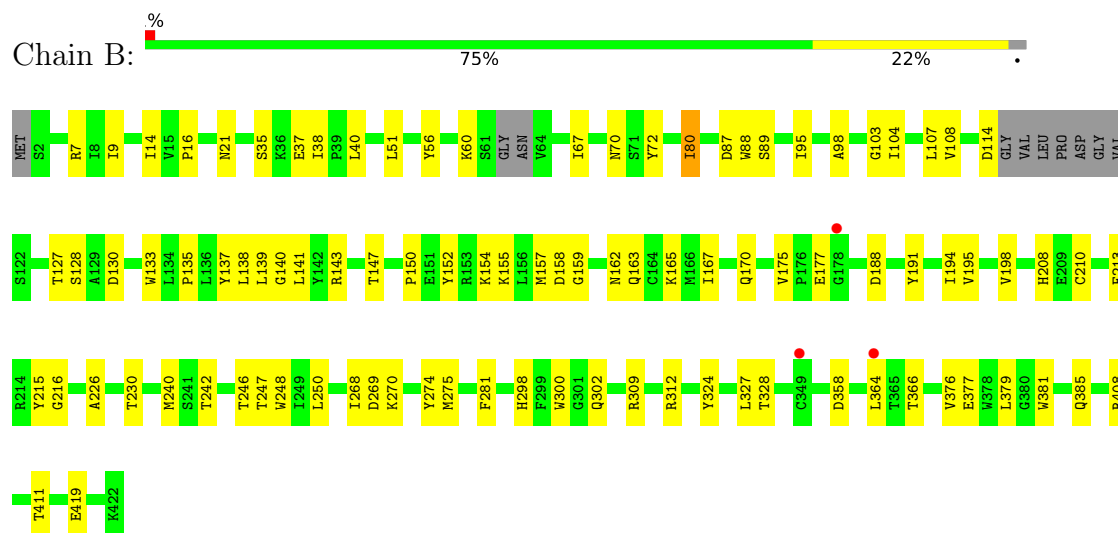
### 3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

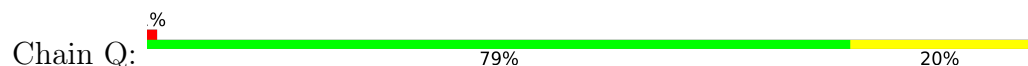
#### • Molecule 1: Nucleoprotein



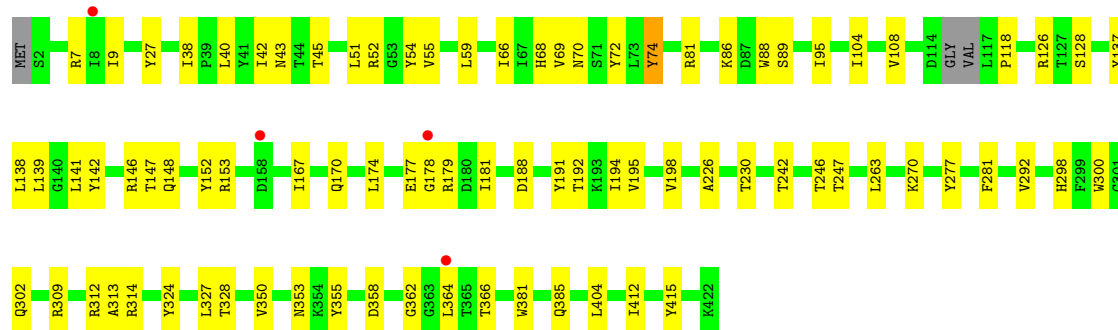
#### • Molecule 1: Nucleoprotein



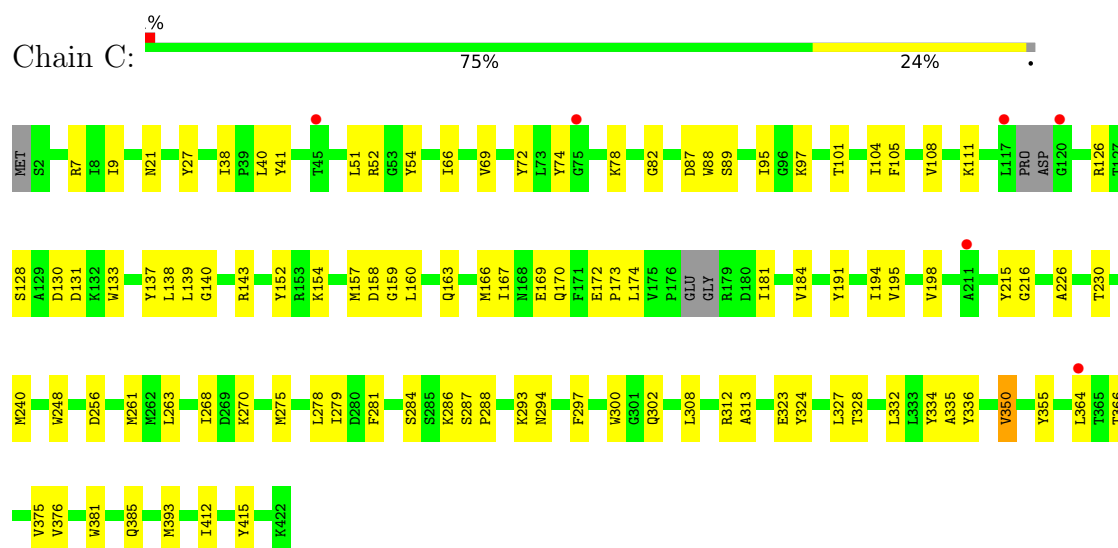
#### • Molecule 1: Nucleoprotein



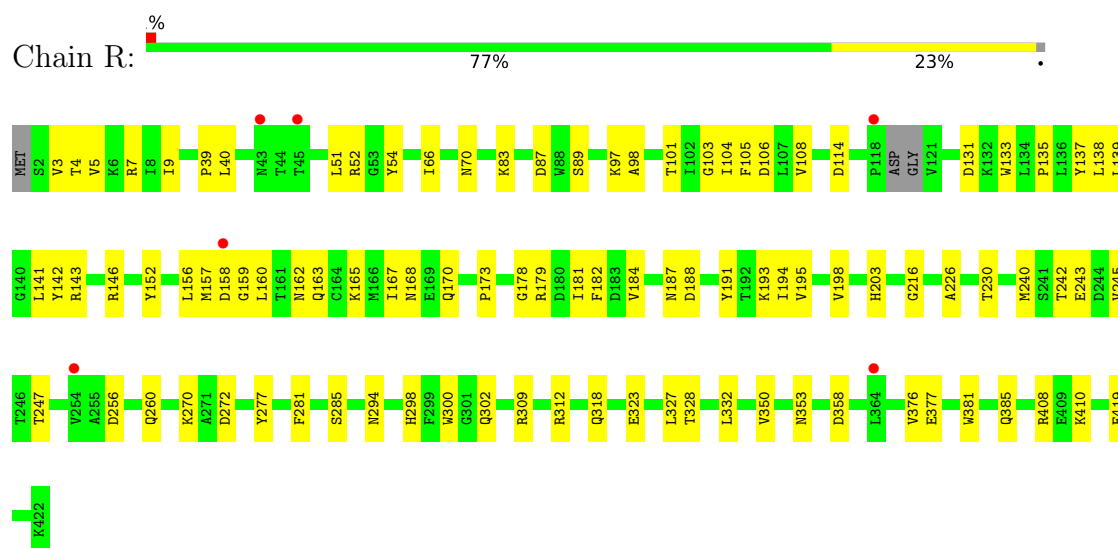




• Molecule 1: Nucleoprotein



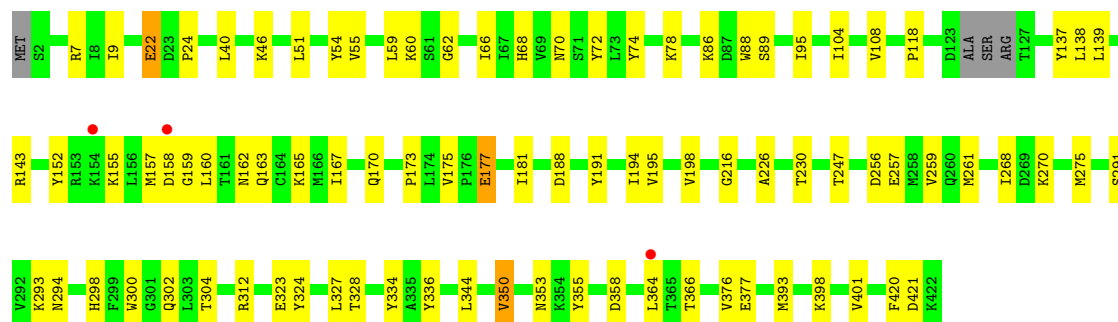
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein

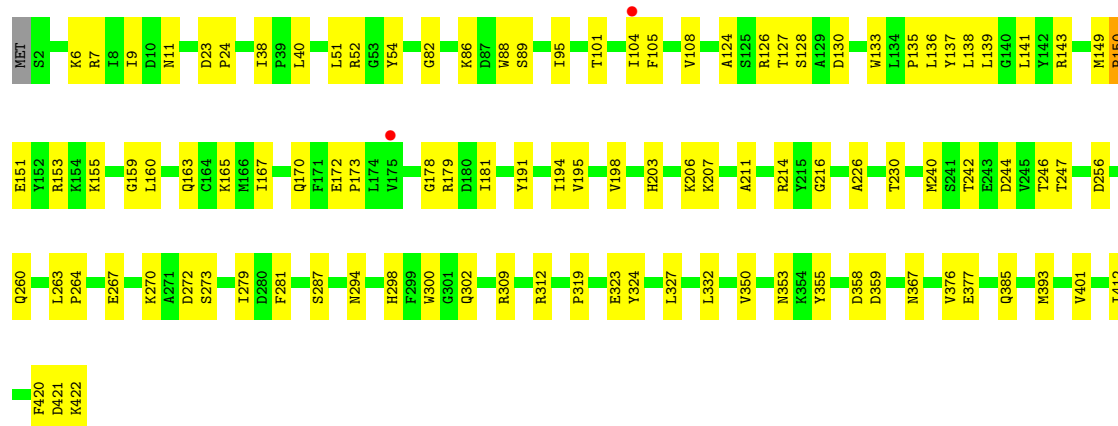






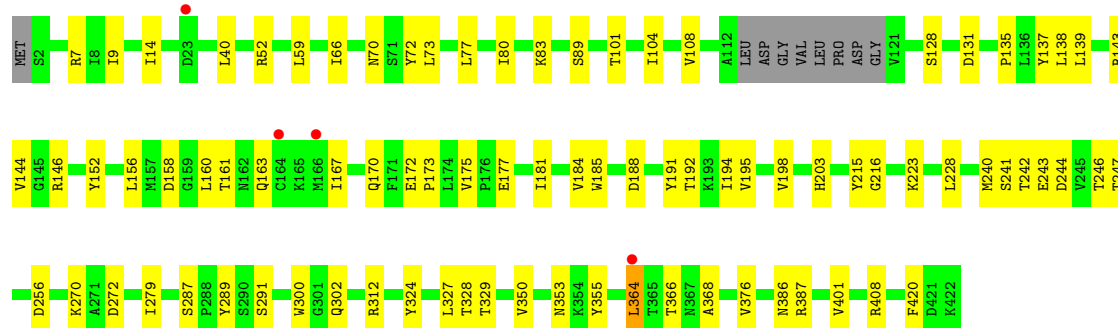
• Molecule 1: Nucleoprotein

Chain S: 75% 24%



• Molecule 1: Nucleoprotein

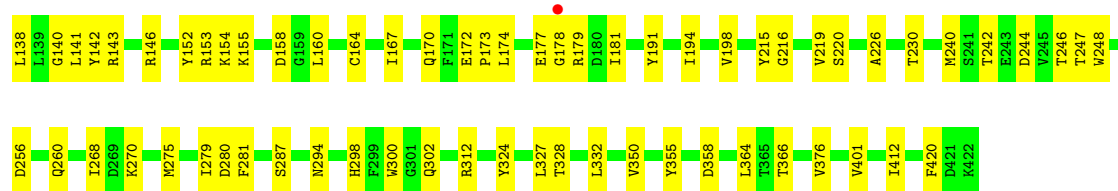
Chain E: 78% 20%



• Molecule 1: Nucleoprotein

Chain T: 77% 23%

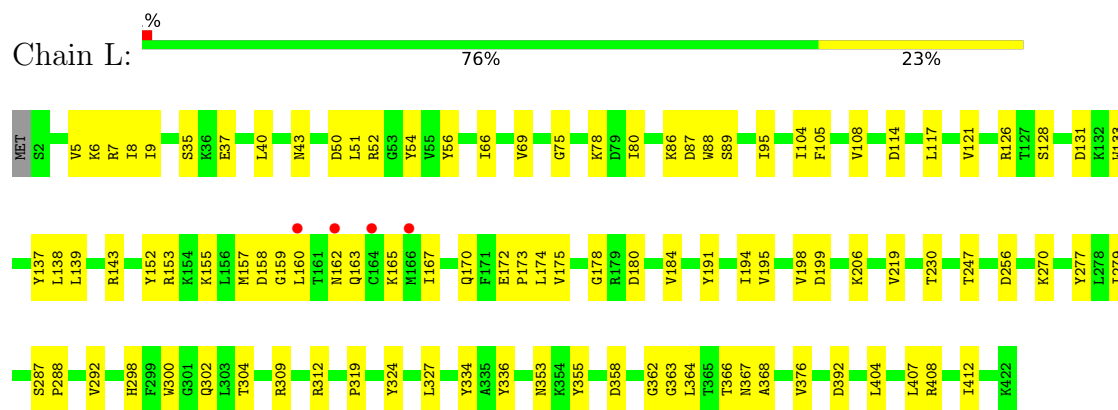




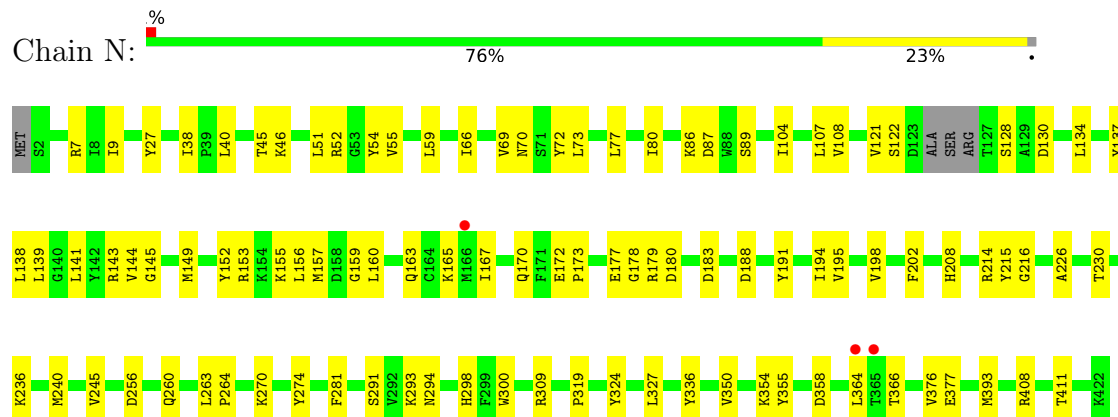
• Molecule 1: Nucleoprotein



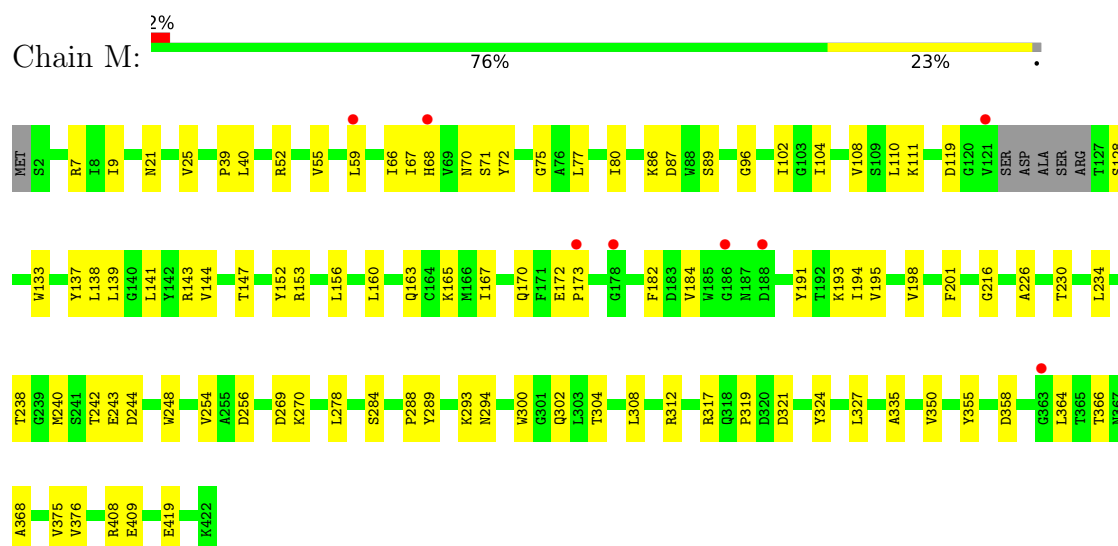
• Molecule 1: Nucleoprotein



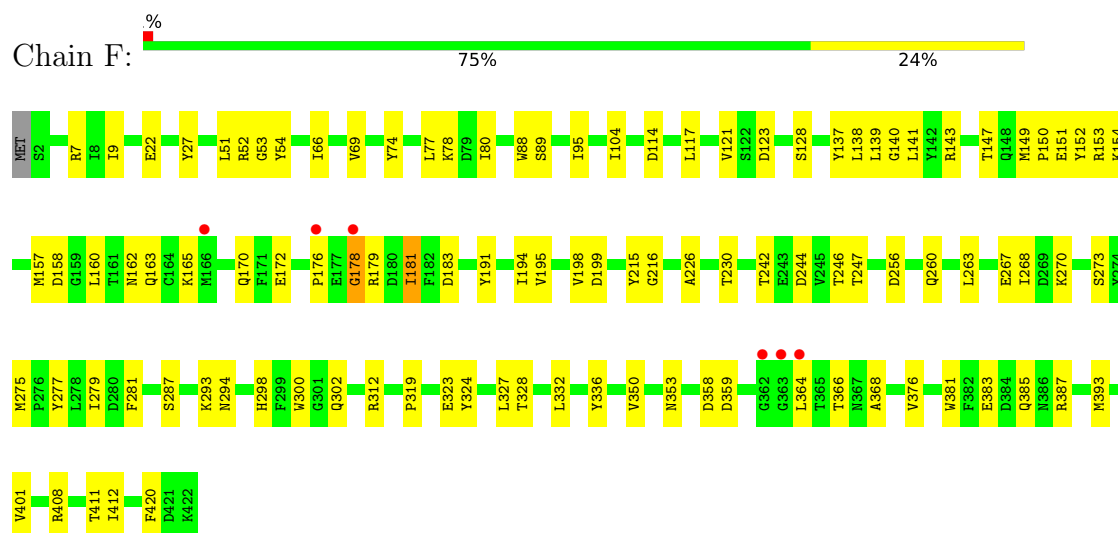
• Molecule 1: Nucleoprotein



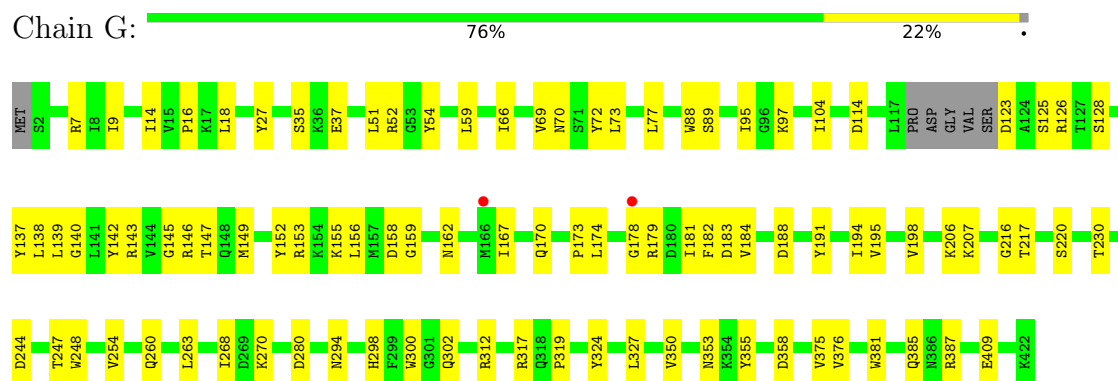
• Molecule 1: Nucleoprotein



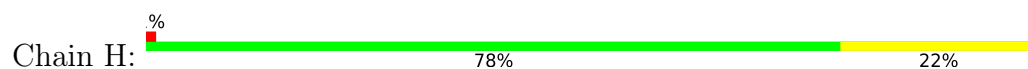
• Molecule 1: Nucleoprotein

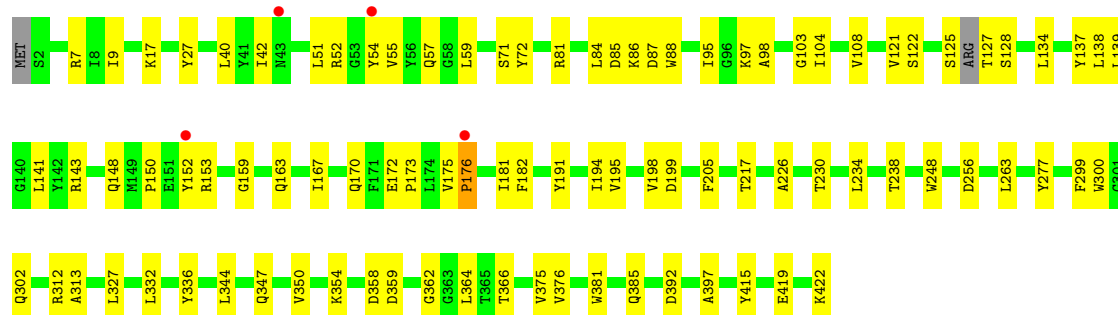


• Molecule 1: Nucleoprotein



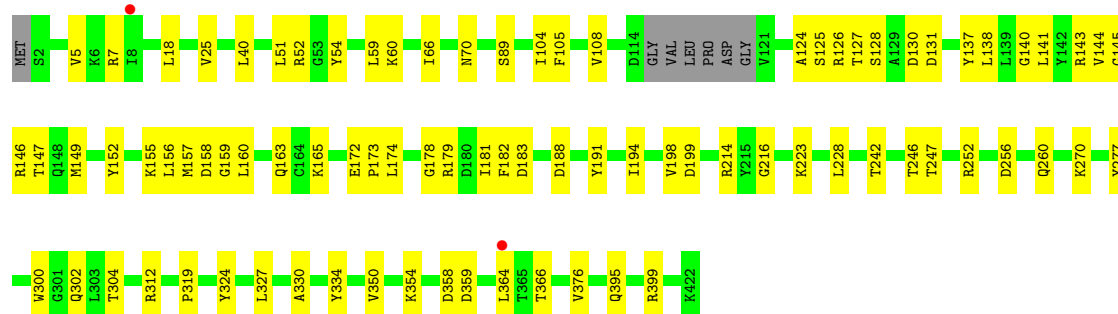
• Molecule 1: Nucleoprotein





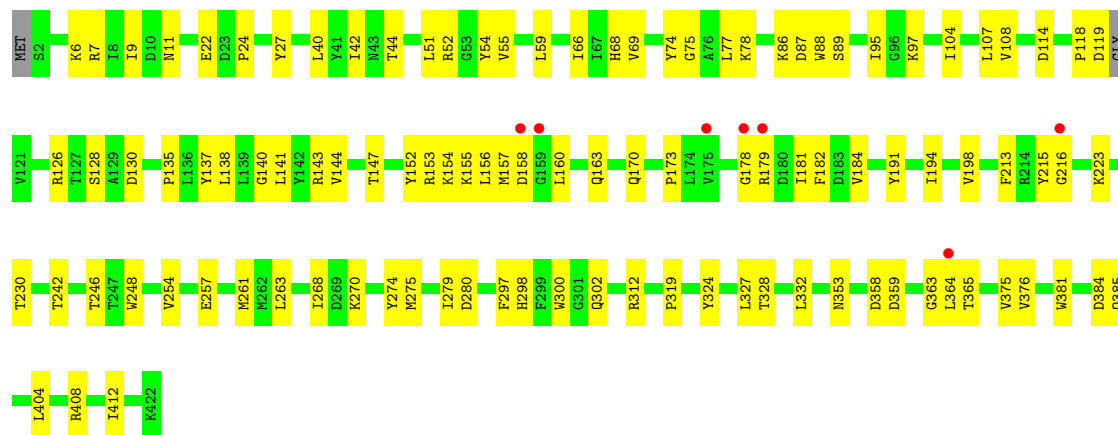
### • Molecule 1: Nucleoprotein

Chain I: 78% 20%



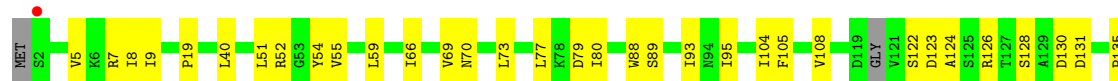
### • Molecule 1: Nucleoprotein

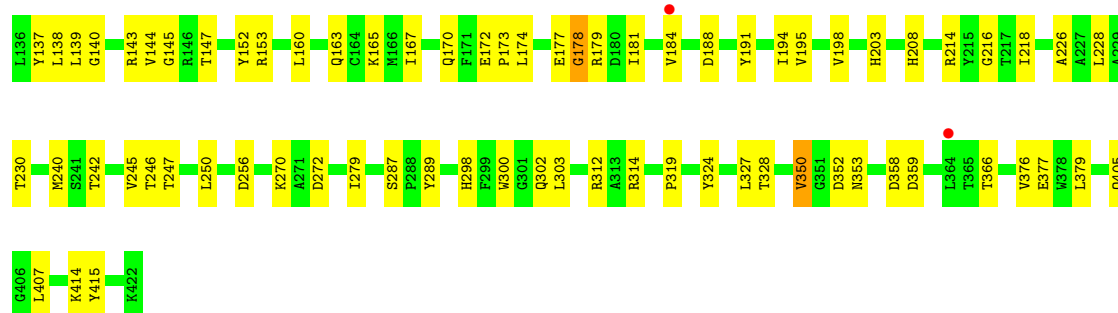
Chain O: 2% 74% 25%



### • Molecule 1: Nucleoprotein

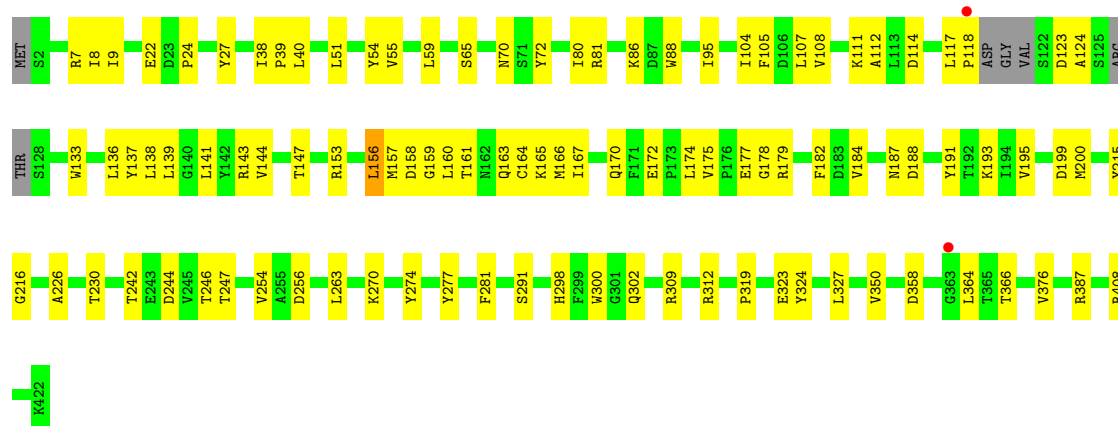
Chain J: 75% 24%





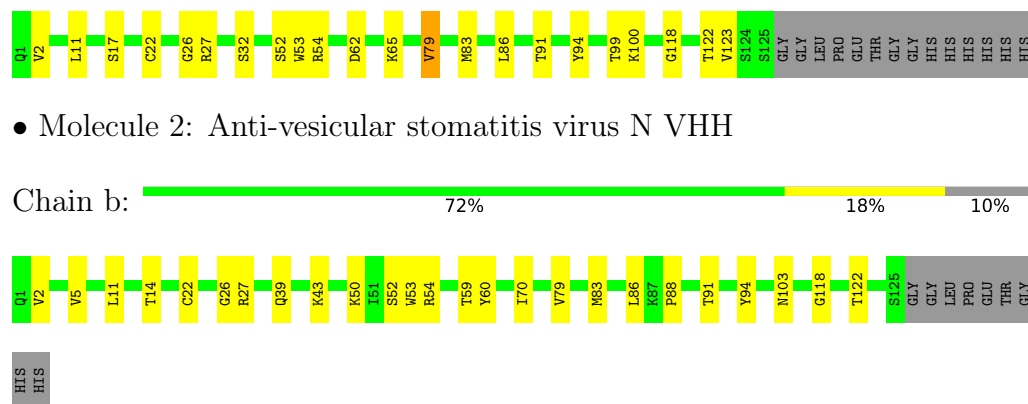
• Molecule 1: Nucleoprotein

Chain A: 75% 24%



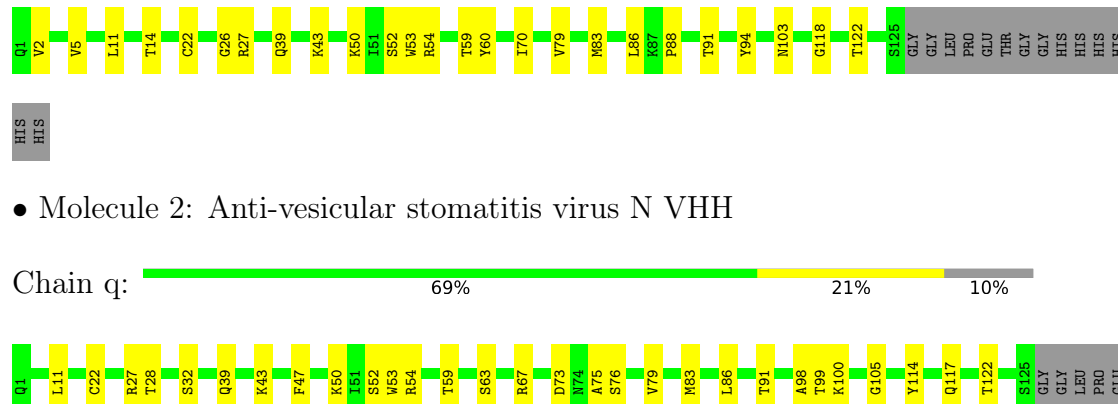
• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain p: 74% 15% 10%



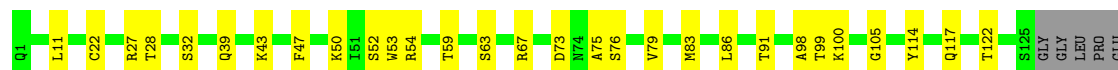
• Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain b: 72% 18% 10%



• Molecule 2: Anti-vesicular stomatitis virus N VHH

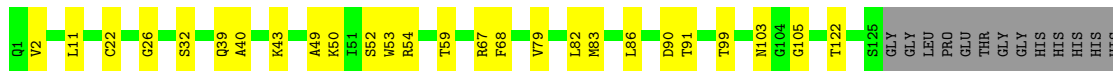
Chain q: 69% 21% 10%



THR  
GLY  
GLY  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain c:  71% 19% 10%



HIS

- Molecule 2: Anti-vesicular stomatitis virus N VHH

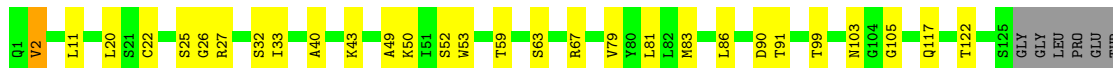
Chain r:  72% 18% 10%



HIS

- Molecule 2: Anti-vesicular stomatitis virus N VHH

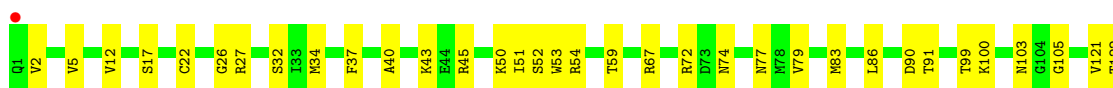
Chain d:  69% 20% 10%

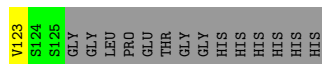


GLY  
GLY  
HIS  
HIS  
HIS  
HIS  
HIS

- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain s:  65% 25% 10%





- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain e:  76% 14% 10%



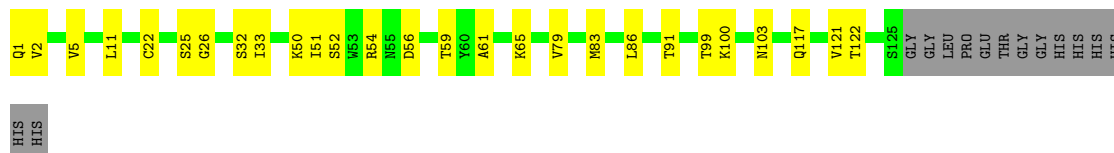
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain t:  73% 17% 10%



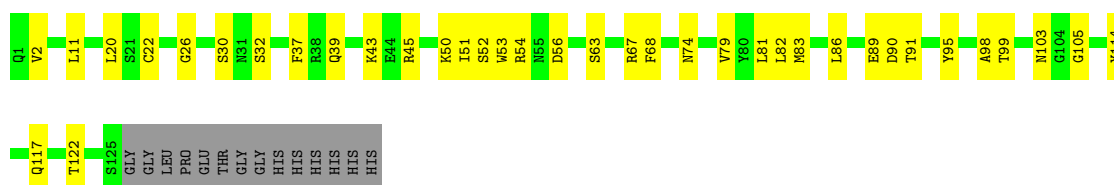
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain k: 71% 19% 10%



- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain l: 63% 27% 10%



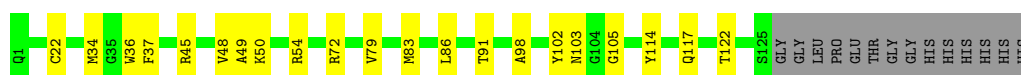
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain n: 65% 25% 10%



- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain m: 75% 15% 10%



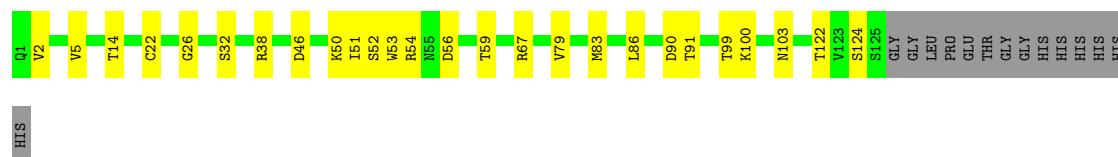
- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain f: 73% 17% 10%



- Molecule 2: Anti-vesicular stomatitis virus N VHH

Chain g: 71% 19% 10%



• Molecule 2: Anti-vesicular stomatitis virus N VHH



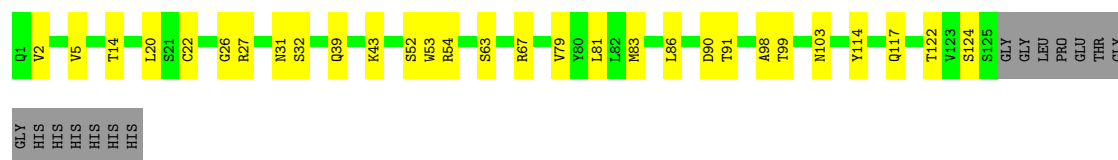
• Molecule 2: Anti-vesicular stomatitis virus N VHH



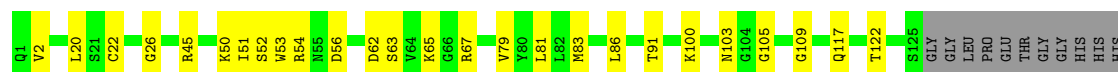
• Molecule 2: Anti-vesicular stomatitis virus N VHH



• Molecule 2: Anti-vesicular stomatitis virus N VHH



• Molecule 2: Anti-vesicular stomatitis virus N VHH







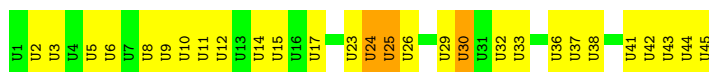
• Molecule 3: RNA (45-MER)

Chain u: 40% 42% 18%



• Molecule 3: RNA (45-MER)

Chain v: 38% 56% 7%



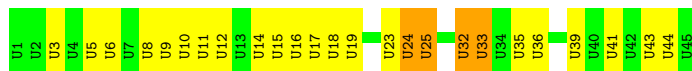
• Molecule 3: RNA (45-MER)

Chain w: 40% 51% 9%



• Molecule 3: RNA (45-MER)

Chain x: 44% 47% 9%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1                                                         | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 147.56Å 156.01Å 217.45Å<br>79.24° 75.66° 62.27°             | Depositor        |
| Resolution (Å)                                                          | 128.35 – 3.20<br>128.35 – 3.20                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.0 (128.35-3.20)<br>91.9 (128.35-3.20)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.20                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.45 (at 3.19Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.11.1_2575                                          | Depositor        |
| R, $R_{free}$                                                           | 0.236 , 0.288<br>0.237 , 0.286                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1990 reflections (0.73%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 56.7                                                        | Xtriage          |
| Anisotropy                                                              | 0.724                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.28 , 5.4                                                  | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.89                                                        | EDS              |
| Total number of atoms                                                   | 89086                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 57.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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     | 0.12         | 0/3364  | 0.31        | 0/4551        |
| 1   | B     | 0.11         | 0/3343  | 0.31        | 0/4521        |
| 1   | C     | 0.10         | 0/3372  | 0.30        | 0/4561        |
| 1   | D     | 0.11         | 0/3380  | 0.30        | 0/4575        |
| 1   | E     | 0.11         | 0/3347  | 0.32        | 0/4528        |
| 1   | F     | 0.11         | 0/3403  | 0.31        | 0/4607        |
| 1   | G     | 0.11         | 0/3369  | 0.33        | 0/4558        |
| 1   | H     | 0.13         | 0/3391  | 0.33        | 0/4590        |
| 1   | I     | 0.11         | 0/3363  | 0.31        | 0/4550        |
| 1   | J     | 0.11         | 0/3398  | 0.31        | 0/4599        |
| 1   | K     | 0.11         | 0/3403  | 0.32        | 0/4607        |
| 1   | L     | 0.11         | 0/3403  | 0.34        | 1/4607 (0.0%) |
| 1   | M     | 0.12         | 0/3366  | 0.30        | 0/4556        |
| 1   | N     | 0.10         | 0/3380  | 0.33        | 0/4575        |
| 1   | O     | 0.11         | 0/3398  | 0.31        | 0/4599        |
| 1   | P     | 0.11         | 0/3355  | 0.31        | 0/4539        |
| 1   | Q     | 0.12         | 0/3391  | 0.33        | 1/4589 (0.0%) |
| 1   | R     | 0.12         | 0/3390  | 0.31        | 0/4588        |
| 1   | S     | 0.13         | 0/3403  | 0.34        | 0/4607        |
| 1   | T     | 0.11         | 0/3403  | 0.31        | 0/4607        |
| 2   | a     | 0.09         | 0/988   | 0.30        | 0/1334        |
| 2   | b     | 0.09         | 0/988   | 0.31        | 0/1334        |
| 2   | c     | 0.10         | 0/988   | 0.31        | 0/1334        |
| 2   | d     | 0.10         | 0/988   | 0.33        | 0/1334        |
| 2   | e     | 0.10         | 0/988   | 0.32        | 0/1334        |
| 2   | f     | 0.10         | 0/988   | 0.30        | 0/1334        |
| 2   | g     | 0.10         | 0/988   | 0.30        | 0/1334        |
| 2   | h     | 0.10         | 0/988   | 0.31        | 0/1334        |
| 2   | i     | 0.10         | 0/988   | 0.32        | 0/1334        |
| 2   | j     | 0.09         | 0/988   | 0.31        | 0/1334        |
| 2   | k     | 0.09         | 0/988   | 0.31        | 0/1334        |
| 2   | l     | 0.09         | 0/988   | 0.30        | 0/1334        |
| 2   | m     | 0.09         | 0/988   | 0.29        | 0/1334        |
| 2   | n     | 0.09         | 0/988   | 0.30        | 0/1334        |

| Mol | Chain | Bond lengths |         | Bond angles |                 |
|-----|-------|--------------|---------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5         |
| 2   | o     | 0.09         | 0/988   | 0.30        | 0/1334          |
| 2   | p     | 0.09         | 0/988   | 0.30        | 0/1334          |
| 2   | q     | 0.09         | 0/988   | 0.30        | 0/1334          |
| 2   | r     | 0.09         | 0/988   | 0.32        | 0/1334          |
| 2   | s     | 0.09         | 0/988   | 0.31        | 0/1334          |
| 2   | t     | 0.09         | 0/988   | 0.33        | 0/1334          |
| 3   | u     | 0.14         | 0/989   | 0.42        | 0/1526          |
| 3   | v     | 0.14         | 0/989   | 0.42        | 0/1526          |
| 3   | w     | 0.14         | 0/989   | 0.42        | 0/1526          |
| 3   | x     | 0.14         | 0/989   | 0.44        | 0/1526          |
| All | All   | 0.11         | 0/91338 | 0.32        | 2/124298 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | H     | 0                   | 1                   |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | Q     | 292 | VAL  | N-CA-C | -6.22 | 106.74      | 112.96   |
| 1   | L     | 292 | VAL  | N-CA-C | -6.12 | 106.84      | 112.96   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | H     | 152 | TYR  | Peptide |

## 5.2 Too-close contacts ⓘ

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     | 3290  | 0        | 3249     | 71      | 0            |
| 1   | B     | 3270  | 0        | 3230     | 64      | 0            |
| 1   | C     | 3299  | 0        | 3265     | 69      | 0            |
| 1   | D     | 3305  | 0        | 3263     | 65      | 0            |
| 1   | E     | 3273  | 0        | 3234     | 58      | 0            |
| 1   | F     | 3327  | 0        | 3287     | 74      | 0            |
| 1   | G     | 3295  | 0        | 3258     | 73      | 0            |
| 1   | H     | 3316  | 0        | 3273     | 60      | 0            |
| 1   | I     | 3289  | 0        | 3249     | 66      | 0            |
| 1   | J     | 3323  | 0        | 3283     | 83      | 0            |
| 1   | K     | 3327  | 0        | 3287     | 65      | 0            |
| 1   | L     | 3327  | 0        | 3287     | 79      | 1            |
| 1   | M     | 3291  | 0        | 3254     | 71      | 0            |
| 1   | N     | 3305  | 0        | 3263     | 71      | 0            |
| 1   | O     | 3323  | 0        | 3283     | 79      | 0            |
| 1   | P     | 3281  | 0        | 3245     | 64      | 0            |
| 1   | Q     | 3316  | 0        | 3274     | 58      | 1            |
| 1   | R     | 3315  | 0        | 3279     | 72      | 0            |
| 1   | S     | 3327  | 0        | 3287     | 77      | 0            |
| 1   | T     | 3327  | 0        | 3287     | 74      | 0            |
| 2   | a     | 968   | 0        | 932      | 16      | 0            |
| 2   | b     | 968   | 0        | 932      | 16      | 0            |
| 2   | c     | 968   | 0        | 932      | 19      | 0            |
| 2   | d     | 968   | 0        | 932      | 20      | 0            |
| 2   | e     | 968   | 0        | 932      | 12      | 0            |
| 2   | f     | 968   | 0        | 932      | 18      | 0            |
| 2   | g     | 968   | 0        | 932      | 17      | 0            |
| 2   | h     | 968   | 0        | 932      | 23      | 0            |
| 2   | i     | 968   | 0        | 932      | 20      | 0            |
| 2   | j     | 968   | 0        | 932      | 19      | 0            |
| 2   | k     | 968   | 0        | 932      | 19      | 0            |
| 2   | l     | 968   | 0        | 932      | 26      | 0            |
| 2   | m     | 968   | 0        | 932      | 14      | 0            |
| 2   | n     | 968   | 0        | 932      | 22      | 0            |
| 2   | o     | 968   | 0        | 932      | 16      | 0            |
| 2   | p     | 968   | 0        | 932      | 15      | 0            |
| 2   | q     | 968   | 0        | 932      | 19      | 0            |
| 2   | r     | 968   | 0        | 932      | 18      | 0            |
| 2   | s     | 968   | 0        | 932      | 26      | 0            |
| 2   | t     | 968   | 0        | 932      | 16      | 0            |
| 3   | u     | 900   | 0        | 451      | 23      | 0            |
| 3   | v     | 900   | 0        | 451      | 17      | 0            |
| 3   | w     | 900   | 0        | 451      | 17      | 0            |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | x     | 900   | 0        | 451      | 17      | 0            |
| All | All   | 89086 | 0        | 85781    | 1619    | 1            |

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 9.

All (1619) 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:D:158:ASP:O    | 1:D:162:ASN:HB2  | 1.45                     | 1.14              |
| 1:M:55:VAL:O     | 1:M:59:LEU:HD13  | 1.63                     | 0.97              |
| 1:G:158:ASP:O    | 1:G:162:ASN:HB2  | 1.66                     | 0.93              |
| 1:L:300:TRP:HB2  | 1:L:327:LEU:HD12 | 1.51                     | 0.93              |
| 1:K:300:TRP:HB2  | 1:K:327:LEU:HD12 | 1.51                     | 0.92              |
| 1:N:157:MET:O    | 1:N:160:LEU:HB2  | 1.72                     | 0.89              |
| 1:G:300:TRP:HB2  | 1:G:327:LEU:HD12 | 1.56                     | 0.86              |
| 1:I:300:TRP:HB2  | 1:I:327:LEU:HD12 | 1.56                     | 0.86              |
| 1:T:74:TYR:O     | 1:T:78:LYS:HB2   | 1.76                     | 0.85              |
| 1:F:149:MET:HG3  | 1:F:150:PRO:HD2  | 1.57                     | 0.85              |
| 1:M:300:TRP:HB2  | 1:M:327:LEU:HD12 | 1.58                     | 0.84              |
| 1:N:55:VAL:O     | 1:N:59:LEU:HB2   | 1.77                     | 0.83              |
| 1:D:300:TRP:HB2  | 1:D:327:LEU:HD12 | 1.60                     | 0.83              |
| 1:Q:300:TRP:HB2  | 1:Q:327:LEU:HD12 | 1.59                     | 0.83              |
| 2:t:39:GLN:NE2   | 2:t:43:LYS:O     | 2.10                     | 0.83              |
| 1:N:300:TRP:HB2  | 1:N:327:LEU:HD12 | 1.61                     | 0.82              |
| 1:C:300:TRP:HB2  | 1:C:327:LEU:HD12 | 1.62                     | 0.81              |
| 1:L:364:LEU:HD23 | 2:l:30:SER:HA    | 1.63                     | 0.81              |
| 1:F:27:TYR:CZ    | 1:F:263:LEU:HD22 | 2.16                     | 0.80              |
| 1:B:300:TRP:HB2  | 1:B:327:LEU:HD12 | 1.63                     | 0.80              |
| 1:H:300:TRP:HB2  | 1:H:327:LEU:HD12 | 1.62                     | 0.79              |
| 1:F:300:TRP:HB2  | 1:F:327:LEU:HD12 | 1.63                     | 0.79              |
| 1:H:175:VAL:HG22 | 1:H:176:PRO:HD2  | 1.65                     | 0.78              |
| 1:H:167:ILE:HG23 | 1:H:170:GLN:HB2  | 1.67                     | 0.77              |
| 1:S:300:TRP:HB2  | 1:S:327:LEU:HD12 | 1.64                     | 0.77              |
| 1:R:300:TRP:HB2  | 1:R:327:LEU:HD12 | 1.64                     | 0.77              |
| 3:u:11:U:H3'     | 3:u:12:U:H5''    | 1.67                     | 0.77              |
| 1:P:300:TRP:HB2  | 1:P:327:LEU:HD12 | 1.67                     | 0.76              |
| 1:G:376:VAL:O    | 2:g:103:ASN:ND2  | 2.19                     | 0.75              |
| 1:I:147:THR:O    | 1:I:179:ARG:NH1  | 2.19                     | 0.75              |
| 1:P:144:VAL:HG11 | 1:P:156:LEU:HG   | 1.69                     | 0.75              |
| 1:D:104:ILE:HD11 | 1:D:198:VAL:HG22 | 1.69                     | 0.75              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:143:ARG:HE   | 1:T:155:LYS:HE3  | 1.48                     | 0.75              |
| 1:G:179:ARG:NH1  | 1:G:183:ASP:OD2  | 2.19                     | 0.75              |
| 1:T:300:TRP:HB2  | 1:T:327:LEU:HD12 | 1.68                     | 0.75              |
| 1:J:70:ASN:ND2   | 1:J:188:ASP:OD2  | 2.19                     | 0.74              |
| 1:J:300:TRP:HB2  | 1:J:327:LEU:HD12 | 1.69                     | 0.74              |
| 1:O:40:LEU:HD12  | 1:O:108:VAL:HG21 | 1.69                     | 0.73              |
| 1:R:133:TRP:HB2  | 1:R:163:GLN:HG3  | 1.70                     | 0.73              |
| 1:K:376:VAL:HG13 | 1:L:355:TYR:HA   | 1.70                     | 0.73              |
| 1:D:376:VAL:O    | 2:d:103:ASN:ND2  | 2.20                     | 0.73              |
| 1:J:376:VAL:O    | 2:j:103:ASN:ND2  | 2.20                     | 0.73              |
| 2:k:91:THR:HG23  | 2:k:122:THR:HA   | 1.71                     | 0.72              |
| 1:J:40:LEU:HD12  | 1:J:108:VAL:HG21 | 1.71                     | 0.72              |
| 1:B:104:ILE:HD11 | 1:B:198:VAL:HG22 | 1.72                     | 0.72              |
| 2:i:39:GLN:NE2   | 2:i:43:LYS:O     | 2.22                     | 0.72              |
| 2:t:91:THR:HG23  | 2:t:122:THR:HA   | 1.72                     | 0.72              |
| 1:N:376:VAL:O    | 2:n:103:ASN:ND2  | 2.23                     | 0.72              |
| 1:H:159:GLY:O    | 1:H:163:GLN:NE2  | 2.23                     | 0.72              |
| 2:q:39:GLN:NE2   | 2:q:43:LYS:O     | 2.23                     | 0.71              |
| 1:D:165:LYS:NZ   | 1:E:184:VAL:O    | 2.23                     | 0.71              |
| 1:N:104:ILE:HD11 | 1:N:198:VAL:HG22 | 1.71                     | 0.71              |
| 1:C:230:THR:HG22 | 1:C:312:ARG:HH22 | 1.55                     | 0.71              |
| 1:I:144:VAL:HG11 | 1:I:156:LEU:HG   | 1.72                     | 0.71              |
| 1:H:376:VAL:O    | 2:h:103:ASN:ND2  | 2.22                     | 0.71              |
| 2:q:91:THR:HG23  | 2:q:122:THR:HA   | 1.72                     | 0.71              |
| 1:E:163:GLN:N    | 1:E:163:GLN:OE1  | 2.23                     | 0.71              |
| 1:E:300:TRP:HB2  | 1:E:327:LEU:HD12 | 1.71                     | 0.71              |
| 1:F:376:VAL:HG12 | 2:f:103:ASN:HD21 | 1.55                     | 0.70              |
| 1:O:68:HIS:NE2   | 1:O:118:PRO:O    | 2.24                     | 0.70              |
| 1:O:279:ILE:HD12 | 1:O:280:ASP:H    | 1.54                     | 0.70              |
| 2:d:91:THR:HG23  | 2:d:122:THR:HA   | 1.73                     | 0.70              |
| 1:S:260:GLN:OE1  | 1:S:294:ASN:ND2  | 2.23                     | 0.70              |
| 1:K:104:ILE:HD11 | 1:K:198:VAL:HG22 | 1.74                     | 0.70              |
| 1:F:256:ASP:OD1  | 1:G:7:ARG:NH2    | 2.25                     | 0.70              |
| 2:s:91:THR:HG23  | 2:s:122:THR:HA   | 1.73                     | 0.70              |
| 2:k:54:ARG:NH1   | 1:L:358:ASP:OD2  | 2.25                     | 0.69              |
| 1:A:40:LEU:HD12  | 1:A:108:VAL:HG21 | 1.73                     | 0.69              |
| 1:Q:302:GLN:OE1  | 1:Q:312:ARG:NH1  | 2.25                     | 0.69              |
| 1:O:300:TRP:HB2  | 1:O:327:LEU:HD12 | 1.74                     | 0.69              |
| 2:j:39:GLN:NE2   | 2:j:43:LYS:O     | 2.25                     | 0.69              |
| 1:J:167:ILE:HG23 | 1:J:170:GLN:HB2  | 1.73                     | 0.69              |
| 1:M:376:VAL:O    | 2:m:103:ASN:ND2  | 2.24                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:j:91:THR:HG23  | 2:j:122:THR:HA   | 1.73                     | 0.69              |
| 1:J:165:LYS:HZ2  | 1:A:184:VAL:HA   | 1.58                     | 0.69              |
| 1:M:40:LEU:HD12  | 1:M:108:VAL:HG21 | 1.75                     | 0.69              |
| 1:G:147:THR:O    | 1:G:153:ARG:NH2  | 2.25                     | 0.69              |
| 1:E:52:ARG:NH1   | 1:E:131:ASP:OD2  | 2.27                     | 0.68              |
| 1:T:155:LYS:NZ   | 3:v:26:U:OP2     | 2.27                     | 0.68              |
| 1:G:376:VAL:HG12 | 2:g:103:ASN:ND2  | 2.08                     | 0.68              |
| 2:q:27:ARG:NH2   | 2:q:28:THR:O     | 2.26                     | 0.68              |
| 1:M:308:LEU:HD11 | 1:M:335:ALA:HA   | 1.75                     | 0.68              |
| 1:O:89:SER:O     | 1:O:270:LYS:NZ   | 2.27                     | 0.68              |
| 2:r:91:THR:HG23  | 2:r:122:THR:HA   | 1.76                     | 0.68              |
| 1:E:40:LEU:HD12  | 1:E:108:VAL:HG21 | 1.74                     | 0.68              |
| 1:P:86:LYS:HD3   | 1:P:87:ASP:H     | 1.57                     | 0.68              |
| 2:n:5:VAL:O      | 2:n:22:CYS:HA    | 1.94                     | 0.68              |
| 1:O:376:VAL:HG12 | 2:o:103:ASN:HD21 | 1.58                     | 0.68              |
| 1:P:167:ILE:HG23 | 1:P:170:GLN:HB2  | 1.75                     | 0.68              |
| 1:M:317:ARG:NH1  | 1:M:409:GLU:O    | 2.26                     | 0.67              |
| 1:S:104:ILE:HD11 | 1:S:198:VAL:HG22 | 1.76                     | 0.67              |
| 1:H:104:ILE:HD11 | 1:H:198:VAL:HG22 | 1.76                     | 0.67              |
| 1:B:230:THR:HG22 | 1:B:312:ARG:HH22 | 1.59                     | 0.67              |
| 1:F:376:VAL:HG12 | 2:f:103:ASN:ND2  | 2.08                     | 0.67              |
| 2:g:2:VAL:HA     | 2:g:26:GLY:HA3   | 1.75                     | 0.67              |
| 2:e:91:THR:HG23  | 2:e:122:THR:HA   | 1.74                     | 0.67              |
| 1:F:137:TYR:HB2  | 1:F:163:GLN:HE22 | 1.60                     | 0.67              |
| 1:A:166:MET:HE2  | 1:A:167:ILE:HG22 | 1.76                     | 0.67              |
| 1:Q:230:THR:HG22 | 1:Q:312:ARG:HH12 | 1.59                     | 0.67              |
| 1:C:302:GLN:OE1  | 1:C:312:ARG:NH2  | 2.27                     | 0.67              |
| 1:S:7:ARG:NH2    | 1:T:256:ASP:OD1  | 2.28                     | 0.67              |
| 1:N:358:ASP:OD2  | 2:m:54:ARG:NH1   | 2.26                     | 0.67              |
| 2:s:2:VAL:HA     | 2:s:26:GLY:HA3   | 1.77                     | 0.67              |
| 1:I:40:LEU:HD12  | 1:I:108:VAL:HG21 | 1.77                     | 0.67              |
| 1:B:7:ARG:NH2    | 1:A:256:ASP:OD1  | 2.27                     | 0.67              |
| 1:T:52:ARG:NH1   | 1:T:131:ASP:OD2  | 2.28                     | 0.67              |
| 1:A:300:TRP:HB2  | 1:A:327:LEU:HD12 | 1.77                     | 0.67              |
| 1:R:104:ILE:HD11 | 1:R:198:VAL:HG22 | 1.77                     | 0.67              |
| 1:S:178:GLY:HA2  | 1:S:181:ILE:HG12 | 1.76                     | 0.67              |
| 1:E:104:ILE:HD11 | 1:E:198:VAL:HG22 | 1.77                     | 0.66              |
| 1:L:56:TYR:OH    | 1:L:126:ARG:NH2  | 2.28                     | 0.66              |
| 1:L:376:VAL:O    | 2:l:103:ASN:ND2  | 2.28                     | 0.66              |
| 1:F:137:TYR:O    | 1:F:141:LEU:HD22 | 1.93                     | 0.66              |
| 2:h:91:THR:HG23  | 2:h:122:THR:HA   | 1.77                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:138:LEU:O    | 1:G:191:TYR:OH   | 2.12                     | 0.66              |
| 1:A:376:VAL:O    | 2:a:103:ASN:ND2  | 2.24                     | 0.66              |
| 1:B:40:LEU:HD12  | 1:B:108:VAL:HG21 | 1.76                     | 0.66              |
| 1:E:256:ASP:OD1  | 1:F:7:ARG:NH2    | 2.27                     | 0.66              |
| 2:n:91:THR:HG23  | 2:n:122:THR:HA   | 1.77                     | 0.66              |
| 1:F:376:VAL:O    | 2:f:103:ASN:ND2  | 2.27                     | 0.66              |
| 1:N:145:GLY:HA2  | 1:N:153:ARG:HH12 | 1.60                     | 0.66              |
| 1:G:14:ILE:HG23  | 1:G:16:PRO:HD3   | 1.77                     | 0.66              |
| 2:p:54:ARG:NH1   | 1:Q:358:ASP:OD2  | 2.29                     | 0.66              |
| 1:C:376:VAL:O    | 2:c:103:ASN:ND2  | 2.29                     | 0.66              |
| 1:E:167:ILE:HG23 | 1:E:170:GLN:HB2  | 1.77                     | 0.66              |
| 2:l:39:GLN:NE2   | 2:l:43:LYS:O     | 2.29                     | 0.66              |
| 2:r:83:MET:HE2   | 2:r:86:LEU:HD21  | 1.78                     | 0.66              |
| 2:l:54:ARG:NH1   | 1:M:358:ASP:OD2  | 2.29                     | 0.66              |
| 1:A:158:ASP:OD1  | 1:A:161:THR:OG1  | 2.14                     | 0.66              |
| 1:L:89:SER:O     | 1:L:270:LYS:NZ   | 2.30                     | 0.65              |
| 1:O:152:TYR:OH   | 3:u:26:U:OP2     | 2.12                     | 0.65              |
| 1:J:144:VAL:O    | 1:J:153:ARG:NH2  | 2.29                     | 0.65              |
| 1:B:167:ILE:HG23 | 1:B:170:GLN:HB2  | 1.76                     | 0.65              |
| 1:E:242:THR:O    | 1:E:246:THR:OG1  | 2.13                     | 0.65              |
| 1:G:143:ARG:HH22 | 3:x:8:U:H3'      | 1.61                     | 0.65              |
| 1:I:59:LEU:HD22  | 1:I:174:LEU:HD11 | 1.79                     | 0.65              |
| 1:J:104:ILE:HD11 | 1:J:198:VAL:HG22 | 1.76                     | 0.65              |
| 2:l:91:THR:HG23  | 2:l:122:THR:HA   | 1.78                     | 0.65              |
| 1:N:51:LEU:HB3   | 1:N:72:TYR:HB2   | 1.79                     | 0.65              |
| 1:B:358:ASP:OD2  | 2:c:54:ARG:NH1   | 2.29                     | 0.65              |
| 1:R:408:ARG:NH2  | 3:v:43:U:OP1     | 2.25                     | 0.65              |
| 2:t:40:ALA:HB3   | 2:t:43:LYS:HB2   | 1.79                     | 0.65              |
| 1:A:319:PRO:O    | 1:A:324:TYR:OH   | 2.10                     | 0.65              |
| 1:Q:137:TYR:O    | 1:Q:141:LEU:HD22 | 1.97                     | 0.65              |
| 1:Q:313:ALA:HB1  | 1:Q:412:ILE:HD11 | 1.78                     | 0.65              |
| 2:o:91:THR:HG23  | 2:o:122:THR:HA   | 1.78                     | 0.65              |
| 2:d:2:VAL:HA     | 2:d:25:SER:O     | 1.97                     | 0.65              |
| 1:K:137:TYR:O    | 1:K:141:LEU:HD22 | 1.96                     | 0.65              |
| 2:o:50:LYS:NZ    | 2:o:105:GLY:O    | 2.23                     | 0.65              |
| 1:I:178:GLY:HA2  | 1:I:181:ILE:HG12 | 1.78                     | 0.65              |
| 1:J:358:ASP:OD2  | 2:a:54:ARG:NH1   | 2.30                     | 0.64              |
| 1:Q:104:ILE:HD11 | 1:Q:198:VAL:HG22 | 1.79                     | 0.64              |
| 1:D:355:TYR:HA   | 1:E:376:VAL:HG13 | 1.78                     | 0.64              |
| 1:Q:178:GLY:HA2  | 1:Q:181:ILE:HG12 | 1.79                     | 0.64              |
| 2:h:63:SER:O     | 2:h:67:ARG:NH2   | 2.28                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:174:LEU:HD11 | 1:C:181:ILE:HG13 | 1.78                     | 0.64              |
| 1:F:358:ASP:OD2  | 2:g:54:ARG:NH1   | 2.30                     | 0.64              |
| 1:K:89:SER:O     | 1:K:270:LYS:NZ   | 2.31                     | 0.64              |
| 1:J:178:GLY:HA2  | 1:J:181:ILE:HD13 | 1.79                     | 0.64              |
| 1:S:40:LEU:HD12  | 1:S:108:VAL:HG21 | 1.80                     | 0.64              |
| 1:N:177:GLU:O    | 1:N:179:ARG:N    | 2.31                     | 0.64              |
| 1:G:143:ARG:HH12 | 3:x:9:U:H5'      | 1.61                     | 0.64              |
| 1:D:167:ILE:HG23 | 1:D:170:GLN:HB2  | 1.79                     | 0.64              |
| 2:a:45:ARG:HH22  | 2:a:109:GLY:HA3  | 1.63                     | 0.64              |
| 1:N:152:TYR:O    | 1:N:155:LYS:HB3  | 1.97                     | 0.64              |
| 1:F:27:TYR:CE2   | 1:F:263:LEU:HD22 | 2.33                     | 0.64              |
| 1:H:332:LEU:HD21 | 1:H:397:ALA:HB2  | 1.80                     | 0.64              |
| 1:I:127:THR:HG22 | 1:I:128:SER:H    | 1.62                     | 0.64              |
| 1:P:56:TYR:OH    | 1:P:126:ARG:NH2  | 2.30                     | 0.63              |
| 2:c:40:ALA:HB3   | 2:c:43:LYS:HB2   | 1.79                     | 0.63              |
| 1:Q:42:ILE:CD1   | 1:Q:74:TYR:HB2   | 2.27                     | 0.63              |
| 1:R:139:LEU:HD22 | 1:R:195:VAL:HG12 | 1.79                     | 0.63              |
| 2:n:54:ARG:NH1   | 1:O:358:ASP:OD2  | 2.31                     | 0.63              |
| 2:i:50:LYS:NZ    | 2:i:105:GLY:O    | 2.28                     | 0.63              |
| 1:J:52:ARG:NH1   | 1:J:131:ASP:OD2  | 2.31                     | 0.63              |
| 2:m:22:CYS:HB3   | 2:m:79:VAL:HG13  | 1.80                     | 0.63              |
| 2:r:11:LEU:HG    | 2:r:122:THR:HB   | 1.80                     | 0.63              |
| 1:N:77:LEU:HD13  | 1:N:104:ILE:HD13 | 1.81                     | 0.63              |
| 1:G:104:ILE:HD11 | 1:G:198:VAL:HG22 | 1.81                     | 0.63              |
| 1:P:256:ASP:OD1  | 1:O:7:ARG:NH2    | 2.30                     | 0.63              |
| 1:E:138:LEU:O    | 1:E:191:TYR:OH   | 2.17                     | 0.63              |
| 2:e:22:CYS:HB3   | 2:e:79:VAL:HG13  | 1.79                     | 0.63              |
| 1:P:376:VAL:HG13 | 1:Q:355:TYR:HA   | 1.80                     | 0.63              |
| 1:D:68:HIS:NE2   | 1:D:118:PRO:O    | 2.31                     | 0.63              |
| 1:N:143:ARG:HB2  | 1:N:216:GLY:HA2  | 1.80                     | 0.63              |
| 1:I:242:THR:O    | 1:I:246:THR:OG1  | 2.16                     | 0.63              |
| 2:c:50:LYS:NZ    | 2:c:105:GLY:O    | 2.28                     | 0.63              |
| 1:I:138:LEU:O    | 1:I:191:TYR:OH   | 2.17                     | 0.63              |
| 1:S:139:LEU:HD22 | 1:S:195:VAL:HG12 | 1.79                     | 0.63              |
| 1:L:7:ARG:NH2    | 1:M:256:ASP:OD1  | 2.30                     | 0.63              |
| 1:F:138:LEU:O    | 1:F:191:TYR:OH   | 2.17                     | 0.63              |
| 1:T:160:LEU:HD21 | 1:T:172:GLU:HB3  | 1.81                     | 0.62              |
| 2:a:83:MET:HE2   | 2:a:86:LEU:HD21  | 1.80                     | 0.62              |
| 1:B:70:ASN:ND2   | 1:B:188:ASP:OD2  | 2.28                     | 0.62              |
| 1:I:179:ARG:NH2  | 1:I:183:ASP:OD1  | 2.32                     | 0.62              |
| 1:J:153:ARG:NH1  | 1:J:179:ARG:O    | 2.31                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:R:137:TYR:O    | 1:R:141:LEU:HD22 | 1.98                     | 0.62              |
| 1:D:376:VAL:HG12 | 2:d:103:ASN:ND2  | 2.14                     | 0.62              |
| 1:D:152:TYR:OH   | 3:w:26:U:OP2     | 2.16                     | 0.62              |
| 1:O:137:TYR:O    | 1:O:141:LEU:HD22 | 1.99                     | 0.62              |
| 2:j:63:SER:O     | 2:j:67:ARG:NH2   | 2.27                     | 0.62              |
| 2:p:62:ASP:HA    | 2:p:65:LYS:HD3   | 1.81                     | 0.62              |
| 1:B:242:THR:O    | 1:B:246:THR:OG1  | 2.16                     | 0.62              |
| 2:d:33:ILE:H     | 2:d:99:THR:HG22  | 1.63                     | 0.62              |
| 1:R:157:MET:HA   | 1:R:160:LEU:HB2  | 1.81                     | 0.62              |
| 2:e:2:VAL:HA     | 2:e:26:GLY:HA3   | 1.79                     | 0.62              |
| 1:P:178:GLY:HA2  | 1:P:181:ILE:HG12 | 1.81                     | 0.62              |
| 1:R:376:VAL:O    | 2:r:103:ASN:ND2  | 2.28                     | 0.62              |
| 1:L:40:LEU:HD12  | 1:L:108:VAL:HG21 | 1.82                     | 0.62              |
| 2:m:91:THR:HG23  | 2:m:122:THR:HA   | 1.82                     | 0.62              |
| 1:T:167:ILE:HG23 | 1:T:170:GLN:HB2  | 1.82                     | 0.62              |
| 2:f:50:LYS:NZ    | 2:f:105:GLY:O    | 2.25                     | 0.62              |
| 1:T:137:TYR:O    | 1:T:141:LEU:HD22 | 2.01                     | 0.61              |
| 2:f:83:MET:HB3   | 2:f:86:LEU:HD21  | 1.82                     | 0.61              |
| 1:P:138:LEU:O    | 1:P:191:TYR:OH   | 2.18                     | 0.61              |
| 1:N:137:TYR:O    | 1:N:141:LEU:HD22 | 1.99                     | 0.61              |
| 1:T:302:GLN:OE1  | 1:T:312:ARG:NH1  | 2.32                     | 0.61              |
| 1:G:178:GLY:HA2  | 1:G:181:ILE:HG12 | 1.82                     | 0.61              |
| 1:I:358:ASP:OD2  | 2:j:54:ARG:NH1   | 2.33                     | 0.61              |
| 1:C:313:ALA:HB1  | 1:C:412:ILE:HD11 | 1.81                     | 0.61              |
| 1:D:157:MET:HA   | 1:D:160:LEU:HB2  | 1.81                     | 0.61              |
| 2:k:100:LYS:NZ   | 1:L:353:ASN:OD1  | 2.34                     | 0.61              |
| 1:L:104:ILE:HD11 | 1:L:198:VAL:HG22 | 1.81                     | 0.61              |
| 1:G:260:GLN:OE1  | 1:G:294:ASN:ND2  | 2.28                     | 0.61              |
| 1:J:302:GLN:OE1  | 1:J:312:ARG:NH2  | 2.34                     | 0.61              |
| 1:D:159:GLY:HA3  | 1:D:163:GLN:HG2  | 1.81                     | 0.61              |
| 2:f:32:SER:OG    | 2:f:99:THR:O     | 2.16                     | 0.61              |
| 1:B:159:GLY:O    | 1:B:163:GLN:HG2  | 2.01                     | 0.61              |
| 2:l:2:VAL:HA     | 2:l:26:GLY:HA3   | 1.82                     | 0.61              |
| 2:t:54:ARG:NH1   | 1:K:358:ASP:OD2  | 2.33                     | 0.61              |
| 2:f:22:CYS:HB3   | 2:f:79:VAL:HG13  | 1.82                     | 0.61              |
| 1:P:139:LEU:HD22 | 1:P:195:VAL:HG12 | 1.81                     | 0.61              |
| 1:E:203:HIS:ND1  | 1:E:272:ASP:OD1  | 2.31                     | 0.61              |
| 2:g:91:THR:HG23  | 2:g:122:THR:HA   | 1.81                     | 0.61              |
| 1:H:40:LEU:HD12  | 1:H:108:VAL:HG21 | 1.83                     | 0.61              |
| 2:d:83:MET:HE2   | 2:d:86:LEU:HD21  | 1.82                     | 0.61              |
| 2:a:91:THR:HG23  | 2:a:122:THR:HA   | 1.82                     | 0.61              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:22:GLU:HB3   | 1:P:24:PRO:HD3   | 1.82                     | 0.60              |
| 2:c:22:CYS:HB3   | 2:c:79:VAL:HG13  | 1.83                     | 0.60              |
| 1:K:138:LEU:O    | 1:K:191:TYR:OH   | 2.18                     | 0.60              |
| 1:N:69:VAL:O     | 1:N:73:LEU:HB2   | 2.00                     | 0.60              |
| 1:O:376:VAL:HG12 | 2:o:103:ASN:ND2  | 2.14                     | 0.60              |
| 1:M:89:SER:O     | 1:M:270:LYS:NZ   | 2.34                     | 0.60              |
| 2:q:83:MET:HE2   | 2:q:86:LEU:HD21  | 1.82                     | 0.60              |
| 2:j:32:SER:OG    | 2:j:99:THR:O     | 2.14                     | 0.60              |
| 1:Q:51:LEU:HB3   | 1:Q:72:TYR:HB2   | 1.82                     | 0.60              |
| 1:Q:138:LEU:O    | 1:Q:191:TYR:OH   | 2.19                     | 0.60              |
| 1:T:143:ARG:HB2  | 1:T:216:GLY:HA2  | 1.83                     | 0.60              |
| 1:F:143:ARG:HB2  | 1:F:216:GLY:HA2  | 1.84                     | 0.60              |
| 1:J:279:ILE:HD11 | 1:J:287:SER:HB2  | 1.84                     | 0.60              |
| 2:d:32:SER:OG    | 2:d:99:THR:O     | 2.15                     | 0.60              |
| 2:n:22:CYS:HB3   | 2:n:79:VAL:HG13  | 1.83                     | 0.60              |
| 2:q:54:ARG:NH1   | 1:R:358:ASP:OD2  | 2.34                     | 0.60              |
| 1:E:279:ILE:HD11 | 1:E:287:SER:HB2  | 1.83                     | 0.60              |
| 1:T:7:ARG:HG2    | 1:T:9:ILE:HG22   | 1.84                     | 0.60              |
| 1:E:70:ASN:ND2   | 1:E:188:ASP:OD2  | 2.34                     | 0.60              |
| 1:K:242:THR:O    | 1:K:246:THR:OG1  | 2.17                     | 0.60              |
| 1:H:358:ASP:OD2  | 2:i:54:ARG:NH1   | 2.35                     | 0.60              |
| 1:I:256:ASP:OD1  | 1:J:7:ARG:NH2    | 2.35                     | 0.60              |
| 1:Q:40:LEU:HD12  | 1:Q:108:VAL:HG21 | 1.84                     | 0.60              |
| 1:S:203:HIS:ND1  | 1:S:272:ASP:OD1  | 2.31                     | 0.60              |
| 1:L:364:LEU:HD22 | 2:l:74:ASN:HB3   | 1.83                     | 0.60              |
| 1:O:163:GLN:NE2  | 1:O:170:GLN:OE1  | 2.34                     | 0.60              |
| 1:P:358:ASP:OD2  | 2:o:54:ARG:NH1   | 2.35                     | 0.60              |
| 2:p:22:CYS:HB3   | 2:p:79:VAL:HG13  | 1.84                     | 0.60              |
| 1:B:127:THR:OG1  | 1:B:128:SER:N    | 2.34                     | 0.60              |
| 2:r:2:VAL:HA     | 2:r:26:GLY:HA3   | 1.83                     | 0.60              |
| 1:N:138:LEU:O    | 1:N:191:TYR:OH   | 2.19                     | 0.60              |
| 1:A:143:ARG:HB2  | 1:A:216:GLY:HA2  | 1.84                     | 0.60              |
| 2:b:22:CYS:HB3   | 2:b:79:VAL:HG13  | 1.83                     | 0.59              |
| 1:L:52:ARG:NH1   | 1:L:131:ASP:OD2  | 2.35                     | 0.59              |
| 1:M:144:VAL:HG11 | 1:M:156:LEU:HB2  | 1.83                     | 0.59              |
| 2:n:39:GLN:NE2   | 2:n:43:LYS:O     | 2.34                     | 0.59              |
| 1:P:38:ILE:HD12  | 1:P:39:PRO:HD2   | 1.84                     | 0.59              |
| 2:f:91:THR:HG23  | 2:f:122:THR:HA   | 1.82                     | 0.59              |
| 2:b:91:THR:HG23  | 2:b:122:THR:HA   | 1.85                     | 0.59              |
| 2:t:83:MET:HB3   | 2:t:86:LEU:HD21  | 1.84                     | 0.59              |
| 1:M:72:TYR:O     | 1:M:75:GLY:N     | 2.35                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:312:ARG:HD2  | 3:x:32:U:C4      | 2.37                     | 0.59              |
| 2:h:22:CYS:HB3   | 2:h:79:VAL:HG13  | 1.85                     | 0.59              |
| 2:b:52:SER:OG    | 2:b:53:TRP:N     | 2.35                     | 0.59              |
| 1:M:167:ILE:HG23 | 1:M:170:GLN:HB2  | 1.84                     | 0.59              |
| 2:i:91:THR:HG23  | 2:i:122:THR:HA   | 1.85                     | 0.59              |
| 1:C:51:LEU:HA    | 1:C:54:TYR:HB2   | 1.85                     | 0.59              |
| 1:K:143:ARG:HB2  | 1:K:216:GLY:HA2  | 1.85                     | 0.59              |
| 1:L:160:LEU:HD11 | 1:L:172:GLU:HG3  | 1.83                     | 0.59              |
| 1:I:228:LEU:HD21 | 1:J:19:PRO:HG2   | 1.84                     | 0.59              |
| 2:i:83:MET:HE2   | 2:i:86:LEU:HD21  | 1.85                     | 0.59              |
| 1:O:376:VAL:O    | 2:o:103:ASN:ND2  | 2.36                     | 0.59              |
| 1:J:123:ASP:OD1  | 1:J:124:ALA:N    | 2.35                     | 0.59              |
| 1:A:51:LEU:HB3   | 1:A:72:TYR:HB2   | 1.85                     | 0.59              |
| 1:C:104:ILE:HD11 | 1:C:198:VAL:HG22 | 1.84                     | 0.59              |
| 1:M:138:LEU:O    | 1:M:191:TYR:OH   | 2.20                     | 0.59              |
| 1:G:358:ASP:OD2  | 2:h:54:ARG:NH1   | 2.36                     | 0.59              |
| 1:J:230:THR:HG22 | 1:J:312:ARG:HH22 | 1.67                     | 0.59              |
| 1:A:242:THR:O    | 1:A:246:THR:OG1  | 2.21                     | 0.59              |
| 2:b:54:ARG:NH1   | 1:A:358:ASP:OD2  | 2.36                     | 0.59              |
| 1:Q:42:ILE:HD11  | 1:Q:74:TYR:HB2   | 1.85                     | 0.59              |
| 2:c:39:GLN:NE2   | 2:c:43:LYS:O     | 2.35                     | 0.59              |
| 1:R:184:VAL:O    | 1:S:165:LYS:NZ   | 2.36                     | 0.59              |
| 1:E:302:GLN:OE1  | 1:E:312:ARG:NH1  | 2.36                     | 0.59              |
| 1:H:139:LEU:HD22 | 1:H:195:VAL:HG12 | 1.83                     | 0.59              |
| 1:E:139:LEU:HD22 | 1:E:195:VAL:HG12 | 1.85                     | 0.58              |
| 1:I:376:VAL:O    | 2:i:103:ASN:ND2  | 2.30                     | 0.58              |
| 1:J:145:GLY:HA2  | 1:J:153:ARG:HH22 | 1.67                     | 0.58              |
| 1:E:152:TYR:OH   | 3:w:35:U:OP2     | 2.18                     | 0.58              |
| 1:M:86:LYS:HD3   | 1:M:87:ASP:H     | 1.68                     | 0.58              |
| 1:L:298:HIS:O    | 1:L:302:GLN:HB2  | 2.03                     | 0.58              |
| 2:i:22:CYS:HB3   | 2:i:79:VAL:HG13  | 1.85                     | 0.58              |
| 1:C:40:LEU:HD12  | 1:C:108:VAL:HG21 | 1.84                     | 0.58              |
| 2:r:54:ARG:NH1   | 1:S:358:ASP:OD2  | 2.36                     | 0.58              |
| 1:C:279:ILE:HD11 | 1:C:287:SER:HB2  | 1.85                     | 0.58              |
| 1:S:206:LYS:HE2  | 3:v:37:U:H4'     | 1.86                     | 0.58              |
| 2:s:22:CYS:HB3   | 2:s:79:VAL:HG13  | 1.84                     | 0.58              |
| 1:H:55:VAL:O     | 1:H:59:LEU:HB2   | 2.04                     | 0.58              |
| 1:I:104:ILE:HD11 | 1:I:198:VAL:HG22 | 1.85                     | 0.58              |
| 1:J:7:ARG:HG2    | 1:J:9:ILE:HG22   | 1.85                     | 0.58              |
| 1:A:88:TRP:CD2   | 1:A:95:ILE:HD11  | 2.38                     | 0.58              |
| 2:d:50:LYS:NZ    | 2:d:105:GLY:O    | 2.27                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:242:THR:O    | 1:T:246:THR:OG1  | 2.18                     | 0.58              |
| 1:M:67:ILE:O     | 1:M:71:SER:OG    | 2.18                     | 0.58              |
| 1:G:319:PRO:O    | 1:G:324:TYR:OH   | 2.17                     | 0.58              |
| 1:P:292:VAL:HG21 | 3:u:12:U:H5'     | 1.86                     | 0.58              |
| 1:Q:153:ARG:NH2  | 1:Q:179:ARG:O    | 2.36                     | 0.58              |
| 2:q:11:LEU:HA    | 2:q:122:THR:O    | 2.04                     | 0.58              |
| 2:q:22:CYS:HB3   | 2:q:79:VAL:HG13  | 1.86                     | 0.58              |
| 1:R:260:GLN:OE1  | 1:R:294:ASN:ND2  | 2.33                     | 0.58              |
| 1:S:367:ASN:OD1  | 1:S:385:GLN:NE2  | 2.28                     | 0.58              |
| 1:R:52:ARG:NH1   | 1:R:131:ASP:OD2  | 2.37                     | 0.58              |
| 1:H:302:GLN:OE1  | 1:H:312:ARG:NH1  | 2.37                     | 0.58              |
| 2:o:22:CYS:HB3   | 2:o:79:VAL:HG13  | 1.85                     | 0.58              |
| 2:t:50:LYS:NZ    | 2:t:105:GLY:O    | 2.33                     | 0.58              |
| 1:J:165:LYS:NZ   | 1:A:187:ASN:HB2  | 2.18                     | 0.58              |
| 2:j:67:ARG:NH1   | 2:j:90:ASP:OD2   | 2.28                     | 0.58              |
| 1:N:230:THR:HG21 | 1:N:298:HIS:ND1  | 2.19                     | 0.57              |
| 2:n:50:LYS:HG2   | 2:n:59:THR:HB    | 1.86                     | 0.57              |
| 2:g:83:MET:HE2   | 2:g:86:LEU:HD21  | 1.86                     | 0.57              |
| 1:O:143:ARG:HH12 | 3:u:27:U:H5'     | 1.68                     | 0.57              |
| 2:a:63:SER:O     | 2:a:67:ARG:NH2   | 2.30                     | 0.57              |
| 2:q:50:LYS:NZ    | 2:q:105:GLY:O    | 2.33                     | 0.57              |
| 1:C:159:GLY:O    | 1:C:163:GLN:NE2  | 2.38                     | 0.57              |
| 1:D:256:ASP:OD1  | 1:E:7:ARG:NH2    | 2.38                     | 0.57              |
| 2:s:83:MET:HE1   | 2:s:121:VAL:HG11 | 1.86                     | 0.57              |
| 1:T:138:LEU:O    | 1:T:191:TYR:OH   | 2.22                     | 0.57              |
| 1:C:376:VAL:HG12 | 2:c:103:ASN:HD21 | 1.69                     | 0.57              |
| 2:e:83:MET:HB3   | 2:e:86:LEU:HD21  | 1.86                     | 0.57              |
| 2:k:2:VAL:HA     | 2:k:26:GLY:HA3   | 1.87                     | 0.57              |
| 1:N:143:ARG:HG2  | 1:N:155:LYS:HZ2  | 1.69                     | 0.57              |
| 1:N:165:LYS:HG2  | 1:M:184:VAL:HG22 | 1.87                     | 0.57              |
| 2:j:83:MET:HB3   | 2:j:86:LEU:HD21  | 1.85                     | 0.57              |
| 1:T:364:LEU:HG   | 1:T:366:THR:HG23 | 1.87                     | 0.57              |
| 1:N:152:TYR:OH   | 3:u:35:U:OP2     | 2.19                     | 0.57              |
| 2:n:2:VAL:HA     | 2:n:26:GLY:HA3   | 1.85                     | 0.57              |
| 2:g:22:CYS:HB3   | 2:g:79:VAL:HG13  | 1.86                     | 0.57              |
| 2:q:32:SER:OG    | 2:q:99:THR:O     | 2.16                     | 0.57              |
| 2:f:2:VAL:HA     | 2:f:26:GLY:HA3   | 1.86                     | 0.57              |
| 2:h:11:LEU:HA    | 2:h:122:THR:O    | 2.04                     | 0.57              |
| 1:O:154:LYS:HA   | 1:O:157:MET:HE2  | 1.86                     | 0.57              |
| 1:O:178:GLY:HA2  | 1:O:181:ILE:HG12 | 1.87                     | 0.57              |
| 1:J:353:ASN:HD22 | 2:a:100:LYS:HE3  | 1.68                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:199:ASP:OD1  | 1:A:277:TYR:OH   | 2.20                     | 0.57              |
| 1:B:143:ARG:HB3  | 1:B:216:GLY:HA2  | 1.86                     | 0.57              |
| 1:D:159:GLY:CA   | 1:D:163:GLN:HG2  | 2.34                     | 0.57              |
| 1:M:25:VAL:HG11  | 1:M:288:PRO:HB3  | 1.87                     | 0.57              |
| 1:G:317:ARG:NH1  | 1:G:409:GLU:O    | 2.37                     | 0.57              |
| 1:B:7:ARG:HG2    | 1:B:9:ILE:HG22   | 1.85                     | 0.57              |
| 2:r:98:ALA:HB3   | 2:r:114:TYR:HB2  | 1.86                     | 0.57              |
| 2:g:50:LYS:HG2   | 2:g:59:THR:HB    | 1.85                     | 0.57              |
| 1:B:140:GLY:HA2  | 1:B:216:GLY:HA3  | 1.87                     | 0.57              |
| 1:C:7:ARG:HG2    | 1:C:9:ILE:HG22   | 1.86                     | 0.57              |
| 1:H:7:ARG:HG2    | 1:H:9:ILE:HG22   | 1.86                     | 0.57              |
| 1:I:137:TYR:HD1  | 1:I:163:GLN:HE22 | 1.50                     | 0.57              |
| 2:j:2:VAL:HA     | 2:j:26:GLY:HA3   | 1.87                     | 0.57              |
| 1:C:376:VAL:HG12 | 2:c:103:ASN:ND2  | 2.20                     | 0.57              |
| 1:S:240:MET:HE2  | 1:S:244:ASP:HB3  | 1.85                     | 0.57              |
| 1:K:7:ARG:NH2    | 1:L:256:ASP:OD1  | 2.25                     | 0.57              |
| 2:c:83:MET:HB3   | 2:c:86:LEU:HD21  | 1.85                     | 0.57              |
| 1:T:152:TYR:OH   | 3:v:26:U:OP2     | 2.23                     | 0.57              |
| 2:k:22:CYS:HB3   | 2:k:79:VAL:HG13  | 1.86                     | 0.57              |
| 1:H:87:ASP:OD1   | 1:H:98:ALA:N     | 2.37                     | 0.57              |
| 1:O:77:LEU:HD11  | 1:O:135:PRO:HB3  | 1.86                     | 0.57              |
| 2:p:83:MET:HE2   | 2:p:86:LEU:HD21  | 1.85                     | 0.56              |
| 1:D:7:ARG:HG2    | 1:D:9:ILE:HG22   | 1.87                     | 0.56              |
| 1:T:72:TYR:OH    | 1:T:131:ASP:OD1  | 2.17                     | 0.56              |
| 1:F:302:GLN:OE1  | 1:F:312:ARG:NH1  | 2.38                     | 0.56              |
| 1:O:7:ARG:HG2    | 1:O:9:ILE:HG22   | 1.85                     | 0.56              |
| 1:J:160:LEU:HD21 | 1:J:172:GLU:HB3  | 1.87                     | 0.56              |
| 1:P:377:GLU:OE2  | 2:p:27:ARG:NH1   | 2.38                     | 0.56              |
| 2:d:22:CYS:HB3   | 2:d:79:VAL:HG13  | 1.85                     | 0.56              |
| 1:T:260:GLN:OE1  | 1:T:294:ASN:ND2  | 2.33                     | 0.56              |
| 1:F:154:LYS:HG2  | 1:F:179:ARG:HH22 | 1.71                     | 0.56              |
| 1:I:149:MET:HB3  | 1:I:152:TYR:HB2  | 1.87                     | 0.56              |
| 2:c:67:ARG:NH1   | 2:c:90:ASP:OD2   | 2.32                     | 0.56              |
| 1:R:51:LEU:HA    | 1:R:54:TYR:HB2   | 1.86                     | 0.56              |
| 1:S:153:ARG:HB2  | 1:S:179:ARG:HH21 | 1.69                     | 0.56              |
| 1:E:144:VAL:HG11 | 1:E:156:LEU:HD12 | 1.86                     | 0.56              |
| 2:k:32:SER:OG    | 2:k:99:THR:O     | 2.16                     | 0.56              |
| 1:L:302:GLN:OE1  | 1:L:312:ARG:NH1  | 2.39                     | 0.56              |
| 2:n:32:SER:OG    | 2:n:99:THR:O     | 2.16                     | 0.56              |
| 1:F:7:ARG:HG2    | 1:F:9:ILE:HG22   | 1.87                     | 0.56              |
| 1:H:350:VAL:HG22 | 1:J:5:VAL:HG22   | 1.87                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:230:THR:HG21 | 1:J:298:HIS:ND1  | 2.20                     | 0.56              |
| 1:J:256:ASP:OD1  | 1:A:7:ARG:NH2    | 2.38                     | 0.56              |
| 1:K:359:ASP:OD1  | 1:K:359:ASP:N    | 2.38                     | 0.56              |
| 1:L:5:VAL:HG22   | 1:N:350:VAL:HG22 | 1.87                     | 0.56              |
| 1:A:22:GLU:HB3   | 1:A:24:PRO:HD3   | 1.88                     | 0.56              |
| 1:Q:139:LEU:HD22 | 1:Q:195:VAL:HG12 | 1.87                     | 0.56              |
| 1:K:279:ILE:HD11 | 1:K:287:SER:HB2  | 1.87                     | 0.56              |
| 1:J:51:LEU:HA    | 1:J:54:TYR:HB2   | 1.86                     | 0.56              |
| 1:A:55:VAL:O     | 1:A:59:LEU:HB2   | 2.05                     | 0.56              |
| 1:P:353:ASN:HD22 | 2:o:100:LYS:HE3  | 1.69                     | 0.56              |
| 1:K:419:GLU:OE2  | 1:L:309:ARG:NE   | 2.38                     | 0.56              |
| 1:N:364:LEU:HG   | 1:N:366:THR:HG23 | 1.87                     | 0.56              |
| 1:O:75:GLY:HA2   | 1:O:78:LYS:HE2   | 1.88                     | 0.56              |
| 2:q:63:SER:O     | 2:q:67:ARG:NH2   | 2.27                     | 0.56              |
| 1:C:163:GLN:HB3  | 1:C:170:GLN:HG3  | 1.88                     | 0.56              |
| 1:M:319:PRO:O    | 1:M:324:TYR:OH   | 2.22                     | 0.56              |
| 1:F:104:ILE:HD11 | 1:F:198:VAL:HA   | 1.86                     | 0.56              |
| 1:O:153:ARG:HD2  | 1:O:179:ARG:HD2  | 1.86                     | 0.56              |
| 1:B:230:THR:HG22 | 1:B:312:ARG:NH2  | 2.21                     | 0.56              |
| 1:C:138:LEU:O    | 1:C:191:TYR:OH   | 2.23                     | 0.56              |
| 1:R:89:SER:O     | 1:R:270:LYS:NZ   | 2.39                     | 0.56              |
| 2:b:2:VAL:HA     | 2:b:26:GLY:HA3   | 1.88                     | 0.56              |
| 1:D:70:ASN:ND2   | 1:D:188:ASP:OD2  | 2.38                     | 0.56              |
| 1:K:139:LEU:HD22 | 1:K:195:VAL:HG12 | 1.88                     | 0.56              |
| 1:L:162:ASN:HA   | 1:L:165:LYS:HD3  | 1.88                     | 0.56              |
| 1:L:376:VAL:HG12 | 2:l:103:ASN:HD21 | 1.71                     | 0.56              |
| 1:G:153:ARG:C    | 1:G:155:LYS:H    | 2.13                     | 0.56              |
| 2:o:32:SER:OG    | 2:o:99:THR:O     | 2.18                     | 0.56              |
| 1:A:7:ARG:HG2    | 1:A:9:ILE:HG22   | 1.86                     | 0.56              |
| 2:s:32:SER:OG    | 2:s:99:THR:O     | 2.16                     | 0.56              |
| 1:G:69:VAL:O     | 1:G:73:LEU:HB2   | 2.05                     | 0.56              |
| 1:H:143:ARG:HH12 | 3:x:18:U:H5'     | 1.71                     | 0.56              |
| 1:O:104:ILE:HD11 | 1:O:198:VAL:HG22 | 1.88                     | 0.56              |
| 1:Q:89:SER:O     | 1:Q:270:LYS:NZ   | 2.39                     | 0.55              |
| 2:n:52:SER:OG    | 2:n:53:TRP:N     | 2.37                     | 0.55              |
| 1:O:279:ILE:HD12 | 1:O:280:ASP:N    | 2.21                     | 0.55              |
| 1:B:139:LEU:HD22 | 1:B:195:VAL:HG12 | 1.86                     | 0.55              |
| 1:B:302:GLN:OE1  | 1:B:312:ARG:NH2  | 2.38                     | 0.55              |
| 1:Q:7:ARG:HG2    | 1:Q:9:ILE:HG22   | 1.88                     | 0.55              |
| 1:Q:324:TYR:O    | 1:Q:328:THR:OG1  | 2.19                     | 0.55              |
| 1:D:139:LEU:HD22 | 1:D:195:VAL:HG12 | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:88:TRP:CD2   | 1:S:95:ILE:HD11  | 2.41                     | 0.55              |
| 1:K:364:LEU:HG   | 1:K:366:THR:HG23 | 1.87                     | 0.55              |
| 1:G:167:ILE:HG23 | 1:G:170:GLN:HB2  | 1.89                     | 0.55              |
| 1:I:140:GLY:HA2  | 1:I:216:GLY:HA3  | 1.87                     | 0.55              |
| 1:I:302:GLN:OE1  | 1:I:312:ARG:NH1  | 2.39                     | 0.55              |
| 1:P:234:LEU:O    | 1:P:238:THR:OG1  | 2.19                     | 0.55              |
| 2:p:32:SER:OG    | 2:p:99:THR:O     | 2.16                     | 0.55              |
| 1:J:139:LEU:HD22 | 1:J:195:VAL:HG12 | 1.88                     | 0.55              |
| 2:r:22:CYS:HB3   | 2:r:79:VAL:HG13  | 1.87                     | 0.55              |
| 1:M:66:ILE:O     | 1:M:70:ASN:ND2   | 2.40                     | 0.55              |
| 2:c:91:THR:HG23  | 2:c:122:THR:HA   | 1.88                     | 0.55              |
| 1:L:408:ARG:HD3  | 3:v:6:U:C4       | 2.42                     | 0.55              |
| 1:O:55:VAL:O     | 1:O:59:LEU:HB2   | 2.05                     | 0.55              |
| 1:R:184:VAL:HA   | 1:S:165:LYS:HZ2  | 1.72                     | 0.55              |
| 1:M:133:TRP:HB2  | 1:M:163:GLN:HG2  | 1.88                     | 0.55              |
| 1:G:153:ARG:HH11 | 1:G:182:PHE:HE1  | 1.55                     | 0.55              |
| 1:A:144:VAL:HG22 | 1:A:156:LEU:HB3  | 1.88                     | 0.55              |
| 1:B:230:THR:HG21 | 1:B:298:HIS:ND1  | 2.22                     | 0.55              |
| 1:C:256:ASP:OD1  | 1:D:7:ARG:NH2    | 2.35                     | 0.55              |
| 2:k:83:MET:HB3   | 2:k:86:LEU:HD21  | 1.88                     | 0.55              |
| 2:g:32:SER:OG    | 2:g:99:THR:O     | 2.15                     | 0.55              |
| 1:O:242:THR:O    | 1:O:246:THR:OG1  | 2.24                     | 0.55              |
| 2:a:51:ILE:HD11  | 2:a:56:ASP:HB3   | 1.89                     | 0.55              |
| 1:P:408:ARG:NH2  | 3:u:16:U:OP1     | 2.25                     | 0.55              |
| 1:S:138:LEU:O    | 1:S:191:TYR:OH   | 2.24                     | 0.55              |
| 1:K:55:VAL:O     | 1:K:59:LEU:HB2   | 2.07                     | 0.55              |
| 2:a:22:CYS:HB3   | 2:a:79:VAL:HG13  | 1.88                     | 0.55              |
| 1:T:160:LEU:O    | 1:T:164:CYS:HB2  | 2.07                     | 0.55              |
| 1:K:126:ARG:HD2  | 1:K:130:ASP:OD2  | 2.07                     | 0.55              |
| 2:l:22:CYS:HB3   | 2:l:79:VAL:HG13  | 1.88                     | 0.55              |
| 1:N:137:TYR:CZ   | 1:N:173:PRO:HD2  | 2.42                     | 0.55              |
| 1:H:51:LEU:HB3   | 1:H:72:TYR:HB2   | 1.89                     | 0.55              |
| 1:J:377:GLU:OE2  | 2:j:27:ARG:NH1   | 2.40                     | 0.55              |
| 1:P:247:THR:HG21 | 1:Q:350:VAL:HG23 | 1.89                     | 0.54              |
| 1:M:39:PRO:O     | 1:M:193:LYS:NZ   | 2.34                     | 0.54              |
| 2:i:5:VAL:O      | 2:i:22:CYS:HA    | 2.07                     | 0.54              |
| 1:N:309:ARG:NE   | 1:M:419:GLU:OE2  | 2.41                     | 0.54              |
| 1:J:138:LEU:O    | 1:J:191:TYR:OH   | 2.24                     | 0.54              |
| 1:B:143:ARG:HE   | 1:B:155:LYS:HD2  | 1.72                     | 0.54              |
| 1:L:206:LYS:NZ   | 3:v:10:U:O3'     | 2.39                     | 0.54              |
| 1:G:376:VAL:HG12 | 2:g:103:ASN:HD21 | 1.72                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:364:LEU:HG   | 1:H:366:THR:HG23 | 1.89                     | 0.54              |
| 1:P:158:ASP:O    | 1:P:162:ASN:N    | 2.41                     | 0.54              |
| 1:D:46:LYS:HD3   | 1:D:54:TYR:HE2   | 1.70                     | 0.54              |
| 1:K:160:LEU:HD11 | 1:K:172:GLU:HG3  | 1.90                     | 0.54              |
| 1:L:7:ARG:HG2    | 1:L:9:ILE:HG22   | 1.90                     | 0.54              |
| 1:O:302:GLN:HB3  | 1:O:412:ILE:HD13 | 1.90                     | 0.54              |
| 2:o:83:MET:HB3   | 2:o:86:LEU:HD21  | 1.88                     | 0.54              |
| 1:R:178:GLY:HA2  | 1:R:181:ILE:HG12 | 1.90                     | 0.54              |
| 1:R:83:LYS:HA    | 1:R:101:THR:HA   | 1.88                     | 0.54              |
| 1:N:167:ILE:HG23 | 1:N:170:GLN:HB2  | 1.87                     | 0.54              |
| 1:G:206:LYS:HE3  | 3:x:10:U:H4'     | 1.88                     | 0.54              |
| 2:h:106:GLU:HB2  | 2:h:110:ARG:HB3  | 1.90                     | 0.54              |
| 1:O:27:TYR:CZ    | 1:O:263:LEU:HD22 | 2.42                     | 0.54              |
| 1:R:103:GLY:N    | 1:R:106:ASP:OD2  | 2.30                     | 0.54              |
| 1:R:167:ILE:HG23 | 1:R:170:GLN:HB2  | 1.90                     | 0.54              |
| 1:T:376:VAL:HG13 | 1:K:355:TYR:HA   | 1.90                     | 0.54              |
| 2:i:51:ILE:HD11  | 2:i:56:ASP:HB3   | 1.90                     | 0.54              |
| 1:B:208:HIS:HD1  | 1:B:210:CYS:H    | 1.55                     | 0.54              |
| 1:C:312:ARG:HD2  | 3:w:14:U:C4      | 2.42                     | 0.54              |
| 2:d:11:LEU:HA    | 2:d:122:THR:O    | 2.07                     | 0.54              |
| 1:K:88:TRP:CD2   | 1:K:95:ILE:HD11  | 2.43                     | 0.54              |
| 1:F:199:ASP:OD2  | 1:F:277:TYR:OH   | 2.24                     | 0.54              |
| 2:g:52:SER:OG    | 2:g:53:TRP:N     | 2.40                     | 0.54              |
| 1:R:70:ASN:ND2   | 1:R:188:ASP:OD2  | 2.37                     | 0.53              |
| 1:E:160:LEU:HD21 | 1:E:172:GLU:HB3  | 1.88                     | 0.53              |
| 1:R:230:THR:HG21 | 1:R:298:HIS:ND1  | 2.23                     | 0.53              |
| 1:S:137:TYR:CZ   | 1:S:173:PRO:HD2  | 2.43                     | 0.53              |
| 1:S:149:MET:HB2  | 1:S:150:PRO:HD2  | 1.91                     | 0.53              |
| 1:T:22:GLU:HB3   | 1:T:24:PRO:HD3   | 1.89                     | 0.53              |
| 1:I:172:GLU:OE2  | 1:I:172:GLU:N    | 2.32                     | 0.53              |
| 1:L:137:TYR:CZ   | 1:L:173:PRO:HD2  | 2.43                     | 0.53              |
| 1:M:77:LEU:HD11  | 1:M:80:ILE:HG12  | 1.90                     | 0.53              |
| 1:H:354:LYS:HD3  | 1:J:8:ILE:HB     | 1.90                     | 0.53              |
| 1:D:138:LEU:O    | 1:D:191:TYR:OH   | 2.25                     | 0.53              |
| 1:J:59:LEU:HD22  | 1:J:174:LEU:HD11 | 1.91                     | 0.53              |
| 1:R:137:TYR:CZ   | 1:R:173:PRO:HD2  | 2.43                     | 0.53              |
| 2:d:67:ARG:NH1   | 2:d:90:ASP:OD2   | 2.38                     | 0.53              |
| 1:T:51:LEU:HA    | 1:T:54:TYR:HB2   | 1.90                     | 0.53              |
| 1:M:104:ILE:HD11 | 1:M:198:VAL:HG22 | 1.91                     | 0.53              |
| 2:m:83:MET:HE2   | 2:m:86:LEU:HD21  | 1.90                     | 0.53              |
| 1:G:59:LEU:HD23  | 1:G:173:PRO:HG2  | 1.90                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:p:2:VAL:HA     | 2:p:26:GLY:HA3   | 1.91                     | 0.53              |
| 1:R:302:GLN:OE1  | 1:R:312:ARG:NH1  | 2.42                     | 0.53              |
| 1:E:364:LEU:HG   | 1:E:366:THR:HG23 | 1.89                     | 0.53              |
| 2:t:67:ARG:NH1   | 2:t:90:ASP:OD2   | 2.23                     | 0.53              |
| 1:N:240:MET:HB2  | 1:N:245:VAL:HG23 | 1.90                     | 0.53              |
| 1:P:152:TYR:OH   | 3:u:17:U:OP2     | 2.26                     | 0.53              |
| 2:a:20:LEU:HD12  | 2:a:81:LEU:HD23  | 1.90                     | 0.53              |
| 1:Q:174:LEU:HG   | 1:Q:178:GLY:HA3  | 1.89                     | 0.53              |
| 1:M:67:ILE:O     | 1:M:71:SER:CB    | 2.56                     | 0.53              |
| 1:F:89:SER:O     | 1:F:270:LYS:NZ   | 2.42                     | 0.53              |
| 1:G:51:LEU:HA    | 1:G:54:TYR:HB2   | 1.90                     | 0.53              |
| 1:H:148:GLN:HA   | 1:H:153:ARG:HH11 | 1.73                     | 0.53              |
| 1:S:7:ARG:HG2    | 1:S:9:ILE:HG22   | 1.90                     | 0.53              |
| 2:s:52:SER:OG    | 2:s:53:TRP:N     | 2.42                     | 0.53              |
| 1:E:291:SER:OG   | 3:w:31:U:OP2     | 2.22                     | 0.53              |
| 1:N:139:LEU:HD22 | 1:N:195:VAL:HG12 | 1.91                     | 0.53              |
| 1:F:279:ILE:HD11 | 1:F:287:SER:HB2  | 1.90                     | 0.53              |
| 1:A:138:LEU:O    | 1:A:191:TYR:OH   | 2.19                     | 0.53              |
| 1:P:364:LEU:HG   | 1:P:366:THR:HG23 | 1.90                     | 0.53              |
| 1:S:38:ILE:HD12  | 1:S:281:PHE:O    | 2.08                     | 0.53              |
| 1:E:408:ARG:NH2  | 3:w:34:U:OP1     | 2.31                     | 0.53              |
| 1:L:158:ASP:OD1  | 1:L:159:GLY:N    | 2.42                     | 0.53              |
| 1:N:293:LYS:O    | 1:N:294:ASN:ND2  | 2.41                     | 0.53              |
| 1:Q:55:VAL:O     | 1:Q:59:LEU:HB2   | 2.08                     | 0.52              |
| 1:C:51:LEU:HB3   | 1:C:72:TYR:HB2   | 1.90                     | 0.52              |
| 1:S:143:ARG:NH2  | 3:v:36:U:OP2     | 2.42                     | 0.52              |
| 1:J:140:GLY:HA2  | 1:J:216:GLY:HA3  | 1.90                     | 0.52              |
| 1:Q:27:TYR:CZ    | 1:Q:263:LEU:HD22 | 2.43                     | 0.52              |
| 1:L:167:ILE:HG23 | 1:L:170:GLN:HB2  | 1.90                     | 0.52              |
| 2:l:32:SER:OG    | 2:l:99:THR:O     | 2.19                     | 0.52              |
| 1:M:304:THR:O    | 1:M:308:LEU:HD13 | 2.09                     | 0.52              |
| 2:i:32:SER:OG    | 2:i:99:THR:O     | 2.16                     | 0.52              |
| 1:J:73:LEU:O     | 1:J:77:LEU:HB2   | 2.10                     | 0.52              |
| 1:L:138:LEU:O    | 1:L:191:TYR:OH   | 2.26                     | 0.52              |
| 1:N:144:VAL:O    | 1:N:153:ARG:NH1  | 2.42                     | 0.52              |
| 1:F:140:GLY:HA2  | 1:F:216:GLY:HA3  | 1.90                     | 0.52              |
| 1:G:302:GLN:OE1  | 1:G:312:ARG:NH1  | 2.42                     | 0.52              |
| 1:J:80:ILE:HG23  | 1:J:208:HIS:HE1  | 1.75                     | 0.52              |
| 1:L:180:ASP:OD1  | 1:L:180:ASP:N    | 2.38                     | 0.52              |
| 2:n:83:MET:HE2   | 2:n:86:LEU:HD21  | 1.92                     | 0.52              |
| 1:A:302:GLN:OE1  | 1:A:312:ARG:NH1  | 2.43                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:89:SER:O     | 1:E:270:LYS:NZ   | 2.42                     | 0.52              |
| 1:K:152:TYR:C    | 1:K:154:LYS:H    | 2.18                     | 0.52              |
| 1:Q:51:LEU:HA    | 1:Q:54:TYR:HB2   | 1.91                     | 0.52              |
| 1:R:152:TYR:OH   | 3:v:44:U:OP2     | 2.19                     | 0.52              |
| 1:L:50:ASP:HB3   | 1:L:54:TYR:HE2   | 1.73                     | 0.52              |
| 1:I:137:TYR:CZ   | 1:I:173:PRO:HD2  | 2.44                     | 0.52              |
| 1:J:137:TYR:CZ   | 1:J:173:PRO:HD2  | 2.44                     | 0.52              |
| 1:R:328:THR:O    | 1:R:332:LEU:HB2  | 2.09                     | 0.52              |
| 1:D:51:LEU:HD23  | 1:D:54:TYR:HD2   | 1.75                     | 0.52              |
| 1:D:358:ASP:OD2  | 2:e:54:ARG:NH1   | 2.42                     | 0.52              |
| 2:t:68:PHE:HA    | 2:t:82:LEU:O     | 2.09                     | 0.52              |
| 1:G:137:TYR:CZ   | 1:G:173:PRO:HD2  | 2.45                     | 0.52              |
| 2:h:2:VAL:HA     | 2:h:26:GLY:HA3   | 1.92                     | 0.52              |
| 1:C:143:ARG:HH12 | 3:w:18:U:H5'     | 1.74                     | 0.52              |
| 1:S:143:ARG:HE   | 1:S:155:LYS:HD3  | 1.74                     | 0.52              |
| 1:N:7:ARG:HG2    | 1:N:9:ILE:HG22   | 1.91                     | 0.52              |
| 1:P:312:ARG:HD2  | 3:u:14:U:C4      | 2.45                     | 0.52              |
| 1:B:138:LEU:O    | 1:B:191:TYR:OH   | 2.27                     | 0.52              |
| 2:r:63:SER:OG    | 2:r:89:GLU:OE2   | 2.26                     | 0.52              |
| 1:E:73:LEU:O     | 1:E:77:LEU:HB2   | 2.10                     | 0.52              |
| 1:F:260:GLN:OE1  | 1:F:294:ASN:ND2  | 2.35                     | 0.52              |
| 1:I:350:VAL:HG23 | 1:J:247:THR:HG21 | 1.92                     | 0.52              |
| 1:O:104:ILE:HD11 | 1:O:198:VAL:HA   | 1.92                     | 0.52              |
| 1:O:135:PRO:HB2  | 1:O:213:PHE:HE2  | 1.75                     | 0.52              |
| 1:Q:43:ASN:OD1   | 1:Q:45:THR:OG1   | 2.22                     | 0.52              |
| 2:d:2:VAL:H      | 2:d:26:GLY:HA3   | 1.75                     | 0.52              |
| 2:d:63:SER:O     | 2:d:67:ARG:NH2   | 2.30                     | 0.52              |
| 2:s:40:ALA:HB3   | 2:s:43:LYS:HB2   | 1.91                     | 0.52              |
| 1:M:293:LYS:O    | 1:M:294:ASN:ND2  | 2.42                     | 0.52              |
| 1:G:69:VAL:HB    | 1:G:138:LEU:HD13 | 1.92                     | 0.52              |
| 1:G:142:TYR:CZ   | 1:G:146:ARG:HD2  | 2.44                     | 0.52              |
| 1:O:66:ILE:HA    | 1:O:69:VAL:HG22  | 1.92                     | 0.52              |
| 1:O:223:LYS:HD3  | 1:O:279:ILE:HD13 | 1.91                     | 0.52              |
| 2:j:20:LEU:HD12  | 2:j:81:LEU:HD23  | 1.92                     | 0.52              |
| 1:C:89:SER:O     | 1:C:270:LYS:NZ   | 2.43                     | 0.51              |
| 1:E:66:ILE:HD12  | 1:E:66:ILE:H     | 1.75                     | 0.51              |
| 1:N:152:TYR:O    | 1:N:155:LYS:CB   | 2.58                     | 0.51              |
| 1:M:242:THR:OG1  | 1:M:243:GLU:OE1  | 2.27                     | 0.51              |
| 1:F:163:GLN:OE1  | 1:F:170:GLN:NE2  | 2.43                     | 0.51              |
| 1:I:89:SER:O     | 1:I:270:LYS:NZ   | 2.42                     | 0.51              |
| 1:I:152:TYR:CZ   | 1:I:155:LYS:HE3  | 2.45                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:a:2:VAL:HA     | 2:a:26:GLY:HA3   | 1.92                     | 0.51              |
| 1:B:364:LEU:HG   | 1:B:366:THR:HG23 | 1.92                     | 0.51              |
| 1:Q:242:THR:O    | 1:Q:246:THR:OG1  | 2.27                     | 0.51              |
| 2:c:83:MET:HE2   | 2:c:86:LEU:HD21  | 1.92                     | 0.51              |
| 1:S:267:GLU:OE1  | 1:S:273:SER:OG   | 2.26                     | 0.51              |
| 1:F:230:THR:HG21 | 1:F:298:HIS:ND1  | 2.26                     | 0.51              |
| 1:H:199:ASP:OD1  | 1:H:277:TYR:OH   | 2.21                     | 0.51              |
| 1:I:157:MET:O    | 1:I:160:LEU:HB2  | 2.09                     | 0.51              |
| 1:I:159:GLY:O    | 1:I:163:GLN:NE2  | 2.30                     | 0.51              |
| 1:E:215:TYR:HD1  | 3:w:36:U:H5'     | 1.75                     | 0.51              |
| 1:O:143:ARG:NH2  | 3:u:27:U:OP2     | 2.42                     | 0.51              |
| 1:R:138:LEU:O    | 1:R:191:TYR:OH   | 2.25                     | 0.51              |
| 1:E:7:ARG:HG2    | 1:E:9:ILE:HG22   | 1.93                     | 0.51              |
| 1:T:38:ILE:HD12  | 1:T:281:PHE:O    | 2.11                     | 0.51              |
| 1:T:152:TYR:CG   | 3:v:24:U:H4'     | 2.45                     | 0.51              |
| 1:M:68:HIS:HE2   | 1:M:119:ASP:HA   | 1.74                     | 0.51              |
| 1:F:319:PRO:O    | 1:F:324:TYR:OH   | 2.19                     | 0.51              |
| 1:F:350:VAL:HG23 | 1:G:247:THR:HG21 | 1.91                     | 0.51              |
| 1:J:93:ILE:HG22  | 1:J:95:ILE:HG23  | 1.92                     | 0.51              |
| 2:j:22:CYS:HB3   | 2:j:79:VAL:HG13  | 1.93                     | 0.51              |
| 1:Q:177:GLU:OE1  | 1:R:168:ASN:ND2  | 2.32                     | 0.51              |
| 1:K:87:ASP:OD1   | 1:K:98:ALA:N     | 2.44                     | 0.51              |
| 1:K:332:LEU:HD22 | 1:K:393:MET:HE2  | 1.93                     | 0.51              |
| 1:N:143:ARG:CZ   | 1:N:155:LYS:HZ1  | 2.24                     | 0.51              |
| 1:N:260:GLN:OE1  | 1:N:294:ASN:ND2  | 2.43                     | 0.51              |
| 1:G:156:LEU:O    | 1:G:159:GLY:N    | 2.43                     | 0.51              |
| 1:J:89:SER:O     | 1:J:270:LYS:NZ   | 2.43                     | 0.51              |
| 1:J:147:THR:HG21 | 1:J:152:TYR:HE2  | 1.75                     | 0.51              |
| 2:l:20:LEU:HD12  | 2:l:81:LEU:HD23  | 1.93                     | 0.51              |
| 1:J:203:HIS:ND1  | 1:J:272:ASP:OD1  | 2.44                     | 0.51              |
| 1:B:268:ILE:HG22 | 1:B:275:MET:HE3  | 1.93                     | 0.51              |
| 1:D:40:LEU:HD12  | 1:D:108:VAL:HG21 | 1.93                     | 0.51              |
| 2:s:54:ARG:NH1   | 1:T:358:ASP:OD2  | 2.44                     | 0.51              |
| 1:K:167:ILE:HG23 | 1:K:170:GLN:HB2  | 1.92                     | 0.51              |
| 1:K:194:ILE:O    | 1:K:198:VAL:HG23 | 2.10                     | 0.51              |
| 1:R:3:VAL:HG22   | 1:R:4:THR:H      | 1.76                     | 0.51              |
| 1:R:7:ARG:HG2    | 1:R:9:ILE:HG22   | 1.93                     | 0.51              |
| 1:R:242:THR:OG1  | 1:R:243:GLU:OE1  | 2.29                     | 0.51              |
| 2:k:33:ILE:HG12  | 2:k:52:SER:HA    | 1.93                     | 0.51              |
| 1:L:279:ILE:HD11 | 1:L:287:SER:HB2  | 1.91                     | 0.51              |
| 1:G:145:GLY:HA2  | 1:G:153:ARG:NH1  | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:137:TYR:CZ   | 1:H:173:PRO:HD2  | 2.46                     | 0.51              |
| 2:i:63:SER:O     | 2:i:67:ARG:NH2   | 2.32                     | 0.51              |
| 1:O:156:LEU:O    | 1:O:160:LEU:HG   | 2.11                     | 0.51              |
| 1:J:314:ARG:NH2  | 1:J:405:GLN:O    | 2.26                     | 0.51              |
| 1:A:136:LEU:HD22 | 1:A:163:GLN:HE21 | 1.75                     | 0.51              |
| 1:P:152:TYR:CZ   | 1:P:155:LYS:HE3  | 2.46                     | 0.51              |
| 1:S:401:VAL:HG21 | 1:S:420:PHE:HB2  | 1.93                     | 0.51              |
| 1:T:172:GLU:OE2  | 1:T:172:GLU:N    | 2.41                     | 0.51              |
| 1:I:312:ARG:HG3  | 3:x:23:U:C2      | 2.46                     | 0.51              |
| 2:r:5:VAL:O      | 2:r:22:CYS:HA    | 2.11                     | 0.51              |
| 1:S:159:GLY:O    | 1:S:163:GLN:HG2  | 2.11                     | 0.51              |
| 1:L:194:ILE:O    | 1:L:198:VAL:HG23 | 2.11                     | 0.51              |
| 1:F:114:ASP:OD1  | 1:F:114:ASP:N    | 2.44                     | 0.51              |
| 1:Q:314:ARG:HE   | 1:Q:404:LEU:HD22 | 1.76                     | 0.50              |
| 1:C:139:LEU:HD22 | 1:C:195:VAL:HG12 | 1.92                     | 0.50              |
| 1:D:376:VAL:HG12 | 2:d:103:ASN:HD21 | 1.75                     | 0.50              |
| 1:S:89:SER:O     | 1:S:270:LYS:NZ   | 2.43                     | 0.50              |
| 1:S:167:ILE:HG23 | 1:S:170:GLN:HB2  | 1.92                     | 0.50              |
| 2:e:52:SER:OG    | 2:e:53:TRP:N     | 2.44                     | 0.50              |
| 1:T:178:GLY:HA2  | 1:T:181:ILE:HG12 | 1.93                     | 0.50              |
| 1:L:366:THR:O    | 1:L:368:ALA:N    | 2.44                     | 0.50              |
| 1:M:144:VAL:O    | 1:M:153:ARG:NH2  | 2.44                     | 0.50              |
| 1:R:5:VAL:HG22   | 1:T:350:VAL:HG22 | 1.92                     | 0.50              |
| 2:s:72:ARG:NH2   | 2:s:74:ASN:OD1   | 2.39                     | 0.50              |
| 1:K:40:LEU:HD12  | 1:K:108:VAL:HG21 | 1.92                     | 0.50              |
| 1:F:165:LYS:HG2  | 1:G:184:VAL:HG22 | 1.93                     | 0.50              |
| 2:o:17:SER:HA    | 2:o:83:MET:O     | 2.11                     | 0.50              |
| 1:D:89:SER:O     | 1:D:270:LYS:NZ   | 2.44                     | 0.50              |
| 2:t:32:SER:OG    | 2:t:99:THR:O     | 2.24                     | 0.50              |
| 1:L:133:TRP:HB2  | 1:L:163:GLN:HG2  | 1.93                     | 0.50              |
| 1:N:54:TYR:CE1   | 1:N:122:SER:HB2  | 2.46                     | 0.50              |
| 1:N:70:ASN:ND2   | 1:N:188:ASP:OD2  | 2.43                     | 0.50              |
| 1:A:139:LEU:HD22 | 1:A:195:VAL:HG12 | 1.92                     | 0.50              |
| 1:D:259:VAL:HG22 | 1:E:14:ILE:HD12  | 1.93                     | 0.50              |
| 1:S:52:ARG:NH1   | 1:S:128:SER:HA   | 2.26                     | 0.50              |
| 1:K:156:LEU:O    | 1:K:160:LEU:HD23 | 2.10                     | 0.50              |
| 1:O:319:PRO:O    | 1:O:324:TYR:OH   | 2.21                     | 0.50              |
| 2:o:49:ALA:HA    | 2:o:59:THR:O     | 2.11                     | 0.50              |
| 3:w:23:U:H2'     | 3:w:25:U:H5''    | 1.94                     | 0.50              |
| 1:D:22:GLU:HB3   | 1:D:24:PRO:HD3   | 1.94                     | 0.50              |
| 2:s:50:LYS:NZ    | 2:s:105:GLY:O    | 2.29                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:184:VAL:HG22 | 1:M:165:LYS:HG2  | 1.94                     | 0.50              |
| 1:F:51:LEU:HA    | 1:F:54:TYR:HB2   | 1.92                     | 0.50              |
| 1:H:336:TYR:OH   | 1:H:392:ASP:OD2  | 2.26                     | 0.50              |
| 1:O:328:THR:O    | 1:O:332:LEU:HB2  | 2.12                     | 0.50              |
| 1:J:359:ASP:OD1  | 1:J:359:ASP:N    | 2.42                     | 0.50              |
| 1:A:254:VAL:HG21 | 1:A:327:LEU:HD11 | 1.94                     | 0.50              |
| 1:P:319:PRO:O    | 1:P:324:TYR:OH   | 2.21                     | 0.50              |
| 1:C:154:LYS:HB2  | 1:C:157:MET:HE2  | 1.92                     | 0.50              |
| 1:D:401:VAL:HG21 | 1:D:420:PHE:HB2  | 1.93                     | 0.50              |
| 1:F:66:ILE:HD12  | 1:F:66:ILE:H     | 1.76                     | 0.50              |
| 1:G:59:LEU:HG    | 1:G:174:LEU:HD11 | 1.94                     | 0.50              |
| 2:g:38:ARG:O     | 2:g:46:ASP:N     | 2.29                     | 0.50              |
| 1:J:137:TYR:HD1  | 1:J:163:GLN:HE22 | 1.60                     | 0.50              |
| 2:a:52:SER:OG    | 2:a:53:TRP:N     | 2.44                     | 0.50              |
| 1:T:38:ILE:HG23  | 1:T:108:VAL:HG12 | 1.93                     | 0.50              |
| 1:L:139:LEU:HD22 | 1:L:195:VAL:HG12 | 1.94                     | 0.50              |
| 1:M:234:LEU:O    | 1:M:238:THR:OG1  | 2.26                     | 0.50              |
| 1:D:74:TYR:O     | 1:D:78:LYS:N     | 2.44                     | 0.50              |
| 1:D:165:LYS:HZ2  | 1:E:184:VAL:HG13 | 1.77                     | 0.50              |
| 2:h:83:MET:HE2   | 2:h:86:LEU:HD21  | 1.94                     | 0.50              |
| 1:I:52:ARG:NH1   | 1:I:131:ASP:OD2  | 2.44                     | 0.50              |
| 3:u:1:U:OP2      | 3:v:44:U:O2'     | 2.20                     | 0.50              |
| 3:u:11:U:C3'     | 3:u:12:U:H5''    | 2.38                     | 0.50              |
| 1:F:74:TYR:O     | 1:F:78:LYS:N     | 2.44                     | 0.49              |
| 2:h:68:PHE:HA    | 2:h:82:LEU:O     | 2.12                     | 0.49              |
| 1:I:152:TYR:CE2  | 1:I:155:LYS:HE3  | 2.47                     | 0.49              |
| 1:P:123:ASP:OD1  | 1:P:124:ALA:N    | 2.43                     | 0.49              |
| 1:E:353:ASN:HD22 | 2:f:100:LYS:HE3  | 1.77                     | 0.49              |
| 1:T:240:MET:HE1  | 1:T:248:TRP:CD1  | 2.47                     | 0.49              |
| 2:t:2:VAL:HA     | 2:t:26:GLY:HA3   | 1.94                     | 0.49              |
| 1:J:143:ARG:HB2  | 1:J:216:GLY:HA2  | 1.94                     | 0.49              |
| 1:B:114:ASP:OD1  | 1:B:114:ASP:N    | 2.43                     | 0.49              |
| 1:B:376:VAL:HG12 | 2:b:103:ASN:HD21 | 1.77                     | 0.49              |
| 1:D:143:ARG:NH1  | 3:w:27:U:OP2     | 2.43                     | 0.49              |
| 2:l:83:MET:HB3   | 2:l:86:LEU:HD21  | 1.94                     | 0.49              |
| 1:F:268:ILE:HG22 | 1:F:275:MET:HE3  | 1.94                     | 0.49              |
| 1:L:35:SER:OG    | 1:L:37:GLU:O     | 2.27                     | 0.49              |
| 2:m:50:LYS:NZ    | 2:m:105:GLY:O    | 2.32                     | 0.49              |
| 1:A:230:THR:HG21 | 1:A:298:HIS:ND1  | 2.27                     | 0.49              |
| 1:P:242:THR:O    | 1:P:246:THR:OG1  | 2.23                     | 0.49              |
| 1:B:152:TYR:HB2  | 3:w:6:U:H1'      | 1.95                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:c:11:LEU:HA    | 2:c:122:THR:O    | 2.12                     | 0.49              |
| 2:r:50:LYS:HG2   | 2:r:59:THR:HB    | 1.94                     | 0.49              |
| 1:D:175:VAL:O    | 1:D:177:GLU:N    | 2.39                     | 0.49              |
| 1:T:89:SER:O     | 1:T:270:LYS:NZ   | 2.46                     | 0.49              |
| 1:T:126:ARG:HD2  | 1:T:130:ASP:OD2  | 2.12                     | 0.49              |
| 1:M:302:GLN:OE1  | 1:M:312:ARG:NH1  | 2.45                     | 0.49              |
| 1:A:159:GLY:HA3  | 1:A:215:TYR:OH   | 2.12                     | 0.49              |
| 3:x:8:U:O2'      | 3:x:10:U:OP2     | 2.27                     | 0.49              |
| 1:P:77:LEU:C     | 1:P:80:ILE:HD11  | 2.37                     | 0.49              |
| 1:T:42:ILE:HD13  | 1:T:74:TYR:HB2   | 1.95                     | 0.49              |
| 1:L:114:ASP:OD1  | 1:L:114:ASP:N    | 2.40                     | 0.49              |
| 1:L:247:THR:HG21 | 1:M:350:VAL:HG23 | 1.95                     | 0.49              |
| 1:M:364:LEU:HG   | 1:M:366:THR:HG23 | 1.94                     | 0.49              |
| 3:u:26:U:O2'     | 3:u:28:U:OP2     | 2.29                     | 0.49              |
| 1:S:149:MET:O    | 1:S:151:GLU:N    | 2.45                     | 0.49              |
| 1:T:17:LYS:HG3   | 1:K:268:ILE:HD11 | 1.95                     | 0.49              |
| 1:M:137:TYR:CZ   | 1:M:173:PRO:HD2  | 2.47                     | 0.49              |
| 1:H:51:LEU:HA    | 1:H:54:TYR:HB2   | 1.94                     | 0.49              |
| 1:O:248:TRP:CD1  | 1:O:375:VAL:HG22 | 2.47                     | 0.49              |
| 1:B:130:ASP:HA   | 1:B:133:TRP:NE1  | 2.28                     | 0.49              |
| 1:T:143:ARG:NE   | 1:T:155:LYS:HE3  | 2.24                     | 0.49              |
| 2:l:50:LYS:NZ    | 2:l:105:GLY:O    | 2.37                     | 0.49              |
| 1:G:220:SER:OG   | 1:G:280:ASP:OD2  | 2.28                     | 0.49              |
| 1:I:395:GLN:O    | 1:I:399:ARG:HG2  | 2.13                     | 0.49              |
| 1:O:138:LEU:O    | 1:O:191:TYR:OH   | 2.30                     | 0.49              |
| 1:Q:88:TRP:CD2   | 1:Q:95:ILE:HD11  | 2.48                     | 0.49              |
| 1:G:89:SER:O     | 1:G:270:LYS:NZ   | 2.46                     | 0.49              |
| 1:J:319:PRO:O    | 1:J:324:TYR:OH   | 2.24                     | 0.49              |
| 1:J:350:VAL:HG23 | 1:A:247:THR:HG21 | 1.95                     | 0.49              |
| 2:b:39:GLN:NE2   | 2:b:43:LYS:O     | 2.36                     | 0.49              |
| 1:Q:364:LEU:HG   | 1:Q:366:THR:HG23 | 1.94                     | 0.49              |
| 2:k:5:VAL:O      | 2:k:22:CYS:HA    | 2.12                     | 0.49              |
| 1:N:256:ASP:OD1  | 1:M:7:ARG:NH2    | 2.42                     | 0.49              |
| 3:x:23:U:O2'     | 3:x:25:U:OP1     | 2.27                     | 0.49              |
| 2:b:83:MET:HB3   | 2:b:86:LEU:HD21  | 1.93                     | 0.48              |
| 1:C:323:GLU:HB2  | 1:C:327:LEU:HD23 | 1.95                     | 0.48              |
| 1:C:355:TYR:HA   | 1:D:376:VAL:HG13 | 1.94                     | 0.48              |
| 1:R:285:SER:O    | 1:S:207:LYS:NZ   | 2.46                     | 0.48              |
| 1:D:293:LYS:O    | 1:D:294:ASN:ND2  | 2.46                     | 0.48              |
| 1:S:376:VAL:O    | 2:s:103:ASN:ND2  | 2.42                     | 0.48              |
| 1:O:302:GLN:OE1  | 1:O:312:ARG:NH1  | 2.42                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:364:LEU:HG   | 1:A:366:THR:HG23 | 1.94                     | 0.48              |
| 1:B:158:ASP:O    | 1:B:162:ASN:HB2  | 2.13                     | 0.48              |
| 2:c:32:SER:OG    | 2:c:99:THR:O     | 2.19                     | 0.48              |
| 1:R:376:VAL:HG13 | 1:S:355:TYR:HA   | 1.95                     | 0.48              |
| 1:T:153:ARG:NH2  | 1:T:179:ARG:HB3  | 2.28                     | 0.48              |
| 1:K:103:GLY:N    | 1:K:106:ASP:OD2  | 2.39                     | 0.48              |
| 1:N:226:ALA:HB3  | 1:N:291:SER:HB3  | 1.94                     | 0.48              |
| 1:B:247:THR:HG21 | 1:A:350:VAL:HG23 | 1.95                     | 0.48              |
| 1:R:66:ILE:H     | 1:R:66:ILE:HD12  | 1.77                     | 0.48              |
| 1:D:230:THR:HG21 | 1:D:298:HIS:ND1  | 2.28                     | 0.48              |
| 1:G:149:MET:HB3  | 1:G:152:TYR:HB3  | 1.95                     | 0.48              |
| 2:g:5:VAL:O      | 2:g:22:CYS:HA    | 2.13                     | 0.48              |
| 2:g:67:ARG:NH1   | 2:g:90:ASP:OD2   | 2.33                     | 0.48              |
| 1:I:194:ILE:O    | 1:I:198:VAL:HG23 | 2.14                     | 0.48              |
| 1:D:364:LEU:HG   | 1:D:366:THR:HG23 | 1.93                     | 0.48              |
| 1:S:124:ALA:C    | 1:S:126:ARG:H    | 2.21                     | 0.48              |
| 1:S:230:THR:HG21 | 1:S:298:HIS:ND1  | 2.28                     | 0.48              |
| 1:L:51:LEU:HA    | 1:L:54:TYR:HB2   | 1.95                     | 0.48              |
| 1:G:52:ARG:NH1   | 1:G:128:SER:HA   | 2.28                     | 0.48              |
| 1:I:359:ASP:OD1  | 1:I:359:ASP:N    | 2.37                     | 0.48              |
| 1:A:51:LEU:HA    | 1:A:54:TYR:HB2   | 1.96                     | 0.48              |
| 1:C:364:LEU:HG   | 1:C:366:THR:HG23 | 1.96                     | 0.48              |
| 1:S:332:LEU:HD22 | 1:S:393:MET:HE2  | 1.95                     | 0.48              |
| 1:E:137:TYR:CZ   | 1:E:173:PRO:HD2  | 2.48                     | 0.48              |
| 1:O:137:TYR:CZ   | 1:O:173:PRO:HD2  | 2.49                     | 0.48              |
| 1:J:165:LYS:HZ3  | 1:A:187:ASN:HB2  | 1.77                     | 0.48              |
| 2:a:62:ASP:HA    | 2:a:65:LYS:HE3   | 1.95                     | 0.48              |
| 1:L:159:GLY:HA3  | 1:L:163:GLN:CD   | 2.38                     | 0.48              |
| 1:A:70:ASN:ND2   | 1:A:188:ASP:OD2  | 2.43                     | 0.48              |
| 2:p:100:LYS:HE3  | 1:Q:353:ASN:HD22 | 1.79                     | 0.48              |
| 1:Q:70:ASN:ND2   | 1:Q:188:ASP:OD2  | 2.41                     | 0.48              |
| 1:D:194:ILE:O    | 1:D:198:VAL:HG23 | 2.13                     | 0.48              |
| 1:S:421:ASP:O    | 1:S:422:LYS:HD3  | 2.13                     | 0.48              |
| 1:K:147:THR:OG1  | 1:K:155:LYS:NZ   | 2.46                     | 0.48              |
| 1:F:178:GLY:HA2  | 1:F:181:ILE:HG12 | 1.96                     | 0.48              |
| 1:I:319:PRO:O    | 1:I:324:TYR:OH   | 2.24                     | 0.48              |
| 1:D:344:LEU:HD11 | 1:E:329:THR:HG22 | 1.96                     | 0.48              |
| 1:K:152:TYR:OH   | 3:v:17:U:OP2     | 2.29                     | 0.48              |
| 1:L:158:ASP:O    | 1:L:162:ASN:HB2  | 2.14                     | 0.48              |
| 1:L:362:GLY:O    | 1:L:364:LEU:N    | 2.47                     | 0.48              |
| 2:l:52:SER:OG    | 2:l:53:TRP:N     | 2.47                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:n:51:ILE:HD11  | 2:n:56:ASP:HB3   | 1.95                     | 0.48              |
| 2:q:73:ASP:HB3   | 2:q:76:SER:HB3   | 1.96                     | 0.48              |
| 1:D:60:LYS:HA    | 1:D:173:PRO:O    | 2.14                     | 0.48              |
| 1:L:143:ARG:HH12 | 3:v:9:U:H5'      | 1.79                     | 0.48              |
| 1:F:158:ASP:HB3  | 1:F:215:TYR:OH   | 2.13                     | 0.48              |
| 1:G:143:ARG:NH1  | 3:x:9:U:H5'      | 2.29                     | 0.48              |
| 1:H:347:GLN:OE1  | 1:I:252:ARG:NH2  | 2.47                     | 0.48              |
| 2:c:2:VAL:HA     | 2:c:26:GLY:HA3   | 1.95                     | 0.48              |
| 1:E:52:ARG:NH1   | 1:E:128:SER:HA   | 2.29                     | 0.48              |
| 1:T:114:ASP:OD1  | 1:T:114:ASP:N    | 2.45                     | 0.48              |
| 2:k:50:LYS:HG2   | 2:k:59:THR:HB    | 1.96                     | 0.48              |
| 1:G:230:THR:HG21 | 1:G:298:HIS:ND1  | 2.29                     | 0.48              |
| 1:O:268:ILE:HG22 | 1:O:275:MET:HE3  | 1.96                     | 0.48              |
| 1:R:158:ASP:OD1  | 1:R:159:GLY:N    | 2.44                     | 0.47              |
| 2:d:40:ALA:HB3   | 2:d:43:LYS:HB2   | 1.96                     | 0.47              |
| 2:s:83:MET:HE2   | 2:s:86:LEU:HD21  | 1.96                     | 0.47              |
| 1:L:159:GLY:HA2  | 1:L:163:GLN:H    | 1.79                     | 0.47              |
| 1:P:143:ARG:HB3  | 1:P:216:GLY:HA2  | 1.96                     | 0.47              |
| 1:B:14:ILE:HG23  | 1:B:16:PRO:HD3   | 1.97                     | 0.47              |
| 1:R:381:TRP:O    | 1:R:385:GLN:HG2  | 2.14                     | 0.47              |
| 1:R:419:GLU:OE2  | 1:S:309:ARG:NE   | 2.39                     | 0.47              |
| 1:K:278:LEU:HA   | 1:K:283:LEU:HD12 | 1.97                     | 0.47              |
| 1:N:80:ILE:HD11  | 1:N:208:HIS:HE2  | 1.79                     | 0.47              |
| 1:N:86:LYS:HG3   | 1:N:87:ASP:H     | 1.78                     | 0.47              |
| 1:G:139:LEU:HD22 | 1:G:195:VAL:HG12 | 1.97                     | 0.47              |
| 1:H:141:LEU:HD12 | 1:H:182:PHE:CZ   | 2.49                     | 0.47              |
| 1:O:144:VAL:HG22 | 1:O:155:LYS:HB3  | 1.95                     | 0.47              |
| 1:A:137:TYR:HD1  | 1:A:163:GLN:OE1  | 1.98                     | 0.47              |
| 1:A:200:MET:HE1  | 1:A:274:TYR:CE1  | 2.49                     | 0.47              |
| 1:P:7:ARG:HG2    | 1:P:9:ILE:HG22   | 1.97                     | 0.47              |
| 1:B:324:TYR:O    | 1:B:328:THR:OG1  | 2.22                     | 0.47              |
| 1:E:192:THR:HA   | 1:E:195:VAL:HG22 | 1.96                     | 0.47              |
| 2:t:83:MET:HE2   | 2:t:86:LEU:HD21  | 1.96                     | 0.47              |
| 1:K:7:ARG:HG2    | 1:K:9:ILE:HG22   | 1.97                     | 0.47              |
| 1:G:7:ARG:HG2    | 1:G:9:ILE:HG22   | 1.96                     | 0.47              |
| 1:G:51:LEU:HB3   | 1:G:72:TYR:HB2   | 1.96                     | 0.47              |
| 1:O:74:TYR:O     | 1:O:78:LYS:HG3   | 2.14                     | 0.47              |
| 3:u:20:U:H2'     | 3:u:21:U:O4'     | 2.15                     | 0.47              |
| 1:P:278:LEU:HD12 | 1:P:284:SER:HB3  | 1.95                     | 0.47              |
| 1:B:137:TYR:O    | 1:B:141:LEU:HG   | 2.14                     | 0.47              |
| 1:Q:42:ILE:HD13  | 1:Q:74:TYR:HB2   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:Q:312:ARG:HD2  | 3:u:5:U:C4       | 2.49                     | 0.47              |
| 1:C:248:TRP:CD1  | 1:C:375:VAL:HG22 | 2.49                     | 0.47              |
| 1:K:132:LYS:HB3  | 1:K:166:MET:HE3  | 1.95                     | 0.47              |
| 1:L:86:LYS:HA    | 1:L:86:LYS:HD3   | 1.63                     | 0.47              |
| 1:O:42:ILE:HD13  | 1:O:74:TYR:HB2   | 1.96                     | 0.47              |
| 1:J:126:ARG:NE   | 1:J:130:ASP:OD2  | 2.41                     | 0.47              |
| 1:A:114:ASP:OD1  | 1:A:114:ASP:N    | 2.46                     | 0.47              |
| 1:P:74:TYR:O     | 1:P:78:LYS:HG3   | 2.15                     | 0.47              |
| 1:B:376:VAL:HG12 | 2:b:103:ASN:ND2  | 2.29                     | 0.47              |
| 1:S:127:THR:HG22 | 1:S:128:SER:H    | 1.78                     | 0.47              |
| 1:S:359:ASP:O    | 2:s:77:ASN:ND2   | 2.47                     | 0.47              |
| 1:E:355:TYR:HA   | 1:F:376:VAL:HG13 | 1.97                     | 0.47              |
| 1:M:288:PRO:HG2  | 1:M:289:TYR:CE2  | 2.50                     | 0.47              |
| 1:F:66:ILE:HA    | 1:F:69:VAL:HG22  | 1.97                     | 0.47              |
| 2:q:50:LYS:HG2   | 2:q:59:THR:HB    | 1.95                     | 0.47              |
| 1:C:160:LEU:HD11 | 1:C:172:GLU:HB3  | 1.95                     | 0.47              |
| 1:D:66:ILE:HD12  | 1:D:66:ILE:H     | 1.80                     | 0.47              |
| 1:E:194:ILE:O    | 1:E:198:VAL:HG23 | 2.14                     | 0.47              |
| 1:T:268:ILE:HG22 | 1:T:275:MET:HE3  | 1.95                     | 0.47              |
| 2:k:100:LYS:HB3  | 2:k:103:ASN:HD22 | 1.79                     | 0.47              |
| 1:L:104:ILE:HG23 | 1:L:105:PHE:CD2  | 2.50                     | 0.47              |
| 1:F:408:ARG:HD3  | 3:w:42:U:C4      | 2.49                     | 0.47              |
| 2:f:49:ALA:HA    | 2:f:59:THR:O     | 2.14                     | 0.47              |
| 1:G:350:VAL:HG22 | 1:I:5:VAL:HG22   | 1.97                     | 0.47              |
| 1:I:124:ALA:O    | 1:I:125:SER:OG   | 2.29                     | 0.47              |
| 1:J:88:TRP:CD1   | 1:J:95:ILE:HG13  | 2.50                     | 0.47              |
| 1:Q:66:ILE:HD12  | 1:Q:66:ILE:H     | 1.79                     | 0.47              |
| 1:C:312:ARG:HG3  | 3:w:14:U:C2      | 2.50                     | 0.47              |
| 1:R:114:ASP:OD1  | 1:R:114:ASP:N    | 2.45                     | 0.47              |
| 1:S:135:PRO:O    | 1:S:139:LEU:HG   | 2.15                     | 0.47              |
| 1:T:66:ILE:HA    | 1:T:69:VAL:HG22  | 1.96                     | 0.47              |
| 1:T:247:THR:HG21 | 1:K:350:VAL:HG23 | 1.97                     | 0.47              |
| 2:k:2:VAL:HA     | 2:k:25:SER:O     | 2.15                     | 0.47              |
| 1:M:156:LEU:O    | 1:M:160:LEU:HG   | 2.14                     | 0.47              |
| 2:f:71:SER:O     | 2:f:79:VAL:HG23  | 2.14                     | 0.47              |
| 1:G:77:LEU:HD13  | 1:G:104:ILE:HD13 | 1.97                     | 0.47              |
| 1:H:194:ILE:O    | 1:H:198:VAL:HG23 | 2.15                     | 0.47              |
| 2:i:20:LEU:HD12  | 2:i:81:LEU:HD23  | 1.96                     | 0.47              |
| 1:P:87:ASP:OD2   | 1:P:97:LYS:HG3   | 2.15                     | 0.47              |
| 1:R:159:GLY:HA2  | 1:R:163:GLN:H    | 1.79                     | 0.47              |
| 2:r:11:LEU:HA    | 2:r:122:THR:O    | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:S:136:LEU:HB3  | 1:S:163:GLN:HE22 | 1.79                     | 0.47              |
| 2:k:83:MET:HE1   | 2:k:121:VAL:HG11 | 1.96                     | 0.47              |
| 1:L:88:TRP:CD2   | 1:L:95:ILE:HD11  | 2.50                     | 0.47              |
| 1:L:319:PRO:O    | 1:L:324:TYR:OH   | 2.26                     | 0.47              |
| 2:l:39:GLN:HB3   | 2:l:95:TYR:HE2   | 1.80                     | 0.47              |
| 2:n:14:THR:N     | 2:n:124:SER:O    | 2.47                     | 0.47              |
| 2:n:37:PHE:CD2   | 2:n:45:ARG:HD3   | 2.50                     | 0.47              |
| 1:G:70:ASN:ND2   | 1:G:188:ASP:OD2  | 2.48                     | 0.47              |
| 1:G:152:TYR:CG   | 3:x:6:U:H4'      | 2.50                     | 0.47              |
| 1:O:52:ARG:NH1   | 1:O:128:SER:HA   | 2.30                     | 0.47              |
| 1:J:366:THR:OG1  | 2:j:31:ASN:OD1   | 2.23                     | 0.47              |
| 2:r:46:ASP:OD1   | 2:r:46:ASP:N     | 2.45                     | 0.47              |
| 1:L:376:VAL:HG12 | 2:l:103:ASN:ND2  | 2.29                     | 0.47              |
| 1:F:158:ASP:OD1  | 1:F:162:ASN:ND2  | 2.48                     | 0.47              |
| 1:I:126:ARG:NE   | 1:I:130:ASP:OD2  | 2.46                     | 0.47              |
| 1:O:86:LYS:HA    | 1:O:86:LYS:HD3   | 1.72                     | 0.47              |
| 1:O:298:HIS:O    | 1:O:302:GLN:HB2  | 2.15                     | 0.47              |
| 1:S:319:PRO:O    | 1:S:324:TYR:OH   | 2.20                     | 0.47              |
| 2:t:17:SER:HA    | 2:t:83:MET:O     | 2.15                     | 0.47              |
| 2:i:14:THR:N     | 2:i:124:SER:O    | 2.48                     | 0.47              |
| 1:J:152:TYR:OH   | 3:x:35:U:OP2     | 2.33                     | 0.47              |
| 1:P:66:ILE:HA    | 1:P:69:VAL:HG22  | 1.97                     | 0.46              |
| 1:R:277:TYR:O    | 1:R:281:PHE:HB2  | 2.15                     | 0.46              |
| 1:M:7:ARG:HG2    | 1:M:9:ILE:HG22   | 1.96                     | 0.46              |
| 1:M:172:GLU:H    | 1:M:172:GLU:CD   | 2.22                     | 0.46              |
| 1:M:269:ASP:OD1  | 1:M:269:ASP:N    | 2.48                     | 0.46              |
| 1:I:199:ASP:OD1  | 1:I:214:ARG:NE   | 2.40                     | 0.46              |
| 1:A:38:ILE:HD12  | 1:A:281:PHE:O    | 2.15                     | 0.46              |
| 1:S:130:ASP:HA   | 1:S:133:TRP:NE1  | 2.30                     | 0.46              |
| 1:T:40:LEU:HD12  | 1:T:108:VAL:HG21 | 1.97                     | 0.46              |
| 1:T:105:PHE:HB3  | 1:T:110:LEU:HD21 | 1.97                     | 0.46              |
| 1:K:228:LEU:HB2  | 1:K:289:TYR:HB3  | 1.97                     | 0.46              |
| 2:l:98:ALA:HB3   | 2:l:114:TYR:HB2  | 1.96                     | 0.46              |
| 1:N:319:PRO:O    | 1:N:324:TYR:OH   | 2.23                     | 0.46              |
| 2:n:112:PHE:O    | 2:n:115:TRP:NE1  | 2.48                     | 0.46              |
| 1:H:350:VAL:HG23 | 1:I:247:THR:HG21 | 1.97                     | 0.46              |
| 1:Q:167:ILE:HG23 | 1:Q:170:GLN:HB2  | 1.96                     | 0.46              |
| 1:D:350:VAL:HG23 | 1:E:247:THR:HG21 | 1.97                     | 0.46              |
| 1:L:199:ASP:OD2  | 1:L:277:TYR:OH   | 2.31                     | 0.46              |
| 2:h:83:MET:HE1   | 2:h:121:VAL:HG11 | 1.98                     | 0.46              |
| 1:O:126:ARG:HH21 | 1:O:130:ASP:CG   | 2.23                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:165:LYS:NZ   | 1:A:184:VAL:O    | 2.47                     | 0.46              |
| 1:P:140:GLY:HA2  | 1:P:216:GLY:HA3  | 1.97                     | 0.46              |
| 1:B:226:ALA:O    | 1:B:230:THR:HG23 | 2.15                     | 0.46              |
| 1:R:7:ARG:NH2    | 1:S:256:ASP:OD1  | 2.44                     | 0.46              |
| 1:T:54:TYR:CE1   | 1:T:122:SER:HB2  | 2.51                     | 0.46              |
| 1:L:50:ASP:HB3   | 1:L:54:TYR:CE2   | 2.51                     | 0.46              |
| 1:M:194:ILE:O    | 1:M:198:VAL:HG23 | 2.16                     | 0.46              |
| 1:G:35:SER:OG    | 1:G:37:GLU:O     | 2.29                     | 0.46              |
| 1:A:226:ALA:HB3  | 1:A:291:SER:HB3  | 1.98                     | 0.46              |
| 1:Q:247:THR:HG21 | 1:R:350:VAL:HG23 | 1.98                     | 0.46              |
| 1:D:226:ALA:HB3  | 1:D:291:SER:HB3  | 1.98                     | 0.46              |
| 1:T:298:HIS:O    | 1:T:302:GLN:HB2  | 2.15                     | 0.46              |
| 2:l:63:SER:O     | 2:l:67:ARG:NH2   | 2.31                     | 0.46              |
| 1:N:153:ARG:O    | 1:N:156:LEU:HB3  | 2.16                     | 0.46              |
| 1:F:364:LEU:HG   | 1:F:366:THR:HG23 | 1.98                     | 0.46              |
| 1:H:85:ASP:OD1   | 1:H:85:ASP:N     | 2.41                     | 0.46              |
| 1:O:119:ASP:OD1  | 1:O:119:ASP:N    | 2.49                     | 0.46              |
| 1:O:158:ASP:HB3  | 1:O:215:TYR:OH   | 2.14                     | 0.46              |
| 1:B:165:LYS:HD2  | 1:C:184:VAL:HG13 | 1.96                     | 0.46              |
| 1:Q:192:THR:HA   | 1:Q:195:VAL:HG22 | 1.96                     | 0.46              |
| 1:C:82:GLY:O     | 1:C:101:THR:HA   | 2.16                     | 0.46              |
| 1:S:6:LYS:NZ     | 1:S:11:ASN:O     | 2.46                     | 0.46              |
| 1:T:244:ASP:O    | 1:T:247:THR:OG1  | 2.32                     | 0.46              |
| 1:N:143:ARG:CB   | 1:N:216:GLY:HA2  | 2.46                     | 0.46              |
| 1:N:143:ARG:HH12 | 3:u:36:U:H5'     | 1.81                     | 0.46              |
| 1:F:267:GLU:OE1  | 1:F:273:SER:OG   | 2.28                     | 0.46              |
| 1:G:66:ILE:HD12  | 1:G:66:ILE:H     | 1.79                     | 0.46              |
| 1:G:254:VAL:HG21 | 1:G:327:LEU:HD11 | 1.97                     | 0.46              |
| 1:I:143:ARG:HE   | 1:I:155:LYS:HE2  | 1.81                     | 0.46              |
| 1:O:51:LEU:HA    | 1:O:54:TYR:HB2   | 1.98                     | 0.46              |
| 1:J:194:ILE:O    | 1:J:198:VAL:HG23 | 2.16                     | 0.46              |
| 1:B:80:ILE:HA    | 1:B:103:GLY:HA2  | 1.97                     | 0.46              |
| 1:B:240:MET:HE1  | 1:B:248:TRP:CD1  | 2.50                     | 0.46              |
| 1:C:66:ILE:HA    | 1:C:69:VAL:HG22  | 1.98                     | 0.46              |
| 1:L:404:LEU:HB3  | 1:L:407:LEU:HD21 | 1.97                     | 0.46              |
| 1:I:52:ARG:NH1   | 1:I:128:SER:HA   | 2.31                     | 0.46              |
| 1:Q:38:ILE:HG23  | 1:Q:108:VAL:HG12 | 1.97                     | 0.46              |
| 2:t:98:ALA:HB3   | 2:t:114:TYR:HB2  | 1.97                     | 0.46              |
| 1:K:27:TYR:CZ    | 1:K:263:LEU:HD22 | 2.51                     | 0.46              |
| 1:K:178:GLY:HA2  | 1:K:181:ILE:HG12 | 1.97                     | 0.46              |
| 2:n:117:GLN:H    | 2:n:117:GLN:CD   | 2.24                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:153:ARG:HH22 | 1:F:183:ASP:CG   | 2.24                     | 0.46              |
| 1:H:226:ALA:O    | 1:H:230:THR:HG23 | 2.16                     | 0.46              |
| 2:i:2:VAL:HA     | 2:i:26:GLY:HA3   | 1.97                     | 0.46              |
| 1:Q:147:THR:HG21 | 1:Q:152:TYR:CE2  | 2.51                     | 0.46              |
| 1:S:194:ILE:O    | 1:S:198:VAL:HG23 | 2.16                     | 0.46              |
| 1:E:181:ILE:O    | 1:E:185:TRP:NE1  | 2.48                     | 0.46              |
| 1:M:67:ILE:HD12  | 1:M:67:ILE:H     | 1.80                     | 0.46              |
| 1:G:114:ASP:OD1  | 1:G:114:ASP:N    | 2.49                     | 0.46              |
| 1:G:355:TYR:HA   | 1:H:376:VAL:HG13 | 1.98                     | 0.46              |
| 1:J:143:ARG:CB   | 1:J:216:GLY:HA2  | 2.46                     | 0.46              |
| 2:j:117:GLN:CD   | 2:j:117:GLN:H    | 2.24                     | 0.46              |
| 1:A:244:ASP:O    | 1:A:247:THR:OG1  | 2.32                     | 0.46              |
| 1:P:230:THR:HG21 | 1:P:298:HIS:ND1  | 2.31                     | 0.46              |
| 1:L:172:GLU:H    | 1:L:172:GLU:CD   | 2.24                     | 0.46              |
| 1:L:178:GLY:C    | 1:L:180:ASP:H    | 2.24                     | 0.46              |
| 1:F:328:THR:O    | 1:F:332:LEU:HB2  | 2.16                     | 0.46              |
| 2:h:50:LYS:HG2   | 2:h:59:THR:HB    | 1.98                     | 0.46              |
| 1:J:66:ILE:HA    | 1:J:69:VAL:HG22  | 1.97                     | 0.46              |
| 1:A:136:LEU:HD22 | 1:A:163:GLN:NE2  | 2.30                     | 0.46              |
| 2:q:117:GLN:H    | 2:q:117:GLN:CD   | 2.24                     | 0.45              |
| 1:C:152:TYR:C    | 1:C:154:LYS:H    | 2.24                     | 0.45              |
| 1:T:59:LEU:HD23  | 1:T:173:PRO:HG2  | 1.99                     | 0.45              |
| 1:T:194:ILE:O    | 1:T:198:VAL:HG23 | 2.16                     | 0.45              |
| 1:F:293:LYS:O    | 1:F:294:ASN:ND2  | 2.49                     | 0.45              |
| 1:G:88:TRP:CD2   | 1:G:95:ILE:HD11  | 2.52                     | 0.45              |
| 1:H:27:TYR:CZ    | 1:H:263:LEU:HD22 | 2.51                     | 0.45              |
| 1:H:125:SER:O    | 1:H:127:THR:OG1  | 2.34                     | 0.45              |
| 1:O:141:LEU:HB3  | 1:O:182:PHE:CG   | 2.51                     | 0.45              |
| 2:b:94:TYR:O     | 2:b:118:GLY:HA2  | 2.16                     | 0.45              |
| 1:C:293:LYS:O    | 1:C:294:ASN:ND2  | 2.48                     | 0.45              |
| 1:T:78:LYS:NZ    | 1:T:79:ASP:OD1   | 2.40                     | 0.45              |
| 1:N:66:ILE:HD12  | 1:N:66:ILE:H     | 1.81                     | 0.45              |
| 2:m:98:ALA:HB3   | 2:m:114:TYR:HB2  | 1.98                     | 0.45              |
| 1:P:70:ASN:ND2   | 1:P:188:ASP:OD2  | 2.49                     | 0.45              |
| 1:P:320:ASP:OD1  | 1:P:410:LYS:NZ   | 2.48                     | 0.45              |
| 1:P:401:VAL:HG21 | 1:P:420:PHE:HB2  | 1.99                     | 0.45              |
| 1:S:422:LYS:HD2  | 1:S:422:LYS:HA   | 1.57                     | 0.45              |
| 1:E:386:ASN:O    | 1:E:387:ARG:HG2  | 2.16                     | 0.45              |
| 1:L:88:TRP:O     | 1:L:95:ILE:HG12  | 2.17                     | 0.45              |
| 2:l:51:ILE:HD11  | 2:l:56:ASP:HB3   | 1.97                     | 0.45              |
| 1:N:194:ILE:O    | 1:N:198:VAL:HG23 | 2.15                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:234:LEU:O    | 1:H:238:THR:OG1  | 2.23                     | 0.45              |
| 1:J:407:LEU:HD13 | 1:J:414:LYS:HA   | 1.97                     | 0.45              |
| 2:j:52:SER:OG    | 2:j:53:TRP:N     | 2.49                     | 0.45              |
| 1:A:157:MET:CG   | 1:A:179:ARG:HH12 | 2.29                     | 0.45              |
| 1:P:55:VAL:O     | 1:P:59:LEU:HG    | 2.16                     | 0.45              |
| 1:P:143:ARG:HD2  | 1:P:219:VAL:HG13 | 1.98                     | 0.45              |
| 1:C:52:ARG:NH1   | 1:C:128:SER:HA   | 2.31                     | 0.45              |
| 1:R:247:THR:HG21 | 1:S:350:VAL:HG23 | 1.98                     | 0.45              |
| 1:D:55:VAL:O     | 1:D:59:LEU:HB2   | 2.16                     | 0.45              |
| 1:S:376:VAL:HG12 | 2:s:103:ASN:ND2  | 2.31                     | 0.45              |
| 2:s:34:MET:HG2   | 2:s:72:ARG:NH1   | 2.30                     | 0.45              |
| 1:K:124:ALA:O    | 1:K:125:SER:OG   | 2.28                     | 0.45              |
| 1:L:8:ILE:HB     | 1:N:354:LYS:HD3  | 1.98                     | 0.45              |
| 1:M:147:THR:HG21 | 1:M:152:TYR:CD2  | 2.51                     | 0.45              |
| 2:f:5:VAL:O      | 2:f:22:CYS:HA    | 2.17                     | 0.45              |
| 1:J:242:THR:O    | 1:J:246:THR:OG1  | 2.28                     | 0.45              |
| 1:J:328:THR:HG21 | 1:J:415:TYR:HE2  | 1.81                     | 0.45              |
| 1:A:136:LEU:HB3  | 1:A:163:GLN:HE21 | 1.81                     | 0.45              |
| 1:Q:126:ARG:HD3  | 1:Q:126:ARG:HA   | 1.68                     | 0.45              |
| 2:q:100:LYS:HE3  | 1:R:353:ASN:ND2  | 2.31                     | 0.45              |
| 1:R:40:LEU:HD12  | 1:R:108:VAL:HG21 | 1.97                     | 0.45              |
| 1:S:143:ARG:HB2  | 1:S:216:GLY:HA2  | 1.99                     | 0.45              |
| 1:N:27:TYR:CZ    | 1:N:263:LEU:HD22 | 2.52                     | 0.45              |
| 1:H:86:LYS:HD3   | 1:H:86:LYS:HA    | 1.80                     | 0.45              |
| 1:O:107:LEU:O    | 1:O:274:TYR:OH   | 2.30                     | 0.45              |
| 2:c:50:LYS:HG2   | 2:c:59:THR:HB    | 1.99                     | 0.45              |
| 1:T:104:ILE:HD11 | 1:T:198:VAL:HG22 | 1.99                     | 0.45              |
| 1:K:267:GLU:OE1  | 1:K:273:SER:OG   | 2.34                     | 0.45              |
| 1:N:51:LEU:HA    | 1:N:54:TYR:HB2   | 1.99                     | 0.45              |
| 1:N:149:MET:O    | 1:N:153:ARG:HG2  | 2.17                     | 0.45              |
| 1:F:383:GLU:CD   | 1:F:387:ARG:HE   | 2.24                     | 0.45              |
| 1:G:194:ILE:O    | 1:G:198:VAL:HG23 | 2.16                     | 0.45              |
| 2:j:98:ALA:HB3   | 2:j:114:TYR:HB2  | 1.98                     | 0.45              |
| 2:p:11:LEU:HA    | 2:p:122:THR:O    | 2.17                     | 0.45              |
| 1:Q:152:TYR:CG   | 3:u:6:U:H4'      | 2.51                     | 0.45              |
| 1:R:270:LYS:HE2  | 1:R:270:LYS:HB3  | 1.81                     | 0.45              |
| 2:r:83:MET:HE1   | 2:r:121:VAL:HG11 | 1.99                     | 0.45              |
| 1:D:165:LYS:HD2  | 1:E:184:VAL:HG13 | 1.98                     | 0.45              |
| 1:S:279:ILE:HD11 | 1:S:287:SER:HB2  | 1.99                     | 0.45              |
| 1:E:83:LYS:HA    | 1:E:101:THR:HA   | 1.98                     | 0.45              |
| 1:F:53:GLY:HA3   | 1:F:123:ASP:HB3  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:151:GLU:HG3  | 1:F:154:LYS:HB2  | 1.98                     | 0.45              |
| 1:I:60:LYS:HD2   | 1:I:60:LYS:HA    | 1.69                     | 0.45              |
| 1:I:146:ARG:HH22 | 1:I:223:LYS:HE3  | 1.80                     | 0.45              |
| 2:p:17:SER:HA    | 2:p:83:MET:O     | 2.16                     | 0.45              |
| 1:C:226:ALA:O    | 1:C:230:THR:HG23 | 2.17                     | 0.45              |
| 2:e:83:MET:HE2   | 2:e:86:LEU:HD21  | 1.97                     | 0.45              |
| 1:K:124:ALA:C    | 1:K:126:ARG:H    | 2.24                     | 0.45              |
| 1:L:302:GLN:HB3  | 1:L:412:ILE:HD13 | 1.97                     | 0.45              |
| 1:F:302:GLN:HB3  | 1:F:412:ILE:HD13 | 1.98                     | 0.45              |
| 1:H:256:ASP:OD1  | 1:I:7:ARG:NH2    | 2.46                     | 0.45              |
| 1:Q:194:ILE:O    | 1:Q:198:VAL:HG23 | 2.17                     | 0.45              |
| 1:C:350:VAL:HG23 | 1:D:247:THR:HG21 | 1.99                     | 0.45              |
| 1:R:194:ILE:O    | 1:R:198:VAL:HG23 | 2.17                     | 0.45              |
| 1:L:376:VAL:HG13 | 1:M:355:TYR:HA   | 1.99                     | 0.45              |
| 2:l:37:PHE:HB3   | 2:l:45:ARG:HD3   | 1.98                     | 0.45              |
| 1:M:139:LEU:HD22 | 1:M:195:VAL:HG12 | 1.98                     | 0.45              |
| 1:M:240:MET:HE2  | 1:M:244:ASP:HB3  | 1.99                     | 0.45              |
| 1:G:206:LYS:HA   | 1:G:206:LYS:HD2  | 1.78                     | 0.45              |
| 1:I:160:LEU:HD21 | 1:I:172:GLU:HB3  | 1.98                     | 0.45              |
| 1:O:87:ASP:OD2   | 1:O:97:LYS:HG3   | 2.17                     | 0.45              |
| 1:O:147:THR:HG21 | 1:O:152:TYR:CD2  | 2.52                     | 0.45              |
| 1:A:174:LEU:HD21 | 1:A:178:GLY:HA3  | 1.98                     | 0.45              |
| 3:v:23:U:H2'     | 3:v:25:U:H5''    | 1.99                     | 0.45              |
| 1:R:104:ILE:HG23 | 1:R:105:PHE:CD2  | 2.52                     | 0.45              |
| 1:N:107:LEU:O    | 1:N:274:TYR:OH   | 2.34                     | 0.45              |
| 2:n:20:LEU:HD12  | 2:n:81:LEU:HD23  | 1.98                     | 0.45              |
| 1:B:38:ILE:HD12  | 1:B:281:PHE:O    | 2.18                     | 0.44              |
| 1:R:39:PRO:O     | 1:R:193:LYS:NZ   | 2.37                     | 0.44              |
| 1:D:137:TYR:CZ   | 1:D:173:PRO:HD2  | 2.51                     | 0.44              |
| 1:D:268:ILE:HG22 | 1:D:275:MET:HE3  | 1.99                     | 0.44              |
| 1:T:279:ILE:HD11 | 1:T:287:SER:HB2  | 1.98                     | 0.44              |
| 2:k:11:LEU:HA    | 2:k:122:THR:O    | 2.16                     | 0.44              |
| 2:k:117:GLN:CD   | 2:k:117:GLN:H    | 2.26                     | 0.44              |
| 1:G:140:GLY:HA2  | 1:G:216:GLY:HA3  | 1.99                     | 0.44              |
| 1:G:387:ARG:NH2  | 1:G:387:ARG:HB2  | 2.33                     | 0.44              |
| 1:P:137:TYR:O    | 1:P:141:LEU:HD13 | 2.17                     | 0.44              |
| 1:P:355:TYR:HA   | 1:O:376:VAL:HG13 | 1.99                     | 0.44              |
| 1:Q:7:ARG:NH2    | 1:R:256:ASP:OD1  | 2.47                     | 0.44              |
| 1:S:376:VAL:HG13 | 1:T:355:TYR:HA   | 1.99                     | 0.44              |
| 1:E:353:ASN:ND2  | 2:f:100:LYS:HE3  | 2.33                     | 0.44              |
| 1:L:159:GLY:CA   | 1:L:163:GLN:H    | 2.30                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:38:ILE:HD12  | 1:N:281:PHE:O    | 2.17                     | 0.44              |
| 1:N:172:GLU:OE2  | 1:N:172:GLU:N    | 2.34                     | 0.44              |
| 1:M:147:THR:HG21 | 1:M:152:TYR:CE2  | 2.52                     | 0.44              |
| 1:F:176:PRO:O    | 1:F:179:ARG:HG2  | 2.17                     | 0.44              |
| 1:H:230:THR:HG22 | 1:H:312:ARG:HH12 | 1.82                     | 0.44              |
| 2:h:61:ALA:O     | 2:h:65:LYS:HG3   | 2.17                     | 0.44              |
| 1:P:313:ALA:HB1  | 1:P:412:ILE:HD11 | 1.98                     | 0.44              |
| 1:B:88:TRP:CD2   | 1:B:95:ILE:HD11  | 2.51                     | 0.44              |
| 1:S:51:LEU:HD23  | 1:S:54:TYR:HD2   | 1.81                     | 0.44              |
| 1:O:223:LYS:HB3  | 1:O:279:ILE:HD11 | 1.99                     | 0.44              |
| 1:P:302:GLN:HB3  | 1:P:412:ILE:HD13 | 1.99                     | 0.44              |
| 1:Q:381:TRP:O    | 1:Q:385:GLN:HG2  | 2.16                     | 0.44              |
| 2:q:98:ALA:HB3   | 2:q:114:TYR:HB2  | 1.98                     | 0.44              |
| 1:R:156:LEU:C    | 1:R:158:ASP:H    | 2.24                     | 0.44              |
| 1:S:82:GLY:O     | 1:S:101:THR:HA   | 2.17                     | 0.44              |
| 1:E:77:LEU:HD12  | 1:E:80:ILE:HD11  | 2.00                     | 0.44              |
| 1:E:240:MET:HE2  | 1:E:244:ASP:HB3  | 1.99                     | 0.44              |
| 1:T:230:THR:HG21 | 1:T:298:HIS:ND1  | 2.33                     | 0.44              |
| 1:K:148:GLN:OE1  | 1:K:148:GLN:N    | 2.49                     | 0.44              |
| 1:L:80:ILE:HD11  | 1:L:104:ILE:HB   | 1.99                     | 0.44              |
| 2:l:68:PHE:HA    | 2:l:82:LEU:O     | 2.18                     | 0.44              |
| 1:N:45:THR:OG1   | 1:N:46:LYS:N     | 2.51                     | 0.44              |
| 1:N:180:ASP:HA   | 1:N:183:ASP:HB2  | 2.00                     | 0.44              |
| 1:F:160:LEU:HD11 | 1:F:172:GLU:HB3  | 1.99                     | 0.44              |
| 1:G:195:VAL:HB   | 1:G:217:THR:HG22 | 2.00                     | 0.44              |
| 1:H:84:LEU:HD23  | 1:H:205:PHE:HZ   | 1.82                     | 0.44              |
| 1:H:381:TRP:O    | 1:H:385:GLN:HG2  | 2.18                     | 0.44              |
| 1:I:155:LYS:O    | 1:I:158:ASP:HB3  | 2.17                     | 0.44              |
| 1:J:214:ARG:HH21 | 1:J:218:ILE:HG13 | 1.82                     | 0.44              |
| 2:q:52:SER:OG    | 2:q:53:TRP:N     | 2.50                     | 0.44              |
| 1:C:172:GLU:H    | 1:C:172:GLU:CD   | 2.24                     | 0.44              |
| 1:D:88:TRP:CD2   | 1:D:95:ILE:HD11  | 2.53                     | 0.44              |
| 1:E:324:TYR:O    | 1:E:328:THR:OG1  | 2.28                     | 0.44              |
| 1:F:154:LYS:HE3  | 1:F:157:MET:HE3  | 1.99                     | 0.44              |
| 1:G:147:THR:HG21 | 1:G:152:TYR:HE2  | 1.82                     | 0.44              |
| 1:P:126:ARG:HA   | 1:P:126:ARG:HD3  | 1.68                     | 0.44              |
| 1:R:203:HIS:ND1  | 1:R:272:ASP:OD1  | 2.48                     | 0.44              |
| 1:R:226:ALA:O    | 1:R:230:THR:HG23 | 2.18                     | 0.44              |
| 1:D:51:LEU:HB3   | 1:D:72:TYR:HB2   | 1.99                     | 0.44              |
| 2:s:37:PHE:CD2   | 2:s:45:ARG:HD3   | 2.52                     | 0.44              |
| 1:T:66:ILE:HD12  | 1:T:66:ILE:H     | 1.82                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:T:302:GLN:HB3  | 1:T:412:ILE:HD13 | 2.00                     | 0.44              |
| 1:T:324:TYR:O    | 1:T:328:THR:OG1  | 2.31                     | 0.44              |
| 1:M:96:GLY:HA3   | 1:M:102:ILE:HD11 | 2.00                     | 0.44              |
| 1:G:244:ASP:O    | 1:G:247:THR:OG1  | 2.33                     | 0.44              |
| 1:G:353:ASN:ND2  | 2:h:100:LYS:HE3  | 2.33                     | 0.44              |
| 1:H:138:LEU:O    | 1:H:191:TYR:OH   | 2.31                     | 0.44              |
| 1:O:97:LYS:HE3   | 1:O:97:LYS:HB2   | 1.85                     | 0.44              |
| 1:A:147:THR:OG1  | 1:A:153:ARG:HG2  | 2.18                     | 0.44              |
| 1:P:419:GLU:CD   | 1:Q:309:ARG:HE   | 2.25                     | 0.44              |
| 1:B:270:LYS:HE2  | 1:B:270:LYS:HB3  | 1.86                     | 0.44              |
| 1:C:332:LEU:HD22 | 1:C:393:MET:HE2  | 1.99                     | 0.44              |
| 2:l:63:SER:OG    | 2:l:89:GLU:OE2   | 2.33                     | 0.44              |
| 1:M:243:GLU:OE1  | 1:M:243:GLU:N    | 2.50                     | 0.44              |
| 2:f:12:VAL:HG21  | 2:f:86:LEU:HD12  | 2.00                     | 0.44              |
| 2:g:14:THR:N     | 2:g:124:SER:O    | 2.51                     | 0.44              |
| 1:H:42:ILE:HD11  | 1:H:71:SER:N     | 2.33                     | 0.44              |
| 1:I:149:MET:HG2  | 3:x:24:U:H1'     | 1.99                     | 0.44              |
| 1:O:384:ASP:OD1  | 2:o:54:ARG:NH2   | 2.50                     | 0.44              |
| 1:S:376:VAL:HG12 | 2:s:103:ASN:HD21 | 1.81                     | 0.44              |
| 1:E:59:LEU:HB3   | 1:E:173:PRO:O    | 2.17                     | 0.44              |
| 1:T:51:LEU:HB3   | 1:T:72:TYR:HB2   | 2.00                     | 0.44              |
| 1:G:27:TYR:CZ    | 1:G:263:LEU:HD22 | 2.52                     | 0.44              |
| 1:J:104:ILE:HG23 | 1:J:105:PHE:CD2  | 2.53                     | 0.44              |
| 1:J:177:GLU:O    | 1:J:179:ARG:N    | 2.50                     | 0.44              |
| 1:B:154:LYS:HE3  | 1:B:157:MET:HG3  | 1.99                     | 0.44              |
| 1:C:133:TRP:HB3  | 1:C:166:MET:HG3  | 1.98                     | 0.44              |
| 1:C:381:TRP:O    | 1:C:385:GLN:HG2  | 2.18                     | 0.44              |
| 1:R:152:TYR:CG   | 3:v:42:U:H4'     | 2.52                     | 0.44              |
| 1:D:257:GLU:O    | 1:D:261:MET:HG3  | 2.18                     | 0.44              |
| 1:N:52:ARG:NH1   | 1:N:128:SER:HA   | 2.33                     | 0.44              |
| 1:N:355:TYR:HA   | 1:M:376:VAL:HG13 | 2.00                     | 0.44              |
| 1:M:143:ARG:HB2  | 1:M:216:GLY:HA2  | 1.99                     | 0.44              |
| 1:J:153:ARG:HE   | 1:J:179:ARG:HD2  | 1.83                     | 0.44              |
| 1:C:286:LYS:NZ   | 3:w:11:U:H5'     | 2.33                     | 0.43              |
| 1:R:142:TYR:O    | 1:R:146:ARG:HG3  | 2.18                     | 0.43              |
| 2:e:6:GLU:HA     | 2:e:21:SER:O     | 2.18                     | 0.43              |
| 1:K:114:ASP:OD1  | 1:K:114:ASP:N    | 2.50                     | 0.43              |
| 1:K:401:VAL:HG21 | 1:K:420:PHE:HB2  | 2.00                     | 0.43              |
| 1:L:52:ARG:NH1   | 1:L:128:SER:HA   | 2.33                     | 0.43              |
| 1:O:194:ILE:O    | 1:O:198:VAL:HG23 | 2.17                     | 0.43              |
| 1:O:324:TYR:O    | 1:O:328:THR:HG23 | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:P:52:ARG:HE    | 1:P:131:ASP:CG   | 2.25                     | 0.43              |
| 1:P:165:LYS:HA   | 1:O:184:VAL:HG21 | 2.00                     | 0.43              |
| 1:P:269:ASP:OD1  | 1:P:269:ASP:N    | 2.50                     | 0.43              |
| 2:p:99:THR:HG22  | 2:p:100:LYS:O    | 2.18                     | 0.43              |
| 2:b:11:LEU:HA    | 2:b:122:THR:O    | 2.18                     | 0.43              |
| 1:Q:142:TYR:O    | 1:Q:146:ARG:HG3  | 2.17                     | 0.43              |
| 1:R:87:ASP:OD1   | 1:R:98:ALA:N     | 2.51                     | 0.43              |
| 2:s:17:SER:HA    | 2:s:83:MET:O     | 2.17                     | 0.43              |
| 2:l:117:GLN:H    | 2:l:117:GLN:CD   | 2.26                     | 0.43              |
| 1:N:336:TYR:CG   | 1:N:393:MET:HG2  | 2.53                     | 0.43              |
| 1:F:244:ASP:O    | 1:F:247:THR:OG1  | 2.34                     | 0.43              |
| 1:C:194:ILE:O    | 1:C:198:VAL:HG23 | 2.18                     | 0.43              |
| 1:D:143:ARG:HB2  | 1:D:216:GLY:HA2  | 2.00                     | 0.43              |
| 1:D:302:GLN:OE1  | 1:D:312:ARG:NH1  | 2.50                     | 0.43              |
| 1:S:302:GLN:OE1  | 1:S:312:ARG:NH1  | 2.51                     | 0.43              |
| 1:T:52:ARG:NH1   | 1:T:128:SER:HA   | 2.33                     | 0.43              |
| 1:T:177:GLU:O    | 1:T:177:GLU:HG2  | 2.18                     | 0.43              |
| 1:G:248:TRP:CE2  | 1:G:375:VAL:HG22 | 2.53                     | 0.43              |
| 1:J:303:LEU:HD22 | 1:J:328:THR:HG22 | 1.99                     | 0.43              |
| 1:A:117:LEU:HA   | 1:A:118:PRO:HD3  | 1.89                     | 0.43              |
| 1:B:21:ASN:OD1   | 1:B:21:ASN:N     | 2.52                     | 0.43              |
| 2:q:47:PHE:HE1   | 2:q:50:LYS:HB3   | 1.83                     | 0.43              |
| 1:S:211:ALA:O    | 1:S:214:ARG:HG2  | 2.18                     | 0.43              |
| 1:S:226:ALA:O    | 1:S:230:THR:HG23 | 2.18                     | 0.43              |
| 2:s:5:VAL:O      | 2:s:22:CYS:HA    | 2.18                     | 0.43              |
| 1:E:143:ARG:CB   | 1:E:216:GLY:HA2  | 2.49                     | 0.43              |
| 1:K:126:ARG:HA   | 1:K:126:ARG:HD3  | 1.74                     | 0.43              |
| 1:K:308:LEU:O    | 1:K:310:SER:N    | 2.50                     | 0.43              |
| 1:L:155:LYS:HD3  | 1:L:155:LYS:HA   | 1.91                     | 0.43              |
| 2:m:36:TRP:HE1   | 2:m:79:VAL:HG22  | 1.83                     | 0.43              |
| 1:H:57:GLN:OE1   | 1:H:122:SER:N    | 2.50                     | 0.43              |
| 1:J:165:LYS:HZ2  | 1:A:184:VAL:CA   | 2.29                     | 0.43              |
| 1:Q:277:TYR:O    | 1:Q:281:PHE:HB2  | 2.19                     | 0.43              |
| 1:C:66:ILE:HD12  | 1:C:66:ILE:H     | 1.83                     | 0.43              |
| 1:C:88:TRP:CE2   | 1:C:95:ILE:HD11  | 2.53                     | 0.43              |
| 1:C:240:MET:SD   | 1:C:334:TYR:OH   | 2.69                     | 0.43              |
| 1:R:318:GLN:O    | 1:R:410:LYS:NZ   | 2.40                     | 0.43              |
| 1:S:160:LEU:HD11 | 1:S:172:GLU:HB3  | 2.01                     | 0.43              |
| 1:T:173:PRO:O    | 1:T:174:LEU:HD22 | 2.19                     | 0.43              |
| 1:K:86:LYS:HD3   | 1:K:86:LYS:HA    | 1.80                     | 0.43              |
| 1:F:359:ASP:OD1  | 1:F:359:ASP:N    | 2.49                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:27:TYR:CZ    | 1:A:263:LEU:HD22 | 2.53                     | 0.43              |
| 1:A:123:ASP:OD1  | 1:A:124:ALA:N    | 2.52                     | 0.43              |
| 1:P:39:PRO:O     | 1:P:193:LYS:NZ   | 2.51                     | 0.43              |
| 1:B:87:ASP:OD1   | 1:B:98:ALA:N     | 2.52                     | 0.43              |
| 1:B:152:TYR:OH   | 3:w:8:U:OP2      | 2.32                     | 0.43              |
| 1:B:309:ARG:HB2  | 1:C:324:TYR:HB2  | 2.01                     | 0.43              |
| 1:D:158:ASP:OD1  | 1:D:159:GLY:N    | 2.51                     | 0.43              |
| 2:d:117:GLN:CD   | 2:d:117:GLN:H    | 2.26                     | 0.43              |
| 1:L:143:ARG:HG3  | 1:L:219:VAL:HG11 | 1.99                     | 0.43              |
| 1:F:194:ILE:O    | 1:F:198:VAL:HG23 | 2.18                     | 0.43              |
| 2:g:51:ILE:HD11  | 2:g:56:ASP:HB3   | 1.99                     | 0.43              |
| 1:H:52:ARG:NH1   | 1:H:128:SER:HA   | 2.33                     | 0.43              |
| 1:C:126:ARG:NE   | 1:C:130:ASP:OD2  | 2.42                     | 0.43              |
| 1:S:137:TYR:O    | 1:S:141:LEU:HD13 | 2.18                     | 0.43              |
| 1:E:401:VAL:HG21 | 1:E:420:PHE:HB2  | 2.00                     | 0.43              |
| 1:T:140:GLY:HA2  | 1:T:216:GLY:HA3  | 2.01                     | 0.43              |
| 1:T:158:ASP:HB2  | 1:T:215:TYR:OH   | 2.18                     | 0.43              |
| 1:K:260:GLN:OE1  | 1:K:294:ASN:ND2  | 2.48                     | 0.43              |
| 1:F:336:TYR:CG   | 1:F:393:MET:HG2  | 2.53                     | 0.43              |
| 1:F:408:ARG:O    | 1:F:411:THR:OG1  | 2.28                     | 0.43              |
| 1:G:158:ASP:O    | 1:G:162:ASN:CB   | 2.52                     | 0.43              |
| 1:H:359:ASP:OD1  | 1:H:359:ASP:N    | 2.49                     | 0.43              |
| 1:J:122:SER:OG   | 1:J:123:ASP:N    | 2.50                     | 0.43              |
| 1:A:164:CYS:HB3  | 1:A:170:GLN:HB3  | 2.00                     | 0.43              |
| 1:P:293:LYS:O    | 1:P:294:ASN:ND2  | 2.52                     | 0.43              |
| 2:b:14:THR:HG23  | 2:b:88:PRO:HD3   | 2.01                     | 0.43              |
| 2:b:50:LYS:HG2   | 2:b:59:THR:HB    | 2.01                     | 0.43              |
| 1:C:308:LEU:HD11 | 1:C:335:ALA:HA   | 2.00                     | 0.43              |
| 2:s:12:VAL:O     | 2:s:123:VAL:HA   | 2.19                     | 0.43              |
| 1:T:126:ARG:HA   | 1:T:126:ARG:HD3  | 1.69                     | 0.43              |
| 1:K:223:LYS:NZ   | 1:K:280:ASP:OD1  | 2.47                     | 0.43              |
| 1:N:263:LEU:HA   | 1:N:264:PRO:HD3  | 1.86                     | 0.43              |
| 1:H:55:VAL:HG23  | 1:H:134:LEU:HD21 | 2.01                     | 0.43              |
| 1:I:364:LEU:HG   | 1:I:366:THR:HG23 | 2.00                     | 0.43              |
| 1:O:152:TYR:CG   | 3:u:24:U:H4'     | 2.54                     | 0.43              |
| 1:A:104:ILE:HG23 | 1:A:105:PHE:CD2  | 2.54                     | 0.43              |
| 1:P:23:ASP:N     | 1:P:24:PRO:HD3   | 2.34                     | 0.43              |
| 1:R:179:ARG:HA   | 1:R:182:PHE:CZ   | 2.54                     | 0.43              |
| 2:s:51:ILE:HD13  | 2:s:72:ARG:HG2   | 2.01                     | 0.43              |
| 2:e:50:LYS:HG2   | 2:e:59:THR:HB    | 2.01                     | 0.43              |
| 1:K:224:ASP:HB2  | 1:K:279:ILE:HG13 | 2.01                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:m:83:MET:HB3   | 2:m:86:LEU:HD21  | 2.01                     | 0.43              |
| 1:O:408:ARG:HD3  | 3:u:24:U:C4      | 2.54                     | 0.43              |
| 2:o:99:THR:HG22  | 2:o:100:LYS:O    | 2.19                     | 0.43              |
| 1:Q:362:GLY:HA3  | 2:q:75:ALA:HB2   | 2.01                     | 0.43              |
| 1:C:261:MET:HE1  | 1:C:297:PHE:CD1  | 2.54                     | 0.43              |
| 1:C:278:LEU:HD12 | 1:C:284:SER:HB3  | 2.00                     | 0.43              |
| 1:C:324:TYR:O    | 1:C:328:THR:OG1  | 2.24                     | 0.43              |
| 2:d:49:ALA:HA    | 2:d:59:THR:O     | 2.18                     | 0.43              |
| 1:K:83:LYS:HE2   | 1:K:83:LYS:HB3   | 1.79                     | 0.43              |
| 1:K:143:ARG:CB   | 1:K:216:GLY:HA2  | 2.47                     | 0.43              |
| 2:k:51:ILE:HD11  | 2:k:56:ASP:HB3   | 2.01                     | 0.43              |
| 2:n:67:ARG:NH1   | 2:n:90:ASP:OD2   | 2.37                     | 0.43              |
| 1:M:21:ASN:OD1   | 1:M:21:ASN:N     | 2.52                     | 0.43              |
| 1:F:139:LEU:HD22 | 1:F:195:VAL:HG12 | 2.01                     | 0.43              |
| 1:H:172:GLU:OE2  | 1:H:172:GLU:N    | 2.31                     | 0.43              |
| 1:O:42:ILE:HG22  | 1:O:44:THR:HG23  | 2.00                     | 0.43              |
| 1:O:230:THR:HG21 | 1:O:298:HIS:ND1  | 2.34                     | 0.43              |
| 1:J:328:THR:HG21 | 1:J:415:TYR:CE2  | 2.54                     | 0.43              |
| 1:A:80:ILE:O     | 1:A:81:ARG:NH1   | 2.44                     | 0.43              |
| 1:B:158:ASP:HB3  | 1:B:215:TYR:OH   | 2.19                     | 0.42              |
| 1:R:184:VAL:HG13 | 1:S:165:LYS:HD2  | 2.00                     | 0.42              |
| 1:E:72:TYR:OH    | 1:E:131:ASP:OD1  | 2.29                     | 0.42              |
| 1:T:328:THR:O    | 1:T:332:LEU:HB2  | 2.19                     | 0.42              |
| 1:K:164:CYS:HA   | 1:K:167:ILE:O    | 2.18                     | 0.42              |
| 1:L:43:ASN:ND2   | 1:L:117:LEU:HD11 | 2.34                     | 0.42              |
| 1:L:336:TYR:OH   | 1:L:392:ASP:OD2  | 2.21                     | 0.42              |
| 1:N:143:ARG:HH11 | 1:N:216:GLY:H    | 1.67                     | 0.42              |
| 2:n:100:LYS:HE3  | 1:O:353:ASN:HD22 | 1.82                     | 0.42              |
| 1:M:226:ALA:O    | 1:M:230:THR:HG23 | 2.19                     | 0.42              |
| 1:F:147:THR:HG21 | 1:F:152:TYR:HE2  | 1.84                     | 0.42              |
| 2:r:100:LYS:HE3  | 1:S:353:ASN:ND2  | 2.34                     | 0.42              |
| 2:s:83:MET:HB3   | 2:s:86:LEU:HD21  | 2.01                     | 0.42              |
| 1:E:241:SER:OG   | 1:E:243:GLU:HG2  | 2.19                     | 0.42              |
| 2:f:117:GLN:CD   | 2:f:117:GLN:H    | 2.27                     | 0.42              |
| 2:i:117:GLN:H    | 2:i:117:GLN:CD   | 2.27                     | 0.42              |
| 1:O:223:LYS:HD3  | 1:O:279:ILE:CD1  | 2.49                     | 0.42              |
| 1:B:89:SER:O     | 1:B:270:LYS:NZ   | 2.52                     | 0.42              |
| 1:C:140:GLY:HA2  | 1:C:216:GLY:HA3  | 2.01                     | 0.42              |
| 1:C:167:ILE:HG22 | 1:C:169:GLU:H    | 1.83                     | 0.42              |
| 1:R:162:ASN:HA   | 1:R:165:LYS:HD3  | 2.01                     | 0.42              |
| 1:K:130:ASP:O    | 1:K:134:LEU:HB2  | 2.19                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:N:51:LEU:HD23  | 1:N:54:TYR:HD2   | 1.84                     | 0.42              |
| 1:N:202:PHE:HB2  | 1:N:214:ARG:HG3  | 2.01                     | 0.42              |
| 1:J:226:ALA:O    | 1:J:230:THR:HG23 | 2.19                     | 0.42              |
| 2:j:83:MET:HE2   | 2:j:86:LEU:HD21  | 2.02                     | 0.42              |
| 1:Q:66:ILE:HA    | 1:Q:69:VAL:HG22  | 2.01                     | 0.42              |
| 1:C:74:TYR:O     | 1:C:78:LYS:N     | 2.52                     | 0.42              |
| 1:C:137:TYR:CZ   | 1:C:173:PRO:HD2  | 2.54                     | 0.42              |
| 1:D:88:TRP:CE2   | 1:D:95:ILE:HD11  | 2.54                     | 0.42              |
| 1:L:304:THR:HG21 | 1:L:334:TYR:CD2  | 2.55                     | 0.42              |
| 1:F:353:ASN:ND2  | 2:g:100:LYS:HE3  | 2.34                     | 0.42              |
| 2:h:38:ARG:HG2   | 2:h:48:VAL:HG13  | 2.01                     | 0.42              |
| 2:h:67:ARG:NH1   | 2:h:90:ASP:OD2   | 2.35                     | 0.42              |
| 2:h:83:MET:HB3   | 2:h:86:LEU:HD21  | 2.01                     | 0.42              |
| 1:O:381:TRP:O    | 1:O:385:GLN:HG2  | 2.19                     | 0.42              |
| 2:b:5:VAL:O      | 2:b:22:CYS:HA    | 2.20                     | 0.42              |
| 1:R:309:ARG:N    | 1:R:309:ARG:HD2  | 2.34                     | 0.42              |
| 1:D:353:ASN:HD22 | 2:e:100:LYS:HE3  | 1.84                     | 0.42              |
| 1:D:398:LYS:HG3  | 1:D:421:ASP:HA   | 2.01                     | 0.42              |
| 1:S:263:LEU:HA   | 1:S:264:PRO:HD3  | 1.90                     | 0.42              |
| 2:e:112:PHE:O    | 2:e:115:TRP:NE1  | 2.52                     | 0.42              |
| 1:K:230:THR:HG21 | 1:K:298:HIS:ND1  | 2.35                     | 0.42              |
| 2:k:83:MET:HE2   | 2:k:86:LEU:HD21  | 2.01                     | 0.42              |
| 2:m:34:MET:HG2   | 2:m:72:ARG:NH1   | 2.34                     | 0.42              |
| 1:F:172:GLU:OE2  | 1:F:172:GLU:N    | 2.27                     | 0.42              |
| 1:I:141:LEU:HD12 | 1:I:182:PHE:CE2  | 2.54                     | 0.42              |
| 1:I:354:LYS:HD3  | 1:A:8:ILE:HB     | 2.00                     | 0.42              |
| 1:A:172:GLU:H    | 1:A:172:GLU:CD   | 2.27                     | 0.42              |
| 2:a:50:LYS:NZ    | 2:a:105:GLY:O    | 2.30                     | 0.42              |
| 2:p:94:TYR:O     | 2:p:118:GLY:HA2  | 2.20                     | 0.42              |
| 1:E:135:PRO:O    | 1:E:139:LEU:HG   | 2.20                     | 0.42              |
| 2:n:33:ILE:HG12  | 2:n:52:SER:HA    | 2.01                     | 0.42              |
| 2:m:48:VAL:HG23  | 2:m:49:ALA:H     | 1.85                     | 0.42              |
| 1:F:242:THR:O    | 1:F:246:THR:OG1  | 2.29                     | 0.42              |
| 1:F:381:TRP:O    | 1:F:385:GLN:HG2  | 2.20                     | 0.42              |
| 1:H:248:TRP:CD1  | 1:H:375:VAL:HG22 | 2.54                     | 0.42              |
| 1:B:194:ILE:O    | 1:B:198:VAL:HG23 | 2.19                     | 0.42              |
| 1:B:298:HIS:O    | 1:B:302:GLN:HB2  | 2.20                     | 0.42              |
| 1:R:142:TYR:HB2  | 1:R:191:TYR:CE2  | 2.55                     | 0.42              |
| 1:R:159:GLY:CA   | 1:R:163:GLN:HB2  | 2.50                     | 0.42              |
| 1:R:187:ASN:CG   | 1:S:165:LYS:HZ3  | 2.26                     | 0.42              |
| 1:D:377:GLU:OE2  | 2:d:27:ARG:NH1   | 2.53                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:t:11:LEU:HA    | 2:t:122:THR:O    | 2.20                     | 0.42              |
| 1:I:52:ARG:HD2   | 1:I:130:ASP:HB2  | 2.01                     | 0.42              |
| 1:P:359:ASP:OD1  | 1:P:359:ASP:N    | 2.49                     | 0.42              |
| 1:C:38:ILE:HD11  | 1:C:281:PHE:O    | 2.19                     | 0.42              |
| 1:C:152:TYR:OH   | 3:w:17:U:OP2     | 2.32                     | 0.42              |
| 1:D:175:VAL:C    | 1:D:177:GLU:H    | 2.27                     | 0.42              |
| 2:s:67:ARG:NH1   | 2:s:90:ASP:OD2   | 2.37                     | 0.42              |
| 1:T:143:ARG:HG3  | 1:T:219:VAL:HG11 | 2.02                     | 0.42              |
| 1:N:226:ALA:O    | 1:N:230:THR:HG23 | 2.20                     | 0.42              |
| 1:F:52:ARG:NH1   | 1:F:128:SER:HA   | 2.35                     | 0.42              |
| 3:x:17:U:O2'     | 3:x:19:U:OP2     | 2.29                     | 0.42              |
| 1:P:84:LEU:HD11  | 1:P:96:GLY:HA3   | 2.02                     | 0.42              |
| 1:P:244:ASP:O    | 1:P:247:THR:OG1  | 2.38                     | 0.42              |
| 1:B:56:TYR:O     | 1:B:60:LYS:HG2   | 2.20                     | 0.42              |
| 1:Q:230:THR:HG21 | 1:Q:298:HIS:ND1  | 2.35                     | 0.42              |
| 1:T:142:TYR:O    | 1:T:146:ARG:HG3  | 2.20                     | 0.42              |
| 2:t:100:LYS:HE3  | 1:K:353:ASN:HD22 | 1.84                     | 0.42              |
| 1:H:141:LEU:HD12 | 1:H:182:PHE:CE2  | 2.54                     | 0.42              |
| 2:h:117:GLN:CD   | 2:h:117:GLN:H    | 2.28                     | 0.42              |
| 1:O:404:LEU:HD23 | 1:O:404:LEU:HA   | 1.96                     | 0.42              |
| 1:P:42:ILE:HD12  | 1:P:42:ILE:HA    | 1.88                     | 0.42              |
| 1:P:153:ARG:HD2  | 1:P:153:ARG:HA   | 1.75                     | 0.42              |
| 1:B:51:LEU:HB3   | 1:B:72:TYR:HB2   | 2.02                     | 0.42              |
| 2:q:99:THR:HG22  | 2:q:100:LYS:O    | 2.20                     | 0.42              |
| 1:R:97:LYS:HB2   | 1:R:97:LYS:HE3   | 1.81                     | 0.42              |
| 1:S:242:THR:O    | 1:S:246:THR:OG1  | 2.36                     | 0.42              |
| 2:t:83:MET:HE1   | 2:t:121:VAL:HG11 | 2.01                     | 0.42              |
| 1:K:181:ILE:HD13 | 1:K:181:ILE:HA   | 1.90                     | 0.42              |
| 2:k:1:GLN:HG2    | 2:k:2:VAL:H      | 1.84                     | 0.42              |
| 1:M:104:ILE:HA   | 1:M:201:PHE:CD1  | 2.54                     | 0.42              |
| 1:M:110:LEU:C    | 1:M:111:LYS:HD2  | 2.45                     | 0.42              |
| 1:M:278:LEU:HD12 | 1:M:284:SER:HB3  | 2.01                     | 0.42              |
| 1:F:401:VAL:HG21 | 1:F:420:PHE:HB2  | 2.00                     | 0.42              |
| 1:H:88:TRP:CD2   | 1:H:95:ILE:HD11  | 2.55                     | 0.42              |
| 1:I:145:GLY:HA2  | 1:I:179:ARG:NH2  | 2.35                     | 0.42              |
| 1:O:135:PRO:HB2  | 1:O:213:PHE:CE2  | 2.55                     | 0.42              |
| 1:O:257:GLU:O    | 1:O:261:MET:HG3  | 2.19                     | 0.42              |
| 2:o:2:VAL:HA     | 2:o:26:GLY:HA3   | 2.02                     | 0.42              |
| 2:a:117:GLN:CD   | 2:a:117:GLN:H    | 2.27                     | 0.42              |
| 1:R:157:MET:HE2  | 1:R:157:MET:HB3  | 1.97                     | 0.41              |
| 2:d:52:SER:OG    | 2:d:53:TRP:N     | 2.54                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:s:99:THR:HG22  | 2:s:100:LYS:O    | 2.20                     | 0.41              |
| 1:K:287:SER:HA   | 1:K:288:PRO:HD3  | 1.93                     | 0.41              |
| 1:L:175:VAL:HG23 | 1:L:178:GLY:HA3  | 2.01                     | 0.41              |
| 1:F:277:TYR:O    | 1:F:281:PHE:HB2  | 2.20                     | 0.41              |
| 1:G:268:ILE:HD11 | 1:H:17:LYS:HG3   | 2.01                     | 0.41              |
| 1:I:70:ASN:ND2   | 1:I:188:ASP:OD2  | 2.39                     | 0.41              |
| 1:I:124:ALA:C    | 1:I:126:ARG:H    | 2.28                     | 0.41              |
| 1:J:52:ARG:NH1   | 1:J:128:SER:HA   | 2.35                     | 0.41              |
| 1:J:143:ARG:NH2  | 3:x:36:U:OP2     | 2.50                     | 0.41              |
| 1:J:350:VAL:C    | 1:J:352:ASP:H    | 2.28                     | 0.41              |
| 1:A:65:SER:OG    | 1:A:118:PRO:HG2  | 2.19                     | 0.41              |
| 1:A:88:TRP:CE2   | 1:A:95:ILE:HD11  | 2.55                     | 0.41              |
| 1:P:135:PRO:O    | 1:P:139:LEU:HG   | 2.20                     | 0.41              |
| 1:Q:52:ARG:NH1   | 1:Q:128:SER:HA   | 2.35                     | 0.41              |
| 1:Q:148:GLN:OE1  | 1:Q:153:ARG:NH1  | 2.54                     | 0.41              |
| 1:E:350:VAL:HG23 | 1:F:247:THR:HG21 | 2.02                     | 0.41              |
| 1:M:408:ARG:NH2  | 3:u:43:U:OP1     | 2.41                     | 0.41              |
| 1:G:125:SER:O    | 1:G:126:ARG:NE   | 2.52                     | 0.41              |
| 1:I:18:LEU:HD23  | 1:I:18:LEU:HA    | 1.93                     | 0.41              |
| 1:O:140:GLY:HA2  | 1:O:216:GLY:HA3  | 2.02                     | 0.41              |
| 1:J:228:LEU:HB2  | 1:J:289:TYR:HB3  | 2.02                     | 0.41              |
| 2:j:5:VAL:O      | 2:j:22:CYS:HA    | 2.19                     | 0.41              |
| 2:j:14:THR:N     | 2:j:124:SER:O    | 2.52                     | 0.41              |
| 1:B:135:PRO:HB2  | 1:B:213:PHE:HE2  | 1.86                     | 0.41              |
| 1:D:62:GLY:HA2   | 1:D:181:ILE:HD11 | 2.00                     | 0.41              |
| 2:s:50:LYS:HG2   | 2:s:59:THR:HB    | 2.02                     | 0.41              |
| 1:E:146:ARG:NH2  | 1:E:223:LYS:HE2  | 2.35                     | 0.41              |
| 1:E:228:LEU:HB2  | 1:E:289:TYR:HB3  | 2.02                     | 0.41              |
| 1:T:137:TYR:CZ   | 1:T:173:PRO:HD2  | 2.55                     | 0.41              |
| 1:M:152:TYR:CG   | 3:u:42:U:H4'     | 2.54                     | 0.41              |
| 2:m:117:GLN:CD   | 2:m:117:GLN:H    | 2.28                     | 0.41              |
| 1:F:77:LEU:O     | 1:F:80:ILE:HG22  | 2.21                     | 0.41              |
| 1:F:368:ALA:O    | 2:f:102:TYR:OH   | 2.28                     | 0.41              |
| 2:f:33:ILE:HG12  | 2:f:52:SER:HA    | 2.02                     | 0.41              |
| 1:I:66:ILE:HD12  | 1:I:66:ILE:H     | 1.85                     | 0.41              |
| 1:I:104:ILE:HG23 | 1:I:105:PHE:CD2  | 2.55                     | 0.41              |
| 1:I:304:THR:HG21 | 1:I:334:TYR:CD2  | 2.55                     | 0.41              |
| 2:i:83:MET:HE1   | 2:i:121:VAL:HG11 | 2.01                     | 0.41              |
| 1:A:387:ARG:NH2  | 1:A:387:ARG:HB2  | 2.35                     | 0.41              |
| 3:x:43:U:H2'     | 3:x:44:U:O4'     | 2.20                     | 0.41              |
| 1:P:321:ASP:OD1  | 1:P:321:ASP:N    | 2.53                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:377:GLU:OE2  | 2:b:27:ARG:NH1   | 2.53                     | 0.41              |
| 1:Q:412:ILE:HA   | 1:Q:415:TYR:HB3  | 2.02                     | 0.41              |
| 1:C:72:TYR:OH    | 1:C:131:ASP:OD1  | 2.24                     | 0.41              |
| 1:C:104:ILE:HG23 | 1:C:105:PHE:CD2  | 2.55                     | 0.41              |
| 1:C:328:THR:HG21 | 1:C:415:TYR:HE2  | 1.85                     | 0.41              |
| 1:D:323:GLU:HB2  | 1:D:327:LEU:HD23 | 2.03                     | 0.41              |
| 1:S:104:ILE:HG23 | 1:S:105:PHE:CD2  | 2.55                     | 0.41              |
| 1:S:377:GLU:OE2  | 2:s:27:ARG:NH1   | 2.53                     | 0.41              |
| 1:T:42:ILE:CD1   | 1:T:74:TYR:HB2   | 2.50                     | 0.41              |
| 1:K:244:ASP:O    | 1:K:247:THR:OG1  | 2.36                     | 0.41              |
| 1:L:174:LEU:HD21 | 1:L:178:GLY:O    | 2.21                     | 0.41              |
| 1:L:230:THR:HG21 | 1:L:298:HIS:ND1  | 2.35                     | 0.41              |
| 2:l:67:ARG:NH1   | 2:l:90:ASP:OD2   | 2.39                     | 0.41              |
| 1:H:97:LYS:HE3   | 1:H:97:LYS:HB2   | 1.85                     | 0.41              |
| 1:I:25:VAL:HG21  | 1:I:260:GLN:NE2  | 2.36                     | 0.41              |
| 1:I:143:ARG:HB2  | 1:I:216:GLY:HA2  | 2.03                     | 0.41              |
| 1:O:254:VAL:HG13 | 1:O:297:PHE:HD2  | 1.86                     | 0.41              |
| 1:O:359:ASP:OD1  | 1:O:359:ASP:N    | 2.49                     | 0.41              |
| 1:J:172:GLU:H    | 1:J:172:GLU:CD   | 2.26                     | 0.41              |
| 1:A:165:LYS:HE2  | 1:A:165:LYS:HB3  | 1.82                     | 0.41              |
| 1:A:270:LYS:HE2  | 1:A:270:LYS:HB3  | 1.90                     | 0.41              |
| 1:Q:86:LYS:HD3   | 1:Q:86:LYS:HA    | 1.79                     | 0.41              |
| 1:C:21:ASN:OD1   | 1:C:21:ASN:N     | 2.54                     | 0.41              |
| 2:c:49:ALA:HA    | 2:c:59:THR:O     | 2.21                     | 0.41              |
| 1:E:368:ALA:O    | 2:e:102:TYR:OH   | 2.26                     | 0.41              |
| 1:T:152:TYR:C    | 1:T:154:LYS:H    | 2.28                     | 0.41              |
| 1:N:159:GLY:O    | 1:N:163:GLN:HG2  | 2.20                     | 0.41              |
| 1:M:270:LYS:HE2  | 1:M:270:LYS:HB3  | 1.87                     | 0.41              |
| 1:F:298:HIS:O    | 1:F:302:GLN:HB2  | 2.20                     | 0.41              |
| 1:G:381:TRP:O    | 1:G:385:GLN:HG2  | 2.20                     | 0.41              |
| 2:i:99:THR:HG22  | 2:i:100:LYS:O    | 2.19                     | 0.41              |
| 1:O:42:ILE:HD11  | 1:O:194:ILE:HD11 | 2.01                     | 0.41              |
| 3:w:17:U:O2'     | 3:w:19:U:OP2     | 2.30                     | 0.41              |
| 1:B:381:TRP:O    | 1:B:385:GLN:HG2  | 2.21                     | 0.41              |
| 1:S:133:TRP:HB2  | 1:S:163:GLN:OE1  | 2.20                     | 0.41              |
| 1:S:206:LYS:HD2  | 1:S:206:LYS:HA   | 1.83                     | 0.41              |
| 1:S:401:VAL:HG23 | 1:S:421:ASP:HB2  | 2.03                     | 0.41              |
| 1:T:172:GLU:H    | 1:T:172:GLU:CD   | 2.28                     | 0.41              |
| 1:L:157:MET:HA   | 1:L:160:LEU:HB2  | 2.01                     | 0.41              |
| 1:L:366:THR:HB   | 2:l:53:TRP:CZ3   | 2.55                     | 0.41              |
| 1:F:88:TRP:CE2   | 1:F:95:ILE:HD11  | 2.56                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:123:ASP:OD1  | 1:G:125:SER:OG   | 2.33                     | 0.41              |
| 1:J:152:TYR:CG   | 3:x:33:U:H4'     | 2.56                     | 0.41              |
| 1:A:133:TRP:HB3  | 1:A:166:MET:SD   | 2.61                     | 0.41              |
| 1:Q:226:ALA:O    | 1:Q:230:THR:HG23 | 2.21                     | 0.41              |
| 1:D:86:LYS:HA    | 1:D:86:LYS:HD3   | 1.87                     | 0.41              |
| 1:D:155:LYS:NZ   | 1:D:155:LYS:HB3  | 2.35                     | 0.41              |
| 1:D:324:TYR:O    | 1:D:328:THR:OG1  | 2.38                     | 0.41              |
| 1:T:220:SER:OG   | 1:T:280:ASP:OD2  | 2.25                     | 0.41              |
| 1:K:157:MET:HA   | 1:K:160:LEU:HB2  | 2.03                     | 0.41              |
| 1:K:254:VAL:HG21 | 1:K:327:LEU:HD11 | 2.03                     | 0.41              |
| 1:N:377:GLU:OE2  | 2:n:27:ARG:NH1   | 2.54                     | 0.41              |
| 1:N:408:ARG:O    | 1:N:411:THR:OG1  | 2.30                     | 0.41              |
| 1:M:110:LEU:HD13 | 1:M:110:LEU:HA   | 1.89                     | 0.41              |
| 1:M:248:TRP:CD1  | 1:M:375:VAL:HG22 | 2.56                     | 0.41              |
| 1:F:226:ALA:O    | 1:F:230:THR:HG23 | 2.21                     | 0.41              |
| 1:I:51:LEU:HA    | 1:I:54:TYR:HB2   | 2.02                     | 0.41              |
| 1:I:174:LEU:HD23 | 1:I:178:GLY:HA3  | 2.02                     | 0.41              |
| 1:O:22:GLU:HB3   | 1:O:24:PRO:HD3   | 2.03                     | 0.41              |
| 1:O:114:ASP:OD1  | 1:O:114:ASP:N    | 2.48                     | 0.41              |
| 1:J:240:MET:HB2  | 1:J:245:VAL:HG23 | 2.03                     | 0.41              |
| 1:A:153:ARG:NH1  | 1:A:179:ARG:O    | 2.54                     | 0.41              |
| 3:v:29:U:H2'     | 3:v:30:U:O4'     | 2.20                     | 0.41              |
| 2:p:91:THR:HG23  | 2:p:122:THR:HA   | 2.02                     | 0.41              |
| 1:B:67:ILE:HD12  | 1:B:67:ILE:H     | 1.86                     | 0.41              |
| 1:C:87:ASP:OD2   | 1:C:97:LYS:HG3   | 2.21                     | 0.41              |
| 2:r:32:SER:OG    | 2:r:99:THR:O     | 2.22                     | 0.41              |
| 1:S:86:LYS:HD3   | 1:S:86:LYS:HA    | 1.90                     | 0.41              |
| 1:S:302:GLN:HB3  | 1:S:412:ILE:HD13 | 2.02                     | 0.41              |
| 1:K:66:ILE:HD12  | 1:K:66:ILE:H     | 1.84                     | 0.41              |
| 1:N:236:LYS:HB3  | 1:M:321:ASP:HB3  | 2.03                     | 0.41              |
| 2:n:83:MET:HB3   | 2:n:86:LEU:HD21  | 2.02                     | 0.41              |
| 1:H:302:GLN:NE2  | 1:H:313:ALA:HA   | 2.36                     | 0.41              |
| 1:H:362:GLY:HA3  | 2:h:75:ALA:HB2   | 2.02                     | 0.41              |
| 2:i:60:TYR:CE1   | 2:i:70:ILE:HG22  | 2.56                     | 0.41              |
| 1:J:177:GLU:C    | 1:J:179:ARG:H    | 2.28                     | 0.41              |
| 1:A:86:LYS:HD3   | 1:A:86:LYS:HA    | 1.89                     | 0.41              |
| 1:A:104:ILE:O    | 1:A:107:LEU:HG   | 2.21                     | 0.41              |
| 3:u:23:U:H2'     | 3:u:25:U:H5''    | 2.02                     | 0.41              |
| 1:P:73:LEU:HD23  | 1:P:73:LEU:HA    | 1.97                     | 0.41              |
| 1:B:107:LEU:O    | 1:B:274:TYR:OH   | 2.34                     | 0.41              |
| 1:B:175:VAL:HG23 | 1:B:177:GLU:H    | 1.86                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:419:GLU:OE2  | 1:A:309:ARG:NE   | 2.51                     | 0.41              |
| 1:Q:68:HIS:NE2   | 1:Q:118:PRO:HG2  | 2.36                     | 0.41              |
| 1:C:27:TYR:CZ    | 1:C:263:LEU:HD22 | 2.56                     | 0.41              |
| 1:C:158:ASP:HB3  | 1:C:215:TYR:OH   | 2.20                     | 0.41              |
| 1:C:336:TYR:CG   | 1:C:393:MET:HG2  | 2.56                     | 0.41              |
| 1:R:143:ARG:HB2  | 1:R:216:GLY:HA2  | 2.03                     | 0.41              |
| 1:R:240:MET:HB2  | 1:R:245:VAL:HG23 | 2.03                     | 0.41              |
| 1:R:377:GLU:OE2  | 2:r:27:ARG:NH1   | 2.53                     | 0.41              |
| 2:r:101:ALA:C    | 2:r:103:ASN:H    | 2.29                     | 0.41              |
| 2:d:20:LEU:HD12  | 2:d:81:LEU:HD23  | 2.02                     | 0.41              |
| 1:S:126:ARG:HA   | 1:S:126:ARG:HD3  | 1.81                     | 0.41              |
| 1:T:153:ARG:HD2  | 1:T:179:ARG:HD2  | 2.03                     | 0.41              |
| 1:L:6:LYS:HB3    | 1:L:6:LYS:HE2    | 1.87                     | 0.41              |
| 1:N:157:MET:HE2  | 1:N:157:MET:HB3  | 1.94                     | 0.41              |
| 1:M:52:ARG:NH1   | 1:M:128:SER:HA   | 2.36                     | 0.41              |
| 1:M:368:ALA:O    | 2:m:102:TYR:OH   | 2.31                     | 0.41              |
| 2:m:37:PHE:CD2   | 2:m:45:ARG:HD3   | 2.56                     | 0.41              |
| 1:F:327:LEU:HD13 | 1:F:327:LEU:HA   | 1.90                     | 0.41              |
| 1:G:143:ARG:HB3  | 1:G:216:GLY:HA2  | 2.03                     | 0.41              |
| 1:H:54:TYR:CE1   | 1:H:121:VAL:HG21 | 2.56                     | 0.41              |
| 1:H:175:VAL:O    | 1:H:176:PRO:C    | 2.63                     | 0.41              |
| 1:H:419:GLU:O    | 1:H:422:LYS:NZ   | 2.40                     | 0.41              |
| 2:h:2:VAL:HG23   | 2:h:25:SER:O     | 2.21                     | 0.41              |
| 1:I:145:GLY:HA2  | 1:I:179:ARG:HH22 | 1.86                     | 0.41              |
| 2:i:78:MET:HE2   | 2:i:78:MET:HB3   | 1.95                     | 0.41              |
| 1:O:6:LYS:NZ     | 1:O:11:ASN:O     | 2.50                     | 0.41              |
| 1:J:55:VAL:O     | 1:J:59:LEU:HG    | 2.20                     | 0.41              |
| 1:A:408:ARG:NH2  | 3:x:43:U:OP1     | 2.38                     | 0.41              |
| 2:p:86:LEU:HB3   | 2:p:123:VAL:HG21 | 2.03                     | 0.41              |
| 1:B:152:TYR:C    | 1:B:154:LYS:H    | 2.28                     | 0.41              |
| 2:b:60:TYR:CE1   | 2:b:70:ILE:HG22  | 2.56                     | 0.41              |
| 1:D:304:THR:HG21 | 1:D:334:TYR:CD2  | 2.56                     | 0.41              |
| 1:D:336:TYR:CG   | 1:D:393:MET:HG2  | 2.56                     | 0.41              |
| 1:S:323:GLU:O    | 1:S:327:LEU:HD23 | 2.21                     | 0.41              |
| 1:E:158:ASP:O    | 1:E:161:THR:HG22 | 2.20                     | 0.41              |
| 1:T:80:ILE:HD12  | 1:T:80:ILE:HA    | 1.86                     | 0.41              |
| 1:L:66:ILE:HA    | 1:L:69:VAL:HG22  | 2.02                     | 0.41              |
| 1:L:270:LYS:HE2  | 1:L:270:LYS:HB3  | 1.86                     | 0.41              |
| 1:F:117:LEU:HD23 | 1:F:117:LEU:HA   | 1.91                     | 0.41              |
| 1:G:97:LYS:HE3   | 1:G:97:LYS:HB2   | 1.82                     | 0.41              |
| 1:H:199:ASP:HB2  | 1:H:217:THR:HB   | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:250:LEU:HD22 | 1:J:379:LEU:HD21 | 2.02                     | 0.41              |
| 1:A:175:VAL:HB   | 1:A:177:GLU:O    | 2.21                     | 0.41              |
| 1:A:376:VAL:HG12 | 2:a:103:ASN:OD1  | 2.21                     | 0.41              |
| 3:w:23:U:O2'     | 3:w:25:U:OP1     | 2.36                     | 0.41              |
| 1:P:226:ALA:O    | 1:P:230:THR:HG23 | 2.21                     | 0.40              |
| 1:B:250:LEU:HD22 | 1:B:379:LEU:HD21 | 2.03                     | 0.40              |
| 1:B:269:ASP:OD1  | 1:B:269:ASP:N    | 2.51                     | 0.40              |
| 1:C:268:ILE:HG22 | 1:C:275:MET:HE3  | 2.02                     | 0.40              |
| 2:c:68:PHE:HA    | 2:c:82:LEU:O     | 2.21                     | 0.40              |
| 1:R:52:ARG:HH11  | 1:R:131:ASP:CG   | 2.29                     | 0.40              |
| 1:R:135:PRO:O    | 1:R:139:LEU:HG   | 2.21                     | 0.40              |
| 1:N:89:SER:O     | 1:N:270:LYS:NZ   | 2.54                     | 0.40              |
| 1:N:130:ASP:O    | 1:N:134:LEU:HB2  | 2.21                     | 0.40              |
| 1:G:18:LEU:HD23  | 1:G:18:LEU:HA    | 1.96                     | 0.40              |
| 1:H:81:ARG:HG2   | 1:H:103:GLY:HA2  | 2.02                     | 0.40              |
| 1:H:344:LEU:HD22 | 1:I:330:ALA:HB2  | 2.03                     | 0.40              |
| 1:A:323:GLU:HB2  | 1:A:327:LEU:HD23 | 2.03                     | 0.40              |
| 1:P:260:GLN:OE1  | 1:P:294:ASN:ND2  | 2.46                     | 0.40              |
| 2:p:52:SER:OG    | 2:p:53:TRP:N     | 2.54                     | 0.40              |
| 1:Q:88:TRP:CE2   | 1:Q:95:ILE:HD11  | 2.57                     | 0.40              |
| 1:S:244:ASP:O    | 1:S:247:THR:OG1  | 2.37                     | 0.40              |
| 1:E:175:VAL:C    | 1:E:177:GLU:H    | 2.28                     | 0.40              |
| 1:K:167:ILE:HG12 | 1:K:169:GLU:H    | 1.85                     | 0.40              |
| 1:L:153:ARG:C    | 1:L:155:LYS:N    | 2.80                     | 0.40              |
| 1:M:67:ILE:O     | 1:M:71:SER:HB2   | 2.20                     | 0.40              |
| 1:M:143:ARG:CB   | 1:M:216:GLY:HA2  | 2.51                     | 0.40              |
| 1:F:270:LYS:HE2  | 1:F:270:LYS:HB3  | 1.85                     | 0.40              |
| 2:o:5:VAL:O      | 2:o:22:CYS:HA    | 2.21                     | 0.40              |
| 1:J:153:ARG:NE   | 1:J:179:ARG:HD2  | 2.37                     | 0.40              |
| 1:B:35:SER:OG    | 1:B:37:GLU:O     | 2.38                     | 0.40              |
| 1:B:147:THR:HG21 | 1:B:155:LYS:NZ   | 2.37                     | 0.40              |
| 1:K:41:TYR:HB2   | 1:K:190:ASN:HD21 | 1.86                     | 0.40              |
| 1:K:79:ASP:HA    | 1:K:81:ARG:HE    | 1.85                     | 0.40              |
| 1:L:75:GLY:HA2   | 1:L:78:LYS:HE3   | 2.03                     | 0.40              |
| 1:L:152:TYR:OH   | 3:v:8:U:OP2      | 2.31                     | 0.40              |
| 1:L:287:SER:HA   | 1:L:288:PRO:HD3  | 1.98                     | 0.40              |
| 1:N:40:LEU:HD12  | 1:N:108:VAL:HG21 | 2.03                     | 0.40              |
| 1:M:327:LEU:HD13 | 1:M:327:LEU:HA   | 1.92                     | 0.40              |
| 2:h:36:TRP:HD1   | 2:h:70:ILE:HD12  | 1.86                     | 0.40              |
| 2:h:73:ASP:HB3   | 2:h:76:SER:HB3   | 2.03                     | 0.40              |
| 1:I:165:LYS:HD2  | 1:J:184:VAL:HA   | 2.03                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:199:ASP:OD2  | 1:I:277:TYR:OH   | 2.34                     | 0.40              |
| 1:O:88:TRP:CE2   | 1:O:95:ILE:HD11  | 2.56                     | 0.40              |
| 1:O:363:GLY:O    | 1:O:365:THR:N    | 2.54                     | 0.40              |
| 1:A:39:PRO:O     | 1:A:193:LYS:NZ   | 2.45                     | 0.40              |
| 3:u:1:U:O4'      | 3:v:45:U:H2'     | 2.21                     | 0.40              |
| 1:C:287:SER:HA   | 1:C:288:PRO:HD3  | 1.95                     | 0.40              |
| 2:c:52:SER:OG    | 2:c:53:TRP:N     | 2.55                     | 0.40              |
| 1:T:401:VAL:HG21 | 1:T:420:PHE:HB2  | 2.03                     | 0.40              |
| 1:N:215:TYR:HD2  | 3:u:36:U:C6      | 2.39                     | 0.40              |
| 1:N:270:LYS:HE2  | 1:N:270:LYS:HB3  | 1.93                     | 0.40              |
| 1:G:153:ARG:NH1  | 1:G:183:ASP:OD1  | 2.55                     | 0.40              |
| 1:J:172:GLU:OE2  | 1:J:172:GLU:N    | 2.38                     | 0.40              |
| 1:A:141:LEU:HD12 | 1:A:182:PHE:CZ   | 2.56                     | 0.40              |
| 1:P:200:MET:HE1  | 1:P:274:TYR:CD2  | 2.57                     | 0.40              |
| 1:B:408:ARG:O    | 1:B:411:THR:OG1  | 2.26                     | 0.40              |
| 1:C:41:TYR:HD1   | 1:C:111:LYS:HB2  | 1.85                     | 0.40              |
| 1:R:323:GLU:O    | 1:R:327:LEU:HD23 | 2.22                     | 0.40              |
| 1:S:23:ASP:N     | 1:S:24:PRO:HD3   | 2.36                     | 0.40              |
| 1:T:226:ALA:O    | 1:T:230:THR:HG23 | 2.22                     | 0.40              |
| 2:k:61:ALA:O     | 2:k:65:LYS:HG3   | 2.21                     | 0.40              |
| 2:l:11:LEU:HA    | 2:l:122:THR:O    | 2.22                     | 0.40              |
| 1:M:141:LEU:HD12 | 1:M:182:PHE:CD2  | 2.56                     | 0.40              |
| 1:M:254:VAL:HG21 | 1:M:327:LEU:HD11 | 2.04                     | 0.40              |
| 1:G:149:MET:HE2  | 1:G:149:MET:HB2  | 1.96                     | 0.40              |
| 1:H:299:PHE:HZ   | 1:H:415:TYR:CE2  | 2.40                     | 0.40              |
| 2:h:99:THR:HG22  | 2:h:100:LYS:O    | 2.20                     | 0.40              |
| 2:i:29:PHE:HB2   | 2:i:74:ASN:ND2   | 2.37                     | 0.40              |
| 1:J:135:PRO:O    | 1:J:139:LEU:HG   | 2.21                     | 0.40              |
| 1:A:111:LYS:HB3  | 1:A:112:ALA:H    | 1.62                     | 0.40              |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:Q:81:ARG:NH1 | 1:L:87:ASP:OD2[1_565] | 2.15                     | 0.05              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 410/422 (97%) | 388 (95%) | 22 (5%) | 0        | 100         | 100 |
| 1   | B     | 406/422 (96%) | 372 (92%) | 32 (8%) | 2 (0%)   | 24          | 59  |
| 1   | C     | 411/422 (97%) | 384 (93%) | 26 (6%) | 1 (0%)   | 43          | 73  |
| 1   | D     | 414/422 (98%) | 383 (92%) | 28 (7%) | 3 (1%)   | 18          | 52  |
| 1   | E     | 409/422 (97%) | 379 (93%) | 29 (7%) | 1 (0%)   | 43          | 73  |
| 1   | F     | 419/422 (99%) | 387 (92%) | 27 (6%) | 5 (1%)   | 10          | 42  |
| 1   | G     | 412/422 (98%) | 379 (92%) | 32 (8%) | 1 (0%)   | 43          | 73  |
| 1   | H     | 416/422 (99%) | 384 (92%) | 29 (7%) | 3 (1%)   | 18          | 52  |
| 1   | I     | 411/422 (97%) | 385 (94%) | 26 (6%) | 0        | 100         | 100 |
| 1   | J     | 416/422 (99%) | 385 (92%) | 28 (7%) | 3 (1%)   | 18          | 52  |
| 1   | K     | 419/422 (99%) | 387 (92%) | 30 (7%) | 2 (0%)   | 24          | 59  |
| 1   | L     | 419/422 (99%) | 388 (93%) | 28 (7%) | 3 (1%)   | 18          | 52  |
| 1   | M     | 412/422 (98%) | 379 (92%) | 33 (8%) | 0        | 100         | 100 |
| 1   | N     | 414/422 (98%) | 386 (93%) | 26 (6%) | 2 (0%)   | 24          | 59  |
| 1   | O     | 416/422 (99%) | 389 (94%) | 26 (6%) | 1 (0%)   | 43          | 73  |
| 1   | P     | 410/422 (97%) | 388 (95%) | 21 (5%) | 1 (0%)   | 43          | 73  |
| 1   | Q     | 415/422 (98%) | 394 (95%) | 20 (5%) | 1 (0%)   | 43          | 73  |
| 1   | R     | 415/422 (98%) | 381 (92%) | 34 (8%) | 0        | 100         | 100 |
| 1   | S     | 419/422 (99%) | 389 (93%) | 29 (7%) | 1 (0%)   | 43          | 73  |
| 1   | T     | 419/422 (99%) | 392 (94%) | 26 (6%) | 1 (0%)   | 43          | 73  |
| 2   | a     | 123/139 (88%) | 115 (94%) | 8 (6%)  | 0        | 100         | 100 |
| 2   | b     | 123/139 (88%) | 120 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 2   | c     | 123/139 (88%) | 119 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 2   | d     | 123/139 (88%) | 118 (96%) | 4 (3%)  | 1 (1%)   | 16          | 50  |
| 2   | e     | 123/139 (88%) | 116 (94%) | 7 (6%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 2   | f     | 123/139 (88%)     | 119 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 2   | g     | 123/139 (88%)     | 117 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 2   | h     | 123/139 (88%)     | 117 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 2   | i     | 123/139 (88%)     | 119 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 2   | j     | 123/139 (88%)     | 119 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 2   | k     | 123/139 (88%)     | 118 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 2   | l     | 123/139 (88%)     | 116 (94%)   | 7 (6%)   | 0        | 100         | 100 |
| 2   | m     | 123/139 (88%)     | 115 (94%)   | 8 (6%)   | 0        | 100         | 100 |
| 2   | n     | 123/139 (88%)     | 117 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 2   | o     | 123/139 (88%)     | 118 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 2   | p     | 123/139 (88%)     | 118 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| 2   | q     | 123/139 (88%)     | 117 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 2   | r     | 123/139 (88%)     | 119 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 2   | s     | 123/139 (88%)     | 117 (95%)   | 6 (5%)   | 0        | 100         | 100 |
| 2   | t     | 123/139 (88%)     | 118 (96%)   | 5 (4%)   | 0        | 100         | 100 |
| All | All   | 10742/11220 (96%) | 10051 (94%) | 659 (6%) | 32 (0%)  | 36          | 68  |

All (32) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | d     | 2   | VAL  |
| 1   | L     | 367 | ASN  |
| 1   | N     | 121 | VAL  |
| 1   | N     | 178 | GLY  |
| 1   | F     | 121 | VAL  |
| 1   | H     | 176 | PRO  |
| 1   | D     | 350 | VAL  |
| 1   | L     | 363 | GLY  |
| 1   | G     | 207 | LYS  |
| 1   | J     | 79  | ASP  |
| 1   | T     | 121 | VAL  |
| 1   | H     | 150 | PRO  |
| 1   | O     | 364 | LEU  |
| 1   | P     | 22  | GLU  |
| 1   | D     | 22  | GLU  |
| 1   | K     | 22  | GLU  |
| 1   | J     | 178 | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 177 | GLU  |
| 1   | E     | 364 | LEU  |
| 1   | K     | 172 | GLU  |
| 1   | F     | 22  | GLU  |
| 1   | B     | 80  | ILE  |
| 1   | Q     | 74  | TYR  |
| 1   | L     | 121 | VAL  |
| 1   | F     | 178 | GLY  |
| 1   | F     | 323 | GLU  |
| 1   | S     | 150 | PRO  |
| 1   | J     | 350 | VAL  |
| 1   | B     | 150 | PRO  |
| 1   | F     | 181 | ILE  |
| 1   | C     | 350 | VAL  |
| 1   | H     | 181 | ILE  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | A     | 358/363 (99%)  | 356 (99%)  | 2 (1%)   | 78          | 84  |
| 1   | B     | 356/363 (98%)  | 356 (100%) | 0        | 100         | 100 |
| 1   | C     | 359/363 (99%)  | 359 (100%) | 0        | 100         | 100 |
| 1   | D     | 360/363 (99%)  | 360 (100%) | 0        | 100         | 100 |
| 1   | E     | 356/363 (98%)  | 356 (100%) | 0        | 100         | 100 |
| 1   | F     | 362/363 (100%) | 362 (100%) | 0        | 100         | 100 |
| 1   | G     | 358/363 (99%)  | 358 (100%) | 0        | 100         | 100 |
| 1   | H     | 361/363 (99%)  | 361 (100%) | 0        | 100         | 100 |
| 1   | I     | 358/363 (99%)  | 358 (100%) | 0        | 100         | 100 |
| 1   | J     | 362/363 (100%) | 362 (100%) | 0        | 100         | 100 |
| 1   | K     | 362/363 (100%) | 361 (100%) | 1 (0%)   | 86          | 88  |
| 1   | L     | 362/363 (100%) | 362 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 1   | M     | 358/363 (99%)   | 358 (100%)  | 0        | 100         | 100 |
| 1   | N     | 360/363 (99%)   | 360 (100%)  | 0        | 100         | 100 |
| 1   | O     | 362/363 (100%)  | 362 (100%)  | 0        | 100         | 100 |
| 1   | P     | 357/363 (98%)   | 357 (100%)  | 0        | 100         | 100 |
| 1   | Q     | 361/363 (99%)   | 361 (100%)  | 0        | 100         | 100 |
| 1   | R     | 361/363 (99%)   | 361 (100%)  | 0        | 100         | 100 |
| 1   | S     | 362/363 (100%)  | 362 (100%)  | 0        | 100         | 100 |
| 1   | T     | 362/363 (100%)  | 362 (100%)  | 0        | 100         | 100 |
| 2   | a     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | b     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | c     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | d     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | e     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | f     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | g     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | h     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | i     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | j     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | k     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | l     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | m     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | n     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | o     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | p     | 101/111 (91%)   | 100 (99%)   | 1 (1%)   | 68          | 80  |
| 2   | q     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | r     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | s     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| 2   | t     | 101/111 (91%)   | 101 (100%)  | 0        | 100         | 100 |
| All | All   | 9217/9480 (97%) | 9213 (100%) | 4 (0%)   | 100         | 100 |

All (4) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | p     | 79  | VAL  |
| 1   | K     | 25  | VAL  |
| 1   | A     | 156 | LEU  |
| 1   | A     | 160 | LEU  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | P     | 190 | ASN  |
| 2   | p     | 31  | ASN  |
| 2   | p     | 74  | ASN  |
| 1   | B     | 68  | HIS  |
| 1   | B     | 260 | GLN  |
| 2   | b     | 31  | ASN  |
| 2   | b     | 120 | GLN  |
| 1   | Q     | 187 | ASN  |
| 1   | Q     | 294 | ASN  |
| 1   | Q     | 367 | ASN  |
| 1   | Q     | 386 | ASN  |
| 2   | q     | 31  | ASN  |
| 1   | C     | 11  | ASN  |
| 1   | C     | 190 | ASN  |
| 1   | C     | 208 | HIS  |
| 1   | C     | 294 | ASN  |
| 1   | C     | 385 | GLN  |
| 2   | c     | 1   | GLN  |
| 2   | c     | 31  | ASN  |
| 1   | R     | 68  | HIS  |
| 1   | R     | 190 | ASN  |
| 1   | R     | 367 | ASN  |
| 2   | r     | 31  | ASN  |
| 1   | D     | 385 | GLN  |
| 2   | d     | 31  | ASN  |
| 1   | S     | 163 | GLN  |
| 1   | S     | 190 | ASN  |
| 2   | s     | 13  | GLN  |
| 2   | s     | 31  | ASN  |
| 1   | E     | 294 | ASN  |
| 1   | E     | 315 | ASN  |
| 2   | e     | 31  | ASN  |
| 2   | e     | 120 | GLN  |
| 1   | T     | 170 | GLN  |
| 2   | t     | 31  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 57  | GLN  |
| 1   | K     | 162 | ASN  |
| 1   | K     | 260 | GLN  |
| 1   | K     | 294 | ASN  |
| 1   | K     | 367 | ASN  |
| 2   | k     | 31  | ASN  |
| 2   | k     | 77  | ASN  |
| 2   | k     | 103 | ASN  |
| 1   | L     | 11  | ASN  |
| 1   | L     | 190 | ASN  |
| 1   | L     | 294 | ASN  |
| 2   | l     | 31  | ASN  |
| 1   | N     | 163 | GLN  |
| 1   | N     | 260 | GLN  |
| 1   | N     | 294 | ASN  |
| 1   | N     | 367 | ASN  |
| 2   | n     | 13  | GLN  |
| 2   | n     | 31  | ASN  |
| 2   | n     | 120 | GLN  |
| 1   | M     | 43  | ASN  |
| 1   | M     | 148 | GLN  |
| 1   | M     | 190 | ASN  |
| 1   | M     | 294 | ASN  |
| 2   | m     | 31  | ASN  |
| 1   | F     | 162 | ASN  |
| 1   | F     | 163 | GLN  |
| 1   | F     | 170 | GLN  |
| 1   | F     | 190 | ASN  |
| 1   | F     | 367 | ASN  |
| 1   | F     | 386 | ASN  |
| 1   | F     | 405 | GLN  |
| 2   | f     | 74  | ASN  |
| 2   | f     | 120 | GLN  |
| 1   | G     | 168 | ASN  |
| 1   | G     | 386 | ASN  |
| 2   | g     | 74  | ASN  |
| 1   | H     | 11  | ASN  |
| 2   | h     | 13  | GLN  |
| 2   | h     | 31  | ASN  |
| 1   | I     | 187 | ASN  |
| 1   | I     | 190 | ASN  |
| 1   | I     | 367 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | i     | 31  | ASN  |
| 1   | O     | 163 | GLN  |
| 1   | O     | 367 | ASN  |
| 1   | O     | 385 | GLN  |
| 2   | o     | 13  | GLN  |
| 2   | o     | 74  | ASN  |
| 1   | J     | 251 | ASN  |
| 1   | J     | 294 | ASN  |
| 2   | j     | 74  | ASN  |
| 1   | A     | 163 | GLN  |
| 1   | A     | 187 | ASN  |
| 1   | A     | 294 | ASN  |
| 1   | A     | 315 | ASN  |
| 2   | a     | 31  | ASN  |
| 2   | a     | 39  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed      | Backbone Outliers | Pucker Outliers |
|-----|-------|---------------|-------------------|-----------------|
| 3   | u     | 44/45 (97%)   | 15 (34%)          | 0               |
| 3   | v     | 44/45 (97%)   | 14 (31%)          | 0               |
| 3   | w     | 44/45 (97%)   | 15 (34%)          | 0               |
| 3   | x     | 44/45 (97%)   | 13 (29%)          | 0               |
| All | All   | 176/180 (97%) | 57 (32%)          | 0               |

All (57) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | u     | 3   | U    |
| 3   | u     | 5   | U    |
| 3   | u     | 11  | U    |
| 3   | u     | 12  | U    |
| 3   | u     | 14  | U    |
| 3   | u     | 15  | U    |
| 3   | u     | 23  | U    |
| 3   | u     | 24  | U    |
| 3   | u     | 25  | U    |
| 3   | u     | 30  | U    |
| 3   | u     | 32  | U    |
| 3   | u     | 33  | U    |
| 3   | u     | 38  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | u     | 41  | U    |
| 3   | u     | 42  | U    |
| 3   | v     | 2   | U    |
| 3   | v     | 3   | U    |
| 3   | v     | 5   | U    |
| 3   | v     | 11  | U    |
| 3   | v     | 12  | U    |
| 3   | v     | 14  | U    |
| 3   | v     | 15  | U    |
| 3   | v     | 24  | U    |
| 3   | v     | 25  | U    |
| 3   | v     | 30  | U    |
| 3   | v     | 32  | U    |
| 3   | v     | 33  | U    |
| 3   | v     | 38  | U    |
| 3   | v     | 41  | U    |
| 3   | w     | 3   | U    |
| 3   | w     | 5   | U    |
| 3   | w     | 12  | U    |
| 3   | w     | 14  | U    |
| 3   | w     | 15  | U    |
| 3   | w     | 21  | U    |
| 3   | w     | 23  | U    |
| 3   | w     | 24  | U    |
| 3   | w     | 25  | U    |
| 3   | w     | 30  | U    |
| 3   | w     | 32  | U    |
| 3   | w     | 33  | U    |
| 3   | w     | 38  | U    |
| 3   | w     | 41  | U    |
| 3   | w     | 42  | U    |
| 3   | x     | 3   | U    |
| 3   | x     | 5   | U    |
| 3   | x     | 11  | U    |
| 3   | x     | 12  | U    |
| 3   | x     | 14  | U    |
| 3   | x     | 15  | U    |
| 3   | x     | 16  | U    |
| 3   | x     | 24  | U    |
| 3   | x     | 25  | U    |
| 3   | x     | 32  | U    |
| 3   | x     | 33  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | x     | 39  | U    |
| 3   | x     | 41  | U    |

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 oligosaccharides 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 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed      | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1   | A     | 416/422 (98%) | 0.03   | 2 (0%) 87 76 | 35, 55, 77, 101       | 0     |
| 1   | B     | 412/422 (97%) | 0.08   | 3 (0%) 84 69 | 36, 64, 85, 93        | 0     |
| 1   | C     | 417/422 (98%) | 0.09   | 6 (1%) 73 54 | 39, 63, 82, 99        | 0     |
| 1   | D     | 418/422 (99%) | 0.06   | 3 (0%) 84 69 | 35, 61, 79, 100       | 0     |
| 1   | E     | 413/422 (97%) | 0.01   | 4 (0%) 79 63 | 34, 56, 77, 89        | 0     |
| 1   | F     | 421/422 (99%) | 0.07   | 6 (1%) 73 54 | 34, 54, 78, 91        | 0     |
| 1   | G     | 416/422 (98%) | 0.04   | 2 (0%) 87 76 | 36, 60, 83, 97        | 0     |
| 1   | H     | 420/422 (99%) | 0.12   | 4 (0%) 79 63 | 34, 64, 85, 93        | 0     |
| 1   | I     | 415/422 (98%) | -0.05  | 2 (0%) 87 76 | 35, 56, 76, 100       | 0     |
| 1   | J     | 420/422 (99%) | 0.02   | 3 (0%) 84 69 | 35, 56, 78, 91        | 0     |
| 1   | K     | 421/422 (99%) | -0.04  | 4 (0%) 79 63 | 34, 55, 76, 85        | 0     |
| 1   | L     | 421/422 (99%) | -0.06  | 4 (0%) 79 63 | 35, 53, 73, 87        | 0     |
| 1   | M     | 416/422 (98%) | 0.21   | 8 (1%) 66 46 | 36, 62, 85, 108       | 0     |
| 1   | N     | 418/422 (99%) | -0.00  | 3 (0%) 84 69 | 37, 60, 82, 96        | 0     |
| 1   | O     | 420/422 (99%) | 0.00   | 7 (1%) 69 49 | 34, 51, 74, 94        | 0     |
| 1   | P     | 414/422 (98%) | -0.02  | 6 (1%) 73 54 | 35, 57, 77, 99        | 0     |
| 1   | Q     | 419/422 (99%) | 0.04   | 4 (0%) 79 63 | 35, 57, 75, 94        | 0     |
| 1   | R     | 419/422 (99%) | 0.05   | 6 (1%) 73 54 | 36, 63, 82, 100       | 0     |
| 1   | S     | 421/422 (99%) | 0.06   | 2 (0%) 87 76 | 36, 61, 83, 101       | 0     |
| 1   | T     | 421/422 (99%) | -0.05  | 1 (0%) 91 85 | 34, 53, 75, 95        | 0     |
| 2   | a     | 125/139 (89%) | -0.07  | 0 100 100    | 35, 51, 66, 75        | 0     |
| 2   | b     | 125/139 (89%) | -0.17  | 0 100 100    | 40, 53, 69, 78        | 0     |
| 2   | c     | 125/139 (89%) | -0.13  | 0 100 100    | 40, 55, 69, 76        | 0     |
| 2   | d     | 125/139 (89%) | -0.13  | 0 100 100    | 39, 52, 65, 76        | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|---------------|-----------------------|-------|
| 2   | e     | 125/139 (89%)     | -0.18  | 0 100 100     | 38, 50, 65, 74        | 0     |
| 2   | f     | 125/139 (89%)     | -0.13  | 0 100 100     | 38, 52, 66, 73        | 0     |
| 2   | g     | 125/139 (89%)     | -0.14  | 0 100 100     | 40, 53, 67, 75        | 0     |
| 2   | h     | 125/139 (89%)     | -0.16  | 1 (0%) 82 67  | 38, 50, 68, 74        | 0     |
| 2   | i     | 125/139 (89%)     | -0.15  | 1 (0%) 82 67  | 37, 48, 67, 78        | 0     |
| 2   | j     | 125/139 (89%)     | -0.11  | 0 100 100     | 35, 49, 62, 70        | 0     |
| 2   | k     | 125/139 (89%)     | -0.25  | 0 100 100     | 37, 48, 66, 76        | 0     |
| 2   | l     | 125/139 (89%)     | -0.19  | 0 100 100     | 38, 51, 65, 79        | 0     |
| 2   | m     | 125/139 (89%)     | -0.09  | 0 100 100     | 39, 53, 68, 76        | 0     |
| 2   | n     | 125/139 (89%)     | -0.20  | 0 100 100     | 41, 54, 71, 79        | 0     |
| 2   | o     | 125/139 (89%)     | 0.01   | 0 100 100     | 37, 51, 64, 73        | 0     |
| 2   | p     | 125/139 (89%)     | -0.19  | 0 100 100     | 37, 51, 68, 76        | 0     |
| 2   | q     | 125/139 (89%)     | -0.15  | 0 100 100     | 37, 50, 70, 78        | 0     |
| 2   | r     | 125/139 (89%)     | -0.18  | 0 100 100     | 40, 53, 65, 83        | 0     |
| 2   | s     | 125/139 (89%)     | -0.20  | 1 (0%) 82 67  | 35, 50, 66, 79        | 0     |
| 2   | t     | 125/139 (89%)     | -0.06  | 1 (0%) 82 67  | 35, 47, 63, 69        | 0     |
| 3   | u     | 45/45 (100%)      | -0.39  | 0 100 100     | 44, 56, 68, 74        | 0     |
| 3   | v     | 45/45 (100%)      | -0.44  | 0 100 100     | 42, 54, 65, 76        | 0     |
| 3   | w     | 45/45 (100%)      | -0.42  | 0 100 100     | 44, 58, 71, 75        | 0     |
| 3   | x     | 45/45 (100%)      | -0.54  | 0 100 100     | 45, 52, 65, 71        | 0     |
| All | All   | 11038/11400 (96%) | -0.02  | 84 (0%) 82 67 | 34, 55, 79, 108       | 0     |

All (84) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | O     | 178 | GLY  | 6.1  |
| 1   | P     | 180 | ASP  | 4.9  |
| 1   | P     | 160 | LEU  | 4.2  |
| 1   | K     | 180 | ASP  | 3.6  |
| 1   | I     | 8   | ILE  | 3.4  |
| 1   | F     | 364 | LEU  | 3.4  |
| 1   | T     | 178 | GLY  | 3.4  |
| 1   | B     | 364 | LEU  | 3.3  |
| 1   | C     | 120 | GLY  | 3.2  |
| 2   | h     | 48  | VAL  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | K     | 364 | LEU  | 3.2  |
| 1   | O     | 364 | LEU  | 3.1  |
| 1   | H     | 152 | TYR  | 3.1  |
| 1   | P     | 63  | ASN  | 3.0  |
| 1   | O     | 159 | GLY  | 3.0  |
| 1   | F     | 178 | GLY  | 2.9  |
| 1   | A     | 363 | GLY  | 2.9  |
| 1   | F     | 166 | MET  | 2.9  |
| 1   | J     | 2   | SER  | 2.9  |
| 1   | M     | 121 | VAL  | 2.8  |
| 1   | E     | 166 | MET  | 2.8  |
| 1   | P     | 363 | GLY  | 2.7  |
| 1   | G     | 178 | GLY  | 2.7  |
| 1   | H     | 176 | PRO  | 2.7  |
| 1   | F     | 176 | PRO  | 2.7  |
| 1   | O     | 175 | VAL  | 2.7  |
| 1   | P     | 161 | THR  | 2.6  |
| 1   | M     | 68  | HIS  | 2.6  |
| 1   | Q     | 364 | LEU  | 2.6  |
| 1   | J     | 364 | LEU  | 2.6  |
| 1   | S     | 104 | ILE  | 2.6  |
| 1   | R     | 43  | ASN  | 2.6  |
| 1   | O     | 158 | ASP  | 2.6  |
| 1   | B     | 178 | GLY  | 2.5  |
| 1   | C     | 364 | LEU  | 2.5  |
| 1   | H     | 43  | ASN  | 2.5  |
| 1   | E     | 364 | LEU  | 2.5  |
| 1   | F     | 363 | GLY  | 2.5  |
| 1   | I     | 364 | LEU  | 2.5  |
| 1   | L     | 160 | LEU  | 2.4  |
| 1   | Q     | 158 | ASP  | 2.4  |
| 1   | C     | 117 | LEU  | 2.4  |
| 1   | N     | 364 | LEU  | 2.4  |
| 2   | s     | 1   | GLN  | 2.4  |
| 1   | M     | 173 | PRO  | 2.4  |
| 1   | Q     | 178 | GLY  | 2.3  |
| 1   | R     | 118 | PRO  | 2.3  |
| 1   | M     | 178 | GLY  | 2.3  |
| 1   | K     | 57  | GLN  | 2.3  |
| 1   | C     | 211 | ALA  | 2.3  |
| 1   | Q     | 8   | ILE  | 2.3  |
| 1   | C     | 45  | THR  | 2.3  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 349 | CYS  | 2.3  |
| 1   | M     | 363 | GLY  | 2.3  |
| 1   | N     | 365 | THR  | 2.2  |
| 1   | R     | 364 | LEU  | 2.2  |
| 1   | F     | 362 | GLY  | 2.2  |
| 1   | L     | 166 | MET  | 2.2  |
| 1   | S     | 175 | VAL  | 2.2  |
| 2   | t     | 48  | VAL  | 2.2  |
| 1   | L     | 164 | CYS  | 2.2  |
| 1   | R     | 45  | THR  | 2.2  |
| 1   | P     | 175 | VAL  | 2.2  |
| 1   | H     | 54  | TYR  | 2.1  |
| 1   | L     | 162 | ASN  | 2.1  |
| 2   | i     | 74  | ASN  | 2.1  |
| 1   | D     | 364 | LEU  | 2.1  |
| 1   | N     | 166 | MET  | 2.1  |
| 1   | M     | 59  | LEU  | 2.1  |
| 1   | M     | 186 | GLY  | 2.1  |
| 1   | D     | 154 | LYS  | 2.1  |
| 1   | C     | 75  | GLY  | 2.1  |
| 1   | O     | 216 | GLY  | 2.1  |
| 1   | A     | 118 | PRO  | 2.1  |
| 1   | R     | 254 | VAL  | 2.1  |
| 1   | D     | 158 | ASP  | 2.1  |
| 1   | R     | 158 | ASP  | 2.0  |
| 1   | E     | 23  | ASP  | 2.0  |
| 1   | K     | 175 | VAL  | 2.0  |
| 1   | G     | 166 | MET  | 2.0  |
| 1   | M     | 188 | ASP  | 2.0  |
| 1   | E     | 164 | CYS  | 2.0  |
| 1   | O     | 179 | ARG  | 2.0  |
| 1   | J     | 184 | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.