



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:01 PM UTC

PDB ID : 4XJN / pdb\_00004xjn  
Title : Structure of the parainfluenza virus 5 nucleocapsid-RNA complex: an insight into paramyxovirus polymerase activity  
Authors : Alayyoubi, M.; Leser, G.P.; Kors, C.A.; Lamb, R.A.  
Deposited on : 2015-01-08  
Resolution : 3.11 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:

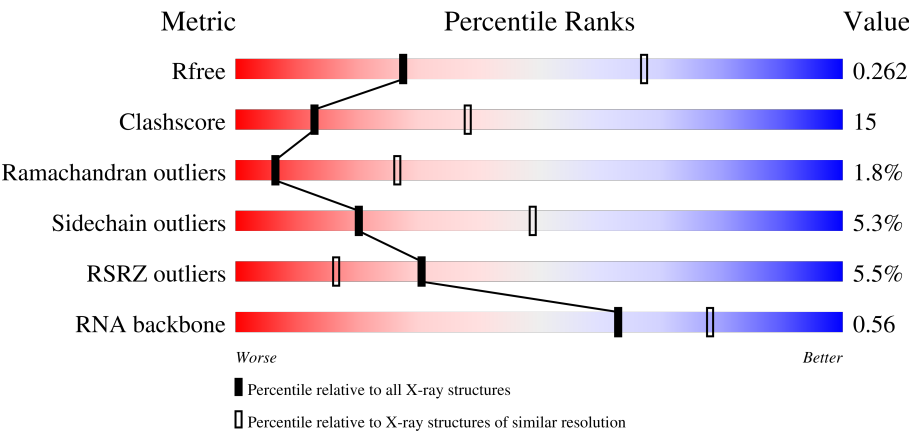
MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson 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 3.11 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                      | 1816 (3.14-3.10)                                      |
| Clashscore            | 190562                      | 1906 (3.14-3.10)                                      |
| Ramachandran outliers | 187476                      | 1802 (3.14-3.10)                                      |
| Sidechain outliers    | 187428                      | 1802 (3.14-3.10)                                      |
| RSRZ outliers         | 180081                      | 1816 (3.14-3.10)                                      |
| RNA backbone          | 3983                        | 1017 (3.34-2.90)                                      |

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     | 525    | <div><div>3%</div><div>47%25%•25%</div></div>  |
| 1   | B     | 525    | <div><div>3%</div><div>50%24%•25%</div></div>  |
| 1   | C     | 525    | <div><div>5%</div><div>47%25%••25%</div></div> |
| 1   | D     | 525    | <div><div>6%</div><div>47%25%•25%</div></div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | E     | 525    |                  |
| 1   | F     | 525    |                  |
| 1   | G     | 525    |                  |
| 1   | H     | 525    |                  |
| 1   | I     | 525    |                  |
| 1   | J     | 525    |                  |
| 1   | K     | 525    |                  |
| 1   | L     | 525    |                  |
| 1   | M     | 525    |                  |
| 2   | N     | 78     |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3   | PB   | B     | 601 | -         | -        | -       | X                |

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 42329 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 Nucleocapsid.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | B     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | C     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | D     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | E     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | F     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | G     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | H     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | I     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | J     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | K     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | L     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |
| 1   | M     | 395      | Total | C    | N   | O   | S  | 16      | 0       | 0     |
|     |       |          | 3135  | 1992 | 541 | 579 | 23 |         |         |       |

There are 208 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| A     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| A     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| A     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| A     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| A     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| A     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| A     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| A     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| A     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| A     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| A     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| A     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| A     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| A     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| B     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| B     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| B     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| B     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| B     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| B     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| B     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| B     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| B     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| B     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| B     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| B     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| B     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| B     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| B     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| B     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| C     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| C     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| C     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| C     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| C     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| C     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| C     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| C     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| C     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| C     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| C     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| C     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| C     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| C     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| C     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| D     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| D     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| D     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| D     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| D     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| D     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| D     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| D     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| D     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| D     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| D     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| D     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| D     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| D     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| D     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| D     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| E     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| E     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| E     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| E     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| E     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| E     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| E     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| E     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| E     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| E     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| E     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| E     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| E     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| E     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| E     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| E     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| F     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| F     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| F     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| F     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| F     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| F     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| F     | -9      | SER      | -      | expression tag | UNP W5QKM4 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| F     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| F     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| F     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| F     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| F     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| F     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| F     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| F     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| F     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| G     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| G     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| G     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| G     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| G     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| G     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| G     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| G     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| G     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| G     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| G     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| G     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| G     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| G     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| G     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| G     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| H     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| H     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| H     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| H     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| H     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| H     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| H     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| H     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| H     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| H     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| H     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| H     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| H     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| H     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| H     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| H     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| I     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| I     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| I     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| I     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| I     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| I     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| I     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| I     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| I     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| I     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| I     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| I     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| I     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| I     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| I     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| I     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| J     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| J     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| J     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| J     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| J     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| J     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| J     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| J     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| J     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| J     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| J     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| J     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| J     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| J     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| J     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| J     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| K     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| K     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| K     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| K     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| K     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| K     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| K     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| K     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| K     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| K     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| K     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| K     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| K     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| K     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| K     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| L     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| L     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| L     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| L     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| L     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| L     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| L     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| L     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| L     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| L     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| L     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| L     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| L     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| L     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| L     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| L     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |
| M     | -15     | HIS      | -      | expression tag | UNP W5QKM4 |
| M     | -14     | HIS      | -      | expression tag | UNP W5QKM4 |
| M     | -13     | HIS      | -      | expression tag | UNP W5QKM4 |
| M     | -12     | HIS      | -      | expression tag | UNP W5QKM4 |
| M     | -11     | HIS      | -      | expression tag | UNP W5QKM4 |
| M     | -10     | HIS      | -      | expression tag | UNP W5QKM4 |
| M     | -9      | SER      | -      | expression tag | UNP W5QKM4 |
| M     | -8      | SER      | -      | expression tag | UNP W5QKM4 |
| M     | -7      | GLY      | -      | expression tag | UNP W5QKM4 |
| M     | -6      | LEU      | -      | expression tag | UNP W5QKM4 |
| M     | -5      | VAL      | -      | expression tag | UNP W5QKM4 |
| M     | -4      | PRO      | -      | expression tag | UNP W5QKM4 |
| M     | -3      | ARG      | -      | expression tag | UNP W5QKM4 |
| M     | -2      | GLY      | -      | expression tag | UNP W5QKM4 |
| M     | -1      | SER      | -      | expression tag | UNP W5QKM4 |
| M     | 0       | HIS      | -      | expression tag | UNP W5QKM4 |

- Molecule 2 is a RNA chain called RNA (78-MER).

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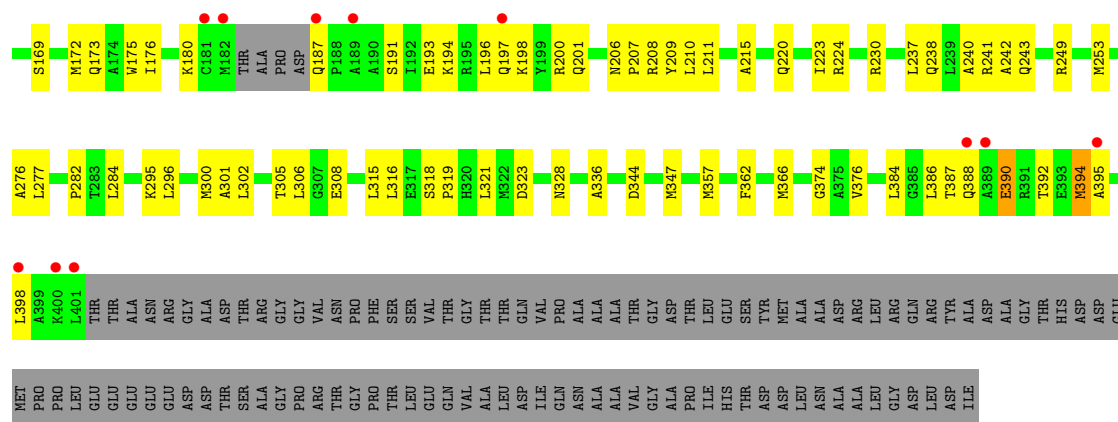
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| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|---------|-------|
| Mol | Chain | Residues | Atoms |     |     |     |    | ZeroOcc | AltConf | Trace |
| 2   | N     | 78       | Total | C   | N   | O   | P  | 0       | 0       | 0     |
|     |       |          | 1560  | 702 | 156 | 624 | 78 |         |         |       |

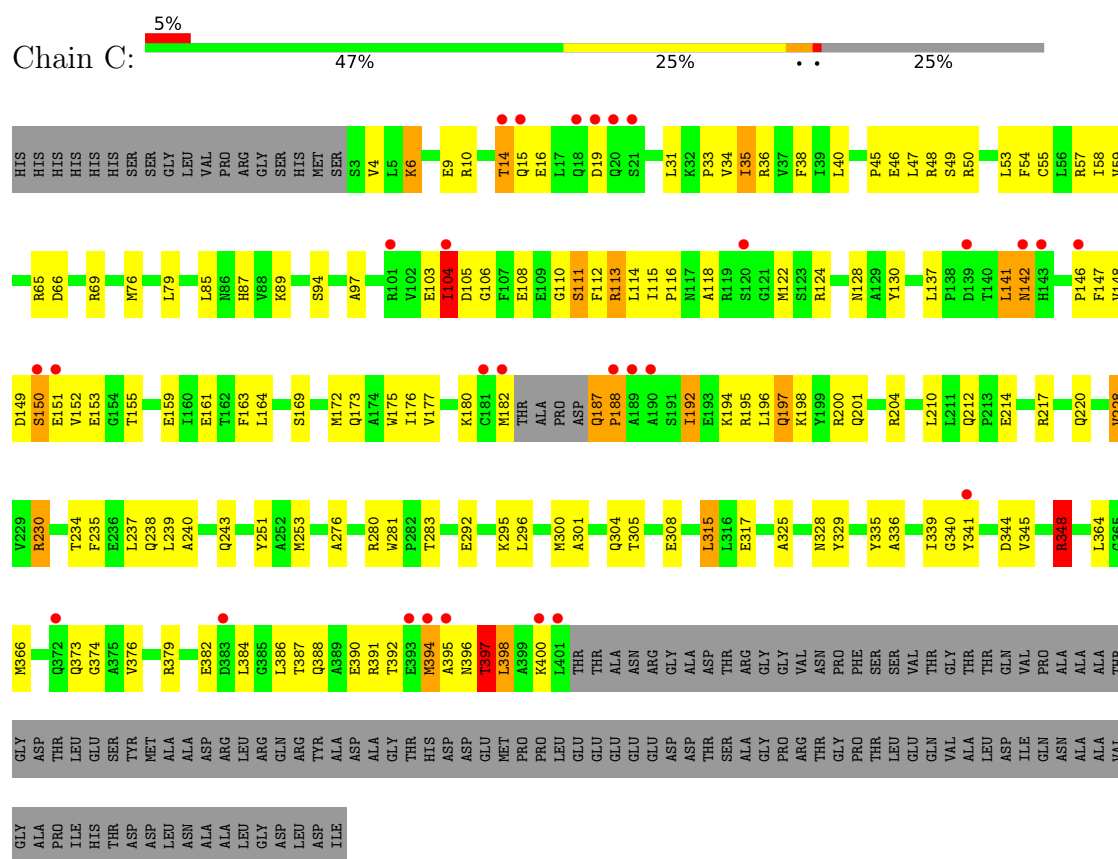
- Molecule 3 is LEAD (II) ION (CCD ID: PB) (formula: Pb).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3   | A     | 1        | Total | Pb | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | B     | 1        | Total | Pb | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | D     | 1        | Total | Pb | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | G     | 1        | Total | Pb | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | H     | 1        | Total | Pb | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 3   | I     | 2        | Total | Pb | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | K     | 2        | Total | Pb | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 3   | M     | 4        | Total | Pb | 0       | 0       |
|     |       |          | 4     | 4  |         |         |
| 3   | N     | 1        | Total | Pb | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

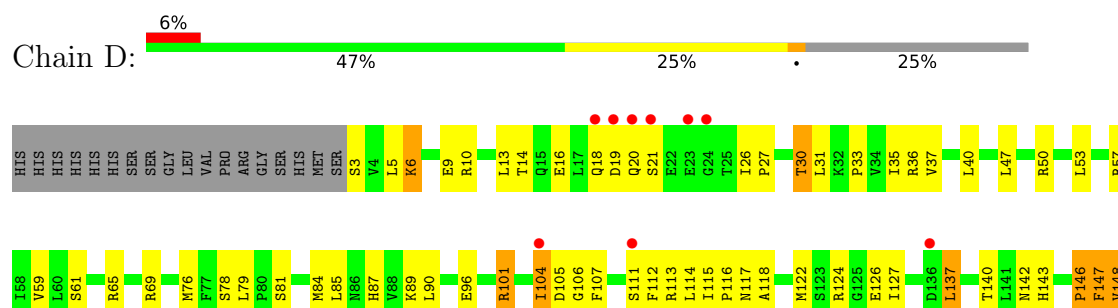


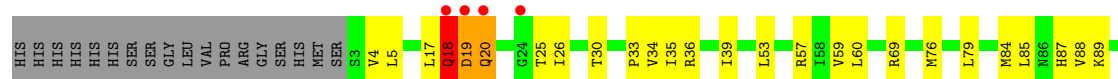


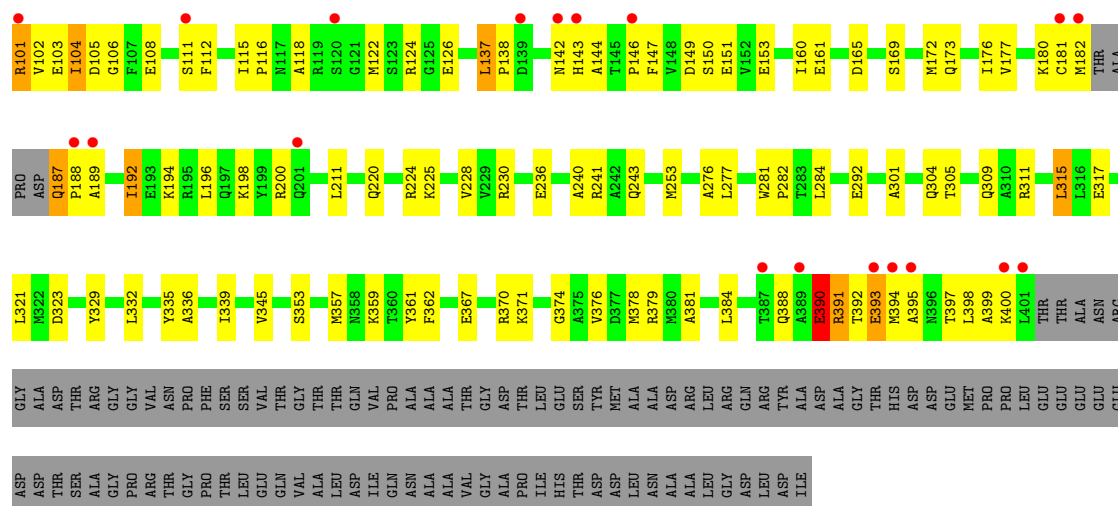
### • Molecule 1: Nucleocapsid



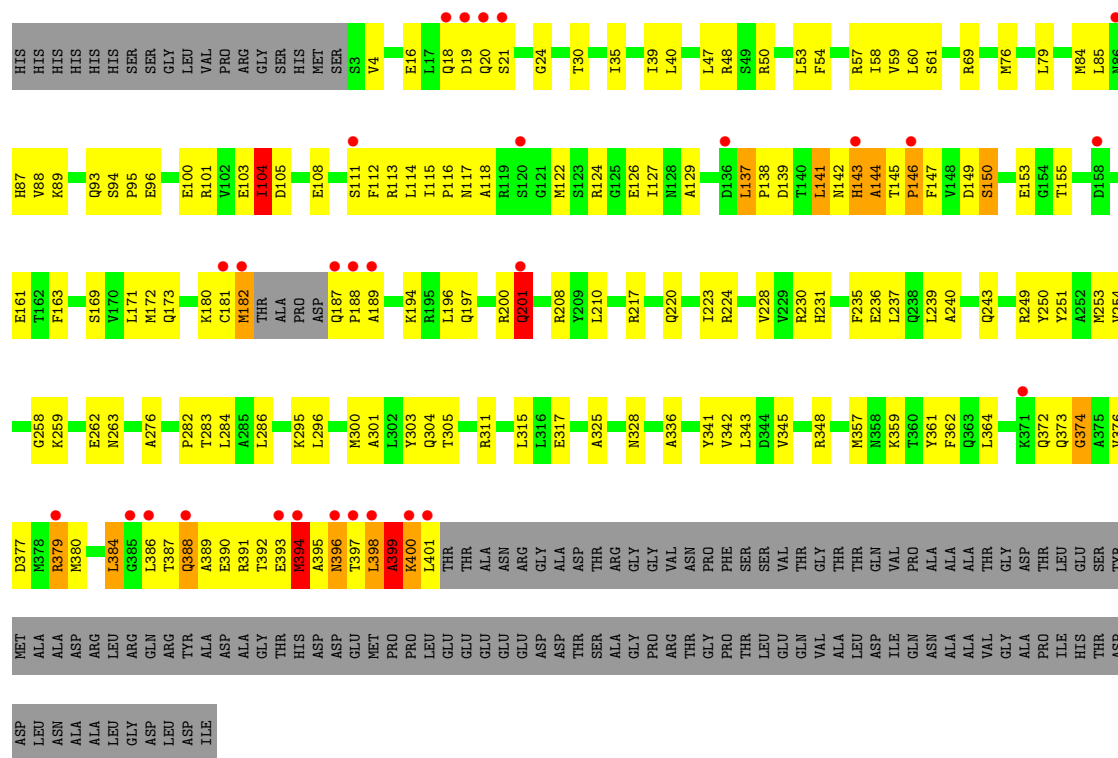
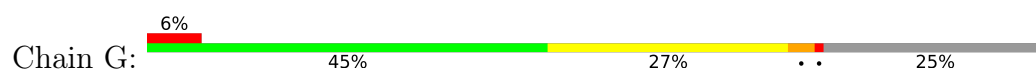
### • Molecule 1: Nucleocapsid



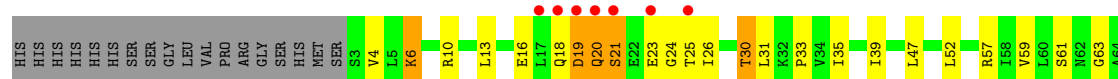


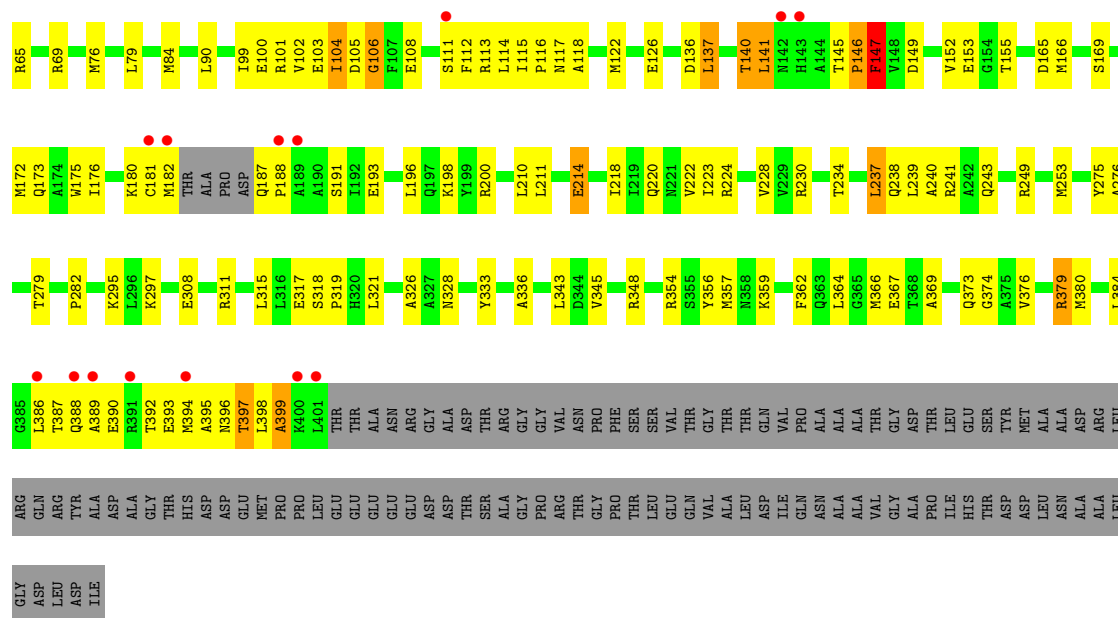


### • Molecule 1: Nucleocapsid

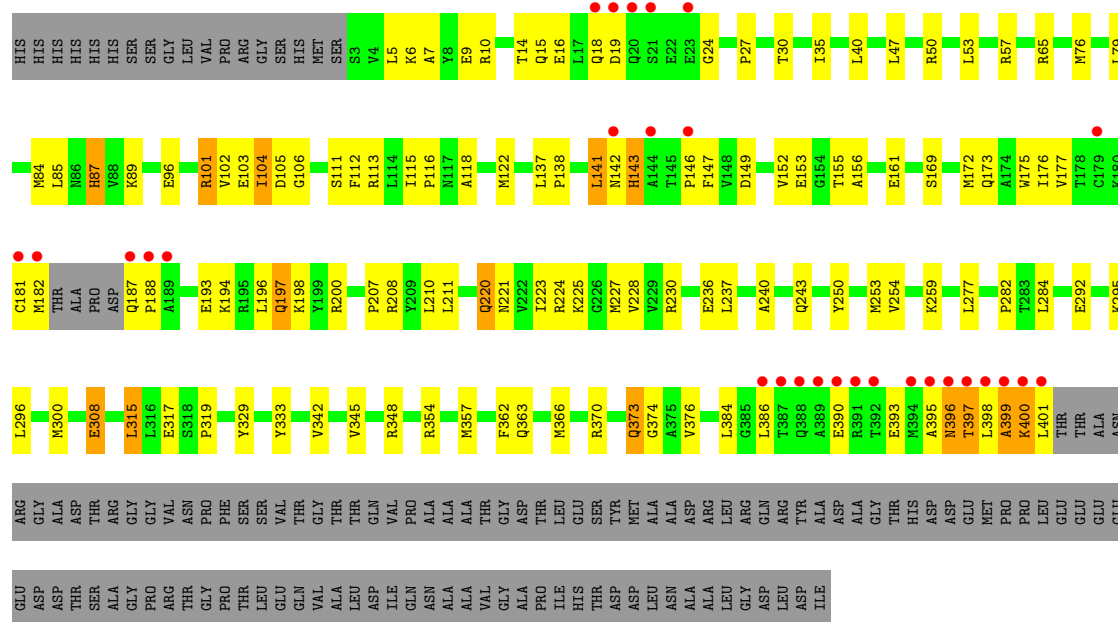


### • Molecule 1: Nucleocapsid

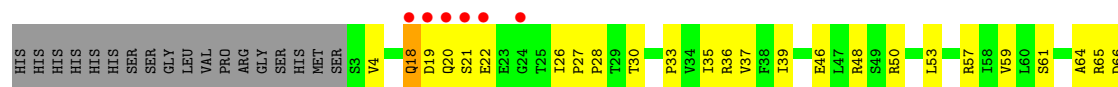


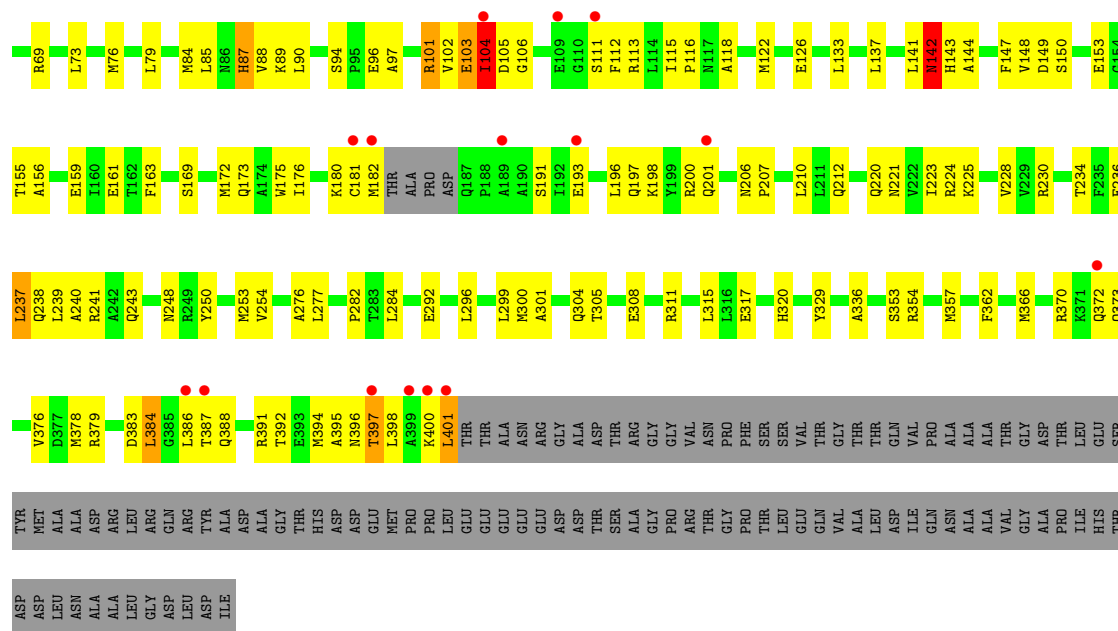


• Molecule 1: Nucleocapsid

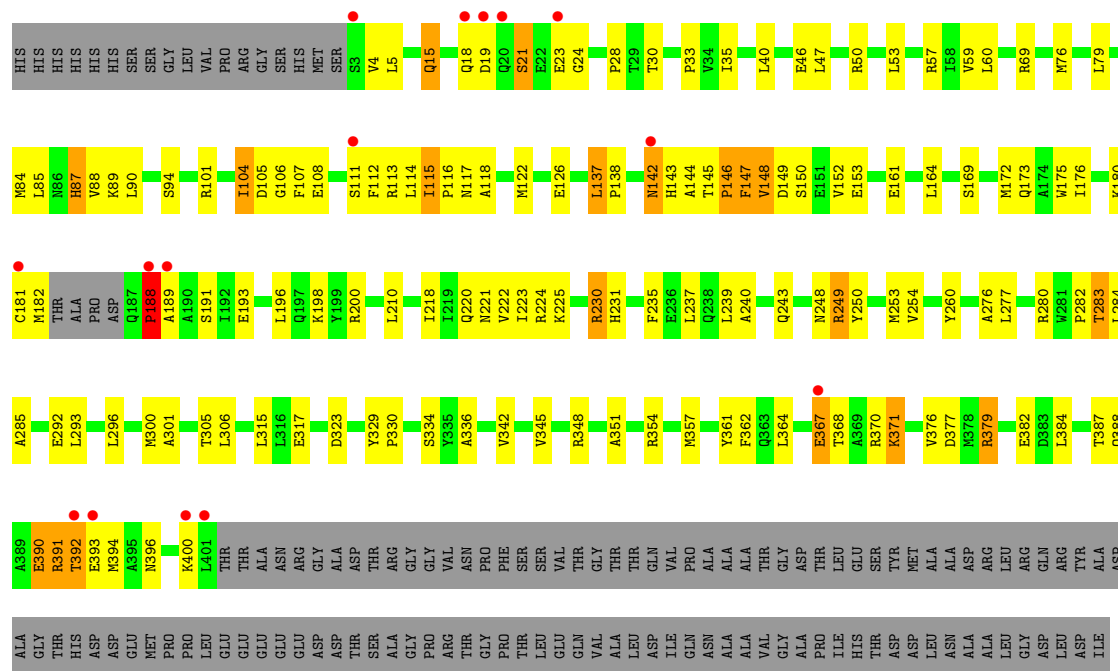


• Molecule 1: Nucleocapsid



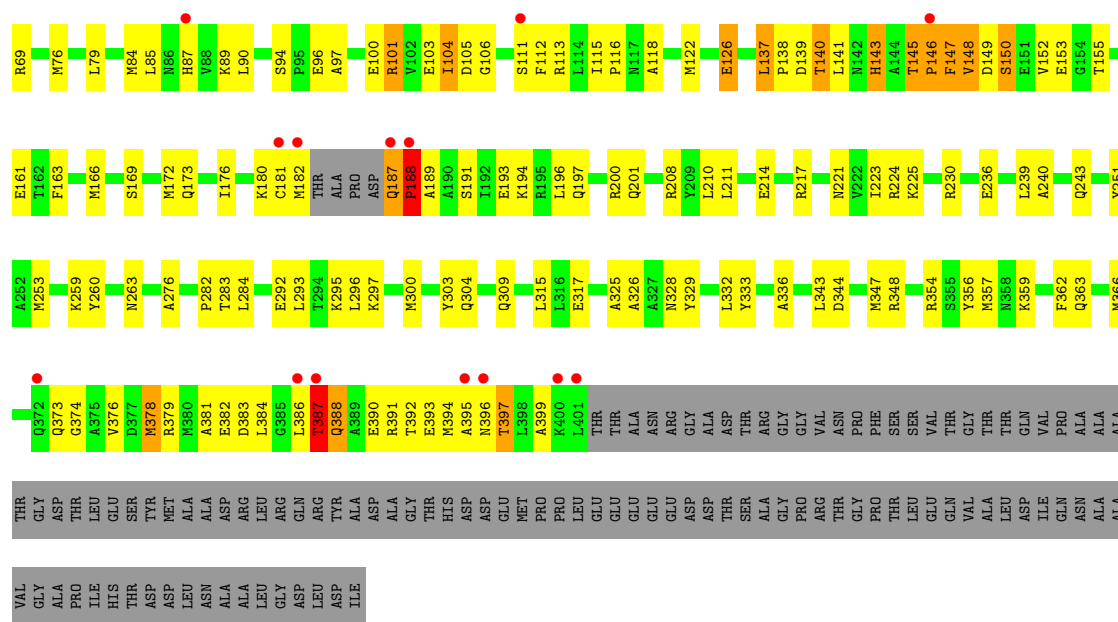


### • Molecule 1: Nucleocapsid

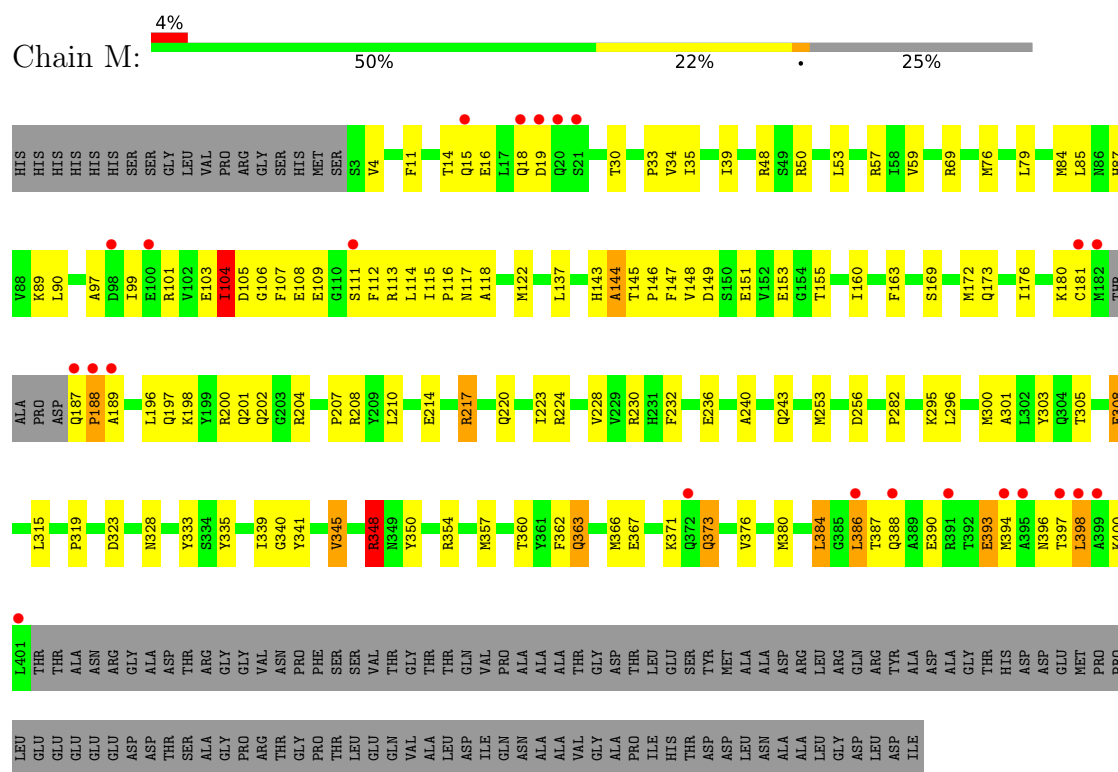


### • Molecule 1: Nucleocapsid





• Molecule 1: Nucleocapsid



• Molecule 2: RNA (78-MER)

Chain N: 67% 28% 5%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 2 2 21                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 205.64Å 309.44Å 233.24Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 45.01 – 3.11<br>45.01 – 3.11                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (45.01-3.11)<br>99.6 (45.01-3.11)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.18                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.51 (at 3.01Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.9_1692                                             | Depositor        |
| R, $R_{free}$                                                           | 0.227 , 0.263<br>0.227 , 0.262                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 7187 reflections (4.87%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 54.2                                                        | Xtriage          |
| Anisotropy                                                              | 0.148                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.31 , 27.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.90                                                        | EDS              |
| Total number of atoms                                                   | 42329                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 46.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PB

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     | 0.59         | 0/3194         | 1.06        | 13/4316 (0.3%)   |
| 1   | B     | 0.59         | 0/3194         | 1.00        | 7/4316 (0.2%)    |
| 1   | C     | 0.70         | 0/3194         | 1.11        | 21/4316 (0.5%)   |
| 1   | D     | 0.63         | 1/3194 (0.0%)  | 1.02        | 14/4316 (0.3%)   |
| 1   | E     | 0.63         | 0/3194         | 1.03        | 17/4316 (0.4%)   |
| 1   | F     | 0.64         | 0/3194         | 1.07        | 11/4316 (0.3%)   |
| 1   | G     | 0.66         | 0/3194         | 1.07        | 18/4316 (0.4%)   |
| 1   | H     | 0.63         | 0/3194         | 1.03        | 14/4316 (0.3%)   |
| 1   | I     | 0.62         | 0/3194         | 1.03        | 14/4316 (0.3%)   |
| 1   | J     | 0.65         | 0/3194         | 1.02        | 11/4316 (0.3%)   |
| 1   | K     | 0.65         | 0/3194         | 0.99        | 12/4316 (0.3%)   |
| 1   | L     | 0.63         | 0/3194         | 1.08        | 22/4316 (0.5%)   |
| 1   | M     | 0.63         | 0/3194         | 1.00        | 9/4316 (0.2%)    |
| 2   | N     | 0.27         | 0/1715         | 0.50        | 2/2648 (0.1%)    |
| All | All   | 0.63         | 1/43237 (0.0%) | 1.02        | 185/58756 (0.3%) |

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   | A     | 0                   | 1                   |
| 1   | B     | 0                   | 1                   |
| 1   | C     | 0                   | 1                   |
| 1   | D     | 0                   | 1                   |
| 1   | E     | 0                   | 2                   |
| 1   | F     | 0                   | 2                   |
| 1   | G     | 0                   | 4                   |
| 1   | I     | 0                   | 2                   |
| 1   | M     | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| All | All   | 0                   | 15                  |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | D     | 188 | PRO  | CA-C  | 5.43 | 1.60        | 1.52     |

All (185) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1   | I     | 400 | LYS  | CB-CA-C | -15.23 | 98.96       | 116.63   |
| 1   | C     | 398 | LEU  | N-CA-C  | -13.55 | 97.21       | 113.88   |
| 1   | F     | 187 | GLN  | CA-C-N  | 13.21  | 136.35      | 119.84   |
| 1   | F     | 187 | GLN  | C-N-CA  | 13.21  | 136.35      | 119.84   |
| 1   | J     | 397 | THR  | N-CA-C  | -11.65 | 98.56       | 111.14   |
| 1   | I     | 400 | LYS  | N-CA-C  | 11.12  | 126.88      | 108.08   |
| 1   | F     | 20  | GLN  | N-CA-C  | -10.54 | 100.37      | 113.02   |
| 1   | G     | 399 | ALA  | N-CA-C  | 9.91   | 131.90      | 110.80   |
| 1   | G     | 394 | MET  | N-CA-C  | -9.32  | 101.67      | 113.23   |
| 1   | H     | 18  | GLN  | N-CA-C  | -9.24  | 95.60       | 110.20   |
| 1   | B     | 104 | ILE  | N-CA-C  | 9.17   | 119.44      | 111.56   |
| 1   | L     | 6   | LYS  | N-CA-C  | -9.08  | 101.33      | 111.14   |
| 1   | A     | 103 | GLU  | CA-C-N  | -9.03  | 113.58      | 123.16   |
| 1   | A     | 103 | GLU  | C-N-CA  | -9.03  | 113.58      | 123.16   |
| 1   | L     | 394 | MET  | N-CA-C  | -8.86  | 101.70      | 111.36   |
| 1   | E     | 147 | PHE  | N-CA-C  | 8.65   | 124.02      | 113.38   |
| 1   | I     | 397 | THR  | N-CA-C  | -8.49  | 101.98      | 111.07   |
| 1   | H     | 397 | THR  | N-CA-C  | -8.22  | 102.28      | 111.07   |
| 1   | K     | 104 | ILE  | N-CA-C  | 8.20   | 119.19      | 111.48   |
| 1   | D     | 104 | ILE  | N-CA-C  | 8.20   | 119.18      | 111.48   |
| 1   | D     | 21  | SER  | N-CA-C  | -8.11  | 102.13      | 110.97   |
| 1   | A     | 18  | GLN  | N-CA-C  | -8.05  | 96.96       | 109.76   |
| 1   | D     | 146 | PRO  | CA-C-O  | -8.05  | 112.23      | 122.13   |
| 1   | H     | 103 | GLU  | CA-C-N  | -7.90  | 115.23      | 122.97   |
| 1   | H     | 103 | GLU  | C-N-CA  | -7.90  | 115.23      | 122.97   |
| 1   | E     | 187 | GLN  | CA-C-N  | -7.81  | 110.08      | 119.84   |
| 1   | E     | 187 | GLN  | C-N-CA  | -7.81  | 110.08      | 119.84   |
| 1   | C     | 397 | THR  | N-CA-C  | 7.75   | 119.72      | 111.28   |
| 1   | G     | 389 | ALA  | N-CA-C  | 7.74   | 119.80      | 111.36   |
| 1   | D     | 20  | GLN  | N-CA-C  | -7.66  | 104.35      | 112.93   |
| 1   | F     | 103 | GLU  | CA-C-N  | -7.59  | 115.41      | 123.08   |
| 1   | F     | 103 | GLU  | C-N-CA  | -7.59  | 115.41      | 123.08   |

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| Mol | Chain | Res | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 1   | C     | 104 | ILE  | N-CA-C      | 7.46  | 118.49      | 111.48   |
| 1   | M     | 388 | GLN  | CA-CB-CG    | 7.30  | 128.69      | 114.10   |
| 1   | L     | 106 | GLY  | N-CA-C      | 7.28  | 120.71      | 110.38   |
| 1   | I     | 400 | LYS  | CA-C-N      | 7.26  | 134.78      | 121.70   |
| 1   | I     | 400 | LYS  | C-N-CA      | 7.26  | 134.78      | 121.70   |
| 1   | M     | 398 | LEU  | N-CA-C      | 7.23  | 119.24      | 111.36   |
| 1   | G     | 104 | ILE  | N-CA-C      | 7.20  | 118.25      | 111.48   |
| 1   | A     | 106 | GLY  | N-CA-C      | 7.18  | 120.57      | 110.38   |
| 1   | G     | 137 | LEU  | CA-C-N      | -7.15 | 112.95      | 120.03   |
| 1   | G     | 137 | LEU  | C-N-CA      | -7.15 | 112.95      | 120.03   |
| 1   | J     | 103 | GLU  | CA-C-N      | -7.09 | 115.92      | 123.08   |
| 1   | J     | 103 | GLU  | C-N-CA      | -7.09 | 115.92      | 123.08   |
| 1   | C     | 104 | ILE  | CA-C-O      | -7.05 | 114.71      | 120.70   |
| 1   | C     | 391 | ARG  | N-CA-C      | -6.98 | 103.67      | 111.28   |
| 1   | J     | 21  | SER  | N-CA-C      | -6.96 | 102.76      | 111.11   |
| 1   | L     | 104 | ILE  | N-CA-C      | 6.86  | 117.46      | 111.56   |
| 1   | C     | 197 | GLN  | CA-CB-CG    | -6.85 | 100.39      | 114.10   |
| 2   | N     | 66  | U    | C2'-C3'-O3' | 6.85  | 119.77      | 109.50   |
| 1   | D     | 18  | GLN  | N-CA-C      | -6.84 | 99.38       | 110.20   |
| 1   | F     | 104 | ILE  | N-CA-C      | 6.75  | 117.37      | 111.56   |
| 1   | H     | 106 | GLY  | N-CA-C      | 6.75  | 119.96      | 110.38   |
| 1   | D     | 137 | LEU  | CA-C-N      | -6.75 | 113.35      | 120.03   |
| 1   | D     | 137 | LEU  | C-N-CA      | -6.75 | 113.35      | 120.03   |
| 1   | L     | 387 | THR  | N-CA-C      | 6.74  | 119.41      | 109.24   |
| 1   | B     | 106 | GLY  | N-CA-C      | 6.64  | 119.81      | 110.38   |
| 1   | C     | 14  | THR  | N-CA-C      | 6.64  | 118.60      | 111.36   |
| 1   | D     | 181 | CYS  | N-CA-C      | 6.61  | 119.48      | 111.82   |
| 1   | H     | 19  | ASP  | CA-C-N      | -6.56 | 112.16      | 122.73   |
| 1   | H     | 19  | ASP  | C-N-CA      | -6.56 | 112.16      | 122.73   |
| 1   | D     | 106 | GLY  | N-CA-C      | 6.49  | 119.60      | 110.38   |
| 1   | H     | 147 | PHE  | N-CA-C      | 6.46  | 124.56      | 110.80   |
| 1   | E     | 181 | CYS  | CA-C-N      | 6.44  | 133.29      | 121.70   |
| 1   | E     | 181 | CYS  | C-N-CA      | 6.44  | 133.29      | 121.70   |
| 1   | A     | 104 | ILE  | N-CA-C      | 6.41  | 116.68      | 111.62   |
| 1   | D     | 373 | GLN  | N-CA-C      | -6.39 | 105.79      | 113.97   |
| 1   | F     | 106 | GLY  | N-CA-C      | 6.33  | 119.36      | 110.38   |
| 1   | K     | 392 | THR  | N-CA-C      | 6.25  | 119.38      | 111.69   |
| 1   | G     | 24  | GLY  | N-CA-C      | 6.23  | 118.64      | 111.36   |
| 1   | G     | 103 | GLU  | CA-C-N      | -6.18 | 116.92      | 122.97   |
| 1   | G     | 103 | GLU  | C-N-CA      | -6.18 | 116.92      | 122.97   |
| 1   | J     | 104 | ILE  | N-CA-C      | 6.17  | 116.87      | 111.56   |
| 1   | C     | 394 | MET  | N-CA-C      | -6.15 | 106.31      | 113.88   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | H     | 104 | ILE  | N-CA-C   | 6.13  | 117.24      | 111.48   |
| 1   | B     | 145 | THR  | CA-C-N   | -6.09 | 112.22      | 119.84   |
| 1   | B     | 145 | THR  | C-N-CA   | -6.09 | 112.22      | 119.84   |
| 1   | I     | 106 | GLY  | N-CA-C   | 6.06  | 118.99      | 110.38   |
| 1   | L     | 366 | MET  | N-CA-C   | -6.04 | 104.62      | 111.14   |
| 1   | C     | 142 | ASN  | CA-C-N   | 6.03  | 133.05      | 121.54   |
| 1   | C     | 142 | ASN  | C-N-CA   | 6.03  | 133.05      | 121.54   |
| 1   | A     | 360 | THR  | N-CA-C   | 6.02  | 117.51      | 111.07   |
| 1   | L     | 397 | THR  | N-CA-C   | -5.99 | 104.66      | 111.07   |
| 1   | J     | 106 | GLY  | N-CA-C   | 5.97  | 118.86      | 110.38   |
| 1   | G     | 201 | GLN  | CA-CB-CG | 5.95  | 126.00      | 114.10   |
| 1   | C     | 398 | LEU  | CB-CA-C  | 5.92  | 118.62      | 109.03   |
| 1   | J     | 101 | ARG  | N-CA-C   | 5.90  | 119.67      | 112.23   |
| 1   | C     | 187 | GLN  | CA-C-N   | 5.90  | 127.21      | 119.84   |
| 1   | C     | 187 | GLN  | C-N-CA   | 5.90  | 127.21      | 119.84   |
| 1   | G     | 399 | ALA  | CA-C-N   | 5.90  | 132.80      | 121.54   |
| 1   | G     | 399 | ALA  | C-N-CA   | 5.90  | 132.80      | 121.54   |
| 1   | E     | 104 | ILE  | N-CA-C   | 5.89  | 117.02      | 111.48   |
| 1   | M     | 340 | GLY  | N-CA-C   | -5.88 | 105.53      | 113.24   |
| 1   | M     | 146 | PRO  | CA-C-O   | -5.88 | 114.96      | 123.07   |
| 1   | E     | 103 | GLU  | CA-C-N   | -5.87 | 117.22      | 122.97   |
| 1   | E     | 103 | GLU  | C-N-CA   | -5.87 | 117.22      | 122.97   |
| 1   | K     | 392 | THR  | CA-C-N   | -5.87 | 112.86      | 122.54   |
| 1   | K     | 392 | THR  | C-N-CA   | -5.87 | 112.86      | 122.54   |
| 1   | C     | 106 | GLY  | N-CA-C   | 5.86  | 118.70      | 110.38   |
| 1   | E     | 106 | GLY  | N-CA-C   | 5.86  | 118.69      | 110.38   |
| 1   | I     | 24  | GLY  | N-CA-C   | 5.85  | 118.21      | 111.36   |
| 1   | A     | 104 | ILE  | CA-C-O   | -5.84 | 115.60      | 120.80   |
| 1   | D     | 146 | PRO  | N-CA-C   | -5.84 | 102.02      | 111.77   |
| 1   | L     | 137 | LEU  | CA-C-N   | -5.82 | 114.27      | 120.03   |
| 1   | L     | 137 | LEU  | C-N-CA   | -5.82 | 114.27      | 120.03   |
| 1   | K     | 106 | GLY  | N-CA-C   | 5.81  | 118.64      | 110.38   |
| 1   | M     | 106 | GLY  | N-CA-C   | 5.81  | 118.63      | 110.38   |
| 1   | L     | 387 | THR  | CA-C-N   | 5.77  | 132.55      | 121.54   |
| 1   | L     | 387 | THR  | C-N-CA   | 5.77  | 132.55      | 121.54   |
| 1   | L     | 188 | PRO  | N-CA-C   | 5.76  | 124.34      | 112.47   |
| 1   | C     | 103 | GLU  | CA-C-N   | -5.76 | 117.32      | 122.97   |
| 1   | C     | 103 | GLU  | C-N-CA   | -5.76 | 117.32      | 122.97   |
| 1   | K     | 101 | ARG  | N-CA-C   | 5.76  | 119.48      | 112.23   |
| 1   | M     | 103 | GLU  | CA-C-N   | -5.74 | 117.28      | 123.08   |
| 1   | M     | 103 | GLU  | C-N-CA   | -5.74 | 117.28      | 123.08   |
| 1   | I     | 104 | ILE  | CA-C-O   | -5.74 | 115.82      | 120.70   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | C     | 348 | ARG  | CA-CB-CG | 5.71  | 125.52      | 114.10   |
| 1   | H     | 20  | GLN  | CA-CB-CG | -5.69 | 102.72      | 114.10   |
| 1   | G     | 374 | GLY  | N-CA-C   | -5.67 | 108.44      | 114.67   |
| 1   | G     | 101 | ARG  | N-CA-C   | 5.66  | 119.36      | 112.23   |
| 1   | A     | 373 | GLN  | N-CA-C   | -5.65 | 107.03      | 114.31   |
| 1   | H     | 399 | ALA  | N-CA-C   | 5.64  | 117.42      | 111.28   |
| 1   | E     | 397 | THR  | N-CA-C   | -5.63 | 98.81       | 110.80   |
| 1   | E     | 20  | GLN  | N-CA-CB  | -5.62 | 102.01      | 110.73   |
| 1   | F     | 142 | ASN  | N-CA-C   | 5.60  | 117.71      | 110.65   |
| 1   | H     | 20  | GLN  | N-CA-C   | -5.59 | 106.35      | 112.72   |
| 1   | G     | 127 | ILE  | N-CA-C   | -5.57 | 105.07      | 110.42   |
| 1   | J     | 18  | GLN  | N-CA-C   | -5.55 | 98.69       | 108.23   |
| 1   | K     | 188 | PRO  | CA-C-N   | 5.53  | 131.66      | 121.70   |
| 1   | K     | 188 | PRO  | C-N-CA   | 5.53  | 131.66      | 121.70   |
| 1   | F     | 101 | ARG  | N-CA-C   | 5.52  | 119.19      | 112.23   |
| 1   | B     | 390 | GLU  | N-CA-C   | 5.52  | 117.38      | 111.36   |
| 1   | D     | 104 | ILE  | CA-C-O   | -5.52 | 116.01      | 120.70   |
| 1   | L     | 140 | THR  | N-CA-C   | -5.47 | 105.86      | 112.54   |
| 1   | D     | 101 | ARG  | N-CA-C   | 5.46  | 119.11      | 112.23   |
| 1   | L     | 373 | GLN  | N-CA-C   | -5.44 | 107.00      | 113.97   |
| 1   | E     | 101 | ARG  | N-CA-C   | 5.43  | 119.08      | 112.23   |
| 1   | E     | 20  | GLN  | CA-CB-CG | 5.42  | 124.93      | 114.10   |
| 1   | F     | 18  | GLN  | CA-CB-CG | 5.41  | 124.92      | 114.10   |
| 1   | I     | 373 | GLN  | N-CA-C   | -5.40 | 107.06      | 113.97   |
| 1   | A     | 397 | THR  | N-CA-C   | 5.39  | 116.96      | 111.14   |
| 1   | C     | 398 | LEU  | CA-C-O   | 5.39  | 125.33      | 119.24   |
| 1   | H     | 389 | ALA  | N-CA-C   | -5.36 | 105.52      | 111.36   |
| 1   | I     | 103 | GLU  | CA-C-N   | -5.35 | 117.73      | 122.97   |
| 1   | I     | 103 | GLU  | C-N-CA   | -5.35 | 117.73      | 122.97   |
| 1   | G     | 379 | ARG  | CB-CG-CD | 5.34  | 123.59      | 111.30   |
| 1   | K     | 137 | LEU  | CA-C-N   | -5.33 | 114.75      | 120.03   |
| 1   | K     | 137 | LEU  | C-N-CA   | -5.33 | 114.75      | 120.03   |
| 1   | C     | 340 | GLY  | N-CA-C   | -5.32 | 106.34      | 112.73   |
| 1   | D     | 140 | THR  | N-CA-C   | -5.32 | 105.89      | 112.38   |
| 1   | F     | 104 | ILE  | CA-C-O   | -5.32 | 115.62      | 120.73   |
| 1   | A     | 150 | SER  | N-CA-C   | 5.30  | 119.23      | 112.87   |
| 1   | I     | 400 | LYS  | CA-CB-CG | 5.28  | 124.66      | 114.10   |
| 1   | M     | 104 | ILE  | N-CA-C   | 5.28  | 116.10      | 111.56   |
| 1   | B     | 104 | ILE  | CA-C-O   | -5.25 | 115.69      | 120.73   |
| 1   | L     | 187 | GLN  | CA-C-N   | 5.24  | 126.39      | 119.84   |
| 1   | L     | 187 | GLN  | C-N-CA   | 5.24  | 126.39      | 119.84   |
| 1   | I     | 101 | ARG  | N-CA-C   | 5.24  | 118.83      | 112.23   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | J     | 142 | ASN  | CA-C-N    | 5.23  | 131.12      | 121.70   |
| 1   | J     | 142 | ASN  | C-N-CA    | 5.23  | 131.12      | 121.70   |
| 1   | B     | 394 | MET  | N-CA-C    | -5.23 | 105.49      | 111.14   |
| 1   | E     | 391 | ARG  | N-CA-C    | 5.23  | 116.79      | 111.14   |
| 1   | L     | 384 | LEU  | N-CA-C    | -5.23 | 106.87      | 113.20   |
| 1   | E     | 79  | LEU  | CA-C-N    | -5.23 | 114.28      | 119.56   |
| 1   | E     | 79  | LEU  | C-N-CA    | -5.23 | 114.28      | 119.56   |
| 2   | N     | 66  | U    | P-O3'-C3' | 5.22  | 128.03      | 120.20   |
| 1   | A     | 181 | CYS  | CA-C-N    | 5.17  | 131.01      | 121.70   |
| 1   | A     | 181 | CYS  | C-N-CA    | 5.17  | 131.01      | 121.70   |
| 1   | C     | 111 | SER  | CA-C-N    | 5.17  | 131.01      | 121.70   |
| 1   | C     | 111 | SER  | C-N-CA    | 5.17  | 131.01      | 121.70   |
| 1   | K     | 21  | SER  | N-CA-C    | -5.17 | 105.54      | 111.07   |
| 1   | H     | 141 | LEU  | N-CA-C    | -5.17 | 102.83      | 110.48   |
| 1   | E     | 371 | LYS  | N-CA-C    | 5.16  | 118.73      | 112.23   |
| 1   | M     | 348 | ARG  | NE-CZ-NH2 | 5.15  | 123.83      | 119.20   |
| 1   | L     | 103 | GLU  | CA-C-N    | -5.14 | 117.89      | 123.08   |
| 1   | L     | 103 | GLU  | C-N-CA    | -5.14 | 117.89      | 123.08   |
| 1   | G     | 19  | ASP  | N-CA-C    | 5.13  | 121.72      | 110.80   |
| 1   | K     | 115 | ILE  | N-CA-C    | -5.13 | 102.47      | 107.55   |
| 1   | A     | 374 | GLY  | N-CA-C    | -5.13 | 109.03      | 114.67   |
| 1   | I     | 104 | ILE  | N-CA-C    | 5.12  | 116.29      | 111.48   |
| 1   | J     | 104 | ILE  | CA-C-O    | -5.09 | 115.84      | 120.73   |
| 1   | L     | 101 | ARG  | N-CA-C    | 5.05  | 118.60      | 112.23   |
| 1   | G     | 104 | ILE  | CA-C-O    | -5.04 | 116.42      | 120.70   |
| 1   | L     | 392 | THR  | CA-C-N    | -5.00 | 114.28      | 122.54   |
| 1   | L     | 392 | THR  | C-N-CA    | -5.00 | 114.28      | 122.54   |

There are no chirality outliers.

All (15) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | A     | 187 | GLN  | Peptide |
| 1   | B     | 117 | ASN  | Peptide |
| 1   | C     | 397 | THR  | Peptide |
| 1   | D     | 188 | PRO  | Peptide |
| 1   | E     | 19  | ASP  | Peptide |
| 1   | E     | 400 | LYS  | Peptide |
| 1   | F     | 17  | LEU  | Peptide |
| 1   | F     | 390 | GLU  | Peptide |
| 1   | G     | 20  | GLN  | Peptide |
| 1   | G     | 396 | ASN  | Peptide |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | G     | 398 | LEU  | Peptide |
| 1   | G     | 399 | ALA  | Peptide |
| 1   | I     | 396 | ASN  | Peptide |
| 1   | I     | 399 | ALA  | Peptide |
| 1   | M     | 393 | GLU  | 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     | 3135  | 0        | 3145     | 99      | 0            |
| 1   | B     | 3135  | 0        | 3145     | 98      | 1            |
| 1   | C     | 3135  | 0        | 3145     | 109     | 1            |
| 1   | D     | 3135  | 0        | 3145     | 106     | 0            |
| 1   | E     | 3135  | 0        | 3145     | 108     | 0            |
| 1   | F     | 3135  | 0        | 3145     | 96      | 0            |
| 1   | G     | 3135  | 0        | 3145     | 121     | 2            |
| 1   | H     | 3135  | 0        | 3145     | 107     | 0            |
| 1   | I     | 3135  | 0        | 3145     | 86      | 2            |
| 1   | J     | 3135  | 0        | 3145     | 113     | 0            |
| 1   | K     | 3135  | 0        | 3145     | 107     | 0            |
| 1   | L     | 3135  | 0        | 3145     | 110     | 1            |
| 1   | M     | 3135  | 0        | 3144     | 94      | 0            |
| 2   | N     | 1560  | 0        | 781      | 22      | 0            |
| 3   | A     | 1     | 0        | 0        | 0       | 0            |
| 3   | B     | 1     | 0        | 0        | 0       | 0            |
| 3   | D     | 1     | 0        | 0        | 0       | 0            |
| 3   | G     | 1     | 0        | 0        | 0       | 0            |
| 3   | H     | 1     | 0        | 0        | 0       | 0            |
| 3   | I     | 2     | 0        | 0        | 0       | 0            |
| 3   | K     | 2     | 0        | 0        | 0       | 1            |
| 3   | M     | 4     | 0        | 0        | 0       | 0            |
| 3   | N     | 1     | 0        | 0        | 1       | 0            |
| All | All   | 42329 | 0        | 41665    | 1255    | 4            |

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 15.

All (1255) 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:188:PRO:HB2  | 1:D:189:ALA:HA   | 1.42                     | 1.00              |
| 1:M:341:TYR:O    | 1:M:348:ARG:NH1  | 1.96                     | 0.98              |
| 1:A:369:ALA:O    | 1:A:373:GLN:NE2  | 1.99                     | 0.95              |
| 1:I:396:ASN:HA   | 1:I:399:ALA:H    | 1.31                     | 0.94              |
| 1:C:348:ARG:H    | 1:C:348:ARG:HD2  | 1.30                     | 0.93              |
| 1:E:397:THR:HG22 | 1:E:400:LYS:HD2  | 1.51                     | 0.93              |
| 1:F:18:GLN:O     | 1:F:20:GLN:N     | 2.00                     | 0.93              |
| 1:I:397:THR:O    | 1:I:400:LYS:HG3  | 1.70                     | 0.90              |
| 1:E:372:GLN:HG3  | 1:E:375:ALA:HB2  | 1.54                     | 0.89              |
| 1:E:393:GLU:O    | 1:E:397:THR:OG1  | 1.91                     | 0.89              |
| 1:I:177:VAL:HB   | 1:I:220:GLN:HG3  | 1.53                     | 0.88              |
| 1:G:201:GLN:HA   | 1:G:201:GLN:HE21 | 1.37                     | 0.88              |
| 1:I:398:LEU:HA   | 1:I:400:LYS:HD3  | 1.55                     | 0.87              |
| 1:J:241:ARG:HH21 | 1:J:308:GLU:HG3  | 1.39                     | 0.86              |
| 1:I:398:LEU:HD23 | 1:I:398:LEU:O    | 1.76                     | 0.86              |
| 1:A:386:LEU:HD11 | 1:E:282:PRO:HB3  | 1.59                     | 0.85              |
| 1:C:214:GLU:OE1  | 1:C:217:ARG:NH1  | 2.09                     | 0.84              |
| 1:G:155:THR:HG21 | 1:G:208:ARG:HH22 | 1.41                     | 0.84              |
| 1:A:367:GLU:HA   | 1:A:370:ARG:HG3  | 1.60                     | 0.83              |
| 1:J:197:GLN:O    | 1:J:201:GLN:HG2  | 1.78                     | 0.83              |
| 1:D:189:ALA:HB3  | 1:D:192:ILE:HD12 | 1.60                     | 0.83              |
| 1:C:396:ASN:OD1  | 1:C:397:THR:N    | 2.12                     | 0.82              |
| 1:B:117:ASN:HB3  | 1:B:119:ARG:H    | 1.43                     | 0.81              |
| 1:E:116:PRO:HB3  | 1:E:122:MET:HE2  | 1.61                     | 0.81              |
| 1:L:333:TYR:OH   | 1:L:354:ARG:NH1  | 2.13                     | 0.81              |
| 1:F:241:ARG:NH1  | 1:F:311:ARG:HE   | 1.80                     | 0.80              |
| 1:K:142:ASN:O    | 1:K:144:ALA:N    | 2.13                     | 0.80              |
| 1:J:20:GLN:HE22  | 1:J:320:HIS:CE1  | 2.01                     | 0.79              |
| 1:E:295:LYS:HZ2  | 1:E:328:ASN:HB2  | 1.47                     | 0.79              |
| 1:E:397:THR:O    | 1:E:400:LYS:N    | 2.13                     | 0.78              |
| 1:A:15:GLN:NE2   | 1:M:303:TYR:HE1  | 1.81                     | 0.78              |
| 1:H:224:ARG:O    | 1:H:230:ARG:NH1  | 2.17                     | 0.78              |
| 1:K:23:GLU:OE1   | 1:K:24:GLY:N     | 2.16                     | 0.78              |
| 1:C:196:LEU:HD23 | 1:C:210:LEU:HD11 | 1.65                     | 0.78              |
| 1:B:386:LEU:HD11 | 1:H:282:PRO:HB3  | 1.66                     | 0.77              |
| 1:J:224:ARG:O    | 1:J:230:ARG:NH1  | 2.17                     | 0.77              |
| 1:J:241:ARG:NH2  | 1:J:308:GLU:HG3  | 1.99                     | 0.76              |
| 1:E:207:PRO:HA   | 1:E:210:LEU:HD13 | 1.67                     | 0.76              |
| 1:J:46:GLU:OE2   | 1:J:50:ARG:NH2   | 2.18                     | 0.76              |
| 1:C:341:TYR:O    | 1:C:348:ARG:NH2  | 2.19                     | 0.76              |
| 1:F:390:GLU:O    | 1:F:393:GLU:N    | 2.15                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:193:GLU:HA   | 1:K:196:LEU:HD12 | 1.68                     | 0.76              |
| 1:D:304:GLN:NE2  | 1:I:14:THR:OG1   | 2.19                     | 0.75              |
| 1:E:311:ARG:HH22 | 1:F:18:GLN:HG3   | 1.51                     | 0.75              |
| 1:G:57:ARG:NH1   | 1:G:153:GLU:OE2  | 2.20                     | 0.75              |
| 1:M:187:GLN:HG2  | 1:M:188:PRO:HD2  | 1.67                     | 0.75              |
| 1:L:386:LEU:HD11 | 1:L:390:GLU:HG2  | 1.67                     | 0.74              |
| 1:M:116:PRO:HB3  | 1:M:122:MET:HE2  | 1.69                     | 0.74              |
| 1:K:224:ARG:O    | 1:K:230:ARG:NH1  | 2.20                     | 0.74              |
| 1:G:386:LEU:HD11 | 1:K:282:PRO:HB3  | 1.69                     | 0.74              |
| 1:I:393:GLU:O    | 1:I:397:THR:OG1  | 2.04                     | 0.74              |
| 1:A:241:ARG:HH12 | 1:A:308:GLU:HG3  | 1.53                     | 0.74              |
| 1:M:341:TYR:C    | 1:M:348:ARG:HH12 | 1.93                     | 0.74              |
| 1:H:16:GLU:OE1   | 1:H:295:LYS:NZ   | 2.18                     | 0.73              |
| 1:G:155:THR:HG21 | 1:G:208:ARG:NH2  | 2.03                     | 0.73              |
| 1:C:116:PRO:HB3  | 1:C:122:MET:HE2  | 1.69                     | 0.73              |
| 1:F:116:PRO:HB3  | 1:F:122:MET:HE2  | 1.71                     | 0.73              |
| 1:K:116:PRO:HB3  | 1:K:122:MET:HE2  | 1.69                     | 0.73              |
| 1:E:397:THR:C    | 1:E:400:LYS:HG3  | 2.12                     | 0.73              |
| 1:E:108:GLU:OE1  | 1:E:124:ARG:NH2  | 2.22                     | 0.73              |
| 1:E:373:GLN:OE1  | 1:F:361:TYR:OH   | 2.06                     | 0.73              |
| 1:I:224:ARG:O    | 1:I:230:ARG:NH1  | 2.22                     | 0.73              |
| 1:D:282:PRO:HB3  | 1:J:386:LEU:HD11 | 1.69                     | 0.72              |
| 1:C:348:ARG:HD2  | 1:C:348:ARG:N    | 2.04                     | 0.72              |
| 1:I:207:PRO:HA   | 1:I:210:LEU:HD12 | 1.71                     | 0.72              |
| 1:A:138:PRO:HD2  | 1:A:141:LEU:HD12 | 1.71                     | 0.72              |
| 1:H:52:LEU:HD23  | 1:H:166:MET:HE3  | 1.70                     | 0.72              |
| 1:H:387:THR:HB   | 1:H:390:GLU:HG3  | 1.71                     | 0.72              |
| 1:A:104:ILE:O    | 1:A:105:ASP:HB2  | 1.89                     | 0.72              |
| 1:D:249:ARG:HA   | 1:I:227:MET:HE1  | 1.71                     | 0.72              |
| 1:K:388:GLN:OE1  | 1:K:388:GLN:N    | 2.21                     | 0.72              |
| 1:E:379:ARG:NH1  | 1:E:383:ASP:OD1  | 2.23                     | 0.72              |
| 1:L:104:ILE:O    | 1:L:105:ASP:HB2  | 1.89                     | 0.71              |
| 1:K:182:MET:SD   | 1:K:221:ASN:ND2  | 2.63                     | 0.71              |
| 1:M:143:HIS:O    | 1:M:145:THR:N    | 2.23                     | 0.71              |
| 1:A:116:PRO:HB3  | 1:A:122:MET:HE2  | 1.71                     | 0.71              |
| 1:I:398:LEU:O    | 1:I:400:LYS:HB2  | 1.90                     | 0.71              |
| 1:L:116:PRO:HB3  | 1:L:122:MET:HE2  | 1.71                     | 0.71              |
| 1:H:333:TYR:OH   | 1:H:354:ARG:NH1  | 2.24                     | 0.71              |
| 1:G:388:GLN:HE21 | 1:G:388:GLN:HA   | 1.55                     | 0.71              |
| 1:J:241:ARG:NH1  | 1:J:311:ARG:HE   | 1.88                     | 0.71              |
| 1:E:397:THR:O    | 1:E:400:LYS:HG3  | 1.91                     | 0.71              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:16:GLU:OE1   | 1:G:295:LYS:NZ   | 2.20                     | 0.71              |
| 1:B:374:GLY:HA3  | 1:B:395:ALA:HA   | 1.73                     | 0.71              |
| 1:B:197:GLN:HE21 | 1:B:201:GLN:HE21 | 1.37                     | 0.70              |
| 1:K:367:GLU:HG2  | 1:K:368:THR:N    | 1.91                     | 0.70              |
| 1:L:379:ARG:O    | 1:L:379:ARG:NH1  | 2.24                     | 0.70              |
| 1:E:150:SER:O    | 1:E:151:GLU:HB2  | 1.89                     | 0.70              |
| 1:L:111:SER:OG   | 1:L:112:PHE:HA   | 1.90                     | 0.70              |
| 1:L:187:GLN:HB2  | 1:L:188:PRO:HD2  | 1.74                     | 0.70              |
| 1:L:57:ARG:NH1   | 1:L:153:GLU:OE1  | 2.25                     | 0.70              |
| 1:A:87:HIS:HE1   | 1:E:28:PRO:HB3   | 1.56                     | 0.70              |
| 1:M:57:ARG:NH1   | 1:M:153:GLU:OE2  | 2.25                     | 0.70              |
| 1:G:393:GLU:O    | 1:G:397:THR:OG1  | 2.07                     | 0.70              |
| 1:I:386:LEU:HD11 | 1:M:282:PRO:HB3  | 1.72                     | 0.70              |
| 1:H:59:VAL:O     | 1:H:69:ARG:NH1   | 2.25                     | 0.70              |
| 1:J:142:ASN:O    | 1:J:212:GLN:NE2  | 2.22                     | 0.70              |
| 1:E:386:LEU:HD21 | 1:F:282:PRO:HB3  | 1.73                     | 0.69              |
| 1:J:238:GLN:NE2  | 1:J:308:GLU:OE1  | 2.25                     | 0.69              |
| 1:H:181:CYS:O    | 1:H:182:MET:HB2  | 1.90                     | 0.69              |
| 1:K:111:SER:OG   | 1:K:112:PHE:HA   | 1.93                     | 0.69              |
| 1:A:224:ARG:O    | 1:A:230:ARG:NH1  | 2.26                     | 0.69              |
| 1:E:388:GLN:N    | 1:E:388:GLN:OE1  | 2.24                     | 0.69              |
| 1:L:396:ASN:HA   | 1:L:399:ALA:HB3  | 1.74                     | 0.69              |
| 1:B:16:GLU:OE1   | 1:B:295:LYS:NZ   | 2.20                     | 0.69              |
| 1:D:16:GLU:OE1   | 1:D:295:LYS:NZ   | 2.21                     | 0.69              |
| 1:M:11:PHE:O     | 1:M:15:GLN:HG2   | 1.93                     | 0.69              |
| 1:E:148:VAL:HG23 | 1:E:212:GLN:HG2  | 1.73                     | 0.68              |
| 1:L:393:GLU:O    | 1:L:397:THR:OG1  | 2.09                     | 0.68              |
| 1:F:111:SER:HB3  | 1:F:112:PHE:HA   | 1.75                     | 0.68              |
| 1:G:374:GLY:HA3  | 1:G:395:ALA:HA   | 1.75                     | 0.68              |
| 1:K:181:CYS:O    | 1:K:182:MET:HB2  | 1.92                     | 0.68              |
| 1:C:9:GLU:OE2    | 1:F:379:ARG:NH2  | 2.27                     | 0.68              |
| 1:G:396:ASN:C    | 1:G:399:ALA:HB2  | 2.17                     | 0.68              |
| 1:K:396:ASN:O    | 1:K:400:LYS:HG2  | 1.94                     | 0.68              |
| 1:C:15:GLN:HE21  | 1:F:304:GLN:HG2  | 1.59                     | 0.68              |
| 1:I:373:GLN:HB2  | 1:I:398:LEU:HD22 | 1.75                     | 0.68              |
| 1:D:116:PRO:HB3  | 1:D:122:MET:HE2  | 1.75                     | 0.68              |
| 1:I:116:PRO:HB3  | 1:I:122:MET:HE2  | 1.75                     | 0.68              |
| 1:I:333:TYR:OH   | 1:I:354:ARG:NH1  | 2.26                     | 0.68              |
| 1:L:53:LEU:HD13  | 1:L:153:GLU:HG2  | 1.76                     | 0.68              |
| 1:G:181:CYS:O    | 1:G:182:MET:HB2  | 1.93                     | 0.68              |
| 1:J:57:ARG:NH1   | 1:J:153:GLU:OE2  | 2.24                     | 0.68              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:196:LEU:HD23 | 1:L:210:LEU:HD11 | 1.74                     | 0.68              |
| 1:F:224:ARG:O    | 1:F:230:ARG:NH1  | 2.27                     | 0.68              |
| 1:H:173:GLN:HE22 | 1:H:211:LEU:HG   | 1.58                     | 0.68              |
| 1:C:38:PHE:HB3   | 1:C:104:ILE:HD12 | 1.76                     | 0.68              |
| 1:G:18:GLN:NE2   | 1:H:308:GLU:OE1  | 2.26                     | 0.68              |
| 1:H:57:ARG:NH1   | 1:H:153:GLU:OE2  | 2.28                     | 0.68              |
| 1:F:393:GLU:O    | 1:F:397:THR:HG23 | 1.95                     | 0.67              |
| 1:G:304:GLN:OE1  | 1:K:15:GLN:NE2   | 2.27                     | 0.67              |
| 1:M:16:GLU:OE1   | 1:M:295:LYS:NZ   | 2.22                     | 0.67              |
| 1:F:241:ARG:HH12 | 1:F:311:ARG:HE   | 1.43                     | 0.67              |
| 1:K:57:ARG:NH1   | 1:K:153:GLU:OE2  | 2.28                     | 0.67              |
| 1:D:177:VAL:HB   | 1:D:220:GLN:HG3  | 1.76                     | 0.67              |
| 1:G:187:GLN:OE1  | 1:G:217:ARG:NH1  | 2.28                     | 0.67              |
| 1:J:141:LEU:O    | 1:J:142:ASN:HB3  | 1.94                     | 0.67              |
| 1:M:187:GLN:CG   | 1:M:188:PRO:HD2  | 2.24                     | 0.67              |
| 1:D:386:LEU:HD11 | 1:I:282:PRO:HB3  | 1.77                     | 0.67              |
| 1:G:282:PRO:HB3  | 1:H:386:LEU:HD11 | 1.76                     | 0.67              |
| 1:I:7:ALA:HA     | 1:I:10:ARG:HE    | 1.60                     | 0.67              |
| 1:I:196:LEU:O    | 1:I:200:ARG:HG3  | 1.95                     | 0.66              |
| 1:J:87:HIS:HE1   | 1:J:236:GLU:CD   | 2.03                     | 0.66              |
| 1:A:15:GLN:NE2   | 1:M:303:TYR:CE1  | 2.61                     | 0.66              |
| 1:C:33:PRO:HB3   | 1:F:161:GLU:HG2  | 1.77                     | 0.66              |
| 1:D:238:GLN:NE2  | 1:D:308:GLU:OE1  | 2.28                     | 0.66              |
| 1:J:181:CYS:O    | 1:J:182:MET:HG2  | 1.96                     | 0.66              |
| 1:M:173:GLN:HE22 | 1:M:210:LEU:HA   | 1.60                     | 0.66              |
| 1:J:282:PRO:HB2  | 1:K:394:MET:HE1  | 1.77                     | 0.66              |
| 1:C:147:PHE:O    | 1:C:149:ASP:N    | 2.28                     | 0.66              |
| 1:J:147:PHE:O    | 1:J:149:ASP:N    | 2.28                     | 0.66              |
| 1:C:187:GLN:HB2  | 1:C:188:PRO:HD2  | 1.77                     | 0.66              |
| 1:B:76:MET:HA    | 1:B:79:LEU:HD12  | 1.78                     | 0.65              |
| 1:G:108:GLU:OE1  | 1:G:124:ARG:NH2  | 2.29                     | 0.65              |
| 1:B:147:PHE:O    | 1:B:149:ASP:N    | 2.26                     | 0.65              |
| 1:D:147:PHE:O    | 1:D:149:ASP:N    | 2.30                     | 0.65              |
| 1:E:224:ARG:O    | 1:E:230:ARG:NH1  | 2.30                     | 0.65              |
| 1:H:393:GLU:O    | 1:H:397:THR:HG23 | 1.96                     | 0.65              |
| 1:D:61:SER:O     | 1:D:69:ARG:NH2   | 2.28                     | 0.65              |
| 1:F:367:GLU:HA   | 1:F:370:ARG:HG3  | 1.78                     | 0.65              |
| 1:I:161:GLU:HG2  | 1:M:33:PRO:HB3   | 1.77                     | 0.65              |
| 1:A:57:ARG:NH1   | 1:A:153:GLU:OE2  | 2.29                     | 0.65              |
| 1:G:116:PRO:HB3  | 1:G:122:MET:HE2  | 1.78                     | 0.65              |
| 1:C:6:LYS:NZ     | 1:C:9:GLU:OE1    | 2.29                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:396:ASN:O    | 1:C:400:LYS:HG3  | 1.97                     | 0.64              |
| 1:I:104:ILE:O    | 1:I:105:ASP:HB2  | 1.98                     | 0.64              |
| 1:L:221:ASN:OD1  | 1:L:224:ARG:NH1  | 2.30                     | 0.64              |
| 1:E:345:VAL:O    | 1:E:348:ARG:HG2  | 1.95                     | 0.64              |
| 1:G:59:VAL:O     | 1:G:69:ARG:NH1   | 2.31                     | 0.64              |
| 1:H:379:ARG:HD2  | 1:H:379:ARG:O    | 1.98                     | 0.64              |
| 1:A:282:PRO:HB3  | 1:M:386:LEU:HD11 | 1.79                     | 0.64              |
| 1:H:105:ASP:CG   | 1:H:117:ASN:HD22 | 2.05                     | 0.64              |
| 1:J:116:PRO:HB3  | 1:J:122:MET:HE2  | 1.78                     | 0.64              |
| 1:B:387:THR:OG1  | 1:B:390:GLU:HG3  | 1.96                     | 0.64              |
| 1:G:104:ILE:O    | 1:G:105:ASP:HB2  | 1.96                     | 0.64              |
| 1:K:249:ARG:HG2  | 1:K:249:ARG:HH11 | 1.63                     | 0.64              |
| 1:L:16:GLU:OE1   | 1:L:295:LYS:NZ   | 2.25                     | 0.64              |
| 1:A:378:MET:O    | 1:A:382:GLU:HG3  | 1.98                     | 0.64              |
| 1:G:377:ASP:OD2  | 1:G:379:ARG:NE   | 2.30                     | 0.63              |
| 1:D:224:ARG:O    | 1:D:230:ARG:NH1  | 2.30                     | 0.63              |
| 1:D:104:ILE:HD11 | 1:D:114:LEU:HD22 | 1.80                     | 0.63              |
| 1:B:180:LYS:NZ   | 1:B:191:SER:OG   | 2.31                     | 0.63              |
| 1:C:50:ARG:HH22  | 1:C:110:GLY:H    | 1.47                     | 0.63              |
| 1:D:53:LEU:HD13  | 1:D:153:GLU:HG2  | 1.80                     | 0.63              |
| 1:E:104:ILE:O    | 1:E:105:ASP:HB2  | 1.98                     | 0.63              |
| 1:G:147:PHE:O    | 1:G:149:ASP:N    | 2.28                     | 0.63              |
| 1:I:40:LEU:HD21  | 1:I:47:LEU:HG    | 1.79                     | 0.63              |
| 1:E:221:ASN:OD1  | 1:E:224:ARG:NH1  | 2.31                     | 0.63              |
| 1:I:401:LEU:HD22 | 1:M:363:GLN:NE2  | 2.13                     | 0.63              |
| 1:C:159:GLU:OE1  | 1:C:161:GLU:HG2  | 1.99                     | 0.63              |
| 1:J:33:PRO:HB3   | 1:K:161:GLU:HG2  | 1.81                     | 0.63              |
| 1:C:76:MET:HA    | 1:C:79:LEU:HD12  | 1.80                     | 0.63              |
| 1:I:308:GLU:N    | 1:I:308:GLU:OE1  | 2.31                     | 0.63              |
| 1:H:116:PRO:HB3  | 1:H:122:MET:HE2  | 1.80                     | 0.62              |
| 1:A:295:LYS:HE2  | 1:A:328:ASN:HB3  | 1.81                     | 0.62              |
| 1:M:147:PHE:C    | 1:M:149:ASP:H    | 2.08                     | 0.62              |
| 1:E:57:ARG:NH1   | 1:E:153:GLU:OE1  | 2.32                     | 0.62              |
| 1:F:104:ILE:O    | 1:F:105:ASP:HB2  | 2.00                     | 0.62              |
| 1:A:59:VAL:O     | 1:A:69:ARG:NH1   | 2.33                     | 0.62              |
| 1:L:240:ALA:O    | 1:L:243:GLN:HG2  | 1.99                     | 0.62              |
| 1:H:240:ALA:O    | 1:H:243:GLN:HG2  | 2.00                     | 0.62              |
| 1:K:188:PRO:CB   | 1:K:189:ALA:HA   | 2.30                     | 0.62              |
| 1:C:390:GLU:O    | 1:C:394:MET:N    | 2.33                     | 0.62              |
| 1:J:104:ILE:O    | 1:J:105:ASP:HB2  | 2.00                     | 0.62              |
| 1:K:392:THR:O    | 1:K:396:ASN:N    | 2.29                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:397:THR:O    | 1:E:399:ALA:N    | 2.33                     | 0.62              |
| 1:M:53:LEU:HD13  | 1:M:153:GLU:HG3  | 1.82                     | 0.62              |
| 1:M:188:PRO:HB3  | 1:M:189:ALA:HB2  | 1.81                     | 0.62              |
| 1:C:87:HIS:HE1   | 1:C:251:TYR:OH   | 1.83                     | 0.61              |
| 1:D:59:VAL:O     | 1:D:69:ARG:NH1   | 2.33                     | 0.61              |
| 1:G:181:CYS:SG   | 3:N:101:PB:PB    | 2.01                     | 0.61              |
| 1:L:224:ARG:O    | 1:L:230:ARG:NH1  | 2.32                     | 0.61              |
| 1:A:147:PHE:O    | 1:A:149:ASP:N    | 2.32                     | 0.61              |
| 1:I:193:GLU:O    | 1:I:197:GLN:HG2  | 2.00                     | 0.61              |
| 1:B:173:GLN:HE22 | 1:B:210:LEU:HA   | 1.64                     | 0.61              |
| 1:B:196:LEU:O    | 1:B:200:ARG:HG3  | 2.00                     | 0.61              |
| 1:G:143:HIS:O    | 1:G:145:THR:N    | 2.33                     | 0.61              |
| 1:C:16:GLU:OE1   | 1:C:295:LYS:HE3  | 2.01                     | 0.61              |
| 1:L:155:THR:OG1  | 1:L:208:ARG:NH2  | 2.34                     | 0.61              |
| 1:L:354:ARG:HH21 | 2:N:36:U:H5      | 1.47                     | 0.61              |
| 1:A:182:MET:SD   | 1:A:221:ASN:ND2  | 2.74                     | 0.61              |
| 1:C:113:ARG:NH2  | 1:C:128:ASN:OD1  | 2.34                     | 0.61              |
| 1:C:187:GLN:N    | 1:C:187:GLN:OE1  | 2.34                     | 0.61              |
| 1:C:280:ARG:NH1  | 1:C:379:ARG:HH12 | 1.98                     | 0.61              |
| 1:C:325:ALA:O    | 1:C:328:ASN:ND2  | 2.30                     | 0.61              |
| 1:C:15:GLN:HE21  | 1:F:304:GLN:CG   | 2.12                     | 0.61              |
| 1:C:388:GLN:O    | 1:C:392:THR:OG1  | 2.18                     | 0.61              |
| 1:F:147:PHE:O    | 1:F:149:ASP:N    | 2.34                     | 0.61              |
| 1:K:240:ALA:O    | 1:K:243:GLN:HG2  | 1.99                     | 0.61              |
| 1:C:108:GLU:OE1  | 1:C:124:ARG:NH2  | 2.33                     | 0.60              |
| 1:D:124:ARG:HG3  | 1:D:124:ARG:HH11 | 1.66                     | 0.60              |
| 1:G:172:MET:SD   | 1:G:253:MET:HG2  | 2.41                     | 0.60              |
| 1:B:238:GLN:NE2  | 1:B:308:GLU:OE1  | 2.34                     | 0.60              |
| 1:E:53:LEU:HD13  | 1:E:153:GLU:HG2  | 1.83                     | 0.60              |
| 1:H:374:GLY:HA3  | 1:H:395:ALA:HA   | 1.83                     | 0.60              |
| 1:J:87:HIS:CE1   | 1:J:236:GLU:CD   | 2.79                     | 0.60              |
| 1:B:242:ALA:O    | 1:H:25:THR:N     | 2.24                     | 0.60              |
| 1:F:173:GLN:HE22 | 1:F:211:LEU:H    | 1.49                     | 0.60              |
| 1:G:143:HIS:CE1  | 1:G:150:SER:HB3  | 2.36                     | 0.60              |
| 1:H:152:VAL:O    | 1:H:155:THR:OG1  | 2.15                     | 0.60              |
| 1:A:196:LEU:O    | 1:A:200:ARG:HG3  | 2.01                     | 0.60              |
| 1:D:363:GLN:HB2  | 1:J:401:LEU:HD21 | 1.84                     | 0.60              |
| 1:E:379:ARG:HD2  | 1:E:379:ARG:O    | 2.01                     | 0.60              |
| 1:J:193:GLU:O    | 1:J:197:GLN:HG3  | 2.01                     | 0.60              |
| 1:L:145:THR:HG22 | 1:L:153:GLU:OE1  | 2.01                     | 0.60              |
| 1:C:283:THR:HG22 | 1:F:394:MET:HG3  | 1.84                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:33:PRO:HB3   | 1:J:161:GLU:HG2  | 1.83                     | 0.60              |
| 1:M:333:TYR:OH   | 1:M:354:ARG:NH1  | 2.34                     | 0.60              |
| 1:B:53:LEU:HD13  | 1:B:153:GLU:HG2  | 1.84                     | 0.60              |
| 1:B:388:GLN:O    | 1:B:392:THR:OG1  | 2.20                     | 0.60              |
| 1:H:311:ARG:HG3  | 1:H:311:ARG:HH11 | 1.65                     | 0.60              |
| 1:M:308:GLU:OE1  | 1:M:308:GLU:N    | 2.27                     | 0.60              |
| 1:B:165:ASP:O    | 1:B:169:SER:OG   | 2.17                     | 0.60              |
| 1:F:374:GLY:HA3  | 1:F:395:ALA:HA   | 1.84                     | 0.60              |
| 1:K:147:PHE:O    | 1:K:149:ASP:N    | 2.32                     | 0.60              |
| 1:G:76:MET:HA    | 1:G:79:LEU:HD12  | 1.84                     | 0.59              |
| 1:K:396:ASN:HB3  | 1:K:400:LYS:HE2  | 1.84                     | 0.59              |
| 1:L:147:PHE:O    | 1:L:149:ASP:N    | 2.34                     | 0.59              |
| 1:D:393:GLU:O    | 1:D:397:THR:HG23 | 2.03                     | 0.59              |
| 1:J:182:MET:HE1  | 1:J:221:ASN:HA   | 1.83                     | 0.59              |
| 1:A:87:HIS:HE1   | 1:E:28:PRO:CB    | 2.16                     | 0.59              |
| 1:D:400:LYS:HD2  | 1:D:400:LYS:O    | 2.03                     | 0.59              |
| 1:A:284:LEU:HD22 | 1:M:380:MET:HE2  | 1.84                     | 0.59              |
| 1:B:197:GLN:NE2  | 1:B:201:GLN:HE21 | 2.00                     | 0.59              |
| 1:G:240:ALA:O    | 1:G:243:GLN:HG2  | 2.01                     | 0.59              |
| 1:J:240:ALA:O    | 1:J:243:GLN:HG2  | 2.03                     | 0.59              |
| 1:I:53:LEU:HD13  | 1:I:153:GLU:HG2  | 1.84                     | 0.59              |
| 1:C:46:GLU:OE2   | 1:C:50:ARG:NH1   | 2.36                     | 0.59              |
| 1:C:53:LEU:HD13  | 1:C:153:GLU:HG2  | 1.83                     | 0.59              |
| 1:C:344:ASP:O    | 1:C:348:ARG:NH1  | 2.36                     | 0.59              |
| 1:C:387:THR:N    | 1:C:390:GLU:OE2  | 2.36                     | 0.59              |
| 1:D:188:PRO:HB2  | 1:D:189:ALA:CA   | 2.24                     | 0.59              |
| 1:G:224:ARG:O    | 1:G:230:ARG:NH1  | 2.36                     | 0.59              |
| 1:H:52:LEU:HD23  | 1:H:166:MET:CE   | 2.33                     | 0.59              |
| 1:L:59:VAL:O     | 1:L:69:ARG:NH1   | 2.36                     | 0.59              |
| 1:E:295:LYS:NZ   | 1:E:299:LEU:HD11 | 2.18                     | 0.58              |
| 1:I:373:GLN:HB2  | 1:I:398:LEU:CD2  | 2.33                     | 0.58              |
| 1:C:240:ALA:O    | 1:C:243:GLN:HG2  | 2.03                     | 0.58              |
| 1:H:173:GLN:NE2  | 1:H:211:LEU:HG   | 2.18                     | 0.58              |
| 1:C:386:LEU:HD11 | 1:L:282:PRO:HB3  | 1.85                     | 0.58              |
| 1:E:308:GLU:OE1  | 1:E:308:GLU:N    | 2.29                     | 0.58              |
| 1:F:59:VAL:O     | 1:F:69:ARG:NH1   | 2.36                     | 0.58              |
| 1:M:400:LYS:HD2  | 1:M:400:LYS:N    | 2.17                     | 0.58              |
| 1:L:52:LEU:HD23  | 1:L:166:MET:CE   | 2.32                     | 0.58              |
| 1:M:207:PRO:HA   | 1:M:210:LEU:CD1  | 2.34                     | 0.58              |
| 1:K:276:ALA:HB2  | 1:K:336:ALA:HB2  | 1.85                     | 0.58              |
| 1:D:104:ILE:O    | 1:D:105:ASP:HB2  | 2.03                     | 0.58              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:345:VAL:O    | 1:H:348:ARG:HG3  | 2.02                     | 0.58              |
| 1:E:240:ALA:O    | 1:E:243:GLN:HG2  | 2.03                     | 0.58              |
| 1:K:59:VAL:O     | 1:K:69:ARG:NH1   | 2.37                     | 0.58              |
| 1:F:182:MET:HE1  | 1:F:220:GLN:HG2  | 1.85                     | 0.58              |
| 1:H:108:GLU:OE2  | 1:H:113:ARG:NE   | 2.26                     | 0.58              |
| 1:C:396:ASN:OD1  | 1:C:397:THR:HG23 | 2.03                     | 0.58              |
| 1:D:388:GLN:O    | 1:D:392:THR:OG1  | 2.21                     | 0.58              |
| 1:H:13:LEU:HD21  | 1:H:297:LYS:HE2  | 1.85                     | 0.58              |
| 1:I:147:PHE:HA   | 1:I:210:LEU:O    | 2.04                     | 0.58              |
| 1:K:393:GLU:HA   | 1:K:396:ASN:HB2  | 1.86                     | 0.58              |
| 1:L:359:LYS:O    | 1:L:363:GLN:HG3  | 2.03                     | 0.58              |
| 1:M:104:ILE:O    | 1:M:105:ASP:HB2  | 2.02                     | 0.58              |
| 1:D:325:ALA:O    | 1:D:328:ASN:ND2  | 2.35                     | 0.58              |
| 1:E:59:VAL:O     | 1:E:69:ARG:NH1   | 2.37                     | 0.58              |
| 1:I:207:PRO:HA   | 1:I:210:LEU:CD1  | 2.34                     | 0.58              |
| 1:K:364:LEU:HD12 | 1:K:367:GLU:OE1  | 2.03                     | 0.58              |
| 1:L:374:GLY:HA3  | 1:L:395:ALA:HA   | 1.86                     | 0.57              |
| 1:J:50:ARG:HH11  | 1:J:111:SER:HB3  | 1.69                     | 0.57              |
| 1:L:76:MET:HA    | 1:L:79:LEU:HD12  | 1.85                     | 0.57              |
| 1:B:224:ARG:O    | 1:B:230:ARG:NH1  | 2.37                     | 0.57              |
| 1:E:169:SER:O    | 1:E:173:GLN:HG3  | 2.04                     | 0.57              |
| 1:L:276:ALA:HB2  | 1:L:336:ALA:HB2  | 1.84                     | 0.57              |
| 1:D:240:ALA:O    | 1:D:243:GLN:HG2  | 2.04                     | 0.57              |
| 1:H:63:GLY:O     | 1:H:65:ARG:NH1   | 2.37                     | 0.57              |
| 1:J:392:THR:O    | 1:J:396:ASN:N    | 2.29                     | 0.57              |
| 1:J:26:ILE:HD12  | 1:J:26:ILE:H     | 1.70                     | 0.57              |
| 1:B:117:ASN:HB3  | 1:B:119:ARG:HB3  | 1.87                     | 0.57              |
| 1:B:249:ARG:HG3  | 1:B:249:ARG:HH11 | 1.69                     | 0.57              |
| 1:E:295:LYS:HZ3  | 1:E:299:LEU:HD11 | 1.69                     | 0.57              |
| 1:M:240:ALA:O    | 1:M:243:GLN:HG2  | 2.04                     | 0.57              |
| 1:A:240:ALA:O    | 1:A:243:GLN:HG2  | 2.05                     | 0.57              |
| 1:B:79:LEU:HA    | 1:B:84:MET:HE3   | 1.87                     | 0.57              |
| 1:F:240:ALA:O    | 1:F:243:GLN:HG2  | 2.03                     | 0.57              |
| 1:M:104:ILE:HD11 | 1:M:114:LEU:HD22 | 1.87                     | 0.57              |
| 1:A:10:ARG:HG2   | 1:A:10:ARG:HH11  | 1.70                     | 0.57              |
| 1:K:104:ILE:O    | 1:K:105:ASP:HB2  | 2.03                     | 0.57              |
| 1:J:59:VAL:O     | 1:J:69:ARG:NH1   | 2.37                     | 0.56              |
| 1:L:396:ASN:HA   | 1:L:399:ALA:CB   | 2.34                     | 0.56              |
| 1:M:224:ARG:O    | 1:M:230:ARG:NH1  | 2.37                     | 0.56              |
| 1:A:190:ALA:O    | 1:A:194:LYS:N    | 2.37                     | 0.56              |
| 1:E:311:ARG:NH2  | 1:F:18:GLN:HG3   | 2.19                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:400:LYS:HZ2  | 1:J:401:LEU:HD13 | 1.70                     | 0.56              |
| 1:B:276:ALA:HB2  | 1:B:336:ALA:HB2  | 1.86                     | 0.56              |
| 1:F:181:CYS:O    | 1:F:182:MET:HG2  | 2.05                     | 0.56              |
| 1:H:104:ILE:O    | 1:H:105:ASP:HB2  | 2.05                     | 0.56              |
| 1:H:137:LEU:HD22 | 1:H:141:LEU:HD12 | 1.87                     | 0.56              |
| 1:B:61:SER:O     | 1:B:69:ARG:NH2   | 2.37                     | 0.56              |
| 1:B:147:PHE:HA   | 1:B:210:LEU:O    | 2.05                     | 0.56              |
| 1:I:147:PHE:O    | 1:I:149:ASP:N    | 2.37                     | 0.56              |
| 1:H:104:ILE:HD11 | 1:H:114:LEU:HD22 | 1.86                     | 0.56              |
| 1:L:6:LYS:HE3    | 1:L:10:ARG:NH2   | 2.21                     | 0.56              |
| 1:D:348:ARG:HD2  | 1:D:348:ARG:O    | 2.05                     | 0.56              |
| 1:E:87:HIS:CE1   | 1:E:232:PHE:HZ   | 2.24                     | 0.56              |
| 1:K:351:ALA:O    | 1:K:354:ARG:NH1  | 2.38                     | 0.56              |
| 1:H:392:THR:HA   | 1:H:395:ALA:HB3  | 1.86                     | 0.56              |
| 1:J:111:SER:HB2  | 1:J:112:PHE:HA   | 1.88                     | 0.56              |
| 1:L:52:LEU:HD23  | 1:L:166:MET:HE3  | 1.86                     | 0.56              |
| 1:L:138:PRO:HG2  | 1:L:141:LEU:HD13 | 1.87                     | 0.56              |
| 1:L:296:LEU:O    | 1:L:300:MET:HG3  | 2.05                     | 0.56              |
| 1:C:390:GLU:OE1  | 1:C:390:GLU:N    | 2.35                     | 0.56              |
| 1:D:177:VAL:HB   | 1:D:220:GLN:CG   | 2.36                     | 0.56              |
| 1:G:201:GLN:HE21 | 1:G:201:GLN:CA   | 2.13                     | 0.56              |
| 1:D:85:LEU:O     | 1:D:89:LYS:HG3   | 2.06                     | 0.55              |
| 1:C:169:SER:O    | 1:C:173:GLN:HG3  | 2.05                     | 0.55              |
| 1:I:111:SER:HB2  | 1:I:112:PHE:HA   | 1.88                     | 0.55              |
| 1:A:111:SER:HB2  | 1:A:112:PHE:HA   | 1.89                     | 0.55              |
| 1:B:175:TRP:CZ3  | 1:B:237:LEU:HD11 | 2.41                     | 0.55              |
| 1:G:387:THR:O    | 1:G:391:ARG:NE   | 2.38                     | 0.55              |
| 1:B:207:PRO:HA   | 1:B:210:LEU:CD1  | 2.36                     | 0.55              |
| 1:E:187:GLN:N    | 1:E:187:GLN:OE1  | 2.40                     | 0.55              |
| 1:L:104:ILE:HG13 | 1:L:105:ASP:N    | 2.21                     | 0.55              |
| 1:F:390:GLU:HA   | 1:F:393:GLU:HB3  | 1.87                     | 0.55              |
| 1:A:111:SER:CB   | 1:A:112:PHE:HA   | 2.37                     | 0.55              |
| 1:G:311:ARG:HH12 | 1:K:15:GLN:HG3   | 1.72                     | 0.55              |
| 1:J:277:LEU:HD23 | 1:J:284:LEU:HD21 | 1.89                     | 0.55              |
| 1:B:296:LEU:O    | 1:B:300:MET:HG3  | 2.07                     | 0.55              |
| 1:C:59:VAL:O     | 1:C:69:ARG:NH1   | 2.39                     | 0.55              |
| 1:G:341:TYR:O    | 1:G:348:ARG:NH1  | 2.38                     | 0.55              |
| 1:J:53:LEU:HD13  | 1:J:153:GLU:HG3  | 1.89                     | 0.55              |
| 1:G:94:SER:OG    | 1:G:231:HIS:ND1  | 2.37                     | 0.55              |
| 1:H:249:ARG:HG3  | 1:H:249:ARG:HH11 | 1.71                     | 0.55              |
| 1:G:399:ALA:HB1  | 1:G:400:LYS:HB3  | 1.88                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:196:LEU:O    | 1:F:200:ARG:HG3  | 2.07                     | 0.55              |
| 1:G:249:ARG:HG3  | 1:G:249:ARG:HH11 | 1.72                     | 0.55              |
| 1:E:142:ASN:O    | 1:E:143:HIS:HB2  | 2.05                     | 0.54              |
| 1:I:277:LEU:HD23 | 1:I:284:LEU:HD21 | 1.88                     | 0.54              |
| 1:C:194:LYS:HD3  | 1:C:194:LYS:N    | 2.22                     | 0.54              |
| 1:E:241:ARG:HD2  | 1:E:312:TYR:OH   | 2.07                     | 0.54              |
| 1:G:388:GLN:HA   | 1:G:388:GLN:NE2  | 2.21                     | 0.54              |
| 1:H:230:ARG:HH21 | 1:H:317:GLU:HG3  | 1.73                     | 0.54              |
| 1:D:221:ASN:OD1  | 1:D:225:LYS:NZ   | 2.32                     | 0.54              |
| 1:J:373:GLN:HG3  | 1:J:398:LEU:HG   | 1.88                     | 0.54              |
| 1:A:79:LEU:HA    | 1:A:84:MET:HE3   | 1.89                     | 0.54              |
| 1:B:197:GLN:HE21 | 1:B:201:GLN:NE2  | 2.03                     | 0.54              |
| 1:D:169:SER:O    | 1:D:173:GLN:HG3  | 2.06                     | 0.54              |
| 1:F:172:MET:O    | 1:F:176:ILE:HG13 | 2.07                     | 0.54              |
| 1:I:398:LEU:HA   | 1:I:400:LYS:CD   | 2.32                     | 0.54              |
| 1:L:193:GLU:O    | 1:L:197:GLN:HG3  | 2.07                     | 0.54              |
| 1:H:145:THR:HG23 | 1:H:146:PRO:O    | 2.08                     | 0.54              |
| 1:I:230:ARG:HH21 | 1:I:317:GLU:HG3  | 1.72                     | 0.54              |
| 1:K:188:PRO:HB2  | 1:K:189:ALA:HA   | 1.90                     | 0.54              |
| 1:J:196:LEU:O    | 1:J:200:ARG:HG3  | 2.07                     | 0.54              |
| 1:B:398:LEU:HD13 | 1:H:364:LEU:HD22 | 1.90                     | 0.54              |
| 1:H:79:LEU:HA    | 1:H:84:MET:HE3   | 1.89                     | 0.54              |
| 1:H:140:THR:HG21 | 1:H:214:GLU:OE1  | 2.08                     | 0.54              |
| 1:B:277:LEU:HD23 | 1:B:284:LEU:HD21 | 1.89                     | 0.54              |
| 1:D:181:CYS:O    | 1:D:182:MET:HG3  | 2.08                     | 0.54              |
| 1:F:53:LEU:HD13  | 1:F:153:GLU:HG2  | 1.89                     | 0.54              |
| 1:B:15:GLN:OE1   | 1:B:15:GLN:HA    | 2.07                     | 0.54              |
| 1:I:57:ARG:NH1   | 1:I:153:GLU:OE2  | 2.40                     | 0.54              |
| 1:J:196:LEU:HD23 | 1:J:210:LEU:HD21 | 1.89                     | 0.54              |
| 1:K:196:LEU:O    | 1:K:200:ARG:HG3  | 2.08                     | 0.54              |
| 1:G:196:LEU:O    | 1:G:200:ARG:HG3  | 2.08                     | 0.53              |
| 1:G:379:ARG:HG3  | 1:G:380:MET:N    | 2.22                     | 0.53              |
| 1:I:155:THR:OG1  | 1:I:208:ARG:NH2  | 2.41                     | 0.53              |
| 1:K:277:LEU:HD23 | 1:K:284:LEU:HD21 | 1.88                     | 0.53              |
| 1:L:172:MET:O    | 1:L:176:ILE:HG13 | 2.07                     | 0.53              |
| 1:A:146:PRO:O    | 1:A:147:PHE:HB2  | 2.08                     | 0.53              |
| 1:J:169:SER:O    | 1:J:173:GLN:HG3  | 2.08                     | 0.53              |
| 1:C:388:GLN:OE1  | 1:C:392:THR:OG1  | 2.25                     | 0.53              |
| 1:D:238:GLN:OE1  | 1:D:309:GLN:NE2  | 2.36                     | 0.53              |
| 1:F:36:ARG:NH1   | 1:F:126:GLU:OE2  | 2.41                     | 0.53              |
| 1:I:111:SER:CB   | 1:I:112:PHE:HA   | 2.39                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:111:SER:CB   | 1:J:112:PHE:HA   | 2.38                     | 0.53              |
| 1:A:111:SER:HA   | 1:A:113:ARG:H    | 1.74                     | 0.53              |
| 1:B:23:GLU:H     | 1:B:23:GLU:CD    | 2.15                     | 0.53              |
| 1:L:61:SER:O     | 1:L:69:ARG:NH2   | 2.40                     | 0.53              |
| 1:L:357:MET:HE1  | 1:L:362:PHE:CD1  | 2.43                     | 0.53              |
| 1:G:372:GLN:NE2  | 1:H:393:GLU:OE2  | 2.40                     | 0.53              |
| 1:K:391:ARG:HG2  | 1:K:392:THR:N    | 2.23                     | 0.53              |
| 1:E:397:THR:HG22 | 1:E:400:LYS:CD   | 2.34                     | 0.53              |
| 1:F:172:MET:SD   | 1:F:253:MET:HG2  | 2.49                     | 0.53              |
| 1:I:79:LEU:HA    | 1:I:84:MET:HE3   | 1.90                     | 0.53              |
| 1:I:296:LEU:O    | 1:I:300:MET:HG3  | 2.08                     | 0.53              |
| 1:J:65:ARG:NH2   | 1:J:66:ASP:OD2   | 2.38                     | 0.53              |
| 1:M:301:ALA:O    | 1:M:305:THR:HG23 | 2.08                     | 0.53              |
| 1:E:10:ARG:HH11  | 1:E:10:ARG:CG    | 2.21                     | 0.53              |
| 1:E:373:GLN:HB3  | 1:E:398:LEU:HD21 | 1.91                     | 0.53              |
| 1:H:180:LYS:NZ   | 1:H:191:SER:OG   | 2.42                     | 0.53              |
| 1:I:111:SER:HA   | 1:I:113:ARG:H    | 1.74                     | 0.53              |
| 1:J:111:SER:HA   | 1:J:113:ARG:H    | 1.73                     | 0.53              |
| 1:K:387:THR:HG22 | 1:K:390:GLU:CD   | 2.33                     | 0.53              |
| 1:A:283:THR:HA   | 1:M:394:MET:SD   | 2.49                     | 0.53              |
| 1:G:384:LEU:HB3  | 1:G:386:LEU:HD23 | 1.91                     | 0.53              |
| 1:I:354:ARG:HH21 | 2:N:78:U:H5      | 1.55                     | 0.53              |
| 1:B:39:ILE:HG12  | 1:B:101:ARG:O    | 2.09                     | 0.53              |
| 1:H:111:SER:HA   | 1:H:113:ARG:H    | 1.74                     | 0.53              |
| 1:K:198:LYS:HE3  | 2:N:64:U:O4'     | 2.09                     | 0.53              |
| 1:J:394:MET:O    | 1:J:398:LEU:N    | 2.32                     | 0.53              |
| 1:A:190:ALA:HB1  | 1:A:194:LYS:HD2  | 1.90                     | 0.52              |
| 1:F:392:THR:C    | 1:F:394:MET:H    | 2.18                     | 0.52              |
| 1:K:94:SER:OG    | 1:K:231:HIS:ND1  | 2.22                     | 0.52              |
| 1:K:175:TRP:CZ3  | 1:K:237:LEU:HD11 | 2.45                     | 0.52              |
| 1:L:39:ILE:HG12  | 1:L:101:ARG:O    | 2.10                     | 0.52              |
| 1:A:182:MET:HE1  | 1:A:217:ARG:O    | 2.09                     | 0.52              |
| 1:D:57:ARG:NH1   | 1:D:153:GLU:OE1  | 2.42                     | 0.52              |
| 1:I:240:ALA:O    | 1:I:243:GLN:HG2  | 2.09                     | 0.52              |
| 1:J:175:TRP:CZ3  | 1:J:237:LEU:HD13 | 2.44                     | 0.52              |
| 1:K:108:GLU:OE1  | 1:K:113:ARG:NE   | 2.35                     | 0.52              |
| 1:E:197:GLN:O    | 1:E:201:GLN:HG2  | 2.09                     | 0.52              |
| 1:H:61:SER:O     | 1:H:69:ARG:NH2   | 2.38                     | 0.52              |
| 1:E:221:ASN:O    | 1:E:225:LYS:HG3  | 2.09                     | 0.52              |
| 1:G:111:SER:HB2  | 1:G:112:PHE:HA   | 1.92                     | 0.52              |
| 1:G:169:SER:O    | 1:G:173:GLN:HG3  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:221:ASN:O    | 1:K:225:LYS:HG3  | 2.10                     | 0.52              |
| 1:M:169:SER:O    | 1:M:173:GLN:HG3  | 2.09                     | 0.52              |
| 1:D:111:SER:HB2  | 1:D:112:PHE:HA   | 1.92                     | 0.52              |
| 1:D:221:ASN:O    | 1:D:225:LYS:HD3  | 2.10                     | 0.52              |
| 1:D:296:LEU:O    | 1:D:300:MET:HG3  | 2.10                     | 0.52              |
| 1:M:155:THR:OG1  | 1:M:208:ARG:NH2  | 2.42                     | 0.52              |
| 1:A:38:PHE:CD1   | 1:A:104:ILE:HD12 | 2.44                     | 0.52              |
| 1:A:213:PRO:HG2  | 1:A:214:GLU:OE2  | 2.10                     | 0.52              |
| 1:E:369:ALA:O    | 1:E:373:GLN:HG2  | 2.10                     | 0.52              |
| 1:J:50:ARG:NH1   | 1:J:111:SER:HB3  | 2.25                     | 0.52              |
| 1:M:373:GLN:HG2  | 1:M:398:LEU:HD21 | 1.91                     | 0.52              |
| 1:B:240:ALA:O    | 1:B:243:GLN:HG2  | 2.10                     | 0.52              |
| 1:C:46:GLU:O     | 1:C:50:ARG:HB2   | 2.10                     | 0.52              |
| 1:D:393:GLU:HA   | 1:D:396:ASN:HB2  | 1.92                     | 0.52              |
| 1:K:180:LYS:NZ   | 1:K:191:SER:OG   | 2.42                     | 0.52              |
| 1:K:122:MET:HG2  | 1:K:126:GLU:OE1  | 2.09                     | 0.52              |
| 1:E:206:ASN:HB3  | 1:E:209:TYR:HD2  | 1.75                     | 0.51              |
| 1:F:388:GLN:C    | 1:F:391:ARG:HB2  | 2.35                     | 0.51              |
| 1:G:397:THR:C    | 1:G:399:ALA:HB2  | 2.35                     | 0.51              |
| 1:J:234:THR:O    | 1:J:238:GLN:HG3  | 2.10                     | 0.51              |
| 1:K:87:HIS:O     | 1:K:90:LEU:HB2   | 2.10                     | 0.51              |
| 1:L:45:PRO:O     | 1:L:49:SER:OG    | 2.23                     | 0.51              |
| 1:L:87:HIS:HE1   | 1:L:251:TYR:OH   | 1.92                     | 0.51              |
| 1:A:284:LEU:CD2  | 1:M:380:MET:HE2  | 2.40                     | 0.51              |
| 1:C:280:ARG:NH1  | 1:C:379:ARG:NH1  | 2.58                     | 0.51              |
| 1:F:79:LEU:HA    | 1:F:84:MET:HE3   | 1.91                     | 0.51              |
| 1:H:147:PHE:HB3  | 1:H:152:VAL:HG11 | 1.93                     | 0.51              |
| 1:J:20:GLN:NE2   | 1:J:320:HIS:CE1  | 2.75                     | 0.51              |
| 1:F:277:LEU:HD23 | 1:F:284:LEU:HD21 | 1.91                     | 0.51              |
| 1:J:87:HIS:CE1   | 1:J:236:GLU:OE2  | 2.64                     | 0.51              |
| 1:M:111:SER:HB2  | 1:M:112:PHE:HA   | 1.91                     | 0.51              |
| 1:M:396:ASN:O    | 1:M:400:LYS:HD3  | 2.11                     | 0.51              |
| 1:B:175:TRP:HZ3  | 1:B:237:LEU:HD11 | 1.74                     | 0.51              |
| 1:D:172:MET:O    | 1:D:176:ILE:HG13 | 2.09                     | 0.51              |
| 1:F:169:SER:O    | 1:F:173:GLN:HG3  | 2.10                     | 0.51              |
| 1:I:374:GLY:HA3  | 1:I:395:ALA:HA   | 1.92                     | 0.51              |
| 1:D:387:THR:OG1  | 1:D:390:GLU:HG3  | 2.10                     | 0.51              |
| 1:I:138:PRO:HD2  | 1:I:141:LEU:HD22 | 1.92                     | 0.51              |
| 1:I:398:LEU:HD23 | 1:I:398:LEU:C    | 2.36                     | 0.51              |
| 1:B:169:SER:O    | 1:B:173:GLN:HG3  | 2.10                     | 0.51              |
| 1:J:223:ILE:O    | 1:J:230:ARG:HD3  | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:76:MET:HA    | 1:M:79:LEU:HD12  | 1.92                     | 0.51              |
| 1:C:198:LYS:HE3  | 2:N:34:U:O4'     | 2.11                     | 0.51              |
| 1:E:230:ARG:HG2  | 1:E:315:LEU:HG   | 1.93                     | 0.51              |
| 1:I:65:ARG:CZ    | 1:I:65:ARG:HB3   | 2.39                     | 0.51              |
| 1:L:223:ILE:O    | 1:L:230:ARG:HD3  | 2.11                     | 0.51              |
| 1:B:111:SER:HB2  | 1:B:112:PHE:HA   | 1.92                     | 0.51              |
| 1:I:40:LEU:HD11  | 1:I:47:LEU:HD21  | 1.92                     | 0.51              |
| 1:F:393:GLU:OE2  | 1:F:394:MET:HE3  | 2.11                     | 0.51              |
| 1:L:169:SER:O    | 1:L:173:GLN:HG3  | 2.11                     | 0.51              |
| 1:B:198:LYS:HE3  | 2:N:46:U:O4'     | 2.10                     | 0.51              |
| 1:C:172:MET:SD   | 1:C:253:MET:HG2  | 2.51                     | 0.51              |
| 1:G:111:SER:HA   | 1:G:113:ARG:H    | 1.75                     | 0.51              |
| 1:K:76:MET:HA    | 1:K:79:LEU:HD12  | 1.94                     | 0.50              |
| 1:D:3:SER:HA     | 1:D:6:LYS:HE3    | 1.91                     | 0.50              |
| 1:D:79:LEU:HA    | 1:D:84:MET:HE3   | 1.93                     | 0.50              |
| 1:G:357:MET:HE3  | 1:G:362:PHE:HB2  | 1.93                     | 0.50              |
| 1:G:361:TYR:OH   | 1:H:373:GLN:OE1  | 2.15                     | 0.50              |
| 1:K:53:LEU:HD13  | 1:K:153:GLU:HG2  | 1.94                     | 0.50              |
| 1:K:87:HIS:CE1   | 1:K:90:LEU:HD22  | 2.46                     | 0.50              |
| 1:K:223:ILE:O    | 1:K:230:ARG:HD3  | 2.12                     | 0.50              |
| 1:M:296:LEU:O    | 1:M:300:MET:HG3  | 2.11                     | 0.50              |
| 1:A:108:GLU:OE1  | 1:A:124:ARG:NH2  | 2.44                     | 0.50              |
| 1:H:111:SER:CB   | 1:H:112:PHE:HA   | 2.42                     | 0.50              |
| 1:J:20:GLN:OE1   | 1:J:320:HIS:HE1  | 1.93                     | 0.50              |
| 1:E:181:CYS:O    | 1:E:182:MET:HG2  | 2.10                     | 0.50              |
| 1:G:79:LEU:HA    | 1:G:84:MET:HE3   | 1.94                     | 0.50              |
| 1:G:283:THR:HG22 | 1:H:394:MET:HG3  | 1.92                     | 0.50              |
| 1:L:379:ARG:NH1  | 1:L:383:ASP:OD2  | 2.41                     | 0.50              |
| 1:C:177:VAL:HG12 | 1:C:192:ILE:HD12 | 1.94                     | 0.50              |
| 1:G:388:GLN:HE21 | 1:G:388:GLN:CA   | 2.24                     | 0.50              |
| 1:M:147:PHE:O    | 1:M:149:ASP:N    | 2.44                     | 0.50              |
| 1:K:172:MET:O    | 1:K:176:ILE:HG13 | 2.11                     | 0.50              |
| 1:A:357:MET:HE1  | 1:A:362:PHE:CD1  | 2.47                     | 0.50              |
| 1:H:196:LEU:O    | 1:H:200:ARG:HG3  | 2.12                     | 0.50              |
| 1:I:175:TRP:CZ3  | 1:I:237:LEU:HD11 | 2.46                     | 0.50              |
| 1:A:76:MET:HA    | 1:A:79:LEU:HD12  | 1.93                     | 0.50              |
| 1:C:104:ILE:O    | 1:C:115:ILE:O    | 2.29                     | 0.50              |
| 1:F:108:GLU:OE1  | 1:F:124:ARG:NH2  | 2.45                     | 0.50              |
| 1:G:111:SER:CB   | 1:G:112:PHE:HA   | 2.42                     | 0.50              |
| 1:H:390:GLU:HA   | 1:H:393:GLU:HB3  | 1.94                     | 0.50              |
| 1:L:187:GLN:HE22 | 1:L:217:ARG:HD2  | 1.77                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:234:THR:O    | 1:D:238:GLN:HG3  | 2.12                     | 0.50              |
| 1:F:76:MET:HA    | 1:F:79:LEU:HD12  | 1.93                     | 0.50              |
| 1:H:111:SER:HB2  | 1:H:112:PHE:HA   | 1.93                     | 0.50              |
| 1:H:187:GLN:HB3  | 1:H:188:PRO:HD2  | 1.92                     | 0.50              |
| 1:H:357:MET:HE1  | 1:H:362:PHE:CD1  | 2.47                     | 0.50              |
| 1:K:104:ILE:HD11 | 1:K:114:LEU:HD22 | 1.94                     | 0.50              |
| 1:K:18:GLN:HG3   | 1:K:19:ASP:N     | 2.26                     | 0.49              |
| 1:K:79:LEU:HA    | 1:K:84:MET:HE3   | 1.92                     | 0.49              |
| 1:K:388:GLN:N    | 1:K:388:GLN:CD   | 2.70                     | 0.49              |
| 1:C:36:ARG:NH2   | 1:C:130:TYR:OH   | 2.45                     | 0.49              |
| 1:D:276:ALA:HB2  | 1:D:336:ALA:HB2  | 1.94                     | 0.49              |
| 1:G:53:LEU:HD13  | 1:G:153:GLU:HG3  | 1.93                     | 0.49              |
| 1:G:161:GLU:HG2  | 1:K:33:PRO:HB3   | 1.94                     | 0.49              |
| 1:A:206:ASN:HB3  | 1:A:209:TYR:HD2  | 1.77                     | 0.49              |
| 1:C:31:LEU:HD13  | 1:F:160:ILE:HD11 | 1.94                     | 0.49              |
| 1:D:111:SER:HA   | 1:D:113:ARG:H    | 1.77                     | 0.49              |
| 1:F:18:GLN:C     | 1:F:20:GLN:H     | 2.15                     | 0.49              |
| 1:G:104:ILE:HD12 | 1:G:114:LEU:HD22 | 1.95                     | 0.49              |
| 1:G:364:LEU:HD22 | 1:H:398:LEU:HD13 | 1.94                     | 0.49              |
| 1:H:173:GLN:OE1  | 1:H:210:LEU:HD12 | 2.13                     | 0.49              |
| 1:B:197:GLN:HA   | 1:B:200:ARG:HB2  | 1.95                     | 0.49              |
| 1:L:143:HIS:CE1  | 1:L:150:SER:HB3  | 2.48                     | 0.49              |
| 1:C:235:PHE:O    | 1:C:239:LEU:HD13 | 2.13                     | 0.49              |
| 1:G:104:ILE:O    | 1:G:115:ILE:O    | 2.29                     | 0.49              |
| 1:I:149:ASP:O    | 1:I:152:VAL:HG22 | 2.13                     | 0.49              |
| 1:K:181:CYS:O    | 1:K:224:ARG:NH1  | 2.45                     | 0.49              |
| 1:M:196:LEU:O    | 1:M:200:ARG:HG3  | 2.13                     | 0.49              |
| 1:C:276:ALA:HB2  | 1:C:336:ALA:HB2  | 1.94                     | 0.49              |
| 1:D:105:ASP:CG   | 1:D:117:ASN:HD22 | 2.21                     | 0.49              |
| 1:E:259:LYS:NZ   | 1:F:323:ASP:OD1  | 2.40                     | 0.49              |
| 1:H:181:CYS:SG   | 2:N:48:U:H1'     | 2.53                     | 0.49              |
| 1:K:145:THR:HG23 | 1:K:146:PRO:O    | 2.12                     | 0.49              |
| 1:E:79:LEU:HA    | 1:E:84:MET:HE3   | 1.93                     | 0.49              |
| 1:G:236:GLU:OE2  | 1:G:251:TYR:OH   | 2.23                     | 0.49              |
| 1:G:276:ALA:HB2  | 1:G:336:ALA:HB2  | 1.95                     | 0.49              |
| 1:H:149:ASP:O    | 1:H:152:VAL:HG12 | 2.12                     | 0.49              |
| 1:I:221:ASN:O    | 1:I:225:LYS:HG3  | 2.13                     | 0.49              |
| 1:J:180:LYS:NZ   | 1:J:191:SER:OG   | 2.46                     | 0.49              |
| 1:A:53:LEU:HD13  | 1:A:153:GLU:HG3  | 1.95                     | 0.49              |
| 1:G:40:LEU:HD21  | 1:G:47:LEU:HB3   | 1.94                     | 0.49              |
| 1:M:198:LYS:HE3  | 2:N:10:U:O4'     | 2.13                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:33:PRO:HB3   | 1:L:161:GLU:HG2  | 1.94                     | 0.49              |
| 1:B:111:SER:HA   | 1:B:113:ARG:H    | 1.77                     | 0.49              |
| 1:D:249:ARG:NH1  | 1:D:253:MET:HE2  | 2.27                     | 0.49              |
| 1:J:172:MET:SD   | 1:J:253:MET:HG2  | 2.53                     | 0.49              |
| 1:A:221:ASN:OD1  | 1:A:224:ARG:NH2  | 2.42                     | 0.48              |
| 1:F:85:LEU:O     | 1:F:89:LYS:HG3   | 2.12                     | 0.48              |
| 1:F:395:ALA:O    | 1:F:399:ALA:HB2  | 2.13                     | 0.48              |
| 1:H:104:ILE:O    | 1:H:115:ILE:O    | 2.31                     | 0.48              |
| 1:H:122:MET:HG2  | 1:H:126:GLU:OE1  | 2.13                     | 0.48              |
| 1:H:388:GLN:O    | 1:H:388:GLN:HG3  | 2.13                     | 0.48              |
| 1:J:85:LEU:O     | 1:J:89:LYS:HG3   | 2.13                     | 0.48              |
| 1:B:111:SER:CB   | 1:B:112:PHE:HA   | 2.43                     | 0.48              |
| 1:A:6:LYS:HD2    | 1:A:6:LYS:HA     | 1.60                     | 0.48              |
| 1:A:31:LEU:HD13  | 1:M:160:ILE:HD11 | 1.96                     | 0.48              |
| 1:A:61:SER:O     | 1:A:69:ARG:NH2   | 2.45                     | 0.48              |
| 1:D:146:PRO:O    | 1:D:147:PHE:HB2  | 2.11                     | 0.48              |
| 1:D:206:ASN:HB3  | 1:D:209:TYR:HD2  | 1.77                     | 0.48              |
| 1:H:172:MET:SD   | 1:H:253:MET:HG2  | 2.52                     | 0.48              |
| 1:M:39:ILE:HG12  | 1:M:101:ARG:O    | 2.12                     | 0.48              |
| 1:A:188:PRO:O    | 1:A:191:SER:HB3  | 2.14                     | 0.48              |
| 1:D:111:SER:CB   | 1:D:112:PHE:HA   | 2.44                     | 0.48              |
| 1:E:172:MET:O    | 1:E:176:ILE:HG13 | 2.13                     | 0.48              |
| 1:G:239:LEU:HD23 | 1:K:28:PRO:HG2   | 1.95                     | 0.48              |
| 1:I:142:ASN:O    | 1:I:143:HIS:HB2  | 2.12                     | 0.48              |
| 1:K:23:GLU:CD    | 1:K:24:GLY:H     | 2.21                     | 0.48              |
| 1:K:104:ILE:HG23 | 1:K:105:ASP:N    | 2.28                     | 0.48              |
| 1:M:79:LEU:HA    | 1:M:84:MET:HE3   | 1.96                     | 0.48              |
| 1:D:241:ARG:HH12 | 1:D:308:GLU:HG3  | 1.79                     | 0.48              |
| 1:F:57:ARG:NH2   | 1:F:144:ALA:O    | 2.47                     | 0.48              |
| 1:G:394:MET:HE2  | 1:K:283:THR:HG23 | 1.95                     | 0.48              |
| 1:I:169:SER:O    | 1:I:173:GLN:HG3  | 2.12                     | 0.48              |
| 1:K:169:SER:O    | 1:K:173:GLN:HG3  | 2.13                     | 0.48              |
| 1:K:182:MET:HA   | 1:K:220:GLN:NE2  | 2.28                     | 0.48              |
| 1:M:14:THR:O     | 1:M:18:GLN:HG2   | 2.13                     | 0.48              |
| 1:A:198:LYS:HE3  | 2:N:16:U:O4'     | 2.13                     | 0.48              |
| 1:B:18:GLN:HG2   | 1:B:19:ASP:N     | 2.28                     | 0.48              |
| 1:C:85:LEU:O     | 1:C:89:LYS:HG3   | 2.14                     | 0.48              |
| 1:D:113:ARG:HG2  | 1:D:127:ILE:HG22 | 1.96                     | 0.48              |
| 1:G:61:SER:O     | 1:G:69:ARG:NH2   | 2.41                     | 0.48              |
| 1:J:61:SER:O     | 1:J:69:ARG:NH2   | 2.40                     | 0.48              |
| 1:L:111:SER:HA   | 1:L:113:ARG:H    | 1.78                     | 0.48              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:L:197:GLN:O   | 1:L:201:GLN:HG3  | 2.14                     | 0.48              |
| 1:L:236:GLU:OE2 | 1:L:251:TYR:OH   | 2.23                     | 0.48              |
| 1:B:223:ILE:O   | 1:B:230:ARG:HD3  | 2.13                     | 0.48              |
| 1:B:390:GLU:O   | 1:B:394:MET:HE2  | 2.13                     | 0.48              |
| 1:C:341:TYR:O   | 1:C:348:ARG:NH1  | 2.46                     | 0.48              |
| 1:F:378:MET:HA  | 1:F:381:ALA:HB3  | 1.95                     | 0.48              |
| 1:C:296:LEU:O   | 1:C:300:MET:HG3  | 2.13                     | 0.48              |
| 1:E:147:PHE:C   | 1:E:148:VAL:O    | 2.55                     | 0.48              |
| 1:G:126:GLU:HA  | 1:G:129:ALA:HB3  | 1.95                     | 0.48              |
| 1:G:197:GLN:O   | 1:G:201:GLN:HB2  | 2.14                     | 0.48              |
| 1:J:76:MET:HA   | 1:J:79:LEU:HD12  | 1.96                     | 0.48              |
| 1:J:292:GLU:HG2 | 1:J:329:TYR:HA   | 1.95                     | 0.48              |
| 1:M:50:ARG:HH21 | 1:M:107:PHE:HB2  | 1.79                     | 0.48              |
| 1:B:104:ILE:O   | 1:B:115:ILE:O    | 2.31                     | 0.48              |
| 1:C:94:SER:HB3  | 1:C:97:ALA:HB2   | 1.96                     | 0.48              |
| 1:G:359:LYS:HD2 | 1:G:359:LYS:O    | 2.14                     | 0.48              |
| 1:J:276:ALA:HB2 | 1:J:336:ALA:HB2  | 1.95                     | 0.48              |
| 1:K:104:ILE:O   | 1:K:115:ILE:O    | 2.32                     | 0.48              |
| 1:E:5:LEU:HG    | 1:M:380:MET:HE1  | 1.96                     | 0.48              |
| 1:K:87:HIS:ND1  | 1:K:90:LEU:HD22  | 2.29                     | 0.48              |
| 1:K:260:TYR:OH  | 2:N:64:U:OP2     | 2.25                     | 0.48              |
| 1:L:122:MET:HG2 | 1:L:126:GLU:OE1  | 2.14                     | 0.48              |
| 1:B:344:ASP:HB3 | 1:B:347:MET:HG2  | 1.96                     | 0.47              |
| 1:C:281:TRP:HZ3 | 1:C:339:ILE:HG23 | 1.79                     | 0.47              |
| 1:D:5:LEU:O     | 1:D:9:GLU:HG3    | 2.14                     | 0.47              |
| 1:E:111:SER:HA  | 1:E:113:ARG:H    | 1.78                     | 0.47              |
| 1:F:194:LYS:HE2 | 2:N:27:U:OP1     | 2.13                     | 0.47              |
| 1:L:378:MET:HE3 | 1:L:378:MET:HB3  | 1.67                     | 0.47              |
| 1:M:345:VAL:O   | 1:M:348:ARG:HD3  | 2.14                     | 0.47              |
| 1:A:319:PRO:HG2 | 1:M:243:GLN:NE2  | 2.29                     | 0.47              |
| 1:G:296:LEU:O   | 1:G:300:MET:HG3  | 2.15                     | 0.47              |
| 1:D:104:ILE:O   | 1:D:115:ILE:O    | 2.33                     | 0.47              |
| 1:E:180:LYS:NZ  | 1:E:191:SER:OG   | 2.46                     | 0.47              |
| 1:F:87:HIS:CE1  | 1:F:236:GLU:OE2  | 2.67                     | 0.47              |
| 1:G:284:LEU:O   | 1:H:380:MET:HE1  | 2.14                     | 0.47              |
| 1:H:23:GLU:OE1  | 1:H:24:GLY:N     | 2.47                     | 0.47              |
| 1:H:180:LYS:HB2 | 1:H:220:GLN:NE2  | 2.29                     | 0.47              |
| 1:K:85:LEU:O    | 1:K:89:LYS:HG3   | 2.13                     | 0.47              |
| 1:A:169:SER:O   | 1:A:173:GLN:HG3  | 2.14                     | 0.47              |
| 1:E:111:SER:CB  | 1:E:112:PHE:HA   | 2.44                     | 0.47              |
| 1:E:161:GLU:HG2 | 1:F:33:PRO:HB3   | 1.95                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:198:LYS:HE3  | 2:N:22:U:O4'     | 2.15                     | 0.47              |
| 1:E:301:ALA:O    | 1:E:305:THR:HG23 | 2.15                     | 0.47              |
| 1:J:225:LYS:HE3  | 1:J:225:LYS:HB3  | 1.68                     | 0.47              |
| 1:M:108:GLU:HG3  | 1:M:115:ILE:HG12 | 1.97                     | 0.47              |
| 1:A:397:THR:HG23 | 1:E:371:LYS:NZ   | 2.29                     | 0.47              |
| 1:B:193:GLU:HA   | 1:B:196:LEU:HD13 | 1.96                     | 0.47              |
| 1:D:197:GLN:O    | 1:D:201:GLN:HG3  | 2.15                     | 0.47              |
| 1:F:230:ARG:HH21 | 1:F:317:GLU:HG3  | 1.80                     | 0.47              |
| 1:A:387:THR:H    | 1:A:390:GLU:HG3  | 1.80                     | 0.47              |
| 1:E:348:ARG:HG3  | 1:E:348:ARG:HH11 | 1.80                     | 0.47              |
| 1:H:180:LYS:HB2  | 1:H:220:GLN:HE21 | 1.79                     | 0.47              |
| 1:I:172:MET:SD   | 1:I:253:MET:HG2  | 2.54                     | 0.47              |
| 1:K:173:GLN:HE22 | 1:K:210:LEU:HA   | 1.79                     | 0.47              |
| 1:A:85:LEU:O     | 1:A:89:LYS:HG3   | 2.15                     | 0.47              |
| 1:A:241:ARG:HH12 | 1:A:308:GLU:CG   | 2.26                     | 0.47              |
| 1:B:57:ARG:NH1   | 1:B:153:GLU:OE2  | 2.47                     | 0.47              |
| 1:D:142:ASN:O    | 1:D:143:HIS:HB2  | 2.15                     | 0.47              |
| 1:F:198:LYS:HE3  | 2:N:28:U:O4'     | 2.15                     | 0.47              |
| 1:F:367:GLU:HG2  | 1:F:371:LYS:HG3  | 1.97                     | 0.47              |
| 1:F:388:GLN:O    | 1:F:391:ARG:HB2  | 2.14                     | 0.47              |
| 1:I:259:LYS:NZ   | 1:M:323:ASP:OD1  | 2.39                     | 0.47              |
| 1:I:292:GLU:HG2  | 1:I:329:TYR:HA   | 1.97                     | 0.47              |
| 1:J:90:LEU:HD21  | 1:J:239:LEU:HD11 | 1.97                     | 0.47              |
| 1:J:366:MET:HE2  | 1:J:370:ARG:HH21 | 1.79                     | 0.47              |
| 1:K:40:LEU:HD11  | 1:K:47:LEU:HD23  | 1.96                     | 0.47              |
| 1:K:107:PHE:CE1  | 1:K:114:LEU:HD23 | 2.49                     | 0.47              |
| 1:L:94:SER:HB3   | 1:L:97:ALA:HB2   | 1.97                     | 0.47              |
| 1:M:387:THR:OG1  | 1:M:390:GLU:HG3  | 2.14                     | 0.47              |
| 1:A:366:MET:HE2  | 1:A:370:ARG:HH21 | 1.80                     | 0.47              |
| 1:C:65:ARG:HE    | 1:F:161:GLU:CD   | 2.22                     | 0.47              |
| 1:C:374:GLY:HA3  | 1:C:395:ALA:HA   | 1.97                     | 0.47              |
| 1:E:111:SER:HB2  | 1:E:112:PHE:HA   | 1.96                     | 0.47              |
| 1:E:306:LEU:HD21 | 1:E:320:HIS:CD2  | 2.50                     | 0.47              |
| 1:B:5:LEU:O      | 1:B:9:GLU:HG3    | 2.15                     | 0.47              |
| 1:E:296:LEU:O    | 1:E:300:MET:HG3  | 2.15                     | 0.47              |
| 1:F:393:GLU:HG2  | 1:F:394:MET:HB2  | 1.96                     | 0.47              |
| 1:H:366:MET:HE2  | 1:H:366:MET:HB3  | 1.79                     | 0.47              |
| 1:I:345:VAL:O    | 1:I:348:ARG:HG3  | 2.14                     | 0.47              |
| 1:M:207:PRO:HA   | 1:M:210:LEU:HD12 | 1.97                     | 0.47              |
| 1:M:400:LYS:N    | 1:M:400:LYS:CD   | 2.78                     | 0.47              |
| 1:D:282:PRO:HG2  | 1:D:372:GLN:NE2  | 2.30                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:188:PRO:HB3  | 1:F:189:ALA:HA   | 1.97                     | 0.47              |
| 1:F:230:ARG:HG2  | 1:F:315:LEU:HG   | 1.96                     | 0.47              |
| 1:G:259:LYS:NZ   | 1:K:323:ASP:OD1  | 2.41                     | 0.47              |
| 1:H:249:ARG:HG3  | 1:H:249:ARG:NH1  | 2.30                     | 0.47              |
| 1:H:384:LEU:HD11 | 1:K:5:LEU:HD11   | 1.97                     | 0.47              |
| 1:I:198:LYS:HE3  | 2:N:4:U:O4'      | 2.14                     | 0.47              |
| 1:K:235:PHE:O    | 1:K:239:LEU:HD13 | 2.15                     | 0.47              |
| 1:L:147:PHE:HA   | 1:L:210:LEU:O    | 2.15                     | 0.47              |
| 1:M:104:ILE:O    | 1:M:115:ILE:O    | 2.33                     | 0.47              |
| 1:A:241:ARG:NH2  | 1:A:311:ARG:HH12 | 2.13                     | 0.46              |
| 1:B:85:LEU:O     | 1:B:89:LYS:HG3   | 2.14                     | 0.46              |
| 1:C:373:GLN:C    | 1:C:398:LEU:HD23 | 2.41                     | 0.46              |
| 1:F:57:ARG:NH1   | 1:F:153:GLU:OE2  | 2.48                     | 0.46              |
| 1:F:276:ALA:HB2  | 1:F:336:ALA:HB2  | 1.97                     | 0.46              |
| 1:K:371:LYS:HD2  | 1:K:371:LYS:HA   | 1.65                     | 0.46              |
| 1:L:193:GLU:HA   | 1:L:196:LEU:HD13 | 1.97                     | 0.46              |
| 1:M:147:PHE:C    | 1:M:149:ASP:N    | 2.74                     | 0.46              |
| 1:C:50:ARG:NH2   | 1:C:110:GLY:H    | 2.11                     | 0.46              |
| 1:D:354:ARG:NH1  | 1:D:356:TYR:OH   | 2.48                     | 0.46              |
| 1:E:10:ARG:HH11  | 1:E:10:ARG:HG2   | 1.80                     | 0.46              |
| 1:F:177:VAL:HG12 | 1:F:192:ILE:CD1  | 2.46                     | 0.46              |
| 1:G:398:LEU:O    | 1:G:401:LEU:HB2  | 2.15                     | 0.46              |
| 1:I:5:LEU:O      | 1:I:9:GLU:HG3    | 2.16                     | 0.46              |
| 1:J:180:LYS:HB2  | 1:J:220:GLN:NE2  | 2.29                     | 0.46              |
| 1:K:292:GLU:HG2  | 1:K:329:TYR:HA   | 1.97                     | 0.46              |
| 1:A:87:HIS:CD2   | 1:A:90:LEU:HD22  | 2.51                     | 0.46              |
| 1:B:104:ILE:HG23 | 1:B:105:ASP:N    | 2.30                     | 0.46              |
| 1:C:57:ARG:NH1   | 1:C:153:GLU:OE2  | 2.49                     | 0.46              |
| 1:D:400:LYS:HD2  | 1:D:400:LYS:C    | 2.39                     | 0.46              |
| 1:E:76:MET:HA    | 1:E:79:LEU:HD12  | 1.97                     | 0.46              |
| 1:F:367:GLU:HG2  | 1:F:371:LYS:HE3  | 1.98                     | 0.46              |
| 1:G:18:GLN:HE22  | 1:H:308:GLU:HA   | 1.79                     | 0.46              |
| 1:H:6:LYS:O      | 1:H:10:ARG:HG3   | 2.15                     | 0.46              |
| 1:A:378:MET:HA   | 1:A:381:ALA:HB3  | 1.98                     | 0.46              |
| 1:F:301:ALA:O    | 1:F:305:THR:HG23 | 2.15                     | 0.46              |
| 1:I:15:GLN:NE2   | 1:I:18:GLN:OE1   | 2.49                     | 0.46              |
| 1:M:111:SER:CB   | 1:M:112:PHE:HA   | 2.45                     | 0.46              |
| 1:A:87:HIS:CE1   | 1:E:28:PRO:HB3   | 2.45                     | 0.46              |
| 1:A:104:ILE:HD13 | 1:A:114:LEU:HD22 | 1.98                     | 0.46              |
| 1:A:104:ILE:HD11 | 1:A:114:LEU:HD13 | 1.97                     | 0.46              |
| 1:G:263:ASN:OD1  | 1:G:303:TYR:OH   | 2.25                     | 0.46              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:399:ALA:HB3  | 1:G:401:LEU:H    | 1.79                     | 0.46              |
| 1:K:249:ARG:NH1  | 1:K:253:MET:HE2  | 2.31                     | 0.46              |
| 1:D:200:ARG:HD2  | 1:D:207:PRO:HG3  | 1.97                     | 0.46              |
| 1:E:39:ILE:HG12  | 1:E:101:ARG:O    | 2.15                     | 0.46              |
| 1:G:283:THR:HA   | 1:H:394:MET:SD   | 2.55                     | 0.46              |
| 1:J:122:MET:HG2  | 1:J:126:GLU:OE1  | 2.16                     | 0.46              |
| 1:E:196:LEU:O    | 1:E:200:ARG:HG3  | 2.16                     | 0.46              |
| 1:H:147:PHE:O    | 1:H:149:ASP:N    | 2.46                     | 0.46              |
| 1:M:111:SER:HA   | 1:M:113:ARG:H    | 1.81                     | 0.46              |
| 1:A:104:ILE:CD1  | 1:A:114:LEU:HD22 | 2.46                     | 0.46              |
| 1:B:295:LYS:HE2  | 1:B:328:ASN:HB3  | 1.98                     | 0.46              |
| 1:C:239:LEU:HD23 | 1:L:28:PRO:HG2   | 1.98                     | 0.46              |
| 1:D:227:MET:HE2  | 1:D:231:HIS:CE1  | 2.50                     | 0.46              |
| 1:H:369:ALA:O    | 1:H:373:GLN:HG2  | 2.16                     | 0.46              |
| 1:B:180:LYS:HB2  | 1:B:220:GLN:HE21 | 1.81                     | 0.46              |
| 1:C:141:LEU:HA   | 1:C:141:LEU:HD12 | 1.81                     | 0.46              |
| 1:C:149:ASP:C    | 1:C:151:GLU:H    | 2.23                     | 0.46              |
| 1:E:373:GLN:HB3  | 1:E:398:LEU:CD2  | 2.45                     | 0.46              |
| 1:H:276:ALA:HB2  | 1:H:336:ALA:HB2  | 1.98                     | 0.46              |
| 1:J:301:ALA:O    | 1:J:305:THR:HG23 | 2.16                     | 0.46              |
| 1:K:147:PHE:HA   | 1:K:210:LEU:O    | 2.16                     | 0.46              |
| 1:L:386:LEU:HD12 | 1:L:386:LEU:HA   | 1.34                     | 0.46              |
| 1:M:384:LEU:HB3  | 1:M:386:LEU:HD23 | 1.96                     | 0.46              |
| 1:A:301:ALA:O    | 1:A:305:THR:HG23 | 2.16                     | 0.46              |
| 1:A:364:LEU:O    | 1:A:368:THR:OG1  | 2.23                     | 0.46              |
| 1:E:386:LEU:HD11 | 1:F:282:PRO:HB3  | 1.98                     | 0.46              |
| 1:G:325:ALA:O    | 1:G:328:ASN:ND2  | 2.44                     | 0.46              |
| 1:J:27:PRO:HB2   | 1:K:248:ASN:HD21 | 1.80                     | 0.46              |
| 1:M:50:ARG:HH22  | 1:M:109:GLU:HA   | 1.81                     | 0.46              |
| 1:M:350:TYR:HE1  | 2:N:6:U:H5"      | 1.81                     | 0.46              |
| 1:D:357:MET:HE1  | 1:D:362:PHE:CD1  | 2.51                     | 0.45              |
| 1:H:90:LEU:HD21  | 1:H:239:LEU:HD11 | 1.98                     | 0.45              |
| 1:M:87:HIS:HE2   | 1:M:236:GLU:CD   | 2.24                     | 0.45              |
| 1:C:196:LEU:O    | 1:C:200:ARG:HG3  | 2.16                     | 0.45              |
| 1:C:230:ARG:HH21 | 1:C:317:GLU:HG3  | 1.82                     | 0.45              |
| 1:E:366:MET:HE2  | 1:E:366:MET:HB3  | 1.86                     | 0.45              |
| 1:F:188:PRO:CB   | 1:F:189:ALA:HA   | 2.47                     | 0.45              |
| 1:G:392:THR:O    | 1:G:395:ALA:HB3  | 2.16                     | 0.45              |
| 1:K:182:MET:HE3  | 1:K:224:ARG:NH1  | 2.31                     | 0.45              |
| 1:L:85:LEU:O     | 1:L:89:LYS:HG3   | 2.16                     | 0.45              |
| 1:M:172:MET:O    | 1:M:176:ILE:HG13 | 2.16                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:M:197:GLN:O    | 1:M:201:GLN:HG2  | 2.16                     | 0.45              |
| 1:M:394:MET:HE3  | 1:M:394:MET:HB2  | 1.58                     | 0.45              |
| 1:A:172:MET:SD   | 1:A:253:MET:HG2  | 2.57                     | 0.45              |
| 1:B:366:MET:HE2  | 1:B:366:MET:HB3  | 1.73                     | 0.45              |
| 1:D:146:PRO:HB2  | 1:D:211:LEU:HD22 | 1.98                     | 0.45              |
| 1:E:199:TYR:OH   | 1:E:256:ASP:OD1  | 2.27                     | 0.45              |
| 1:F:390:GLU:CA   | 1:F:393:GLU:HB3  | 2.46                     | 0.45              |
| 1:G:239:LEU:HD23 | 1:K:28:PRO:CG    | 2.47                     | 0.45              |
| 1:G:377:ASP:OD1  | 1:G:379:ARG:HG2  | 2.17                     | 0.45              |
| 1:K:301:ALA:O    | 1:K:305:THR:HG23 | 2.16                     | 0.45              |
| 1:M:87:HIS:CE1   | 1:M:232:PHE:HZ   | 2.34                     | 0.45              |
| 1:C:57:ARG:NH1   | 1:C:153:GLU:OE1  | 2.48                     | 0.45              |
| 1:C:149:ASP:O    | 1:C:151:GLU:N    | 2.42                     | 0.45              |
| 1:C:335:TYR:CZ   | 1:C:339:ILE:HD11 | 2.51                     | 0.45              |
| 1:D:78:SER:O     | 1:D:81:SER:OG    | 2.34                     | 0.45              |
| 1:D:181:CYS:O    | 1:D:224:ARG:NH1  | 2.50                     | 0.45              |
| 1:H:165:ASP:O    | 1:H:169:SER:OG   | 2.24                     | 0.45              |
| 1:J:79:LEU:HA    | 1:J:84:MET:HE3   | 1.98                     | 0.45              |
| 1:L:30:THR:HG22  | 1:L:31:LEU:O     | 2.16                     | 0.45              |
| 1:L:180:LYS:NZ   | 1:L:191:SER:OG   | 2.50                     | 0.45              |
| 1:A:107:PHE:CE1  | 1:A:114:LEU:HD23 | 2.51                     | 0.45              |
| 1:A:148:VAL:HG12 | 1:A:212:GLN:HG2  | 1.99                     | 0.45              |
| 1:B:65:ARG:NH2   | 1:L:161:GLU:OE2  | 2.40                     | 0.45              |
| 1:C:396:ASN:CG   | 1:C:397:THR:N    | 2.74                     | 0.45              |
| 1:E:104:ILE:O    | 1:E:115:ILE:O    | 2.33                     | 0.45              |
| 1:I:76:MET:HA    | 1:I:79:LEU:HD12  | 1.98                     | 0.45              |
| 1:I:85:LEU:O     | 1:I:89:LYS:HG3   | 2.16                     | 0.45              |
| 1:J:296:LEU:O    | 1:J:300:MET:HG3  | 2.16                     | 0.45              |
| 1:K:249:ARG:HH11 | 1:K:249:ARG:CG   | 2.28                     | 0.45              |
| 1:A:147:PHE:HA   | 1:A:210:LEU:O    | 2.17                     | 0.45              |
| 1:B:116:PRO:HB3  | 1:B:122:MET:HE2  | 1.98                     | 0.45              |
| 1:B:237:LEU:O    | 1:B:241:ARG:HG2  | 2.17                     | 0.45              |
| 1:E:366:MET:O    | 1:E:370:ARG:HG3  | 2.16                     | 0.45              |
| 1:G:142:ASN:O    | 1:G:143:HIS:CB   | 2.65                     | 0.45              |
| 1:I:398:LEU:CA   | 1:I:400:LYS:HD3  | 2.38                     | 0.45              |
| 1:B:282:PRO:HB3  | 1:L:386:LEU:CD2  | 2.47                     | 0.45              |
| 1:C:292:GLU:HG2  | 1:C:329:TYR:HA   | 1.98                     | 0.45              |
| 1:F:388:GLN:HB3  | 1:F:391:ARG:HD3  | 1.98                     | 0.45              |
| 1:J:142:ASN:OD1  | 1:J:142:ASN:C    | 2.59                     | 0.45              |
| 1:K:357:MET:HE3  | 1:K:362:PHE:HB2  | 1.98                     | 0.45              |
| 1:A:46:GLU:HA    | 1:A:157:TRP:HB2  | 1.97                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:76:MET:HA    | 1:D:79:LEU:HD12  | 1.97                     | 0.45              |
| 1:D:364:LEU:HD22 | 1:J:398:LEU:HD13 | 1.99                     | 0.45              |
| 1:I:181:CYS:O    | 1:I:182:MET:HG2  | 2.16                     | 0.45              |
| 1:K:218:ILE:O    | 1:K:222:VAL:HG23 | 2.17                     | 0.45              |
| 1:A:296:LEU:O    | 1:A:300:MET:HG3  | 2.17                     | 0.45              |
| 1:C:113:ARG:HH11 | 1:C:124:ARG:NH2  | 2.15                     | 0.45              |
| 1:D:57:ARG:NH1   | 1:D:153:GLU:OE2  | 2.50                     | 0.45              |
| 1:E:14:THR:O     | 1:E:18:GLN:N     | 2.50                     | 0.45              |
| 1:I:104:ILE:O    | 1:I:115:ILE:O    | 2.34                     | 0.45              |
| 1:M:214:GLU:OE1  | 1:M:217:ARG:NH2  | 2.50                     | 0.45              |
| 1:C:40:LEU:HD21  | 1:C:47:LEU:HB3   | 1.99                     | 0.45              |
| 1:C:172:MET:O    | 1:C:176:ILE:HG13 | 2.16                     | 0.45              |
| 1:F:321:LEU:HD23 | 1:F:321:LEU:HA   | 1.69                     | 0.45              |
| 1:G:105:ASP:OD2  | 1:G:117:ASN:HA   | 2.17                     | 0.45              |
| 1:L:325:ALA:O    | 1:L:328:ASN:ND2  | 2.42                     | 0.45              |
| 1:M:87:HIS:O     | 1:M:90:LEU:HB2   | 2.17                     | 0.45              |
| 1:M:180:LYS:HB2  | 1:M:220:GLN:NE2  | 2.31                     | 0.45              |
| 1:A:181:CYS:O    | 1:A:182:MET:HB2  | 2.17                     | 0.44              |
| 1:A:384:LEU:HD11 | 1:F:5:LEU:HD11   | 1.99                     | 0.44              |
| 1:B:282:PRO:HB3  | 1:L:386:LEU:HD21 | 1.98                     | 0.44              |
| 1:D:27:PRO:HB2   | 1:J:248:ASN:HD21 | 1.82                     | 0.44              |
| 1:D:104:ILE:HG23 | 1:D:105:ASP:N    | 2.32                     | 0.44              |
| 1:I:172:MET:O    | 1:I:176:ILE:HG13 | 2.17                     | 0.44              |
| 1:I:250:TYR:O    | 1:I:254:VAL:HG23 | 2.18                     | 0.44              |
| 1:J:357:MET:HE1  | 1:J:362:PHE:CD1  | 2.52                     | 0.44              |
| 1:L:13:LEU:HD21  | 1:L:297:LYS:HE2  | 1.99                     | 0.44              |
| 1:L:263:ASN:OD1  | 1:L:303:TYR:OH   | 2.29                     | 0.44              |
| 1:B:45:PRO:O     | 1:B:49:SER:OG    | 2.35                     | 0.44              |
| 1:B:321:LEU:HD23 | 1:B:321:LEU:HA   | 1.81                     | 0.44              |
| 1:D:149:ASP:C    | 1:D:151:GLU:H    | 2.25                     | 0.44              |
| 1:D:230:ARG:HG2  | 1:D:315:LEU:HG   | 1.99                     | 0.44              |
| 1:F:57:ARG:HG2   | 1:F:137:LEU:HD11 | 2.00                     | 0.44              |
| 1:G:40:LEU:HD11  | 1:G:47:LEU:HD23  | 1.98                     | 0.44              |
| 1:G:108:GLU:CD   | 1:G:124:ARG:HH22 | 2.25                     | 0.44              |
| 1:G:141:LEU:HD12 | 1:G:141:LEU:HA   | 1.77                     | 0.44              |
| 1:I:223:ILE:O    | 1:I:230:ARG:HD3  | 2.17                     | 0.44              |
| 1:I:357:MET:HE1  | 1:I:362:PHE:CD1  | 2.52                     | 0.44              |
| 1:J:148:VAL:H    | 1:J:212:GLN:HE21 | 1.64                     | 0.44              |
| 1:L:260:TYR:OH   | 2:N:40:U:OP2     | 2.26                     | 0.44              |
| 1:B:172:MET:O    | 1:B:176:ILE:HG13 | 2.16                     | 0.44              |
| 1:C:180:LYS:HB2  | 1:C:220:GLN:NE2  | 2.32                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:104:ILE:HD11 | 1:D:114:LEU:CD2  | 2.47                     | 0.44              |
| 1:D:165:ASP:O    | 1:D:169:SER:OG   | 2.22                     | 0.44              |
| 1:I:16:GLU:OE1   | 1:I:295:LYS:NZ   | 2.27                     | 0.44              |
| 1:J:141:LEU:HD23 | 1:J:141:LEU:HA   | 1.71                     | 0.44              |
| 1:L:90:LEU:HD21  | 1:L:239:LEU:HD11 | 1.99                     | 0.44              |
| 1:A:273:LEU:HB3  | 1:E:8:TYR:CE1    | 2.53                     | 0.44              |
| 1:B:249:ARG:HG3  | 1:B:249:ARG:NH1  | 2.30                     | 0.44              |
| 1:C:48:ARG:HB3   | 1:C:163:PHE:CZ   | 2.51                     | 0.44              |
| 1:E:147:PHE:O    | 1:E:148:VAL:HB   | 2.17                     | 0.44              |
| 1:F:367:GLU:CD   | 1:F:371:LYS:HE3  | 2.42                     | 0.44              |
| 1:G:373:GLN:HB2  | 1:G:398:LEU:HD22 | 1.99                     | 0.44              |
| 1:H:218:ILE:O    | 1:H:222:VAL:HG23 | 2.18                     | 0.44              |
| 1:K:296:LEU:O    | 1:K:300:MET:HG3  | 2.17                     | 0.44              |
| 1:A:180:LYS:HB2  | 1:A:220:GLN:HE21 | 1.82                     | 0.44              |
| 1:A:284:LEU:O    | 1:A:284:LEU:HD23 | 2.17                     | 0.44              |
| 1:A:398:LEU:HA   | 1:A:401:LEU:HB2  | 1.99                     | 0.44              |
| 1:C:234:THR:O    | 1:C:238:GLN:HG3  | 2.18                     | 0.44              |
| 1:D:6:LYS:HD2    | 1:D:10:ARG:HH21  | 1.83                     | 0.44              |
| 1:F:122:MET:HG2  | 1:F:126:GLU:OE1  | 2.18                     | 0.44              |
| 1:G:85:LEU:O     | 1:G:89:LYS:HG3   | 2.18                     | 0.44              |
| 1:G:146:PRO:O    | 1:G:147:PHE:HB2  | 2.17                     | 0.44              |
| 1:G:210:LEU:HD23 | 1:G:210:LEU:HA   | 1.83                     | 0.44              |
| 1:H:275:TYR:O    | 1:H:279:THR:OG1  | 2.23                     | 0.44              |
| 1:I:400:LYS:HE3  | 1:I:401:LEU:HB2  | 2.00                     | 0.44              |
| 1:L:188:PRO:HB2  | 1:L:189:ALA:H    | 1.42                     | 0.44              |
| 1:C:295:LYS:HZ3  | 1:C:328:ASN:HB3  | 1.83                     | 0.44              |
| 1:D:27:PRO:HB2   | 1:J:248:ASN:ND2  | 2.33                     | 0.44              |
| 1:D:223:ILE:O    | 1:D:230:ARG:HD3  | 2.18                     | 0.44              |
| 1:E:276:ALA:HB2  | 1:E:336:ALA:HB2  | 1.99                     | 0.44              |
| 1:E:343:LEU:HD11 | 1:E:373:GLN:NE2  | 2.33                     | 0.44              |
| 1:F:104:ILE:O    | 1:F:115:ILE:O    | 2.35                     | 0.44              |
| 1:J:353:SER:O    | 1:J:354:ARG:HG2  | 2.18                     | 0.44              |
| 1:A:73:LEU:HD22  | 1:A:77:PHE:HE2   | 1.83                     | 0.44              |
| 1:A:260:TYR:OH   | 2:N:16:U:OP2     | 2.29                     | 0.44              |
| 1:D:146:PRO:O    | 1:D:147:PHE:CB   | 2.65                     | 0.44              |
| 1:D:230:ARG:HH21 | 1:D:317:GLU:HG3  | 1.83                     | 0.44              |
| 1:E:230:ARG:HH21 | 1:E:317:GLU:HG3  | 1.83                     | 0.44              |
| 1:G:301:ALA:O    | 1:G:305:THR:HG23 | 2.18                     | 0.44              |
| 1:J:137:LEU:HD22 | 1:J:141:LEU:HD12 | 2.00                     | 0.44              |
| 1:J:397:THR:O    | 1:J:400:LYS:N    | 2.38                     | 0.44              |
| 1:L:386:LEU:CD1  | 1:L:390:GLU:HG2  | 2.43                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:387:THR:HG23 | 1:L:388:GLN:HG2  | 1.99                     | 0.44              |
| 1:B:301:ALA:O    | 1:B:305:THR:HG23 | 2.17                     | 0.44              |
| 1:C:111:SER:HB2  | 1:C:112:PHE:HA   | 2.00                     | 0.44              |
| 1:E:223:ILE:O    | 1:E:230:ARG:HD3  | 2.18                     | 0.44              |
| 1:F:39:ILE:HD11  | 1:F:88:VAL:HG21  | 2.00                     | 0.44              |
| 1:H:47:LEU:HD21  | 1:H:106:GLY:HA2  | 2.00                     | 0.44              |
| 1:L:116:PRO:HB3  | 1:L:122:MET:CE   | 2.46                     | 0.44              |
| 2:N:1:U:P        | 2:N:78:U:O3'     | 2.76                     | 0.44              |
| 1:B:180:LYS:HB2  | 1:B:220:GLN:NE2  | 2.32                     | 0.44              |
| 1:E:50:ARG:HH21  | 1:E:107:PHE:HB2  | 1.82                     | 0.44              |
| 1:E:295:LYS:HE3  | 1:E:328:ASN:HB3  | 1.99                     | 0.44              |
| 1:I:40:LEU:HD11  | 1:I:47:LEU:CD2   | 2.47                     | 0.44              |
| 1:J:64:ALA:HB2   | 1:J:133:LEU:HD21 | 2.00                     | 0.44              |
| 1:J:210:LEU:HD23 | 1:J:210:LEU:HA   | 1.89                     | 0.44              |
| 1:K:105:ASP:CG   | 1:K:117:ASN:HD22 | 2.26                     | 0.44              |
| 1:A:374:GLY:HA3  | 1:A:395:ALA:HA   | 2.00                     | 0.43              |
| 1:C:283:THR:HA   | 1:F:394:MET:SD   | 2.58                     | 0.43              |
| 1:D:187:GLN:HB2  | 1:D:188:PRO:HD2  | 2.00                     | 0.43              |
| 1:D:210:LEU:HD23 | 1:D:211:LEU:O    | 2.17                     | 0.43              |
| 1:H:396:ASN:HA   | 1:H:399:ALA:HB3  | 2.00                     | 0.43              |
| 1:L:87:HIS:O     | 1:L:90:LEU:HB2   | 2.18                     | 0.43              |
| 1:M:223:ILE:O    | 1:M:230:ARG:HD3  | 2.18                     | 0.43              |
| 1:B:394:MET:HE2  | 1:B:394:MET:HB2  | 1.83                     | 0.43              |
| 1:C:175:TRP:CZ3  | 1:C:237:LEU:HD11 | 2.53                     | 0.43              |
| 1:C:364:LEU:HD22 | 1:F:398:LEU:HD13 | 2.00                     | 0.43              |
| 1:G:396:ASN:CG   | 1:G:399:ALA:HA   | 2.43                     | 0.43              |
| 1:J:65:ARG:HG3   | 1:J:66:ASP:H     | 1.83                     | 0.43              |
| 1:K:46:GLU:OE2   | 1:K:50:ARG:NE    | 2.51                     | 0.43              |
| 1:K:377:ASP:OD1  | 1:K:379:ARG:HG3  | 2.19                     | 0.43              |
| 1:C:394:MET:SD   | 1:L:283:THR:HA   | 2.58                     | 0.43              |
| 1:D:148:VAL:HG12 | 1:D:149:ASP:N    | 2.33                     | 0.43              |
| 1:F:357:MET:HE1  | 1:F:362:PHE:CD1  | 2.52                     | 0.43              |
| 1:G:39:ILE:HD11  | 1:G:88:VAL:HG21  | 2.00                     | 0.43              |
| 1:G:390:GLU:O    | 1:G:394:MET:HB3  | 2.19                     | 0.43              |
| 1:H:210:LEU:HD12 | 1:H:210:LEU:HA   | 1.83                     | 0.43              |
| 1:L:172:MET:SD   | 1:L:253:MET:HG2  | 2.57                     | 0.43              |
| 1:C:104:ILE:O    | 1:C:105:ASP:CB   | 2.66                     | 0.43              |
| 1:D:172:MET:SD   | 1:D:253:MET:HG2  | 2.57                     | 0.43              |
| 1:F:187:GLN:HA   | 1:F:188:PRO:HD2  | 1.76                     | 0.43              |
| 1:J:28:PRO:CG    | 1:K:239:LEU:HD23 | 2.48                     | 0.43              |
| 1:J:65:ARG:HG3   | 1:J:66:ASP:N     | 2.33                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:104:ILE:O    | 1:J:115:ILE:O    | 2.36                     | 0.43              |
| 1:L:200:ARG:HE   | 1:L:200:ARG:HB3  | 1.56                     | 0.43              |
| 1:M:393:GLU:OE1  | 1:M:396:ASN:HB3  | 2.19                     | 0.43              |
| 1:A:96:GLU:O     | 1:A:96:GLU:HG3   | 2.18                     | 0.43              |
| 1:C:152:VAL:O    | 1:C:155:THR:OG1  | 2.27                     | 0.43              |
| 1:D:124:ARG:HG3  | 1:D:124:ARG:NH1  | 2.33                     | 0.43              |
| 1:E:85:LEU:O     | 1:E:89:LYS:HG3   | 2.17                     | 0.43              |
| 1:E:90:LEU:HD21  | 1:E:239:LEU:HD11 | 2.00                     | 0.43              |
| 1:G:380:MET:HG2  | 1:K:285:ALA:HA   | 2.01                     | 0.43              |
| 1:H:253:MET:HE3  | 1:H:253:MET:HB2  | 1.91                     | 0.43              |
| 1:H:392:THR:HA   | 1:H:395:ALA:CB   | 2.48                     | 0.43              |
| 1:A:187:GLN:C    | 1:A:189:ALA:HA   | 2.43                     | 0.43              |
| 1:A:322:MET:HE3  | 1:A:322:MET:HB3  | 1.91                     | 0.43              |
| 1:D:155:THR:OG1  | 1:D:208:ARG:NH2  | 2.51                     | 0.43              |
| 1:D:357:MET:HE3  | 1:D:362:PHE:HB2  | 2.00                     | 0.43              |
| 1:D:384:LEU:HB3  | 1:D:386:LEU:HD23 | 2.00                     | 0.43              |
| 1:G:394:MET:HA   | 1:G:397:THR:HB   | 2.00                     | 0.43              |
| 1:H:198:LYS:HE3  | 2:N:52:U:O4'     | 2.19                     | 0.43              |
| 1:J:250:TYR:O    | 1:J:254:VAL:HG23 | 2.18                     | 0.43              |
| 1:K:306:LEU:HD23 | 1:K:306:LEU:HA   | 1.81                     | 0.43              |
| 1:L:292:GLU:HB3  | 1:L:332:LEU:HD12 | 2.00                     | 0.43              |
| 1:L:292:GLU:HG2  | 1:L:329:TYR:HA   | 2.01                     | 0.43              |
| 1:M:48:ARG:HB3   | 1:M:163:PHE:CZ   | 2.53                     | 0.43              |
| 1:M:295:LYS:HE2  | 1:M:328:ASN:HB3  | 2.00                     | 0.43              |
| 1:C:304:GLN:HG2  | 1:L:15:GLN:HE22  | 1.83                     | 0.43              |
| 1:G:235:PHE:O    | 1:G:239:LEU:HD13 | 2.18                     | 0.43              |
| 1:J:400:LYS:HG2  | 1:J:401:LEU:N    | 2.33                     | 0.43              |
| 1:L:15:GLN:HA    | 1:L:18:GLN:HB3   | 2.00                     | 0.43              |
| 1:L:230:ARG:HH21 | 1:L:317:GLU:HG3  | 1.82                     | 0.43              |
| 1:M:85:LEU:O     | 1:M:89:LYS:HG3   | 2.19                     | 0.43              |
| 1:A:105:ASP:CG   | 1:A:117:ASN:HD22 | 2.27                     | 0.43              |
| 1:B:207:PRO:HA   | 1:B:210:LEU:HD12 | 2.00                     | 0.43              |
| 1:B:323:ASP:OD1  | 1:L:259:LYS:NZ   | 2.47                     | 0.43              |
| 1:E:122:MET:HG2  | 1:E:126:GLU:OE1  | 2.19                     | 0.43              |
| 1:G:230:ARG:HH21 | 1:G:317:GLU:HG3  | 1.83                     | 0.43              |
| 1:H:223:ILE:O    | 1:H:230:ARG:HD3  | 2.18                     | 0.43              |
| 1:K:280:ARG:CZ   | 1:K:379:ARG:HH21 | 2.32                     | 0.43              |
| 1:L:386:LEU:O    | 1:L:391:ARG:NH2  | 2.52                     | 0.43              |
| 1:M:180:LYS:HB2  | 1:M:220:GLN:HE21 | 1.84                     | 0.43              |
| 1:A:10:ARG:HG2   | 1:A:10:ARG:NH1   | 2.34                     | 0.43              |
| 1:A:136:ASP:HB3  | 1:A:137:LEU:H    | 1.70                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:161:GLU:HG2  | 1:H:33:PRO:HB3   | 2.00                     | 0.43              |
| 1:B:206:ASN:HB3  | 1:B:209:TYR:HD2  | 1.83                     | 0.43              |
| 1:C:104:ILE:HG22 | 1:C:105:ASP:N    | 2.34                     | 0.43              |
| 1:I:87:HIS:HE1   | 1:I:236:GLU:OE2  | 2.02                     | 0.43              |
| 1:L:221:ASN:O    | 1:L:225:LYS:HG3  | 2.18                     | 0.43              |
| 1:M:367:GLU:OE2  | 1:M:371:LYS:NZ   | 2.40                     | 0.43              |
| 1:A:221:ASN:O    | 1:A:225:LYS:HG3  | 2.18                     | 0.43              |
| 1:A:223:ILE:O    | 1:A:230:ARG:HD3  | 2.19                     | 0.43              |
| 1:C:35:ILE:HD13  | 1:C:228:VAL:HG21 | 2.00                     | 0.43              |
| 1:C:195:ARG:NH2  | 2:N:33:U:OP2     | 2.51                     | 0.43              |
| 1:G:94:SER:HA    | 1:G:95:PRO:HD3   | 1.90                     | 0.43              |
| 1:G:357:MET:HE1  | 1:G:362:PHE:CD1  | 2.53                     | 0.43              |
| 1:I:366:MET:HE2  | 1:I:366:MET:HB3  | 1.89                     | 0.43              |
| 1:K:94:SER:HG    | 1:K:231:HIS:HD1  | 1.55                     | 0.43              |
| 1:K:250:TYR:O    | 1:K:254:VAL:HG23 | 2.19                     | 0.43              |
| 1:B:108:GLU:HG3  | 1:B:115:ILE:HG12 | 2.00                     | 0.42              |
| 1:C:111:SER:CB   | 1:C:112:PHE:HA   | 2.49                     | 0.42              |
| 1:E:339:ILE:O    | 1:E:343:LEU:HB2  | 2.19                     | 0.42              |
| 1:F:390:GLU:O    | 1:F:391:ARG:C    | 2.61                     | 0.42              |
| 1:G:237:LEU:HA   | 1:G:237:LEU:HD23 | 1.74                     | 0.42              |
| 1:J:241:ARG:HH12 | 1:J:311:ARG:HH21 | 1.65                     | 0.42              |
| 1:J:299:LEU:HD23 | 1:J:299:LEU:HA   | 1.83                     | 0.42              |
| 1:K:146:PRO:HB2  | 1:K:147:PHE:H    | 1.66                     | 0.42              |
| 1:L:15:GLN:HA    | 1:L:18:GLN:CB    | 2.49                     | 0.42              |
| 1:M:107:PHE:CE1  | 1:M:114:LEU:HD23 | 2.54                     | 0.42              |
| 1:D:40:LEU:HD11  | 1:D:47:LEU:HD23  | 2.01                     | 0.42              |
| 1:E:61:SER:O     | 1:E:69:ARG:NH2   | 2.46                     | 0.42              |
| 1:G:394:MET:HE3  | 1:G:394:MET:HB2  | 1.80                     | 0.42              |
| 1:I:243:GLN:NE2  | 1:M:319:PRO:HG2  | 2.35                     | 0.42              |
| 1:I:400:LYS:NZ   | 1:M:360:THR:HG22 | 2.34                     | 0.42              |
| 1:J:94:SER:HB3   | 1:J:97:ALA:HB2   | 2.00                     | 0.42              |
| 1:D:198:LYS:HE3  | 2:N:76:U:O4'     | 2.18                     | 0.42              |
| 1:E:48:ARG:HB3   | 1:E:163:PHE:CZ   | 2.55                     | 0.42              |
| 1:E:140:THR:HB   | 1:E:214:GLU:OE1  | 2.19                     | 0.42              |
| 1:G:57:ARG:NH2   | 1:G:144:ALA:O    | 2.51                     | 0.42              |
| 1:K:172:MET:SD   | 1:K:253:MET:HG2  | 2.59                     | 0.42              |
| 1:L:10:ARG:O     | 1:L:14:THR:HG23  | 2.19                     | 0.42              |
| 1:L:326:ALA:HB3  | 1:L:356:TYR:OH   | 2.19                     | 0.42              |
| 2:N:4:U:H2'      | 2:N:5:U:O4'      | 2.20                     | 0.42              |
| 1:B:73:LEU:HD23  | 1:B:73:LEU:HA    | 1.89                     | 0.42              |
| 1:B:197:GLN:HG2  | 1:B:201:GLN:HG3  | 2.01                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:148:VAL:H    | 1:D:212:GLN:HG3  | 1.84                     | 0.42              |
| 1:E:230:ARG:NH2  | 1:E:317:GLU:HG3  | 2.34                     | 0.42              |
| 1:F:165:ASP:O    | 1:F:169:SER:OG   | 2.26                     | 0.42              |
| 1:H:47:LEU:CD2   | 1:H:106:GLY:HA2  | 2.49                     | 0.42              |
| 1:H:104:ILE:HD11 | 1:H:114:LEU:CD2  | 2.50                     | 0.42              |
| 1:J:172:MET:O    | 1:J:176:ILE:HG13 | 2.20                     | 0.42              |
| 1:K:390:GLU:O    | 1:K:394:MET:HB3  | 2.20                     | 0.42              |
| 1:B:104:ILE:O    | 1:B:105:ASP:HB2  | 2.18                     | 0.42              |
| 1:C:54:PHE:CZ    | 1:C:58:ILE:HD11  | 2.54                     | 0.42              |
| 1:D:187:GLN:OE1  | 1:D:217:ARG:NE   | 2.51                     | 0.42              |
| 1:G:143:HIS:CD2  | 1:G:143:HIS:C    | 2.97                     | 0.42              |
| 1:G:155:THR:CG2  | 1:G:208:ARG:HH22 | 2.22                     | 0.42              |
| 1:L:388:GLN:CD   | 1:L:388:GLN:H    | 2.27                     | 0.42              |
| 1:M:59:VAL:O     | 1:M:69:ARG:NH1   | 2.52                     | 0.42              |
| 1:M:202:GLN:OE1  | 1:M:204:ARG:NH1  | 2.52                     | 0.42              |
| 1:A:172:MET:O    | 1:A:176:ILE:HG13 | 2.20                     | 0.42              |
| 1:B:357:MET:HE1  | 1:B:362:PHE:CD1  | 2.54                     | 0.42              |
| 1:C:65:ARG:HG2   | 1:C:66:ASP:H     | 1.84                     | 0.42              |
| 1:C:394:MET:O    | 1:C:397:THR:OG1  | 2.37                     | 0.42              |
| 1:D:107:PHE:CE1  | 1:D:114:LEU:HD23 | 2.55                     | 0.42              |
| 1:E:376:VAL:CG2  | 1:E:381:ALA:HB2  | 2.50                     | 0.42              |
| 1:G:113:ARG:HD2  | 1:G:124:ARG:HH12 | 1.84                     | 0.42              |
| 1:H:104:ILE:HG23 | 1:H:105:ASP:N    | 2.34                     | 0.42              |
| 1:H:193:GLU:HA   | 1:H:196:LEU:HD12 | 2.02                     | 0.42              |
| 1:J:198:LYS:HE3  | 2:N:70:U:O4'     | 2.20                     | 0.42              |
| 1:A:26:ILE:HA    | 1:A:27:PRO:HD3   | 1.89                     | 0.42              |
| 1:B:20:GLN:HE22  | 1:B:302:LEU:HD11 | 1.85                     | 0.42              |
| 1:B:55:CYS:O     | 1:B:59:VAL:HG23  | 2.20                     | 0.42              |
| 1:B:306:LEU:HD23 | 1:B:306:LEU:HA   | 1.80                     | 0.42              |
| 1:C:187:GLN:HB2  | 1:C:188:PRO:CD   | 2.49                     | 0.42              |
| 1:C:230:ARG:HG2  | 1:C:315:LEU:HG   | 2.01                     | 0.42              |
| 1:G:180:LYS:HB2  | 1:G:220:GLN:NE2  | 2.33                     | 0.42              |
| 1:H:136:ASP:HB3  | 1:H:137:LEU:H    | 1.75                     | 0.42              |
| 1:I:315:LEU:HD12 | 1:I:315:LEU:HA   | 1.92                     | 0.42              |
| 1:J:84:MET:O     | 1:J:88:VAL:HG23  | 2.19                     | 0.42              |
| 1:M:97:ALA:HB2   | 1:M:228:VAL:HG13 | 2.02                     | 0.42              |
| 1:C:182:MET:HE2  | 1:C:220:GLN:HG2  | 2.02                     | 0.42              |
| 1:C:204:ARG:HG2  | 1:C:253:MET:HE2  | 2.00                     | 0.42              |
| 1:I:224:ARG:HG3  | 1:I:225:LYS:N    | 2.34                     | 0.42              |
| 1:L:14:THR:O     | 1:L:18:GLN:N     | 2.53                     | 0.42              |
| 1:L:52:LEU:HD23  | 1:L:166:MET:HE2  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:57:ARG:NH1   | 1:L:153:GLU:CD   | 2.78                     | 0.42              |
| 1:L:79:LEU:HA    | 1:L:84:MET:HE3   | 2.02                     | 0.42              |
| 1:L:96:GLU:O     | 1:L:96:GLU:HG3   | 2.20                     | 0.42              |
| 1:M:172:MET:SD   | 1:M:253:MET:HG2  | 2.60                     | 0.42              |
| 1:C:10:ARG:O     | 1:C:14:THR:HG23  | 2.20                     | 0.42              |
| 1:E:243:GLN:HA   | 1:F:25:THR:O     | 2.19                     | 0.42              |
| 1:E:308:GLU:O    | 1:E:311:ARG:HG3  | 2.20                     | 0.42              |
| 1:F:357:MET:HE3  | 1:F:362:PHE:HB2  | 2.01                     | 0.42              |
| 1:H:230:ARG:NH2  | 1:H:317:GLU:HG3  | 2.35                     | 0.42              |
| 1:J:87:HIS:O     | 1:J:90:LEU:HB2   | 2.20                     | 0.42              |
| 1:A:352:PHE:O    | 1:A:354:ARG:HG2  | 2.20                     | 0.42              |
| 1:D:26:ILE:HA    | 1:D:27:PRO:HD3   | 1.89                     | 0.42              |
| 1:G:60:LEU:O     | 1:G:138:PRO:HD3  | 2.20                     | 0.42              |
| 1:G:143:HIS:O    | 1:G:143:HIS:CG   | 2.73                     | 0.42              |
| 1:H:326:ALA:HB3  | 1:H:356:TYR:OH   | 2.20                     | 0.42              |
| 1:I:50:ARG:NH1   | 1:I:111:SER:OG   | 2.53                     | 0.42              |
| 1:J:33:PRO:HD3   | 1:K:164:LEU:HD12 | 2.01                     | 0.42              |
| 1:J:143:HIS:O    | 1:J:144:ALA:HB3  | 2.20                     | 0.42              |
| 1:J:366:MET:HE2  | 1:J:366:MET:HB3  | 1.94                     | 0.42              |
| 1:J:378:MET:SD   | 1:J:391:ARG:NH1  | 2.93                     | 0.42              |
| 1:K:357:MET:HE1  | 1:K:362:PHE:CD1  | 2.55                     | 0.42              |
| 1:L:343:LEU:HD12 | 1:L:343:LEU:HA   | 1.91                     | 0.42              |
| 1:M:198:LYS:HZ3  | 1:M:256:ASP:CG   | 2.27                     | 0.42              |
| 1:M:357:MET:HE3  | 1:M:362:PHE:HB2  | 2.00                     | 0.42              |
| 1:B:141:LEU:O    | 1:B:143:HIS:HA   | 2.20                     | 0.41              |
| 1:E:207:PRO:HA   | 1:E:210:LEU:CD1  | 2.45                     | 0.41              |
| 1:E:344:ASP:HB3  | 1:E:347:MET:HG2  | 2.02                     | 0.41              |
| 1:F:60:LEU:O     | 1:F:138:PRO:HD3  | 2.19                     | 0.41              |
| 1:F:281:TRP:HZ3  | 1:F:339:ILE:HG23 | 1.85                     | 0.41              |
| 1:F:292:GLU:HG2  | 1:F:329:TYR:HA   | 2.02                     | 0.41              |
| 1:I:96:GLU:HG3   | 1:I:96:GLU:O     | 2.20                     | 0.41              |
| 1:J:230:ARG:HH21 | 1:J:317:GLU:HG3  | 1.85                     | 0.41              |
| 1:L:181:CYS:O    | 1:L:182:MET:HB2  | 2.20                     | 0.41              |
| 1:C:345:VAL:O    | 1:C:348:ARG:HD3  | 2.21                     | 0.41              |
| 1:C:384:LEU:HB3  | 1:C:386:LEU:HD23 | 2.00                     | 0.41              |
| 1:E:357:MET:HE1  | 1:E:362:PHE:CD1  | 2.54                     | 0.41              |
| 1:E:386:LEU:CD2  | 1:F:282:PRO:HB3  | 2.47                     | 0.41              |
| 1:G:147:PHE:HA   | 1:G:210:LEU:O    | 2.19                     | 0.41              |
| 1:H:295:LYS:HE2  | 1:H:328:ASN:HB3  | 2.03                     | 0.41              |
| 1:K:60:LEU:O     | 1:K:138:PRO:HD3  | 2.20                     | 0.41              |
| 1:A:36:ARG:NH2   | 1:A:126:GLU:OE2  | 2.43                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:104:ILE:O    | 1:A:115:ILE:O    | 2.38                     | 0.41              |
| 1:A:366:MET:HE2  | 1:A:366:MET:HB3  | 1.92                     | 0.41              |
| 1:B:26:ILE:HA    | 1:B:27:PRO:HD3   | 1.85                     | 0.41              |
| 1:B:147:PHE:O    | 1:B:148:VAL:HG12 | 2.20                     | 0.41              |
| 1:E:343:LEU:HD12 | 1:E:343:LEU:HA   | 1.69                     | 0.41              |
| 1:F:57:ARG:NH1   | 1:F:153:GLU:OE1  | 2.54                     | 0.41              |
| 1:F:315:LEU:HD12 | 1:F:315:LEU:HA   | 1.89                     | 0.41              |
| 1:G:50:ARG:NH1   | 1:G:111:SER:HB3  | 2.35                     | 0.41              |
| 1:H:237:LEU:O    | 1:H:241:ARG:HG2  | 2.20                     | 0.41              |
| 1:H:396:ASN:HA   | 1:H:399:ALA:H    | 1.85                     | 0.41              |
| 1:B:28:PRO:HB3   | 1:L:87:HIS:NE2   | 2.36                     | 0.41              |
| 1:D:248:ASN:HD21 | 1:I:27:PRO:HB2   | 1.85                     | 0.41              |
| 1:G:48:ARG:HB3   | 1:G:163:PHE:CZ   | 2.56                     | 0.41              |
| 1:G:104:ILE:HG22 | 1:G:105:ASP:N    | 2.35                     | 0.41              |
| 1:H:136:ASP:O    | 1:H:137:LEU:HB2  | 2.19                     | 0.41              |
| 1:I:173:GLN:HE22 | 1:I:211:LEU:H    | 1.68                     | 0.41              |
| 1:J:28:PRO:HG2   | 1:K:239:LEU:HD23 | 2.02                     | 0.41              |
| 1:J:37:VAL:O     | 1:J:101:ARG:O    | 2.38                     | 0.41              |
| 1:L:378:MET:HA   | 1:L:381:ALA:HB3  | 2.01                     | 0.41              |
| 1:B:243:GLN:HA   | 1:H:25:THR:O     | 2.20                     | 0.41              |
| 1:D:87:HIS:CD2   | 1:D:90:LEU:HD22  | 2.56                     | 0.41              |
| 1:D:96:GLU:O     | 1:D:96:GLU:HG3   | 2.20                     | 0.41              |
| 1:D:241:ARG:HH12 | 1:D:308:GLU:CG   | 2.34                     | 0.41              |
| 1:F:390:GLU:HG3  | 1:F:393:GLU:HB3  | 2.01                     | 0.41              |
| 1:G:223:ILE:O    | 1:G:230:ARG:HD3  | 2.21                     | 0.41              |
| 1:I:101:ARG:O    | 1:I:102:VAL:C    | 2.63                     | 0.41              |
| 1:K:146:PRO:O    | 1:K:148:VAL:N    | 2.54                     | 0.41              |
| 1:K:330:PRO:O    | 1:K:334:SER:OG   | 2.27                     | 0.41              |
| 1:L:344:ASP:HB3  | 1:L:347:MET:HG2  | 2.03                     | 0.41              |
| 1:B:384:LEU:HB3  | 1:B:386:LEU:HD23 | 2.02                     | 0.41              |
| 1:D:30:THR:HG22  | 1:D:31:LEU:O     | 2.20                     | 0.41              |
| 1:E:241:ARG:NH1  | 1:E:308:GLU:HB2  | 2.35                     | 0.41              |
| 1:F:149:ASP:O    | 1:F:151:GLU:N    | 2.51                     | 0.41              |
| 1:F:335:TYR:CZ   | 1:F:339:ILE:HD11 | 2.55                     | 0.41              |
| 1:H:152:VAL:HG13 | 1:H:153:GLU:N    | 2.36                     | 0.41              |
| 1:H:172:MET:O    | 1:H:176:ILE:HG13 | 2.21                     | 0.41              |
| 1:J:206:ASN:HA   | 1:J:207:PRO:HD3  | 1.94                     | 0.41              |
| 1:J:392:THR:HA   | 1:J:395:ALA:HB3  | 2.01                     | 0.41              |
| 1:K:84:MET:O     | 1:K:88:VAL:HG23  | 2.20                     | 0.41              |
| 1:L:48:ARG:HB3   | 1:L:163:PHE:CZ   | 2.56                     | 0.41              |
| 1:M:335:TYR:CZ   | 1:M:339:ILE:HD11 | 2.55                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:39:ILE:HD11  | 1:A:88:VAL:HG21  | 2.02                     | 0.41              |
| 1:B:15:GLN:NE2   | 1:L:303:TYR:CE1  | 2.89                     | 0.41              |
| 1:D:14:THR:OG1   | 1:J:304:GLN:NE2  | 2.53                     | 0.41              |
| 1:G:104:ILE:HD13 | 1:G:104:ILE:HA   | 1.83                     | 0.41              |
| 1:H:76:MET:HA    | 1:H:79:LEU:HD12  | 2.01                     | 0.41              |
| 1:I:177:VAL:HB   | 1:I:220:GLN:CG   | 2.39                     | 0.41              |
| 1:J:101:ARG:O    | 1:J:102:VAL:C    | 2.63                     | 0.41              |
| 1:J:180:LYS:HB2  | 1:J:220:GLN:HE21 | 1.85                     | 0.41              |
| 1:K:293:LEU:HD23 | 1:K:293:LEU:HA   | 1.89                     | 0.41              |
| 1:K:345:VAL:O    | 1:K:348:ARG:HD3  | 2.20                     | 0.41              |
| 1:L:173:GLN:HE22 | 1:L:211:LEU:H    | 1.67                     | 0.41              |
| 1:M:400:LYS:CD   | 1:M:400:LYS:H    | 2.34                     | 0.41              |
| 1:E:141:LEU:HD12 | 1:E:141:LEU:HA   | 1.80                     | 0.41              |
| 1:E:386:LEU:HA   | 1:E:386:LEU:HD12 | 1.83                     | 0.41              |
| 1:G:96:GLU:HG3   | 1:G:96:GLU:O     | 2.20                     | 0.41              |
| 1:J:48:ARG:HB3   | 1:J:163:PHE:CZ   | 2.56                     | 0.41              |
| 1:L:146:PRO:O    | 1:L:148:VAL:N    | 2.53                     | 0.41              |
| 1:A:94:SER:HA    | 1:A:95:PRO:HD3   | 1.91                     | 0.41              |
| 1:B:5:LEU:HD21   | 1:L:284:LEU:HD21 | 2.03                     | 0.41              |
| 1:B:211:LEU:HB3  | 1:B:215:ALA:HB3  | 2.02                     | 0.41              |
| 1:B:318:SER:HA   | 1:B:319:PRO:HD3  | 1.93                     | 0.41              |
| 1:C:55:CYS:O     | 1:C:59:VAL:HG23  | 2.20                     | 0.41              |
| 1:D:37:VAL:O     | 1:D:101:ARG:O    | 2.38                     | 0.41              |
| 1:D:65:ARG:NE    | 1:J:159:GLU:OE1  | 2.54                     | 0.41              |
| 1:E:172:MET:SD   | 1:E:253:MET:HG2  | 2.60                     | 0.41              |
| 1:F:101:ARG:O    | 1:F:102:VAL:C    | 2.64                     | 0.41              |
| 1:G:54:PHE:CZ    | 1:G:58:ILE:HD11  | 2.56                     | 0.41              |
| 1:G:87:HIS:HE1   | 1:G:251:TYR:OH   | 2.04                     | 0.41              |
| 1:G:143:HIS:C    | 1:G:145:THR:H    | 2.29                     | 0.41              |
| 1:G:250:TYR:O    | 1:G:254:VAL:HG23 | 2.21                     | 0.41              |
| 1:G:343:LEU:HD12 | 1:G:343:LEU:HA   | 1.93                     | 0.41              |
| 1:H:379:ARG:HD2  | 1:H:379:ARG:C    | 2.46                     | 0.41              |
| 1:I:141:LEU:HD12 | 1:I:141:LEU:HA   | 1.92                     | 0.41              |
| 1:I:155:THR:HG22 | 1:I:156:ALA:N    | 2.35                     | 0.41              |
| 1:J:22:GLU:OE1   | 1:J:22:GLU:N     | 2.32                     | 0.41              |
| 1:J:73:LEU:HD23  | 1:J:73:LEU:HA    | 1.94                     | 0.41              |
| 1:M:363:GLN:O    | 1:M:366:MET:HB2  | 2.21                     | 0.41              |
| 1:M:396:ASN:OD1  | 1:M:397:THR:N    | 2.54                     | 0.41              |
| 1:A:187:GLN:HB3  | 1:A:188:PRO:HD2  | 2.02                     | 0.41              |
| 1:A:276:ALA:HB2  | 1:A:336:ALA:HB2  | 2.01                     | 0.41              |
| 1:C:366:MET:HE2  | 1:C:366:MET:HB3  | 1.87                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:180:LYS:HB2  | 1:F:220:GLN:NE2  | 2.36                     | 0.41              |
| 1:F:292:GLU:HB3  | 1:F:332:LEU:HD12 | 2.03                     | 0.41              |
| 1:F:359:LYS:HA   | 1:F:359:LYS:HD2  | 1.88                     | 0.41              |
| 1:G:39:ILE:CD1   | 1:G:88:VAL:HG21  | 2.51                     | 0.41              |
| 1:G:286:LEU:HD23 | 1:G:286:LEU:HA   | 1.89                     | 0.41              |
| 1:H:30:THR:HG22  | 1:H:31:LEU:O     | 2.21                     | 0.41              |
| 1:H:39:ILE:HG12  | 1:H:101:ARG:O    | 2.21                     | 0.41              |
| 1:J:387:THR:HG22 | 1:J:388:GLN:H    | 1.86                     | 0.41              |
| 1:M:105:ASP:OD1  | 1:M:117:ASN:ND2  | 2.46                     | 0.41              |
| 1:M:181:CYS:HA   | 1:M:224:ARG:HD3  | 2.03                     | 0.41              |
| 1:B:4:VAL:HG21   | 1:L:293:LEU:HB3  | 2.03                     | 0.40              |
| 1:B:172:MET:SD   | 1:B:253:MET:HG2  | 2.61                     | 0.40              |
| 1:D:173:GLN:HE22 | 1:D:210:LEU:HA   | 1.86                     | 0.40              |
| 1:D:230:ARG:NH2  | 1:D:317:GLU:HG3  | 2.36                     | 0.40              |
| 1:D:243:GLN:NE2  | 1:I:319:PRO:HG2  | 2.36                     | 0.40              |
| 1:D:393:GLU:HG3  | 1:D:396:ASN:HB2  | 2.02                     | 0.40              |
| 1:E:214:GLU:O    | 1:E:218:ILE:HG13 | 2.22                     | 0.40              |
| 1:G:171:LEU:HD23 | 1:G:171:LEU:HA   | 1.90                     | 0.40              |
| 1:H:175:TRP:CZ3  | 1:H:237:LEU:HD13 | 2.56                     | 0.40              |
| 1:H:308:GLU:H    | 1:H:308:GLU:HG2  | 1.64                     | 0.40              |
| 1:H:343:LEU:HD12 | 1:H:343:LEU:HA   | 1.95                     | 0.40              |
| 1:J:27:PRO:HB2   | 1:K:248:ASN:ND2  | 2.36                     | 0.40              |
| 1:M:57:ARG:NH2   | 1:M:144:ALA:O    | 2.53                     | 0.40              |
| 1:C:53:LEU:HD23  | 1:C:53:LEU:HA    | 1.86                     | 0.40              |
| 1:C:164:LEU:HD12 | 1:L:33:PRO:HD3   | 2.02                     | 0.40              |
| 1:E:148:VAL:O    | 1:E:149:ASP:C    | 2.63                     | 0.40              |
| 1:G:182:MET:HE1  | 1:G:217:ARG:O    | 2.21                     | 0.40              |
| 1:H:234:THR:O    | 1:H:238:GLN:HG3  | 2.21                     | 0.40              |
| 1:J:39:ILE:HG12  | 1:J:101:ARG:O    | 2.21                     | 0.40              |
| 1:J:57:ARG:NH1   | 1:J:153:GLU:CD   | 2.79                     | 0.40              |
| 1:J:96:GLU:O     | 1:J:96:GLU:HG3   | 2.21                     | 0.40              |
| 1:J:155:THR:HG22 | 1:J:156:ALA:N    | 2.36                     | 0.40              |
| 1:J:384:LEU:HB3  | 1:J:386:LEU:HD23 | 2.03                     | 0.40              |
| 1:K:230:ARG:HH21 | 1:K:317:GLU:HG3  | 1.86                     | 0.40              |
| 1:L:140:THR:OG1  | 1:L:214:GLU:HG2  | 2.22                     | 0.40              |
| 1:L:210:LEU:HD12 | 1:L:210:LEU:HA   | 1.94                     | 0.40              |
| 1:M:366:MET:HE2  | 1:M:366:MET:HB3  | 1.71                     | 0.40              |
| 1:A:293:LEU:HD23 | 1:A:293:LEU:HA   | 1.90                     | 0.40              |
| 1:B:36:ARG:NH2   | 1:B:130:TYR:OH   | 2.54                     | 0.40              |
| 1:B:107:PHE:CE1  | 1:B:114:LEU:HD23 | 2.56                     | 0.40              |
| 1:B:155:THR:OG1  | 1:B:208:ARG:NH2  | 2.55                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:45:PRO:O     | 1:C:49:SER:OG    | 2.38                     | 0.40              |
| 1:C:295:LYS:NZ   | 1:C:328:ASN:HB3  | 2.36                     | 0.40              |
| 1:F:194:LYS:HB3  | 1:F:194:LYS:HE3  | 1.78                     | 0.40              |
| 1:K:361:TYR:O    | 1:K:364:LEU:HB3  | 2.22                     | 0.40              |
| 1:L:253:MET:HE3  | 1:L:253:MET:HB2  | 1.94                     | 0.40              |
| 1:A:175:TRP:CH2  | 1:A:233:LEU:HD22 | 2.57                     | 0.40              |
| 1:A:277:LEU:HD23 | 1:A:284:LEU:HD11 | 2.02                     | 0.40              |
| 1:B:15:GLN:NE2   | 1:L:303:TYR:HE1  | 2.20                     | 0.40              |
| 1:B:20:GLN:HE22  | 1:B:302:LEU:CD1  | 2.35                     | 0.40              |
| 1:B:113:ARG:HD2  | 1:B:124:ARG:HH12 | 1.86                     | 0.40              |
| 1:C:148:VAL:H    | 1:C:212:GLN:HG3  | 1.86                     | 0.40              |
| 1:C:301:ALA:O    | 1:C:305:THR:HG23 | 2.21                     | 0.40              |
| 1:C:304:GLN:HG2  | 1:L:15:GLN:NE2   | 2.36                     | 0.40              |
| 1:D:149:ASP:O    | 1:D:151:GLU:N    | 2.53                     | 0.40              |
| 1:H:318:SER:HA   | 1:H:319:PRO:HD3  | 1.97                     | 0.40              |
| 1:I:401:LEU:CD2  | 1:M:363:GLN:NE2  | 2.84                     | 0.40              |
| 1:K:111:SER:HA   | 1:K:113:ARG:H    | 1.87                     | 0.40              |
| 1:L:104:ILE:O    | 1:L:115:ILE:O    | 2.39                     | 0.40              |
| 1:A:14:THR:O     | 1:A:18:GLN:N     | 2.53                     | 0.40              |
| 1:B:316:LEU:HD23 | 1:B:316:LEU:HA   | 1.88                     | 0.40              |
| 1:E:26:ILE:HA    | 1:E:27:PRO:HD3   | 1.92                     | 0.40              |
| 1:E:396:ASN:OD1  | 1:E:396:ASN:C    | 2.64                     | 0.40              |
| 1:G:258:GLY:O    | 1:G:262:GLU:HG3  | 2.21                     | 0.40              |
| 1:H:321:LEU:HD23 | 1:H:321:LEU:HA   | 1.87                     | 0.40              |
| 1:J:379:ARG:NH1  | 1:J:383:ASP:OD2  | 2.54                     | 0.40              |

All (4) 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:L:100:GLU:OE2 | 3:K:601:PB:PB[3_555]   | 1.86                     | 0.34              |
| 1:G:139:ASP:OD1 | 1:I:200:ARG:NH2[7_545] | 2.13                     | 0.07              |
| 1:B:119:ARG:NH1 | 1:G:100:GLU:OE1[3_555] | 2.17                     | 0.03              |
| 1:C:150:SER:OG  | 1:I:396:ASN:ND2[8_455] | 2.18                     | 0.02              |

## 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     | 391/525 (74%)   | 372 (95%)  | 12 (3%)  | 7 (2%)   | 6           | 26 |
| 1   | B     | 391/525 (74%)   | 376 (96%)  | 13 (3%)  | 2 (0%)   | 24          | 55 |
| 1   | C     | 391/525 (74%)   | 371 (95%)  | 13 (3%)  | 7 (2%)   | 6           | 26 |
| 1   | D     | 391/525 (74%)   | 374 (96%)  | 11 (3%)  | 6 (2%)   | 8           | 30 |
| 1   | E     | 391/525 (74%)   | 372 (95%)  | 9 (2%)   | 10 (3%)  | 4           | 19 |
| 1   | F     | 391/525 (74%)   | 370 (95%)  | 13 (3%)  | 8 (2%)   | 6           | 24 |
| 1   | G     | 391/525 (74%)   | 367 (94%)  | 15 (4%)  | 9 (2%)   | 5           | 21 |
| 1   | H     | 391/525 (74%)   | 373 (95%)  | 11 (3%)  | 7 (2%)   | 6           | 26 |
| 1   | I     | 391/525 (74%)   | 371 (95%)  | 14 (4%)  | 6 (2%)   | 8           | 30 |
| 1   | J     | 391/525 (74%)   | 372 (95%)  | 15 (4%)  | 4 (1%)   | 12          | 39 |
| 1   | K     | 391/525 (74%)   | 371 (95%)  | 12 (3%)  | 8 (2%)   | 6           | 24 |
| 1   | L     | 391/525 (74%)   | 370 (95%)  | 12 (3%)  | 9 (2%)   | 5           | 21 |
| 1   | M     | 391/525 (74%)   | 372 (95%)  | 12 (3%)  | 7 (2%)   | 6           | 26 |
| All | All   | 5083/6825 (74%) | 4831 (95%) | 162 (3%) | 90 (2%)  | 6           | 26 |

All (90) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 19  | ASP  |
| 1   | A     | 118 | ALA  |
| 1   | A     | 188 | PRO  |
| 1   | A     | 359 | LYS  |
| 1   | C     | 118 | ALA  |
| 1   | C     | 188 | PRO  |
| 1   | D     | 19  | ASP  |
| 1   | D     | 118 | ALA  |
| 1   | D     | 147 | PHE  |
| 1   | D     | 188 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 19  | ASP  |
| 1   | E     | 118 | ALA  |
| 1   | E     | 148 | VAL  |
| 1   | E     | 151 | GLU  |
| 1   | E     | 188 | PRO  |
| 1   | E     | 398 | LEU  |
| 1   | E     | 400 | LYS  |
| 1   | F     | 18  | GLN  |
| 1   | F     | 19  | ASP  |
| 1   | F     | 118 | ALA  |
| 1   | F     | 143 | HIS  |
| 1   | F     | 391 | ARG  |
| 1   | G     | 143 | HIS  |
| 1   | G     | 144 | ALA  |
| 1   | G     | 188 | PRO  |
| 1   | G     | 400 | LYS  |
| 1   | H     | 118 | ALA  |
| 1   | I     | 118 | ALA  |
| 1   | I     | 188 | PRO  |
| 1   | J     | 118 | ALA  |
| 1   | K     | 118 | ALA  |
| 1   | K     | 143 | HIS  |
| 1   | L     | 118 | ALA  |
| 1   | L     | 188 | PRO  |
| 1   | L     | 388 | GLN  |
| 1   | M     | 118 | ALA  |
| 1   | M     | 144 | ALA  |
| 1   | M     | 148 | VAL  |
| 1   | M     | 188 | PRO  |
| 1   | A     | 143 | HIS  |
| 1   | B     | 137 | LEU  |
| 1   | C     | 19  | ASP  |
| 1   | C     | 114 | LEU  |
| 1   | E     | 143 | HIS  |
| 1   | E     | 397 | THR  |
| 1   | F     | 146 | PRO  |
| 1   | G     | 21  | SER  |
| 1   | G     | 118 | ALA  |
| 1   | H     | 19  | ASP  |
| 1   | H     | 146 | PRO  |
| 1   | I     | 19  | ASP  |
| 1   | I     | 146 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 19  | ASP  |
| 1   | K     | 146 | PRO  |
| 1   | K     | 188 | PRO  |
| 1   | L     | 143 | HIS  |
| 1   | L     | 146 | PRO  |
| 1   | M     | 19  | ASP  |
| 1   | M     | 151 | GLU  |
| 1   | B     | 146 | PRO  |
| 1   | C     | 137 | LEU  |
| 1   | C     | 146 | PRO  |
| 1   | C     | 150 | SER  |
| 1   | D     | 150 | SER  |
| 1   | F     | 150 | SER  |
| 1   | G     | 146 | PRO  |
| 1   | J     | 150 | SER  |
| 1   | K     | 150 | SER  |
| 1   | L     | 150 | SER  |
| 1   | F     | 137 | LEU  |
| 1   | G     | 189 | ALA  |
| 1   | H     | 21  | SER  |
| 1   | H     | 147 | PHE  |
| 1   | I     | 143 | HIS  |
| 1   | J     | 142 | ASN  |
| 1   | K     | 147 | PHE  |
| 1   | L     | 147 | PHE  |
| 1   | A     | 137 | LEU  |
| 1   | K     | 137 | LEU  |
| 1   | L     | 137 | LEU  |
| 1   | D     | 137 | LEU  |
| 1   | E     | 137 | LEU  |
| 1   | G     | 137 | LEU  |
| 1   | H     | 137 | LEU  |
| 1   | K     | 142 | ASN  |
| 1   | I     | 137 | LEU  |
| 1   | M     | 137 | LEU  |
| 1   | L     | 145 | THR  |
| 1   | H     | 102 | VAL  |
| 1   | A     | 102 | VAL  |

### 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     | 334/435 (77%)   | 316 (95%)  | 18 (5%)  | 20          | 48 |
| 1   | B     | 334/435 (77%)   | 322 (96%)  | 12 (4%)  | 31          | 59 |
| 1   | C     | 334/435 (77%)   | 316 (95%)  | 18 (5%)  | 20          | 48 |
| 1   | D     | 334/435 (77%)   | 316 (95%)  | 18 (5%)  | 20          | 48 |
| 1   | E     | 334/435 (77%)   | 315 (94%)  | 19 (6%)  | 18          | 47 |
| 1   | F     | 334/435 (77%)   | 315 (94%)  | 19 (6%)  | 18          | 47 |
| 1   | G     | 334/435 (77%)   | 316 (95%)  | 18 (5%)  | 20          | 48 |
| 1   | H     | 334/435 (77%)   | 316 (95%)  | 18 (5%)  | 20          | 48 |
| 1   | I     | 334/435 (77%)   | 316 (95%)  | 18 (5%)  | 20          | 48 |
| 1   | J     | 334/435 (77%)   | 318 (95%)  | 16 (5%)  | 23          | 52 |
| 1   | K     | 334/435 (77%)   | 312 (93%)  | 22 (7%)  | 15          | 41 |
| 1   | L     | 334/435 (77%)   | 316 (95%)  | 18 (5%)  | 20          | 48 |
| 1   | M     | 334/435 (77%)   | 318 (95%)  | 16 (5%)  | 23          | 52 |
| All | All   | 4342/5655 (77%) | 4112 (95%) | 230 (5%) | 20          | 49 |

All (230) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | VAL  |
| 1   | A     | 87  | HIS  |
| 1   | A     | 104 | ILE  |
| 1   | A     | 148 | VAL  |
| 1   | A     | 151 | GLU  |
| 1   | A     | 194 | LYS  |
| 1   | A     | 217 | ARG  |
| 1   | A     | 221 | ASN  |
| 1   | A     | 230 | ARG  |
| 1   | A     | 342 | VAL  |
| 1   | A     | 345 | VAL  |
| 1   | A     | 348 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 359 | LYS  |
| 1   | A     | 373 | GLN  |
| 1   | A     | 376 | VAL  |
| 1   | A     | 379 | ARG  |
| 1   | A     | 384 | LEU  |
| 1   | A     | 393 | GLU  |
| 1   | B     | 19  | ASP  |
| 1   | B     | 21  | SER  |
| 1   | B     | 23  | GLU  |
| 1   | B     | 26  | ILE  |
| 1   | B     | 34  | VAL  |
| 1   | B     | 35  | ILE  |
| 1   | B     | 87  | HIS  |
| 1   | B     | 150 | SER  |
| 1   | B     | 187 | GLN  |
| 1   | B     | 194 | LYS  |
| 1   | B     | 315 | LEU  |
| 1   | B     | 376 | VAL  |
| 1   | C     | 4   | VAL  |
| 1   | C     | 6   | LYS  |
| 1   | C     | 34  | VAL  |
| 1   | C     | 35  | ILE  |
| 1   | C     | 104 | ILE  |
| 1   | C     | 113 | ARG  |
| 1   | C     | 141 | LEU  |
| 1   | C     | 142 | ASN  |
| 1   | C     | 192 | ILE  |
| 1   | C     | 197 | GLN  |
| 1   | C     | 201 | GLN  |
| 1   | C     | 228 | VAL  |
| 1   | C     | 230 | ARG  |
| 1   | C     | 308 | GLU  |
| 1   | C     | 315 | LEU  |
| 1   | C     | 348 | ARG  |
| 1   | C     | 376 | VAL  |
| 1   | C     | 382 | GLU  |
| 1   | D     | 6   | LYS  |
| 1   | D     | 13  | LEU  |
| 1   | D     | 30  | THR  |
| 1   | D     | 35  | ILE  |
| 1   | D     | 36  | ARG  |
| 1   | D     | 50  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 126 | GLU  |
| 1   | D     | 148 | VAL  |
| 1   | D     | 220 | GLN  |
| 1   | D     | 228 | VAL  |
| 1   | D     | 315 | LEU  |
| 1   | D     | 342 | VAL  |
| 1   | D     | 367 | GLU  |
| 1   | D     | 370 | ARG  |
| 1   | D     | 371 | LYS  |
| 1   | D     | 376 | VAL  |
| 1   | D     | 384 | LEU  |
| 1   | D     | 393 | GLU  |
| 1   | E     | 4   | VAL  |
| 1   | E     | 10  | ARG  |
| 1   | E     | 18  | GLN  |
| 1   | E     | 20  | GLN  |
| 1   | E     | 22  | GLU  |
| 1   | E     | 30  | THR  |
| 1   | E     | 34  | VAL  |
| 1   | E     | 35  | ILE  |
| 1   | E     | 104 | ILE  |
| 1   | E     | 141 | LEU  |
| 1   | E     | 214 | GLU  |
| 1   | E     | 228 | VAL  |
| 1   | E     | 309 | GLN  |
| 1   | E     | 315 | LEU  |
| 1   | E     | 370 | ARG  |
| 1   | E     | 376 | VAL  |
| 1   | E     | 388 | GLN  |
| 1   | E     | 391 | ARG  |
| 1   | E     | 401 | LEU  |
| 1   | F     | 4   | VAL  |
| 1   | F     | 18  | GLN  |
| 1   | F     | 19  | ASP  |
| 1   | F     | 26  | ILE  |
| 1   | F     | 30  | THR  |
| 1   | F     | 34  | VAL  |
| 1   | F     | 35  | ILE  |
| 1   | F     | 192 | ILE  |
| 1   | F     | 225 | LYS  |
| 1   | F     | 228 | VAL  |
| 1   | F     | 309 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 315 | LEU  |
| 1   | F     | 345 | VAL  |
| 1   | F     | 353 | SER  |
| 1   | F     | 376 | VAL  |
| 1   | F     | 384 | LEU  |
| 1   | F     | 390 | GLU  |
| 1   | F     | 393 | GLU  |
| 1   | F     | 400 | LYS  |
| 1   | G     | 4   | VAL  |
| 1   | G     | 30  | THR  |
| 1   | G     | 35  | ILE  |
| 1   | G     | 93  | GLN  |
| 1   | G     | 104 | ILE  |
| 1   | G     | 141 | LEU  |
| 1   | G     | 150 | SER  |
| 1   | G     | 182 | MET  |
| 1   | G     | 194 | LYS  |
| 1   | G     | 201 | GLN  |
| 1   | G     | 228 | VAL  |
| 1   | G     | 315 | LEU  |
| 1   | G     | 342 | VAL  |
| 1   | G     | 345 | VAL  |
| 1   | G     | 376 | VAL  |
| 1   | G     | 384 | LEU  |
| 1   | G     | 388 | GLN  |
| 1   | G     | 394 | MET  |
| 1   | H     | 4   | VAL  |
| 1   | H     | 6   | LYS  |
| 1   | H     | 20  | GLN  |
| 1   | H     | 21  | SER  |
| 1   | H     | 26  | ILE  |
| 1   | H     | 30  | THR  |
| 1   | H     | 35  | ILE  |
| 1   | H     | 99  | ILE  |
| 1   | H     | 100 | GLU  |
| 1   | H     | 140 | THR  |
| 1   | H     | 214 | GLU  |
| 1   | H     | 228 | VAL  |
| 1   | H     | 237 | LEU  |
| 1   | H     | 315 | LEU  |
| 1   | H     | 359 | LYS  |
| 1   | H     | 367 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 376 | VAL  |
| 1   | H     | 379 | ARG  |
| 1   | I     | 6   | LYS  |
| 1   | I     | 30  | THR  |
| 1   | I     | 35  | ILE  |
| 1   | I     | 87  | HIS  |
| 1   | I     | 141 | LEU  |
| 1   | I     | 187 | GLN  |
| 1   | I     | 194 | LYS  |
| 1   | I     | 197 | GLN  |
| 1   | I     | 220 | GLN  |
| 1   | I     | 228 | VAL  |
| 1   | I     | 308 | GLU  |
| 1   | I     | 315 | LEU  |
| 1   | I     | 342 | VAL  |
| 1   | I     | 363 | GLN  |
| 1   | I     | 370 | ARG  |
| 1   | I     | 376 | VAL  |
| 1   | I     | 384 | LEU  |
| 1   | I     | 390 | GLU  |
| 1   | J     | 4   | VAL  |
| 1   | J     | 18  | GLN  |
| 1   | J     | 30  | THR  |
| 1   | J     | 35  | ILE  |
| 1   | J     | 36  | ARG  |
| 1   | J     | 87  | HIS  |
| 1   | J     | 103 | GLU  |
| 1   | J     | 104 | ILE  |
| 1   | J     | 142 | ASN  |
| 1   | J     | 228 | VAL  |
| 1   | J     | 237 | LEU  |
| 1   | J     | 315 | LEU  |
| 1   | J     | 372 | GLN  |
| 1   | J     | 376 | VAL  |
| 1   | J     | 384 | LEU  |
| 1   | J     | 401 | LEU  |
| 1   | K     | 4   | VAL  |
| 1   | K     | 15  | GLN  |
| 1   | K     | 21  | SER  |
| 1   | K     | 30  | THR  |
| 1   | K     | 35  | ILE  |
| 1   | K     | 87  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | K     | 148 | VAL  |
| 1   | K     | 152 | VAL  |
| 1   | K     | 230 | ARG  |
| 1   | K     | 249 | ARG  |
| 1   | K     | 283 | THR  |
| 1   | K     | 315 | LEU  |
| 1   | K     | 342 | VAL  |
| 1   | K     | 367 | GLU  |
| 1   | K     | 370 | ARG  |
| 1   | K     | 371 | LYS  |
| 1   | K     | 376 | VAL  |
| 1   | K     | 379 | ARG  |
| 1   | K     | 382 | GLU  |
| 1   | K     | 384 | LEU  |
| 1   | K     | 390 | GLU  |
| 1   | K     | 391 | ARG  |
| 1   | L     | 9   | GLU  |
| 1   | L     | 15  | GLN  |
| 1   | L     | 30  | THR  |
| 1   | L     | 34  | VAL  |
| 1   | L     | 35  | ILE  |
| 1   | L     | 126 | GLU  |
| 1   | L     | 139 | ASP  |
| 1   | L     | 148 | VAL  |
| 1   | L     | 152 | VAL  |
| 1   | L     | 194 | LYS  |
| 1   | L     | 304 | GLN  |
| 1   | L     | 309 | GLN  |
| 1   | L     | 315 | LEU  |
| 1   | L     | 348 | ARG  |
| 1   | L     | 376 | VAL  |
| 1   | L     | 378 | MET  |
| 1   | L     | 382 | GLU  |
| 1   | L     | 387 | THR  |
| 1   | M     | 4   | VAL  |
| 1   | M     | 30  | THR  |
| 1   | M     | 34  | VAL  |
| 1   | M     | 35  | ILE  |
| 1   | M     | 99  | ILE  |
| 1   | M     | 104 | ILE  |
| 1   | M     | 217 | ARG  |
| 1   | M     | 308 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | M     | 315 | LEU  |
| 1   | M     | 345 | VAL  |
| 1   | M     | 348 | ARG  |
| 1   | M     | 363 | GLN  |
| 1   | M     | 373 | GLN  |
| 1   | M     | 376 | VAL  |
| 1   | M     | 384 | LEU  |
| 1   | M     | 386 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 87  | HIS  |
| 1   | A     | 173 | GLN  |
| 1   | A     | 220 | GLN  |
| 1   | B     | 197 | GLN  |
| 1   | B     | 220 | GLN  |
| 1   | B     | 328 | ASN  |
| 1   | B     | 363 | GLN  |
| 1   | C     | 15  | GLN  |
| 1   | C     | 87  | HIS  |
| 1   | C     | 143 | HIS  |
| 1   | C     | 187 | GLN  |
| 1   | C     | 243 | GLN  |
| 1   | D     | 15  | GLN  |
| 1   | D     | 87  | HIS  |
| 1   | D     | 220 | GLN  |
| 1   | D     | 304 | GLN  |
| 1   | D     | 320 | HIS  |
| 1   | D     | 363 | GLN  |
| 1   | E     | 15  | GLN  |
| 1   | E     | 197 | GLN  |
| 1   | F     | 173 | GLN  |
| 1   | F     | 220 | GLN  |
| 1   | F     | 304 | GLN  |
| 1   | G     | 87  | HIS  |
| 1   | G     | 143 | HIS  |
| 1   | G     | 201 | GLN  |
| 1   | G     | 220 | GLN  |
| 1   | G     | 304 | GLN  |
| 1   | G     | 388 | GLN  |
| 1   | H     | 20  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 220 | GLN  |
| 1   | I     | 87  | HIS  |
| 1   | I     | 142 | ASN  |
| 1   | I     | 173 | GLN  |
| 1   | J     | 15  | GLN  |
| 1   | J     | 20  | GLN  |
| 1   | J     | 143 | HIS  |
| 1   | J     | 220 | GLN  |
| 1   | J     | 304 | GLN  |
| 1   | J     | 320 | HIS  |
| 1   | K     | 15  | GLN  |
| 1   | L     | 87  | HIS  |
| 1   | L     | 173 | GLN  |
| 1   | L     | 187 | GLN  |
| 1   | L     | 388 | GLN  |
| 1   | M     | 20  | GLN  |
| 1   | M     | 220 | GLN  |
| 1   | M     | 363 | GLN  |
| 1   | M     | 373 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed    | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 2   | N     | 77/78 (98%) | 8 (10%)           | 2 (2%)          |

All (8) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 18  | U    |
| 2   | N     | 22  | U    |
| 2   | N     | 28  | U    |
| 2   | N     | 48  | U    |
| 2   | N     | 49  | U    |
| 2   | N     | 58  | U    |
| 2   | N     | 61  | U    |
| 2   | N     | 67  | U    |

All (2) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 48  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | N     | 66  | U    |

## 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](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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     | 395/525 (75%)   | 0.27   | 15 (3%)   | 44  | 25  | 13, 41, 98, 139       | 3 (0%)  |
| 1   | B     | 395/525 (75%)   | 0.23   | 18 (4%)   | 37  | 20  | 14, 40, 99, 140       | 3 (0%)  |
| 1   | C     | 395/525 (75%)   | 0.35   | 28 (7%)   | 22  | 11  | 12, 40, 102, 139      | 3 (0%)  |
| 1   | D     | 395/525 (75%)   | 0.28   | 30 (7%)   | 20  | 10  | 13, 39, 99, 137       | 3 (0%)  |
| 1   | E     | 395/525 (75%)   | 0.28   | 16 (4%)   | 41  | 23  | 14, 40, 101, 140      | 3 (0%)  |
| 1   | F     | 395/525 (75%)   | 0.31   | 23 (5%)   | 29  | 15  | 14, 40, 99, 137       | 3 (0%)  |
| 1   | G     | 395/525 (75%)   | 0.30   | 29 (7%)   | 21  | 11  | 13, 38, 98, 141       | 3 (0%)  |
| 1   | H     | 395/525 (75%)   | 0.27   | 21 (5%)   | 32  | 17  | 14, 39, 98, 140       | 3 (0%)  |
| 1   | I     | 395/525 (75%)   | 0.30   | 29 (7%)   | 21  | 11  | 13, 38, 98, 138       | 3 (0%)  |
| 1   | J     | 395/525 (75%)   | 0.26   | 21 (5%)   | 32  | 17  | 13, 39, 98, 141       | 3 (0%)  |
| 1   | K     | 395/525 (75%)   | 0.18   | 15 (3%)   | 44  | 25  | 14, 39, 98, 139       | 3 (0%)  |
| 1   | L     | 395/525 (75%)   | 0.25   | 19 (4%)   | 35  | 19  | 12, 40, 102, 137      | 3 (0%)  |
| 1   | M     | 395/525 (75%)   | 0.23   | 23 (5%)   | 29  | 15  | 14, 39, 99, 139       | 3 (0%)  |
| 2   | N     | 78/78 (100%)    | -0.23  | 0         | 100 | 100 | 35, 44, 50, 54        | 0       |
| All | All   | 5213/6903 (75%) | 0.26   | 287 (5%)  | 30  | 16  | 12, 40, 102, 141      | 39 (0%) |

All (287) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | M     | 19  | ASP  | 9.4  |
| 1   | L     | 19  | ASP  | 8.8  |
| 1   | D     | 19  | ASP  | 8.7  |
| 1   | B     | 19  | ASP  | 8.6  |
| 1   | I     | 19  | ASP  | 8.5  |
| 1   | G     | 19  | ASP  | 8.5  |
| 1   | J     | 19  | ASP  | 8.3  |
| 1   | E     | 19  | ASP  | 8.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 19  | ASP  | 7.9  |
| 1   | K     | 19  | ASP  | 7.9  |
| 1   | F     | 19  | ASP  | 7.1  |
| 1   | H     | 19  | ASP  | 6.5  |
| 1   | J     | 18  | GLN  | 6.0  |
| 1   | G     | 181 | CYS  | 5.9  |
| 1   | K     | 367 | GLU  | 5.7  |
| 1   | C     | 19  | ASP  | 5.3  |
| 1   | A     | 188 | PRO  | 5.1  |
| 1   | I     | 392 | THR  | 4.8  |
| 1   | E     | 20  | GLN  | 4.8  |
| 1   | J     | 401 | LEU  | 4.8  |
| 1   | L     | 401 | LEU  | 4.7  |
| 1   | G     | 188 | PRO  | 4.6  |
| 1   | C     | 20  | GLN  | 4.6  |
| 1   | D     | 401 | LEU  | 4.6  |
| 1   | G     | 396 | ASN  | 4.5  |
| 1   | H     | 20  | GLN  | 4.4  |
| 1   | F     | 181 | CYS  | 4.4  |
| 1   | J     | 20  | GLN  | 4.3  |
| 1   | K     | 20  | GLN  | 4.2  |
| 1   | C     | 21  | SER  | 4.1  |
| 1   | L     | 181 | CYS  | 4.1  |
| 1   | F     | 389 | ALA  | 4.1  |
| 1   | A     | 187 | GLN  | 4.1  |
| 1   | L     | 20  | GLN  | 4.0  |
| 1   | M     | 20  | GLN  | 3.9  |
| 1   | D     | 397 | THR  | 3.9  |
| 1   | I     | 142 | ASN  | 3.9  |
| 1   | E     | 401 | LEU  | 3.9  |
| 1   | E     | 181 | CYS  | 3.8  |
| 1   | D     | 21  | SER  | 3.8  |
| 1   | L     | 187 | GLN  | 3.7  |
| 1   | C     | 120 | SER  | 3.7  |
| 1   | I     | 391 | ARG  | 3.7  |
| 1   | B     | 401 | LEU  | 3.7  |
| 1   | G     | 189 | ALA  | 3.7  |
| 1   | I     | 188 | PRO  | 3.7  |
| 1   | F     | 393 | GLU  | 3.7  |
| 1   | A     | 20  | GLN  | 3.7  |
| 1   | K     | 18  | GLN  | 3.6  |
| 1   | I     | 18  | GLN  | 3.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 18  | GLN  | 3.5  |
| 1   | D     | 20  | GLN  | 3.5  |
| 1   | C     | 143 | HIS  | 3.5  |
| 1   | H     | 189 | ALA  | 3.5  |
| 1   | G     | 187 | GLN  | 3.5  |
| 1   | B     | 20  | GLN  | 3.5  |
| 1   | D     | 393 | GLU  | 3.5  |
| 1   | C     | 401 | LEU  | 3.5  |
| 1   | C     | 181 | CYS  | 3.4  |
| 1   | A     | 388 | GLN  | 3.4  |
| 1   | J     | 189 | ALA  | 3.3  |
| 1   | I     | 401 | LEU  | 3.3  |
| 1   | K     | 401 | LEU  | 3.3  |
| 1   | K     | 111 | SER  | 3.3  |
| 1   | C     | 182 | MET  | 3.3  |
| 1   | H     | 401 | LEU  | 3.3  |
| 1   | L     | 18  | GLN  | 3.3  |
| 1   | H     | 21  | SER  | 3.3  |
| 1   | I     | 181 | CYS  | 3.3  |
| 1   | G     | 111 | SER  | 3.2  |
| 1   | C     | 139 | ASP  | 3.2  |
| 1   | D     | 394 | MET  | 3.2  |
| 1   | I     | 388 | GLN  | 3.2  |
| 1   | L     | 372 | GLN  | 3.2  |
| 1   | I     | 389 | ALA  | 3.2  |
| 1   | G     | 136 | ASP  | 3.2  |
| 1   | A     | 181 | CYS  | 3.1  |
| 1   | B     | 181 | CYS  | 3.1  |
| 1   | H     | 181 | CYS  | 3.1  |
| 1   | K     | 188 | PRO  | 3.1  |
| 1   | D     | 387 | THR  | 3.1  |
| 1   | M     | 187 | GLN  | 3.1  |
| 1   | G     | 143 | HIS  | 3.1  |
| 1   | J     | 201 | GLN  | 3.1  |
| 1   | J     | 22  | GLU  | 3.1  |
| 1   | I     | 182 | MET  | 3.1  |
| 1   | A     | 401 | LEU  | 3.1  |
| 1   | G     | 18  | GLN  | 3.0  |
| 1   | D     | 389 | ALA  | 3.0  |
| 1   | L     | 15  | GLN  | 3.0  |
| 1   | I     | 189 | ALA  | 3.0  |
| 1   | H     | 111 | SER  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | H     | 18  | GLN  | 2.9  |
| 1   | F     | 401 | LEU  | 2.9  |
| 1   | J     | 109 | GLU  | 2.9  |
| 1   | L     | 111 | SER  | 2.9  |
| 1   | D     | 396 | ASN  | 2.9  |
| 1   | I     | 21  | SER  | 2.9  |
| 1   | M     | 401 | LEU  | 2.9  |
| 1   | A     | 190 | ALA  | 2.9  |
| 1   | I     | 387 | THR  | 2.9  |
| 1   | M     | 395 | ALA  | 2.9  |
| 1   | J     | 21  | SER  | 2.8  |
| 1   | A     | 189 | ALA  | 2.8  |
| 1   | I     | 390 | GLU  | 2.8  |
| 1   | E     | 188 | PRO  | 2.8  |
| 1   | M     | 188 | PRO  | 2.8  |
| 1   | G     | 182 | MET  | 2.8  |
| 1   | C     | 188 | PRO  | 2.8  |
| 1   | I     | 397 | THR  | 2.8  |
| 1   | J     | 182 | MET  | 2.8  |
| 1   | A     | 87  | HIS  | 2.8  |
| 1   | I     | 187 | GLN  | 2.8  |
| 1   | J     | 181 | CYS  | 2.7  |
| 1   | I     | 398 | LEU  | 2.7  |
| 1   | L     | 386 | LEU  | 2.7  |
| 1   | F     | 111 | SER  | 2.7  |
| 1   | F     | 395 | ALA  | 2.7  |
| 1   | B     | 388 | GLN  | 2.7  |
| 1   | M     | 18  | GLN  | 2.7  |
| 1   | H     | 182 | MET  | 2.7  |
| 1   | F     | 400 | LYS  | 2.7  |
| 1   | C     | 146 | PRO  | 2.7  |
| 1   | D     | 390 | GLU  | 2.7  |
| 1   | L     | 400 | LYS  | 2.6  |
| 1   | M     | 181 | CYS  | 2.6  |
| 1   | M     | 397 | THR  | 2.6  |
| 1   | I     | 395 | ALA  | 2.6  |
| 1   | D     | 182 | MET  | 2.6  |
| 1   | I     | 146 | PRO  | 2.6  |
| 1   | B     | 189 | ALA  | 2.6  |
| 1   | G     | 386 | LEU  | 2.6  |
| 1   | D     | 111 | SER  | 2.6  |
| 1   | M     | 21  | SER  | 2.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 18  | GLN  | 2.6  |
| 1   | K     | 23  | GLU  | 2.6  |
| 1   | B     | 395 | ALA  | 2.6  |
| 1   | M     | 111 | SER  | 2.6  |
| 1   | C     | 15  | GLN  | 2.6  |
| 1   | G     | 20  | GLN  | 2.6  |
| 1   | I     | 20  | GLN  | 2.6  |
| 1   | M     | 388 | GLN  | 2.6  |
| 1   | G     | 385 | GLY  | 2.6  |
| 1   | C     | 142 | ASN  | 2.6  |
| 1   | C     | 151 | GLU  | 2.6  |
| 1   | F     | 394 | MET  | 2.5  |
| 1   | H     | 143 | HIS  | 2.5  |
| 1   | E     | 18  | GLN  | 2.5  |
| 1   | D     | 181 | CYS  | 2.5  |
| 1   | B     | 187 | GLN  | 2.5  |
| 1   | D     | 398 | LEU  | 2.5  |
| 1   | I     | 386 | LEU  | 2.5  |
| 1   | F     | 387 | THR  | 2.5  |
| 1   | M     | 398 | LEU  | 2.5  |
| 1   | L     | 395 | ALA  | 2.5  |
| 1   | G     | 393 | GLU  | 2.5  |
| 1   | I     | 23  | GLU  | 2.5  |
| 1   | J     | 387 | THR  | 2.5  |
| 1   | B     | 197 | GLN  | 2.5  |
| 1   | A     | 118 | ALA  | 2.5  |
| 1   | C     | 395 | ALA  | 2.5  |
| 1   | C     | 393 | GLU  | 2.5  |
| 1   | L     | 396 | ASN  | 2.5  |
| 1   | F     | 146 | PRO  | 2.5  |
| 1   | F     | 20  | GLN  | 2.5  |
| 1   | C     | 189 | ALA  | 2.4  |
| 1   | M     | 98  | ASP  | 2.4  |
| 1   | L     | 21  | SER  | 2.4  |
| 1   | L     | 146 | PRO  | 2.4  |
| 1   | D     | 24  | GLY  | 2.4  |
| 1   | H     | 389 | ALA  | 2.4  |
| 1   | M     | 189 | ALA  | 2.4  |
| 1   | B     | 400 | LYS  | 2.4  |
| 1   | D     | 355 | SER  | 2.4  |
| 1   | G     | 397 | THR  | 2.4  |
| 1   | L     | 188 | PRO  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 24  | GLY  | 2.4  |
| 1   | H     | 394 | MET  | 2.4  |
| 1   | G     | 401 | LEU  | 2.4  |
| 1   | K     | 393 | GLU  | 2.4  |
| 1   | G     | 394 | MET  | 2.4  |
| 1   | B     | 21  | SER  | 2.4  |
| 1   | E     | 111 | SER  | 2.4  |
| 1   | A     | 142 | ASN  | 2.3  |
| 1   | F     | 143 | HIS  | 2.3  |
| 1   | C     | 372 | GLN  | 2.3  |
| 1   | M     | 386 | LEU  | 2.3  |
| 1   | M     | 100 | GLU  | 2.3  |
| 1   | C     | 400 | LYS  | 2.3  |
| 1   | H     | 391 | ARG  | 2.3  |
| 1   | B     | 389 | ALA  | 2.3  |
| 1   | F     | 189 | ALA  | 2.3  |
| 1   | I     | 399 | ALA  | 2.3  |
| 1   | M     | 182 | MET  | 2.3  |
| 1   | A     | 359 | LYS  | 2.3  |
| 1   | F     | 101 | ARG  | 2.3  |
| 1   | F     | 182 | MET  | 2.3  |
| 1   | E     | 398 | LEU  | 2.3  |
| 1   | F     | 201 | GLN  | 2.3  |
| 1   | D     | 23  | GLU  | 2.3  |
| 1   | C     | 14  | THR  | 2.3  |
| 1   | I     | 394 | MET  | 2.3  |
| 1   | G     | 120 | SER  | 2.3  |
| 1   | K     | 3   | SER  | 2.3  |
| 1   | H     | 17  | LEU  | 2.3  |
| 1   | H     | 388 | GLN  | 2.3  |
| 1   | M     | 372 | GLN  | 2.3  |
| 1   | D     | 395 | ALA  | 2.3  |
| 1   | J     | 24  | GLY  | 2.3  |
| 1   | D     | 386 | LEU  | 2.3  |
| 1   | G     | 21  | SER  | 2.3  |
| 1   | J     | 372 | GLN  | 2.3  |
| 1   | D     | 161 | GLU  | 2.2  |
| 1   | D     | 104 | ILE  | 2.2  |
| 1   | E     | 389 | ALA  | 2.2  |
| 1   | J     | 399 | ALA  | 2.2  |
| 1   | M     | 399 | ALA  | 2.2  |
| 1   | B     | 398 | LEU  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 18  | GLN  | 2.2  |
| 1   | F     | 142 | ASN  | 2.2  |
| 1   | M     | 15  | GLN  | 2.2  |
| 1   | E     | 151 | GLU  | 2.2  |
| 1   | G     | 158 | ASP  | 2.2  |
| 1   | H     | 25  | THR  | 2.2  |
| 1   | I     | 400 | LYS  | 2.2  |
| 1   | F     | 120 | SER  | 2.2  |
| 1   | F     | 18  | GLN  | 2.2  |
| 1   | D     | 136 | ASP  | 2.2  |
| 1   | C     | 190 | ALA  | 2.2  |
| 1   | F     | 188 | PRO  | 2.2  |
| 1   | G     | 400 | LYS  | 2.2  |
| 1   | L     | 387 | THR  | 2.2  |
| 1   | D     | 388 | GLN  | 2.2  |
| 1   | E     | 346 | ASN  | 2.2  |
| 1   | K     | 181 | CYS  | 2.2  |
| 1   | H     | 400 | LYS  | 2.2  |
| 1   | K     | 392 | THR  | 2.2  |
| 1   | B     | 104 | ILE  | 2.2  |
| 1   | A     | 182 | MET  | 2.2  |
| 1   | D     | 400 | LYS  | 2.2  |
| 1   | H     | 142 | ASN  | 2.2  |
| 1   | I     | 396 | ASN  | 2.2  |
| 1   | K     | 189 | ALA  | 2.2  |
| 1   | E     | 13  | LEU  | 2.1  |
| 1   | B     | 111 | SER  | 2.1  |
| 1   | G     | 371 | LYS  | 2.1  |
| 1   | D     | 189 | ALA  | 2.1  |
| 1   | J     | 111 | SER  | 2.1  |
| 1   | H     | 188 | PRO  | 2.1  |
| 1   | D     | 392 | THR  | 2.1  |
| 1   | E     | 392 | THR  | 2.1  |
| 1   | B     | 182 | MET  | 2.1  |
| 1   | M     | 394 | MET  | 2.1  |
| 1   | G     | 379 | ARG  | 2.1  |
| 1   | C     | 150 | SER  | 2.1  |
| 1   | B     | 86  | ASN  | 2.1  |
| 1   | G     | 86  | ASN  | 2.1  |
| 1   | G     | 398 | LEU  | 2.1  |
| 1   | H     | 386 | LEU  | 2.1  |
| 1   | C     | 101 | ARG  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | L     | 182 | MET  | 2.1  |
| 1   | E     | 189 | ALA  | 2.1  |
| 1   | G     | 146 | PRO  | 2.1  |
| 1   | C     | 104 | ILE  | 2.1  |
| 1   | I     | 179 | CYS  | 2.1  |
| 1   | M     | 391 | ARG  | 2.1  |
| 1   | A     | 103 | GLU  | 2.1  |
| 1   | E     | 16  | GLU  | 2.1  |
| 1   | H     | 23  | GLU  | 2.1  |
| 1   | L     | 87  | HIS  | 2.1  |
| 1   | F     | 139 | ASP  | 2.1  |
| 1   | J     | 397 | THR  | 2.1  |
| 1   | G     | 201 | GLN  | 2.1  |
| 1   | J     | 193 | GLU  | 2.1  |
| 1   | J     | 400 | LYS  | 2.0  |
| 1   | K     | 400 | LYS  | 2.0  |
| 1   | D     | 391 | ARG  | 2.0  |
| 1   | E     | 386 | LEU  | 2.0  |
| 1   | J     | 386 | LEU  | 2.0  |
| 1   | C     | 394 | MET  | 2.0  |
| 1   | C     | 383 | ASP  | 2.0  |
| 1   | J     | 104 | ILE  | 2.0  |
| 1   | K     | 142 | ASN  | 2.0  |
| 1   | I     | 144 | ALA  | 2.0  |
| 1   | C     | 341 | TYR  | 2.0  |
| 1   | G     | 388 | GLN  | 2.0  |
| 1   | D     | 193 | GLU  | 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 3   | PB   | B     | 601 | 1/1   | 0.63 | 0.40 | 194,194,194,194            | 0     |
| 3   | PB   | M     | 602 | 1/1   | 0.78 | 0.38 | 171,171,171,171            | 0     |
| 3   | PB   | M     | 603 | 1/1   | 0.90 | 0.09 | 83,83,83,83                | 1     |
| 3   | PB   | M     | 604 | 1/1   | 0.90 | 0.11 | 76,76,76,76                | 1     |
| 3   | PB   | H     | 601 | 1/1   | 0.92 | 0.06 | 59,59,59,59                | 1     |
| 3   | PB   | G     | 601 | 1/1   | 0.92 | 0.28 | 113,113,113,113            | 0     |
| 3   | PB   | D     | 601 | 1/1   | 0.93 | 0.08 | 82,82,82,82                | 1     |
| 3   | PB   | N     | 101 | 1/1   | 0.93 | 0.06 | 57,57,57,57                | 1     |
| 3   | PB   | A     | 601 | 1/1   | 0.95 | 0.09 | 70,70,70,70                | 1     |
| 3   | PB   | M     | 601 | 1/1   | 0.95 | 0.20 | 83,83,83,83                | 0     |
| 3   | PB   | I     | 601 | 1/1   | 0.96 | 0.25 | 94,94,94,94                | 0     |
| 3   | PB   | K     | 602 | 1/1   | 0.98 | 0.14 | 62,62,62,62                | 0     |
| 3   | PB   | I     | 602 | 1/1   | 0.98 | 0.24 | 94,94,94,94                | 0     |
| 3   | PB   | K     | 601 | 1/1   | 0.99 | 0.12 | 56,56,56,56                | 0     |

## 6.5 Other polymers

There are no such residues in this entry.